Quantum Mechanics found in a nutshell.

Updated 2021-04-29 I leave the Mahan Course

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www.leennoordzij.me

dr.l.noordzij@leennoordzij.nl

Exercises, Remarks and Questions.
Based on *Quantum Mechanics in a Nutshell* by Mahan.
References will be made to *Quantum Mechanics, The Theoretical Minimum* by Susskind, *The Feynman Lectures on Physics* and *The Principles of Quantum Mechanics* by Dirac.

1.Introduction.

In this chapter Mahan summarizes some basics of Quantum Mechanics. Having consummated for example Susskind's book, this chapter is accessible.

Remark: On page 4 in paragraph 1.3 reference is made to the Schrödinger equation. The equation number should read (1.6) instead of (1.8), a printing error.
On top of page 5 Eq. (1.15) is given: $b_n = \int d^3\, r f(\boldsymbol{r})\phi_n(\boldsymbol{r})$. I think this Eq. should read $b_n = \int d^3\, r f(\boldsymbol{r})\phi_{\boldsymbol{n}}^*(\boldsymbol{r})$. Then you will find with Eq. (1.12), after substitution of Eq. (1.14) in the latter expression for b_n, $b_n = b_n$.
In paragraph 1.52 on The Heisenberg Representation, Eq. (1.59) should read:
$\psi^\dagger(\boldsymbol{r}, t) = \psi^*(\boldsymbol{r}, t = 0)e^{itH/\hbar}$.

Homework:

Homework 1,2.

Exercise 1. Prove that

$e^L a e^{-L} = a + [L, a] + \frac{1}{2!}[L, [L, a]] + \frac{1}{3!}\Big[L, \big[L, [L, a]\big]\Big] + \cdots$

where (a, L) are any operators.

Use will be made of the Taylor series expansion $e^x = \sum_{r=0}^{\infty} \frac{x^r}{r!}$. **(C1.1)**

After expansion of $e^L a e^{-L}$ into Taylor series of the operators, the above sum of commutators can be found. Well, this is not exactly a proof. It is a demonstration that the expansion works. How to prove it in a more formal way? That is not so easily done.
Taking a close look at the expansion in commutators for example the third expression of the commutators on the right hand side, you will find

$\frac{1}{3!}\Big[L, \big[L, [L, a]\big]\Big] = \frac{1}{3!}\sum_{k=0}^{3} \binom{3}{k} L^{3-k}\, a(-L)^k$. This indicates a general expression for the n^{th} expression: $\frac{1}{n!}\big[L, \ldots .\big[L, [L, a]\big] \ldots .\big] = \frac{1}{n!}\sum_{k=0}^{n} \binom{n}{k} L^{n-k}\, a(-L)^k$, **(C1.2)**

where the dots on the left-hand side of **(C1.2)** indicates: L, [and the dots on the right-hand side:].

Now something can be done with induction. So we assume **(C1.2)** to be true and then prove it for $n + 1$. First, let's illustrate induction for the fourth expression of commutators:

$\frac{1}{4!}\Big[L, [L, \big[L, [L, a]\big]\big]\Big] = \frac{1}{4!}\sum_{k=0}^{4} \binom{4}{k} L^{4-k}\, a(-L)^k$. **(C1.3)**

The left-hand side of **(C1.3)** can be written as

$\Big[L, [L, \big[L, [L, a]\big]\big]\Big] = L\Big[L, \big[L, [L, a]\big]\Big] - \Big[L, \big[L, [L, a]\big]\Big]L$, **(C1.4)**

where we neglect $\frac{1}{4!}$, since this factor sows up at the left-hand – and right-hand side. With $\Big[L, \big[L, [L, a]\big]\Big] = \sum_{k=0}^{3} \binom{3}{k} L^{3-k}\, a(-L)^k$, the right-hand side of **(C1.4)** can be written as:

$\Big[L, [L, \big[L, [L, a]\big]\big]\Big] = \sum_{k=0}^{3} \binom{3}{k} L^{4-k}\, a(-L)^k - \sum_{k=0}^{3} \binom{3}{k} L^{3-k}\, a(-L)^{k+1}$. **(C1.5)**

After some algebra collecting the expressions for $k = 0, k = 1, k = 2$ and $k = 3$ we obtain: $L^4 a - 4L^3 aL + 6L^2 aL^2 - 4LaL^3 + aL^4$. Well, it comes as no surprise, this equals $\sum_{k=0}^{4} \binom{4}{k} L^{4-k}\, a(-L)^k$. Induction works here.

Now for $n + 1$:

$\frac{1}{(n+1)!}\big[L, [L, \ldots .\big[L, [L, a]\big] \ldots .]\big] = \frac{1}{(n+1)!}\sum_{k=0}^{n+1} \binom{n+1}{k} L^{n+1-k}\, a(-L)^k$. **(C1.6)**

Again we neglect $\frac{1}{(n+1)!}$.

With **(C1.2)** the left-hand side of **(C1.6)** becomes:

$\sum_{k=0}^{n}\binom{n}{k} L^{n+1-k}\, a(-L)^k + \sum_{k=0}^{n}\binom{n}{k} L^{n-k}\, a(-L)^{k+1}$, **(C1.7)**
where we have included $+L$ into L^{n+1-k} and $-L$ into $(-L)^{k+1}$. The first term of this expression $(k=0)$ gives $L^{n+1}a$, the last one $(k=n)$ gives $a(-L)^{n+1}$.
What about the k term? Well, after carefully inspecting **(C1.7)** you need two terms: $\binom{n}{k} L^{n+1-k}a(-L)^k$ and $\binom{n}{k-1} L^{n-(k-1)}a(-L)^k (= \binom{n}{k-1} L^{n+1-k}a(-L)^k)$. So, we need the k term, the left part of **(C1.7)**, and the $(k-1)$term, the right part of **(C1.7)** in order to obtain equal powers of the operators. So collecting equal powers of the operators, the k term of **(C1.7)** finally reads: $\{\binom{n}{k} + \binom{n}{k-1}\}L^{n+1-k}a(-L)^k$. From a straightforward procedure the term between {} becomes: $\frac{(n+1)!}{k!(n+1-k)!} = \binom{n+1}{k}$.
To summarize: The first term is $L^{n+1}a$, the k term is $\binom{n+1}{k} L^{n+1-k}a(-L)^k$ and the last one is $a(-L)^{n+1}$. We know after collecting the terms, this can be written as $\sum_{k=0}^{n+1}\binom{n+1}{k} L^{n+1-k}\, a(-L)^k$. By induction we have proven **(C1.6)** to be correct.

Exercise 2. If F is any operator that does not explicitly depend on time, show that $\frac{\partial\langle F\rangle}{\partial t} = 0$ in an eigenstate of H with discrete eigenvalues.
With Eq. 1.52 we have $\frac{\partial}{\partial t}\langle F\rangle(t) = \frac{i}{\hbar}\langle[H,F]\rangle$. For the time independent Schrödinger equation we have with eigenvectors $|E_j\rangle$ and eigenvalues ε_j: $H|E_j\rangle = \varepsilon_j|E_j\rangle$. The eigenvalues of the Hermitian operator H are real. So Eq. 1.52 can be written as:

$$\frac{\partial}{\partial t}\langle F\rangle(t) = \frac{i}{\hbar}\langle[H,F]\rangle = \frac{i}{\hbar}\langle E_j|[HF-FH]|E_j\rangle = \frac{i}{\hbar}\langle E_j|\varepsilon_{j(}F-F)\varepsilon_j|E_j\rangle =$$
$$= \frac{i\varepsilon_j}{\hbar}\langle E_j|(F-F)|E_j\rangle.$$

And $\frac{i\varepsilon_j}{\hbar}\langle E_j|(F-F)|E_j\rangle = 0$.

Remark: In the above exercise we learned that for any operator not explicitly depending on time the time derivative is zero in an eigenstate of the Hamiltonian operator with discrete eigenvalues. In addition, we can add this applies also for a more general state when the set of eigenvectors is complete. The general state vector $|A\rangle$, say, can be expanded in the eigenvector base. Then again: $\frac{\partial}{\partial t}\langle F\rangle(t) = \frac{i}{\hbar}\langle A|[HF-FH]|A\rangle = 0$. Note: $|A\rangle$ can be written as: $|A\rangle = \sum\alpha_j\,|E_j\rangle$ and $\langle A|[HF-FH]|A\rangle = \sum\langle E_j\,|\alpha_j^*\varepsilon_j(F-F)\sum\varepsilon_j\,\alpha_j|E_j\rangle$.

2. One Dimension.

This chapter is about the one-dimensional Schrödinger equation, the square well, the harmonic oscillator and various types of potential all leading to exact solutions.

2.1 Square well.

Remark: In section 2.1 Mahan introduced the expression: binding energy. It is clear that there is a direct relation between binding energy and de eigenvalues.
Mahan started this section with the square well of infinite positive potential- “walls” and width a. Inside this well, $0 < x < a$, the potential $V(x)$ is zero.

The Schrödinger equation Eq. (2.3) is: $\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+E\right)\psi=0$.
The boundary conditions are: $\psi(x)=0$, at $x=0$ and $\psi(x)=0$ at $x=a$.
No solutions exist for $E<0$. Mahan gives the physical meaning of this statement. The mathematics are: for $E<0$, the solution of the above wave equation is similar to Eq. (2.27): $\psi(x)=C_3e^{-\alpha x}+C_4e^{\alpha x}$. So for $x=0$,
$C_3=-C_4$ and for $x=a$, $C_3(e^{-\alpha x}-e^{\alpha x})=0$. With $a\neq 0$, $C_3=0$: no solution for $E<0$.
As mentioned above inside the well the potential $V(x)$ is zero. This is not of vital importance. We could have set inside the well $V(x)$ equal to a positive value, V_1 say, or a negative one, V_2 say. In the first case, V_1, to find solutions $-V_1+E>0$ and in the second one $V_2+E>0$.
The second example is equivalent to the first.
The third example is for a potential well/box $V(x)$ given by Eq. (2.23) and Figure 2.2.
$V(x)=\infty$ for $x<0$, $V(x)=-V_0$ for $0<x<a$ and $V(x)=0$ for $a<x$; V_0 is positive.
Mahan discussed bound states first. A bound state describes a system where a particle is subject to a potential such that the particle has a tendency to remain localized in one or more regions of space. Caveat: in Eq.(2.24) it is less confusing to write $p=p_B$ for bound states with eigenvalues $E=E_B$.
Again for $x<0$, $\psi(x)=0$.
In the region $a<x$ with $V(x)=0$, the Schrödinger equation is $\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+E\right)\psi=0$.
With $E<0$, bound states, the eigen function decays exponentially. For $0<x<a$ the Schrödinger equation is $\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-V(x)+E\right)\psi=0$, where $V(x)=-V_0$, and $V_0+E>0$.
With $V_0+E>0$ the boundary conditions can be fulfilled and the general solutions are given by Eqs. (2.25) and (2.27). A bound state is found for $0<E+V_0<V_0$. Mahan found a minimum eigenvalue $E>-V_0+\frac{\pi^2}{4}E_a$ with $E_a=\frac{\hbar^2}{2ma^2}$. In Eq. (2.36) Mahan defined the *strength of the potential:* $g^2=\frac{V_0}{E_a}$ and he introduced a dimensionless binding energy ε through $E=-\varepsilon V_0$. Plug ε and g^2 into $E>-V_0+\frac{\pi^2}{4}E_a$ and we obtain $\varepsilon<1-(\frac{\pi}{2g})^2$. Then with $\varepsilon>0$ the expression for ε is $0<\varepsilon<1-(\frac{\pi}{2g})^2$. Now we see that the smallest or minimum binding energy is found for $\varepsilon\to 0$, then $g=\frac{\pi}{2}$. This is also the minimum value for g or minimum critical value g_c as represented by Eq. (2.38). Mahan derived the minimum value of the coupling strength g_c with help of Eq. (2.37).
In the middle of page 20 Mahan writes:"…the two equations in (2.24)-2.26), except now $\alpha^2=-k^2<0$. " This is confusing. α is related with bound states E_B and k is related with continuous states E_k. So $\alpha^2\neq -k^2$.
At the bottom of page 21 Mahan used the expression "unrenormalized". I was not aware Mahan has discussed the subject of renormalization.

The fourth example with constant potentials discussed by Mahan is, when a particle reflects at a barrier. The transmission is discussed for a particle entering from the right and from the left (Fig. 2.4). The equations derived by Mahan are extended to the transmission and reflection of a barrier of any shape and thickness. In Fig. 2.5, the fifth example, a barrier of any shape(height) and thickness is represented by a grey box. I think to find expressions for

R_L, T_{RL} , etc, expressed in the amplitude of the incoming wave and the wave numbers k and p, the geometry of the barrier has to be known. In the text below Figure 2.5 the equations for the fifth example are the same as for a step function potential.
Fig. 2.5 consists of two parts: **(a)** and **(b).** The text below Eq.(2.72) : "In figure 2.5b, take the complex conjugate of the wave coming from the left". Looking at what Mahan did, the complex conjugate of the left incoming wave in Fig. 2.5**(a)** is taken, given in Eq. (2.73). Furthermore Mahan stated: "Since Schrödinger's equation is invariant under complex conjugate operation….". The Hamiltonian is invariant too?
In addition Mahan mentioned: "In fact, the complex conjugate is the time- reversal operation….". Is there a time reversal operator? Time is not explicitly present.
Mahan constructed the complex conjugate by multiplying the two eigen functions representing the particle entering from the right and the left by R_L^* and T_{LR}^* respectively. Why these two coefficients? I will come back to this question later on.
From the resulting equations he derived for example: $T_{RL} = \frac{p}{k} T_{LR}$, Eq.(2.81).
Now, look at Eq. (2.70) example four, there we see: $T' = \frac{p}{k} T$. This is the same as the result in Eq.(2.81), example number five.
Let us return to example four and use the same procedure as used in example five. We do not use the matching at $x = 0$. We find:
for $x < 0$: $I^* = |R|^2 + T^* T'$ **(C2.1)**
and $R^* = R^* I$. So $I = 1$, and $I^* = 1$;
for $x > 0$: $T^* R' + R^* T = 0$ **(C2.2)**
and $T^* = T^* I'$. So $I' = 1$, and $|I'|^* = 1$.
Now we look at the conservation of currents.
For a particle entering from the left, with the notation of Mahan:
$v_p |T|^2 + v_k |R|^2 = v_k |I|^2$. **(C2.3)**
For a particle entering from the right:
$v_k |T'|^2 + v_p |R'|^2 = v_p |I'|^2$. **(C2.4)**
With $I^* = 1$, Eq. **(C2.1)** can be written as $1 = |R|^2 + T^* T'$ equivalent to Eq. 2.77.
Eq. **(C2.2)** can be written as: $R' = -\frac{R^*}{T^*} T$ being equivalent to Eq. 2.82.
With $I = 1$, **(C2.3)** and the notation of Mahan: $|T|^2 = \frac{k}{p}(1 - |R|^2)$ **(C2.5)**
equivalent to Eq. 2.79
With $I' = 1$, **(C2.4)** and the notation of Mahan: $|T'|^2 = \frac{p}{k}(1 - |R'|^2)$ **(C2.6)**
equivalent to Eq. 2.80.
The above equations give the solution $|T'| = \frac{p}{k} |T|$, equivalent to Eq. 2.77.
From Eq. (2.53) we learn with the assumptions $E > V_0$ and $V_0 > 0$, k^2 to be larger than p^2. What does that mean for R and T with $I = 1$given in Eqs. (2.56) and (2.57)? Well, it looks like T is larger than one. What is the physical meaning of that? Does the particle wave, the transmitted one get a kind of boost from the positive potential step?
Above I raised the question why Mahan used the coefficients R_L^* and T_{LR}^* to construct the "time-reversed state" ψ_L^*. With the amplitudes of the incoming waves from the right and from the left equal to unity and equating ψ_L^* equal to $A\psi_L + B\psi_R$ the general coefficients are found to be $A = R_L^*$ and $B = T_{RL}^*$. Use has been made of the equations (2.71), (2.72) and

(2.73.). Furthermore for $x > 0$, the coefficient of e^{ipx} in the expression for ψ_L^* is forced to zero. Consequently $R_L^* T_{LR} + T_{LR}^* R_R = 0$. This leads directly to Eq. (2.82). See also Eq.(2.76).

Homework 1, 2, 3, 4, 5, 6, 7.

Exercise 1.

Derive the numerical value in eV for the bound-state energy E of an electron in the one-dimensional square-well potential:

$$V(x) = \begin{cases} -V_0 \; for \; |x| < b \\ \;0 \;\; for \; |x| > b \end{cases}$$

where $b = 1.0$ Å and $V_0 = 1.0$ eV. What is the critical value of coupling strength g_c for this potential?

To begin with: when the potential is symmetric, the eigenfunctions are either of even or odd parity(Mahan, page 17). Even parity eigenfunctions are in this case cosine functions. Odd parity eigenfunctions are sine functions. The Schrödinger equation:

for $|x| < b$: $\frac{d^2\psi(x)}{dx^2} + \beta^2\psi(x) = 0$ and $\beta^2 = \frac{2m}{\hbar}(V_0 + E)$. This gives the solution for

$\psi(x) = C_1 \sin(\beta x) + C_2 \cos(\beta x)$ **(C.2.9)**

for $|x| > b$: $\frac{d^2\psi(x)}{dx^2} - \alpha^2\psi(x) = 0$ and $\alpha^2 = -\frac{2m}{\hbar^2}E$.

$\psi(x) = C_3 e^{-\alpha x} + C_4 e^{\alpha x}$ or $\psi(x) = C_3 e^{-\alpha|x|}$. **(C.2.10)**

Now we start with even parity eigenfunctions:

So $|x| < b$: $\psi(x) = C_2 \cos(\beta x)$ and **(C.2.11)**

$|x| > b$: $\psi(x) = C_3 e^{-\alpha|x|}$, ψ vanishes for $x \to \infty$. **(C.2.12)**

We match both functions and their derivatives at $x = b$ (matching at $-b$ creates no new information): with Eqs. **(C.2.11)** and **(C.2.12)** :

$C_2 \cos(\beta b) = C_3 e^{-\alpha b}$ and $C_2 \beta \sin(\beta b) = C_3 \alpha e^{\alpha b}$. Dividing this two expressions leads to the eigenvalue equation: $\tan(\beta b) = \frac{\alpha}{\beta}$ or $\tan\left(\sqrt{\frac{V_0+E}{E_b}}\right) = \sqrt{\frac{-E}{V_0+E}}$ and $E_b = \frac{\hbar^2}{2mb^2}$. Bound states exist for $-V_0 < E < 0$. So, the tangent function is positive: $0 < \sqrt{\frac{E+V_0}{E_b}} < \frac{\pi}{2}$. The left-hand side of this expression produces no new information. The right-hand side leads to

$E < -V_0 + \frac{\pi^2}{4} E_b$. **(C2.13)**

The lower bound state can be found for $E > -V_0$. The upper bound state is given by Eq. **(C2.13)**. What about the factor $\frac{\pi^2}{4} E_b$? Let us look at the numerical value. Using the mass of the electron we have: $E_b = 3{,}75$ eV. Bound state can be found for:

$-1 < E < 8.24$ eV. The upper bound is positive, consequently, $-1 < E < 0$. Well, this could have been said on beforehand. Are there bound states actually? Look again at Eq. **(C.2.13).** We also have $-V_0 < E < 0$. So $-V_0 < E < -V_0 + \frac{\pi^2}{4} E_b$. This is inconclusive.

Using $E = -\varepsilon V_0$ and $g^2 = \frac{V_0}{E_b}$, the eigenvalue equation $\tan\left(\sqrt{\frac{V_0+E}{E_b}}\right) = \sqrt{\frac{-E}{V_0+E}}$, can be written as : $\tan\left(\sqrt{g^2(1-\varepsilon)}\right) = \sqrt{\frac{\varepsilon}{1-\varepsilon}}$. The critical binding is found for $\varepsilon \to 0$. Then $\tan(g) = 0$ and the minimum value of $g_c = 0$.

g is defined as $g^2 = \frac{V_0}{E_b}$. With numerical values: $g^2 = \frac{1}{3.75}$ or $g = 0.52$
Now we apply the odd parity eigenfunction:
$|x| < b$: $\psi(x) = C_1 \sin(\beta x)$. **(C.2.14)**
Again we match both functions and their derivatives, Eqs. **(C2.14)** and **(C2.12)**, at $x = b$ (matching at $-b$ gives no new information): $C_1 \sin(\beta b) = C_3 e^{-\alpha b}$ and $C_1 \beta \cos(\beta b) = -C_3 \alpha e^{\alpha b}$. Dividing these two expressions: $\tan(\beta b) = -\frac{\beta}{\alpha}$.
Then the minimum eigenvalue is found from $\sqrt{\frac{E+V_0}{E_b}} > \frac{\pi}{2}$ or $E > -V_0 + \frac{\pi^2}{4} E_b$. Plug in the numerical values and $E > 8.24$ eV. Since E has to be < 0 we conclude: no bound states. The potential well is too shallow.
What about the critical value of the coupling strength g_c?
g is defined as $g^2 = \frac{V_0}{E_b}$. With numerical values: $g^2 = \frac{1}{3.75}$ or $g = 0.52$.
For the odd parity eigenfunction we can use the minimum coupling strength or minimum potential strength g_c , given by Eq. (2.38), $g_c = \frac{\pi}{2}$. Consequently $g < g_c$ and there are no bound states.
What conclusion can be drawn? Only a bound state of the even parity type?
Well, according to Fitzpatrick, no odd parity bound states can be found for $g < g_c$.

Exercise 2.
Make a graph similar to Figure 2.8 of the solutions of Eq. (2.37) over the range of $0 < g < 10$. Show that new bound state start at $g_{cn} = \pi(n + \frac{1}{2})$.
Remark: I think Figure 2.8 should read Figure 2.10 after reading the text.
As given by Mahan, the eigenvalue equation Eq. (2.37) can be solved for various values of g using graph paper or with help of a computer.
The lowest bound state started at $g_c = \frac{\pi}{2}$.
Eq. (2.38) states that the eigenvalues start at the following critical values: $g_c = \frac{\pi}{2}(2n + 1) = \pi\left(n + \frac{1}{2}\right)$. I think that Eq.(2.33) also gives the maximum eigenvalue. So, Eq.(2.34) becomes $\pi(n + 1) > \sqrt{\frac{V_0+E}{E_a}} > \frac{\pi}{2}(2n + 1)$. So $-V_0 + \pi^2 E_a > E > -V_0 + \frac{\pi^2}{4} E_a$.
By computing, numerical or graphical, the solutions of the eigenvalue equation $\tan\sqrt{g^2(1-\varepsilon)} = -\sqrt{\frac{1-\varepsilon}{\varepsilon}}$ for the various values of g, you can check the critical values of $g = g_{cn} = \pi(n + \frac{1}{2})$. An eigenvalue by inspection: $\varepsilon = 1$. This eigenvalue is found with all calculations. For $g > \frac{\pi}{2}$ you will find additional values for ε.
For example: $g = 2$, we have $\varepsilon = 1.02$ and $\varepsilon = 1$. For $g = \frac{5\pi}{3}$, you will find for ε: $0.508, 0.875$ and 1 (With help of WolframAlpha).

Exercise 3.

A particle in a one-dimensional square well of infinite sides is confined to the interval $0 < x < L$. The eigenfunctions are given in Eq. (2.19). Prove the relation $\sum_{n=1}^{\infty} \phi_n(x)\phi_n(x') = C\delta(x-x')$, by evaluating the summation, and determine the constant C.

So prove $\frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi x'}{L}\right) = C\delta(x-x')$. **(C.2.15)**

For the left-hand side of **(C.2.15)** we write:

$$\frac{2}{L}\sum_{n=0}^{\infty}\frac{1}{4}\left(e^{\frac{-in\pi(x-x')}{L}} + e^{\frac{in\pi(x-x')}{L}} - e^{\frac{in\pi(x+x')}{L}} - e^{\frac{-in\pi(x+x')}{L}}\right).$$

Change the sign of n in the first and fourth term in the above expression, then we have:

$$\frac{1}{2L}\sum_{n=-\infty}^{\infty}\left(e^{\frac{in\pi(x-x')}{L}} - e^{\frac{in\pi(x+x')}{L}}\right). \qquad \textbf{(C.2.16)}$$

We use the delta function representation[1] for the expression in **(C2.16)** and obtain, using $\delta\left[\frac{\pi(x-x')}{L}\right] = \frac{L}{\pi}\delta(x-x')$ (Dirac), :

$$\frac{1}{2\pi}\left(\delta(x-x') - \delta(x+x')\right).$$

We know $0 < x < L$. Likewise, $0 < x' < L$, consequently

$\delta(x+x') = 0$ for $0 < x < L$. This finally leads to:

$\frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi x'}{L}\right) = \delta(x-x')$. So $C = 1$.

Exercise 4.

For the potential shown in Figure 2.1, prove Eq. (2.51) by doing the integral. ψ_b and ψ_k are the bound and continuum eigenfunctions.

Remark: I think Figure 2.2 is meant, since figure 2.1 illustrates bound sates only.

The integral for orthogonality reads: $0 = \int_0^{\infty} \psi_B\psi_k\, dx$, Eq. (2.51). This equation is correct for real wave functions. In general, the orthogonality relation is given by Eq.(1.12). Then Eq.(2.51) is $0 = \int_0^{\infty} \psi_B^*\psi_k\, dx$.

The bound states are given by Eq.(2.29):

$$\psi_B = \begin{cases} 0\,, & x < 0 \\ C_1 \sin(p_B x)\,, & 0 < x < a \\ C_3 e^{-\alpha x}, & a < x \end{cases}$$

The continuum states are given by Eq.(2.42):

$$\psi_k = \begin{cases} a_1 \sin(p_k x), & 0 \\ D\sin(kx+\delta)\,, & a < x \end{cases}$$

Mahan used δ as a phase shift in Eq.(2.42). To find out about the continuum- and bound wave functions to be orthogonal we calculate the constants C_1, etc. of the wave functions. For the bound states the procedure to find the constant by means of normalization is rather straightforward as shown by Mahan.

C_1 is given in Eq.(2.244): $C_1 = \sqrt{2}\left(a - \frac{\sin(2p_B a)}{2p} + \frac{\sin^2(p_B a)}{\alpha}\right)^{-1/2}$, **(C.2.17)**

where p and α are given by Eqs.(2.24) and (2.25).

With Eq.(2.30): $C_3 = C_1 \sin(p_B a) e^{\alpha a}$. **(C.2.18)**

For the continuum states delta function normalization is used, discussed in section 2.8.3 by

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[1] $\delta(x-a) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} e^{ik(x-a)}$, *Algebraic and Analytical Methods*, www.dlmf.nist.govn

Mahan. The delta function is represented by:

$2\pi\delta(\mathrm{k}-\mathrm{k}') = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}x(\mathrm{k}-\mathrm{k}')}\mathrm{d}x.$

In section 2.8.3, Mahan derived the normalization constant $\mathrm{D} = 2$. So, with Eq.(2.47) we find for a_1: $\mathrm{a}_1 = 2\frac{\sin(\mathrm{ka}+\delta)}{\sin(\mathrm{p_k a})}$. **(C.2.19)**

Now with the constants for the wave functions we can try to prove :

$0 = \int_0^{\infty} \psi_\mathrm{B}\psi_\mathrm{k}\,\mathrm{d}x.$

"All solutions of the Schrödinger's equation must be orthogonal to all others with the same potential energy function", Mahan page 22.

We have the expressions for the wave functions. So let us find out about the orthogonality. Is the following equality true:

$0 = \int_0^{\mathrm{a}} \mathrm{C}_1 \sin(\mathrm{p_B}x)\,\mathrm{a}_1 \sin(\mathrm{p_k}x)\mathrm{d}x + \int_{\mathrm{a}}^{\infty} \mathrm{C}_3\,\mathrm{e}^{-\alpha x}\mathrm{D}\sin(\mathrm{k}x+\delta)\mathrm{d}x\,.$ **(C.2.20)**

The first integral is reads:

$\frac{\mathrm{C_1 a_1}}{2}\Big(\frac{1}{\mathrm{p_B}-\mathrm{p_k}}\sin(\mathrm{p_B}-\mathrm{p_k})\,\mathrm{a} - \frac{1}{\mathrm{p_B}+\mathrm{p_k}}\sin(\mathrm{p_B}+\mathrm{p_k})\mathrm{a}\Big).$ **(C.2.21)**

The second integral in **(C.2.20)** is evaluated by means of integration by parts.

This results into:

$(1+\frac{\alpha^2}{\mathrm{k}^2})\int_{\mathrm{a}}^{\infty} \mathrm{e}^{-\alpha x}\sin(\mathrm{k}x+\delta)\,\mathrm{d}x = \frac{1}{\mathrm{k}}\mathrm{e}^{-\mathrm{a}\alpha}(\frac{\alpha}{\mathrm{k}}\sin(\mathrm{ka}+\delta)+\cos(\mathrm{ka}+\delta)).$

Caveat: with Eq.(2.26) and Eq.(2.41) we could find $\left(1+\frac{\alpha^2}{\mathrm{k}^2}\right) = 0$. However, keep in mind for α bound states $\mathrm{E} = \mathrm{E_B} < 0$ and for k continuous states $\mathrm{E} = \mathrm{E_k} > 0$.

Substitute the integral $\int_{\mathrm{a}}^{\infty}$… and **(C.2.21)** into **(C.2.20)** and find out whether the right-hand side of **(C.2.20)** is 0. To this end we use Eq.(2.30), **(C.2.19)** and $\mathrm{D} = 2$.

$\frac{\mathrm{C}_1\sin(\mathrm{ka}+\delta)}{\sin(\mathrm{p_k a})}\Big(\frac{1}{\mathrm{p_B}-\mathrm{p_k}}\sin(\mathrm{p_B}-\mathrm{p_k})\,\mathrm{a} - \frac{1}{\mathrm{p_B}+\mathrm{p_k}}\sin(\mathrm{p_B}+\mathrm{p_k})\mathrm{a}\Big) +$

$+\frac{2\mathrm{kC}_1\sin(\mathrm{p_B a})}{\mathrm{k}^2+\alpha^2}\Big(\frac{\alpha}{\mathrm{k}}\sin(\mathrm{ka}+\delta)+\cos(\mathrm{ka}+\delta)\Big) = 0\ ?$ **(C.2.22)**

We divide **(C.2.22)** by C_1 and $\sin(\mathrm{ka}+\delta)$, both $\neq 0$, then we have

$\frac{1}{\sin(\mathrm{p_k a})}\Big(\frac{1}{\mathrm{p_B}-\mathrm{p_k}}\sin(\mathrm{p_B}-\mathrm{p_k})\,\mathrm{a} - \frac{1}{\mathrm{p_B}+\mathrm{p_k}}\sin(\mathrm{p_B}+\mathrm{p_k})\mathrm{a}\Big) +$

$+\frac{2\mathrm{k}\sin(\mathrm{p_B a})}{\mathrm{k}^2+\alpha^2}\Big(\frac{\alpha}{\mathrm{k}}+\cot(\mathrm{ka}+\delta)\Big) = 0\ ?$ **(C.2.23)**

Substitute into **(C.2.23)** , $\frac{1}{\tan(\mathrm{ka}+\delta)} = \frac{\mathrm{p_k}}{\mathrm{k}}\frac{1}{\tan(\mathrm{p_k a})}$, Eq.(2.49), and multiply by $\sin(\mathrm{p_k a})$

$\frac{1}{\sin(\mathrm{p_k a})}(\frac{1}{\mathrm{p_B}-\mathrm{p_k}}\sin((\mathrm{p_B}-\mathrm{p_k})\mathrm{a}) - \frac{1}{\mathrm{p_B}+\mathrm{p_k}}\sin((\mathrm{p_B}+\mathrm{p_k})\mathrm{a})) + \frac{2\mathrm{k}\sin(\mathrm{p_B a})}{\mathrm{k}^2+\alpha^2}(\frac{\alpha}{\mathrm{k}}+ +\cot(\mathrm{ka}+\delta))\ .$

We are still trying to find out whether this expression is zero.

Rewrite this expression by expending the two first sin functions:

$\frac{\mathrm{p_k}\sin(\mathrm{p_B a})\cot(\mathrm{p_k a})-\mathrm{p_B}\cos(\mathrm{p_B a})}{\mathrm{p_B^2}-\mathrm{p_k^2}} + \frac{2\mathrm{k}\sin(\mathrm{p_B a})}{\mathrm{k}^2+\alpha^2}\Big(\frac{\alpha}{\mathrm{k}}+\cot(\mathrm{ka}+\delta)\Big) = 0\ ?$ **(C.2.24)**

What about the factor $\frac{(\mathrm{p_B^2}-\mathrm{p_k^2})}{(\mathrm{k}^2+\alpha^2)}$? Back to some physics. With the Eqs. (2.24), (2.26) and (2.41): $\frac{(\mathrm{p_B^2}-\mathrm{p_k^2})}{(\mathrm{k}^2+\alpha^2)} = -1$. Substitute this result into **(C2.24)** :

$(\mathrm{p_k}\sin(\mathrm{p_B a})\cot(\mathrm{p_k a}) - \mathrm{p_B}\cos(\mathrm{p_B a})) +$

$-\mathrm{k}\sin(\mathrm{p_B a})\left(\cot(\mathrm{ka}+\delta)+\frac{\alpha}{\mathrm{k}}\right) = 0\ ?$ **(C2.25)**

Now $\frac{1}{\tan(\mathrm{ka}+\delta)} = \frac{\mathrm{p_k}}{\mathrm{k}}\frac{1}{\tan(\mathrm{p_k a})}$, Eq.(2.49). Substitute this into **(C2.25)** :
$\mathrm{p_k}\frac{\sin(\mathrm{p_B a})}{\tan(\mathrm{p_k a})} - \mathrm{p_B}\cos(\mathrm{p_b a}) - \mathrm{p_k}\frac{\sin(\mathrm{p_B a})}{\tan(\mathrm{p_k a})} - \alpha\sin(\mathrm{p_B a}) = 0?$
Well, this results into: $\tan(\mathrm{p_B a}) + \frac{\mathrm{p_B}}{\alpha} = 0?$ Eq.(2.30): it is zero indeed and
$0 = \int_0^\infty \psi_\mathrm{B}\psi_\mathrm{k}\,\mathrm{dx}$.

Exercise 5.
Consider in one dimension the solutions of the Schrödinger's equation for the half-space problem and $V_0 > 0$:

$$V(x) = \begin{cases} V = \infty \ , x \leq 0 \\ V_0 \ , 0 < x < a \\ V = 0, x > a \end{cases}$$

Find an expression for the phase shift $\delta(k)$ for the two cases (a) $0 < E < V_0$ and (b) $V_0 < E$.
a) $0 < E < V_0$ and $V_0 > 0$. "Bound states". These are no real bound states.
$0 < x < a$:
Schrödinger's equation: $\frac{d^2\psi(x)}{dx^2} - \alpha^2\psi(x) = 0$ and $\alpha^2 = \frac{2m}{\hbar^2}(V_0 - E_B)$.
The general solution is $\psi(x) = C_1 e^{-\alpha x} + C_2 e^{\alpha x}$.
For $x = 0$, $V(x) = \infty$, so $\psi = 0$ and we have $C_1 = -C_2$.
The wave function is $\psi(x) = C_1(e^{-\alpha x} - e^{\alpha x}) = -2C_1\sinh(\alpha x)$. **(C.2.26)**
$x > a$**:**
$\frac{d^2\psi(x)}{dx^2} + E_B\psi(x) = 0$. With general solution expressed with help of phase shift δ:
$\psi(x) = a_1\sin(k_B x + \delta)$ and $k_B = \sqrt{\frac{2m}{\hbar^2}E_B}$.
At $x = a$ the wave function **(C.2.26)** and its derivative are continuous:
$-2C_1\sinh(\alpha a) = a_1\sin(k_B a + \delta)$, **(C.2.27)**
$-2\alpha C_1\cosh(\alpha a) = k_B a_1\cos(k_B a + \delta)$. **(C.2.28)**
Divide these two equations and we have $\frac{\tanh(\alpha a)}{\alpha} = \frac{\tan(k_B a + \delta)}{k_B}$.
The phase shift is $\delta = -k_B a + \arctan\left[\frac{k_B}{\alpha}\tanh(\alpha a)\right]$. **(C.2.29)**
b) Now $V_0 < E_k$. Continuous states.
$0 < x < a$:
Schrödinger's equation: $\frac{d^2\psi(x)}{dx^2} + p^2\psi(x) = 0$ and $p^2 = \frac{2m}{\hbar^2}(E_k - V_0)$.
For $x = 0$, we have $\psi = 0$ and $\psi(x) = a_2\sin(px)$.
$x > a$:
the wave function is $\psi(x) = D\sin(k_k x + \gamma)$ and $k_k^2 = \frac{2m}{\hbar^2}E_k$.
At $x = a$ the wave function and its derivative are continuous:
$a_2\sin(pa) = D\sin(k_k a + \gamma)$,
$a_2\mathrm{p}\sin(px) = Dk_k\cos(k_k a + \gamma)$.

Again, divide these two equations and we find $\frac{\tan{(pa)}}{p} = \frac{\tan(k_k a+\gamma)}{k_k}$.
The phase shift is $\gamma = -k_k a + \arctan{[\frac{k_k}{p}\tan(pa)]}$.

Exercise 6.
Consider a particle of energy $E > V_0 > 0$ approaching a potential step from the left.
The Hamiltonians in the two regions are:

$$H\begin{cases} \frac{p^2}{2m_L}\ , x < 0 \\ \frac{p^2}{2m_R} + V_0\ , x > 0 \end{cases}$$

where $m_L \neq m_R$ and $V(x) = V_0\boldsymbol{\Theta}(x)$. $\boldsymbol{\Theta}(x)$ is the Heaviside function.
Find the amplitude of the transmitted (T) and reflected wave (R), by matching at $x = 0$ the amplitude of the wave function and the derivative $\frac{1}{m_L}\frac{d\psi_L}{dx} = \frac{1}{m_R}\frac{d\psi_R}{dx}$. Show that this choice of matching conserves the current of particles.
For $x < 0$: $\frac{d^2\psi_L}{dx^2} + E\psi_L = 0$, and $k^2 = \frac{2m_L E}{\hbar^2}$.
Then $\psi_L = Ie^{ikx} + Re^{-ikx}$.
For $x > 0$: $\frac{d^2\psi_R}{dx^2} + (E - V_0)\psi_R = 0$, and $p^2 = \frac{2m_R}{\hbar^2}(E - V_0)$.
Then $\psi_R = Te^{ipx}$. Now at $x = 0$, $\psi_L = \psi_R$ and
$I + R = T$. **(C.2.30)**
Furthermore: $\frac{1}{m_L}\frac{d\psi_L}{dx} = \frac{1}{m_R}\frac{d\psi_R}{dx}$ at $x = 0$ and
$\frac{k}{m_R}(I - R) = \frac{p}{m_R}T$. **(C.2.31)**
With **(C.2.30)** and **(C.2.31)** we find:
$R = I\frac{km_R - pm_L}{km_R + pm_L}$. **(C.2.32)**
$T = 2I\frac{km_R}{km_R + pm_L}$. **(C.2.33)**
Now we check the matching of the derivatives by calculating the particle currency given by Eq.(2.58): $j = \frac{\hbar}{2mi}[\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}]$, the current operator.
The incoming particle: $\psi_i(x) = Ie^{ikx}$, then $j_i = \frac{\hbar k}{m_L}|I|^2$. **(C.2.34)**
The reflected wave : $\psi_r = Re^{-ikx}$, then $j_r = -\frac{\hbar k}{m_L}|R|^2$. **(C.2.34)**
The transmitted wave: $\psi_t = Te^{ipx}$, then $j_t = \frac{\hbar p}{m_R}|T|^2$. **(C.2.36)**
With $j_t - j_r = j_i$ and the equations **(C.2.32)**-**(C.2.36)** we indeed find the proposed matching condition justified.

Exercise 7.
A particle of mass m moves in a one-dimensional square-well potential with walls of infinite height: the particle is constrained in the region $L/2 < x < L/2$.
a. What are the eigenvalues and eigenfunctions of the two lowest states in energy?
b. What is the expectation value of the energy for a state that is an equal mixture of these two states?

c. For the state in (b), what is the probability, as a function of time, that the particle is in the right-hand side of the well?

a) See Mahan page 17. The wave function:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left[k_n\left(x+\frac{L}{2}\right)\right], \qquad \textbf{(C.2.37)}$$

with $k_n = \frac{n\pi}{L}$, and $E_n = \frac{\hbar^2 k_n^2}{2m}$.

So $\psi_n = \sqrt{\frac{2}{L}}\left[\sin\left(\frac{n\pi}{L}x\right)\cos\left(\frac{n\pi}{2}\right) + \cos\left(\frac{n\pi}{L}x\right)\sin\left(\frac{n\pi}{2}\right)\right]$.

As we see, the boundary conditions are fulfilled.

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad n \text{ is even,} \qquad \textbf{(C.2.38)}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right) \quad n \text{ is odd.} \qquad \textbf{(C.2.39)}$$

The eigenfunctions are:

$$\psi_1(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right) \text{ and } \psi_2(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right), \qquad \textbf{(C.2.40)}$$

The eigenvalues are, Eq. (2.12) and (2.13):

$$E_1 = \frac{\hbar^2\pi^2}{2mL^2}, \text{ and } E_2 = 4E_1. \qquad \textbf{(C.2.41)}$$

b) The expectation value of the energy for a state that is an equal mixture of the two states in **(C.2.40).**

The mixed state: $\psi_m = a(\psi_1(x) + \psi_2(x))$. The factor a is found by normalization.

$\psi_m = \frac{1}{\sqrt{L}}[\cos\left(\frac{\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right)]$

$\int_{-L/2}^{L/2} |\psi_m|^2\, dx = 1$. Substituting the two wave functions **(C.2.40)** and we find $a = \frac{1}{\sqrt{L}}$.

$$\text{So } \psi_m = \frac{1}{\sqrt{L}}[\cos\left(\frac{\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right)]. \qquad \textbf{(C.2.42)}$$

The expectation value for the energy:

$$\langle H\rangle = \int_{-L/2}^{L/2} \psi_m^*\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi_m dx. \qquad \textbf{(C.2.43)}$$

So the expectation value of the Hamiltonian will produce the expectation value of the energy.

Reminder: in Dirac notation of bra's , kets, eigenvectors and eigenvalues we have $\langle H\rangle = \langle\Psi|H|\Psi\rangle = \langle\Psi|E|\Psi\rangle = E\langle\Psi|\Psi\rangle = E$.

We substitute **(C.2.42)** into **(C.2.43)** and find:

$$\langle H\rangle = \frac{\hbar^2 5\pi^2}{2m2L^2} = E_m. \qquad \textbf{(C.2.44)}$$

We see $\langle H\rangle = E_m = \frac{1}{2}(E_1 + E_2)$.

c) For the state in (b), ψ_m, what is the probability, as a function of time, that the particle is in the right-hand side of the well, $0 < x < L/2$?

It is about time-dependency.

So we have to return to **(C.2.40)** and include $e^{-iE_n t/\hbar}$, where $n = 1$ and $n = 2$.

With **(C.2.42)** :

$$\psi_m = \frac{1}{\sqrt{L}}[\cos\left(\frac{\pi x}{L}\right)e^{-iE_1 t/\hbar} + \sin\left(\frac{2\pi x}{L}\right)e^{-iE_2 t/\hbar}], \qquad \textbf{(C.2.45)}$$

and

E_1 and E_2 given in **(C.2.41)** .

The probability as a function of time to find that the particle is in the right-hand side of the well, $0 < x < L/2$, is:

$P(t) = \int_0^{L/2} \psi_m^* \, \psi_m dx.$

Substitute **(C.2.45)** into $P(t)$, you will obtain after some goniometrical manipulation:

$P(t) = \frac{1}{2} + \frac{4}{3\pi}\cos[\frac{(E_1 - E_2)t}{\hbar}]$.

Hence with two states we will find time dependency for the probability.

2.2 Linear potentials.

In section 2.2 Mahan deals with linear potentials. The Schrödinger equation is converted into an Airy's equation.

Below Eq. (2.94) Mahan writes: "The last line shows that the integrand is an exact differential, which vanishes at both end points. The value of the sine function as $t \to \infty$ is not obvious, since it oscillates. However, it is to be zero anyway". For any unbound state?

In Fig. 2.6 the potential (a) and the wave function (b) is shown. There is no numerical relation between (a) and (b) . The energy level in (a) is not an eigenvalue. It illustrates the point where $z = 0$, the turning point.

Homework 8.

Exercise 8.

Derive an equation for the eigenvalues of the potential $V(x) = F|x|$, where $F > 0$ for values $-\infty < x < \infty$.

So we have a wedge, ramp, type symmetrical potential well with infinite walls.

Schrödinger's equation is $\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + (-F|x| + E)\psi(x) = 0.$

Keep in mind: "When the potential is symmetric, the eigen functions are either of even or odd parity"(Mahan).

We use the transformations of Eq. (2.85) and (2.86):

$x_0 = (\frac{\hbar^2}{2m})^{1/3}$,

$z = \frac{|x| - E/F}{x_0}$.

Schrödinger's equation reads: $\left(\frac{d^2}{dz^2} - z\right)\psi(z) = 0$. This is Airy's equation and the solution is

$\psi(z) = C_1 Ai(\frac{|x| - \frac{E}{F}}{x_0}).$

The eigenvalues of the eigenfunctions for $\psi(x)$ with odd parity are found with:

$\psi(0) = 0 = C_1 Ai(\frac{-E}{x_{0F}})$. The allowed eigenvalues for odd parity are:

$z_2 = -2.3381, 4 = -4.0879, z_6 = -5.5206, z_8 = -6.7867$, etc.

The eigenvalues of the eigenfunctions with even parity are found with:

$\frac{d\psi}{dx} = 0 = \frac{d}{dx}Ai(\frac{|x| - \frac{E}{F}}{x_0})$, at $x = 0$. The allowed eigenvalues are:

$z_1 = -1.0188, z_3 = -3.2482, z_5 = -4.8201, z_7 = -6.1633$, etc.
The above values for zeros z_n can be found from tables (Abramowitz and Stegun) or with help of WolframAlpha. Also a few values are given by Mahan page 29. As in the example given by Mahan for linear potentials $z_n < 0$, consequently $E_n(= -x_0 F z_{n)}) > 0$.

2.3 Harmonic oscillator.

Remark: On top of page 30 Mahan mentioned the question about the polynomial as a solution to the Hamiltonian on page 29. Solution to the Hamiltonian or the solution to the Schrödinger equation?
Mahan gave the eigen values and eigenvectors(functions) of the Schrödinger equation in the Eqs. (2.107-2.109). "A differential equation is a mathematical problem that is incompletely specified: the boundary conditions are needed to completely determine the eigenfunctions", Mahan. Which are the boundary conditions for the harmonic oscillator where the potential exists over all space? The potential is a symmetric function, consequently we find even parity eigenfunctions for $\frac{d\psi}{dx} = 0$, at $x = 0$; odd parity eigenfunctions are found for $\psi(0) = 0$. In addition, for $x \to \infty$, $V(x) \to \infty$, so $\psi(x) = 0$. Do these conditions produce the Hermite polynomials, the eigenvalues and the eigenvectors(functions) as solutions? Or are there just the Hermite polynomial's for $n = \frac{1}{2}(\varepsilon_n - 1)$?
Schrödinger's equation is:$\left[\frac{d^2}{d\xi^2} - \xi^2 + \varepsilon\right]\psi = 0$. Now we substitute the Hermite polynomial for the bound state $\psi_n = C_n H_n(\xi) e^{-\xi^2/2}$ into the Schrödinger's equation and obtain:
$-H_n - 2\xi\frac{dH_n}{d\xi} + \frac{d^2 H_n}{d\xi^2} + \varepsilon_n H_n = 0$. The constants drop out of the differential equation.
With help of Eq.(2.112) we rewrite the differential equation.
$\frac{dH_n}{d\xi} = 2nH_{n-1}$. Consequently: $\frac{d^2 H_n}{d\xi^2} = 2n\frac{dH_{n-1}}{d\xi} = 4n^2 H_{n-2}$. We substitute this result into $-H_n - 2\xi\frac{dH_n}{d\xi} + \frac{d^2 H_n}{d\xi^2} + \varepsilon_n H_n = 0$ and obtain $(\varepsilon_n - 1)H_n - 4n(\xi H_{n-1} - nH_{n-2}) = 0$.
With help of equation (2.111), $\xi H_n = \frac{1}{2}H_{n+1} + nH_{n-1}$, the equation for the eigenvalues is $\varepsilon_n = 2n + 1$. So the Hermite polynomials are solutions to Schrödinger's equation. The constant C_n is found by normalization : $1 = \int_{-\infty}^{\infty} d\xi \psi_n^* \psi_n$ and orthogonality is found by $0 = \int_{-\infty}^{\infty} d\xi \psi_n^* \psi_l$. This can be written as $\delta_{nl} = \int_{-\infty}^{\infty} d\xi \psi_n^* \psi_l$. With help of generating functions C_1 is found and equals N_n. This approach differs from what has been written on page 31 and 32. It differs indeed. Mahan writes on page 31: "Generating functions are useful for evaluating integrals of harmonic oscillator functions. They will used to prove (2.115): $I_{nl} = \int_{-\infty}^{\infty} d\xi \psi_n^*(\xi)\psi_l(\xi) = N_n N_l \int_{-\infty}^{\infty} d\xi H_n(\xi) H_l(\xi) e^{-\xi^2}$, Eq.(2.118)". I assume Mahan means to prove the first part $I_{nl} = \int_{-\infty}^{\infty} d\xi \psi_n^*(\xi)\psi_l(\xi)$, since the second part represent the integral of the wave functions in terms of Hermite polynomials. So, the second equality sign is an identity. I further assume I_{nl} to be the unity matrix. So, what is Mahan basically doing? I think to prove $I_{nl} = \delta_{nl}$. This is what he concluded on page 32. I think this is quantum mechanics upside down. $\delta_{nl} = \int_{-\infty}^{\infty} d\xi \psi_n^* \psi_l$ is part of the physics: the probability to find a particle in the whole interval is 1. Furthermore, the bound states are orthogonal. Even

orthonormal after normalization.
Mahan derived Eq. (2.124): $\int_{-\infty}^{\infty} d\xi H_n(\xi)H_l(\xi)e^{-\xi^2} = \frac{\delta_{nl}}{N_n^2}$. Well, plugging into this equation the unknown constant C_n, we have $\int_{-\infty}^{\infty} \frac{1}{C_n C_l}\psi_n(\xi)\psi_l\,(\xi)d\xi = \frac{\delta_{nl}}{N_l N_n}$, and $C_n = N_n$. This is concluded by Mahan: "….., and also derives the value of the normalization constant N_n".
Let's have a look once more at Schrödinger's equation is:$\left[\frac{d^2}{d\xi^2} - \xi^2 + \varepsilon\right]\psi = 0$.Playing with WolframAlpha you will find for $n = 0, \varepsilon = 1$:
$\psi = C_2\sqrt{\pi}e^{-\xi^2/2}erfi(\xi) + C_1 e^{-\xi^2/2}$, where $erfi(\xi) = \frac{2}{\sqrt{\pi}}\int_0^{\xi} e^{t^2}dt$. Consequently $C_2 = 0$ and $C_1 = N_0$. So $\psi_0 = N_0 H_0 e^{-\xi^2/2}$, even parity.
For $n = 1, \varepsilon = 3$ a solution is produced which is not so easy to recognise:
$\psi_1 = C_2 D_{-2}\left(i\sqrt{2}\xi\right) + C_1 D_1(\sqrt{2}\xi)$. The D_n-functions can be found in Whittaker and Watson. There, the relation with the Whittaker function $W_{k,j}$ can be found. Abramowitz and Stegun list the Whittaker function too. Again in the above expression for ψ_1 , $C_2 = 0$ and
$\psi_1 = N_1 2\xi e^{-\xi^2/2}$, odd parity.
For $n = 2, \varepsilon = 5$, WolframAlpha produces again error functions and a Gaussian function, the wave function ψ_2 is of even parity.

Susskind found the entire energy spectrum, eigenvalues, without solving the differential equation. Based on the sometimes called ladder operator developed by Dirac. Susskind did not solve the differential equation. On the other hand he just proposed as ground state a Gaussian distribution and found in this way the lowest ground energy E_0 .

At the bottom of page 31, above Eq. (2.119), in the line on the two generating functions $e^{-\xi^2}$, has to be included. See Eq. (2.121).
Now we will pay some attention to deriving Eqs. (2.128) and (2.129).
We write Eq. (2.111) as $\xi H_n = \frac{1}{2}H_{n+1} + nH_{n-1}$, Eq.(2.127). This equation is converted into eigenfunctions by multiplying Eq. (2.127) with the appropriate factor given in Eq. (2.108). Then on the left of Eq. (2.127) appears $\xi\psi_n$. On the right appears $N_n \exp(-\xi^2)$ with the Hermite polynomials
Mahan converted N_n on the right of the resulting equation to N_{n+1} and N_{n-1} respectively with help of Eq. (2.109).
The result for N_{n+1} is: $N_n = \sqrt{2(n+1)}N_{n+1}$, and for N_{n-1}: $N_n = \sqrt{\frac{1}{2n}}N_{n-1}$. We use both expressions for N_n. N_{n+1} with H_{n+1} and N_{n-1} with H_{n-1}.
Then $N_n n H_{n-1} = \sqrt{\frac{n}{2}}N_{n-1}H_{n-1}$ and $N_n\frac{1}{2}H_{n+1} = \sqrt{\frac{n+1}{2}}N_{n+1}H_{n+1}$, where we left $\exp(-\xi^2)$ out of account on both sides of these expressions. In using Eq. (2.108) for the right hand side of Eq. (2.127) with the above expressions including $\exp(-\xi^2)$ you will obtain Eq. (2.128) and consequently Eq. (2.129). The latter equation is given in the Dirac notation.
Nota bene: keep in mind, by converting N_n to $N_{n\pm1}$, we used Eq. (2.109) and
$N_{n+1} = [\sqrt{\pi}(n+1)!\,2^{n+1}]^{-1/2} = [2(n+1)\sqrt{\pi}(n!)2^n]^{-1/2} = [2(n+1)]^{-1/2}N_n$, etc.

With Eq. (2.129) Mahan derived the matrix element of Eq. (2.125) $\langle n|x|l\rangle$. In Eq. (2.130), e.g., $\delta_{n,l+1} = 1$ for $l + 1 = n$, or $l = n - 1$.
In order to derive the Hamiltonian, expressions such as $\xi^2|n\rangle$ are needed. The basis for that is Eq. (2.129). For the Hamiltonian we need also the derivative $\frac{d}{dx} = \frac{1}{x_0}\frac{d}{d\xi}$.
In Eq. (2.136) we find $\frac{d}{d\xi}H_n (= 2nH_{n-1})$ by differentiating H_n given in Eq.(2.113) and using Eq.(2.111).
Like we did for the matrix element of x, Eq. (2.139) for the matrix element for p is constructed. For the Hamiltonian we need the second derivative of the wave function. I consider the subscript of the Kronecker Delta in Eq. (2.140) a bit confusing.
Finally, Eq.(2.144), the eigenvalues are found: $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$. To me the relation between the boundary conditions for the differential equation of the quantum harmonic oscillator and the eigenvalues is not clear.
By plugging ψ_n of Eq. (2.108) into the Schrödinger equation, using Eqs. (2.110)-(2.112) you can find the expression for ε_n at $\xi = 0$.
First derive $\frac{d}{d\xi}\psi_n$: $\frac{d}{d\xi}\psi_n = -\xi\psi_n + 2n\frac{N_n}{N_{n-1}}\psi`_{n-1}$ where use has been made of Eq. (2.136).
To find the second derivative differentiate this expression once more and we arrive at:

$$\frac{d^2}{d\xi^2}\psi_n = -\psi_n - \xi\frac{d}{d\xi}\psi_n - 2n\xi\frac{N_n}{N_{n-1}}\psi_{n-1} + 4n(n-1)N_n e^{\frac{\xi^2}{2}}H_{n-2}. \qquad \textbf{(C2.46)}$$

This expression can be rewritten with help of the recursion relation Eq. (2.111):

$$H_{n-2} = \frac{\xi}{n}(\frac{\xi}{n}H_n - \frac{1}{2(n-1)}H_{n+1} - \frac{1}{2(n-1)}H_n \, . \qquad \textbf{(C.2.47)}$$

With Eq. (2.108), **(C2.46)** and **(C2.47)** we have for Schrödinger's equation:

$$-\psi_n(2n+1) - \xi\frac{d}{d\xi}\psi_n - 2n\xi\frac{N_n}{N_{n-1}}\psi_{n-1} + 4\xi^2\frac{n-1}{n}\psi_n - 2n\frac{N_n}{N_{n+1}}\psi_{n+1} - \xi^2\psi_n + \varepsilon\psi_n = 0.$$

For even parity,$\psi_n \neq 0$, at $\xi = 0$, this this gives: $\varepsilon = 2n + 1$.

Homework 11, 13, 14.

Exercise 11.
Find the exact eigenvalues for the potential

$$V(x) = \begin{cases} \infty & x < 0 \\ \dfrac{1}{2}Kx^2 & x > 0 \end{cases}$$

Hint: With a little thought, the answer may be found by doing no derivation.
A little thought:
For the above potential function we have $\psi(x) = 0$ at $x = 0$.
Mahan dealt with the Schrödinger's equation in section 2.3: the Harmonic oscillator. There the potential function is $V(x) = \frac{Kx^2}{2}$ for $-\infty < x < \infty$. A symmetrical potential function where we can find odd parity and even parity wave functions. The general solution is given in terms of Hermite H polynomials. In this exercise we do not have a symmetrical potential function and the boundary condition is: $\psi(0) = 0$. And this is the only boundary condition at $x = 0$.
From the recursion relations we have $\frac{1}{2}H_{n+1}(0) = -nH_{n-1}$ and $H_1 = 0$. Furthermore $H_0(0) = 1$ and $H_2(0) = -2$. So we learn for n is odd and nonnegative $\psi(0) = 0$, and n is

even $\psi(0) \neq 0$. Use has been made of the general solution for $\psi_n(\xi) = N_n H_n(\xi) e^{-\xi^2/2}$, Eq.(2.108), and $N_n \neq 0$.
The eigenvalues are $E_n = \hbar\omega(n + \frac{1}{2})$ for n is odd.
I do not know whether or not I gave sufficient little thought. Well, look at this problem from a different perspective. We have the harmonic oscillator and the infinite potential "wall" at $x = 0$. So, we know $\psi(0) = 0$. The boundary condition leading to odd parity solutions for the wave function. Consequently, we can mirror the oscillator at $x = 0$. Picture that and we immediately have the exact eigenvalues for the mirrored situation:
the eigenvalues are $E_n = \hbar\omega(n + \frac{1}{2})$ for n is odd.

Exercise 13.
Evaluate the following integral for the harmonic oscillator using generating functions:

$M_{nl} = \int_{-\infty}^{\infty} dx \phi_n(x) x \phi_l(x)$.
Evaluate to prove something? To prove what?
M_{nl} is the matrix element of the observable represented by the position operator. To evaluate means: find $\frac{x_0}{\sqrt{2}}[\sqrt{n}\delta_{n,l+1} + \sqrt{(n+1)}\delta_{n,l-1}]$?
As Mahan writes: "Generating functions are useful in evaluating integrals of harmonic oscillator functions". In the section of the harmonic oscillator Mahan evaluated the matrix element $\langle n|x|l\rangle = M_{nl}$ of the position operator. This is done with the Dirac approach with bra's and kets.
a). We could follow the procedure of page 31 for the normalization.
$\phi_n(x) = \frac{1}{\sqrt{x_0}}\psi_n\left(\frac{x}{x_0}\right) = \frac{1}{\sqrt{x_0}}\psi_n(\xi)$.
Then we evaluate the integral $M_{nl} = x_0 \int_{-\infty}^{\infty} d\xi \psi_n(\xi) \xi \psi_l(\xi)$ using generator functions
With the Hermite polynomials this becomes: $M_{nl} = x_0 N_l N_n \int_{-\infty}^{\infty} d\xi H_n(\xi) \xi H_l(\xi) e^{-\xi^2}$.
Using Eqs.(2.109) and(2.111) the integral becomes:
$M_{nl} = N_l N_n \int_{-\infty}^{\infty} d\xi [H_n \frac{N_{l+1}}{N_l}\sqrt{\frac{l+1}{2}} H_{l+1} + H_n \frac{N_{l-1}}{N_l}\sqrt{\frac{l}{2}} H_{l-1}] e^{-\xi^2}$.
Now we make use of: $\int_{-\infty}^{\infty} d\xi H_n(\xi) H_l(\xi) e^{-\xi^2} = \frac{\delta_{nl}}{N_l N_n}$. Then we find for the matrix element:
$M_{nl} = \frac{x_0}{\sqrt{2}}[\sqrt{l+1}\delta_{n,l+1} + \sqrt{l}\delta_{n,l-1}]$, or $M_{nl} = \frac{1}{\sqrt{2}}[\sqrt{n}\delta_{n,l+1} + \sqrt{n+1}\delta_{n,l-1}]$. Well, this is Eq.(2.130). Did I use generating functions or not? See the discussion in the above section 2.3 on the harmonic oscillator.
b).On the other hand we could proceed as follows:
We have $M_{nl} = x_0 N_l N_n \int_{-\infty}^{\infty} d\xi H_n(\xi) \xi H_l(\xi) e^{-\xi^2}$. Multiply both generating functions, Eqs. (2.119) and (2.120) and include $\xi e^{-\xi^2}$. Then integrate over all ξ, we obtain with the expression for M_{nl}: $\sum_{n,l}^{\infty} \frac{z^n y^l}{n!l!} \frac{M_{n,l}}{N_n N_l} = \sqrt{\pi} x_0 (z + y) e^{2zy}$. Well, what do you prefer?

Exercise 14.
Evaluate the following integral for the harmonic oscillator using generating functions:
$M_{nl}(q) = \int_{-\infty}^{\infty} dx \phi_n(x) \phi_l(x) e^{iqx}$.

With generating functions follow the procedure b) of exercise 13.

a) $\sum_{n,l}^{\infty} \frac{z^n y^l}{n!l!} \frac{M_{n,l(q)}}{N_n N_l} = \sqrt{\pi} e^{2zy + i(z+y)qx_0 - q^2 x_0^2/4}$.

b) Another approach. We have: $M_{nl}(q) = N_l N_n \int_{-\infty}^{\infty} d\xi H_n(\xi) H_l(\xi) e^{-\xi^2} e^{iqx_0\xi}$. For convenience we substitute: $a = iqx_0$. Then:

$M_{nl}(q) = N_l N_n e^{\frac{a^2}{4}} \int_{-\infty}^{\infty} d\xi H_n(\xi) H_l(\xi) e^{-(\xi - a)^2} = e^{\frac{a^2}{4}} \delta_{nl} = e^{-q^2 x_0^2/4} \delta_{nl}$.

2.4 Raising and Lowering Operators.

Remark: *I refer here again to the work of Dirac and the "ladder operator".*

Eq. (2.180): C is found with the selection of A and B.

The operator for finding the observables, energy levels, is the Hamiltonian $\boldsymbol{H}$ which can be written as Eq. (2.173): $\boldsymbol{H} = \omega\hbar(\boldsymbol{a}^\dagger \boldsymbol{a} + \frac{1}{2})$. So, the raising and lowering operators are acting together. How to measure their effects separately?

Homework 15, 16.

Exercise 15.

For the harmonic oscillator, evaluate the following (s is constant):

a. $[a, H]$

b. $[a^\dagger, H]$

c. $e^{sH} a e^{-sH}$

d. $e^{sH} a^\dagger e^{-sH}$

ad a) For the Hamiltonian we use: $H = \hbar\omega(a^\dagger a + \frac{1}{2})$.

$[a, H] = aH - Ha = \hbar\omega(aa^\dagger a - a^\dagger aa) = \hbar\omega(aa^\dagger - a^\dagger a)a = \hbar\omega a = \frac{\hbar\omega}{\sqrt{2}}(\xi + \frac{d}{d\xi})$ with $\xi = x/x_0$.

ad b) Similar to ad a): $[a^\dagger, H]$= $\hbar\omega a^\dagger(aa^\dagger - a^\dagger a) = \hbar\omega a^\dagger = \frac{\hbar\omega}{\sqrt{2}}(\xi - \frac{d}{d\xi})$.

ad c) $e^{sH} a e^{-sH} = \frac{1}{\sqrt{2}} e^{sH} \left(\xi + \frac{d}{d\xi}\right) e^{-sH} = \frac{1}{\sqrt{2}} e^{sH} \left(\xi e^{-sH} - s e^{-sH} \frac{dH}{d\xi}\right) = \frac{1}{\sqrt{2}}(\xi - s\frac{dH}{d\xi})$.

With $H = \frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \frac{1}{2} K x^2$.

ad d) $e^{sH} a^\dagger e^{-sH} = \frac{1}{\sqrt{2}} e^{sH} \left(\xi - \frac{d}{d\xi}\right) e^{-sH} = \frac{1}{\sqrt{2}} e^{sH} \left(\xi e^{-sH} + s e^{-sH} \frac{dH}{d\xi}\right) = \frac{1}{\sqrt{2}}(\xi + s\frac{dH}{d\xi})$.

Exercise 16.

The *squeezed state* is the operator (λ is a constant) $S(\lambda) = N(\lambda) e^{\lambda a^\dagger}$. This is also called a *coherent state.*

a. Find the normalization constant $N(\lambda)$ such that $\langle 0 | S^\dagger S | 0 \rangle = 1$.

I assume $N(\lambda)$ and λ to be complex and $S(\lambda)$ Hermitian.

Now $\langle 0 | S^\dagger S | 0 \rangle = |N|^2 \left\langle 0 \middle| e^{\lambda^* a} e^{\lambda a^\dagger} \middle| 0 \right\rangle$. Since the exponentials are separated, we need not to apply the Feynman-Glauber Theorem. With help of the Eqs. (2.157), (2.160) or (2.182)-(2.184) we have: $M_{00} = |N|^2 \left\langle 0 \middle| e^{\lambda^* a} e^{\lambda a^\dagger} \middle| 0 \right\rangle = |N|^2 \langle 0 | 0 \rangle$. Consequently $|N|^2 = 1$.

b. Evaluate the commutator $[a, S]$.

For the commutator we write: $aS - Sa = N\sum_{k=0}^{\infty} a\frac{(\lambda a^\dagger)^k}{k!} - N\sum_{k=0}^{\infty}\frac{(\lambda a^\dagger)^k}{k!}a$. Collecting equal exponents of k we finally obtain $[a, S] = \lambda N\sum_{k=0}^{\infty}\frac{\lambda^k}{k!}(a^\dagger)^k = \lambda N e^{\lambda a^\dagger} = \lambda S$.

Use has been made of: $aa^\dagger - a^\dagger a = 1$ or $aa^\dagger = a^\dagger a + 1$. Furthermore use has been made of induction. In order to prove :

$$\sum_{k=1}^{\infty} a\frac{(\lambda a^\dagger)^k}{k!} - \sum_{k=1}^{\infty}\frac{(\lambda a^\dagger)^k}{k!}a = \lambda\sum_{k=1}^{\infty}\frac{\lambda^{k-1}}{(k-1)!} \qquad \textbf{(C.2.48)}$$

we presume this expression to be correct for $k = m$ and prove that the expression is true for $k = m + 1$.

So is the following $m + 1$ expression correct:

$\frac{a(\lambda a^\dagger)^{m+1}}{(m+1)!} - \frac{(\lambda a^\dagger)^{m+1}a}{(m+1)!} = \frac{\lambda(\lambda a^\dagger)^m}{m!}$? Let's find out. We can rewrite the latter expression by using $aa^\dagger = a^\dagger a + 1$. Then we obtain:

$\frac{\lambda a^\dagger}{m+1}\left\{\frac{a(\lambda a^\dagger)^m}{m!} - \frac{(\lambda a^\dagger)^m a}{m!}\right\} + \frac{\lambda(\lambda a^\dagger)^m}{(m+1)m!} = \frac{\lambda(\lambda a^\dagger)^m}{m!}$? The expression between {} is just the m-th term of the commutator $(aS - Sa)$, the left-hand side of **(C.2.48)**. This equals according to the presumption of induction $\frac{\lambda(\lambda a^\dagger)^{m-1}}{(m-1)!}$.

So $\frac{\lambda a^\dagger}{m+1}\left\{\frac{\lambda(\lambda a^\dagger)^{m-1}}{(m-1)!}\right\} = \frac{\lambda(\lambda a^\dagger)^m}{m!}$?

Rearranging and dividing by λ^{m+1} we arrive at $m(a^\dagger)^m + (a^\dagger)^m = (m+1)(a^\dagger)^m$.

Et voilà $(m+1)\left(a^\dagger\right)^m = (m+1)(a^\dagger)^m$.

c. Evaluate the commutator $[a^\dagger, S]$.

Since S is a power series in $a^\dagger$, $[a^\dagger, S]$ commute and equals 0.

Or $a^\dagger S - S a^\dagger = a^\dagger e^{\lambda a^\dagger} - e^{\lambda a^\dagger}a^\dagger = \sum_{k=0}^{\infty}[\frac{a^\dagger(\lambda a^\dagger)^k}{k!} - \frac{(\lambda a^\dagger)^k a^\dagger}{k!}] = 0$.

d. Show that $S|0\rangle$ is an eigenstate of the lowering operator a and find its eigenvalue.

So we have to prove $aS|0\rangle = S_0 S|0\rangle$, where the eigenvalue is indicated by S_0.

Above(ad. b) we found $aS - Sa = \lambda S$. Then $aS|0\rangle = (\lambda S + Sa)|0\rangle$. We know $a|0\rangle = 0$.

Consequently $aS|0\rangle = \lambda S|0\rangle$. We may conclude $S|0\rangle$ to be an eigenstate and $S_0 = \lambda$ to be its eigenvalue.

2.5 Exponential Potential.

Both bound states and continuum states are discussed.

2.5.1 Bound States.

In the section on bound states the exponent β in the second term in Eq.(2.201) should have the minus sign.

Homework 9.

Exercise 9.

Derive the equation for the bound states of the potential $V(x) = -V_0 e^{-2|x|/a}$, for all $-\infty < x < \infty$ and $V_0 > 0$.

The derivation follows closely the procedure of exercise 8 with respect to a symmetrical

potential. Due to this symmetry, the wave function is described by Eq.(2.198). The solution to this differential equation of section 2.5.1(Mahan) can be used for the eigenvalues of odd parity wave functions.
The equation for the bound states : $J_\beta(g) = 0$, Eq.(2.203). β, g and E_a are given by Eqs. (2.195)-(2.197).
The equation for even parity wave functions is found from the condition $\frac{d\psi}{dx} = 0$ at $x = 0.$
So $\frac{d}{dx} J_\beta(ge^{-|x|/a})$=0. With this equation you can also find some additional critical values of the coupling strength g_c. These values are:
$g_c = 3.8317,\ 7.0156,\ 10.1734$, etc.(See Fig. 2.10). These values are found with WolframAlpha and are equal to the values found from $J_1(g) = 0$.
For $\beta \neq 0$, I could only find solutions(with WolframAlpha) for integer values of β. For example:
$\beta = 2$, we find with $J_2(g) = 0$: $g = 5.1356,\ 8.4172,\ 11.7960$, etc.

2.5.2 Continuum States.

Eq. (2.210) describes continuum states. Mahan writes: "The prefactor in front is inserted to make $\psi(k.x)$ a real function….". The wave function in general is not a real function. Mahan wanted to make the wave function real.
Eq.(2.12) represents a wave going to the left and a wave going to the right. The latter can be interpreted as a reflected wave due to the infinite exponential potential barrier.
In order to find Eq. (2.213) use has been made of: $\Gamma(z^*) = (\Gamma(z))^*$ (Abramowitz and Stegun): the complex conjugate of the gamma function equals the gamma function with complex argument..
Then you will obtain: $\frac{1}{\Gamma(1+iK)} = \frac{1}{|\Gamma(1+iK)|}[\frac{\Gamma(1+iK)}{\Gamma(1-iK)}]^{-1/2}$,
and $\frac{1}{\Gamma(1-iK)} = \frac{1}{|\Gamma(1+iK)|}[\frac{\Gamma(1+iK)}{\Gamma(1-iK)}]^{1/2}$.

The second term in Eq.(2.212) can also be rewritten using a phase factor:
$\frac{\left(\frac{g}{2}\right)^{-iK}}{\Gamma(1-iK)} = \frac{e^{i\gamma}}{|\Gamma(1+iK)|}$, then $e^{i\gamma} = \frac{\left(\frac{g}{2}\right)^{-iK}}{\Gamma(1-iK)}|\Gamma(1+iK)|$. With help of the above expression for $\frac{|\Gamma(1+iK)|}{\Gamma(1-iK)}$, we can find for $\gamma = -Kln\left(\frac{g}{2}\right) - \frac{i}{2}\ln[\frac{\Gamma(1+iK)}{\Gamma(1-iK)}]$. May be it comes as no surprise: $\gamma = \delta$ (Eq.(2.214) and Eq.(2.212) can be written as Eq.(2.215).
On page 44 Mahan writes below Eq.(2.218): "The current $j(x)$ does not depend on x since all the cross terms cancel to zero." Well, this is a mathematical argument. A physical argument is: there is nothing at $x \to \infty$ that can create a dependency on x.
It is confusing to use δ to express the phase shift; top page 44 and 53.
Does $\psi(k, x)$ in Eq. (2.221) represent a real wave function?

Homework 10, 12.

Exercise 10.
Find the transmission coefficient of a continuum wave going from left to right for the potential $V(x) = -V_0 e^{-2|x|/a}$.

For a continuum wave we have $E > 0$ and Schrödinger's equation is
$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + (E - V)\psi(x) = 0.$ **(C.2.49)**
$E - V = E + V_0 e^{-2|x|/a}$. **(C.2.50)**
We transform the wave equation with $y = e^{-|x|/a}$ and use the definitions of Eq.(2.206).
We arrive at the following Schrödingers equation:
$\left(y^2\frac{d^2}{dy^2} + y\frac{d}{dy} + g^2y^2 + K^2\right)\psi(y) = 0.$ **(C.2.51)**
Now what to do?
First we know that we are considering a continuum wave going from the left to the right. We might expect the particle wave not to be trapped in the potential sink or well, $E > 0$.
For $x \to -\infty$ and $V(x) \to 0$, we can approximate the wave function by $\psi(x) = Ie^{ikx}$, with $k^2 = \frac{2mE}{\hbar^2}$ and I is the amplitude. For $x \to \infty$ we can approximate the wave function, the transmitted wave, by $\psi(x) = Te^{ikx}$. T is the amplitude.
Since no particles are created or disappear $|I| = |T|$. There only can be a phase factor between the two waves. Define the transmission coefficient as $\frac{|T|}{|I|}$, then the coefficient equals 1. There is no reflection at the potential well.
could we look at the problem in another way? Well, we have equation **(C.2.51)** . Rewrite this equation as: $\left(y^2\frac{d^2}{dy^2} + y\frac{d}{dy} - (ig)^2y^2 + K^2\right)\psi(y) = 0.$
We can use Eq.(2.212)-Mahan-for a wave going to the write. Due to the term with ig instead of g the phase factor changes with a factor $-Ki\pi/2$ for the incoming wave as well as for the transmitted wave. So, the transmission coefficient is 1.

Exercise 12.
Consider the potential in one dimension:
$V(x) = g\frac{\hbar^2}{2mx^2}$, where $g > 0$ is a dimensionless parameter and solve for $x > 0$.
a. Find the solution to Schrödinger's equation.
b. Derive the phase shift by considering the form of the eigenfunction at large positive x.
Hint: Try a solution of the form $\sqrt{x}J_\nu(kx)$ and use the fact that
$\lim_{z\to\infty} J_\nu(z) = \sqrt{\frac{2}{\pi z}}\cos\left[z - \frac{\pi}{2}\left(\nu + \frac{1}{2}\right)\right].$
a) Schrödinger's equation: $\left(\frac{d^2}{dx^2} - \frac{g}{x^2} + k^2\right)\psi(x) = 0$, with $k^2 = \frac{2mE}{\hbar^2}$. At $x = 0$, $\psi(0) = 0$ since $V(x) \to \infty$. Now there is an infinite potential barrier at $x = 0$, we may expect at $x \to \infty$ with a particle wave going to the left a reflected particle wave similar to the example of section 2.5.2 (Mahan).
Mahan proposes a solution of the form $\sqrt{x}J_\nu(kx)$. After substitution of this particular Bessel function you will find a relation between ν and g.
Substitution of z for kx Schrödinger's equation reads: $\left(\frac{d^2}{dz^2} - \frac{g}{z^2} + 1\right)\psi(z) = 0$. Playing with this equation using WolframAlpha for various values of g, for example $g = 1/4$, you will find as a solution: $\psi(z) = C_1\sqrt{z}J_{\frac{1}{\sqrt{2}}}(z) + C_2\sqrt{z}Y_{\frac{1}{\sqrt{2}}}(z).$ **(C.2.52)**
After playing with various values of g you could guess a relation between ν and g. This is

shown in the table below.

g	v	ν^2	
3	$\sqrt{13}/2$	$13/4$	$g = \nu^2 - \frac{1}{4}$
2.01	1.503		
2	?		
1.99	1.497		
1	$\sqrt{5}/2$	5/4	$g = \nu^2 - \frac{1}{4}$
1/2	$\sqrt{3}/2$	3/4	$g = \nu^2 - \frac{1}{4}$
1/4	$1/\sqrt{2}$	1/2	$g = \nu^2 - \frac{1}{4}$
1/8	$\sqrt{3}/2\sqrt{2}$	3/8	$g = \nu^2 - \frac{1}{4}$

For $g = 2$, I put a question mark into the table since with Wolfram Alpha I got the following expression:

$$\psi(z) = \frac{\sqrt{2}}{\pi} C_1 \left[\frac{\sin(z)}{z} - \cos(z)\right] + \frac{\sqrt{2}}{\pi} C_2\left[-\sin(z) - \frac{\cos(z)}{z}\right]. \qquad \textbf{(C.2.53)}$$

Again by substituting $g = 2.01$ and $g = 1.99$ into Schrödinger's equation I found with WolframAlpha the values for ν as given in the table. Now you could guess ν to be 1.5. With a sort of reverse engineering you will obtain (Chisholm and Morris):

$\sqrt{z}J_{3/2} = \sqrt{\frac{2}{\pi}}\left[\frac{\sin(z)}{z} - \cos(z)\right]$, so $\nu = 3/2$ indeed.

To have $\psi = 0$ at $z \to 0$ for any value of ν, C_2 =0 in equation **(C.2.52)** for $\psi(z)$.

However, $g = 2$ is a special case as shown in **(C.2.53).** For this value of g no solution exists.

The other way: with help of Abramowitz and Stegun in the section on "Other differential equations" in the chapter on Bessel functions, you will find the differential equation $w''(z) + \left(\lambda^2 - \frac{\nu^2 - \frac{1}{4}}{z^2}\right) w(z) = 0$. The solution of this equation is, among other solutions: $w = z^{\frac{1}{2}} J_\nu(\lambda z)$. Now for our Schrödinger's equation $\lambda = 1$ and $\nu^2 - \frac{1}{4} = g$. Well, that is all there is. Playing with WolframAlpha creates a lot of fun.

b) The eigenfunction at large positive x is given by Mahan(see above) and can also be found in Abramowitz and Stegun. Then the phase shift is $\frac{\pi}{2}(\nu + \frac{1}{2})$. Or written in the parameters of Schrödinger's equation: $\frac{\pi}{2}(\frac{1}{2} + \sqrt{g + \frac{1}{4}})$.

2.6 Delta-Function Potential.

In Eq. (2.225) the expression containing $E\psi(x_0)$ vanishes due to: $\lim_{\varepsilon \to 0} -\frac{2m2\varepsilon}{\hbar^2} E\psi(x_0)$.

In Eqs. (2.234) and (2.235) the subscript B indicates bound states, I presume.

Homework 17, 18, 19.

Exercise 17.

Find the transmission and reflection coefficients, from left to right, of a particle scattering of the potential $V(x) = V_0\Theta(x) + \lambda\delta(x), \lambda > 0$ in one dimension, where $E > V_0$. Find the transmission and reflection coefficients from right to left and verify the relations the

relations found from time reversal.
The barrier described above I consider to be one of the barriers as described by Mahan on top of page 25.
Schrödinger's equation is $\frac{d^2\psi}{d^2x} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi = 0$. There are no bound states.
Nb.: a delta-function potential I consider to be a potential of infinite height and infinite thinness. My first thought was: there is no transmission. Well, then I supposed the infinite thinness sufficient for tunnelling).
We start with a particle wave from the left. The wave function is:

$\psi = Ie^{ikx} + Re^{-ikx},\ x < 0, k^2 = \frac{2m}{\hbar^2}E,$ **(C.2.54)**

and for the transmitted wave

$\psi = Te^{ipx}, x > 0, p^2 = \frac{2m}{\hbar^2}(E - V_0).$ **(C.2.55)**

For convenience we denote $\frac{2m}{\hbar^2} : b$.
Now we go to the barrier and apply the matching condition ψ to be continuous, consequently $I + R = T$. **(C.2.56)**
The continuity of the wave function is a bit more subtle due to the delta function type of barrier as described by Mahan on page 46. We approach the barrier on very small distance ε and eventually take $\varepsilon \to 0$, and obtain:

$(\frac{d\psi}{dx})_{+\varepsilon} - \left(\frac{d\psi}{dx}\right)_{-\varepsilon} = \lambda b\psi(0),$ **(C.2.57)**

where the contribution to the integral $\int_{-\varepsilon}^{\varepsilon} dx[E - V(x)]\psi(x)$ by $E - V_0\Theta$(x) vanishes at the interval $-\varepsilon < x < \varepsilon$ for $\varepsilon \to 0$.
With **(C.2.54)** and **(C.2.55)** we find for the derivative with $\varepsilon \to 0$:

$ipT - ikI + ikR = \lambda b(I + R) = \lambda bT.$ **(C.2.58)**

Without losing any information we set $I = 1$. We find for R and T:

$R = \frac{k^2 - p^2 - (\lambda b)^2 - 2i\lambda kb}{(k+p)^2 + (\lambda b)^2}.$ **(C.2.59)**

$T = \frac{2k(k+p) - 2i\lambda kb}{(k+p)^2 + (\lambda b)^2}.$ **(C.2.60)**

For $\lambda = 0$ **,** the ordinary step function potential barrier, we find the reflection and transmission coefficient as given by Mahan: Eqs. (2.56) and (2.57) with $I = 1$. So the influence of the delta-function potential is represented by a phase shift:

$\phi = \arctan\left(\frac{-2i\lambda kb}{(k+p)^2 + (\lambda b)^2}\right),$

and a reduction of the refection amplitude. The amount of reduction depends on the amplitude λ of the delta function.
Now the particle wave from the right.

$\psi' = I'e^{-ipx} + R'e^{ipx}, x > 0,$ **(C.2.61)**

and for the transmitted wave

$\psi' = T'e^{-ikx}.$ **(C.2.62)**

The matching conditions give, completely similar to the particle wave from the left,

$I' + R' = T'$, and **(C.2.63)**

$-ipI' + ipR' + ikT' = \lambda b(I' + R') = \lambda bT'.$ **(C.2.64)**

Again we set $I' = 1$, then we find for R' and T':

$R' = \frac{p^2-k^2-(\lambda b)^2-2i\lambda pb}{(k+p)^2+(\lambda b)^2}$, **(C.2.65)**

$T' = \frac{2p(k+p)-2i\lambda pb}{(k+p)^2+(\lambda b)^2}$. **(C.2.66)**

For $\lambda = 0$ we find the reflection and transmission coefficient as given by Mahan : Eqs. (2.68) and (2.69). For $\lambda > 0$ there is a phase shift $\phi' = \arctan\left(\frac{-2i\lambda pb}{(k+p)^2+(\lambda b)^2}\right)$ and a reduction of the reflection amplitude.

To conclude this exercise we will verify the relations for the refection and transmission coefficient by the time reversal procedure as described by Mahan on page 25 and 26. From this procedure we have :

$|R|^2 + T^*T' = 1$, **(C.2.67)**

and

$R'T^* + R^*T = 0$. **(C.2.68)**

As an example I will use **(C.2.66)** to verify the expressions for the refection and transmission coefficient. Substitute **(C.2.58)**, the complex conjugate of **(C.2.59)** and **(C.2.65)** into **(C.2.66)** and find out whether the following expression is correct:

$1 = \frac{(k^2-p^2-(\lambda b)^2)^2+(2\lambda kb)^2+4pk(k+p)^2+pk(2\lambda b)^2}{((k+p)^2+(\lambda b)^2)^2}$? Well, it is

Exercise 18.

Consider in one dimension the bound states of a particle in the pair of delta-function potentials $(W > 0)$:

$V(x) = -W[\delta(x+a) + \delta(x-a)]$. A sort of double potential sink.

Derive the eigenvalue equation for all possible bound states.

$a > 0$.

Schrödinger's equation is: $\frac{d^2\psi}{d^2x} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi = 0$.

We are looking for bound states: $E < 0$.

Away from the singularity, for bound states, $|x| \to \infty$, we have $\psi \to 0$ and $V(x) = 0$.

Schrödinger's equation is $\frac{d^2\psi}{d^2x} - \alpha^2\psi = 0$, and $\alpha^2 = -\frac{2m}{\hbar^2}E$.

So for $x \to \infty$, the particle wave equation is: $\psi = Ae^{-\alpha|x|}$, **(C.2.69)**

where A is a constant to be determined.

Now for $-a < x < a$ still away from the singularity, $E < 0$ and $V(x) = 0$.

The solution of Schrödinger's equation is: $\psi = Ce^{-\alpha x} + De^{\alpha x}$. **(C.2.70)**

The matchings condition at $|x| = a$ are ψ to be continuous and for the derivative we have something similar to Eq. (2.225), with $\lambda = -W$.

Keep in mind: $\frac{d|x|}{dx} = -1$ for $x < 0$.

Since the potential function is symmetric we have two solutions: a wave function of even parity and a wave function of odd parity.

Let us start with even parity.

For even parity we have at $x = 0$, $\frac{d\psi}{dx} = 0$. With **(C.2.70)** this leads to $C = D$.

Now matching at $x = -a$: $\psi(-a) = C\big(e^{-\alpha|a|} + e^{\alpha|a|}\big) = Ae^{-\alpha|a|}$. **(C.2.71)**

For the derivative we have to treat the singularity carefully.

So $(\frac{d\psi}{dx})_{-a+\varepsilon} - \left(\frac{d\psi}{dx}\right)_{-a-\varepsilon} = -\frac{2mW}{\hbar^2}\psi(-a)$. **(C.2.72)**

The derivative $\left(\frac{d\psi}{dx}\right)_{-a-\varepsilon} = \alpha A e^{-\alpha|a|}$. **(C.2.73)**

The derivative $(\frac{d\psi}{dx})_{-a+\varepsilon} = C\left(\alpha e^{-\alpha|a|} - \alpha e^{\alpha|a|}\right)$. **(C.2.74)**

Then **(C.2.72)** gives $C\left(\alpha e^{-\alpha|a|} - \alpha e^{\alpha|a|}\right) - \alpha A e^{-\alpha|a|} = -\frac{2mW}{\hbar^2}\psi(-a)$. **(C.2.75)**

In addition we use **(C.2.71)** to find for $C = \frac{Ae^{-\alpha|a|}}{e^{-\alpha|a|}+e^{\alpha|a|}}$. **(C.2.76)**

The matching at $x = a$ gives the same results as it should for a symmetric potential.

Keep in mind: $\frac{d|x|}{dx} = 1$ for $x > 0$.

Finally we obtain with help of **(C.2.71)**, **(C.2.75)** and **(C.2.76)** for even parity the following eigenvalue equation:

$\alpha\left(1 + \frac{\sinh(\alpha a)}{\cosh(\alpha a)}\right) = \frac{2mW}{\hbar^2}$. **(C.2.77)**

This equation for α gives just 1 eigenvalue.

Now for odd parity.

For odd parity we have at $x = 0, \psi = 0$. With **(C.2.66)** this leads to $C = -D$. Then similar to the procedure for even parity we find the following eigenvalue equation:

$\alpha\left(1 + \frac{\cosh(\alpha a)}{\sinh(\alpha a)}\right) = \frac{2mW}{\hbar^2}$. **(C.2.78)**

This equation for α gives again 1 eigenvalue.

So for this exercise for a pair of delta-functions we found two eigenvalues.

Note: with Dirac we know $\delta(x+a) + \delta(x-a)$ *to be equal to* $2a\delta(x^2 - a^2)$. *By using the latter delta-function, the process of finding the eigenvalues is not a lot easier.*

Exercise 19.

Consider the problem of a delta-function potential outside of an infinite barrier at the origin ($a > 0$):

$V(x) = \begin{cases} \infty & x \leq 0 \\ W\delta(x-a) & x > 0 \end{cases}$.

a. Find an analytic expression for the phase shift as a function of k.

b. Plot this on a piece of graph paper for the range $0 < ka < 2\pi$ when $g \equiv \frac{2maW}{\hbar^2} = 1$.

ad. a. When we mirror this problem at $x = 0$ and set $W > 0$ the odd parity solution $\psi(0) = 0$ of exercise 18 appears. Then $\alpha\left(1 + \frac{\cosh(\alpha a)}{\sinh(\alpha a)}\right) = -\frac{2mW}{\hbar^2}$. This leads to negative and or complex values of α. So we look for oscillatory type of wave functions.

For $0 < x < a$: $\psi = A\sin(kx)$ with $k^2 = \frac{2m}{\hbar^2}E$.

For $a < x$: $\psi = D\sin(kx + \phi)$ where ϕ represents the phase shift.

At $x = 0$ the particle wave function vanishes.

At $x = a$ we have to deal with the singularity of the delta-function:

$(\frac{d\psi}{dx})_{a+\varepsilon} - \left(\frac{d\psi}{dx}\right)_{a-\varepsilon} = \frac{2mW}{\hbar^2}\psi(a)$. **(C.2.79)**

Furthermore $\psi(a) = Asin(ka) = Dsin(ka + \phi)$. **(C.2.80)**

We find for (**C.2.75)** with help of the derivatives of both wave functions:

$kDcos(ka + \phi) - kAcos(ka) = \frac{2mW}{\hbar^2}Asin(ka)$. **(C.2.81)**

(C.2.80) gives $D = \frac{Asin(ka)}{sin(ka+\phi)}$. Substitution of this expression into **(C.2.81)** finally leads to:

$cotan(ka+\phi) = cotan(ka) + \frac{2mW}{k\hbar^2}$. **(C.2.82)**

Then we can write for the phase shift, using the definition of $g \equiv \frac{2maW}{\hbar^2}$,

$\phi = -ka + cotan^{-1}(cotan(ka) + \frac{g}{ak})$. **(C.2.83)**

ad. b. Now we can plot ϕ as a function of ka with $0 < ka < 2\pi$ and $g = 1$.

Some values of the phase shift: $ak = 0,\ \phi = 0;\ ak = 0.1,\ \phi = -0.05;$

$ak = \frac{\pi}{4},\ \phi = -0.37;\ ak = \pi,\ \phi = -\pi;\ ak = 6.2,\ \phi = -6.28$ and $ak = 2\pi,\ \phi = -2\pi$.

2.7 Number of Solutions.

In this section Mahan gives some examples of shapes of potential function and the solutions of the Schrödinger equation.

2.8 Normalization.

In this section Mahan derives the general method for normalization of the wave function. Various examples as presented in the foregoing sections illustrates the method of normalization.

Homework 20, 21, 22.

Exercise 20.

20.Consider the one-dimensional Schrödinger equation with a delta-function potential $V(x) = W\delta(x)$. For each value of $E > 0$ construct two wave functions that are orthogonal to each other and normalized according to delta-function normalization.

,We can create a particle wave function as a sum of the wave function from the left ψ_L and a wave function from the right ψ_R.

With $k^2 = \frac{2mE}{\hbar^2}$,

$\psi_L = Ie^{ikx} + Re^{-ikx}$ for $x < 0$, **(C.2.84)**

$\psi_L = Te^{ikx}$ for $x > 0$. **(C.2.85)**

Matching at $x = 0$ gives for the wave function ψ_L:

$I + R = T$, **(C.2.86)**

For the derivative we have to take into account the singularity and we obtain:

$ikT - ikI + ikR = Wb\psi(0)$, **(C.2.87)**

with $b = \frac{2m}{\hbar^2}$.

With **(C.2.86)** and **(C.2.87)** we obtain:

$R = \frac{-(Wb)^2 - i2kWb}{(Wb)^2 + (2k)^2}$, and **(C.2.88)**

$T = \frac{(2k)^2 - i2kWb}{(Wb)^2 + (2k)^2}$. **(C.2.89)**

For the wave from the right we have, in a similar way:

$R_r = \frac{-(Wb)^2 - i2kWb}{(Wb)^2 + (2k)^2}$, and **(C.2.90)**

$T_r = \frac{(2k)^2 - i2kWb}{(Wb)^2 + (2k)^2}$. **(C.2.91)**

We can proceed in two ways. We can create a wave function ψ by :

$\psi = \psi_L + \psi_R$ or we choose the wave from the left as a particle wave function of which we have to find out how to normalize this function by means of delta-function normalization instead of the sum wave function. Take notice of the following: I have set in the derivation of the reflection and transmission coefficient $I = 1$. No information is lost in this way.
Let us work with a wave going to the right. To normalize this wave, we need another oscillatory wave function with a wave number $k' \neq k$. Delta-function normalization means
$\int_{-\infty}^{\infty} \psi_L^* (k', x)\psi_L(k, x)dx = 2\pi\delta(k - k'),$ **(C.2.92)**
It is immediately clear that the problem of orthogonality is solved.
We have $\psi_L^* = e^{-ik'x} + R^* e^{ik'x}$ for $x < 0,$ **(C.2.93)**
and $\psi_L^* = T^* e^{-ik'x}$ for $x > 0.$ **(C.2.94)**
Keep in mind R^* and T^* to be functions of k' , **(C.2.88)** and **(C.2.89).**
Plug **(C.2.84)**, (**C.2.85)**, **(C.2.93)**,and **(C.2.94)** into **(C.2.92)**:
$\int_{-\infty}^{0} dx(e^{ix(k-k')} + R^* e^{ix(k'+k)} + Re^{-ix(k'+k)} + RR^* e^{ix(k'-k)}) + \int_{0}^{\infty} dxTT^* e^{ix(k-k')}.$
Let's look at the various expressions in this integral. Mahan writes on page 54 the terms with $(k' + k)$ do not contribute to the above expression. The integral with the transmission coefficients can be written as: $\int_{-\infty}^{0} dxTT^* e^{-ix(k-k')}$. Finally the normalization expression reduces into:
$\int_{-\infty}^{0} dx(e^{ix(k-k')} + RR^* e^{ix(k'-k)} + TT^* e^{-ix(k-k')}).$ **(C.2.95)**
Now the question is, does this integral equals the integral with the cosine function and consequently the delta-function:
$\int_{-\infty}^{0} dx(e^{ix(k-k')} + RR^* e^{-ix(k-k')} + TT^* e^{-ix(k-k')}) = 2\int_{-\infty}^{0} \cos[(k - k')x]dx =$
$2\pi\delta(k - k')$?
Well, only for $RR^* + TT^* = 1$ or when we had included the amplitude of the wave function form the left for $II^* = 1$ and $RR^* + TT^* = II^*$. When we substitute the expressions for the transmission and reflection coefficients into $RR^* + TT^* = 1$, we obtain a complex equation for k' as a function of k. After inspection you will find $k' = k$ to be the only solution, as it should be. If we try to find out whether a left going wave is orthonormal to another left going wave you will find again $k' = k$ as is should be. We have unbound states so E is continuous and so is k.

Exercise 21.
21.Find the formula for the normalization coefficient C_1 for the bound-state wave function in Eq.(2.29). Then find the numerical value for the bound state shown in Figure 2.2.
Note: *in Figure 2.2 the potential function is shown. So, I think Mahan indicates the bound state wave function in figure 2.3.*
Eq. (2.29): $\psi(x) = \begin{cases} 0 & x < 0 \\ C_1 \sin(px) & 0 < x < a \\ C_3 e^{-\alpha x} & a < x \end{cases}$
$p^2 = \frac{2m}{\hbar^2}(V_0 + E)$, and $\alpha^2 = -\frac{2m}{\hbar^2}E$.
The formula for normalization of the above mentioned bound state reads:
$1 = \int_{0}^{\infty} dx\, |\psi|^2 = C_1^2 \int_{0}^{a} sin^2(px)dx + C_3^2 \int_{a}^{\infty} e^{-2\alpha x}dx = \frac{C_1^2}{2}[a - \frac{1}{2p}\sin(2pa) + \frac{\sin^2(p\alpha)}{\alpha}].$
See Eq.(2.244).

What is the numerical value for C_1? The relevant numbers are given at the bottom of page 21: $a = 2.0$ Å, $V_0 = 4.0$ eV, $E = -0.48$ eV, $m = 9.109 \times 10^{-31}$ kg. Furthermore $\hbar = 1.055 \times 10^{-34}$ Js, and 1eV= 1.602×10^{-19} J.
With these values you can find the numerical value of C_1 . C_1 has the dimension of the reciprocal square root of length.

Exercise 22
A one-dimensional Hamiltonian has a ground-state eigenfunction of
$\psi_0(x) = \frac{A}{\cosh\left(\frac{x}{a}\right)}$,
where (a, A) are constants. Assume that $V(x) \to 0$ as $|x|/a \gg 1$.
a. What is A?
b. What is the exact eigen value?
c. What is the exact potential.
What is A? Well, $\int_{-\infty}^{\infty} |\psi_0|^2 \, dx = 1$, the equation for A is: $A^2 a \int_{-\infty}^{\infty} d\left(\frac{x}{a}\right) \frac{1}{cosh^2\left(\frac{x}{a}\right)} = 1$.
For this integral we have: $aA^2 \tanh\left(\frac{x}{a}\right) |_{-\infty}^{\infty} = 1$. Consequently $A = \sqrt{\frac{1}{2a}}$.
Now the exact eigenvalue and the exact potential.
Schrödinger's equation for the ground state:
$\frac{d^2\psi_0}{dx^2} + \frac{2m}{\hbar^2}\left(E_0 - V(x)\right)\psi_0 = 0$, with $E_0 < V(x)$. After substitution of the ground-state into the wave equation we arrive at: $2tanh^2\left(\frac{x}{a}\right) - 1 + \frac{2m}{\hbar^2}\left(E_0 - V(x)\right)a^2 = 0$. After rearranging we obtain: $E_0 - V(x) = \frac{\hbar^2}{2ma^2} - \frac{\hbar^2}{2ma^2} 2tanh^2\left(\frac{x}{a}\right)$.
We know E_0 to be a number and $V(x)$ to be a function of x and $V(x)$ has to vanish for $|x|/a \gg 1$. This leads to the following expression for $E_0 - V(x)$:
$E_0 - V(x) = -\frac{\hbar^2}{2ma^2} + \frac{\hbar^2}{ma^2}\left(1 - tanh^2\left(\frac{x}{a}\right)\right)$. So, finally we have:
for the bound-state eigenvalue $E_0 = -\frac{\hbar^2}{2ma^2}$,
for the potential: $V(x) = \frac{\hbar^2}{ma^2}\left(1 - tanh^2\left(\frac{x}{a}\right)\right)$.

Remark: For continuous states delta function normalisation is applied. There you have to realize: $|\psi|^2 = \psi^*(k', x)\psi(k, x)$. Furthermore, it is confusing that δ is used both for the delta function and the phase shift. Just below Eq. (2.266) Mahan writes: "Note that there is no complex conjugate (ψ^*) in the above integral, since for the half-space problems the eigenfunctions are always real." This clarifies to some extent the remark below Eq. (2.210) about the wave function to be a real function.
Eq. (2.271) is obtained by rewriting Eq. (2.264). This result is substituted in Eq. (2.270). Subsequently the constant C of Eq. (2.265) is found.

2.9 Wave Packets.

In this section Mahan discusses groups of particles: wave packets.

Dirac defines a wave packet in relation with Heisenberg's principle of uncertainty.

In Eq. (2.287) Mahan gives a Gaussian wave packet in momentum representation.

Homework 23.

Exercise 23.

Derive a wave packet for photons ($\omega = ck$) using (a) a Gaussian packet, and (b) a Lorentzian packet.

a. In section 2.9 on Wave Packets the case of nonrelativistic particles is discussed. A photon is certainly not a nonrelativistic particle. In the sections preceding section 2.9 relativistic particles are not dealt with. A nonrelativistic Schrödinger equation has been studied. Maybe we are allowed just to use $\omega = ck$ to study the effect of a relativistic particle. Working with $\omega = ck$ in Eq. (2.287) we obtain for the wave packet:

$\Psi(k_0, x, t) = A\Delta\sqrt{2\pi}\exp\left[-(x-ct)^2\frac{\Delta^2}{2} + ik_0(x-ct)\right]$.

The velocity of the wave packet is c. This comes as no surprise.

The particle density is: $\rho(k_0, x, t) = |\Psi|^2 = 2\pi A^2\Delta^2\exp\left[-(x-ct)^2\Delta^2\right]$.

The probability a particle contributing to the density is 1, so:

$\int_{-\infty}^{\infty} dx\, \rho(k_0, x, t) = 1$. Consequently, $A = \frac{1}{\pi^{3/4}\sqrt{2\Delta}}$.

And $\Psi(k_0, x, t) = \sqrt{\frac{\Delta}{\sqrt{\pi}}}e^{ik_0(x-ct)}exp\left[-(x-ct)^2\Delta^2\right]$.

b. The Lorentzian wave packet. In the preceding text I could not find anything about such a wave packet. It belongs to a basic course in Quantum Mechanics. On the other hand, I can hardly assume a Lorentzian wave packet to be a Gaussian wave packet under Lorentz transformation. The photon is moving with velocity c. In the new frame of reference with a transformed x , $\Psi(k_0, x, t)$ could read

$\Psi(k_0, x, t) = \sqrt{\frac{\Delta}{\sqrt{\pi}}}e^{ik_0(x)}exp\left[-(x)^2\Delta^2\right]$.

On page 34 in the section of raising and lowering operators, Mahan mentioned photons obeying harmonic oscillator statistics. He will discuss this in chapter 8. May be in that chapter I find some answers.

Well, could it be possible $\psi(x) = \sqrt{\lambda}e^{-\lambda|x|}$ to represent the Lorentzian wave packet? Well, it most probably is. On www.mathworld.wolfram.com I found the Lorentzian function $L(x)$ to be: $L(x) = \frac{1}{\pi}\frac{\frac{1}{2}\Gamma}{(x-x_0)^2+(\frac{1}{2}\Gamma)^2}$, where Γ is a parameter specifying the width.

In momentum space : $L(k) = \frac{1}{\pi}\frac{\frac{1}{2}\Gamma}{(k-k_0)^2+(\frac{1}{2}\Gamma)^2}$, or with Δ, this reads $L(k) = \frac{1}{\pi}\frac{\frac{1}{2}\Delta}{(k-k_0)^2+(\frac{1}{2}\Delta)^2}$.

The factor ½ could be absorbed by Δ . Applying Fourier transformation to $\psi(x) = \sqrt{\lambda}e^{-\lambda|x|}$, we obtain a function similar to $L(k)$.

Now with Eq. (2.287) we have for the Lorentzian wave packet:

$\Psi(k_0, x, t) = A\int_{-\infty}^{\infty} dk\, \frac{\Delta}{(k-k_0)^2+(\Delta)^2} exp[ik(x-ct)]$.

Now we use $k - k_0 = z$ to integrate:

$\Psi(k_0,x,t) = Aexp[ik_0(x-ct)]\int_{-\infty}^{\infty} dz\,\frac{\Delta}{(z)^2+(\Delta)^2}exp[iz(x-ct)]$.
Insert in this expression $x' = (x-ct)$. This results into:
$\Psi(k_0,x,t) = Aexp[ik_0x']\int_{-\infty}^{\infty} dz\,\frac{\Delta}{\Delta^2+z^2}exp[izx']$. With help of Fourier transformation, we can evaluate the integral. Neglecting a constant the integral is: $e^{-\Delta|x'|}$. Finally we obtain for the wave packet: $\Psi(k_0,x,t) = Aexp[-\Delta|x-ct|]\exp[ik(x-ct)]$.
Normalization leads rather straight forward to: $A = \sqrt{\Delta}$, and the wave packet is:
$\Psi(k_0,x,t) = \sqrt{\Delta}\,exp[-\Delta|x-ct|]\exp[ik(x-ct)]$.

Homework

The exercises are dealt with in the various section related to the subject matter.

3. Approximate Methods.

In this chapter Mahan deals with two approximate methods. As Mahan indicates, these methods are still worthwhile even working with numerical solutions of Schrödinger's equation. These approximate solutions can be used as a first estimate for a numerical solution.

3.1 WKBJ.

In this section Mahan treated the so-called WKBJ method. As Mahan mentioned: "….The main idea behind WKBJ is to treat ħ as a "small" parameter, and to expand the eigenfunction in a series in this parameter…….".
As an example, the half space problem is discussed.
On page 66 Mahan writes: "the momentum $p(x)$ approaches in the limit, $x \to \infty$, $\hbar k$.
Keep in mind: for $x \to \infty, V(x) \to 0$ and so $p(x) = \sqrt{2mE}$. With $k^2 = \frac{2mE}{\hbar^2}$, we obtain $p = \hbar k$.
In Eq. (3.23) Mahan presents the eigenfunction for $x \to \infty$. Delta-function normalization is used for this eigenfunction. In chapter 2 page 53 the eigenfunction is written as: $\lim_{x\to\infty}\psi(k,x) = C(k)\sin(kx+\delta)$, where δ represents the phase shift. On pages 53-54 Mahan derived $C(k) = 2$.. So with Eq. (3.23) the factor $\frac{D}{\sqrt{\hbar k}} = 2$.
On page 67 Mahan found the WKBJ phase shift for aa exponential function $V(x) = V_0e^{-2x/a}$.
An indefinite integral has to be solved and it could be done exactly. This solution is found by substitution: $y = \sqrt{E - V_0z}$, and integration by partial fractions. The integral to be evaluated: $-2\int\frac{y^2}{E-y^2}dy$. Resulting into the integration of: $\int 2dy - \int\frac{dy\sqrt{E}}{\sqrt{E}+y} - \int\frac{dy\sqrt{E}}{\sqrt{E}-y}$.
Mahan concludes this section with: "The WKBJ is an excellent method of describing the motion of particles except those states with the lowest energy."
On page 68: "There are no bound states for the repulsive exponential potential, which is why

the phase shifts simply go to zero". Well, in section 2.5.2 continuum states and the repulsive potential is analysed. No bound states, just continuum states. No bound states at all. The phase shifts simply do not disappear. The phase shift $\delta = m\pi$ for $k = 0$, *Levinson's theorem.* The eigenfunction for $x \to \infty$ is given for the exponential potential by Eq. (2.215). $\lim_{x\to\infty} \psi(x) = \frac{2C}{|\Gamma(1+iK)|} \sin\,(kx + \delta)$. For $\delta = m\pi$, $\sin(kx + \delta) = (-1)^m \sin\,(kx)$. Finally, for $k = 0, \sin(kx) = 0$, and we have no states at all. So, what is the meaning of this?

Homework 1, 2, 3, 4, 12.

Exercise 1.

Use WKBJ to calculate the phase shift of a particle in the one-dimensional potential $V(x) = 0, x > 0$ and $V(x) = |Fx|, x < 0$.

At $x = -b$, $E = V(-b)$, and $p(-b) = 0$; $x = -b$ is the turning point.

For $x < -b$, we have a particle wave function like the one in Eq.(3.19).

We leave this wave function and focus attention at the wave function describing the phase shift and $V(x) < E$. The particle wave function is given in Eq. (3.20):

$\psi(x) = \frac{D}{\sqrt{p(x)}} \sin[\frac{1}{\hbar}\int_{-b}^{x} dx' p(x') + \beta]$.

Let us look evaluate this wave function for $-b < x < 0$.

$p(x) = \sqrt{2m(E + |F|x)}$ and the wave function is

$\psi(x) = \frac{D}{\sqrt{p(x)}} \sin\,[\frac{2\sqrt{2m}}{3\hbar|F|}(E + |F|x)^{\frac{3}{2}} + \frac{\pi}{4}]$; $\beta = \frac{\pi}{4}$ is explained on page 66.

For $x > 0$ and $x \to \infty$ we have a right and a left going wave differing by a phase factor as described on page 44. This wave function can be written as:

$\psi(k, x) = -2iIe^{i\delta} \sin(kx + \delta)$, Eq.(2.221). And $k^2 = \frac{2mE}{\hbar^2}$, $V(x) = 0$.

At $x = 0$ we match the wave functions from both intervals: $-b < x < 0$ and $x > 0$.

This results into: $\frac{D}{\sqrt{\hbar k}} \sin\left(\frac{2E}{3|F|}k + \frac{\pi}{4}\right) = -2iIe^{i\delta} \sin\delta$. Mahan denotes $-2iIe^{i\delta}$ to be a prefactor($\equiv C$,say). So: $\sin\delta = \frac{D}{C\sqrt{\hbar k}} \sin\left(\frac{2E}{3|F|}k + \frac{\pi}{4}\right)$.

The next step is to match the derivatives of the wave functions in both intervals at $x = 0$.

Divide both expressions to eliminate (C, D) and $\delta(k) = \text{arccotan}\,(E, |F|, k)$:

$\delta = arccotan[-\frac{1}{4k}\frac{|F|}{E} + cotan\left(\frac{2E}{3|F|}k + \frac{\pi}{4}\right)]$.

Remark: This is not a very elegant expression for the phase shift. Is there something wrong? On page 66 Mahan writes: "Recall that the phase shift is defined as:

$\lim_{x\to\infty} \psi(x) = 2\sin(kx + \delta)$. Then: $\delta_{WKBJ}(k) = \frac{\pi}{4} + \lim_{x\to\infty}[\frac{1}{\hbar}\int_{-b}^{x} dx'\, p(x') - kx]$.

Now the integral runs from $-b$ through 0 to x.

So $\delta_{WKBJ}(k) = \frac{\pi}{4} + \lim_{x\to\infty}[\frac{2E}{3|F|}k + kx - kx]$ and $\delta_{WKBJ}(k) = \frac{\pi}{4} + \frac{2E}{3|F|}k$. This differs from the δ, a few lines above, with the number $-\frac{1}{4k}\frac{|F|}{E}$. How come? Does the phase factor and consequently the wave function change when approaching the ramp at $x > 0$? Well, the answer to this question is given by Mahan. It is just the definition of the phase shift. Evaluating the phase integral, the wave functions and the derivatives of the wave functions at $x = 0$ leads to an identity and consequently does not create new information. So, the approach presented above the remark is wrong! And $\delta_{WKBJ}(k)$ given above is the right answer.

Exercise 2.
Use WKBJ to calculate the phase shift of a particle in the one-dimensional potential $V(x) = 0, x > 0$ and $V(x) = Kx^2/2, x < 0$.
At $x = -b$, $E = V(-b)$, and $p(-b) = 0$; $x = -b$ is the turning point.
Let us evaluate the wave function for $-b < x < 0$.
$p(x) = \sqrt{2m(E - Kx^2/2)}$ and $b = \sqrt{\frac{2E}{K}}$.
The particle wave function is: $\psi(x) = \frac{D}{\sqrt{p(x)}} \sin[\frac{1}{\hbar}\int_{-b}^{x} dx' p(x') + \frac{\pi}{4}]$.
With the substitution: $x = \sqrt{\frac{2E}{K}} \sin\alpha$, we obtain for the wave function:
$\psi(\alpha) = \frac{D}{\sqrt{p(\alpha)}} \sin[k\sqrt{\frac{2E}{K}}(\frac{\alpha}{2} + \frac{1}{4}\sin 2\alpha + \frac{\pi}{4}) + \frac{\pi}{4}]$, use has been made of $\sin\alpha = -1$at $x = -\sqrt{\frac{2E}{K}}$ -the turning point.
For $x > 0$ and $x \to \infty$ we have a right and a left going wave differing by a phase factor as described on page 44. This wave function can be written as:
$\psi(k, x) = -2iIe^{i\delta}\sin(kx + \delta)$, Eq.(2.221). And $k^2 = \frac{2mE}{\hbar^2}$, $V(x) = 0$. Mahan denotes $-2iIe^{i\delta}$ to be a prefactor($\equiv C$,say).
Now we match the wave function and their derivatives at $x = 0$, or $\sin\alpha = 0$. Express the wave function for $x > 0$ in α. With $\frac{d}{dx} = \frac{d}{d\alpha}\frac{d\alpha}{dx}$, the expression for the phase shift is, leaving out the details,:

$$\delta = \arctan\{\frac{k\sqrt{\frac{2E}{K}}}{k\sqrt{\frac{2E}{K}} + \frac{\pi}{4}} \tan[\frac{\pi}{4}(k\sqrt{\frac{2E}{K}} + 1)]\}. \qquad \textbf{(C.3.1)}$$

Remark: Well, as you can imagine, I arrive at a similar remark as made at the end of exercise 1. So $\delta_{WKBJ}(k) = \frac{\pi}{4} + \lim_{x\to\infty}[kb\frac{\pi}{4} + kx - kx]$ and $\delta_{WKBJ}(k) = \frac{\pi}{4}\left(k\sqrt{\frac{2E}{K}} + 1\right)$. Again this differs from the phase factor derived a few lines before. See the remark at the bottom of exercise 2. The matching I did perform at $x = 0$ is wrong. When executed in a correct way the matching leads to an identity and creates no new information. So $\delta_{WKBJ}(k) = \frac{\pi}{4}\left(k\sqrt{\frac{2E}{K}} + 1\right)$ is the correct answer. **(C.3.1)** is wrong.

Exercise 3.
Use WKBJ to derive an equation for the phase shift $\delta(k)$ of an electron in the one-

dimensional potential ($V_0 > 0, a > 0$):

$$V(x) = \begin{cases} \infty & x \leq 0 \\ -V_0\left(1-\frac{x}{a}\right) & 0 < x < a \\ 0 & a < x \end{cases}$$

Remark: I assume the phase shift to be calculated for $E > 0$. For $E < 0$ and $|E| < V_0$, we find bound states very similar to those described by Mahan on page 75 in the section on Discontinuous Potentials.

At $x \leq 0$ we have $\psi = 0$.

For $0 < x < a$ we need to evaluate $\psi(x) = \frac{D}{\sqrt{p(x)}}\sin[\frac{1}{\hbar}\int_0^x dx' p(x')]$. Notice: no phase factor $\pi/4$ since we are working with a discontinuous potential at $x = 0$. For $a < x$ we have $\psi(k,x) = -2iIe^{i\delta}\sin(kx+\delta)$, Eq.(2.221). And $k^2 = \frac{2mE}{\hbar^2}$, $V(x) = 0$. Mahan denotes $-2iIe^{i\delta}$ to be a prefactor($\equiv C$,say).

The wave function on the interval $0 < x < a$, becomes:

$$\psi(x) = \frac{D}{(2m(E+V_0\left(1-\frac{x}{a}\right))^{1/4}}\sin[\frac{1}{\hbar}\sqrt{2m(E+V_0)}\{\frac{2a(E+V_0)}{3V_0}\left(1-\left(1-\frac{xV_0}{a(E+V_0)}\right)^{\frac{3}{2}}\right)\}]\ .$$

Now the hard work begins. Matching the wave functions and their derivatives at $x = a$. Leaving out the details, the result is:

$$\delta = -ka + arccotan\left[\frac{V_0}{4kaE} + cotan\left\{\frac{2}{3}ka\frac{E}{V_0}\left(\left(1+\frac{V_0}{E}\right)^{\frac{3}{2}}-1\right)\right\}\right]. \qquad \textbf{(C.3.2)}$$

Remark: A continuing story.

$\delta_{WKBJ}(k) = \frac{\pi}{4} + \lim_{x\to\infty}[\frac{1}{\hbar}\int_{-b}^{x} dx'\, p(x') - kx]$. With the above potential we find:

$\delta_{WKBJ}(k) = \lim_{x\to\infty}[\frac{2}{3}ka\frac{E}{V_0}\left(\left(1+\frac{V_0}{E}\right)^{\frac{3}{2}}-1\right) + kx - ka - kx]$ and

$\delta_{WKBJ}(k) = -ka + \frac{2}{3}ka\frac{E}{V_0}\left(\left(1+\frac{V_0}{E}\right)^{\frac{3}{2}}-1\right)$.

I have to pay attention to the phenomena described in the remarks at the end of the above two exercises. I did and the answer is given by Mahan: “The asymptotic expression $\delta_{WKBJ}(k)$ for $x \to \infty$ has to be used”. Correctly matching the wave function and the derivatives of the wave functions at $x = a$ leads to an identity. So, the above answer for δ **(C.3.2)** is wrong!

The correct answer is :

$$\delta_{WKBJ}(k) = -ka + \frac{2}{3}ka\frac{E}{V_0}\left(\left(1+\frac{V_0}{E}\right)^{\frac{3}{2}}-1\right).$$

Exercise 4.

The phase $\phi = \Theta(x) + \beta$ has $\beta = \frac{\pi}{4}$ for potentials with smooth turning points, and $\beta = 0$ for an infinite step potential. Examine the value of $\beta(k)$ for a finite step potential. Solve exactly, as in chapter 2, the eigenfunctions for the potential:

$$V(x) = \begin{cases} V_0 & x < 0 \\ 0 & x > 0 \end{cases}$$

for $0 < E < V_0$. For $x > 0$ the eigenfunction has the form $\sin(kx+\delta)$. In this case $\delta(k) = \beta(k)$. For what value of E/V_0 is $\beta = \pi/4$?

For $x < 0$ the Schrödinger's equation is :$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0$, and $\alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$. Then we find for the wave equation: $\psi = A_1 e^{-\alpha x} + A_2 e^{\alpha x}$. Preventing ψ from becoming infinite for $x \to -\infty$ we have: $\psi = A_2 e^{\alpha x}$.
For $x > 0$ the Schrödinger's equation is :$\frac{d^2\psi}{dx^2} + k^2\psi = 0$, and $k^2 = \frac{2m}{\hbar^2}E$. The wave equation consists of an incoming and reflected wave: $\psi = A_3 e^{-ikx} + A_4 e^{ikx}$. The potential step does not create or destroy particles. The particle current for $x < 0$ is zero. So $|A_3| = |A_4|$. The amplitudes differ by a phase factor and we write:
$A_4 = -A_3 e^{2i\delta}$. Mahan page 44. Consequently $\psi = -A_3 2ie^{i\delta}\sin(kx + \delta)$ and $\delta(k) = \beta(k)$.
Now we match both wave functions at $x = 0$:
$A_2 = -2iA_3 e^{i\delta}\sin\delta$ and with the derivative $A_2\alpha = -2iA_3 e^{i\delta}k\cos\delta$. The quotient of both expressions gives: $\beta = \delta = \arctan(\frac{k}{\alpha})$.
We set $\beta = \pi/4 = \arctan(\frac{k}{\alpha})$. So $\tan\beta = \frac{\sqrt{2}}{2} = \frac{k}{\alpha}$. With the expressions for k and α we finally obtain: $\frac{E}{V_0} = 1/3$.

Exercise 12.
For the potential $V(x)$
$$V(x) = \begin{cases} \infty & x < 0 \\ -\frac{e^2}{x} & 0 < x \end{cases}$$
use WKBJ to derive an expression for the continuum eigenfunction.
So we have a repulsive wall at $x = 0$, a discontinuous potential. There is an incoming and a reflective wave. The eigenfunction is written as the sine of a phase integral and a phase angle. We have no turning point at $x = 0$. The incoming and reflected wave have the same amplitude; no particle will disappear. The wave function is:
$\psi(x) = \frac{D}{\sqrt{p(x)}}\sin[\frac{1}{\hbar}\int_0^x dx' p(x') + \beta]$, Eq. (3.20). For a repulsive wall $\beta = 0$; a discontinuous potential.

$p(x) = \sqrt{2m(E - V(x))} = \sqrt{2m(E + \frac{e^2}{x})}$. For $x \to \infty, p = \sqrt{2mE} = \hbar k$.

The phase integral: $\int_0^x dx' p(x') = e^2\sqrt{\frac{2m}{E}}\int_0^{Ex/e^2} dy\sqrt{\frac{1+y}{y}}$. This expression can be written as:

$e^2\sqrt{\frac{2m}{E}}[\left\{\frac{Ex}{e^2}\left(1 + \frac{Ex}{e^2}\right)\right\}^{\frac{1}{2}} + \ln\{(\frac{Ex}{e^2})^{\frac{1}{2}} + \left(1 + \frac{Ex}{e^2}\right)^{\frac{1}{2}}\}]$, (Abramowitz and Stegun).
For $x \to \infty$ The wave function $\psi(x) = 2\sin kx$. No phase shift for $\lim_{x\to\infty}\psi(x)$.
The amplitude D in the expression for the wave function is found by means of Delta-function normalization (page 66,Mahan): $D = 2\sqrt{\hbar k}$.
This is also illustrated by: $\delta_{WKBJ}(k) = \lim_{x\to\infty}[\frac{1}{\hbar}\int_0^x dx' p(x') - kx] = 0$.
The expression for the continuum eigen function becomes:
$$\psi(x) = \frac{2}{\sqrt{1+\frac{e^2}{Ex}}}\sin(\frac{e^2}{E}k[\left\{\frac{Ex}{e^2}\left(1 + \frac{Ex}{e^2}\right)\right\}^{\frac{1}{2}} + \ln\{(\frac{Ex}{e^2})^{\frac{1}{2}} + \left(1 + \frac{Ex}{e^2}\right)^{\frac{1}{2}}\}]).$$

3.2 Bound States by WKBJ.

In this section it is shown how to find eigenfunctions and eigenvalues with the WKBJ approximation. This is done for one dimensional problems. Examples are given in this section.

To find the bound states, for a potential with a smooth minimum Mahan actually implies two solutions for continuum states: Eqs. (3.40) and (3.41). That is not what I expected to do. Nevertheless, it works. Mahan finds discrete-bound-states. Then Mahan gives a few examples.

3.2.1 Harmonic Oscillator

The eigenvalue equation for the harmonic oscillator is:

$\int dx[m(2E_n - Kx^2)]^{1/2} = \pi\hbar(n+\frac{1}{2})$. After evaluating the integral, the expression for E_n is the expression found in chapter 2. Then Mahan writes: "The poor quality of the WKBJ eigenfunction at turning points does not affect the quality of the eigenvalue." The poor quality? Is this equal to the statement that the WKBJ is an excellent method of describing the motion of particles except those states with the lowest energy?

In Eq. (3.142) the m should be deleted. A printing error.

3.2.2 Morse Potential

Schrödinger's equation can be solved exactly. Mahan will show this in chapter 5. The basic equation for WKBJ is: $\pi\hbar\left(n+\frac{1}{2}\right) = \sqrt{2mAa}\int_{y_2}^{y_1}\frac{dy}{y}[(y_1-y)(y-y_2)]^{1/2}$, where y_1 and y_1 are the turning points.

Mahan gave the result of the integration and mentioned the use of standard tables. With help of the WolframAlpha app it is just fun to find the result yourself. It starts with the substitution: $u = y - \frac{y_2+y_1}{2}$, followed by the use of goniometric relations, other substitutions, particle fractions and finally use of the relation $tan^{-1}(x) + tan^{-1}\left(\frac{1}{x}\right) = \frac{\pi}{2}$.

The final result is : $\frac{\pi}{2}\left(y_1 + y_2 - 2\sqrt{y_1y_2}\right) = \frac{\pi}{2}(\sqrt{y_1} - \sqrt{y_2})^2$.

3.2.3 Symmetric Ramp

In chapter 2 the ramp has been discussed and exact solutions for the bound waves are found.

The eigenvalue equation for the ramp is: $\pi\hbar\left(n+\frac{1}{2}\right) = \sqrt{2m}\int dx\sqrt{E_n - F|x|}$.

Furthermore: $E_n = E_F[\frac{3\pi}{4}\left(n+\frac{1}{2}\right)]^{2/3}$, and $E_F = (\frac{\hbar^2F^2}{2m})^{1/3}$, Eqs. (3.71) and (3.72).

Mahan writes at the bottom of page 73: "The potential $V(x) = F|x|$ is symmetric $[V(-x) = V(x)]$. The eigenfunctions can be separated into even and odd parity. In WKBJ, the solutions with even values of integer n have even parity [$\psi(-x) = \psi(x)$; Mahan writes $V(-x) = V(x)$. I think this to be a printing error], while those with odd values of n have odd parity [$\psi(-x) = -\psi(x)$]". Well, let's have a look. The eigenfunction is, Eq. (3.46):

$\psi(x) = \frac{-(-1)^{n+1}C_L}{\sqrt{p(x)}}\sin\phi_R(x)$, where $p(x) = \sqrt{2m(E_n - F|x|)}$. For ϕ_R we have Eq. (3.44): $\phi_R = \Theta_R + \frac{\pi}{4}$, and, Eq. (3.43), $\Theta_R(x) = \frac{1}{\hbar}\int_x^{b_R} dx'\, p(x')$. b_R is the turning point of the potential shown at the right-hand side of Figure 3.3. For example we take $x > 0$, and obtain for $\Theta_R(x) = \sqrt{2m}\frac{2}{3F\hbar}(E_n - Fx)^{3/2}$. At $x = 0$, after rearranging: $\Theta_R(0) = \frac{1}{2}\pi(n + \frac{1}{2})$.
For the eigenfunction we write:

$\psi(x) = \frac{-(-1)^{n+1}C_L}{\sqrt{p(x)}}\sin\left(\Theta_R(x) + \frac{\pi}{4}\right) = \frac{-(-1)^{n+1}C_L}{2\sqrt{p(x)}}\sqrt{2}\{\sin(\Theta_R(x)) + \cos(\Theta_R(x))\}$. It is not clear to me how to separate this eigenfunction into even and od parity, in spite of $\Theta_R(x)$ depending on E_n and consequently on n.
We can write for n is even: $\psi(x) = \frac{C_L}{2\sqrt{p(x)}}\sqrt{2}\{\sin(\Theta_R(x)) + \cos(\Theta_R(x))\}$, and for n is odd: $\psi(x) = \frac{-C_L}{2\sqrt{p(x)}}\sqrt{2}\{\sin(\Theta_R(x)) + \cos(\Theta_R(x))\}$. The eigenfunction just changes sign. Well, by inspection you find, with help of the above expression for $\Theta_R(0)$: for n is even $\psi(0) \neq 0$, and for n is odd , $\psi(0) = 0$. The latter values of the eigenfunction at $x = 0$ indicate even and odd parity. We could go a small step further by expanding $\Theta_R(x)$ near $x \to 0$. Then we have: $\Theta_R(x) = \frac{2\sqrt{2m}}{3F\hbar}E_n^{\frac{3}{2}}(1 - \frac{3Fx}{2E_n})$. With the expressions for E_n and E_F, Eqs. (3.71) an (3.72), we find $\sin\,(\Theta_R(x) + \frac{\pi}{4})$ to be: $\sin\,(\frac{\pi}{2}(n+1) - \frac{\sqrt{2mE_n}}{\hbar}x)$. Now we have for n is odd a function of odd parity: $\sin\,(\frac{\sqrt{2mE_n}}{\hbar}x)$ and for n is even a function of even parity: $\cos\,(\frac{\sqrt{2mE_n}}{\hbar}x)$.
In this section Mahan also discussed the exact solutions in terms of Airy function as given in Chapter 2. The eigenvalue equations are given and can be compared with the equations in Homework 8 of the same chapter.

3.2.4 Discontinuous Potentials.

In this section Mahan dealt with two examples: A particle in a box and the half-space linear potential.
For the particle in a box WKBJ gives the exact eigenvalue. The eigenfunction is also exact. For a particle in a box we use Eq. (3.15) and find with help of the boundary conditions: $\psi = 0$ at $x = 0 \;\; \to \;\; A_1 = -A_2$ and for $\psi = 0$ at $x = L \to \;\; E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{L})^2$. For the eigenfunction we have, with $p = \sqrt{2mE_n}$, $\psi_n = \frac{2iA_1}{(2mE_n)^{1/4}}\sin\,(kx)$, where $k = \frac{n\pi}{L}$. To conclude with normalization: $\frac{2iA_1}{(2mE_n)^{1/4}} = \sqrt{\frac{2}{L}}$.
As Mahan writes: “The eigenfunction is exact”. What does this mean for the higher order terms in the WKBJ expansion? For example, what is the contribution of σ_2 in Eq. (3.6)? With help of Eq. (3.8) you will find σ_2 to be a $constant$ and in the expansion of $\psi(x)$, the contribution is: $\exp\,(\frac{\hbar}{i}constant)$. So, this term contributes as a phase factor. This leads to the conclusion “The eigenfunction is exact”, is valid for the standard WKBJ where $O(\hbar^2)$ and higher order are neglected.

The eigenvalue equation for the half-space linear potential is similar to the potential found for the symmetric ramp given in the preceding section.

Homework 5, 6, 11.

Exercise 5.

Use WKBJ to find the eigenvalue of bound states in the one-dimensional potential:

$$V(x)\begin{cases} = 0 & |x| < a \\ = \dfrac{K}{2}(|x| - a)^2 & |x| > a \end{cases}$$

This potential to some extent $(a = 0)$ resembles the harmonic oscillator. We need to evaluate the phase integral between the turning points b_L and b_R. The potential function is symmetric so we evaluate $2\int_0^{b_R} p(x)dx = \pi\hbar(n + \frac{1}{2})$.

For the integral we write: $2[\int_0^a dx\sqrt{2mE_n} + \int_a^{b_R} dx\sqrt{2m\left(E_n - \frac{K}{2}(x-a)^2\right)}]$ where $b_R = a + \sqrt{\frac{2E_n}{K}}$. Now we have all the ingredients to evaluate the phase integral available. Then $\pi\hbar\left(n + \frac{1}{2}\right) = 2[\int_0^a dx\sqrt{2mE_n} + \int_a^{b_R} dx\sqrt{2m\left(E_n - \frac{K}{2}(x-a)^2\right)}]$,with help of $x = a + \sqrt{\frac{2E_n}{K}}\sin\alpha$, we finally obtain for E_n:

$$E_n = \hbar\left(n + \frac{1}{2}\right)\sqrt{\frac{K}{m}} + \frac{4a^2}{\pi^2}K + \frac{2a}{\pi}\sqrt{\left[\frac{(2aK)^2}{\pi^2} + 2K\hbar\left(n + \frac{1}{2}\right)\sqrt{\frac{K}{m}}\right]}.$$

For $a = 0$ the harmonic oscillator is recovered; Eq. (3.57).

Exercise 6.

Use WKBJ to find the bound-state energies E_n in the symmetric quartic potential $V(x) = Kx^4$. *Hint:*

$\int_0^1 dy\sqrt{1-y^4} = \frac{\Gamma(\frac{1}{4})\Gamma(\frac{3}{2})}{4\Gamma(\frac{7}{4})} = 0.8740$. Just for curiosity. This hint is based on the Beta Function:

$\int_0^1 dy\sqrt{1-y^4} = \frac{\Gamma(\frac{1}{4})\Gamma(\frac{3}{2})}{4\Gamma(\frac{7}{4})} = \frac{\Gamma(\frac{1}{4})\Gamma(\frac{3}{2})}{4\Gamma(\frac{1}{4}+\frac{3}{2})} = \frac{1}{4}B\left(\frac{1}{4},\frac{3}{2}\right) = \int_0^1 dt\, t^{-3/4}\,(1-t)^{1/2}$ and $t = y^4$ (Abramowitz and Stegun).

Now the physical part: the potential is symmetric so $2\int_0^{b_R} dx\sqrt{2m(E_n - Kx^4)^{\frac{1}{2}}} = \hbar\pi(n + \frac{1}{2})$, with turning point $b_R = (\frac{E_n}{K})^{1/2}$. After substitution of $y = (\frac{K}{E_n})^{1/4}x$ the equation for the eigenvalues becomes: $2\sqrt{2mE_n}\left(\frac{E_n}{K}\right)^{\frac{1}{4}}\int_0^1 dy(1-y^4)^{\frac{1}{2}} = \hbar\pi\left(n + \frac{1}{2}\right)$. With the above expression for the Beta Function the equation for bound-states energies E_n is:

$E_n = [\frac{\hbar\pi(n+\frac{1}{2})}{1.748}]^{4/3}(\frac{1}{4}\frac{K}{m^2})^{1/3}$.

Exercise 11.
For the half-space potential

$$V(x) = \begin{cases} \infty & x < 0 \\ -\frac{e^2}{x} & 0 < x \end{cases}$$

find all the bound-state energies by WKBJ.
We have a half-space potential and a discontinuous potential at $x = 0$, since $V(0) = \infty$.
With the phase integral given in Eq. (3.87):
$\frac{\pi}{4} + \frac{1}{\hbar}\int_0^{b_R} dxp(x) = \pi(n+1)$, we can find the bound-energies. Now we have:
$p(x) = \sqrt{2m(E_n + \frac{e^2}{x})}$, where $E_n < 0$. For convenience we substitute $E_n = -E$. The turning point $b_R = \frac{e^2}{E}$. For the phase integral we find by substituting $\frac{xE}{e^2} = y$,
$\frac{e^2\sqrt{2m}}{\sqrt{E}}\int_0^1 dy\sqrt{\frac{1-y}{y}} = \pi\hbar(n+\frac{3}{4})$. With help of a table of integrals or with WolframAlpha app or with substitution and partial fractions you finally obtain:
$\int_0^1 dy\sqrt{\frac{1-y}{y}} = \frac{\pi}{2}$. The phase integral gives as a result for $E_n = -E = -\frac{1}{4}\frac{2me^4}{\hbar^2(n+\frac{3}{4})^2}$.
For $n = 0$, $E_0 = -\frac{4}{9}\frac{2me^4}{\hbar^2}$. Well, this can hardly be called a close approximation of the exact eigenvalue for the ground state: $E = -\frac{1}{4}\frac{2me^4}{\hbar^2}$. I expected to find with WKBJ something like: $E_0 = -\frac{2}{9}\frac{2me^4}{\hbar^2}$. I did not.

3.3 Electron Tunneling.

WKBJ is used to calculate the tunneling rate of particles through potential barriers. Mahan mentioned WKBJ to be an accurate method of obtaining tunneling rates. An example is presented.
I do not know why Mahan used E for the states of the electrons and for the external potential of the electric field.

Homework 15, 16.

Exercise 15.
At the interface between a metal and a semiconductor, a Scottky barrier is formed due to a depletion region. The potential function is
$V(x) = A(x_0 - x)^2$ for $0 < x < x_0$
$= 0$ for $x > x_0, x < 0$
where $x = 0$ is the interface; the metal is at $x < 0$ and the semiconductor at $x > 0$. Use WKBJ to calculate the tunneling exponent $2\int dx\alpha(x)$ of an electron with energy E, $[Ax_0^2 > E > 0]$ going from the metal to the semiconductor.
Remark: is the factor 2 in the tunneling exponent $2\int dx\alpha(x)$ relevant?

We have a potential barrier $V(x) > E$, and $2\alpha(x) = \frac{\sqrt{2m}}{\hbar}\int_0^x dx' \sqrt{V(x') - E}$. Eq. (3.92).
With tunneling we have a evanescent wave without phase factors.

The turning point of the right-hand side is found for $V - E = 0$: $x = x_0 - \sqrt{\frac{E}{A}} = b_R$.

So we have to evaluate: $2\alpha = \int_0^{b_R} dx\sqrt{A(x_0 - x)^2 - \mathrm{E}}$.

After some manipulations with the integral and using $\beta = \sqrt{\frac{Ax_0^2}{E}}$, we obtain with help of a table of integrals: $2\alpha = \frac{1}{2}[\beta\sqrt{\beta^2 - 1} - \ln(\beta + \sqrt{\beta^2 - 1})]$.

Exercise 16.
A potential $V(x)$ is an inverted parabola:
$V(x) = K(a^2 - x^2), |x| < a$ and $V(x) = 0\,, |x| > a$.
Remark: An inverted parabola? Convex? It is a parabola.
Calculate the WKBJ tunneling exponent $\alpha = \int k(x)dx$, for values of $0 < E < Ka^2$.
There are two turning points b_R andb_L.
We have to evaluate : $\alpha = \frac{\sqrt{2mK}}{\hbar}\int_{b_L}^{b_R} dx\sqrt{a^2 - x^2 - \frac{E}{K}}$.
We substitute $\beta = \pm\sqrt{a^2 - \frac{E}{K}}$ in the expression for α and with the turning points where the square root equals 0 we find: $\alpha = \frac{\sqrt{2mK}}{\hbar}\int_{-\beta}^{\beta} dx\sqrt{\beta^2 - x^2}$. The integral can be found from a table of integrals(Abramowitz and Stegun) and with WolframAlpha.
The result is: $\alpha = \frac{\pi}{2}\sqrt{\frac{2mE^2}{\hbar^2 K}}(\frac{a^2K}{E} - 1)$.

3.4 Variational Theory.

As mentioned by Mahan the Variational method is useful for finding the eigenfunction and eigenvalue of the lowest bound state of a Hamiltonian. First the theory is explained, followed by two examples: the half-space potential and the harmonic oscillator.

3.4.1 Half-Space Potential

The variational method is about assuming the trial function and find the lowest possible energy functional. The result with the variational method is not as precise as the WKBJ method for the same potential.
On page 79 Mahan introduced the functional $\mathcal{E}(\phi)$; ϕ is the trial function. "The best eigenvalue is the lowest value of $\mathcal{E}(\phi)$." On the same page Mahan explained how to find the minimum energy by varying the parameters on which $\mathcal{E}(\phi)$ depends. Mahan gives the resulting equations to find the parameters $a_1, \ldots\ldots m$, Eqs. (3.114) – (3.117). Well, I do not understand these equations to be the equations to find the minimum energy. On page 81 Mahan illustrates the optimization procedure for a single parameter α and the optimization equation is : $0 = \frac{d\mathcal{E}}{d\alpha}$. So I think Eq. (3.114) should read : $0 = \frac{\partial\mathcal{E}}{\partial a_1}$, and so on. See also www.hitoshi.berkeley.edu , 221A Lecture Notes- Variational Method.
In this section Mahan illustrated the variational method for the linear half-space potential:

$V(x) = Fx$. The trial function $\phi = Axe^{-\alpha x}$ has been used. This results into the trial eigenfunction given in Eq. (3.137): $\psi(x) = \frac{Ax}{\sqrt{I}} \exp\left[-\alpha_0 x\right]$. Mahan concludes: “The prefactor has the correct normalization”. Meaning: $I = 2! \frac{A^2}{(2\alpha_0)^3}$. Use has been made of Eq. (3.129) with α replaced by α_0, where α_0 is found from the optimization procedure.

3.4.2 Harmonic Oscillator in One Dimension.

A Gaussian trial function is chosen. The result equals the exact eigenvalue and eigenfunction for the ground state.

Homework 7, 8, 9, 10,13, 14.

Exercise 7.

Use the trial eigenfunction $\phi = Ax \exp[-(\alpha x)^p]$ to find the lowest eigenvalue for the half-space linear potential for $p = \frac{3}{2}$ and $p = 2$. Which of the three exponents $p = \left(1, \frac{3}{2}, 2\right)$ gives the lowest eigenvalue?

The trial function depends on two parameters: α and p. Mahan mentioned on page 80: “Most of our examples have only one variational parameter, since with two or more one has to minimize on the computer. “ So, I suppose this to be the reason to perform the optimization $0 = \frac{\partial \mathcal{E}}{\partial \alpha}$ for a given value of p . Well, I will present the complete picture and at the end I will substitute a value for p.

I shall start with the integral $I = \int dx |\phi|^2$.

Make use of the substitution $|\alpha x|^p = y$ and $2y = z$. The integral I becomes:

$$I = \frac{A^2}{\alpha^3 p} (\frac{1}{2})^{3/p} \int_0^\infty dz(z)^{\frac{3-p}{p}} \exp(-z) = \frac{A^2}{\alpha^3 p} \left(\frac{1}{2}\right)^{\frac{3}{p}} \Gamma(\frac{3}{p}) \ . \qquad \textbf{(C.3.3)}$$

Now you will notice that finding $0 = \frac{d\mathcal{E}}{dp}$, is a lot of work.

Substitute $p = 1$ in **(C.3.3)** and you will find Eq.(3.129); $\Gamma(3) = 2!$. Again, the WolframAlpha app is of great help.

Now the Hamiltonian. First the potential energy $PE = \int dx V(x) \, |\phi|^2$. The half space linear potential: $V(x) = Fx$. We use the substitutions given above for x and y:

$$PE = \frac{A^2 F}{\alpha^4 p} (\frac{1}{2})^{4/p} \int_0^\infty dz(z)^{\frac{4-p}{p}} \exp(-z) = \frac{A^2 F}{\alpha^4 p} \left(\frac{1}{2}\right)^{\frac{4}{p}} \Gamma(\frac{4}{p}) \ . \qquad \textbf{(C.3.4)}$$

Substitute $p = 1$ in **(C.3.4)** and you will recover Eq. (3.131).

The kinetic energy: $KE = \frac{\hbar^2}{2m} \int dx |\frac{d\phi}{dx}|^2$. Again using the substitution for x and y :

$$KE = \frac{\hbar^2}{2m} \frac{A^2}{\alpha p} (\frac{1}{2})^{1/p} \left[\int_0^\infty dz(z)^{\frac{1-p}{p}} e^{-z} + p \int_0^\infty dz(z)^{\frac{1}{p}} e^{-z} + \frac{p^2}{4} \int_0^\infty dz(z)^{\frac{1+p}{p}} e^{-z} \right] =$$

$$\frac{\hbar^2}{2m} \frac{A^2}{4\alpha} \left(\frac{1}{2}\right)^{\frac{1}{p}} p\Gamma(\frac{1+2p}{p}) \ . \qquad \textbf{(C.3.5)}$$

For $p = 1$, **(C.3.5)** gives Eq.(3.130).

The energy functional: $\mathcal{E}(\phi) = \frac{KE+PE}{I}$. We substitute the expressions for KE, PE and I into the $\mathcal{E}(\phi)$ and obtain: $\frac{\frac{\hbar^2}{2m4}\frac{A^2}{\alpha}\left(\frac{1}{2}\right)^{\frac{1}{p}} p\Gamma\left(\frac{1+2p}{p}\right)+\frac{A^2F}{\alpha^4 p}\left(\frac{1}{2}\right)^{\frac{4}{p}}\Gamma(\frac{4}{p})}{\frac{A^2}{\alpha^3 p}\left(\frac{1}{2}\right)^{\frac{3}{p}}\Gamma(\frac{3}{p})}$, after rearranging this becomes:

$$\mathcal{E}(\alpha,p) = \frac{\frac{\hbar^2}{2m}\frac{\alpha^2}{4}\left(\frac{1}{2}\right)^{\frac{-2}{p}} p^2\Gamma\left(\frac{1+2p}{p}\right)+\frac{F}{\alpha}\left(\frac{1}{2}\right)^{\frac{1}{p}}\Gamma(\frac{4}{p})}{\Gamma(\frac{3}{p})}. \qquad \textbf{(C.3.6)}$$

This equation illustrates the remark by Mahan to have one variational parameter. Now we vary $\mathcal{E}$ with α for some values of p. For obvious reasons we write **(C.3.6)** as:
$\mathcal{E}(\alpha) = \frac{\hbar^2\alpha^2}{2m}K(p) + \frac{F}{\alpha}P(p)$, and with $\frac{\partial\mathcal{E}}{\partial\alpha} = 0$, $\alpha_0 = (\frac{Fm}{\hbar^2}\frac{P(p)}{K(p)})^{1/3}$.

$$\text{Furthermore: } \frac{P(p)}{E(p)} = \frac{4\left(\frac{1}{2}\right)^{\frac{3}{p}}\Gamma(\frac{4}{p})}{p^2\Gamma(\frac{1+2p}{p})}. \qquad \textbf{(C.3.7)}$$

For $p = 1, \frac{P(p)}{E(p)} = \frac{3}{2}$, Eq. (3.134),
and $p = \frac{3}{2}, \frac{P(p)}{E(p)} = \frac{8\sqrt{2}}{9}$; and $p = 2, \frac{P(p)}{E(p)} = \frac{1}{6\sqrt{2\pi}}$.
Now we substitute the general expression for $\alpha_0 = (\frac{Fm}{\hbar^2}\frac{P(p)}{K(p)})^{1/3}$ into **(C.3.6)** with **(C.3.7)** we obtain:

$$\mathcal{E}(\alpha_0) = \frac{E_F}{\Gamma(\frac{3}{p})}[p^2 2^{\frac{6-8p}{3p}}\left(\frac{P(p)}{K(p)}\right)^{\frac{2}{3}}\Gamma\left(\frac{1+2p}{p}\right) + 2^{\frac{p-3}{3p}}\left(\frac{K(p)}{P(p)}\right)^{\frac{1}{3}}\Gamma\left(\frac{4}{p}\right)], \qquad \textbf{(C.3.8)}$$

and $E_F = (\frac{\hbar^2 F^2}{2m})^{1/3}$, Eq. (3.72).
Finally, the Question is: does $p = 1$produces the lowest approximation of the ground state? Well, for $p = 1$ we find with **(C.3.7)** and **(C.3.8)** $\mathcal{E}(\alpha_0) = 2.476\, E_F$, Eq. (3.136), for $p = \frac{2}{3}, \mathcal{E}(\alpha_0) = 2.671\, E_F$ and for $p = 2, \mathcal{E}(\alpha_0) = 2.792\, E_F$. So $p = 1$ gives the best approximation for the three given values of p. Whether this represents the best approximation for the given trial function is not clear. Then we have to calculate in addition $\frac{\partial\mathcal{E}}{\partial p} = 0$, substitute α_0 in the resulting equation and find the lowest possible value for p. May be the equation for p is relatively easy found. However we have to solve this equation numerical with help of a computer program.

Exercise 8.
Use the variational method to find the ground-state energy of the following potential $(-\infty < x < \infty)$:
$V(x) = -V_0 \exp\,[-\left(\frac{x}{a}\right)^2]$,
$g = \frac{2ma^2V_0}{\hbar^2} = \sqrt{8}$.
Choose your own trial function, and obtain a numerical answer for the binding energy as a fraction of V_0.
At $x = 0$ the potential well is most "attractive" and a trial function must reflect the probability to find a particle at $x = 0$ to be maximal for the ground state. So a trial function could be: $\phi = A\exp[-\frac{1}{2}(\frac{\alpha x}{a})^2]$. Now, similar to exercise 7 we calculate I:

$I = \int dx|\phi|^2 = \int_{-\infty}^{\infty} dxA^2 \exp[-(\frac{\alpha x}{a})^2] = \frac{A^2 a}{\alpha}\sqrt{\pi}$. (Normalization).
For the potential energy we find:

$PE = \int dxV(x)\,|\phi|^2 = -A^2V_0\sqrt{\pi}\sqrt{\frac{a^2}{1+\alpha^2}}$.

The kinetic energy:

$KE = \frac{\hbar^2}{2m}\int dx|\frac{d\phi}{dx}|^2 = \frac{\hbar^2A^2}{2ma}\alpha\frac{1}{2}\sqrt{\pi}$.

With I, PE and KE the energy potential is:

$\mathcal{E}(\alpha) = \frac{\hbar^2\alpha^2}{2ma^2}\frac{1}{2} - V_0\frac{\alpha}{\sqrt{1+\alpha^2}}$, or with g, as defined above:

$\frac{\mathcal{E}(\alpha)}{V_0} = \alpha^2\sqrt{2} - \frac{\alpha}{\sqrt{1+\alpha^2}}$.

So $\frac{d\mathcal{E}}{d\alpha} = 0 = 2\sqrt{2}\alpha - \frac{1}{(1+\alpha^2)^{3/2}}$.

We have to solve $2(1+\alpha^2)\alpha^{\frac{2}{3}} = 1$. With the WolframAlpha app this is easy. You will find one real solution and two complex solutions.

The real solution is : $\alpha = 0.30849$. Then we find for $\frac{\mathcal{E}(\alpha)}{V_0} = -0.3351$. A negative fraction as it should be since V_0 is a positive number. Is this the best approximation? We could vary the power of α, or choose another trial function like the Lorentzian function: $\frac{\alpha}{x^2+1}$. I leave it here.

Exercise 9.

Use the following trial function $\phi(x) = Ax\exp(-\alpha x)$ to find the ground-state energy variationally for the half-space potential:

$$V(x) = \begin{cases} \infty & x < 0 \\ -\frac{e^2}{x} & 0 < x \end{cases}$$

Where e and m are the charge and mass of an electron.
For this exercise we can use some results of section 3.4.1.

Normalization: $I = \int_0^{\infty} dxA^2\,x^2\exp(-2\alpha x) = \frac{2!A^2}{(2\alpha)^3}$. Eq. (3.129).

Kinetic energy: $KE = \frac{\hbar^2A^2}{2m}\int_0^{\infty} dx(1-\alpha x)^2\exp(-2\alpha x) = \frac{\hbar^2A^2}{2m}\frac{1}{4\alpha}$. Eq. (3.130).

Potential energy: $PE = -A^2\int_0^{\infty} dx\frac{e^2}{x}\exp(-2\alpha x) = -\frac{A^2e^2}{4\alpha^2}$.

The energy functional is: $\mathcal{E}(\alpha) = \frac{\hbar^2}{2m}\alpha^2 - e^2\alpha$. Variation $\mathcal{E}$ with respect to α, then with $\frac{d\mathcal{E}}{d\alpha} = 0$, we have $\alpha = \frac{1}{2}\frac{2me^2}{\hbar^2}$. With this value for α the ground-state energy is :

$\mathcal{E} = -\frac{1}{4}\frac{2me^4}{\hbar^2}$. A negative value as it should be.

Exercise 10.

Show that the $\phi(x)(= Ax\exp(-\alpha x))$ for the half-space potential:

$$V(x) = \begin{cases} \infty & x < 0 \\ -\frac{e^2}{x} & 0 < x \end{cases}$$

is an exact eigenstate of the Hamiltonian, and find its eigenvalue. To this end we substitute $\phi(x) = Ax \exp(-\alpha x)$ into, $0 = -(\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{e^2}{x} + E)\phi(x)$. The result is:
$E = -\frac{1}{4}\frac{2me^4}{\hbar^2}$.

Exercise 13.
Use the variational method to find the eigenvalue of the harmonic oscillator with the trial eigenfunction $\phi = Ax \exp[-\alpha^2 x^2/2]$.
Remark: In section 3.4.2 Mahan gave the example trial function for the ground state $\phi = A \exp[-\alpha^2 x^2/2]$. With variation of the energy functional the ground state wave function is: $\psi_0 = \sqrt{\frac{\alpha_0}{\sqrt{\pi}}} \exp[-\alpha_0^2 x^2/2]$ and $\alpha_0^4 = \frac{mK}{\hbar^2}$. (Keep in mind the amplitude A of the ground state differs from the A of $\phi = Ax \exp[-\alpha^2 x^2/2]$.)
This result, ψ_0 , is the exact result for the ground state $n = 0$. This is nice. However, not knowing the exact result to find the "best approximation" is a bit more challenging.
With the best approximation of the ground state are we allowed to use the raising operator to find the excited states?
Back to the exercise.
Normalization: $I = A^2 \int_{-\infty}^{\infty} dx\, x^2 \exp[-\alpha^2 x^2] = \frac{A^2\sqrt{\pi}}{2\alpha^3}$.
Potential Energy: $PE = \frac{KA^2}{2}\int_{-\infty}^{\infty} dx x^4 \exp[-\alpha^2 x^2] = \frac{3KA^2\sqrt{\pi}}{8\alpha^5}$.
Kinetic Energy: $KE = \frac{\hbar^2 A^2}{2m}\int_{-\infty}^{\infty} dx |\frac{d\phi}{dx}|^2 = \frac{\hbar^2 A^2}{2m}\int_{-\infty}^{\infty} dx (1-\alpha^2 x^2)^2 \exp[-\alpha^2 x^2] =$
$= \frac{\hbar^2 A^2}{2m}\frac{3\sqrt{\pi}}{4\alpha}$.
The energy functional: $\mathcal{E} = \frac{KE+PE}{I} = \frac{\hbar^2}{2m}\frac{3}{2}\alpha^2 + K\frac{3}{4\alpha^2}$.
Variation with respect to α : $\frac{d\mathcal{E}}{d\alpha} = 0 = \frac{\hbar^2}{2m}3\alpha - K\frac{3}{2\alpha^3}$.
This leads to: $\alpha_1^2 = \sqrt{\frac{mK}{\hbar^2}} (= \alpha_0^2)$, Eq. (3.145). Substitute this value into the energy functional and we finally obtain: $\mathcal{E} = \frac{3}{2}\hbar\sqrt{\frac{K}{m}} = \frac{3}{2}\hbar\omega$. This results is presented in section 3.4.2. This eigenvalue is the exact value of the first exited state $n = 1$. As mentioned by Mahan the trial function $\phi = Ax \exp[-\alpha^2 x^2/2]$ is orthogonal to the ground state trial function $\phi = A \exp[-\alpha^2 x^2/2]$.
By evaluating the integral: $A^2 \int_{-\infty}^{\infty} dx \exp[-\alpha^2 x^2/2]\, x \exp[-\alpha^2 x^2/2]$, we find the orthogonality. Normalization leads to $A = \sqrt{\frac{2\alpha_1^3}{\sqrt{\pi}}}$. So the wave function for the exited state is
$\psi_1 = x\sqrt{\frac{2\alpha_1^3}{\sqrt{\pi}}} \exp[-\frac{1}{2}\alpha_1^2 x^2] = \sqrt{\frac{2\alpha_0^3}{\sqrt{\pi}}} x \exp[-\frac{1}{2}\alpha_0^2 x^2] = \alpha_0\sqrt{2}x\psi_0$.
This can be written as: $\psi_1 = \sqrt{\frac{2m\omega}{\hbar}}\; x\psi_0$.
Remark: there is something troubling me. In chapter 10 of "The Theoretical Minimum" Susskind dealt with the harmonic oscillator. He used a trial function for the ground state and with help of the raising operator calculated the first two excited states(pages 339 and 340).

Susskind found: $\psi_1(x) = 2i\omega x e^{-\frac{\omega}{2\hbar}x^2}$*, where* $e^{-\frac{\omega}{2\hbar}x^2}$ *is the ground-state wave function;* $\omega = \sqrt{\frac{K}{m}}$*. Compare the Susskind wave function with the Mahan wave function for the ground state and you obtain:* $\alpha_0^2 = \frac{\omega}{\hbar}$*. On the other hand :* $\alpha_0^2 = \sqrt{\frac{mK}{\hbar^2}} = m\frac{\omega}{\hbar}$*. Well, Susskind did not normalize the ground-state wave function. So, to make a correct comparison you have to use normalization. That does not save the day. Since Susskind used an "x" different from that used by Mahan. Susskind used:* $x = \sqrt{m}\, y$*. Where* y *represents the real world. In addition Susskind ignored a factor* $-i/\omega\hbar$*. Plugging this factor back into the exited state, this state becomes normalized again.*

Exercise 14.
Use the variational method to solve for the ground-state eigenvalue of the quartic potential $V(x) = Kx^4$ using a Gaussian trial wave function.
A Gaussian trial wave function: $\phi = A\exp(-\frac{1}{2}\alpha^2 x^2)$.
Normalization: $I = \int_{-\infty}^{\infty} dx|\phi|^2 = \frac{A^2}{\alpha}\sqrt{\pi}$, Eq. (3.140).
Kinetic Energy : $KE = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx|\frac{d\phi}{dx}|^2 = \frac{\hbar^2\alpha A^2}{4m}\sqrt{\pi}$, Eq. (3.141).
Potential Energy: $PE = \int_{-\infty}^{\infty} dx\, V(x)\,|\phi|^2 = \frac{3KA^2}{4\alpha^5}\sqrt{\pi}$.
The energy functional: $\mathcal{E} = \frac{KE+PE}{I} = \frac{\hbar^2}{4m}\alpha^2 + \frac{3K}{4}\frac{1}{\alpha^4}$.
Variation of the energy functional with respect to α:
$\frac{d\mathcal{E}}{d\alpha} = 0 = \frac{\hbar^2}{2m}\alpha - 3K\frac{1}{\alpha^5}$, gives for the ground-state value of α: $\alpha_0^6 = \frac{6Km}{\hbar^2}$.
So we finally find for the eigenvalue: $\mathcal{E}_0 = \frac{1}{2}\left(\frac{3K\hbar^4}{2m^2}\right)^{\frac{1}{3}}(2^{\frac{2}{3}} + 1)$.
The eigenfunction: $\psi_0 = \sqrt{\frac{\alpha_0}{\sqrt{\pi}}}\exp[-\frac{1}{2}\alpha_0^2 x^2]$. This ground-state eigenfunction is similar to that of the harmonic oscillator. This is not surprising: the potential function for the quartic potential is similar to the function for the harmonic oscillator. The quartic potential produces a different α_0 .

Homework.

The exercises can be found in the relevant sections.

4. Spin and Agular Momentum

In this chapter the eigenfunctions and eigenvalues for both spin and angular momentum are derived. Mahan mentioned the derivation to be based on the Heisenberg approach, i.e. the operator method.

In the introduction to this chapter Mahan mentioned the major contributors to the angular momentum are spin ($\vec{s}$) and the orbital angular momentum ($\vec{l}$). Adding angular momentum in quantum mechanics is not a straightforward addition since the three components of $\vec{j} = \vec{l} + \vec{s}$ are quantized. In this chapter attention is paid to orbital or orbital and spin components of angular momentum.

The eigenvalues for $\vec{l}$ and $\vec{s}$ are derived.

Mahan concluded this introduction with: "…….. formulas are valid for all values of angular momentum. They apply equally well to spin or orbital motion."

Question: What does "…. Apply equally well … " mean?

4.1 Operators, Eigenvalues, and Eigenfunctions

Mahan presented the expressions for orbital angular momentum. The expressions of the components M_x, M_y and M_z for orbital angular momentum $\vec{M}(= \vec{l}?)$.

4.1.1 Commutation Relations

In this section Mahan showed the orbital angular momentum not to commute. As a reminder: a simple example is $x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x = [x\frac{\partial}{\partial x}, \frac{\partial}{\partial x}x] \neq 0$. In deriving Eqs. (4.8)-(4.10) use has been made of e.g. : $yp_x - p_xy = 0$, and $xz - zx = 0$. Furthermore $[p_z, z] = -[z, p_z]$, and $[z, p_z] = i\hbar$.

Keep in mind, page 88,: The components of spin angular momentum ($\vec{s}$) obey the commutation relations presented in Eqs. (4.8)-(4.10). Mahan: "In fact, the components of any kind of angular momentum obey these relationships"; the Eqs. (4.8)-(4.10). So $\vec{j}$ the total angular momentum obeys these relationships.

To find Eq. (4.11) use has been made of Eqs. (4.12) and (4.17) : $[M_z^2, M_z] = 0$,

$\left[M_x^2 + M_y^2, M_z\right] = 0$

$\left[M_x^2 + M_y^2, M_z\right] + [M_z^2, M_z] = \left(M_x^2 + M_y^2\right)M_z - M_z\left(M_x^2 + M_y^2\right) + M_z^2M_z - M_zM_z^2 = \left(M_x^2 + M_y^2 + M_z^2\right)M_z - M_z\left(M_x^2 + M_y^2 + M_z^2\right) = M^2M_z - M_zM^2 = [M^2, M_z] = 0$,

Eq. (4.11).

On top of page 89: "Each eigenvalue is assigned a symbol: j with M^2 and m with M_z". In the introduction to this chapter $\vec{j}$ is used for the total angular momentum. A bit confusing? Keep in mind: M is used for the angular momentum. The eigenstates for M^2 and M_z are represented by $|j, m\rangle$.

4.1.2 Raising and Lowering Operators

Mahan introduced the raising and lowering operators, $L^\dagger$ and L for the orbital momentum operators. Well, here both are just definitions. Two new machines (Wheeler, Feynman's mentor). It appears later on these newly defined operators work as raising and lowering operators.

For example $[M^2, L] = 0$: $[M^2, L] = \left[M^2, M_x - iM_y\right] = [M^2, M_x] - i[M^2, M_y]$, and with Eq. (4.18) this expression equals 0. Keep in mind the way commutation brackets work! So, Eq. (4.25) is easily found without all the multiplications and using Eq. (4.8): $\left[M_x, M_y\right] = i\hbar M_z$, and, e.g., $[M_x, M_x] = 0$.

4.1.3 Eigenfunctions and Eigenvalues

Below the heading of this section: “The next step is to solve the operator relations…..” . To solve the operator relations?

A basic relation in this section is: $\langle j, m|j', m'\rangle = \delta_{jj'}\delta_{mm'}$, Eq. (4.31), where $|j, m\rangle$ are eigenstates and j is the eigenvalue symbol of the orbital angular momentum M^2 and m is the eigenvalue symbol of the z- component of M, M_z. Question: For a given j , m can vary? j and m are both in the same range?

The expression for the expectation value and matrix element are presented, Eqs. (4.32) and (4.33).

Mahan writes, just below Eq. (4.33): “In the next section the state $|j, m\rangle$ is given an explicit representation in term of matrices.” Well, I thought matrices to be related with operators and $|j, m\rangle$ to be a vector related with states.

Just above Eq. (4.35) you can find f_j'. I think this should read $f_{j'}$.

In deriving matrix elements of commutation relations like Eq. (4.37) Mahan used: $f_{j'}L^\dagger - L^\dagger f_j = f_{j'}L^\dagger - f_jL^\dagger + f_jL^\dagger - L^\dagger f_j = \left(f_{j'} - f_j\right)L^\dagger + \left[f_j, L^\dagger\right] = \left(f_{j'} - f_j\right)L^\dagger$, since $\left[f_j, L^\dagger\right] = 0$. As given by Mahan: f_j is a dimensionless quantity. With help of this expression Mahan calculates the matrix elements giving Eq. (4.37). Then Mahan evaluated the matrix elements of the commutator: $[M_z, L^\dagger] = \hbar L^\dagger$, Eq.(4.27).

In order to derive Eq. (4.41) use has been made of $L^\dagger m = mL^\dagger$. Here m is a number.

In Eq. (4.42) Mahan presents the matrix element of the raising operator: $L^\dagger_{j',m'm} = \delta_{m'=m+1}\hbar q_j(m)$. In Eq. (4.43) this matrix element is represented as: $L^\dagger_{j',m'm} = \delta_{jj'}\delta_{m',m+1}\hbar q_j(m)$. A minor difference since $m' = m + 1$? In Eq. (4.44) Mahan presented the matrix elements for the lowering operator. These are found by the Hermitian conjugate of the raising operator. A shortcut. Below Eq. (4.44) Mahan writes: “ Now m' is on the right(in the ket), while m is on the left(in the bra). Since $m' = m + 1$, the operator L lowers the value of the number m”. Well, this is fine. Below Eq. (4.42) Mahan writes: “….,
$m' = m + 1$ The raising operator $L^\dagger$ raises the value of m.” . What confuses me is the discussion in this section to be about the matrix elements, the elements of the machinery, and not about the operators, the machine itself.

Question: is there a convention about the raising operator operating on the ket and the lowering operator on the bra?

No, let us go back to the shortcut, take a look at the procedure to derive $L^\dagger$ and use this procedure to derive L. You will arrive at the equivalent expression for L in eq. 4.36): $0 = \hbar^2\left(f_{j'} - f_j\right)\langle j', m'|L|j, m\rangle$. So also for L we have $\langle j', m'|L|j, m\rangle = \delta_{jj'}L_{j',m'm}$. Now we evaluate $[M_z, L] = -\hbar L$, Eq. (4.26). And similar to Eqs. (4.40) and (4.41) we finally obtain: $\hbar(m' - m + 1)L_{j',m'm} = 0$. This expression vanishes for $m' = m - 1$. If for $m' \neq m - 1$, the matrix element $L_{j',m'm} = 0$. If $m' = m - 1$, the matrix element does not vanish, but is still unknown (Mahan’s formulation for $L^\dagger_{j',m'm}$ in Eq. (4.42)). There the unknown becomes the function $q_j(m)$. Are we allowed to write $L_{j',m'm} = \delta_{m'=m-1}\hbar q_j^*(m - 1)$? $q_j^*(m)$ is the complex conjugate of $q_j(m)$. I do not know. My first thought is $L_{j',m'm} = \delta_{m'=m-1}\hbar r_j(m)$ where the relation between r_j and q_j has to be found with an additional relation L is the Hermitian conjugate of $L^\dagger$.

What represents the difference between Eq. (4.44), the short cut, and $L_{j',m'm} = \delta_{m'=m-1}\hbar q_j^*(m-1)$? Different m and m'? Or interchange m for m'?
Let us have a look at the matrix elements of L, Eq. (4.44). We interchange m for m'. Then we obtain: $\langle j',m'|L|j,m\rangle = \delta_{j'j}\delta_{m,m-1}\hbar q^*(m-1)$, since $m' = m-1$ by interchanging m for m'.
In Eq. (4.45) use is made of Eq. (4.19): $M_z|m\rangle = \hbar m|m\rangle$ and $\langle j,m|j,m\rangle = 1$.
On page 92 Mahan derived an additional expression by using the identity operator for de matrix elements of the raising and lowering operators. Well, for me it is was an exercise in subtleties. Especially, the way the raising and lowering operators affected the quantum number m . At first I was misled by the statement at page 91, below Eq. (4.42): "…… $m' = m+1$. The raising operator $L^\dagger$ raises the value of m." Is this a proof?
Below Eq.(4.44) : "Since $m' = m+1$, the operator L lowers the value of the quantum number m." Is this a proof?
So, to obtain Eq. (4.49) by using the above statements in the matrix elements of Eq. (4.48) I got nowhere. Then I realized for the first term in Eq. (4.48) $m' = m+1$ indeed. However, for the second term, I have to switch m' for m and obtain $m' = m-1$.
At the bottom of page 92 Mahan writes: "So far it has been proved that when $L^\dagger$ operates upon an eigenstate………..". Well, what I learned is that the discussion was about the matrix elements and not about operators. It is not easy to become a quantum machinist. I almost got lost in operators.
On page 93 Mahan presented the results for the matrix elements of the raising and lowering operators. There he introduced the upper limit n_u of n for the raising operator and the lower limit n_l of n of the lowering operator. Furthermore a number $N = m + n_u$ and a number $N = n_l - m - 1$. Then Mahan equates both N to find the limiting value of the quantum number m: $m = \frac{1}{2}(n_l - 1 - n_u)$, Eq. (4.69). Apparently both values of N are equal. Why is that? Since:
$a_0 = (n_l - m)(n_l - m - 1) = (m + n_u)(m + n_u + 1)$, and $N = n_l - m - 1$, we have $a_0 = N(N+1) = (m + n_u)(m + n_u + 1)$. This again gives $N = m + n_u$, leading to $m = \frac{1}{2}(n_l - 1 - n_u)$. Or the other way around: equating a_0 for both the numbers n_u and n_l, we find $m = \frac{1}{2}(n_l - 1 - n_u)$. So $N = m + n_u$ and $N = n_l - m - 1$.
The quantity of N is the largest possible value of m or the lowest value of $n_u = 0$. Mahan writes, page 94",: "The largest negative value of m is $-N$." Or the highest value of $n_l = 1$.
At the bottom of page 94 j is identified with N. "Identified" means?
On top of page 95 Mahan summarized the results of this section and compared the results for the harmonic oscillator with those for the angular momentum. In the text at the end of this section Mahan writes: "For the angular momentum, the commutator is another operator: $[L, L^\dagger] = 2\hbar M_z$." I think the operator is: : $[L, L^\dagger] = -2\hbar M_z$, Eq. (4.25). A printing error.
In this section a "c-number" is mentioned: Dirac's nomenclature.

Homework 1.

The harmonic oscillator has
$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$,

$[a, a^\dagger] = 1,\ \ [a^\dagger, a^\dagger] = 0,\ \ [a, a] = 0.$
Starting from just these operator relations, derive the eigenvalue spectrum of the harmonic oscillator. In chapter 2 Mahan discussed the harmonic oscillator. There he derived $a^\dagger a|n\rangle = n|n\rangle$. When we use this we obtain at once the eigenvalue spectrum E_n with: $H|n\rangle = E_n|n\rangle$. So, I assume we need to follow a different approach.
We have: $\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|n\rangle = E_n|n\rangle$, Schrödinger's equation with eigenvalue E_n and eigenvector $|n\rangle$. Let us rewrite Schrödinger's equation: $a^\dagger a|n\rangle = (\frac{E_n}{\hbar\omega} - \frac{1}{2})|n\rangle$. Now I use Susskind's notation: $a^\dagger a = N$ and denote $(\frac{E_n}{\hbar\omega} - \frac{1}{2}) \equiv \lambda_n$ to be the eigenvalue of N . *What follows you can find in Susskind's chapter on the harmonic oscillator and the raising and lowering operators. Caveat: Susskind used* $a^\dagger a|n\rangle = n|n\rangle$. We do not do that.
Mahan mentioned above to start with the given operators. Well, to find the spectrum of eigenvalues we need to find in what way the spectrum is build.
Susskind wrote: "The trick is to find an induction procedure……..". Without that trick I was not able to find the asked for spectrum. So, we consider a new vector: $a^\dagger|n\rangle$ and prove this vector to be an eigenvector of N.
So, we start with $N(a^\dagger|n\rangle)$. Change this expression into: $\left[a^\dagger N - \left(a^\dagger N - N a^\dagger\right)\right]|n\rangle$. The expression in parentheses resembles a commutator. Susskind derived this commutator to be: $a^\dagger N - N a^\dagger = [a^\dagger, N] = -a^\dagger$.Then $N\left(a^\dagger|n\rangle\right) =: \left[a^\dagger N - \left(a^\dagger N - N a^\dagger\right)\right]|n\rangle = a^\dagger(N+1)|n\rangle$. We have defined $N|n\rangle$, to be $\lambda_n|n\rangle$. So $N\left(a^\dagger|n\rangle\right) = (\lambda_n - 1\ )\left(a^\dagger|n\rangle\right)$.
We conclude $\left(a^\dagger|n\rangle\right)$ to be an eigenvector of N with eigenvalue $(\lambda_n - 1)$. The same procedure can be followed for the new vector $(a|n\rangle)$. Now you need the commutator $[a, N] = a$, which can be found in Susskind. Briefly summarizing Susskind: writing in full the commutator $[a, N] = aN - Na = aa^\dagger a - a^\dagger a a = \left(aa^\dagger - a^\dagger a\right)a$. The commutator in parentheses equals 1, then $[a, N] = a$. For the lowering operator we obtain in this way: $N(a|n\rangle) = (\lambda_n - 1)(a|n\rangle)$. Keep in mind: in the Hamiltonian you will find the raising and lowering operator operating in tandem and not separately. With the operators separated we have proven the eigen values of the harmonic oscillator to decrease or increase by an integer step equal 1. No more no less. We can do a bit more however. We know the lowering process not to continue since the lowest possible state is the ground state larger than 0. The order of magnitude can be found by analysing the Heisenberg uncertainty relation. Let us denote this number of steps to be m . We denote the lowest state by the vector $|0\rangle$ and the eigen value by E_0.
For this state vector we have: $\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|0\rangle = E_0|0\rangle$. Or, $\hbar\omega a^\dagger a|0\rangle + \frac{\hbar\omega}{2}|0\rangle = E_0|0\rangle$. Now we know $\hbar\omega a^\dagger\, a|0\rangle = 0$, so: $E_0 = \frac{\hbar\omega}{2}$, the ground state.
By lowering λ_n with m integer steps, say, we have $\lambda_n - m = 0$. Here we have shown λ_n to be an integer. Without loss of generality we may replace m by n, $n \in \mathbb{N}$.
So $\frac{E_n}{\hbar\omega} - \frac{1}{2} - n = \lambda_n - n = 0$ and $E_n = \hbar\omega(n + \frac{1}{2})$, the eigenvalue spectrum.
May be it comes as a surprise, started with $\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|n\rangle = E_n|n\rangle$ and using $\frac{E_n}{\hbar\omega} - \frac{1}{2} - n = 0$, or $\frac{E_n}{\hbar\omega} - \frac{1}{2} = n$, we have $a^\dagger a|n\rangle = n|n\rangle$, proven by Mahan in Chapter 2 and defined by Susskind in Chapter 10.

How do the raising and lowering operators affect the eigenstates?
We have found $a^{\dagger}a|n\rangle = n|n\rangle$ and used the trick demonstrated by Susskind:
$a^{\dagger}a(a^{\dagger}|n\rangle) = (n+1)(a^{\dagger}|n\rangle)$, so we can write $a^{\dagger}|n\rangle = |n+1\rangle$. In a similar way you will find:
$a|n\rangle = |n-1\rangle$.
Or having found $N|n\rangle = n|n\rangle$, then obviously $N|n+1\rangle = (n+1)|n+1\rangle$. In a similar way:
$N|n-1\rangle = (n-1)|n-1\rangle$.

4.2 Representations

The subject matter of this section is to represent operators and eigenfunctions by specific functions.
On page 95 and the following pages you will find various representations of operators and eigenstates.
As a reminder: $|j,m\rangle$ is an eigenstate of M^2 and M_z; page 89. So $|j,m\rangle$ is not a product state or an entangled/combined state.
First Mahan dealt with
$j = \frac{1}{2}$.
The spin up and spin down denomination is mentioned by Mahan on page 96.
In this case for the spin: $j = \frac{1}{2}$ and $s = \frac{1}{2}$, where the orbital momentum is represented by $l = 0$. See the introduction of Chapter 4.
Kets are represented by column vectors and Bras are represented by row vectors.
I learned about the spin states by Susskind.
For example, by Susskind, the up spin $|u\rangle$ is given by the column vector representation $\begin{pmatrix}1\\0\end{pmatrix}$.
Let us do a little exercise for the z −coordinate. We do know the operator: the Pauli matrix σ_z and we want to find the column vector representation of $|j,m\rangle$. In general we have for the elements of this representation $\begin{pmatrix}a\\b\end{pmatrix}$ The eigenvalues of $\sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$ are ± 1. We choose 1 and have $\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} = \begin{pmatrix}a\\b\end{pmatrix}$. Consequently the column vector representation is $\begin{pmatrix}a\\0\end{pmatrix}$. Normalization leads to $a = 1$. So, finally we have: $\begin{pmatrix}1\\0\end{pmatrix}$, spin up. Similarly, for the eigenvalue -1 and column vector representation $\begin{pmatrix}c\\d\end{pmatrix}$: $\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\begin{pmatrix}c\\d\end{pmatrix} = -\begin{pmatrix}c\\d\end{pmatrix}$. Then the vector is $\begin{pmatrix}0\\d\end{pmatrix}$. With normalization we find for spin down: $\begin{pmatrix}0\\1\end{pmatrix}$.
On page 96 Mahan noticed the factors $q_j(m)$ to be zero or one. From $m = \frac{1}{2}$ to be the highest possible value of m and $m = -\frac{1}{2}$ the lowest possible value, we have $N = m$. With Eqs. (4.58) and Eqs. (4.63) $q_j(m) = 0$. So, Eqs (4.91) and (4.92) are found.
Then $j = 1$.
Now we have three states: $|1,1\rangle$, $|1,0\rangle$ and $|1,-1\rangle$.
Then Mahan derived the values for $q_j(m)$ with Eq. (4.58) and $a_0 = N(N+1)$ where N is the largest value of m. In addition $j = N$, see bottom of page 94. So $q_j(m)$ is given by Eq. (4.94).
Mahan writes: : “These values immediately give the raising and lowering matrices…..”.

Well, being familiar with constructing the matrices the result is immediately understood.

On the other hand by writing for: $L^{\dagger} = \begin{pmatrix} a\ b\ c \\ d\ e\ f \\ g\ h\ i \end{pmatrix}$ and operate this matrix on the column vector representations of the three states, you will find the elements of the raising and lowering operators. Keep in mind the raising and lowering operators being mutual Hermitian conjugates. An example of the exercise is: $L \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$.

In the next step Mahan derived the angular momentum operators.

M_x and M_y are given by Eq. (4.28) expressed in raising and lowering operators and $[L, L^{\dagger}] = 2\hbar M_z$.

Subsequently Mahan gives the r-space representation.

Mahan started this part of representations with the remark: "…., it is easy to construct…". Reading textbooks and finding sentences like "…it is easy to show…" makes me shudder.

At the bottom of page 98 Mahan presented the angular momentum state in terms of spherical harmonics Eq. (4.117): $|l, m\rangle = D_{lm} r^l P_l^{|m|}(\theta) e^{im\phi}$.

In this expression r^l is plugged into the spherical harmonic function $Y_l^m(\theta, \phi)$ and a part of the factor C_{lm} is used. Without explanation. Why? Or should one read chapter 5 in the first place? Well, on top of page 99 there you will find the explanation. The factor is cancelled out by normalization. This can be found by comparing Eqs. (4.116), (4.118) and (4.119). Additionally, a look at chapter 5 is helpful. The wave function in terms of spherical harmonics is given as representation of the eigenstate.

On page 99 Mahan writes: "If one knows the Legendre polynomials $P_l(\theta)$ then one can construct………..". Well, the relation between associated Legendre polynomials and Legendre polynomials reads: $P_l^m(\mu) = (-1)^m (1-\mu^2)^{\frac{m}{2}} \frac{d^m}{d\mu^m} P_l(\mu)$, and $P_l(\mu) = \frac{1}{2^l l!} \frac{d^l}{d\mu^l} (\mu^2 - 1)^l$, and $\mu = \cos\theta$. (Chisholm and Morris, www.chimica.it , www.ucl.ac.uk).

With this knowledge you will find $|0,0\rangle = 1$.

Mahan used the raising operator for the eigenvector $|2,0\rangle$ and obtained $|2,1\rangle = -\sqrt{\frac{3}{2}}\, z(x+iy)$, where the raising operator is applied to $\frac{1}{2}[2z^2 - x^2 - y^2]$. Then he arrived at the eigenfunction given above for $|2,1\rangle$. Well, you could think this eigenfunction can be found with the spherical harmonic functions: $|l, m\rangle = D_{lm} r^l P_l^{|m|}(\theta) e^{im\phi}$.

$|2,1\rangle = D_{21} r^2 P_2^1(\theta) e^{i\phi}$, Eq. (4.117).

With Eq. (4.118): $D_{21} = -\sqrt{\frac{(2-1)!}{(2+1)!}} = -\frac{1}{\sqrt{3}}$.

Furthermore $P_2^1(\mu) = -(1-\mu^2)^{\frac{1}{2}} \frac{d}{d\mu} P_2(\mu)$ and $P_2(\mu) = \frac{1}{2^2 2!} \frac{d^2}{d\mu^2} (\mu^2 - 1)^2 = \frac{1}{2}(3\mu^2 - 1)$.

So $P_2^1(\mu) = -3\mu(1-\mu^2)^{\frac{1}{2}}$. We know $\mu = \cos\theta$.

Then $P_2^1(\theta) = -3\sin\theta\cos\theta$, where we took the positive value of the square root. We obtain for $|2,1\rangle = \sqrt{3}\, r^2 \sin\theta \cos\theta\, e^{i\phi}$. This we write in the following way with help of spherical coordinates: $|2,1\rangle = \sqrt{3}\, r\cos\theta\ \ r\sin\theta\, e^{i\phi} = \sqrt{3}\, z(x+iy)$. Alas, comparing this with Eq. (4.127), $|2,1\rangle = -\sqrt{\frac{3}{2}}\, z(x+iy)$, the result in the line above differs a factor $-\frac{1}{\sqrt{2}}$

form Eq. (4.127). I cannot find my error. I leave it here.
Below Eq. (4127) Mahan writes: “Note that this (Eq. (4.127), Nz) procedure gives the correct normalization of the eigen function.” So with Eqs. (4.119) and (4.127) :
$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \langle l,m|l,m\rangle = \frac{3}{2}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta z^2\,(x+iy)(x-iy)$. This can be written with spherical coordinates: $\frac{3}{2}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta\ \sin\theta r^2\cos\theta^2\, r^2\sin\theta^2\, e^{i\phi}e^{-i\phi} = \frac{4\pi}{5}r^4$, as it should be.
I leave this section with a question. We learned the eigenstates to be normalized. An additional cheque is are the eigenstates orthogonal? Let us take for example the states $|1{,}1\rangle$ and $|1,-1\rangle$. Well, using equation (4.121) and (4.123):
$\langle 1,-1|1{,}1\rangle = -\frac{1}{2}\left(r\sin\theta e^{-i\phi}\right)^{*} r\sin\theta e^{i\phi}$.
This expression is not zero. The two eigenstates are not orthogonal. Do we have to construct a orthogonal basis by making a linear combination of these two eigenvectors? May be.

Homework 2, 3, 4.

Exercise 2.
Prove the following result, where $\vec{\sigma} = \left(\sigma_x, \sigma_y, \sigma_z\right)$ are Pauli spin matrices, and $\vec{A} = (A_x, A_y, A_z)$ and $\vec{B} = (B_x, B_y, B_z)$ are ordinary vectors:
$(\vec{\sigma}.\vec{A}\,)(\vec{\sigma}.\vec{B}) = \vec{A}.\vec{B}\, I + i\vec{\sigma}.(\vec{A}\times\vec{B}\,)$, Eq. (4.174).
In this equation I is the identity matrix.
$\vec{\sigma}$ behaves like a three vector.
We define $\vec{C} = \vec{A}\times\vec{B}$, then
$C_x = A_yB_z - A_zB_y$,
$C_y = A_zB_x - A_xB_z$ and
$C_z = A_xB_y - A_yB_x$.
$\vec{A}.\vec{B} = A_xB_x + A_yB_y + A_zB_z \equiv D$.
$i\vec{\sigma}.\left(\vec{A}\times\vec{B}\,\right) = i\sigma_xC_x + i\sigma_yC_y + i\sigma_zC_z$.
$\vec{\sigma}.\vec{A} = \sigma_xA_x + \sigma_yA_y + \sigma_zA_z$.
$\vec{\sigma}.\vec{B} = \sigma_xB_x + \sigma_yB_y + \sigma_zB_z$.
$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
So:
$\vec{\sigma}.\vec{A} = \begin{pmatrix} A_z & (A_x - iA_y) \\ (A_x + iA_y) & -A_z \end{pmatrix}$, and

$\vec{\sigma}.\vec{B} = \begin{pmatrix} B_z & (B_x - iB_y) \\ (B_x + iB_y) & -B_z \end{pmatrix}$.

$\vec{A}.\vec{B}\, I = \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}$.
$i\vec{\sigma}.\left(\vec{A}\times\vec{B}\,\right) = i\begin{pmatrix} C_z & (C_x - iC_y) \\ (C_x + iC_y) & -C_z \end{pmatrix}$.
Now we have all the matrices to prove Eq. (4.174). Plug these matrices into Eq. (4.174) and

you find the correctness of this equation.
A nice exercise in matrix and vector algebra.

Exercise 3.
Construct a matrix representation for the $j = \frac{3}{2}$ angular momentum.
$j = \frac{3}{2}$, so $m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$.
These values give the raising and lowering operators, the elements of which are found by $q_j(m) = \sqrt{j(j+1) - m(m+1)}$ and the Eqs. (4.42) and (4.42):
$q_j(\frac{3}{2}) = 0,\ q_j\left(\frac{1}{2}\right) = \sqrt{3}, q_j\left(-\frac{1}{2}\right) = 2, q_j\left(-\frac{3}{2}\right) = \sqrt{3}$.
Then $L^\dagger = \hbar \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}$, and $L = \hbar \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$.
With Eq. 4.25 we have $2\hbar M_z = -[L, L^\dagger]$. Plugging the raising and lowering operators into this equation we find: $M_z = \frac{\hbar}{2} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}$. Is this result to be expected? Well, M_z is diagonal with elements $\hbar m$.
Furthermore, $M_x = \frac{1}{2}\left(L^\dagger + L\right)$, and $M_y = \frac{i}{2}(L - L^\dagger)$.
So, $M_x = \frac{\hbar}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$, and $M_y = \frac{i\hbar}{2} \begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$.
Now $M^2 = M_x^2 + M_y^2 + M_z^2$, or with Eq. (4.30): $M^2 = \frac{1}{2}\left(L^\dagger L + L L^\dagger\right) + M_z^2$.
We substitute the matrices into the equation for M^2 and find: $M^2 = \hbar^2 \frac{15}{4} I$. Again, is this result to be expected? Yes it is. Bottom of page 94: The eigenvalue of M^2 is just $\hbar^2 a_0$.
And $a_0 = j(j+1) = \frac{15}{4}$.
So far I did not pay attention to the column vector representation of the eigenstates. These are the eigenstates of M_z and M^2.
Eq. (4.76): $M_z|j, m\rangle = \hbar m|j, m\rangle$. For the four eigenvalues $\hbar m$ we can obtain the column vector representation of the eigenstates with the as yet unknown elements $a, b. c$ and d:
$\frac{\hbar}{2} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \hbar m \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$. Then plugging the various values for m into this equation and apply normalization we obtain:

$|j,3/2\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$, $|j,1/2\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$, $|j,-1/2\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$, and $|j,-3/2\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$.
All these column vectors are also eigenvectors of M^2.

Exercise 4.
Construct an r-space representation for the eigenstates with $j = 3$.
$j = 3$, so we have $m = 3, 2, 1, 0 - 1, -2$ and -3.
We follow the recipe of Mahan: “If one knows the Legendre polynomial $P_3(\theta)$,then one can construct the rest of the basis set using raising and lowering operators Eq. (4.107)-(4.109).”
That is to say, we first construct the eigenstate $|3{,}0\rangle$ and subsequently find all the others.
$P_3(\theta)$ is the Legendre polynomial for $m = 0$.
With help of the Eqs. (4.117) and (4.118) you find $|3{,}0\rangle = r^3 P_3(\theta)$.
Then: $L^\dagger|3,m\rangle = \hbar q_j(m)|j,m+1\rangle$ (4.59)
and $L|3,m\rangle = \hbar q_j(m-1)|3,m-1\rangle$ (4.60)
Furthermore $q_j(m) = \sqrt{12 + m(m+1)}$. (4.58)
For the Legendre polynomial we have (Chisholm and Morris): with $\mu = \cos\theta$ and $P_3(\mu) = \frac{1}{48}\frac{d^3}{d\mu^3}(\mu^2 - 1)^3$ the polynomial is
$P_3(\theta) = \frac{1}{2}(3cos^3(\theta) - 1)$. Then we can write for $|3{,}0\rangle = \frac{1}{2}(3z^3 - (x^2 + y^2 + z^2)^{\frac{3}{2}})$. Now apply the raising operator on the polynomial representation of $|3{,}0\rangle$. This operator is given in Eq. (4.109) : $L^\dagger = \hbar[z\left(\frac{\partial}{dx} + i\frac{\partial}{\partial y}\right) - (x + iy)\frac{\partial}{dz}]$ The result of this operation is:
$L^\dagger|3{,}0\rangle = -\hbar 3z^2(x + iy)$ and with Eq. (4.59): $L^\dagger|3{,}0\rangle = \hbar 2\sqrt{3}\,|3{,}1\rangle$. Equating both expressions for $L^\dagger|3{,}0\rangle$ we obtain the new eigenstate $|3{,}1\rangle = -\frac{\sqrt{3}}{2}z^2(x + iy)$.
Now we look for the eigenstate $m = -1$. So, with the given recipe and Eq. (4.60):
$L|3{,}0\rangle = \hbar q_3(-1)|3,-1\rangle = \hbar 2\sqrt{3}|3,-1\rangle$. Apply the lowering operator on the polynomial representation of the eigenstate $|3{,}0\rangle$. This operator is given in Eq. (4.107):
$L = -\hbar[z\left(\frac{\partial}{dx} - i\frac{\partial}{\partial y}\right) - (x - iy)\frac{\partial}{dz}]$. The result of this operation finally is:
the new eigenstate $|3,-1\rangle = \frac{\sqrt{3}}{2}z^2(x - iy)$. For the next step we apply the Mahan recipe on the eigenstates $|3{,}1\rangle$ and $|3,-1\rangle$. Then we find the new eigenstates $|3{,}2\rangle$ and $|3,-2\rangle$.
These are: $|3{,}2\rangle = \sqrt{\frac{3}{10}}\,z(x + iy)^2$ and $|3,-2\rangle = \sqrt{\frac{3}{10}}\,z(x - iy)^2$. In a similar way we have for the eigenstates $|3{,}3\rangle = -\frac{1}{2\sqrt{5}}(x + iy)^3$ and $|3,-3\rangle = \frac{1}{2\sqrt{5}}(x - iy)^3$.
Here I mentioned the question I raised in section 4.2 about orthogonality. Well, again you will see, for example $\langle 3{,}1|3{,}0\rangle \neq 0$. So, do we have to construct a orthogonal basis by linear combinations of the above derived eigenstates?

4.3 Rigid Rotations.

In this sections Mahan deals with rigid rotors.
The first example is about a hollow bead mass sliding around a horizontal circle with fixed radius R. For the Hamiltonian the only variable is θ .

A second example is the rotation of an object around a fixed axis.
In the third place Mahan dealt with the rotation of a spherical top. There the operator M^2 derived in section 4.2 is used: $M^2 = \hbar^2 l(l+1)$. Eq. (4.135). The relation between M^2 and the kinetic energy $\hat{T}$ is given in Eq. (4.144): $\hat{T} = \frac{M^2}{2I}$, where I is the moment of inertia for a spherical top (and not the identity matrix). So the eigenvalues are:
$E_l = \frac{\hbar^2}{2I} l(l+1)$, Eq. (4.145).
Now the spherical top. For a particular value of l , $m = 2l+1$. This results from the associated Legendre polynomials: $-l \leq m \leq l$, then $m \leq 2l+1$ (Wikipedia.org). Also on page 94 in the section on eigenfunctions and eigenvalues you will find $-N \leq m \leq N$, where N is the largest allowed value of m and number of allowed values of $m = 2N+1$.
Another special case is a diatomic molecule of identical atoms.
On page 102 at the end of this section Mahan writes: “The difference between this case(the diatomic molecule, Nz), and the spherical top, is the degeneracy of each energy level. For the spherical top it is $(2l+1)$, while for the diatomic molecule it is one.”
Degeneracy: “In quantum Mechanics an energy level is said to be degenerate if it corresponds to two or more different measurable states of a quantum system”, Wikipedia.org .
So the diatomic molecule has one eigenstate, $m = 0$, for one energy level l.
At the bottom of page 101 the notation is a bit confusing. M is used for the mass of the nuclei and for the momentum operator. In Eq. (4.146) it is clear M to be the momentum operator. The expression with m^2 in Eq.(4.147) is found with help of Eq. (4.76) by operating M_z on $M_z|j,m\rangle = \hbar m|j,m\rangle$, resulting into: $M_z^2|j,m\rangle = \hbar^2 m^2|j,m\rangle$.

Homework 5, 6.

Exercise 5.
Calculate the moment of inertia $I_\perp$ for a diatomic molecule when it is rotating on axis perpendicular to the line between the two nuclei. Then calculate the value of $E_\perp = \hbar^2/2I_\perp$ in temperature units ($T_1 = E_\perp/k_B$) for the three diatomic molecules H_2, N_2 and O_2. The value for the nuclear separation can be found in the *Handbook of Chemistry and Physics.*
This exercise is completely dealt with in section 4.3-Rigid Rotations- and the diatomic molecule.
The eigenvalues are: $E_\perp = \frac{\hbar^2}{2}\frac{l(l+1)}{I_\perp}$, where $m = 0$, assuming ordinary temperatures.
Furthermore $I_\perp = 2Mass(\frac{d}{2})^2$, with $Mass$ the mass of the atom and d the separation of the two atoms. In temperature units the eigenvalues are: $T_1 = \frac{\hbar^2}{2k_B}\frac{l(l+1)}{2Mass(\frac{d}{2})^2}$.
For all three diatomic molecules the numbers in the expression for T_1 can be found in the *Handbook of Chemistry and Physics.*
Well, so far nothing has been said about the potential energy. Since the centre of mass is chosen to be the rotation axis potential energy can be treated as a constant.

Exercise 6.
A molecule consist of four atoms in a perfect square of side a and atomic mass Ms. What are

the eigenvalues of rigid rotation in three dimensions?
We choose the x- and y- axis to be in the plane of the four atoms. These axis intersect at the diagonals of the perfect square. The z- axis is perpendicular to this plane at the intersection. Now we have for the moments of inertia $I_x = I_y = 4Ms(\frac{a}{2})^2 = Ms\, a^2$ and

$I_z = 4Ms(\frac{a\sqrt{2}}{2})^2 = 2Msa^2 = 2I_x = 2I_y$.

For the kinetic energy $\hat{T} = \frac{1}{2}\left[\frac{M_x^2}{I_x} + \frac{M_y^2}{I_y} + \frac{M_z^2}{I_z}\right] = \frac{1}{2}\left[\frac{M^2}{I_x} - \frac{M_z^2}{2I_x}\right]$.

The eigenstates are the spherical harmonics $Y_l^m(\theta, \phi)$.

We have, similar to Eq. (4.147): $\hat{T}Y_l^m(\theta, \phi) = \frac{ħ^2}{2}\left[\frac{l(l+1)}{I_x} - \frac{m^2/2}{I_x}\right] Y_l^m(\theta, \phi)$.

The four atomic molecule has the eigenvalues and eigenfunctions:

$\hat{T}Y_l^m(\theta, \phi) = \frac{ħ^2}{2}\frac{l(l+1)-m^2/2}{a^2Ms} Y_l^m(\theta, \phi)$.

In this exercise I took the centre of mass of the molecule for the position of the coordinates origin. Consequently the potential energy is a constant. However, translating the coordinate origin to one of the four atoms has some effect. Keeping the gravity field acting in the direction of the z – axis, potential energy is again a constant. The moment of inertia is affected. The structure of the expression for the eigenvalues is the same: $\frac{ħ^2}{2}\left[\frac{l(l+1)}{I_x} - \frac{m^2/2}{I_x}\right]$.

4.4 The Addition of Angular Momentum.

This section is about product states of spin and angular momentum.
With Eq. (4.150) Mahan introduced the product state: $|j_1, m_1\rangle|j_2, m_2\rangle$.
The first example(there is no second example in this section) of such a product state introduced on page 103 is a two spin system denoted by (α, β) . α_j is the spin-up particle j and β_j the spin-down particle.

So α_j can be represented by $\begin{pmatrix}1\\0\end{pmatrix}$ and β_j by $\begin{pmatrix}0\\1\end{pmatrix}$. Keep in mind a constant has to be included related to the *Clebsch-Gordon coefficients*(C-G) which are presented at page 105.
So the eigenstate for the total angular momentum M for the two spins aligned upwards becomes:

$|J, M\rangle = |1,1\rangle = (C - G)\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = (C - G)\begin{pmatrix}1\\0\\0\\0\end{pmatrix} = \alpha_1\alpha_2$, where $\otimes$ denotes the tensor product.

In Eq. (4.153) Mahan gives the inner product $\langle J, M|J, M\rangle = \langle j_1, m_1|j_1, m_1\rangle\langle j_2, m_2|j_2, m_2\rangle$.
This follows from: $\langle j_1, m_1|j_1, m_1\rangle\langle j_2, m_2|j_2, m_2\rangle = \langle j_1, m_1|\langle j_2, m_2|j_1, m_1\rangle|j_2, m_2\rangle$.
Here are neglected for the time being the *Clebsch-Gordon coefficients*. For the both spins

upwards this becomes $\langle J,M|J,M\rangle = (1\ 0\ 0\ 0\ )\begin{pmatrix}1\\0\\0\\0\end{pmatrix} = 1$. I suppose Mahan has written for convenience: $\langle J,M|J,M\rangle = \langle 1,1|1,1\rangle = \langle\alpha_1|\alpha_1\rangle\langle\alpha_2|\alpha_2\rangle$.
On page 104 Mahan derived the states for the two spin product state.
There are four states, three are derived by Mahan. The fourth follows from the other three.
Let us have a look:

$|1,1\rangle = \alpha_1\alpha_2 = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$,

$|1,-1\rangle = \beta_1\beta_2 = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$,

$|1,0\rangle = \frac{1}{\sqrt{2}}(\beta_1\alpha_2 + \alpha_1\beta_2) = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}$.

For this state $M = 0$. Since $M = m_1 + m_2$, the value for M can be found by $m_1 = \frac{1}{2}$ and $m_2 = -\frac{1}{2}$ or by $m_1 = -\frac{1}{2}$ and $m_2 = \frac{1}{2}$. This is the reason to have $\frac{1}{\sqrt{2}}(\beta_1\alpha_2 + \alpha_1\beta_2)$.

And now the fourth state $|0,0\rangle$ which we represent by the general column vector $\begin{pmatrix}a\\b\\c\\d\end{pmatrix}$.

These four states are orthogonal, so $(1\ 0\ 0\ 0)\begin{pmatrix}a\\b\\c\\d\end{pmatrix} = 0$, and $a = 0$. Similarly you will find $d = 0$. And with $\frac{1}{\sqrt{2}}(0\ 1\ 1\ 0)\begin{pmatrix}0\\b\\c\\0\end{pmatrix} = 0$, we have $b = -c$. Finally normalizing $\begin{pmatrix}0\\b\\-b\\0\end{pmatrix}$, we obtain $b = \pm\frac{1}{\sqrt{2}}$. Let us take the minus sign (as Mahan mentioned the choice to be arbitrary, phase ambiguity) and we can write for the fourth state vector as a tensor product:
$|0,0\rangle = \frac{1}{\sqrt{2}}(\beta_1\alpha_2 - \alpha_1\beta_2)$.
Remark: *In Susskind this four state vectors are called triplets(of degeneracy 3) and a singlet(no degeneracy). Instead of $\alpha_1\alpha_2$ and $\beta_1\beta_2$ for the first two states Susskind used $\alpha_1\alpha_2 + \beta_1\beta_2$ and $\alpha_1\alpha_2 - \beta_1\beta_2$. Susskind used u for the up-spin d for the down-spin.*

In table 4.1 on page 105 Mahan summarized the results. I think the text of this table should read: **Vector addition of a two spin system of $\left(\frac{1}{2}\right) \times \left(\frac{1}{2}\right)$ gives state $|J = 1, M\rangle|J = 0, 0\rangle$.**
In Eq. (4.161) you will find:
$\langle 0,0|0,0\rangle = \frac{1}{2}\langle(\beta_1\alpha_2 - \alpha_1\beta_2)\ (\beta_1\alpha_2 - \alpha_1\beta_2)\rangle$. Well, I don't understand $\langle\quad\rangle$ on the right-

hand side of this expression. Most certainly it does not represent a mean value or an expectation value. May be the vertical bar in the middle of this expression is missing. I suppose it to be a printing error. Furthermore as far as I am concerned, the equality $\langle 0,0|0,0\rangle = \frac{1}{2}\langle(\beta_1\alpha_2 - \alpha_1\beta_2)|(\beta_1\alpha_2 - \alpha_1\beta_2)\rangle =$
$\frac{1}{2}[\langle\alpha_1|\alpha_1\rangle\langle\beta_2|\beta_2\rangle + \langle\alpha_2|\alpha_2\rangle\langle\beta_1|\beta_1\rangle]$ is not so easily understood. (Nb. : I substituted a vertical bar in the second term of the above expression).

We have $|0,0\rangle = \frac{1}{\sqrt{2}}(\beta_1\alpha_2 - \alpha_1\beta_2) = -\frac{1}{\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\right) =$
$= -\frac{1}{\sqrt{2}}(|\alpha_1\rangle\otimes|\beta_2\rangle - |\beta_1\rangle\otimes|\alpha_2\rangle)$.

Then $\langle 0,0|0,0\rangle = \frac{1}{2}\left[(0\ 1 - 1\ 0)\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}\right] = 1 = \ (\langle\alpha_1|\otimes\langle\beta_2| - \langle\beta_1|\otimes\langle\alpha_2|)(|\alpha_1\rangle\otimes\beta_2\rangle -$
$|\beta_1\rangle\otimes|\alpha_2\rangle) = \ \langle\alpha_1|\otimes\langle\beta_2|\alpha_1\rangle\otimes|\beta_2\rangle - \langle\beta_1|\otimes\langle\alpha_2|\alpha_1\rangle\otimes|\beta_2\rangle -$
$\langle\alpha_1|\otimes\langle\beta_2|\beta_1\rangle\otimes|\alpha_2\rangle + \langle\beta_1|\otimes\langle\alpha_2|\beta_1\rangle\otimes|\alpha_2\rangle$.

In the tensor product space we have composite vectors for which we have in general
$\langle\alpha_i|\otimes\langle\beta_i|\alpha_j\rangle\otimes|\beta_j\rangle = \delta_{\alpha_i\alpha_j}\delta_{\beta_i\beta_j}$.

Consequently $\langle 0,0|0,0\rangle = \frac{1}{2}[\langle\alpha_1|\otimes\langle\beta_2|\alpha_1\rangle\otimes|\beta_2\rangle + \langle\beta_1|\otimes\langle\alpha_2|\beta_1\rangle\otimes|\alpha_2\rangle]$.

This can be written as $= \frac{1}{2}[\langle\alpha_1|\alpha_1\rangle\langle\beta_2|\beta_2\rangle + \langle\alpha_2|\alpha_2\rangle\langle\beta_1|\beta_1\rangle]$, Eq. (4.162).

On page 106 Mahan gave some examples of product states.
Keep in mind: $M = m_1 + m_2$, the maximum value $J = j_1 + j_2$ and the minimum value of $J = |j_1 - j_2|$. So the vector addition $(\frac{3}{2})\times(1)$ has the values $j_1 = 3/2$ and $j_2 = 1, m_1 = 3/2$ and $m_2 = 1$.
Eq. (4.170) is $\sum_{|j_1-j_2|}^{j_1+j_2}(2J+1) = (2j_1+1)(2j_2+1)$. For a particular composite system, $(4)\times(2)$ say, this equality is shown to be correct. In general you will find the expression for J to be correct by writing down the summation. Then the number of steps is $(2j_2+1)$. By doing the summation twice: starting with the maximum value and with the minimum value you will find the summation to be the number of steps times $(2j_1+1)$. Well, as you noticed, I proved the sum of an arithmetic series to be : $\frac{1}{2}(2j_2+1)[2(j_1-j_2)+1+2(j_1+j_2)+1]$.
So for $j_1 > j_2$ this sum equals the right-hand side of Eq. (4.170).
For $j_1 < j_2$ the sum of the arithmetic series is: $\frac{1}{2}(2j_1+1)[2(j_2-j_1)+1+2(j_1+j_2)+1]$.
Again this equals the right-hand-side of Eq. (4.170).
$j_1 = j_2$ needs no further explanation.

Remark:

Let us return to the example of two systems, each spin $\mathbf{\frac{1}{2}}$. The system is denoted by:
$\left(\frac{1}{2}\right)\times\left(\frac{1}{2}\right)$. The basis for vector addition is Eq. (4.150):
$|J,M\rangle = \sum_{m_1,m_2}(C-B)|j_1,m_1\rangle\otimes|j_2,m_2\rangle$, Eq. (4.150)
where $(C-B)$ are the Clebsch-Gordon coefficients.
Now max $J = \frac{1}{2}+\frac{1}{2} = 1$ and min $J = \left|\frac{1}{2}-\frac{1}{2}\right| = 0$.

The first state is $|J,M\rangle = |1,1\rangle$.
With $M = 1$, and $M = m_1 + m_2$, we have $m_1 = \frac{1}{2}, m_2 = \frac{1}{2}$ and a single $(C - B) = C_1$.
So $|J,M\rangle = |1,1\rangle = C_1\,|\frac{1}{2},\frac{1}{2}\rangle \otimes |\frac{1}{2},\frac{1}{2}\rangle$.
With column vector representation of the state $|\frac{1}{2},\frac{1}{2}\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, we have

$$C_1\,|\tfrac{1}{2},\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2},\tfrac{1}{2}\rangle = C_1\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = C_1\begin{pmatrix}1\\0\\0\\0\end{pmatrix}.$$

Normalizing this state : $C_1 = 1$.
The second state is $|J,M\rangle = |1,-1\rangle$.
we have $m_1 = \frac{1}{2}, m_2 = \frac{1}{2}$ and a single $(C - B) = C_1$.
With $M = -1$, and $M = m_1 + m_2$, we have $m_1 = -\frac{1}{2}, m_2 = -\frac{1}{2}$ and a single $(C - B) = C_2$.
So $|J,M\rangle = |1,-1\rangle = C_2\,|\frac{1}{2},-\frac{1}{2}\rangle \otimes |\frac{1}{2},-\frac{1}{2}\rangle$.
With column representation of the state $|\frac{1}{2},-\frac{1}{2}\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, and normalization : $C_2 = 1$.
The third state $|J,M\rangle = |1,0\rangle$.
Now we have two sets m_1 and m_2.
With $M = 0, m_1 = \frac{1}{2}, m_2 = -\frac{1}{2}$, and $m_1 = -\frac{1}{2}, m_2 = \frac{1}{2}$.
So $|J,M\rangle = |1,0\rangle = C_3\,|\frac{1}{2},\frac{1}{2}\rangle \otimes |\frac{1}{2},-\frac{1}{2}\rangle + C_4\,|\frac{1}{2},-\frac{1}{2}\rangle \otimes |\frac{1}{2},\frac{1}{2}\rangle$.
Let us apply the lowering operator on $|1,1\rangle$ in order to find an additional expression for $|J,M\rangle = |1,0\rangle$.
For $L|J,M\rangle$ we use: $L|J,M\rangle = \hbar\sqrt{J(J+1) - M(M-1)}|J,M-1\rangle$. (4.79)
So $L|1,1\rangle = \hbar\sqrt{2}|1,0\rangle$. In addition we apply L on $|\frac{1}{2},\frac{1}{2}\rangle \otimes |\frac{1}{2},\frac{1}{2}\rangle = |1,1\rangle$. On page 104 Mahan used the chain rule for this expression. The reasoning for this L contains derivatives. Well, this may be straight forward but not to me. Why is that? Image L to be in the matrix representation $L|J,M\rangle$. We know $|J,M\rangle$ can be represented in this case in a column: a column representation with 4 elements. Consequently L is a 4×4 matrix. Apply the chain rule on $|\frac{1}{2},\frac{1}{2}\rangle \otimes |\frac{1}{2},\frac{1}{2}\rangle$: $\left[L\,|\frac{1}{2},\frac{1}{2}\rangle\right] \otimes |\frac{1}{2},\frac{1}{2}\rangle + |\frac{1}{2},\frac{1}{2}\rangle \otimes [L\,|\frac{1}{2},\frac{1}{2}\rangle]$, we see the lowering operator applied to a column vector with 2 elements. So L in $L\,|\frac{1}{2},\frac{1}{2}\rangle$ acts as a 2×2 matrix. How come? Well, L itself can be considered as a tensor product of two 2×2 matrices:
$L = L_1 \otimes L_2$ and $\left[L_1 \otimes L_2\ \ |\frac{1}{2},m_1\rangle\right] \otimes |\frac{1}{2},m_2\rangle + |\frac{1}{2},m_1\rangle \otimes [L_1 \otimes L_2\ \ |\frac{1}{2},m_2\rangle]$,
L_1 operates on m_1 and L_2 on m_2. In this way I understand the product rule works. *This interpretation is based on Susskind's Theoretical Minimum.*
With help of this interpretation I can continue to apply the product rule as given above:
$\left[L\,|\frac{1}{2},\frac{1}{2}\rangle\right] \otimes |\frac{1}{2},\frac{1}{2}\rangle + |\frac{1}{2},\frac{1}{2}\rangle \otimes [L\,|\frac{1}{2},\frac{1}{2}\rangle]$.
With help of Eq. (4.79) $L\,|\frac{1}{2},\frac{1}{2}\rangle = \hbar\,|\frac{1}{2},-\frac{1}{2}\rangle$.

So $L|1{,}1\rangle = \hbar\sqrt{2}|1{,}0\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle + \hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle$. This results finally into:

$|1{,}0\rangle = \frac{1}{\sqrt{2}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle + \frac{1}{\sqrt{2}}\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle$.

Comparing this result with the expression $|1{,}0\rangle = C_3\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + C_4\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$,
we have $C_3 = \frac{1}{\sqrt{2}}$, and $C_4 = \frac{1}{\sqrt{2}}$.
The fourth eigenstate $|J,M\rangle = |0{,}0\rangle$.
Again there are two sets for m_1 and m_2.
With $M = 0, m_1 = \frac{1}{2}, m_2 = -\frac{1}{2}$, and $m_1 = -\frac{1}{2}, m_2 = \frac{1}{2}$.
So $|J,M\rangle = |0{,}0\rangle = C_5\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + C_6\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$.
The coefficients are found from orthogonality with the other states: $C_5 = \frac{1}{\sqrt{2}}$ and $C_6 = -\frac{1}{\sqrt{2}}$.

Homework 7, 8, 9.

Exercise 7.
Derive a table of Clebsch-Gordon coefficients for $(\frac{1}{2}) \times (1)$ and also $(\frac{1}{2}) \times (\frac{3}{2})$.
The basis equation for this exercise is Eq. (4.150).
I will show some results for $(\frac{1}{2}) \times (1)$.
Eq. (4.150): $|J,M\rangle = \sum_{m_1,m_2}(CGcoefs)\,|j_1,m_1\rangle \otimes |j_2,m_2\rangle$.
We have: $j_1 = \frac{1}{2}$, and $m_1 = \frac{1}{2}$ and $-\frac{1}{2}$; $j_2 = 1$, and $m_2 = 1, 0$ and -1.
The maximum value of $J = j_1 + j_2 = \frac{3}{2}$, the minimum value of $J = |j_1 - j_2| = \frac{1}{2}$.
We start with $|J,M\rangle = \left|\frac{3}{2},\frac{3}{2}\right\rangle$.
So $\left|\frac{3}{2},\frac{3}{2}\right\rangle = \sum_{m_1,m_2}(CGcoefs)\left|\frac{1}{2},m_1\right\rangle \otimes |1,m_2\rangle$.
We know $M = m_1 + m_2$. Since $M = \frac{3}{2}$, we only have $m_1 = \frac{1}{2}$ and $m_2 = 1$. Consequently there is just one Clebsch-Gordon coefficient ($CGcoefs$), denoted by C.
Then $\left|\frac{3}{2},\frac{3}{2}\right\rangle = C\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes |1{,}1\rangle$. Normalizing gives $C = 1$. This is demonstrated by the results of section 4.2 in Mahan. With column vector representation and tensor multiplication:

$\left|\frac{3}{2},\frac{3}{2}\right\rangle = C\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\\0\end{pmatrix} = C\begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix}$. The inner product: $\left\langle\frac{3}{2},\frac{3}{2}\middle|\frac{3}{2},\frac{3}{2}\right\rangle = C^2(1\;0\;0\;0\;0\;0)\begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix} = 1$

and $C = \pm 1$. We will continue using $C = +1$.
We have found one coefficient.
The above column representation of the eigenstates reminds us applying the raising or lowering operator to be a tensor product of two matrices. One matrix a 2×2 matrix and the other a 3 × 3 matrix. The 2 × 2 matrix only operating on the 2 column vector representation and the 3 × 3 matrix only operating on the 3 column vector representation.
This reasoning of matrix application and tensor products I based on Susskind "The Theoretical Minimum".

Next $\left|\frac{3}{2},\frac{1}{2}\right\rangle = \sum_{m_1,m_2}(CGcoefs)\left|\frac{1}{2},m_1\right\rangle \otimes |1,m_2\rangle$. Now with the constraint $M = m_1 + m_2$, $M = \frac{1}{2}$, we have two values for m_1 and m_2: $m_1 = -\frac{1}{2}$, $m_2 = 1$, and $m_1 = \frac{1}{2}, m_2 = 0$.

So : $\left|\frac{3}{2},\frac{1}{2}\right\rangle = C_1\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes |1,0\rangle + C_2\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes |1,1\rangle$. **(C4.1)**

We follow the procedure by Mahan and apply the lowering operator L to $\left|\frac{3}{2},\frac{3}{2}\right\rangle$ to find another expression for $\left|\frac{3}{2},\frac{1}{2}\right\rangle$. To this end we use Eq. (4.79):

$L|j,m\rangle = \hbar\sqrt{j(j+1)-m(m-1)}\,|j,m-1\rangle$. Eq. (4.79)

Then: $L\left|\frac{3}{2},\frac{3}{2}\right\rangle = \hbar\sqrt{3}\left|\frac{3}{2},\frac{1}{2}\right\rangle$. We know already $\left|\frac{3}{2},\frac{3}{2}\right\rangle = C\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes |1,1\rangle$, with $C = 1$.

All we have to do is to apply the lowering operator on this tensor product and use the product rule to apply the operator:

$L\left|\frac{3}{2},\frac{3}{2}\right\rangle = L\left(\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes |1,1\rangle\right) = L\left(\left|\frac{1}{2},\frac{1}{2}\right\rangle\right) \otimes |1,1\rangle + \left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes L(|1,1\rangle)$.

With help of Eq. (4.79): $L\left|\frac{3}{2},\frac{3}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes |1,1\rangle + \left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \hbar\sqrt{2}\,|1,0\rangle$, since we already found $L\left|\frac{3}{2},\frac{3}{2}\right\rangle = \hbar\sqrt{3}\left|\frac{3}{2},\frac{1}{2}\right\rangle$, we equate the latter expressions for $L\left|\frac{3}{2},\frac{3}{2}\right\rangle$, with the expression of one line above and have : $L\left|\frac{3}{2},\frac{3}{2}\right\rangle = \hbar\sqrt{3}\left|\frac{3}{2},\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes |1,1\rangle + \left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \hbar\sqrt{2}\,|1,0\rangle$, and we have for the new eigenstate $\left|\frac{3}{2},\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes |1,1\rangle + \frac{\sqrt{2}}{\sqrt{3}}\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes |1,0\rangle$. Now compare this expression with **(C4.1)** and you find $C_1 = \frac{\sqrt{2}}{\sqrt{3}}$ and $C_2 = \frac{1}{\sqrt{3}}$.

The next eigenstate can be found with help of the lowering operator applied to $\left|\frac{3}{2},\frac{1}{2}\right\rangle$ or by starting with $|J,M\rangle = \left|\frac{3}{2},-\frac{3}{2}\right\rangle$. For this we have only one set of m_1 and m_2.

$M = -\frac{3}{2}$, and with $M = m_1 + m_2$, $m_1 = -\frac{1}{2}$ and $m_2 = -1$.

However, I prefer to apply the raising operator to $\left|\frac{3}{2},-\frac{3}{2}\right\rangle$.

So we start with: $\left|\frac{3}{2},-\frac{3}{2}\right\rangle = \sum_{m_1,m_2}(CGcoefs)\left|\frac{1}{2},m_1\right\rangle \otimes |1,m_2\rangle$.

We know $M = m_1 + m_2$. Since $M = -\frac{3}{2}$, we only have $m_1 = -\frac{1}{2}$ and $m_2 = -1$.

Consequently there is just one Clebsch-Gordon coefficient ($CGcoefs$), de noted by C_7.

Then : $\left|\frac{3}{2},-\frac{3}{2}\right\rangle = C_7\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes |1,-1\rangle$.

Normalisation gives: $C_7 = 1$.

Now apply $L^\dagger\left|\frac{3}{2},-\frac{3}{2}\right\rangle$.

Then with Eq. (4.78): $L^\dagger\left|\frac{3}{2},-\frac{3}{2}\right\rangle = \hbar\sqrt{3}\left|\frac{3}{2},-\frac{1}{2}\right\rangle$. **(C4.2)**

Next apply Eq. (4.150): $\left|\frac{3}{2},-\frac{1}{2}\right\rangle = \sum_{m_1,m_2}(CGcoefs)\left|\frac{1}{2},m_1\right\rangle \otimes |1,m_2\rangle$. With the constraint $M = m_1 + m_2$, $M = -\frac{1}{2}$, we have again two values for m_1 and m_2: $m_1 = -\frac{1}{2}$, $m_2 = 0$, and $m_1 = \frac{1}{2}, m_2 = -1$.

So: $|\frac{3}{2},-\frac{1}{2}\rangle = C_5\,|\frac{1}{2},\frac{1}{2}\rangle \otimes |1,-1\rangle + C_6\,|\frac{1}{2},-\frac{1}{2}\rangle \otimes |1,0\rangle$. **(C4.3)**

We apply the raising operator again to $|\frac{3}{2},-\frac{3}{2}\rangle = C\,|\frac{1}{2},-\frac{1}{2}\rangle \otimes |1,-1\rangle,\ C = +1$.

$L^{\dagger}|\frac{3}{2},-\frac{3}{2}\rangle = L^{\dagger}[|\frac{1}{2},-\frac{1}{2}\rangle \otimes |1,-1\rangle]$. With the product rule we have:

$L^{\dagger}|\frac{3}{2},-\frac{3}{2}\rangle = [L^{\dagger}\,|\frac{1}{2},-\frac{1}{2}\rangle] \otimes |1,-1\rangle + |\frac{1}{2},-\frac{1}{2}\rangle \otimes [L^{\dagger}|1,-1\rangle]$.

With: $L^{\dagger}\,|j,m\rangle = \hbar\sqrt{j(j+1)-m(m+1)}\,|j,m+1\rangle$, Eq. (4.78)

$L^{\dagger}|\frac{3}{2},-\frac{3}{2}\rangle = \hbar\,|\frac{1}{2},\frac{1}{2}\rangle \otimes |1,-1\rangle + \hbar\sqrt{2}\,|\frac{1}{2},-\frac{1}{2}\rangle \otimes |1,0\rangle$. Now equate this expression with **(C4.2)** and we obtain $|\frac{3}{2},-\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}|\frac{1}{2},\frac{1}{2}\rangle \otimes |1,-1\rangle + \frac{\sqrt{2}}{\sqrt{3}}|\frac{1}{2},-\frac{1}{2}\rangle \otimes |1,0\rangle$. **(C4.4)**

Compare this expression with **(C4.3)** and you find $C_5 = \frac{1}{\sqrt{3}}$ and $C_6 = \frac{\sqrt{2}}{\sqrt{3}}$.

We have found the *Clebsch-Gordon coefficients* of $(\frac{1}{2}) \times (1)$ for $J = \frac{3}{2}$.

As a cheque I will apply the raising operator on $|\frac{3}{2},-\frac{1}{2}\rangle$, **(C4.4)** , and compare the result with $|\frac{3}{2},\frac{1}{2}\rangle$. The latter state is found by using the lowering operator on the former page.

With Eq. (4.78) we find $L^{\dagger}\,|\frac{3}{2},-\frac{1}{2}\rangle = \hbar 2|\frac{3}{2},\frac{1}{2}\rangle$. **(C4.5)**

Now we apply the raising operator on **(C4.4)**, use the product rule and Eq. (4.78) to obtain:

$L^{\dagger}\,|\frac{3}{2},-\frac{1}{2}\rangle = \hbar[\frac{2}{\sqrt{3}}|\frac{1}{2},-\frac{1}{2}\rangle \otimes |1,1\rangle + \frac{2\sqrt{2}}{\sqrt{3}}|\frac{1}{2},\frac{1}{2}\rangle \otimes\ |1,0\rangle]$ equate this expression with **(C4.5)** and we have $|\frac{3}{2},\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}|\frac{1}{2},-\frac{1}{2}\rangle \otimes |1,1\rangle + \frac{\sqrt{2}}{\sqrt{3}}|\frac{1}{2},\frac{1}{2}\rangle \otimes\ |1,0\rangle$, as before.

For the product state $(\frac{1}{2}) \times (1)$ we did not consider the product states $|J,M\rangle = |\frac{1}{2},\frac{1}{2}\rangle$ and $|J,M\rangle = |\frac{1}{2},-\frac{1}{2}\rangle$.

From this product state we know $j_1 = \frac{1}{2}$ and $j_2 = 1$, and for $M = \pm\frac{1}{2}$ there are for each value of M two sets of m_1 and m_2. Knowing these values the Clebsch-Gordon coefficients are found with the above procedure.

The other product state to investigate is $(\frac{1}{2}) \times (\frac{3}{2})$. So $j_1 = \frac{1}{2}$ and $j_2 = \frac{3}{2}$.

The maximum value of $J = 2$ and the minimum value of $J = 1$.

$|J,M\rangle = |2,2\rangle, |2,1\rangle, |2,0\rangle, |2,-1\rangle, |2.-2\rangle$, and

$|J,M\rangle = |1,1\rangle, |1,0\rangle, |1,-1\rangle$.

$m_1 = \frac{1}{2}, -\frac{1}{2},$

$m_2 = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{3}{2}, -\frac{3}{2}.$

The above procedure can be applied in a straightforward way.

I leave this exercise.

Exercise 8.

Derive a table of Clebsch- Gordon coefficients for $(1) \times (1)$. List only states with $m \geq 0$.

So $j_1 = 1$, and $j_2 = 1$. Here we have max $J = 2$ and min $J = 0$.

$|J, M\rangle = |2,2\rangle, |2,1\rangle, |2,0\rangle, |2,-1\rangle, |2.-2\rangle$, and
$|J, M\rangle = |0,0\rangle$.
Furthermore
$m_1 = 1, 0, -1$.
$m_2 = 1, 0, -1$.
Only $m_1 = 1, 0$, and $m_2 = 1, 0$, have to be considered.
The constraint $M = m_1 + m_2$ completes the information we need.
The procedure of exercise 7 can be applied in a straightforward way.
I leave this exercise.

Exercise 9.
Write down the angular momentum states obtained by combining three spin $\frac{1}{2}$ states.
Treat the particles as distinguishable.
Remark: this part of homework is not clear to me. Is the exercise about a three particle system with spin $\frac{1}{2}$? Chapter 4 is about spin and angular momentum. Citing Mahan: "……..The many particle aspects are deferred until chapter 9. The present chapter is concerned with understanding the properties of only one or two separate components of angular momentum". The two separate components of angular momentum: spin and orbital angular momentum? In the section on **The Addition of Angular Momentum** Mahan mentioned two systems each with spin $\frac{1}{2}$. Further on he mentioned the spins of the components. I considered this two be a two particles.
The only way out for me is this exercise is about three particles each with spin $\frac{1}{2}$.
Let us assume this to be correct.
We have three particles each represented by a state $|j, m\rangle$.
With one spin system we have two(2) states; with a system of two particles we have four(2^2) states and with a system of three distinguishable particles we have eight(2^3) states.
In general we can write for this combined state: $|j_1, m_1\rangle \otimes |j_2, m_2\rangle \otimes |j_3, m_3\rangle$.
We know m_i to be $\pm 1/2$. For the up-state we use $|u\rangle$, for the down-state we use $|d\rangle$ as Susskind did. Let us use a condensed notation. For example the particles in the up-state: $|uuu\rangle$. Then the other states are: $|uud\rangle$, $|udd\rangle$, $|ddd\rangle$, $|ddu\rangle$, $|duu\rangle$, $|dud\rangle$ and $|udu\rangle$.
Again, for example $|udd\rangle \to |u\rangle \otimes |d\rangle \otimes |d\rangle$.

Homework.

The exercises can be found in the relevant sections.

5. Two and Three Dimensions.

In this chapter techniques presented in the previous chapters are applied. Exact and approximate methods are given.

5.1 Plane Waves in Three Dimensions.

In this section Mahan starts the discussion on plane waves $\psi(\boldsymbol{r})$ and potential energy $V = 0$. Spherical coordinates are used. Spherical harmonics are used as solutions to Schrödinger's equation. With the operator equation for M^2, Eq. (4.134), and the eigenvalue equation,

Eq. (4.135), $\nabla^2\psi(\boldsymbol{r}) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) - \frac{l(l+1)}{r^2}\psi$. **(C5.1)**
In this equation $\psi(\boldsymbol{r}) = R(r)Y_l^m(\theta,\phi)$. (5.14)
We met the function $Y_l^m(\theta,\phi)$, a spherical harmonic, in chapter 4, section 4.2 on representations. In the Eqs. (5.8) – (5.10) Mahan showed some examples for $l = 0, 1, 2$ and $-l \leq m \leq l$.
With the spherical harmonic given the only function to be found is $R(r)$.
The resulting Schrödinger equation expressed in $R(r)$ is:
$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{l(l+1)}{r^2}R + \frac{2m}{\hbar^2}ER = 0$. **(C5.2)**
In **(C5.2)** E represents the kinetic energy: $E = \frac{\hbar^2k^2}{2m}$. (5.15)
On page 110 Mahan presented the solutions in terms of spherical Bessel functions for the radial function R_l, where the subscript l is introduced for obvious reasons. At the bottom of page 110, Eqs (5.20) - (5.25) some properties of spherical Bessel functions are given.
On page 111 the spherical Hankel functions are introduced as well. With help of Eq. (5.20), two Hankel functions are given.
At the bottom of page 111 Mahan introduced the generating function for spherical Bessel functions. On the next page Mahan the expansion of the plane wave solution is given. For me it is not clear to what purpose this expansion is given. On this page the addition theorem for momentum is mentioned, Eq. (5.38). I do not know where this theorem has been proven. In section 4.4 the addition of angular momentum is discussed. Eq. (4.150) represents the relation for addition. The theorem has not been mentioned. I just except the theorem.
Remark: Looking for more information on the addition theorem I found the answer. The addition theorem is about the addition of spherical harmonics (www.scipp.ucsc.edu). Information on the addition theorem can also be found In Whittaker and Watson, chapter 18 section 4. A new proof of the addition theorem for the Legendre polynomial.

Below Eq.(5.39) writes: “The last bracket is $2\cos(\theta - \theta'')$ … … ". I think this should be: “The last bracket is $2\cos(\phi - \phi'')$.....”. A printing error I suppose.
In his lectures Fitzpatrick dealt with the example of an Infinite Spherical Well. This example is shown in the second exercise of Homework.

Due to the length of chapter 5 I first work on exercise 1 of Homework.

Homework: 1, 2.

Exercise 1 . Verify the addition theorem for $l = 2$.
The addition theorem: $(2l+1)P_l(\theta') = 4\pi\sum_{m=-l}^{m=l} Y_l^m(\theta,\phi)Y_l^{m*}(\theta'',\phi'')$. The various angles are defined on page 112.
For $l = 2$ we have:
$5P_2(\theta') = 4\pi\sum_{m=-2}^{m=2} Y_2^m Y_2^{m*}$.
All the elements of the right-hand side are given in the Eqs. (5.8)-(5.10).
Furthermore the Legendre polynomial $P_2(\theta') = \frac{1}{2}[3(\cos\theta')^2 - 1]$. (4.124)
We also need Eq. (5.34), the relation between $\theta', \theta, \theta'', \phi$ and ϕ''. With all the ingredients the exercise becomes an exercise in goniometrical manipulations.

We could choose a goniometric “Light” approach. This approach is based upon the alignment of the vectors $\boldsymbol{k}$ and $\boldsymbol{r}$. This is just one of the possible values of θ'.
Then the addition theorem becomes:
$5P_2(0) = 4\pi \sum_{m=-2}^{2} |Y_2^m|^2$, (C5.3)
with $\theta' = 0$ the angle between $\boldsymbol{k}$ and $\boldsymbol{r}$. Again all the ingredients are available. Eq. (4.124), $P_2(0) = 1$, and $Y_2^0, Y_2^{\pm 1}$, and $Y_2^{\pm 2}$ are given by Eqs. (5.8)-(5.10). The summation on the right-hand side of (C5.3): $\frac{5}{4}(3cos^2\theta - 1)^{\,2} + 15sin^2\theta cos^2\theta + \frac{15}{4}sin^4\theta = 5$. So for this particular situation the addition theorem is verified with $l = 2$.
Another approach for this “Light” case is to rewrite the addition theorem with associate Legendre polynomials.
So for $\theta' = 0$ the theorem reads:$1 = \sum_{m=-2}^{2} \frac{(2-|m|)!}{(2+|m|)!} |P_2^m|^2$. (C5.4)
$P_2(x) = \frac{1}{8}\frac{d^2}{dx^2}[(x^2-1)^2]$ (C5.5)

>

and
$P_2^m(x) = (-1)^m(1-x^2)^{\frac{m}{2}}\frac{d^m}{dx^m}P_2(x)$. (C5.6)
$P_2(x)$ with (C5.5) becomes: $P_2(x) = \frac{1}{2}(3x^2-1)$.
Now we can derive all the expressions for P_2^m and substitute these in (C5.4) to obtain $[\frac{1}{2}(3x^2-1)]^2 + \frac{1}{3}\left[3x(1-x^2)^{\frac{1}{2}}\right] + \frac{1}{12}[3(1-x^2)]^2$. After some manipulations we find this expression to be equal 1. Another verification of the addition theorem.

Exercise 2.
Find the exact eigenvalue equation for any value of angular momentum for a particle in a spherical well:
$V(r) = \begin{cases} 0 & 0 < r < a \\ \infty & a < r \end{cases}$.
The equations describing this potential are given in the Eqs. (5.63) and (5.64) with the above values for $V(r)$ or Eq. (5.16) with $V(r) = 0$.
Then in the spherical well we have the solution Eq. (5.19). Since the solution $y_l(kr)$ diverges at $r = 0$, the solution for the radial part of the wave equation is: $R_l(kr) = C_1 j_l(kr)$. And $k^2 = \frac{2mE}{\hbar^2}$. The constant C_1 is found from boundary and initial conditions(Mahan). As written by Mahan on page 16 the function $j_l(kr)$ must be forced to vanish at $r = a$. This will give us the eigenvalues. For some values of l these are given in the table below, b).
a. What is the specific result for $l = 0$?
The specific result for the radial part of the wave function is $j_0(kr) = \frac{\sin kr}{kr}$, Eq. (5.20).
At $r = a : j_0(ka) = \frac{\sin ka}{ka}$, consequently $k_n a = n\pi$. So $k_n = \frac{n\pi}{a}$. The eigenvalues are: $E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{a})^2$.
b. Look up a table of zeros of spherical Bessel functions (e.g., *Handbook of Mathematical Functions*). Use these data to list, in order, the six lowest eigenvalues considering all possible values of angular momentum. Remark: what does all possible values mean? On page 109 Mahan writes: “The most frequently used spherical harmonics are those with small values of

(l, m)."

This does not bring me any further, since what does small values mean? $l = 0,1,2$?

For $l = 0$ you will find again the numerical values for $k_n a = n\pi$, $n = 1,2,3,4,5,6$.

And the six lowest eigenvalues are: $E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{a})^2$, $n = 1,2,3,4,5,6$..

For $l = 1$ and 2 you will find the numerical values for $k_n a$, $n = 1,2,3,4,5,6$.

zeros	$l = 0$	$l = 1$	$l = 2$
$n =$	$ka =$	$ka =$	$ka =$
1	π	4.4934	5.7635
2	2π	7.7252	9.9050
3	3π	10.9041	12.3229
4	4π	14.0662	15.5146
5	5π	17.2208	18.6890
6	6π	20.3713	21.8539

And the eigenvalues are : $E_n = \frac{\hbar^2}{2ma^2}(ka)^2$.

Let us return to the expression: "All possible values of angular momentum". With Eq. (5.63) I suppose to find bound states for $\frac{\hbar^2}{2mr^2} l(l+1) < E \left(= \frac{\hbar^2}{2ma^2}(ka)^2\right)$.

Let us plug some numerical values into this equation. With r of order a and ka of order 10 we have $l^2 < 100$ or $l < 10$. Well, in the above table I gave the values for three values of l. Assuming the upper limit of l to be correct I have still a couple of values of l to go. I leave it here.

5.2 Plane Waves in Two Dimensions

In this section Mahan presented the general plane wave solutions to the eigenvalue equation. The solutions are given in terms of Bessel functions and Neumann functions. The generating function for the Bessel function is also given.

5.3 Central potentials

In this case the potential $V(r)$ depends just on the magnitude of $\boldsymbol{r}$. These potentials are spherical symmetric. The eigenvalue equation will be treated in two and three dimensions.

5.3.1 Central Potentials in 3D

Eq. (5.57) has been derived from Eq. (5.55), where use has been made of Eq.(5.12). The latter equation is fund from Eqs. (4.134) and (4.135). In the line above Eq. (5.69) Mahan writes: "Here the most general solution is Eq. (5.19)…". Caveat. I consider this a bit confusing since this solution is given for the differential equation with $V(r) = 0$.

On page 116 Mahan gave as an example the attractive three dimensional square well. On page 117 Mahan matches the solution of the Schrödinger equation at the boundary of the potential well and obtained the expression for the phase shift δ_l. In Eq. (5.78) Mahan uses δ instead of δ_l. A printing error I suppose.

Just below Eq. (5.79) Mahan writes: “It’s an interesting exercise to evaluate this expression (Eq. (5.78) or Eq. (5.79), Nz) for $l = 0$…”. Let us give it a try.
For this we use Eq.(5.20).
Then $j_0(z) = \frac{\sin z}{z}$, $j_0'(z) = -\frac{\sin z}{z^2} + \frac{\cos z}{z}$, $y_0(z) = -\frac{\cos z}{z}$, and $y_0'(z) = \frac{\sin z}{z^2} + \frac{\sin z}{z}$, the prime denotes derivative and $z = pa$ or ka.
We substitute these expressions in to Eq. (5.78) and after carefully manipulating the following expression is found: $\frac{\tan ka + \tan \delta_0}{k(1 - \tan \delta_0 \tan ka)} = \frac{\tan pa}{p}$.
With help of the goniometrical relation $\tan(\alpha + \beta) = \frac{\tan \alpha + \tan \beta}{1 - \tan \alpha \tan \beta}$ the expression Eq. (5.80) is found. The result of the one-dimensional well; Eq. (2.49).
Mahan concluded this section with the expressions for the second example: the repulsive three dimensional square well.
Another example of a central potential is the 3-D harmonic oscillator. In textbooks you will find the this oscillator to be analysed in a Cartesian frame. The Hamiltonian is a sum of 3 independent oscillators. The eigenvalues are a sum of the 1-D eigenvalues. With this result the degeneracy is calculated. The results are reviewed in “Quantum Harmonic Oscillator”, www.en.m.wikipedia.org .

Homework: 3, 4, 5, 6, 7, 14, 15, 17.

Exercise 3.
A deuteron is a bound state of a neutron and a proton. Fermi calculated the binding energy assuming the nuclear forces could be approximated by a spherical square well of depth $V(r) = -V_0$ for $r < a$ and $V(r) = 0$ for $r > a$. His values were $V_0 = 36$ MeV and $a = 2.0$ fm (femtometer: 10^{-15} m). What numerical value did Fermi get for the bound-state energy, in MeV?
Hint: Use the reduced mass in relative coordinates. For a classical rehearsal of reduced mass see: www.en.m.Wikipedia.org : Two-body problem. For the reduced mass concept for quantum mechanics see Steane.
Now with reduced mass and relative coordinates the Schrödinger equation in radial direction is separable. It separates into an equation for the motion of the centre of mass and a separate equation for the motion expressed in the relative coordinate $\boldsymbol{r} = \boldsymbol{r_p} - \boldsymbol{r_n}$. The subscripts p and n denote the proton and neutron respectively. In the analysis I suppose the centre of mass to be stationary.
The reduced mass $\mu = \frac{m_p m_n}{m_p + m_n}$.
The solution for $a > r$ and $V_l(r) = -V_o + \frac{\hbar^2}{2\mu r^2} l(l+1)$ is, Eq. (5.19):

$$R_l(kr) = C_1 j_l(kr) = C_1 \sqrt{\frac{\pi}{2kr}} J_{l+\frac{1}{2}}(kr), \qquad \text{(C5.7)}$$

with $k = \{\frac{2\mu}{\hbar^2}(V_0 + E)\}^{1/2} > 0$.
For $r > a$ and $V_0 = 0$ we have the solution

$$R_l(\alpha r) = B k_l(\alpha r) = B \sqrt{\frac{\pi}{2\alpha r}} K_{l+\frac{1}{2}}(\alpha r). \qquad \text{(C5.8)}$$

$K_{l+\frac{1}{2}}$ is the modified Bessel function of the third kind.

$\alpha^2 = -\frac{2\mu}{\hbar^2}E, E < 0.$

For large r the modified Bessel functions $I_{l+1/2}$ and $I_{-l-\frac{1}{2}}$ diverge(Abramowitz and Stegun).

In order to find the eigenvalues for the bound states we have to match $R_l(kr)$ and $R_l(\alpha r)$ and their derivatives at $r = a$.

This results into:

with (C5.7) and (C5.8): $C_1\sqrt{\frac{\pi}{2kr}}J_{l+\frac{1}{2}}(ka) = B\sqrt{\frac{\pi}{2\alpha r}}K_{l+\frac{1}{2}}(\alpha a).$

The derivatives can be found from Abramowitz an Stegun. We could use the general expressions. However, the exercise is about to find a number for the bound-state energy. So let us start with $l = 0$.

Then $C_1 j_0(ka) = \ Bk_0(\alpha a)$.

With Eq. (5.20) $j_0(ka) = \frac{\sin ka}{ka}$. (C5.9)

And with Abramowitz and Stegun $k_0(\alpha a) = \frac{\pi}{2}\left[\frac{\cosh \alpha a}{\alpha a} - \frac{\sinh \alpha a}{\alpha a}\right]$. (C5.10)

So $C_1\frac{\sin ka}{ka} = B\frac{\pi}{2}[\frac{\cosh \alpha a}{\alpha a} - \frac{\sinh \alpha a}{\alpha a}]$.

This can be $C_1\frac{\sin ka}{ka} = -B\frac{\pi}{2}\frac{e^{-\alpha a}}{\alpha a}$. (C5.11)

For the derivatives at $r = a$, we find

$C_1\left[\frac{\cos ka}{a} - \frac{\sin ka}{ka^2}\right] = -B\frac{\pi}{2}[-\frac{e^{-\alpha a}}{a} - \frac{e^{-\alpha a}}{\alpha a^2}]$. (C5.12)

Again as in chapter 2 by dividing Eqs. (5.11) and (5.12) the constants cancel and we finally found the equation for the eigenvalue with $l = 0$.

So $ka \cot ka = -\alpha a$.

This can be written as $\frac{\tan ka}{k} = -\frac{1}{\alpha}$. (C5.13)

Well this looks familiar. The one dimensional square well Eq. (2.32).

We can plug in the analysis of page 19 of Mahan end rewrite (C5.13) as

$\tan\sqrt{g^2(1-\varepsilon)} = -\sqrt{\frac{1-\varepsilon}{\varepsilon}}$, Eq. (2.37).

In this expression $E = -\varepsilon V_0$ and $g^2 = \frac{V_0}{E_a} = \frac{2\mu V_0 a^2}{\hbar^2}$.

However, this exercise is about to find a number for the bound-state energy. So we have to calculate g^2.

The reduced mass: $\mu = \frac{m_p m_n}{m_p + m_n}$. We need the mass of the proton and of the neutron. In this exercise, as a reasonable approximation, I will use the same value for the neutron and the proton. $m_p = 1.673\ 10^{-27}$ kg. So the reduced mass $\mu = m_p/2$. The potential V_0 is expressed in Joules: $V_0 = 5.767\ 10^{-12}$ Joules.

$E_a = \frac{\hbar^2}{2\mu a^2} = \frac{\hbar^2}{m_p a^2} = \frac{1.113\ 10^{-68}}{6.692\ 10^{-57}} = 1.663\ 10^{-12}$ Joules .

Finally we have $g^2 = \frac{V_0}{E_a} = 3.468$. Then Eq. (2.37) gives as a solution $\varepsilon = .056$, where use has been made of WolframAlpha.

Then we have for the eigenvalue $E = -0.323\ 10^{-12}$Joules.

Or, $E = -3.039$ MeV for $l = 0$. We found $-V_0 < E < 0$.

Reminder: $\varepsilon = 1$ is the trivial solution of Eq. (2.37).

What about $l = 1$?
The expressions become a bit more complicated. We need the expressions for spherical Bessel functions and modified spherical Bessel functions. I present here the result for the eigenvalue equation: $\frac{k^2 \tan ka}{ka - \tan ka} = \frac{\alpha^2}{\alpha a + 1}$. This expression can be rewritten in terms of g^2 and ε.
And we obtain $\tan \sqrt{g^2(1-\varepsilon)} = \frac{\varepsilon\sqrt{g^2(1-\varepsilon)}}{1+(1-\varepsilon)\sqrt{g^2\varepsilon}}$.
Solve this equation for ε and you will find $\varepsilon = 1$. Out of the range of allowed values of ε.
So the value for the bound-state energy is: $E = -3.039$ MeV. So with $l = 0$ this means the orbital angular momentum is zero.

Exercise 4.
Calculate the s-wave ($l = 0$) phase shift for a repulsive ($V_0 > 0$) square-well potential:

$V(r) = \{V_0 \;\; 0 < r < a$ and
$V(r) = \{0 \;\; a < r$.
Then assume that $V_0 > E > 0$ and find the limit of the phase shift $\delta_0(k)$ in the limit $V_0 \to \infty$.
Mahan dealt with the repulsive potential in section 5.31. The general solution is presented at the top of page 118. So "inside" the repulsive potential the eigenfunction is a decaying one.
Using the notation of Mahan, we have for $0 < r < a$:
$R(r) = Ai_l(\alpha r)$,
with $\alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$.
i_l is the modified spherical Bessel function of the first kind. For $l = 0$ we have
$i_0 = \frac{\sinh \alpha r}{\alpha r}$.
For $a < r$ we have $R(r) = C[j_l(kr) - \tan(\delta_l)y_l(kr)]$, Eq.(5.86).
j_l and y_l are spherical Bessel functions.
$k^2 = 2mE/\hbar^2$.
For $l = 0$ we have $R(r) = C[j_0(kr) - \tan(\delta_0)y_0(kr)]$.
Expressions for $j_0(kr)$ and $y_0(kr)$ are:
$j_0(kr) = \frac{\sin kr}{kr}$, and $y_0(kr) = -\frac{coskr}{kr}$.
By matching the eigenfunctions at the boundary $r = a$ we find the eigenvalue equation and the expression for $\delta_0(k)$.
Matching the functions for $R(r)$ at $r = a$:
$$A\frac{\sinh \alpha a}{\alpha a} = C[\frac{\sin ka}{ka} + \tan(\delta_0)\frac{coska}{ka}] \,. \qquad \text{(C5.14)}$$
For the derivative of $R(r)$ at $r = a$ we have:
$$A\left[\frac{\cosh \alpha a}{a} - \frac{\sinh \alpha a}{\alpha a^2}\right] = C[\frac{coska}{a} - \frac{\sin ka}{ka^2} - \tan(\delta_0)\{\frac{\sin ka}{a} + \frac{coska}{ka^2}\}] \,. \qquad \text{(C5.15)}$$
Now we divide the two Eqs. (C5.14) and (C5.15) and obtain
$$\tan(\delta_0) = \frac{k \tanh \alpha a - \alpha \tan ka}{k \tan ka \tanh \alpha a + \alpha} \,. \qquad \text{(C5.16)}$$
Now $V_0 \to \infty$ and $0 < E < V_0$ what will δ_0 looks like?
Well, $V_0 \to \infty$: we may expect $\alpha^2 = \frac{2m}{\hbar^2}(V_0 - E) \to \infty$. So with (C5.16) we expect $\tan(\delta_0) = -\tan ka$, or $\delta_0 = -ka \pm n\pi$.
This result for the phase shift can be found directly by the condition for the radial part of the

wave function to vanish at $r = a$. Then with (C5.14): $\frac{\sin ka}{ka} + \tan(\delta_0)\frac{coska}{ka} = 0$. This results into: $\tan(\delta_0) = -\ \tan ka$. As it should.
This exercise is a prelude for exercise 5

Exercise 5.

The hard-sphere potential in 3D has $V(r) = \infty$ for $r < a$ and $V = 0$ for $a < r$. This potential forces the radial wave function to vanish at $r = a$, $R(a) = 0$. Derive the formula for the phase shift $\delta_l(k)$ for all angular momentum. Use it to derive simple expressions for the phase shift for $l = 0$ and $l = 1$.
A lot of work has already done in exercise 4.
The expression for the phase shift is given by Eq. (5.86):
$R(r) = C[j_l(kr) - \tan(\delta_l)y_l(kr)]$.
So with $R(a) = 0$, we have
$\tan\delta_l\,(k) = \frac{j_l(ka)}{y_l(ka)}$. (C5.17)
Now derive the phase shift for $l = 0$ and $l = 1$.
For $l = 0$, we have with (C5.17) , $j_0(z) = \frac{\sin z}{z}$, and $y_0(z) = -\frac{\cos z}{z}$:
$\delta_0(k) = \tan^{-1}(-\tan(ka)) + n\pi$.
This result has been obtained in exercise 4.
For $l = 1$, we have with (C5.17), $j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}$, and $y_1(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z}$,
$\delta_1(k) = \tan^{-1}[\frac{ka - \tan ka}{1 + ra\tan ka}]$.
Use has been made of Eq.(5.20).

Exercise 6.

In three dimensions, a spherically symmetric potential has the form of a delta function away from the origin: $V(r) = -\lambda\delta(r - a)$, where λ is appositive constant.
a. Find the eigenvalue equation for an s-wave bound state($l = 0$).
b. Show that λ has to have a minimum value for bound states to exist. What is that value?
a. First we consider $r \to \infty$, away from the singularity.
We are looking for bound states: $E < 0$ and $\alpha^2 = -\frac{2m}{\hbar^2}E$.
Similar to what has been found in exercise 3 we have:
$R_l(\alpha r) = Bk_l(\alpha r) = B\sqrt{\frac{\pi}{2\alpha r}}K_{l+\frac{1}{2}}(\alpha r)$, Eq. (C5.8), with $l = 0$ representing the decaying s-wave.
Then for $l = 0$: $R_0(\alpha r) = B\,\frac{\pi}{2}\left[\frac{\cosh\alpha r}{\alpha r} - \frac{\sinh\alpha r}{\alpha r}\right] = B\,\frac{\pi}{2}\frac{e^{-\alpha r}}{\alpha r}$. (C5.18)

(Abramowitz and Stegun).
Now $r < a$, away from the singularity.
$R_0(\alpha r) = A\sqrt{\frac{\pi}{\alpha r}}I_{\frac{1}{2}}(\alpha r)$, (C5.19)
Where $I_{\frac{1}{2}}(\alpha r)$ is the modified spherical Bessel function of the first kind.
And $\sqrt{\frac{\pi}{\alpha r}}I_{\frac{1}{2}}(\alpha r) = \frac{\sinh\alpha r}{\alpha r}$. (C5.20)

We match the wave functions given by Eqs. (C5.18)-(C5.20) at : $r = a$

$$A\frac{\sinh \alpha a}{\alpha a} = B\frac{\pi}{2}\frac{e^{-\alpha a}}{\alpha a} \ . \tag{C5.21}$$

In Chapter 2.6 we learned to deal with the delta-function potential.
The matching at the singularity reads(bottom of page 45):

$$(\frac{dR}{dr})_{r=a+\epsilon} - \left(\frac{dR}{dr}\right)_{r=a-\epsilon} = -\frac{2m\lambda}{\hbar^2}R(a)\ , \tag{C5.22}$$

with $\epsilon \to 0$.
Alas, (C5.22) is wrong. Why is that? Well, to apply the matching procedure for the derivative at the singularity using the one-dimensional case, we need Eq. (5.64):
$0 = [\frac{d^2}{dr^2} - \frac{2m}{\hbar^2}(V_l(r) - E))]\chi(r)$, where $\chi(r) = rR(r)$.
Then the matching condition at the singularity for the derivative, similar to the one-dimensional case, is:

$$(\frac{d\chi}{dr})_{r=a+\epsilon} - \left(\frac{d\chi}{dr}\right)_{r=a-\epsilon} = -\frac{2m\lambda}{\hbar^2}\chi(a). \tag{C5.23}$$

So (C5.22) should have been:

$$(R + r\frac{dR}{dr})_{r=a+\epsilon} - \left(R + r\frac{dR}{dr}\right)_{r=a-\epsilon} = -\frac{2m\lambda}{\hbar^2}R(a).$$

We need to find and evaluate the eigenvalue equation for α. So it is a bit more convenient to deal with (C5.23).
For $a < r$:

$$\chi(r) = Ce^{-\alpha r}. \tag{C5.24}$$

For $a > r$:

$$\chi(r) = D(e^{\alpha r} - e^{-\alpha r}). \tag{C5.25}$$

Matching (C5.24) and (C5.25) at $a = r$:

$$D = C\frac{e^{-\alpha a}}{e^{\alpha a} - e^{-\alpha a}}. \tag{C5.26}$$

Substitute (C.4.24) and (C5.25) into (C5.23) gives:

$$\alpha Ce^{-\alpha a} + \alpha D(e^{\alpha a} + e^{-\alpha a}) = \frac{2m\lambda}{\hbar^2}Ce^{-\alpha a}. \tag{C5.27}$$

With (C5.26) we rewrite (C5.27) and find:

$$\frac{2m\lambda}{\hbar^2} = \alpha(1 + \frac{1}{\tanh \alpha a}). \tag{C5.28}$$

This represents the eigenvalue equation for an s-wave bound state.
b. Now show λ to have a minimum value for bound states to exist.
To find out about this existence we rearrange (C5.28):

$$\frac{2ma\lambda}{\hbar^2} = \alpha a(1 + \frac{1}{\tanh \alpha a}). \tag{C5.29}$$

Keep in mind $\alpha a > 0$.
Differentiate the right-hand side of (C5.29) with respect to αa and set the resulting equation equal to 0. Then: $\left(1 + \frac{1}{\tanh \alpha a}\right)\left(1 + \alpha a(1 - \frac{1}{\tanh \alpha a})\right) = 0$. This leads to

$$\tanh \alpha a = \frac{\alpha a}{1-\alpha a} \text{ or } \frac{\cosh \alpha a}{\sinh \alpha a} = \frac{1-\alpha a}{\alpha a}. \tag{C5.30}$$

The solution of (C5.30) gives us $\alpha a = 0$. Keep in mind we have in (C5.29) the quotient $\frac{\alpha a}{\tanh \alpha a}$, we find the minimum value of $\frac{2ma\lambda}{\hbar^2}$ to be equal 1. The second derivative with respect to αa of $\frac{2ma\lambda}{\hbar^2}$ gives us a positive infinite value. So we have a minimum? Alas, $\alpha a = 0$. So

there are no bound states.
Let us have another look at the minimum value $\frac{2ma\lambda}{\hbar^2} = 1.$ We can rewrite this in the following way: $\frac{2m\lambda}{\hbar^2} = 1/a$. So, what happens for $a \rightarrow 0$? I think exercise 7 deals with this limit.

Exercise 7.
Does an attractive three dimensional delta-function potential bind a particle in three dimensions? Explain your answer. Use atomic units so that the Hamiltonian is
$H = -\nabla^2 - \beta\delta^3(\vec{r})$, where $\beta > 0$ is a constant. So the delta function potential is an attractive potential.
The differential equation for the radial component $rR = \chi$ of the wave function is
$(\nabla^2 + \beta\delta^3(\vec{r}) + E)\chi = 0$, (C5.30)
with $E < 0$. We set $\alpha^2 = -E$.
Away from the singularity $R \rightarrow 0$ for $r \rightarrow \infty$.
So for $r \rightarrow \infty$, $\chi = Ae^{-\alpha r}$ or $R = A\frac{e^{-\alpha r}}{r}$, with A a constant.
Now comes a more difficult part: $R = A\frac{e^{-\alpha r}}{r}$, diverges for $r \rightarrow 0$. So what does the solution looks like for $r \rightarrow 0$? On page 115 in the section on central potentials, Mahan mentioned the close connection between one dimension and three dimensions. So can we use the analysis of the one dimensional case of section 2.6 on delta-function potentials? Intuitively we expect one bound state and one eigenvalue, similar to the one-dimensional case.
Let us isolate the "black hole" by encapsulating the singularity with a sphere of radius ϵ with $\epsilon \rightarrow 0$. Now integrate Eq. (C5.30) over this small volume:
$\int \nabla^2\chi dV = -\int E\chi dV - \int \beta\delta^3(\vec{r})\chi \, \mathrm{dV}$.
With help of Gauss theorem the volume integral on the left-hand side can be replaced by a surface integral over the gradient:
$\int \nabla\chi dA = -\int E\chi dV - \int \beta\delta^3(\vec{r})\chi \, \mathrm{dV}$.
Evaluating the integrals gives:
$\int \nabla\chi dA = -\,\alpha A 4\pi\epsilon^2$.
The integrals on the right-hand side are:
$\int E\chi dV = E\chi(0)\frac{4}{3}\pi\epsilon^3$ and $\int \beta\delta^3(\vec{r})\chi \, \mathrm{dV} = \beta\chi(0)\frac{4}{3}\pi\epsilon^3$.
Since $\epsilon \rightarrow 0$, the left-hand side and the right-hand side of
$\int \nabla^2\chi dV = -\int E\chi dV - \int \beta\delta^3(\vec{r})\chi \, \mathrm{dV}$ are both zero.
No conclusion can be drawn from this evaluation. So we stay with our intuition: one bound state and eigenvalue similar to the one-dimensional results presented on page 45(Mahan).

Exercise 14.
Solve the exact eigenvalues and eigen states of the three-dimensional harmonic oscillator using spherical coordinates and central potential $V(r) = \frac{Kr^2}{2}$.
Hint: Set $z = \frac{r^2 m\omega}{\hbar}$ and find the equation for $G(z)$, where$\chi(r) = z^{\frac{l+1}{2}}e^{-\frac{z}{2}}G(z)$.
We are dealing with a 3-D central potential. The differential equation is:
$0 = \left[\frac{d^2}{dr^2} - \frac{2m}{\hbar^2}\frac{K}{2}r^2 - \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}E\right]\chi(r).$ (C5.3.1.1)

In this equation $\omega = \sqrt{\frac{K}{m}}$, then we write $\frac{2m}{\hbar^2}\frac{K}{2} = \left(\frac{m\omega}{\hbar}\right)^2 = \gamma^2$ and $\varepsilon = \frac{2m}{\hbar^2}E$. With these expressions (C5.3.1.1) can be written as: $0 = [\frac{d^2}{dr^2} - \gamma^2 r^2 - \frac{l(l+1)}{r^2} + \varepsilon]\,\chi(r)$. (C5.3.1.2)
Mahan proposes a coordinate transformation $z = \frac{r^2 m\omega}{\hbar} = \gamma r^2$.
With this transformation we obtain: $\frac{d}{dr} = 2\gamma r\frac{d}{dz}$, and $\frac{d^2}{dr^2} = 2\gamma\frac{d}{dz} + 4\gamma z\frac{d^2}{dz^2}$. Substitute these transformations into (C5.3.1.2): $\left[4z\frac{d^2}{dz^2} + 2\frac{d}{dz} - z - \frac{l(l+1)}{z} + \frac{\varepsilon}{\gamma}\right]\chi(z) = 0$. (C5.3.1.3)
Furthermore, Mahan proposed a trial function $\chi(z) = z^{\frac{l+1}{2}}e^{-\frac{z}{2}}G(z)$. We substitute this function into (C5.3.1.3) and then a tedious job arises. The result is:
$2\frac{d\chi}{dz} = z^{\frac{l+1}{2}}e^{-\frac{z}{2}}\left[\{(l+1)z^{-1} - 1\}G + 2\frac{dG}{dz}\right]$.
$4z\frac{d^2\chi}{dz^2} = z^{\frac{l+1}{2}}e^{-\frac{z}{2}}[\{(l^2-1)z^{-1} - 2(l+1) + z\}G + \{2(l+1) - 2z + 2(l+1) - 2z\}\frac{dG}{dz} + 4z\frac{d^2G}{dz^2}]$.
We plug these expressions with the trial function into (C5.3.1.3), cancel $z^{\frac{l+1}{2}}e^{-\frac{z}{2}}$, we finally obtain a differential equation for G:
$z\frac{d^2G}{dz^2} + \left(l + \frac{3}{2} - z\right)\frac{dG}{dz} - \left(\frac{2l+3}{4} - \frac{\varepsilon}{4\gamma}\right)G = 0$. (C5.3.1.4)
This equation resembles the standard differential equation satisfied by the confluent hypergeometric function $F(a, b, z)$, where:
$a = \frac{2l+3}{4} - \frac{\varepsilon}{4\gamma}$,
$b = l + \frac{3}{2}$, and $z = \frac{r^2 m\omega}{\hbar} = \gamma r^2$.
Similar to the analysis of section 5.4.3(Mahan), G becomes:
$G(r) = C_1 F(\frac{2l+3}{4} - \frac{\varepsilon}{4\gamma}, l + \frac{3}{2}, \gamma r^2)$. (C5.3.1.5)
C_1 is a constant.
This expression diverges at large values of r because of the exponential factor $e^{\gamma r^2}$. Similar to the analysis at page 122(Mahan) the series for F are truncated after n terms. The consequence is a to be negative integer or zero. The requirement a to be a negative integer or zero is:
$-n_r = a = \frac{2l+3}{4} - \frac{\varepsilon}{4\gamma}$, this eigenvalue equation gives, with, $\varepsilon = \frac{2m}{\hbar^2}E$ and $\gamma = \frac{m\omega}{\hbar}$,
$E_{n_r l} = \hbar\omega(2n_r + l + \frac{3}{2})$. (C5.3.1.6)
This expression shows the degeneracy: when $2n_r + l$ is considered to have a integer value n_r, l and m vary. This results into varies eigenfunction for one eigenvalue $E_{n_r l}$. See also the next exercise 15.
The eigenfunction for the 3-D harmonic oscillator is:
$\psi_{nlm}(r, \theta, \phi) = C_2 r^l e^{-\frac{\gamma r^2}{2}} L_{n_r}^{l+\frac{1}{2}}(\gamma r^2) Y_l^m(\theta, \phi)$.
C_2 is found by normalizing the eigenfunction.

Exercise 15.
For the 3-D harmonic oscillator, what is the degeneracy $G(N)$(do not confuse the above

function $G(r)$ with the degeneracy) of each level? That is, how many different states, as a function of N, have the same energy $\hbar\omega(N+\frac{3}{2})$?

Exercise 14 resulted into the energy eigenvalues: $E_{n_r l} = \hbar\omega(2n_r + l + \frac{3}{2})$. So, $N = 2n_r + l$. All states with the same N have the same eigenvalue. Then for a given N, choose a particular l. We have $2n_r = N - l$. There are $N - l + 1$ possible values of $2n_r$. Caveat: $N - l$ has to be even. $n_r : n_r \in \mathbb{N}$ and $0 \leq n_r \leq N - l$ this results into:

$G(N) = \sum_{l=0}^{N} N - l + 1 = \frac{(N+1)(N+2)}{2}$. (www.en.wikipedia.org).

This analysis is based on the 3-D independent oscillators. In the same Wikipedia summary this result is also based on the 3-D isotropic harmonic oscillator.

Another approach is based on counting, finding a pattern and induction.

Let us start with counting.

With $N, n_r$and $l \in \mathbb{N}$, and $m \in \mathbb{Z}$ we make the following set of states:

$N = 0, 2n_r = 0, l = 0, m = 0$:one eigenstate the ground state.

$N = 1, 2n_r = 0, l = 1, m = -1,0,1$: 3 eigenstates, $G(N) = 3$.

$$N = 2, \left\{\begin{matrix} 2n_r = 0, l = 2, m = -2,-1,0,1,2 \\ 2n_r = 2, l = 0, m = 0 \end{matrix}\right\} : G(N) = 6.$$

$$N = 3, \left\{\begin{matrix} 2n_r = 0, l = 3, m = -3,-2,-1,01,2,3 \\ 2n_r = 2, l = 1, m = -1,0,1 \end{matrix}\right\} : G(N) = 10.$$

$$N = 4, \left\{\begin{matrix} 2n_r = 0, l = 4, m = -4,-3,-2,-1,0,1,2,3,4 \\ 2n_r = 2, l = 2, m = -2,-1,0,1,2 \end{matrix}\right\} : G(N) = 15.$$

A pattern? Well, it appears $G(N) = G(N-1) + N + 1$. This recurrence relation can be translated into a direct relation for $G(N)$. Then we have $G(N) = N + 1 + N + \cdots 0$. This series add up to: $\sum_{k=0}^{N+1} k = \frac{(N+1)(N+2)}{2}$.

Now we assume $G(N)$ to be true, what about $G(N+1)$?

With $G(N+1) = N + 2 + N + 1 + N + \cdots 0 = \sum_{k=0}^{N+2} k = \frac{(N+2)(N+3)}{2} = \frac{((N+1)+1)((N+1)+2)}{2}$.

So $G(N+1)$ is true under the assumption $G(N)$ to be true. So $G(N)$ is true for all N.

Exercise 17.

Kratzer's molecular potential has a minimum at $V(r = a) = -D$ and simulates the binding of two atoms: $V(r) = D[(\left(\frac{a}{r}\right)^2 - 2\left(\frac{a}{r}\right)]$.

Find the exact eigenvalue spectrum for bound states in three dimensions.

Remark: as in exercise 3 we work with reduced mass and relative coordinates.

The reduced mass $\mu = \frac{m_p m_n}{m_p + m_n}$. The two atoms necessarily do not have the same mass. So, I will work with μ.

The differential equation describing the above problem is given by Eq. (5.64):

$$0 = \left[\frac{d^2}{dr^2} - \frac{2\mu D a^2}{\hbar^2 r^2} - \frac{l(l+1)}{r^2} + \frac{4\mu D a}{\hbar^2 r} + \frac{2\mu}{\hbar^2}E\right]\chi(r). \tag{C5.3.1.7}$$

We rewrite this differential equation in dimensionless form. The unit length we take the Bohr radius a_0 and the unit of energy E_{Ry}, with mass the reduced mass.

We are looking for bound states so $E < 0$, set $E = -E_n$, and $\varepsilon = \frac{E_n}{E_{Ry}}$.

(C5.3.1.7) becomes: $$0 = \left[\frac{d^2}{d\rho^2} - \frac{Da^2}{E_{Ry}a_0^2\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2Da}{E_{Ry}a_0\rho} - \varepsilon\right]\chi(r). \tag{C5.3.1.8}$$

We can deal with this equation as shown in the section on Coulomb Potentials.
On the other hand we choose for a sort of short cut. Equate $-\frac{Da^2}{E_{Ry}a_0^2\rho^2}-\frac{l(l+1)}{\rho^2}=-\frac{A(A+1)}{\rho^2}$.
A mathematical short cut.

$$A=-\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{Da^2}{E_{Ry}a_0^2}+l(l+1)}. \qquad \text{(C5.3.1.9)}$$

Substitute this into (C5.3.1.8) and obtain :

$$0=\left[\frac{d^2}{d\rho^2}-\frac{A(A+1)}{\rho^2}+\frac{2Da}{E_{Ry}a_0\rho}-\varepsilon\right]\chi(r). \qquad \text{(C5.3.1.10)}$$

This equation resembles the equation for bound states of the hydrogen atom, Eq. (5.99).
From section 5.4.3 we derive the eigenfunction:

$$\chi(r)=C_1\rho^{A(A+1)}e^{-\rho\sqrt{\varepsilon}}F(A+1-\frac{Da}{E_{Ry}a_0\sqrt{\varepsilon}}\ ,2A+2\ ,2\rho\sqrt{\varepsilon}\ ). \qquad \text{(C5.3.1.11)}$$

Using the analysis for the eigenvalue equation on page 122. We find:
$n=n_r+1=\frac{Da}{E_{Ry}a_0\sqrt{\varepsilon}}-A$. This expression represents an integer.

So $\varepsilon=\frac{(\frac{Da}{E_{Ry}a_0})^2}{(n-A)^2}\rightarrow E_n=\frac{(\frac{Da}{E_{Ry}a_0})^2}{(n-A)^2}E_{Ry}$,
with A given by (C5.3.1.9).

Now we leave this exercise. In section 5.5.1 we use the potential of this exercise(Kratzer's molecular potential) to apply WKBJ in order to find the eigenvalues.

5.3.2 Central Potential in 2D

Mahan mentioned the derivation to be quite similar in two dimensions.
In this section Mahan used the dimensionless coupling constant g. This constant has been introduced as the potential strength Eq. (2.196). At the bottom of page 41 the potential strength is called the coupling constant.

Homework 8.

Exercise 8.
Find the exact eigenvalue for any value of angular momentum for a particle in a circular square well in two dimensions:

$$V(\rho)=\begin{cases} 0 & 0<\rho<0 \\ \infty & a<\rho \end{cases}.$$

Look up a table of zeros of Bessel functions(Abramowitz and Stegun). Use these data to list, in order, the six lowest eigenvalues considering all possible values of angular momentum.
Remark: what does all possible values mean? On page 109 Mahan writes: "The most frequently used spherical harmonics are those with small values of (l,m)."
The differential equation for the radial part $R(\rho)$ of the wave function is given by Eq. (5.44):
$\left(\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\frac{n^2}{\rho^2}+k^2\right)R(\rho)=0$, where $k^2=\frac{2mE}{\hbar^2}$. The general wave equation for this particular potential well is: $\psi(k,\rho,\theta)=\sum_n D_n(k)J_n(k\rho)e^{in\theta}$, n is the angular momentum. The eigenvalue equation is found from the zeros of $J_n(k\rho)$ at $k\rho=ka$ since $\psi(k,\rho,\theta)$ is forced to zero at $\rho=a$.

zeros	$n = 0$	$n = 1$	$n = 2$
$s =$	$ka =$	$ka =$	$ka =$
1	2.405	3.382	5.136
2	5.520	7.016	8.417
3	8.654	10.173	11.620
4	11.792	13.324	14.796
5	14.931	16.471	17.960
6	18.071	19.616	21,117

From Abramowitz and Stegun we can find the zeros up to $n = 8$, page 409.

5.4 Coulomb Potentials.

Mahan mentioned the Coulomb potentials to occur often in physics. For example, $V(r) = -Ze^2/4\pi\varepsilon_0 r$. Continuum solutions are the only allowed solutions for repulsive potentials. Attractive potentials have bound and continuum states.

5.4.1 Bound States.

The differential equation describing the bound states are satisfied by *confluent hypergeometric functions*. Mahan writes; “All eigenfunctions of the Coulomb potential involve these functions”. Mahan explained these functions in section 5.4.2

5.4.2 Confluent Hypergeometric Functions.

The hypergeometric functions are presented. Asymptotic representations are given.

Homework 9, 12.

Exercise 9.

Use the series definition of the confluent hypergeometric function $F(a, b, z)$ to show it obeys its differential equation. The series definition:

$$F(a, b, z) = \sum_{n=0} \frac{z^n}{n!}\frac{(a)_n}{(b)_n}, \qquad \text{(C5.31)}$$

$$(a)_n = a(a + 1) \ldots (a + n - 1), \qquad \text{(C5.32)}$$

and the differential equation

$$0 = z\frac{d^2F}{dz^2} + (b - z)\frac{dF}{dz} - aF. \qquad \text{(C5.33)}$$

Well, plug F, its first and second derivative into (C5.33) equate equal powers of z and conclude the factors of equal powers are zero. Of course you do that for just a few powers of z. However, it is not particularly satisfying to do this n times.

So what to do? Plug the expression for F into (C5.33). You will find two powers of $z : z^{n-1}$ and z^n. In the series of z^n there is z^{n-1}. So what to do next is collect all the powers of z^{n-1}.

With (C.5.31) the following expression is obtained:

$$z^{n-1}\left[\frac{n(n-1)}{n!}\frac{(a)_n}{(b)_n} - \frac{(n-1)}{n!}\frac{(a)_{n-1}}{(b)_{n-1}} + \frac{bn}{n!}\frac{(a)_n}{(b)_n} - \frac{a}{(n-1)!}\frac{(a)_{n-1}}{(b)_{n-1}}\right]. \qquad \text{(C5.34)}$$

We know $(a)_n = a(a + 1) \ldots (a + n - 1)$.

So $(a)_{n-1} = a(a + 1) \ldots (a + n - 2)$, (C5.35)

and

$$(a)_n = (a)_{n-1}(a + n - 1). \qquad \text{(C5.36)}$$

Similar for $(b)_n$

We have all the ingredients to show the series to obey the differential equation.

Substitute (C5.36) into (C5.34) and we find:
$\frac{z^n}{(n-1)!}\frac{(a)_{n-1}}{(b)_{n-1}}\frac{1}{b+n-1}[(n-1)(a+n-1)-(n-1)(b+n-1)+b(a+n-1)-a(b+n-1)]$. (C5.37)
The expression between brackets adds up to 0.

Exercise 12.
Find the exact eigenvalue and eigenfunction of the s-wave ground state of an electron in the potential $V(r) = -\frac{e^2}{a+r}$, where a is a positive constant and e is the charge of the electron.
Taking into account the potential, this exercise is on a coulomb potential in 3-D.
The eigen function is: $\psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$.
With $\chi(r) = rR(r)$ and $l = 0$, the differential equation for the radial component of the wave function is: $0 = (\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}\frac{e^2}{a+r} + \frac{2m}{\hbar^2}E)\chi$. For bound states $E < 0$ and with $a_0 = \frac{\hbar^2}{me^2}$, , $E_{Ry} = \frac{\hbar^2}{2ma_0{}^2}$ and $\varepsilon = -\frac{E}{E_{Ry}}$ this differential equation becomes : $\left(\frac{d^2}{d\rho^2} + \frac{2}{\rho+\frac{a}{a_0}} - \varepsilon\right)\chi(\rho) = 0.$
Substitute in this equation γ for $\rho + a/a_0$. This leads to the following differential equation: $\left(\frac{d^2}{d\gamma^2} + \frac{2}{\gamma\gamma} - \varepsilon\right)\chi(\gamma) = 0$, similar to Eq. (5.99) with $l = 0$. Then the analysis of the confluent hypergeometric functions can be applied.
And $\chi(\gamma) = C\gamma e^{-\gamma\sqrt{\varepsilon}}F(1-\frac{1}{\sqrt{\varepsilon}}, 2\ , 2\gamma\sqrt{\varepsilon})$. With Laguerre polynomials: $F = \frac{n_{r!}}{(2)_{n_r}}L^1_{n_r}(\frac{2\gamma}{n})$.
As a reminder: $L_m^\alpha(x) = \sum_{i=0}^m \binom{m+\alpha}{m-i}\frac{(-x)^i}{i!}$. Taken all the ingredients together we obtain:
$\chi(\gamma) = C\gamma e^{-\gamma\sqrt{\varepsilon}}\frac{n_{r!}}{(2)_{n_r}}\sum_{i=0}^{n_r}\binom{n_r+1}{n_r-i}\frac{(-\frac{2\gamma}{n})^i}{i!}$, with $\gamma = \frac{1}{a_0}(a+r)$.
Some additional relations are: $-n_r = 1 - \frac{1}{\sqrt{\varepsilon}} = 1 - n$ and $(2)_{n_r} = (n_r+1)!$.
The eigenvalues for the s-wave ground state are $E_n = -\frac{E_{Ry}}{n^2}$.
The hydrogen atom is highly degenerative (Fitzpatrick). Many different states with possess the same energy. E_n is only dependent on n and not on l and m.

For the eigenfunction we have $\psi_n(\vec{r}) = C\frac{1}{a_0}(a/r+1)\frac{1}{n_r+1}\sum_{i=0}^{n_r}\binom{n_r+1}{n_r-i}\frac{\left(-\frac{2(a+r)}{a_0 n}\right)^i}{i!}P_0(\theta)$, where $P_0(\theta)$, is the associated Legendre polynomial and $P_0(\theta)$=1 (Chisholm and Morris).

5.4.3. Hydrogen Eigenfunctions

In this section the eigenfunctions and eigenvalues are derived as an example of the Coulomb Potentials and the confluent Hypergeometric Functions.
The eigenvalue Eq. (5.121) shows $n_r + l + 1$ to be an integer. Consequently $\frac{Z}{\sqrt{\varepsilon}}$ has to be an integer, n, say.
The hydrogen atom is highly degenerative as illustrated by Eq. (5.123). E_n is only dependent on n, with n the principal quantum number(Fitzpatrick).
On page 123: $\frac{n_{r!}}{(2l+2)_{n_r}}$ is absorbed in the prefactor N, Eqs. (5.125) and (5.127).
In Eq. (5.125) we find the expression: $\frac{n_r!}{(2l+2)_{n_r}}$, where n_r is the radial quantum number. Since n_r can become 0, we have to consider $(2l+2)_0$ I could not find this case. However, I

assume $(2l+2)_0 = 1$. In the examples given in the text you can conclude this assumption to be true.
In Eq. (5.128) a do not understand the factor ρ^2 in the integrand. It looks like the normalization of $\chi(\rho)$. I understand $R(\rho)$ to be the real-world radial wave function. This is not really a problem, the factor ρ^2 is related with the coordinate transformation as presented at the top of page 109. Eq. (5.128) can be written as $1 = \int_0^\infty \chi(\rho)d\rho$. χ has no direct physical interpretation. However, $|\chi|^2$ has. $|\chi|^2 = r^2|R|^2$ is the probability density for finding the electron(particle) at r anywhere in the spherical shell of radius r and thickness dr (Steane, A.). So a shell with volume $4\pi r^2 dr$.
Basically in deriving some normalized functions for R_{nl}, Mahan suggests the radial part of the wave function can be normalized separately from the angular part. I understood normalization to be about the wave function $\psi_{nl}(r,\theta,\phi)$.
Consequently, $\int_0^\infty \int_0^\pi \int_0^{2\pi} \psi^* \psi r^2 \sin\theta \, dr d\theta d\phi = 1$.
Then an additional problem arises. Which spherical function should we use? Is it $Y_l^m = C_{lm}P_l^{|m|}(\theta)e^{im\phi}$, Eqs. (4.115) and (4.116) or $|l,m\rangle = D_{lm}P_l^{|m|}(\theta)e^{im\phi}$, Eqs. (4.117) and (4.118)? For the ground state wave function the difference is just a factor $1/\sqrt{4\pi}$.
For example let us normalize the ground state wave function with $|l,m\rangle = |0{,}0\rangle$. In that case $D_{lm} = 1$ and the normalization expression reads:$\int_0^\infty |R_{1,0}|^2 \, 4\pi r^2 dr$. Then with the normalization factor $N_{1,0}$ the latter expression becomes, using Eq. (5.127) and $\rho = r/a_0$: ${N_{1,0}}^2 4\pi \int_0^\infty dr e^{-r/a_0} r^2 = 1$ and we obtain $N_{1,0} = \frac{1}{\sqrt{\pi a_0^3}}$. See eq. (5.140). On the other hand, with Y_0^0 , $N_{1,0} = \frac{2}{\sqrt{a_0^3}}$. I cannot explain this away. Can we explain this difference due to plane waves, section 5.1, and other waves, section 5.4? We will encounter this problem for sure in exercise 13 below. On the other hand I do not know when to use Y_l^m or $|l,m\rangle$. I suppose it to be written somewhere in the text. Then to me it is hidden in plain sight.
What will give us an idea is to analyse the examples given by Mahan. Let us analyse the matrix element example on top of page 124: $\langle 2p_z|z|1s\rangle, n=2, l=1, m=0$,
and $z == r\cos\theta$, for the ket $n=1, l=0, m=0$. I will use the spherical harmonics.
So for $n=1, l=0, m=0$ we have $R_{1,0} = 2e^{-\rho}$, with and $Y_0^0 = \sqrt{\frac{1}{4\pi}}$. So expect $\psi_{1,0} = \frac{1}{\sqrt{\pi}}e^{-\rho}$. Comparing this with Eq. (5.140) a factor $\frac{1}{\sqrt{a_0^3}}$ is "missing". The question is: is $\psi_{1,0}$ properly normalized? To find out we calculate $\int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_{1,0}^* \psi_{1,0} r^2 \sin\theta \, dr d\theta d\phi$ and we find this integral to be a_0^3, a sort of Rydberg volume. We need an additional normalization factor $\frac{1}{\sqrt{a_0^3}}$. This results into $\psi_{1,0} = \frac{1}{\sqrt{\pi a_0^3}}e^{-\rho}$, Eq. (5.140). When we analyse the bra $\langle 2p_z|$ in a similar way, the result is the need to normalize $\psi_{2,1}$. Doing this, again we find the additional normalization factor $\frac{1}{\sqrt{a_0^3}}$. The expression for $\psi_{2,1} = \frac{r\cos\theta}{\sqrt{32\pi a_0^5}}e^{-r/2a_0}$, Eq. (5.141). The conclusion is : even $R_{n,l}$ and Y_l^m to be separately normalised, we need to normalize the wave function $\psi_{n,l}$. With this analysis I will use Y_l^m in the exercises.

In addition I don't know under what condition I am allowed to use a separate normalization, radial normalization and angular normalization, or not. I assume an additional normalization of the resulting wave function.
On page 124 Mahan derived the two eigenfunctions ϕ for particular values of n, l and m. To prevent confusion about the notation for the eigenfunctions I prefer ψ instead of ϕ. See Eq. (5.56).
So $\psi_{1s} = \cdots$ Eq. (5.141), and $\psi_{2ps} = \cdots$ Eq. (5.141).

Homework 10, 11, 13.

Exercise 10.
Use confluent hypergeometric functions to find the exact solution to the Hamiltonian of the hydrogen atom in one dimension. *Hint:* $\phi(x = 0) = 0$. Remark: I prefer to use ψ for the wave function.
The differential equation for the 0ne-dimensional hydrogen atom($Z = 1$) is:
$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{e^2}{x} + E\right)\psi(x) = 0$.
With $a_0 = \frac{\hbar^2}{me^2}$, $E_{Ry} = \frac{\hbar^2}{2ma_0{}^2}$, $\varepsilon = -\frac{E}{E_{Ry}}$ and $\rho = \frac{x}{a_0}$ this differential equation becomes:
$\left(\frac{d^2}{d\rho^2} + \frac{2}{\rho} - \varepsilon\right)\psi(\rho) = 0$. (C5.38)
Eq. (C5.38) is equal to Eq. (5.99) with $l = 0$.
In our case of the hydrogen atom the parameter $a = -n_r$. See Mahan page 122.
As mentioned by Mahan, the confluent hypergeometric function for $a = -n_r$ is identical to an associated Laguerre polynomial. With $l = 0$, the Laguerre polynomial is:
$L^1_{n_r}(x) = \sum_{i=0}^{n_r} \binom{n_r + 1}{n_r - i} \frac{(-x)^i}{i!}$, (C5.39)
(Warnaar).
So with Eq. (5.125) $F\left(-n_r, 2, \frac{2\rho}{n}\right) = \frac{n_{r!}}{(2)_{n_r}} L^1_{n_r}\left(\frac{2\rho}{n}\right)$. (C5.40)
The solution to the Hamiltonian of the hydrogen atom in one dimension with Eq. (5.119) and (C5.40) is : $\psi(\rho) = C_1 \rho e^{-\rho/n} L^1_{n_r}\left(\frac{2\rho}{n}\right)$. (C5.41)
The factor $\frac{n_{r!}}{(2)_{n_r}}$ is absorbed into C_1.
In the 3-D case $\rho e^{-\rho/n}$ is $e^{-\rho/n}$.
Now as an example we look for the ground state wave function $n = 1 (n_r = 0)$ and find the value for C_1 by normalization. With $n = 1$, $L^1_{n_r}\left(\frac{2\rho}{n}\right) = 1$.
Then $1 = \int_{-\infty}^{\infty} C_1^2 \rho^2 e^{-2\rho}\, d\rho$. Due to symmetry this becomes: $1 = 2\int_0^{\infty} C_1^2 \rho^2 e^{-2\rho}\, d\rho$.
And $C_1 = \sqrt{2}$. The ground state wave function in one dimension is:
$\psi_1(x) = \frac{\sqrt{2}}{a_0} x e^{-x/a_0}$.
The eigenvalue, $\varepsilon = 1$, is: $E = -E_{Ry}$.
In using WolframAlpha with $\varepsilon = 1$: you will find at once:

$\psi_1(x) = C_1 x e^{-x}$.

Exercise 11.
Solve the Hamiltonian for the bound states of the hydrogen atom in two dimensions. Find

the eigenvalues. Hint: Use polar coordinates(ρ, θ), and the solution for $R(\rho)$ involves confluent hypergeometric functions.

This exercise is about a central potential in 2-D, about a Coulomb potential and the Hydrogen atom.

In section 5.3.2 the differential equation for the radial wave function is given:

$$\left\{\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} - \frac{n^2}{\rho^2} - \frac{2m}{\hbar^2}[V(\rho) - E]\right\} R(\rho) = 0 \,. \qquad \text{Eq. (5.87)}$$

The wave function has the form $\psi_n = R(\rho)e^{in\theta}$(Eq.(5.43), where $n \in \mathbb{Z}$.

Caveat: Now ρ is the non-dimensionless radial coordinate.

With $\chi_n(\rho) = \sqrt{\rho}R(\rho)$ we obtain Eq. (5.94):

$$\left\{\frac{d^2}{d\rho^2} - \frac{n^2 - 1/4}{\rho^2} - \frac{2m}{\hbar^2}[V(\rho) - E]\right\} \chi_n(\rho) = 0 \,. \qquad \text{Eq. (5.94)}$$

We rewrite Eq. (5.94) as in section 5.4.1 on Bound states, using

$a_0 = \frac{\hbar^2}{me^2}$, $E_{Ry} = \frac{\hbar^2}{2ma_0{}^2}$, $\varepsilon = -\frac{E}{E_{Ry}}$, $V(\rho) = -\frac{Ze^2}{\rho}$, $Z = 1$ and $\rho = \frac{x}{a_0}$

and we obtain $\left\{\frac{d^2}{dx^2} - \frac{n^2 - \frac{1}{4}}{x^2} + \frac{2}{x} - \varepsilon\right\} \chi_n(x) = 0 \,.$ (C5.41)

To find $\chi_n(x)$ we make use of (C5.41) resembling Eq. (5.99) except for the factor $n^2 - 1/4$. With help of the substitution $t = n - 1/2$ we finally find for the differential equation (C5.41): $\left\{\frac{d^2}{dx^2} - \frac{t(t+1)}{x^2} + \frac{2}{x} - \varepsilon\right\} \chi_n(x) = 0.$ (C5.42)

This is equivalent to Eq. (5.99) equating $Z = 1$.

Similar to the analysis of the sections 5.4.2 and 5.4.3, the solution to the differential equation can be expressed in an associated Laguerre polynomial.

So the confluent hypergeometric function $F(a, b, z) = \frac{(-a)!}{b_{(-a)}} L_{-a}^{(b-1)}(z)$. (C5.43)

In (C5.4.3) $-q_r = a = t + 1 - \frac{1}{\sqrt{\varepsilon}}$, $b = 2t + 2$, $z = 2\rho\sqrt{\varepsilon}/a_0$ and $q = \frac{1}{\sqrt{\varepsilon}} = q_r + t + 1$.

The Laguerre polynomial: $L_{q_r}^{2t+1}(z) = \sum_{i=0}^{q_r} \binom{q_r + 2t + 1}{q_r - i} \frac{(-z)^i}{i!}$. (C5.44)

The radial eigenfunction in two dimensions becomes, with Eq. (5.119), (C5.43) and (C.5.44):

$$R(\rho) = \frac{\chi_n(\rho)}{\sqrt{\rho}} = C(\rho/a_0)^{t+1/2} e^{-\rho\sqrt{\varepsilon}} \frac{q_r!}{(2t+2)_{q_r}} L_{q_r}^{2t+1}\left(\frac{2\rho}{q}\right).$$

$$\psi_{n,q_r} = R_{q_r}(\rho)e^{in\theta} = C(\rho/a_0)^n e^{-\rho\sqrt{\varepsilon}/a_0} \frac{q_r!}{(2n+1)_{q_r}} \sum_{i=0}^{q_r} \binom{q_r + 2n}{q_r - i} \frac{(-\rho\sqrt{\varepsilon}/a_0)^i}{i!}, \qquad \text{(C5.45)}$$

with $\rho = \frac{x}{a_0}$.

The prefactor C is found by normalization and depends on the quantum numbers. The eigenvalues $E_{n,q_r} = -\frac{E_{Ry}}{(q_r + n + 1/2)^2}$.

So for the ground state we have $E_0 = -4E_{Ry}$. The same result is found with the WKBJ approximation, section 5.5.3 Two Dimensions, page 130.

Exercise 13.

Using hydrogen bound-state wave functions, evaluate the following integrals, which are given using Dirac notation:

a. $\langle 1s|2p_z\rangle$

b. $\langle 1s|p_z|2p_z\rangle$

c. $\langle 1s|z|3p_z\rangle$
ad a. $\langle 1s|2p_z\rangle$: we have to use the relevant wave function to find out about this inner product. The nomenclature $1 \rightarrow n = 1, s \rightarrow l = 0$ and $2 \rightarrow n = 2, p \rightarrow l = 1, z \rightarrow m = 0$. So we have to evaluate the integral: $\int_0^\pi \int_0^\infty R_{1,0}R_{2,1}Y_0^0\, Y_1^0 r^2 \sin\theta\, dr d\theta \int_0^{2\pi} d\phi$. (C5.4.3.1)
At the beginning of this section I discussed the choice of type of wave function. In this exercise I use the expressions of Mahan.

$Y_0^0 = \frac{1}{\sqrt{4\pi}}$, $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, Eqs. (5.8) and (5.9) and $R_{1,0}, R_{2,1}$ are given by Eqs. (5.129) and (5.132) respectively.
In Eq. (5.4.3.1) will use $r = \rho a_0$, since R is given in terms of ρ.
So $R_{1,0} = 2e^{-\rho}$ and $R_{2,1} = \frac{\rho}{\sqrt{4!}}e^{-\frac{\rho}{2}}$.
with the above expressions (C5.4.3.1) becomes:
$\frac{a_0^3}{2\sqrt{2}}\int_0^\pi \int_0^\infty \rho^3 e^{-\frac{\rho 3}{2}} \cos\theta \sin\theta\, d\rho d\theta$. (C5.4.3.2)
The factor in front of the integral is not correct. The wave functions $\psi_{1,0}$ and $\psi_{2,1}$have to be normalized. See the discussion at the beginning of this section. At least factors $\frac{1}{\sqrt{\pi a_0^3}}$ and $\frac{1}{\sqrt{32\pi a_0^5}}$ are missing.
This does not matter.
Evaluate the integral and you see immediately the result to be 0:
$\int_0^\pi \sin\theta \cos\theta\, d\theta = 0$.
Did we expect this? Well, the inner product is about two orthogonal wave functions.
ad b. $\langle 1s|p_z|2p_z\rangle$: a matrix element. Is it? The ket and the bra are two different wave functions. However, does p_z represent an element of an operator? Well, I think it represents the angular wave function. So, evaluating the integral $\langle 1s|p_z|2p_z\rangle$ most certainly leads to a 0. This is necessary, however not sufficient. Let us find out.
We will write down the complete integral:
$\psi_{1,0} = \frac{1}{\sqrt{\pi a_0^3}}e^{-\rho}$, (Eq. (.140)), $\psi_{2,1} = \frac{r\cos\theta}{\sqrt{32\pi a_0^5}}$, (Eq. (.141)) and $p_z = Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, (Eq. (5.9)).
Then we have $\langle 1s|p_z|2p_z\rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} \sqrt{\frac{3}{4\pi}}\cos\theta \frac{r\cos\theta}{\sqrt{32\pi a_0^5}} e^{-\frac{r}{2a_0}} r^2 \sin\theta dr d\theta d\phi$.
Well, this integral $\neq 0$, since $\int_0^\pi (\cos\theta)^2 \sin\theta\, d\theta = \frac{2}{3}$, $\int_0^{2\pi} d\phi = 2\pi$ and the “radial” integral is 32/27. The “matrix element” is: $\frac{16}{27\sqrt{6\pi}}$. So, not zero as I expected it to be.
The question is : what does $|p_z|$ represent? It is not a state vector $p_z = Y_1^0$ which I used to do the calculations. Does it represent the angular momentum operator? Then with the eigenvalue of $M^2 \rightarrow l(l+1)\hbar^2$ and $l = 1, m = 0$ we have $p_z = \hbar\sqrt{l(l+1)}$. Using this we find $\int_0^\pi \cos\theta \sin\theta\, d\theta = 0$ and $\langle 1s|p_z|2p_z\rangle$ vanishes. As it should. Since with $p_z = \hbar\sqrt{l(l+1)}$, $\langle 1s|p_z|2p_z\rangle$ becomes: $\hbar\sqrt{l(l+1)}\langle 1s|2p_z\rangle$. With the inner product of ad a) $\hbar\sqrt{l(l+1)}\langle 1s|2p_z\rangle = 0$. Quite a conundrum.

ad c. $\langle 1s|z|3p_z\rangle$: this clearly represent the matrix element of the position operator.

$\psi_{1s} = \psi_{1,0} = \frac{1}{\sqrt{\pi a_0^3}} e^{-\rho}$, Eq. (5.140).

$|3p_z\rangle = \psi_{3,1}$, with $m = 0$.

$\psi_{3,1}$ contains $R_{3,1}$(Eq. (5.133) and $Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$. In addition the product of these two functions has to be normalized. This normalization is the usual procedure. The constant is found to be $\frac{12}{\sqrt{a_0^3}}$. This results into the following expression for the wave equation:

$$\psi_{3,1} = \frac{3\sqrt{2}}{\sqrt{a_0^3}} \left(\frac{2}{3}\right)^3 \rho(1 - \frac{\rho}{6}) e^{-\rho} \cos\theta. \qquad \text{(C5.4.3.3)}$$

Now we need to evaluate, using $z = r\cos\theta$ and $r = \rho a_0$, using Eq. (5.140) and (C5.4.3.3): $\int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_{1,0}\ r\cos\theta\, \psi_{3,1} r^2 \sin\theta\, dr d\theta\, d\phi$. Using the ingredients given above, this integral yields: $\langle 1s|z|3p_z\rangle = 3.58\ a_0$. An expression with the dimension of length as it should be.

5.4.4 Continuum States.

For continuum states $E > 0$. This affects the radial eigenfunction.

5.5 WKBJ

5.5.1 Three Dimensions

As Mahan mentioned there are two major changes with respect to the one dimensional case. In three dimensions the radial function $\chi(r)$ is found. Furthermore the potential function contains the centrifugal barrier, Eq. (5.63): $V_l(r0 = V(r) + \frac{\hbar^2}{2mr^2} l(l+1)$. The second term on the right hand side represents the centrifugal barrier.

In this section Mahan introduced a slightly modified centrifugal barrier, Eq. (5.152), $\left(l + \frac{1}{2}\right)$ replaces $(l+1)$.

$\alpha(r)$ in Eq. (5.153) is similar to the “α” in the one dimensional case, Eq. (3.17), except for the centrifugal barrier.

Keep in mind $\sqrt{r} \exp\left[\left(l + \frac{1}{2}\right) \ln r\right] = r^{l+1}$, Eqs. (5.156) and (5.157).

When $E > V_l$ Eq. (158) should be $p(r) = \sqrt{2m[E - V(r)] - \frac{\hbar^2}{2mr^2}(l + \frac{1}{2})^2}$. A printing error.

Homework 18, 19.

Exercise 18.

Use WKBJ to find the eigenvalues of the potential of exercise 17.

The potential, Kratzer’s molecular potential, reads: . $V(r) = D[(\left(\frac{a}{r}\right)^2 - 2\left(\frac{a}{r}\right)]$.

Kratzer’s molecular potential has a minimum at $V(r = a) = -D$ and simulates the binding of two atoms.

Remark: as in exercise 3 we work with reduced mass and relative coordinates.

The reduced mass $\mu = \frac{m_p m_n}{m_p + m_n}$. The two atoms necessarily do not have the same mass. So I

work with μ.
With WKBJ in 3-D we use $\chi(r)$ for the radial function.
The potential we use for this three dimensional problem is:

$$V_l = D[\left(\left(\frac{a}{r}\right)^2 - 2\left(\frac{a}{r}\right)\right] + \frac{\hbar^2}{2mr^2}(l+\tfrac{1}{2})^2. \qquad \text{(C5.5.1.1)}$$

The differential equation describing the above problem is:

$$0 = \left[\frac{d^2}{dr^2} - \frac{2\mu Da^2}{\hbar^2 r^2} - \frac{(l+\frac{1}{2})^2}{r^2} + \frac{4\mu Da}{\hbar^2 r} + \frac{2\mu}{\hbar^2}E\right]\chi(r). \qquad \text{(C5.5.1.2)}$$

Rewrite this differential equation in dimensionless form. The unit length we take the Bohr radius a_0 and the unit of energy E_{Ry}, with mass the reduced mass.
We are looking for bound states so $E < 0$, set $E = -E_n$, and $\varepsilon = \frac{E_n}{E_{Ry}}$.
The differential equation is:

$$0 = (\frac{d^2}{d\rho^2} - \frac{1}{4\rho^2} - \frac{Da^2}{E_{Ry}a_0^2\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2Da}{E_{Ry}a_0\rho} - \varepsilon)\chi(\rho).$$

With $E > V$ we have a right (b_R) and a left hand(b_L) turning point. The equation for momentum gives us

$$\sqrt{\varepsilon}\int_{b_L}^{b_R}\frac{d\rho}{\rho}[-\rho^2 + \frac{2Da\rho}{\varepsilon E_{Ry}a_0} - \frac{1}{\varepsilon}\left(l+\frac{1}{2}\right)^2 - \frac{Da^2}{\varepsilon E_{Ry}a_0^2}]^{1/2} = \pi(n_r+\tfrac{1}{2}). \qquad \text{(C5.5.1.2)}$$

Mahan: “The factor within the square root is a quadratic expression, which has two roots $b_{R,L}$. The turning points….”.
We rewrite (C5.5.1.4) in the following way: $\pi\left(n_r+\frac{1}{2}\right) = \sqrt{\varepsilon}\int_{b_L}^{b_R}\frac{d\rho}{\rho}\sqrt{(b_R-\rho)(\rho-b_L)}$,

where $b_{R,L} = \frac{Da}{\varepsilon E_{Ry}a_0} \pm \sqrt{(\frac{2Da}{\varepsilon E_{Ry}a_0})^2 - \frac{1}{\varepsilon}\left(l+\frac{1}{2}\right)^2 - \frac{Da^2}{\varepsilon E_{Ry}a_0^2}}$. (C5.5.1.3)

The integral $\int_{b_L}^{b_R}\frac{d\rho}{\rho}\sqrt{(b_R-\rho)(\rho-b_L)}$ is given in Chapter 3-Mahan, a standard integral:
$\int_{b_R}^{b_R}\frac{d\rho}{\rho}\sqrt{(b_R-\rho)(\rho-b_L)} = \frac{\pi}{2}(b_L+b_R-2\sqrt{b_Rb_L})$.
Then $\pi\left(n_r+\frac{1}{2}\right) = \sqrt{\varepsilon}\frac{\pi}{2}(b_L+b_R-2\sqrt{b_Rb_L})$. Substitute (C5.5.1.3) into this equation:

$$\pi\left(n_r+\frac{1}{2}\right) = \sqrt{\varepsilon}\frac{\pi}{2}\left[\frac{2Da}{\varepsilon E_{Ry}a_0} - 2\sqrt{\frac{1}{\varepsilon}\left(l+\frac{1}{2}\right)^2 + \frac{Da^2}{\varepsilon E_{Ry}a_0^2}}\right]. \qquad \text{(C5.5.1.4)}$$

$$n_r+\frac{1}{2} = \frac{Da}{\sqrt{\varepsilon}E_{Ry}a_0} - \sqrt{\left(l+\frac{1}{2}\right)^2 + \frac{Da^2}{E_{Ry}a_0^2}}. \qquad \text{(C5.5.1.5)}$$

Set $A = -\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{Da^2}{E_{Ry}a_0^2} + l(l+1)}$, plug this into (C5.5.1.5) with $l(l+1)+\frac{1}{4} = \left(l+\frac{1}{2}\right)^2$, we have $n_r+\frac{1}{2} = \frac{Da}{\sqrt{\varepsilon}E_{Ry}a_0} - \frac{1}{2} - A$. So for the eigenvalues we finally obtain:
$E_n = \frac{(\frac{Da}{E_{Ry}a_0})^2}{(n-A)^2}E_{Ry}$, with $n_r + 1 = n$. The same result we found in exercise 17 for the eigenvalues.

Exercise 19.

Use the three dimensional form of WKBJ to obtain the eigenvalues of the three dimensional harmonic oscillator. What is the lowest eigenvalue. (See exercise 14: Solve the exact eigenvalues and eigen states of the three-dimensional harmonic oscillator using spherical coordinates and central potential $V(r) = \frac{Kr^2}{2}$.

The result: the exact eigen values are $E_{n_rl} = \hbar\omega(2n_r + l + \frac{3}{2})$.)

With the potential $V(r) = \frac{Kr^2}{2}$ we have $V_l = \frac{Kr^2}{2} + \frac{\hbar^2}{2mr^2}(l + \frac{1}{2})^2$. Eq. (5.152)

Now $E > \frac{Kr^2}{2} + \frac{\hbar^2}{2mr^2}(l + \frac{1}{2})^2 > 0$.

The equation for momentum is: $p(r) = \sqrt{2m\left[E - \frac{Kr^2}{2}\right] - \frac{\hbar^2}{2mr^2}(l + \frac{1}{2})^2}$. Eq. (5.158)

Caveat: Eq. (5.158) reads $p(r) = \sqrt{2m[V(r) - E] - \frac{\hbar^2}{2mr^2}(l + \frac{1}{2})^2}$. I think this to be wrong.

The equation for momentum should be: $p(r) = \sqrt{2m[-V(r) + E] - \frac{\hbar^2}{2mr^2}(l + \frac{1}{2})^2}$.

Furthermore $\int_{-b_R}^{b_R} dr\, p(r) = \pi\hbar(n_r + \frac{1}{2})$. Eq. (5.161)

This equation gives us the eigenvalues.

We substitute $K = m\omega^2$, $z = (m\omega)^2 r^2$ and $dr = \frac{dz}{2m\omega\sqrt{z}}$ into Eq. (5.161), we obtain using the expression Eq. (5.158),

$\int_{b_L}^{b_R} \frac{dz}{2m\omega z}\sqrt{2mE_{n_rl}z - z^2 - (m\omega\hbar)^2(l + \frac{1}{2})^2} = \pi\hbar(n_r + \frac{1}{2})$. (C5.5.1.6)

The turning points $b_{R,L}$ are found following a similar procedure given by Mahan page 128.

They are : $b_{R,L} = mE_n \pm \sqrt{(mE_{n_rl})^2 - (m\omega\hbar\left(l + \frac{1}{2}\right))^2}$. (C5.5.1.7)

Integrating (C5.5.1.6), standard integral, $\frac{\pi}{4m\omega}[b_R + b_L - 2\sqrt{b_L b_R}] = \pi\hbar(n_r + \frac{1}{2})$. Substitute the value for the turning points, (C5.5.1.7), into this expression and we have for the eigenvalues: $E_{n_rl} = \hbar\omega(2n_r + l + \frac{3}{2})$. (C5.5.1.8)

The lowest eigenvalue, $n_r = 0$ and $l = 0$, is $\hbar\omega\frac{3}{2}$. Three times the value of the 1-D eigenvalue. As it should be.

5.5.2 3D Hydrogen Atom.

The WKBJ method produces the exact eigenvalue for this classical problem. However, keep in mind to use the adjusted centrifugal barrier.

Homework 16.

Exercise 16.

The WKBJ method gave poor results for the hydrogen atom in 1-D. In 3-D we had to add a potential term $\delta V = \frac{\hbar^2}{8mr^2}$ to get a good answer. Try the same thing in 1-D. Add the potential δV(with x instead of r) to the potential of the 1-D hydrogen atom. Show that (a) this gives the proper form of the WKBJ wave function at small x, and (b) it gives the correct eigenvalue using WKBJ.

Remark: The hydrogen atom: “In 3-D we had to add a potential term $\delta V = \frac{\hbar^2}{8mr^2}$ to get a good answer (Mahan)”. Did we? Can I find this approach in Chapter 5? In section 5.5.2 3D-Hydrogen Atom no $\delta V = \frac{\hbar^2}{8mr^2}$ has been added. Aha, it is subtle. The potential term $\delta V = \frac{\hbar^2}{8mr^2}$ has been added in the 3-D WKBJ method. Look at Eq. (5.152): $V_l = V(r) + \frac{\hbar^2}{2mr^2}(l+\frac{1}{2})^2 = V(r) + \frac{\hbar^2}{2mr^2}l(l+1) + \frac{\hbar^2}{8mr^2}$. The last term in this expression represents the repulsive part of the potential.

At the end of the 3-D Hydrogen atom section, after deriving E_n, Mahan writes: “The WKBJ method with this additional term produces the exact eigenvalue for this classic problem”.

First I start with the 1-D case without the additional repulsive potential included and look for the exact solution.

1-D Hydrogen Atom with confluent hypergeometric functions. The Hamiltonian:

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{e^2}{x} + E\right)\psi(x) = 0\,. \tag{C5.5.2.1}$$

Substitute $a_0 = \frac{\hbar^2}{me^2}$, $E_{Ry} = \frac{\hbar^2}{2ma_0^2} = \frac{e^2}{2a_0}$, $\varepsilon = -\frac{E}{E_{Ry}}$, and $x = \rho a_0$ into (C5.5.2.1) and obtain:

$$0 = (\frac{d^2}{d\rho^2} + \frac{2}{\rho} - \varepsilon)\psi(\rho). \tag{C5.5.2.2}$$

Well, (C5.5.2.2) reminds you of the equation for the radial function χ of section 5.4.1 Bound States and Coulomb potentials (Mahan) with $l = 0$. Then we can use the analysis of this section and section 5.4.3 and find $\psi = C_1\rho e^{-\rho\sqrt{\varepsilon}}F(1-\frac{1}{\sqrt{\varepsilon}}; 2; 2\rho\sqrt{\varepsilon})$. (C5.5.2.3)

What is illustrative: plug (C5.5.2.2) into the WolframAlpha App and you will find the same answer. If you do not trust the result start the analysis of page 120(Mahan). For small values of ρ the differential equation is $0 = (\frac{d^2}{d\rho^2} + \frac{2}{\rho})\psi(\rho)$ and $\psi(\rho) \propto \rho$. For large values of ρ the equation is $0 = (\frac{d^2}{d\rho^2} - \varepsilon)\psi(\rho)$, with the same result as Mahan presented. The trial function becomes, analogous to Eq. (5.102): $\rho e^{-\rho\sqrt{\varepsilon}}G(\rho)$, and so on.

With (C5.5.2.3) we can find the eigenvalues with the analysis of page 122 by Mahan. $1-\frac{1}{\sqrt{\varepsilon}}$, has to be negative or zero : $1-\frac{1}{\sqrt{\varepsilon}} = -n_r$. This eigenvalue equation results into: $E_{n_r} = \frac{E_{Ry}}{(n_r+1)^2}$, and the ground state $n_r = 0$, with $E_0 = E_{Ry}$.

Secondly.

Mahan mentioned the WKBJ method to give poor results. Let us find out.

So back to the equation (C.5.5.2.1) $\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{e^2}{x} + E\right)\psi(x) = 0\,.$

With $p(x) = \sqrt{2m(E - V(x)}$ and the analysis of chapter 3 section 3.1(Mahan) we have: the eigenfunction for $x < b$, left from the turning point, with $E(= -E_n) < 0$,

$$\psi(x) = \frac{D}{\sqrt{p(x)}}\sin[\frac{1}{\hbar}\int_x^b dx' p(x') + \beta]. \tag{Eq.(3.20)}$$

Is there a need to evaluate the integral in Eq. (3.20)? Well, for $x \to 0$, $\frac{1}{\sqrt{p(x)}} \to 0$ due to the Coulomb potential.

What does $p(x)$ look like? $p(x) = \sqrt{2m}\sqrt{(Ex + e^2)/x}$. With E_n we write this expression as follows: $p(x) = \sqrt{2mE_n}\sqrt{(\frac{e^2}{E_n} - x)/x}$. The integral in Eq.(3.20) results with this expression for $p(x)$ into: $\sqrt{2mE_n}\{\left[x'\left(\frac{e^2}{E_n}-x'\right)\right]-\frac{e^2}{2E_n}\left[\sin^{-1}\left(\frac{-2x'+\frac{e^2}{E_n}}{\frac{e^2}{E_n}}\right)\right]\}|_x^b$. (C5.2.2.4)

Where use has been made of standard integrals (Abramowitz and Stegun).

We know b to be $b=\frac{e^2}{E_n}$, the turning point. Now let $x\to 0$ and substitute the values for b and x into the expression (C5.2.2.4). We obtain for $\sin[\frac{1}{\hbar}\int_x^b dx'p(x')+\beta]$ with $\beta=\frac{\pi}{4}$

$\sin[\pi\,(\frac{1}{4}-\frac{e^2}{\hbar}\sqrt{\frac{2m}{E_n}})]$. We know already for $x\to 0$, $\frac{1}{\sqrt{p(x)}}\to 0$. However we could also force $\sin[\pi\,(\frac{1}{4}-\frac{e^2}{\hbar}\sqrt{\frac{2m}{E_n}})]$ to be zero. Then $\frac{1}{4}-\frac{e^2}{\hbar}\sqrt{\frac{2m}{E_n}}=n$.

Remark: $\beta=\frac{\pi}{4}$ is discussed in chapter 3(Mahan).

With $E_{Ry}=\frac{me^4}{2\hbar^2}$, $\frac{1}{4}-\frac{e^2}{\hbar}\sqrt{\frac{2m}{E_n}}=n$ becomes :$\frac{E_n}{E_{Ry}}=\frac{2}{(n-\frac{1}{4})^2}$.

A poor result indeed.

Thirdly we will work with an repulsive term added to the Coulomb potential. We have to show this gives the proper form of the WKBJ wave function at small x and the correct eigenvalue.

Questions: what does Mahan mean by the proper result for small x? The WKBJ approximation, Eq. (3.20) and (C5.2.2.4), for small x gives $\psi(x)\propto(x)^{5/4}$, without the repulsive term.

I will compare the result of WKBJ, the repulsive term included, with the exact result of the expression (C5.2.2.3). Assuming this comparison to be correct.

So, back to the exercise with the additional potential term.

Schrödinger's equation is: $\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{e^2}{x}-\frac{\hbar^2}{8mx^2}+E\right)\psi(x)=0$. (C5.5.2.5)

Now we have a potential similar to the one shown in Figure 5.2(Mahan). With $E<0$ there are two turning points, a left one and a right one.

Substitute $a_0=\frac{\hbar^2}{me^2}$, $E_{Ry}=\frac{\hbar^2}{2ma_0^2}=\frac{e^2}{2a_0}$, $\varepsilon=-\frac{E}{E_{Ry}}$, and $x=\rho a_0$ into (C5.5.2.5) and obtain:

$0=(\frac{d^2}{d\rho^2}+\frac{2}{\rho}-\frac{1}{4\rho^2}-\varepsilon)\psi(\rho)$. (C5.5.2.6)

An interlude: The exact solution of this differential equation is

$\psi(\rho)=C_1\left(2\rho\sqrt{\varepsilon}\right)^{\frac{1+\sqrt{2}}{2}}e^{-\rho\sqrt{\varepsilon}}F(\frac{1+\sqrt{2}}{2}-\frac{1}{\sqrt{\varepsilon}};1+\sqrt{2};2\rho\sqrt{2})$. (C5.5.2.7)

This equation has been found with the WolframAlpha App. There the solution is given in term of Whittaker's function M. Applying the analysis of sections 5.4.1-5.4.3 the same result can be found.

Another approach: Let us forget about the physics for a while and compare (C5.5.2.6) with Eq. (5.99) to find $l(l+1)=\frac{1}{4}$ and $l=\frac{\sqrt{2}-1}{2}$, just a number. The solution of Eq. (5.99) for Coulomb Potentials is represented by Eq. (5..118) with a hyper geometric function.

Substitute $l=\frac{\sqrt{2}-1}{2}$ into that equation and you will find again (C5.5.2.7). Completely similar to the analysis of page 122 for the eigenvalues we have the eigenvalue equation :

$-n_r=\frac{1}{2}\left(1+\sqrt{2}\right)-\frac{1}{\sqrt{\varepsilon}}$. Remark: the right hand side of this expression has to be an integer.

The eigenvalues resulting from this equation are: $E_{n_r} = \frac{E_{Ry}}{(n_r+\frac{1}{2}(1+\sqrt{2}))^2}$. Not nearly close to the exact solution with just the Coulomb Potential: $E_{n_r} = \frac{E_{Ry}}{(n_r+1)^2}$. So far for the exact solution with the repulsive potential included. End of the interlude.

The last part of this exercise is to apply WKBJ for the solution of the differential equation with the repulsive potential included. We will use the analysis of Chapter 3, section 3.1 on Bound States of WKBJ, page 70 Mahan.

The solution for the wave equation, from Mahan, $\psi_L = \psi_R = \frac{C_R}{\sqrt{p(x)}}\sin(\phi_R)$, Eq. (3.48)

with $\phi_R = \frac{\pi}{4} + \frac{1}{\hbar}\int_{b_L}^{b_R} dx' p(x')$. Eq. (3.44)

And $p(x) = \sqrt{2m(E - V(x))}$. (C5.5.2.8)

For bound states $E < 0$. For the eigenvalues we denote $E = -E_n$. Plug the Coulomb potential and the repulsive potential into (C5.5.2.8) and obtain:

$p(x) = \sqrt{2m(\frac{e^2}{x} - \frac{\hbar^2}{8mx^2} - E_n)}$. (C5.5.2.9)

Between the turning points b_L and b_R $E > V$ and the character of ψ_R is sinusoidal as represented by Eq. (3.48). The eigenvalues are found> The eigenvalues are found from the total phase $\phi_T = \frac{\pi}{2} + \frac{1}{\hbar}\int_{b_L}^{b_R} dx' p(x') = m\pi$. Eq. (3.45)

Following the analysis of page 70 we have for the eigenvalue equation:

$\int_{b_L}^{b_R} dx' p(x') = \pi\hbar(n + \frac{1}{2})$.

The next step is to plug into this equation the expression (C5.5.2.9) and we obtain the following eigenvalue equation:

$\int_{b_L}^{b_R} dx \sqrt{2m(\frac{e^2}{x} - \frac{\hbar^2}{8mx^2} - E_n)} = \pi\hbar(n + \frac{1}{2})$. (C5.5.2.10)

The turning points b_R and b_L are found by $\left(\frac{e^2}{x} - \frac{\hbar^2}{8mx^2} - E_n\right) = 0$,

$b_{R,L} = \frac{e^2}{2E_n}[1 \pm \left(1 - \frac{E_n}{16E_{Ry}}\right)^{\frac{1}{2}}]$. (C5.5.2.11)

Use have been made of $E_{Ry} = \frac{me^4}{2\hbar^2}$.

The integral in (C5.5.2.10) can be found from tables on standard integrals(Abramowitz and Stegun). This is represented by the integral in Eqs. (3.62)-(3.64).

So $\sqrt{2mE_n}\int_{b_L}^{b_R} dx \sqrt{(\frac{e^2 x}{E_n} - \frac{\hbar^2}{8mE_n} - x^2)} = \pi\hbar(n + \frac{1}{2})$.

With the turning points this expression becomes:

$\sqrt{2mE_n}\int_{b_L}^{b_R} dx \frac{1}{x}\sqrt{(b_R - x)(x - b_L)} = \pi\hbar(n + \frac{1}{2})$. (C5.5.2.12)

$\int_{b_L}^{b_R} dx \frac{1}{x}\sqrt{(b_R - x)(x - b_L)} = (\sqrt{b_R} - \sqrt{b_L})^2 = \frac{\pi}{2}[b_R + b_L - 2\sqrt{b_R b_L}]$.

We need to evaluate the expression (See Eq. (3.63)) with help of (C5.5.2.11) :

$(\sqrt{b_R} - \sqrt{b_L})^2 = [b_R + b_L - 2\sqrt{b_R b_L}] = \frac{e^2}{E_n}[1 - \frac{1}{2}\sqrt{\frac{E_n}{E_{Ry}}}]$.

Then with (C5.5.2.12) we finally obtain the eigenvalue equation:

$\sqrt{\frac{E_{Ry}}{E_n}} = n + 1$, or $\frac{E_n}{E_{Ry}} = (\frac{1}{n+1})^2$. The same result as with the hypergeometric functions, the exact solution for the Hamiltonian without the additional term. There we used n_r instead of n.

Do these results also produce the proper form of WKBJ for small x? I assume Mahan asks to compare the WKBJ with the exact solution at small x. Well from the exact solution we find for small x using (C5.5.2.3):

$\psi \propto x$.

For the WKBJ we just apply the analysis of page 65(Mahan) with small x. Now $E < V$ and $E > 0$. Following Mahan we find:

$$\psi(x) = \frac{A_1}{\sqrt{\alpha(x)}}\exp\{-\frac{1}{\hbar}\int_x^b dx'\alpha(x')\}, \qquad \text{(C5.5.2.13)}$$

With $\alpha(x) = \sqrt{2m[V(x) - E]}$, $V(x) = \frac{\hbar^2}{8mx^2} - \frac{e^2}{x}$, and b the turning point.

For small x only the term $\frac{\hbar^2}{8mx^2}$ contributes in (C5.5.2.13). Then $\alpha(x) = \frac{\hbar}{2x}$ and $-\frac{1}{\hbar}\int_x^b dx'\alpha(x')\} = \frac{1}{2}\ln\frac{x}{b}$. Plug these results into (C5.5.2.13) and we obtain:

$\psi(x) \propto \sqrt{x}\exp(\ln(\frac{x}{b})^{1/2}$. So $\psi(x) \propto x$. The same results as we obtained for the exact solution without the repulsive term.

It is time to leave this exercise.

5.5.3 Two Dimension.

In two dimension there is no need for an adjusted centrifugal barrier.

The WKBJ approximation gives the exact result. See exercise 11 in the section on Hydrogen eigenfunctions, section 5.4.3.

At the end of this section, page 130, Mahan writes: “The lowest eigenvalue is $E_0 = -4E_R$.” This should be: $E_0 = -4E_{Ry}$, a printing error.

5.6 Hydrogen -like Atoms.

In this section, as the title indicates, we are harvesting the knowledge gained on the hydrogen atom.

5.6.1 Quantum Defect.

The question to be answered is: to what extend can we apply the Rydberg series for hydrogen-like atoms? The approximation is expressed in a so-called effective quantum number $n^* = n - C_l(n)$, Eq. (5.194). Here $C_l(n)$ is defined as the quantum defect.

Mahan uses the expression Rydberg series. I suppose this to be the eigenvalue series expressed in the Rydberg energy. This relates with the effective quantum number:

$E_n = -\frac{Z_i^2 E_{Ry}}{(n^*)^2}$, where Z_i is the charge of the ion. In table 5.1(Mahan) you can find the effective quantum numbers and eigenvalues for various states of Lithium and Potassium.

Homework 20.

Exercise 20.

Construct a table of effective quantum numbers n^* for the ns series of KI and CaII. CaII means one electron outside of the closed shell in calcium. The data can be found on the physics library shelf in C.E. Moore, *Atomic Energy Levels* (QC453.M58, Vol. 1).

Remark: ns series? KI? Potassium with one electron outside of the closed shell in potassium?
Since I have no access to the library reference shelf I searched on the internet and found the *Handbook of Atomic Spectra Data*, by Sansonetti, J.E. and Martin W.C. , American Institute of Physics [DOI : 10.1063/1.1800011].
Now I just give in order to produce the table the procedure to follow.
For the spectra, i.e. the wave length $\lambda(\text{Å})$ given by the spectra data we find $E_n = \frac{2\pi\hbar c}{\lambda}$. With $E_n = -\frac{Z_i^2 E_{Ry}}{(n^*)^2}$, and a given value of Z_i calculate n^*. Finally, $C_l(n) = n - n^*$, where n is given in the data.

5.6.2 WKBJ Derivation.

WKBJ is used to derive the origin of the quantum defect $C_l(n)$ (Mahan).
The analysis similar to the hydrogen atom can be used and the exact eigenvalue is found with the effective quantum number.

5.6.3 Expectation values.

Mahan showed the results obtained for the hydrogen eigen values, now with the effective quantum number. A good approximation is found for $\langle r^2 \rangle$.

5.7 Variational Theory.

Mahan: “The variational theory for two and three dimensions is similar to the theory for one dimension, chapter 3”.
Choosing a suitable trial function is key.

5.7.1 Hydrogen Atom: $n = 1$.

In this section Mahan analysed the ground state of the hydrogen atom with the trial function: $\phi_2(r) = A\exp[-\frac{1}{2}\alpha^2 r^2]$, Eq. (5.214). Mahan concluded this trial function to be a poor approximation for the ground state eigenfunction.

Homework 21, 24.

Exercise 21.
Use the variational method to determine the eigenvalue of the ground state of the hydrogen atom in two dimensions. Choose your own trial function.
For the ground state we have no angular momentum and the trial function depends just on r.
The exact solution is found with the exercise 11 in section 5.4.3 Hydrogen Eigenfunctions.
For the two dimensional problem I choose the eigenfunction to be: $\psi = Ae^{-\alpha r}$. We have to evaluate three integrals: normalization, kinetic energy and potential energy. Having done this the energy functional is optimized. With the trial function $\psi = Ae^{-\alpha r}$:
Normalization: $I = \int_0^\infty 2\pi r dr |\psi|^2 = 2\pi A^2 \int_0^\infty r dr\, e^{-2\alpha r} = 2\pi (\frac{A}{\alpha})^2$,

Kinetic energy: $KE = \frac{\hbar^2}{2m}\int_0^\infty 2\pi r dr\, |\vec{\nabla}\psi|^2 = \frac{\hbar^2}{2m} 2\pi (A\alpha)^2 \int_0^\infty r dr\, e^{-2\alpha r} = \frac{\pi\hbar^2}{8m} A^2$,
and

Potential energy: $PE = \int_0^\infty 2\pi r dr V(r)|\psi|^2 = -2\pi(eA)^2 \int_0^\infty dr\, e^{-2\alpha r} = -\frac{\pi(eA)^2}{\alpha}$.
Now we plug these three expressions into the energy functional:
$E(\psi) = \frac{KE+PE}{I} = \frac{\hbar^2}{2m}\alpha^2 - 2\alpha e^2$. (C5.7.1.1)
We find the minimum value of E by: $0 = \frac{dE}{d\alpha} = \frac{\hbar^2}{m}\alpha - 2e^2$. The resulting value for α from this equation is: $\alpha = \frac{4me^2}{2\hbar^2} = \frac{2}{a_0}$. (C5.7.1.2)
We substitute (C5.7.1.2) and $E_{Ry} = \frac{e^2}{2a_0} = \frac{\hbar^2}{2ma_0^2}$ into (C5.7.1.1) and obtain:
$E = -4E_{Ry}$.
The same result as obtained with the WKBJ in two dimensions and exercise 11, the exact solution.

Exercise 24.
Use the variational method to solve for the ground-state energy of a hydrogen atom in a constant electric field F along the $\hat{z}$-direction. The Hamiltonian is
$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} - eFr\cos\theta$.
Use a trial wave function of the form
$\psi(r,\theta) = Ae^{-r/a}[1 - \lambda\frac{r}{a}\cos\theta]$. Eq. (5.345)
where a is the Bohr radius and λ is the variational parameter.
a. Find the value of λ that minimizes the energy.
b. Express the energy as a function of F.
c. Expand (b) in power series in F about $F = 0$. If α is the polarizability, the correct answer has the form
$E(F) = -(?)E_{Ry} - \frac{\alpha}{2}F^2 + O(F^4)$.
What value for α is predicted by the variational procedure?
ad a. We start with the normalization integral:
$I = \int d^3 r|\psi(r,\theta)|^2$.
Plug $\psi(r,\theta)$ into I. We have:
$I = A^2\int_0^\infty\int_0^\pi\int_0^{2\pi} e^{-2r/a}\,(1 - \lambda\frac{r}{a}\cos\theta)^2 r^2\sin\theta drd\theta d\phi$. (C5.7.1.3)
This gives: $I = \pi A^2 a^3(1+\lambda^2)$. (C5.7.1.4)
The kinetic expectation value:
$KE = -\frac{\hbar^2}{2m}\int d^3 r\,\psi^*\nabla^2\psi = KE = \frac{\hbar^2}{2m}\int d^3 r[\left|\frac{\partial\psi}{\partial r}\right|^2 + \left|\frac{\partial\psi}{r\partial\theta}\right|^2]$.
Substitute the trial function Eq. (5.345) into KE and we find :
$KE = \frac{\hbar^2}{2ma^2}A^2\int_0^\infty\int_0^\pi\int_0^{2\pi} e^{-2r/a}[(1+\lambda\cos\theta - \lambda\frac{r}{a}\cos\theta)^2 + (\lambda\sin\theta)^2]r^2\sin\theta drd\theta d\phi$.
For KE we obtain:
$KE = \frac{\hbar^2}{2m}\pi A^2 a\left(1+\lambda^2\right)$. (C5.7.1.5)
The expectation value for potential energy:
$PE = -\int d^3 r\,\psi^*(\frac{e^2}{r} + eFr\cos\theta)\,\psi$.
Hence :
$PE = -A^2\int_0^\infty\int_0^\pi\int_0^{2\pi} e^{-2r/a}\,(1 - \lambda\frac{r}{a}\cos\theta)^2(\frac{e^2}{r} + eFr\cos\theta)\,r^2\sin\theta drd\theta d\phi$.
For PE we obtain:

$PE = -2\pi A^2[\frac{e^2a^2}{2}\left(1+\frac{\lambda^2}{2}\right) - \lambda eFa^4].$ (C5.7.1.6)

The energy functional is:

$\mathcal{E}(\lambda) = \frac{KE+PE}{I}$. Substitute (C5.7.1.4), (C5.7.1.5) and (C5.7.1.6) into the expression for the functional and $\mathcal{E}(\lambda) = -E_{Ry} + \frac{\frac{e^2}{2}\lambda^2+2\lambda eFa^2}{a(1+\lambda^2)}$, (C5.7.1.7)

where use have been made of: $E_{Ry} = \frac{\hbar^2}{2ma^2} = \frac{e^2}{2a}$.

After setting $\frac{d\mathcal{E}}{d\lambda} = 0$, we find $\lambda_{1,2} = \frac{e}{4Fa^2} \pm \frac{e}{4Fa^2}\sqrt{1+(\frac{4Fa^2}{e})^2}$. Small values of F indicates

$\lambda = \frac{e}{4Fa^2} - \frac{e}{4Fa^2}\sqrt{1+(\frac{4Fa^2}{e})^2}$. (C5.7.1.8)

With (C5.7.1.7) we have the energy as a function of F.

ad c. Now we expand $\mathcal{E}$ in power series of F for $F \to 0$.

We start with λ: $\lambda = -\frac{2Fa^2}{e}[1 - \frac{1}{4}\left(\frac{4Fa^2}{e}\right)^2 + O(F^4)]$. (C5.7.1.9)

Substitute this value of λ up to orderF^4 into (C5.7.1.7):

$\mathcal{E}(\lambda) = -E_{Ry} - 2a^3F^2 + O(F^4)$.

Now with α the polarizability and $\mathcal{E}(F) = -E_{Ry} - \frac{\alpha}{2}F^2 + O(F^4)$, we may conclude $\alpha = 4a^3$.

The exact value of $\alpha = \frac{9}{2}a^3$.

5.7.2 Hydrogen Atom: $l = 1$.

In this section Mahan applied the variational method with angular momentum, $l = 1$. The exact result is found. Mahan concluded the variational method to be suited. However, in a restricted way. For each case l must be different.

5.7.3 Helium Atom.

"The ground state can be accurately described by the variational method" (Mahan).

The nucleus of the system is regarded as fixed. No effects of reduced mass are included. The $(1s)$: $n = 1, l = 0$ state is considered. The electrons have antiparallel spin, Pauli's exclusion principle is applied and the electrons are in the singlet state:

$|0{,}0\rangle = \frac{1}{\sqrt{2}}[\alpha_1\beta_2 - \alpha_2\beta_1]$. Eq. (5.235)

See also section (4.4) The Addition of Agular momentum (Mahan).

Mahan first dealt with the solution without the electron-electron interaction. Then the ground state is the sum of the system with one electron-nucleus interaction and $Z = 2$. Hence the ground state $E_g = -8E_{Ry}$. Eq. (5.243)

On page 141 Mahan presents the experimental result to be: $E_g = -5.808E_{Ry}$. The electron-electron interaction is supposed to be essential. To find the energy functional an additional

integral has to be included representing electron-electron interaction.
The trial function used by Mahan reads: $\phi(r_1, r_2) = A\exp[-\frac{\alpha(r_1+r_2)}{a_0}]$. Here α is the parameter to minimize the energy functional, a_0 is the Bohr radius, $\phi(r_1, r_2)$ is the orbital(radial?) wave function and r_1, r_2 represent the positions of the two electrons. I assume $\hat{r}_1$ represents the unit vector the position of the electron.
Remark: In Eq. (5.244) Mahan presents the normalization integral. The subscript 1 and 2 for the radial coordinated has been deleted. So it is the product of two normalisation integrals.
Finally after minimizing the energy functional Mahan found $E_g = -5.695E_{Ry}$, a 2% deviation of the experimental value.
There are other approaches for this problem. For example by Fitzpatrick. This author started with a trial function equal to the ground state wave function of the hydrogen atom with $Z = 2$. The expectation value $\langle H \rangle$ is calculated and this results in the ground state eigenvalue of $E_g = -5.5E_{Ry}$. "The trial wave function treats the electrons as *non-interacting* particles. In reality, we would expect one electron to partially shield the nuclear charge from the other, and *vice versa."* (Fitzpatrick). Then Fitzpatrick introduced a new trial wave function with Z as parameter. And uses the variational method (Like Mahan used α.) This results into: $Z = \frac{27}{16}$, where Mahan found $\alpha_0 = \frac{27}{16}$.

Homework 22, 23, 25.

Exercise 22.
Use the variational theory to solve for the ground-state energy of two $1s$ electrons in a Coulomb potential of charge Z. The result for $Z = 2$ should reproduce the helium result in section 5.7.
a. $Z = 1$: Does H^- exist? What do you predict for its binding energy?
b. $Z = 3$: Compare with the Li^+ ion, whose experimental ionization energies are 75.3 and 121.8 eV for the two electrons.
For this exercise use has been made of the results of section 5.7.3 Helium atom. The Hamiltonian is almost complete similar to the one presented in Eq. (5.240). The only thing to do is to replace the factor 2 in the coulomb potential by Z. As a consequence replace the factor 8 in Eq. (5.251), the potential energy, by $4Z$. The energy functional becomes:
$E(\alpha) = (2\alpha^2 - 4Z\alpha + \frac{5}{4}\alpha)$. (C5.7.3.1)
Minimize this functional with respect to α: $\alpha = Z - \frac{5}{16}$. (C5.7.3.2)
ad a) $Z = 1$:
$\alpha = Z - \frac{5}{16} = \frac{11}{16}$. With this value for α, (C5.7.3.1) gives: $E(\alpha) = -2\left(\frac{11}{16}\right)^2 E_{Ry} = -.945E_{Ry} > -E_{Ry}$.
So there is a bound energy for the hydrogen anion and the anion can exist.
ad b) $Z = 3$:
Now $\alpha = Z - \frac{5}{16} = \frac{45}{16}$. With this value for α, (C5.7.3.1) gives: $E(\alpha) = 7.3359E_{Ry}$.
For the Li^+ ion we find 75.3 eV $< 7.3359E_{Ry} <$ 121.8 eV.

Exercise 23.

Use the variational method to find the ground-state energy of two particles in one dimension bound to a delta-function potential, and which interact with a delta-function potential:

$$H = -\frac{ħ^2}{2m}\left[\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right] - \lambda[\delta(x_1)+\delta(x_2)-\delta(x_1-x_2)]. \qquad \text{(C5.7.3.3)}$$

Dirac: "Thus $\delta(x)$ is not a quantity which can be generally used in mathematical analysis like an ordinary function, but its use must be confined to certain simple types of expressions for which it is obvious that no inconsistency can arise".

We use the trial function:

$$\psi(x_1,x_2) = Ae^{-\frac{\alpha(|x_1|+|x_2|)}{a_0}}, \qquad \text{(C5.7.3.4)}$$

where a_0 represents the Bohr radius and the trial function is cusp-shaped. This shape results from the Delta-Function Potential, see section 2.6(Mahan).

The normalization integral in the variational theory is:

$$I = \int dx_1 \int dx_2\, |\psi(x_1,x_2)|^2. \qquad \text{(C5.7.3.5)}$$

With (C5.7.3.4) I can be written as: $I = A^2 \int dx_1 \int dx_2 \left[e^{-\frac{2\alpha(|x_1|+|x_2|)}{a_0}}\right]$. This is a product of two integrals with a symmetric integrand, hence:

$$I = A^2 4\int_0^\infty dx_1 e^{-\frac{2\alpha x_1}{a_0}} \int_0^\infty dx_2 e^{-\frac{2\alpha x_2}{a_0}} = 4A^2\left[\int_0^\infty dx e^{-\frac{2\alpha x}{a_0}}\right]^2 = A^2\left(\frac{a_0}{\alpha}\right)^2. \qquad \text{C(5.7.3.6)}$$

The expectation value for the two particle system is:

For the two particle system we find:

$$KE = -\frac{ħ^2}{2m}\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \left[\psi_1^* \frac{d^2}{dx_1^2}\psi_1 + \psi_2^* \frac{d^2}{dx_2^2}\psi_2\right]. \qquad \text{(C5.7.3.7)}$$

So $KE = 2\frac{ħ^2}{2m}\left[2\int_0^\infty dx \left|\frac{d\psi}{dx}\right|^2\right]^2$. (C5.7.3.8)

With the trial function (C5.7.3.4) , (C5.7.3.8) becomes:

$$KE = 2\frac{ħ^2}{2m}\frac{\alpha^2}{a_0^2}\left[2\int_0^\infty dx|\psi|^2\right]^2. \qquad \text{(C5.7.3.9)}$$

$KE = \frac{ħ^2}{m}\frac{\alpha^2}{a_0^2}4A^2\left[\int_0^\infty dx\, e^{-\frac{2\alpha x}{a_0}}\right]^2$. With (C5.7.3.6) the expectation value of the kinetic energy is $KE = \frac{ħ^2}{m}\frac{\alpha^2}{a_0^2}I$. (C5.7.3.10)

Now the expectation value of the potential energy:

$$PE = -\int dx_1 \int dx_2\, |\psi(x_1,x_2)|^2\{\lambda[\delta(x_1)+\delta(x_2)-\delta(x_1-x_2)]\}. \qquad \text{(C5.7.3.11)}$$

With the trial function $\psi(x_1,x_2) = Ae^{-\frac{\alpha(|x_1|+|x_2|)}{a_0}}$, (C5.7.3.11) can be written as:

$$PE = -\lambda A^2\left\{\int_{-\infty}^{\infty} dx_1\delta(x_1)e^{-\frac{2\alpha|x_1|}{a_0}}\int_{-\infty}^{\infty} dx_2\, e^{-\frac{2\alpha|x_2|}{a_0}} + \right.$$

$$\left.\int_{-\infty}^{\infty} dx_2\delta(x_2)e^{-\frac{2\alpha|x_2|}{a_0}}\int_{-\infty}^{\infty} dx_1\, e^{-\frac{2\alpha|x_1|}{a_0}} - \int_{-\infty}^{\infty} dx_1\int_{-\infty}^{\infty} dx_2\left[e^{-\frac{2\alpha(|x_1|+|x_2|)}{a_0}}\right]\delta(x_1-x_2)\right\}.$$

The expression with $\delta(x_1-x_2)$ gives a contribution for $x_1 = x_2$. Hence:

$PE = -\lambda A^2\left[2\frac{a_0}{\alpha}-(\frac{a_0}{\alpha})^2\right]$. Using the normalization integral (C5.7.3.6)

$$PE = -\lambda\left(\frac{\alpha}{a_0}\right)^2 I\left[2\frac{a_0}{\alpha}-(\frac{a_0}{\alpha})^2\right]. \qquad \text{(C5.7.3.12)}$$

Finally we obtain for the energy functional:

$$E(\alpha) = \frac{KE+PE}{I} = 2\left(\frac{\alpha}{a_0}\right)^2 \frac{\hbar^2}{2m} - \lambda(2\frac{\alpha}{a_0} - 1)\ . \qquad \text{(C5.7.3.13)}$$

The variational parameter is α. Then with $\frac{dE(\alpha)}{d\alpha} = 0$ we will find the value for α giving the smallest value of $E(\alpha)$.

$$\alpha = \frac{m\lambda}{\hbar^2}. \qquad \text{(C5.7.3.14)}$$

For the eigenvalue, the ground-state energy, of the two particles with a delta-function potential:

$$E = -\lambda^2 \frac{m^2}{\hbar^2 a_0}\left(2 - \frac{1}{a_0}\right) + \lambda. \qquad \text{(C5.7.3.15)}$$

Let's look at the just obtained result and compare this result with the expression for the ground state of a single particle in a delta-function potential as given in chapter 2(Mahan). We set $a_0 = 1$ in (C5.7.3.15) and $\lambda = W$.

Then we have $E = -W^2 \frac{m^2}{\hbar^2} + W$. Hence $-W^2 \frac{m^2}{\hbar^2}$ is twice the ground state energy of the single particle(Eq. (2.235)) and $+W$ reduces the effect of the attractive part of the two particles. By the way: $\alpha = \frac{m\lambda}{\hbar^2} = \frac{mW}{\hbar^2}$, the result given in Eq. (2.333).

Exercise 25.

Consider the Hamiltonian of an electron of charge e bound in a three-dimensional harmonic oscillator potential, which is also subject to a static field $\vec{F}$. The potential energy is:

$$V(\vec{r}) = \frac{K}{2} r^2 - e\vec{F}.\vec{r}\ .$$

Find the exact eigenvalue spectrum. What is the polarizability α of a charged particle bound in a harmonic oscillator potential?

As we can see we are not dealing with a central potential. Hence we cannot apply the techniques of this chapter 5. How to proceed? Well, we are free to choose the direction of the electric field to be in the $\hat{z}$-direction. Then it appears feasible to use a Cartesian frame, since the Schrödinger's equation is separable.

We have:

$$\left[\frac{\hbar^2}{2m}\nabla^2 - \frac{K}{2}(x^2 + y^2 + z^2) + eFz + E\right]\psi(x,y,z) = 0, \qquad \text{(5.7.3.16)}$$

where we set $E = E_x + E_y + E_z$ and $\psi(x,y,z) = \psi_1(x)\psi_2(y)\psi_3(z)$.Plugging these expressions into (5.7.3.16) and separation gives three equations:

$$\left[\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{K}{2}x^2 + E_x\right]\psi_1(x) = 0, \qquad \text{(C5.7.3.17)}$$

$$\left[\frac{\hbar^2}{2m}\frac{d^2}{dy^2} - \frac{K}{2}y^2 + E_y\right]\psi_2(y) = 0, \text{ and} \qquad \text{(C5.7.3.18)}$$

$$\left[\frac{\hbar^2}{2m}\frac{d^2}{dz^2} - \frac{K}{2}z^2 + eFz + E_z\right]\psi_3(z) = 0.$$

The first two equations represent the 1-D harmonic oscillator.

The oscillator in the z-direction can be manipulated in such a way leading to an equation resembling the equation of the harmonic oscillator. Let's have a look.

The equation for $\psi_3(z)$ is written as: $\left[\frac{2}{K}\frac{\hbar^2}{2m}\frac{d^2}{dz^2} - z\left(z - \frac{eF}{K} - \frac{eF}{K}\right) + \frac{2}{K}E_z\right]\psi_3(z) = 0$

With the transformation $u = z - \frac{eF}{K}$, the latter differential equation becomes:

$\left[\frac{2}{K}\frac{\hbar^2}{2m}\frac{d^2}{du^2} - \left\{u^2 - \left(\frac{eF}{K}\right)^2\right\} + \frac{2}{K}E_z\right]\psi_3(u) = 0.$

Hence:

$\left[\frac{\hbar^2}{2m}\frac{d^2}{du^2} - \frac{K}{2}u^2 + (E_z + \frac{e^2F^2}{2K})\right]\psi_3(u) = 0.$ (C5.7.3.19)

Now most of the work has been done. We see that the static electric field changes the eigenvalue in the z-direction into $(E_z + \frac{e^2F^2}{2K})$. So with the result of exercise 14 where we calculated the of eigenvalues for a 3-D harmonic oscillator, without an electric field, we finally obtain:

$E = \hbar\omega\left(2n_r + l + \frac{3}{2}\right) + \frac{e^2}{2K}F^2,$

with $\omega = \sqrt{\frac{K}{m}}$.

If the polarizability α is defined similar to the polarizability of hydrogen atom, then $\frac{\alpha}{2} = -\frac{e^2}{2K}$.

Remark: In the above exercise we found the exact solution. Hence there is no need to find an approximation by means of the variational method.

Nevertheless let's give it a try, just out of curiosity.

As a trial function we choose $\psi(r,\theta) = Ae^{-\frac{\left(\frac{r}{r_0}\right)^2}{2}}(1 - \lambda\frac{r}{r_0}\cos\theta)$, (C5.7.3.20)

where we define $r_0 = \sqrt{\frac{\hbar}{m\omega}}$, and $\omega = \sqrt{\frac{K}{m}}$ (Mahan page 30). (C5.7.3.21)

Normalization:

$I = A^2\int_0^\infty\int_0^\pi\int_0^{2\pi} e^{-(\frac{r}{r_0})^2}\,(1 - \lambda\frac{r}{r_0}\cos\theta)^2\, r^2\sin\theta d\phi d\theta dr.$ (C5.7.3.22)

With $r = Rr_0$ and the trial function C(5.7.3.20), we find for I:

$I = A^2\pi^{\frac{3}{2}}r_0^3\left(1 + \frac{1}{2}\lambda^2\right).$ (C5.7.3.23)

The kinetic energy,

$KE = \frac{\hbar^2}{2m}\int_0^\infty\int_0^\pi\int_0^{2\pi}[\left|\frac{\partial\psi}{\partial r}\right|^2 + \left|\frac{\partial\psi}{r\partial\theta}\right|^2]r^2\sin\theta d\phi d\theta dr.$ (C5.7.3.24)

With the trial function C(5.7.3.20) and (C5.7.3.21) becomes:

$KE = A^2\pi^{\frac{3}{2}}r_0^3\omega\hbar\left(\frac{3}{4} + \frac{5}{8}\lambda^2\right).$ (C5.7.3.25)

The potential energy:

$PE = A^2\int_0^\infty\int_0^\pi\int_0^{2\pi} e^{-(\frac{r}{r_0})^2}\,(1 - \lambda\frac{r}{r_0}\cos\theta)^2\,(\frac{K}{2}r^2 - eFr\cos\theta)\,r^2\sin\theta d\phi d\theta dr.$

We finally obtain the expression for the energy functional:

$\mathcal{E} = \frac{KE+PE}{I} = \frac{\omega\hbar\left(\frac{3}{4}+\frac{5}{8}\lambda^2\right)+Kr_0^2\left(\frac{3}{4}+\frac{5}{8}\lambda^2\right)-\lambda eFr_0}{1+\frac{\lambda^2}{2}}.$ (C5.7.3.26)

(C5.7.3.21) gives $Kr_0^2 = \omega\hbar$. Substitute this into (C5.7.3.26):

$\mathcal{E} = \frac{3}{2}\omega\hbar + \frac{\frac{1}{2}\omega\hbar\lambda^2-\lambda eFr_0}{1+\frac{\lambda^2}{2}}.$ (C5.7.3.27)

Then $\frac{d\mathcal{E}}{d\lambda} = 0 = \lambda^2 + 2\frac{\omega\hbar}{eFr_0}\lambda - 2 = 0$, gives:

for λ to be finite : $\lambda = -\frac{\omega\hbar}{eFr_0} + \frac{\omega\hbar}{eFr_0}\sqrt{1 + 2(\frac{eFr_0}{\omega\hbar})^2}$. (C5.7.3.28)

For small F we find for λ from (C5.7.3.28):

$\lambda = \frac{eFr_0}{\omega\hbar}$. Substitute this value of λ into (C5.7.3.27) and we finally obtain:

$$\mathcal{E} = \frac{3}{2}\omega\hbar - \frac{e^2}{K}F^2, \tag{C5.7.3.29}$$

Where use has been made of (C5.7.3.21).

Now we find for the polarizability α: $\frac{\alpha}{2} = -\frac{e^2}{K}$.

Hence with the variational method we find a polarizability being a factor 2 too large.

5.8 Free Particles in a Magnetic Field.

In this section Mahan discussed a free particle in a static magnetic field.

5.8.1 Gauges.

Magnetic fields are introduced into Schrödinger's equation. Now we find a vector potential in the Hamiltonian. The Hamiltonian is derived and justified in Chapter 8. There it is shown the momentum to be equal to

$\boldsymbol{p} = m\boldsymbol{v} + \frac{q}{c}\boldsymbol{A}$.

The magnetic field $\boldsymbol{B}$ is given by $\boldsymbol{B} = \nabla \times \boldsymbol{A}$.

Mahan presented three vector potentials.

Mahan has chosen a particular gauge and presented the Hamiltonian for a particle of charge q and mass m in a constant magnetic field B:

$$H_a = \frac{1}{2m}[\left(p_x + \frac{qB}{c}y\right)^2 + p_y^2 + p_z^2]\ . \tag{5.275}$$

The subscript a denotes the choice of gauge.

5.8.2 Eigenfunctions and Eigenvalues

H_a does not depend on x and z. They can be considered as constants of motion(Boccio, 9.7.38) and can be replaced by their eigenvalues.

The eigenfunctions for x and z are plane wave functions. Then the Hamiltonian has been solved for the variable y. Mahan showed this to represent a harmonic oscillator and presented the eigenvalues end eigenfunctions. The quantum number $k_x$determines the centre of oscillations.

Mahan showed the results another example of another example of the vector potential. The Hamiltonian depends in that case explicitly on x.

Homework 26, 27, 28.

Exercise 26.

Find the eigenfunctions and eigenstates(? Eigenvalues?)of an electron confined to two dimensions that is subject to an electric field and magnetic field ($\vec{F} \perp \vec{B}$). The Hamiltonian is

$$H = \frac{1}{2m}\left[p_x^2 + \left(p_y - \frac{eBx}{c}\right)^2\right] - eFx.$$

We will apply the results of the 3-D case(section 5.8.2) to the 2-D case. Keep in mind we are dealing with another gauge: $\boldsymbol{A} = B(0, x, 0)$, Eq. (5.273). By applying Eq. (5.282) for the 2-D case, we find:

$$H_b\psi_b(x,y) = \frac{e^{ik_y y}}{\sqrt{L_y}}\left[\frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2(x - x_0)^2 - eFx\right]f(x), \tag{C5.8.2.1}$$

where $\omega_c = \frac{eB}{mc}$, $x_0 = \frac{\hbar c k_y}{eB}$ and $k_y = \sqrt{\frac{2mE_y}{\hbar^2}}$.

Now let us take care of the expression between brackets in (C5.8.2.1):

$$\frac{p_x^2}{2m} + \frac{1}{2} m\omega_c^2 (x - x_0)^2 - \frac{eFx}{2m} = \frac{p_x^2}{2m} + \frac{1}{2} m\omega_c^2 (x - x_0)^2 - eF(x - x_0) - eFx_0.$$

The right hand side can be written as:

$$\frac{p_x^2}{2m} + \frac{1}{2} m\omega_c^2 (x - x_0)\left[(x - x_0) - \frac{eF}{m(\omega_c)^2} - \frac{eF}{m(\omega_c)^2}\right] - eFx_0. \tag{C5.8.2.2}$$

Define $\xi = (x - x_0) - \frac{eF}{m(\omega_c)^2}$ and substitute ξ into (C5.8.2.2), the expression between brackets in (C5.8.2.1) becomes $\frac{p_\xi^2}{2m} + \frac{m\omega_c^2}{2}\xi^2 - \frac{1}{2} m\omega_c^2 \left(\frac{eF}{m(\omega_c)^2}\right)^2 - eFx_0$, (C5.8.2.3)

the first two terms represent the harmonic oscillator, the last two terms represent a shift in the eigenvalues E_n .

The eigenvalues are: $E_n = \hbar\omega_c(n + \frac{1}{2}) - \frac{1}{2} m\omega_c^2 \left(\frac{eF}{m(\omega_c)^2}\right)^2 - eFx_0.$ (C5.8.2.4)

With $\omega_c = \frac{eB}{mc}$ and $x_0 = \frac{\hbar c k_y}{eB}$, (C5.8.2.4) can be written as:

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right) - \frac{mF^2}{2B^2} - \hbar c k_y \frac{F}{B}. \tag{C5.8.2.5}$$

This result can be found with Boccio(9.7.38).The eigenfunction becomes:

$$\psi_b(x, y) = \frac{e^{ik_y y}}{\sqrt{L_y}} f(\xi),$$

with $\xi = x - x_0 - \frac{eF}{m(\omega_c)^2}$. $f(\xi)$ are the oscillator eigenfunctions and $x_0 + \frac{eF}{m(\omega_c)^2}$ determines the centre of oscillations.

Exercise 27.

Consider the Hamiltonian of an electron confined to move only in the (xy)-plane. There is a magnetic field in the z-direction and a quadratic potential in the (xy)-plane. Show that in the symmetric gauge the Hamiltonian can be written as

$$H = \frac{1}{2m}\left[\left(p_x + \frac{eB}{2c}y\right)^2 + \left(p_y - \frac{eB}{2c}x\right)^2\right] + \frac{K}{2}(x^2 + y^2).$$

Solve this Hamiltonian exactly using polar coordinates. The problem was originally solved by V. Fock.

The symmetric gauge, Eq. (5.274):

$$\boldsymbol{A} = \frac{B}{2}(-y, x, 0).$$

Mahan presented the Hamiltonian for a charged particle in Eq. (5.268):

$$H = \frac{1}{2m}\left[\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}(\boldsymbol{r})\right]^2 + V(\boldsymbol{r}),$$

where the Pauli interaction is left out of this expression.

For the symmetric gauge $\boldsymbol{A}(\boldsymbol{r}) = -\frac{1}{2}\boldsymbol{r} \times \boldsymbol{B}$, $\boldsymbol{B} = (0,0,B)$ and $\boldsymbol{r} = (x, y, z)$.

$A_x = -\frac{1}{2}(yB - z.0)$,

$A_y = -\frac{1}{2}(z.0 - xB)$, and

$A_z = -\frac{1}{2}(0 - 0)$.

Hence Eq. (5.268) becomes:

$$H = \frac{1}{2m}\left[\left(p_x + \frac{eB}{2c}y\right)^2 + \left(p_y - \frac{eB}{2c}x\right)^2\right] + \frac{K}{2}(x^2 + y^2). \tag{C5.8.2.6}$$

We rewrite (C5.8.2.6):

$$H = \frac{1}{2m}\left[p_x^2 + \frac{eB}{2c}yp_x + \left(\frac{eB}{2c}y\right)^2 + p_y^2 - \frac{eB}{2c}xp_y + \left(\frac{eB}{2c}x\right)^2\right] + \frac{K}{2}(x^2 + y^2), \tag{C5.8.2.7}$$

keep in mind $p_x \frac{eB}{2c} y = 0$, and $p_y \frac{eB}{2c} x = 0$.

So we obtain for the wave function $\psi(x,y)$:

$$\left\{-\frac{\hbar^2}{2m}\nabla^2+\frac{eB}{4mc}\left(yp_x-xp_y\right)+\left(\frac{K}{2}+\frac{1}{2m}\left(\frac{eB}{2c}\right)^2\right)(x^2+y^2)\right\}\psi(x,y)=E\psi(x,y). \qquad \text{(C5.8.2.8)}$$

When $M_z=xp_y-yp_x=0$, Eq. (4.1) Chapter 4 Mahan, the wave equation (C5.8.2.8) is:

$$\left\{-\frac{\hbar^2}{2m}\nabla^2+\left(\frac{K}{2}+\frac{1}{2m}\left(\frac{eB}{2c}\right)^2\right)(x^2+y^2)\right\}\psi(x,y)=E\psi(x,y). \qquad \text{(C5.8.2.9)}$$

We use a modified "spring" constant $\frac{K_B}{2}=\frac{K}{2}+\frac{1}{2m}\left(\frac{eB}{2c}\right)^2$.

Part of this exercise is to solve the Hamiltonian exactly using polar coordinates. Why polar coordinates? I will deal with this question later on.

Let us work on polar coordinates, using the results of section 5.2(Mahan),

$$\nabla^2\psi(r,\theta)=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}. \qquad \text{Eq.(5.42)}$$

In polar coordinates xp_y-yp_x becomes: $-i\hbar\frac{\partial}{\partial\theta}$. Now the resulting Schrödinger equation is separable.

The general solution for angular momentum n can be written as

$$\psi_n=R(r)e^{in\theta}. \qquad \text{Eq.(5.43)}$$

For central potentials we substitute $R(r)=\frac{1}{\sqrt{r}}\chi(r)$, (Mahan).

With Eq. (5.43) and $R(r)=\frac{1}{\sqrt{r}}\chi(r)$, (C5.8.2.8) becomes

$$\left\{\frac{d^2}{dr^2}-\frac{n^2-\frac{1}{4}}{r^2}-\frac{2m}{\hbar^2}\left[\frac{K_B}{2}r^2-E_r\right]\right\}\chi_n=0. \qquad \text{(C5.8.2.10}$$

This equation comes close to (C5.3.1.1) of exercise 14.

We rewrite (C5.8.2.10) with:

$$\omega_B=\sqrt{\frac{K_B}{m}},\ \frac{2m}{\hbar^2}\frac{K_B}{2}=\left(\frac{m\omega_B}{\hbar}\right)^2=\gamma_B^2,\text{ and }\varepsilon=\frac{2m}{\hbar^2}E_r$$

$$\left\{\frac{d^2}{dr^2}-\frac{n^2-\frac{1}{4}}{r^2}-\gamma_B^2r^2+\varepsilon\right\}\chi_n=0. \qquad \text{(C5.8.2.11)}$$

Now we follow the analysis of Exercise 14:

In (C5.3.1.2) we have the term $\frac{l(l+1)}{r^2}$ instead of $\frac{n^2-\frac{1}{4}}{r^2}$. Then, from an algebraic point of view, we can substitute $n=\pm\left(l+\frac{1}{2}\right)$ in (C5.8.2.11).

For the eigenfunction ψ_n we obtain:

$$\psi_n(r,\theta)=C_1r^ne^{-\frac{\gamma_Br^2}{2}}L_{n_r}^{2n}(\gamma_Br^2)e^{in\theta}, \qquad \text{(C5.8.2.12)}$$

where n_r is the radial quantum number , $R(r)=\frac{1}{\sqrt{r}}\chi(r)$ has been substituted and the prefactor C_1 is the normalization coefficient. $L_{n_r}^{2n}$, is an associated Laguerre polynomial and the positive value of n has been taken.

Now for the eigenvalues of the radial part of the wave equation. In the three dimensional case we have

$$E_{n_rl}=\hbar\omega\left(2n_r+l+\frac{3}{2}\right). \qquad \text{(C5.3.1.6)}$$

Hence for the 2-D case(it is not a real two dimensional case), with $n=\left(l+\frac{1}{2}\right)$, we have

$$E_{n_rn}=\hbar\omega_B(2n_r+n+1).$$

Finally, let's look at the angular part of the wave equation.

The result of the separation of Schrödinger equation gives for the angular part:

$$-n\frac{eB}{2c\hbar}=\frac{2m}{\hbar^2}E_\theta. \qquad \text{(C5.8.2.13)}$$

We define $\omega_c=\frac{eB}{2mc}$ and $E_\theta=-\frac{1}{2}\hbar\omega_cn$. (C5.8.2.14)

Hence , for the 2-D we find:

$E_{2-D} = \hbar\omega_B(2n_r + n + 1) - \frac{1}{2}\hbar\omega_c n.$ (C5.8.2.15)

Having a zero “spring” constant K, (C5.8.2.15) reduces into: $E_{2-D} = \hbar\omega_c\left(2n_r + \frac{1}{2}n + 1\right)$.

Remark: In a Cartesian frame Schrödinger equation is not separable. Since $M_z = xp_y - yp_x \neq 0$.

As mentioned before: we are not dealing with a 2-D case. See section 5.8.4 on the Quantum Hall Effect(Mahan). The particle is confined to a plane. A lattice.

Exercise 28.

Consider the Hamiltonian of an electron confined to move only in the (xy)-plane. There is a magnetic field in the z-direction. Consider the Hamiltonian in the symmetric gauge:

$H = \frac{1}{2m}\left[\left(p_x + \frac{eB}{2c}y\right)^2 + \left(p_y - \frac{eB}{2c}x\right)^2\right]$.

Show that the wave function $|n\rangle = A(x - iy)^n\exp[-\frac{x^2+y^2}{4l^2}]$ is an exact eigenstate of this Hamiltonian and of the z-component of angular momentum. What is the eigenvalue?

A lot of work has already been done in exercise 27.

We rewrite the Hamiltonian and the wave function $|n\rangle$ in polar coordinates(r, θ) and find:

$\frac{\hbar^2}{2m}[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} - \frac{r^2}{l^2} + i\frac{\omega_c}{\hbar}\frac{\partial}{\partial\theta}]$. (C5.8.2.16)

In this expression $\omega_c = \frac{eB}{2mc}$, and $l^2 = \frac{\hbar}{m\omega_c} = \frac{\hbar c}{eB}$.

Now we can use the results of exercise 27 and we have for the wave function resulting from the operation $H\psi = E\psi$:

$\psi_n(r,\theta) = C_1 r^n e^{-\frac{\gamma_c r^2}{2}} L_{n_r}^{2n}(\gamma_c r^2)e^{in\theta}$, (C5.8.2.17)

where $\gamma_c = \frac{m\omega_c}{2\hbar} = \frac{1}{2l^2}$. The “spring” constant $K = 0$.

We need to compare (C5.8.2.17) with $|n\rangle = A(x - iy)^n\exp[-\frac{x^2+y^2}{4l^2}]$.

We rewrite $|n\rangle$ in polar coordinates and obtain:

$|n\rangle = A(r)^n\exp[-\frac{r^2}{4l^2}]e^{-in\theta}$.

From comparing this expression for the wave function with (C.5.8.2.17) we set the associated Laguerre polynomial equal 1, substitute $\gamma_c = \frac{1}{2l^2}$ in (C5.8.2.17) and we find:

$\psi_n(r,\theta) = C_1 r^n e^{-\frac{r^2}{4l^2}}e^{in\theta}$.

We have a little more work to do. Substituting $-\theta$ for θ in the Hamiltonian (C.5.8.2.16), $i\frac{\omega_c}{\hbar}\frac{\partial}{\partial\theta}$ changes into $-i\frac{\omega_c}{\hbar}\frac{\partial}{\partial\theta}$, (C5.8.2.17) becomes $\psi_n(r,\theta) = C_1 r^n e^{-\frac{r^2}{4l^2}}e^{-in\theta}$. So what we basically did is separating the wave function $\psi_n(r,\theta)$ into a radial wave function as we did in exercise 27 and an angular wave function $e^{-in\theta}$.

Another approach is to choose polar coordinates:

$x = \cos\theta$ and $y = -\sin\theta$.The Hamiltonian is $\frac{\hbar^2}{2m}[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} - \frac{r^2}{l^2} - i\frac{\omega_c}{\hbar}\frac{\partial}{\partial\theta}]$.

The eigen value of this operator becomes, with E_θ (Exercise 27) changing sign : $E_\theta = +\frac{1}{2}\hbar\omega_c n$.

The eigenvalues of the Hamiltonian are: $\hbar\omega_c\left(2n_r + \frac{3}{2}n + 1\right)$.

Now the eigenvalues of the momentum operator M_z . We rewrite the operator in polar coordinates:

$M_z = xp_y - yp_x = i\hbar\frac{\partial}{\partial\theta}$, where we used $x = \cos\theta$ and $y = -\sin\theta$.

Use this operator for the eigen state $|n\rangle$ (in polar coordinates) and we find: $M_z\,|n\rangle = \hbar\mathrm{n}\,|n\rangle$.

Hence the state $|n\rangle$ is an eigenstate of the Hamiltonian with eigenvalues $\hbar\omega_c\left(2n_r + \frac{3}{2}n + 1\right)$ and an eigenstate of the angular momentum operator with eigenvalues $\hbar n$. In chapter 4 the angular momentum is dealt with. We could have applied the results for the momentum operator: Eq. (4.76), Mahan.

5.8.3 Density of States

The subject matter is about solid state physics. The Hamiltonian of a free particle in a magnetic field is applied to obtain the density of states. In the limiting case the density of state of a three-dimensional free particle system is obtained. With respect to the subject matter, I suppose the basis for the density of states is presented in an undergraduate course.

5.8.4 Quantum Hall Effect.

In this section an example of particles in a magnetic field is presented. It is about semiconductor superlattices.
On page 148 Mahan introduced "curvature" which is described as an effective mass m^*. This is given in Eq. (5.303). I do not know where this can be found in previous chapters.
We know for plane waves k is defined as $E = \frac{\hbar^2 k^2}{2m}$.
In addition the spin is included in the Hamiltonian for a particular gauge and the effect on the eigenvalues is given by the term $-m\Delta$. In do not know where to find this in the previous sections.
Reading this section I think there should be a reference to additional reading on the subject matter.

5.8.5 Flux Quantization

The final section of this chapter deals with the flux quantization in the centre of hollow cylinders and super conductivity.

Homework.

The exercises can be found in the relevant sections of this chapter.

6. Matrix Methods and Perturbation Theory.

6.1 H and H_o

Solving Hamiltonians perturbation theory is a very helpful tool.
I repeat a few characteristics given by Mahan:

- Find an Hamiltonian H_0 which can be solved exactly. This Hamiltonian should resemble the exact problem H as much as possible.
- Its eigenfunctions should be simple functions that are easy to generate and integrate.

Hence $H = H_0 + V$,
where V is considered to be the perturbation. Usually small compared to H_0.
The evaluation of matrix elements is an essential feature of this chapter.

6.2 Matrix Methods.

In this section Mahan presented the fundamental equation of the matrix method.
Mahan discussed the practicalities of the matrix method. The problem with this method is encountered in the infinite dimensions of the matrix. Hence the matrix need to be truncated.
In the next section Mahan presented the determinant of a 2×2 matrix.
In this general section on the matrix method I shall derive the 2×2 matrix. I will apply the Dirac notation.
First, Mahan presented in this section the general method.
For H_0 we have $H_0|\phi_n\rangle = E_n^{(0)}|\phi_n\rangle$ (C.6.2.1)
and for the Hamiltonian $H|\psi_n\rangle = E_n|\psi_n\rangle$. (C.6.2.2)
With $H = H_0 + V$, we have
$(H_0 + V)|\psi_n\rangle = E_n|\psi_n\rangle$. (C.6.2.3)
Now we expand $|\psi_n\rangle$ into $|\phi_n\rangle$:
$|\psi_n\rangle = \langle\phi_1|\psi_n\rangle|\phi_1\rangle + \langle\phi_2|\psi_n\rangle|\phi_2\rangle$, (C.6.2.4)
hence $(H_0 + V)|\psi_n\rangle = \langle\phi_1|\psi_n\rangle(H_0 + V)|\phi_1\rangle + \langle\phi_2|\psi_n\rangle(H_0 + V)|\phi_2\rangle$. (C.6.2.5)
Mahan considered ϕ_m eigen functions of H_0.
To illustrate the general approach I used $m = 1{,}2$.
As a reminder: Mahan expanded $|\psi_n\rangle = C_{n1}|\phi_1\rangle + C_{n2}|\phi_2\rangle$. (C.6.2.4a)
Multiply (C.6.2.4a) on the left and the right with $\langle\phi_1|$ and you find $C_{n1} = \langle\phi_1|\psi_n\rangle$.
Multiplying (C.6.2.4a) similarly with $\langle\phi_2|$, you will find $C_{n2} = \langle\phi_2|\psi_n\rangle$.
Multiply (C.6.2.5) with $\langle\phi_1|$ and we obtain:
$\langle\phi_1|\,(H_0 + V)|\psi_n\rangle = \langle\phi_1|\psi_n\rangle\langle\phi_1|\,(H_0 + V)|\phi_1\rangle + \langle\phi_2|\psi_n\rangle\langle\phi_1|\,(H_0 + V)|\phi_2\rangle$. (C.6.2.6)
Plug equation (C.6.2.1) into (C.6.2.6):
$\langle\phi_1|\,(H_0 + V)|\psi_n\rangle = \langle\phi_1|\psi_n\rangle(E_1^{(0)} + V_{11}) + \langle\phi_2|\psi_n\rangle V_{12}$, (C.6.2.7)
where V_{ij} is shorthand for the matrix element $\langle\phi_i|V|\phi_j\rangle$.
In addition $\langle\phi_i|\phi_j\rangle = \delta_{ij}$.
Multiply (C.6.2.3) on both sides with $\langle\phi_1|$:
$\langle\phi_1|\,(H_0 + V)|\psi_n\rangle = \langle\phi_1|\,E_n|\psi_n\rangle$. (C.6.2.7a)
Subtract the equations (C.6.2.7) and (C.6.2.7a) we obtain:
$\langle\phi_1|\psi_n\rangle\left(E_1^{(0)} - E_n + V_{11}\right) + \langle\phi_2|\psi_n\rangle V_{12} = 0$. (C.6.2.8)
Now we multiply (C.6.2.5) with $\langle\phi_2|$ and we find completely similar to (C.6.2.8):
$\langle\phi_2|\psi_n\rangle\left(E_2^{(0)} - E_n + V_{22}\right) + \langle\phi_1|\psi_n\rangle V_{21} = 0$. (C.6.2.9)
Keep in mind $\langle\phi_l|\psi_n\rangle$ equals C_{ln}, Eq. (6.6) Mahan.
(C.6.2.8) an (C.6.2.9) are two coupled equations for $\langle\phi_1|\psi_n\rangle$ and $\langle\phi_2|\psi_n\rangle$.
In matrix presentation:

$$\begin{pmatrix} E_1^{(0)} - E_n + V_{11} & V_{12} \\ V_{21} & E_2^{(0)} - E_n + V_{22} \end{pmatrix} \begin{pmatrix} \langle\phi_1|\psi_n\rangle \\ \langle\phi_2|\psi_n\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \qquad \text{(C.6.2.10)}$$

The eigenvalues E_n are found with the determinant:

$$\begin{vmatrix} E_1^{(0)} - E_n + V_{11} & V_{12} \\ V_{21} & E_2^{(0)} - E_n + V_{22} \end{vmatrix} = 0. \qquad \text{(C.6.2.11)}$$

Since the Hamiltonian is Hermitian $V_{12} = {V_{21}}^*$.
For a $m \times m$ matrix the diagonal element is:
$E_k^{(0)} - E_n + V_{kk}$,
and the other elements are V_{lk} with $l, k = 1(1)m$.
Eq. (6.14): $0 = \det\left|\left[E_l^{(0)} - \lambda\right]\delta_{lm} + V_{lm}\right|$
represents the elements of the determinant. Through this short-hand notation it becomes clear V_{ll} to be part of the diagonal and $\lambda (= E_n)$ represents the eigenvalues.
The matrix method as presented in this section is not about perturbation. It is not a particular perturbation method. V is dealt with as a part of the Hamiltonian.
Mahan discussed the problems with matrix methods: the dimensionality is infinite.
In practice the matrix is truncated. Convergence tested.

6.2.1 2×2

In this section we will deal with the eigenvalues of (C.6.2.11) for $n = 2$.
For this 2×2 case, the perturbation is considered to be small: $V_{12} \ll E_1 - E_2$.
Mahan dropped the superscript of $E_{1,2}^{(0)}$. The two eigenvalues are second order in V_{12}, see Eq.(6.17) page 160.
Mahan mentioned the case where the states $|\phi_1\rangle$ and $|\phi_2\rangle$ have the same eigenvalue:
$E_1 = E_2$, and : $V_{11} = V_{22}$.
What is not clear to me: $V_{11} = V_{22}$. Is that just an assumption? I suppose so.

6.2.2 Coupled Spins

Coupled Spins: I suppose it's about entanglement.
This is another example of the matrix method. It is helpful to read again Chapter 4 on momentum and spin. The relation for the momentum operator are applicable to the spin operator. In this section Mahan first solved the Hamiltonian exactly. He used, what he called a trick to do the job to find the exact solution.
Mahan mentioned, just above Eq. (6.27): *"…….gives two possible states, $S = 0$ or $S = 1$:….."*.
Eq. (6.27): $E_S = A\hbar^2[S(S+1) - \frac{3}{2}]$.
These are the eigenvalues I suppose.
This section is about the addition of angular momentum and entangled spins. The *Clebsch-Gordon coefficients* are given in Table 4.1.
Let's have a look at the eigenstates. For a two spin entangled system there are two states: the singlet state and the triplet state. We will present these state in the column vector representation(Chapter 4). So we have to find the tensor products of the two spin states. There are four basis column vectors. For convenience I use the notation of Susskind: u for up and d for down spins.

Hence: $|u \otimes u\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$, $|u \otimes d\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$, $|d \otimes u\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ and

$$|d \otimes d\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

These states make up the eigenstates.

For the singlet eigenstate (Susskind notation): $|sing\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$, for one of the three triplets we have for $|Tripl\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$.

The $\frac{1}{\sqrt{2}}$ factor is obtained with normalization.

Now we can prove the singlet and triplets to be eigenvectors of

$$H = 2A\vec{s_1}.\vec{s_2}\,, \qquad \text{(Eq.6.23)}$$

where s_j represents one of the Pauli matrices of particle j. However, I consider it to be a bit more elegant to find the eigenvectors in a straightforward way(See www.leennoordzij.me).

The tensor product of the matrices in Eq. (6.23) gives for the Hamiltonian, with the Eqs. (4.80)- (4.81) and the factor $\frac{\hbar}{2}$, 4× 4 matrix:

$$2A\frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \qquad \text{(C6.2.2.1)}$$

of which the eigenvalues λ_i are found from the determinant leading to the polynomial:

$(1-\lambda)^2((1+\lambda)^2-4)=0$,

with two roots $\lambda_i=1$ and root $\lambda_i=-3$.

Now let us find the eigenvectors. Let’s start with the eigenvalue -3 and assume the components of the column vector representation of the eigenvector to be a,b,c and d. Then:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = -3\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix},$$ applying matrix vector multiplication and equating:

$a = -3a, \rightarrow a = 0, d = -3d, \rightarrow d = 0$, and $b = -c$.

With normalization,

$bb^* + cc^* = 1, b = \frac{1}{\sqrt{2}}$, and $c = -\frac{1}{\sqrt{2}}$.

Now which eigenvector can we construct given these components? The eigenvector is

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}.$$

This is the column vector representation of the singlet.

Hence with the eigenvalue equation for the wave function ψ:
$H\psi = E\psi$, and (C6.2.2.1)
we have $E = -\frac{3}{2}A\hbar^2$, the same result as is found with the trick method of Mahan.
In, not exactly, the same way for the eigenvalue $+1$ you will find the energy level $E = \frac{1}{2}A\hbar^2$ for the three triplets. Let us see what happens:
So what about the three eigenvectors with eigenvalue +1?

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix},$$

applying matrix vector multiplication and equating the corresponding components:
$a = a, d = d$, and $b = c$.

The eigenvector isnu $\begin{pmatrix} a \\ b \\ b \\ d \end{pmatrix}$ and the normalization condition is:

$a^*a + 2b^*b + d^*d = 1$. This represents three equations. In addition we have the orthogonality condition, giving us three equations en plus. Alas, there are nine unknowns. However, we derived the singlet eigenvector, giving us another three equations based on the orthogonality condition. This should be sufficient since the vector space is a four dimensional vector space. It is not sufficient, since no new information is created. Hence we have to assume some vector components. This is done with simplicity in mind.
Starting with a simple eigenvector where $a = 0$ and $d = 0$, and b is real, we find for the first eigenvector with eigenvalue $+1$ the triplet $\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$. The other two are found by setting $b = 0$ and $a = d$, and $b = 0$ and $a = -d$. This produces the eigenvectors, the other two triplets. Finally the orthogonality of the four state vectors can be verified.

As mentioned by Mahan the trick method is not always straightforward. The matrix method is straightforward. I think the matrix and determinant as given above are part of the matrix method. We will see.
For the matrix method Mahan used the notation of Chapter 4 in this case of a two spin system, a neutron and an electron system say.
The Hamiltonian is given in Eq. (6.23) and rewritten in terms of raising and lowering operators: Eq. (6.32). To derive this expression for the Hamiltonian use has been made of the similarity of angular momentum and spin operators:
Hence $s_j^{(+)} = s_{jx} + is_{jy}$, and $s_j^{(-)} = s_{jx} - is_{jy}$.
The matrix elements of the Hamiltonian in Eq. (6.32) are found with the operators given in Eq. (6.33).

So $s_1^{(+)}s_2^{(-)} = \hbar^2 \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \hbar^2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$

and $s_1^{(-)}s_2^{(+)} = \hbar^2\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}\otimes\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix} = \hbar^2\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}$.

Furthermore $s_{1z}s_{2z} = \frac{\hbar^2}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\otimes\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar^2}{2}\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}$.

Now we plug these three matrices into the Hamiltonian given in Eq. (6.32) and find (C.6.2.2.1):

$$H = \begin{pmatrix}A\frac{\hbar^2}{2} & 0 & 0 & 0\\ 0 & -A\frac{\hbar^2}{2} & A\hbar^2 & 0\\ 0 & A\hbar^2 & -A\frac{\hbar^2}{2} & 0\\ 0 & 0 & 0 & A\frac{\hbar^2}{2}\end{pmatrix}.$$

Remark: What is a bit confusing to me is Mahan denoting the matrix elements by V_{ij} (on top of page 162). Keep in mind this V_{ij} is not the same as the matrix elements of V in Eq. (6.5).
The matrix representation of this Hamiltonian H leads to the four eigenvalues.
Remark: what is also not clear to me why Mahan uses $M = m_1 + m_2$ instead of using $S = s_1 + s_2$.

Homework 1,2,3.

Exercise 1.
Find the eigenvalues of a 3 × 3 matrix for which all matrix elements are identical:
$E_j^{(0)} = A,\ V_{lm} = V$.
According to the matrix method:

$$H = H_0 + V \qquad \text{Eq. (6.5)}$$

and

$$H_0\phi_n = E_n^{(0)}\phi_n$$

$$H\psi_n = E_n\psi_n\ ,$$

we have with Eq. (6.14) the general determinant for the eigenvalues.
First the matrix:

$$\begin{pmatrix}A+V & V & V\\ V & A+V & V\\ V & V & A+V\end{pmatrix}.$$

Some elements of the matrix are more identical.
The equation for the eigenvalues:

$$\begin{vmatrix}A+V-\lambda & V & V\\ V & A+V-\lambda & V\\ V & V & A+V-\lambda\end{vmatrix} = 0.$$

The polynomial for λ is:

$(A+V-\lambda)^3 - 3V^3(A+V-\lambda) + 2V^3 = 0.$
We rewrite this equation as:
$(A-\lambda)^2(A+3V-\lambda) = 0.$
The eigenvalues are:
$\lambda_1 = A,$ and $\lambda_2 = A+3V.$

Exercise 2.

Evaluate Eq. (6.23) for the case that $\overrightarrow{s_1}$ has spin-1 and $\overrightarrow{s_2}$ has spin-$\frac{1}{2}$. Do the problem two ways: (i) using the trick method, and (ii) using the matrix method.
The Hamiltonian represented by Eq. (6.23) is about coupled spins: $H = 2A\overrightarrow{s_1} . \overrightarrow{s_2}$
"Evaluate": I suppose it is about eigenvalues and eigenvectors.
With the trick method come the results of chapter 4 *On the Addition of Angular Momentum.*
In exercise 7 of that chapter we calculated the Clebsch-Gordon coefficients for a $(\frac{1}{2}) \times (1)$ coupled spin system.
Now in this exercise we have to do the $(1) \times (\frac{1}{2})$ job. Are the Clebsch-Gordon(C-G) coefficients the same as for the $(\frac{1}{2}) \times (1)$ system? What about the matrix $\overrightarrow{s_1} \otimes \overrightarrow{s_2}$?
Let us find out.
(i) The Trick Method.
As given by Mahan: the trick method uses the total spin $\vec{S}$ to be $\vec{S} = \overrightarrow{s_1} + \overrightarrow{s_2}.$
with Eq. (6.26) the Hamiltonian reads:
$H = A\hbar^2[S(S+1) - s_1(s_1+1) - s_2(s_2+1)]$,

Where use has been made of $\vec{S}.\vec{S} = \hbar^2 S(S+1)$ for spins.
There are two possible states: the maximum value $S = s_1 + s_2 = \frac{3}{2}$, and the minimum value of $S = |s_1 - s_2| = \frac{1}{2}$.
Now we will work on the (C-G) coefficients for $(1) \times (\frac{1}{2})$.
Using the notation of Mahan Eq. (4.150) Chapter 4 $|J,M\rangle = \sum_{m_1,m_2} CG|j_1,m_1\rangle \otimes |j_2,m_2\rangle$,
we evaluate $j_1 = 1$ with $m_1 = 1,0,-1$,
and
$j_2 = \frac{1}{2}$ with $m_2 = \frac{1}{2}, -\frac{1}{2}$.
We start with $|J,M\rangle = \left|\frac{3}{2},\frac{3}{2}\right\rangle$.
Then: $\left|\frac{3}{2},\frac{3}{2}\right\rangle = \sum_{m_1,m_2} CG|1,m_1\rangle \otimes \left|\frac{1}{2},m_2\right\rangle$.
$M = m_1 + m_2$, with $M = \frac{3}{2}$ we have $m_1 = 1$ and $m_2 = \frac{1}{2}$.
So $\left|\frac{3}{2},\frac{3}{2}\right\rangle = CG|1,1\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$. (C.6.2.2.2)

With column vector representation (C6.2.2.2) is written as :

$$|\tfrac{3}{2},\tfrac{3}{2}\rangle = CG|1,1\rangle \otimes |\tfrac{1}{2},\tfrac{1}{2}\rangle = CG\begin{pmatrix}1\\0\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix} = CG\begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix}.$$

Applying normalization $(CG)^2 = 1$ and CG$= \pm 1$.
Hence we obtained two states:

$$|\tfrac{3}{2},\tfrac{3}{2}\rangle = \pm|1,1\rangle \otimes |\tfrac{1}{2},\tfrac{1}{2}\rangle. \qquad \text{(C.6.2.2.3)}$$

We continue with the positive value. The negative one is not considered: just a phase difference of $i\pi$.
Now we evaluate $|\tfrac{3}{2},\tfrac{1}{2}\rangle = \sum_{m_1,m_2} CG|1,m_1\rangle \otimes |\tfrac{1}{2},m_2\rangle$.
$M = \frac{1}{2}$, and we have two sets of m_1 and m_2: $m_1 = 1, m_2 = -\frac{1}{2}$ and $m_1 = 0, m_2 = \frac{1}{2}$.

$$|\tfrac{3}{2},\tfrac{1}{2}\rangle = CG_1|1,0\rangle \otimes |\tfrac{1}{2},\tfrac{1}{2}\rangle + CG_2|1,1\rangle \otimes |\tfrac{1}{2},-\tfrac{1}{2}\rangle, \qquad \text{(C.6.2.2.4)}$$

with column representation $|\tfrac{3}{2},\tfrac{1}{2}\rangle = \begin{pmatrix}0\\CG_2\\CG_1\\0\\0\\0\end{pmatrix}$.

Normalization: $(CG_2)^2 + (CG_1)^2 = 1$.
Next we apply the lowering operator on $|\tfrac{3}{2},\tfrac{3}{2}\rangle$, and with help of Eq. (4.79) we obtain:

$$L\,|\tfrac{3}{2},\tfrac{3}{2}\rangle = \hbar\sqrt{3}\,|\tfrac{3}{2},\tfrac{1}{2}\rangle. \qquad \text{(C.6.2.2.5)}$$

Then using the lowering operator again, (6.2.2.3 produces with Eq.(4.79) and the chain rule:

$$L\,|\tfrac{3}{2},\tfrac{3}{2}\rangle = L(|1,1\rangle \otimes |\tfrac{1}{2},\tfrac{1}{2}\rangle) = \left\{\hbar\sqrt{2}(|1,0\rangle \otimes |\tfrac{1}{2},\tfrac{1}{2}\rangle) + \hbar(|1,1\rangle \otimes |\tfrac{1}{2},-\tfrac{1}{2}\rangle)\right\}.$$

This result is equated to (6.2.2.5) giving:

$$|\tfrac{3}{2},\tfrac{1}{2}\rangle = \{\tfrac{\sqrt{2}}{\sqrt{3}}\left(|1,0\rangle \otimes |\tfrac{1}{2},\tfrac{1}{2}\rangle\right) + \tfrac{1}{\sqrt{3}}\left(|1,1\rangle \otimes |\tfrac{1}{2},-\tfrac{1}{2}\rangle\right)\}. \qquad \text{(C.6.2.2.6)}$$

Do compare this result with (6.2.2.4) and:
$CG_1 = \frac{\sqrt{2}}{\sqrt{3}}$ and $CG_2 = \frac{1}{\sqrt{3}}$. These coefficients and (6.2.2.4) produce another state.
This result is similar to the result of exercise 7 in chapter 4 except for the order of tensor multiplication. With column vector representation it follows $|\tfrac{3}{2},\tfrac{1}{2}\rangle$ to be normalized.
The following state to be to be evaluated is

$$|\tfrac{3}{2},-\tfrac{1}{2}\rangle = \sum_{m_1,m_2} CG|1,m_1\rangle \otimes |\tfrac{1}{2},m_2\rangle.$$

For convenience we first evaluate :

$$|\tfrac{3}{2},-\tfrac{3}{2}\rangle = \sum_{m_1,m_2} CG|1,m_1\rangle \otimes |\tfrac{1}{2},m_2\rangle.$$

$M = -\frac{3}{2}$, so $m_1 = -1$ and $m_2 = -\frac{1}{2}$.

Hence $\left|\frac{3}{2},-\frac{3}{2}\right\rangle = CG_5|1,-1\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle$. (C.6.2.2.7)

Similar to the evaluation of the first state we $CG_5 = 1$, and

$\left|\frac{3}{2},-\frac{3}{2}\right\rangle = |1,-1\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle$. (C.6.2.2.8)

By applying the raising operator $L^\dagger \left|\frac{3}{2},-\frac{3}{2}\right\rangle$ and using Eq. (4.78) we find:

$L^\dagger \left|\frac{3}{2},-\frac{3}{2}\right\rangle = \hbar\sqrt{3}\left|\frac{3}{2},-\frac{1}{2}\right\rangle$. (C.6.2.2.9)

Now, back to $\left|\frac{3}{2},-\frac{1}{2}\right\rangle = \sum_{m_1,m_2} CG|1,m_1\rangle \otimes \left|\frac{1}{2},m_2\right\rangle$.

$M = -\frac{1}{2}$, and we have two sets of m_1 and m_2: $m_1 = 0, m_2 = -\frac{1}{2}$ and $m_1 = -1, m_2 = \frac{1}{2}$.

Hence :

$\left|\frac{3}{2},-\frac{1}{2}\right\rangle = CG_3|1,0\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + CG_4|1,-1\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$. (C.6.2.2.10)

We know the procedure and apply $L^\dagger$ on (C.6.2.2.8) and the chain rule:
with Eq. (4.78) we find

$L^\dagger \left|\frac{3}{2},-\frac{3}{2}\right\rangle = \hbar\sqrt{2}|1,0\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + \hbar|1,-1\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$.

Equate this expression with (C.6.2.2.9), then

$\left|\frac{3}{2},-\frac{1}{2}\right\rangle = \frac{\sqrt{2}}{\sqrt{3}}\left(|1,0\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle\right) + \frac{1}{\sqrt{3}}\left(|1,-1\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle\right)$. (C.6.2.2.11)

So we have 4 states for $J = \frac{3}{2}$.

We have still 2 state vectors to go: $J = \frac{1}{2}$. We start with $\left|\frac{1}{2},\frac{1}{2}\right\rangle$.

$M = \frac{1}{2}$, and we have two sets of m_1 and m_2: $m_1 = 1, m_2 = -\frac{1}{2}$ and $m_1 = 0, m_2 = \frac{1}{2}$.

The state vector is:

$\left|\frac{1}{2},\frac{1}{2}\right\rangle = CG_6|1,1\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + CG_7|1,0\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$. (C.6.2.2.12)

With normalization : $(CG_6)^2 + (CG_7)^2 = 1$. We need some additional information. Well, orthogonality is the other constraint: apply the orthogonality of $\left|\frac{3}{2},\frac{1}{2}\right\rangle$ of (C.6.2.2.6) and $\left|\frac{1}{2},\frac{1}{2}\right\rangle$ of (C.6.2.2.12) , we find $CG_7 = \frac{1}{\sqrt{3}}$ and $CG_6 = -\frac{\sqrt{2}}{\sqrt{3}}$.

So $\left|\frac{1}{2},\frac{1}{2}\right\rangle = -\frac{\sqrt{2}}{\sqrt{3}}\left|1,1\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + \frac{1}{\sqrt{3}}\ |1,0\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$. (C.6.2.2.13)

The fifth state,

The final state to obtain is $\left|\frac{1}{2},-\frac{1}{2}\right\rangle$.

$M = -\frac{1}{2}$, and we have two sets of m_1 and m_2: $m_1 = 0, m_2 = -\frac{1}{2}$ and $m_1 = -1, m_2 = \frac{1}{2}$.

The state vector is:

$\left|\frac{1}{2},-\frac{1}{2}\right\rangle = CG_8|1,0\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + CG_9|1,-1\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$. (C.6.2.2.14)

Normalization: $(CG_8)^2 + (CG_9)^2 = 1$.

Orthogonality: $\left|\frac{3}{2},-\frac{1}{2}\right\rangle$ of (C.6.2.2.15) and $\left|\frac{1}{2},-\frac{1}{2}\right\rangle$ of (C.6.2.2.14).

We find: $CG_8 = \frac{1}{\sqrt{3}}$ and $CG_9 = -\frac{\sqrt{2}}{\sqrt{3}}$.

The final state:

$$\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = \tfrac{1}{\sqrt{3}}\ |1,0\rangle \otimes \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle - \tfrac{\sqrt{2}}{\sqrt{3}}\ |1,-1\rangle \otimes \left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle. \qquad \text{(C.6.2.2.15)}$$

We found the 6 states for the 6- dimensional vector space. Quite an evaluation. Now, what about the eigenvalues? Well, with the 6×6 matrix we could do the job. However, I consider this to be the second part of the evaluation: the matrix method.

With the trick method, the Hamiltonian is (Eq. (2.26)):

$H = A\hbar^2[S(S+1) - s_1(s_1+1) - s_2(s_2+1)]$.

For the $(1) \times (\frac{1}{2})$ coupled spin system we have:

$J(=S) = \frac{3}{2}$ and $J(=S) = \frac{1}{2}$; $s_1 = 1$ and $s_2 = 1/2$.

With these values the Hamiltonian gives two eigenvalues:

$E_{1/2} = -2A\hbar^2$ and $E_{3/2} = A\hbar^2$.

For $J(=S) = \frac{3}{2}$, we have 4 states and degeneracy of 4;

for $J(=S) = \frac{1}{2}$, we have two states with degeneracy of 2.

(ii) The Matrix Method.

We have a 6×6 matrix.

$\overrightarrow{s_1}$ is represented by a 3×3 matrix given by the Eqs. (4.100)-(4.102) in Chapter 4 and $\overrightarrow{s_2}$ is represented by 2×2 matrix based on the Pauli matrices given in Eqs. (4.80) and (4.81) multiplied by $\hbar/2$. The resulting matrix representation of the Hamiltonian is found by tensor multiplication $\overrightarrow{s_1} \otimes \overrightarrow{s_2}$.

$$H = A\hbar^2\left\{\tfrac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \tfrac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}.$$

Resulting into the matrix:

$$H = A\hbar^2 \begin{pmatrix} 1 & 0 & 0 & & & \\ 0 & -1 & \sqrt{2} & & 0 & \\ 0 & \sqrt{2} & 0 & & & \\ & & & 0 & \sqrt{2} & 0 \\ & 0 & & \sqrt{2} & -1 & 0 \\ & & & 0 & 0 & 1 \end{pmatrix}.$$

The matrix elements are H_{ij} .

$H_{11} = H_{66} = 1$ and $H_{22} = H_{55} = -1$. (C.6.2.2.16)

The 4 off diagonal elements are: $H_{23} = H_{32} = H_{45} = H_{54} = \sqrt{2}$. (C.2.2.2.17)

All the elements to be multiplied by the factor $A\hbar^2$.

The determinant for the eigenvalues λ is, with $A\hbar^2 = B$,:

$$\begin{vmatrix} B-\lambda & 0 & 0 & & & \\ 0 & -B-\lambda & B\sqrt{2} & & 0 & \\ 0 & B\sqrt{2} & -\lambda & & & \\ & & & -\lambda & B\sqrt{2} & 0 \\ & 0 & & B\sqrt{2} & -B-\lambda & 0 \\ & & & 0 & 0 & B-\lambda \end{vmatrix} = 0. \qquad \text{(C.6.2.2.18)}$$

The determinant has Block diagonal form with two separated blocks.
The first block and the second block both produces:
$(\lambda - B)^2 = 0$, and $(\lambda + 2B) = 0$.
So one eigenvalue: $\lambda = A\hbar^2$and degeneracy of 4, the other eigenvalue $\lambda = -2A\hbar^2$ and degeneracy of 2. This result we also found with the Trick method.
The eigenstates? We need to find 4 states with eigen value $A\hbar^2$ and 2 states with eigenvalue $-2A\hbar^2$.
Let us start with $\lambda = -2A\hbar^2$. We use a column representation of the eigenvectors and determine the elements.

$$\begin{pmatrix} 1 & 0 & 0 & & & \\ 0 & -1 & \sqrt{2} & & 0 & \\ 0 & \sqrt{2} & 0 & & & \\ & & & 0 & \sqrt{2} & 0 \\ & 0 & & \sqrt{2} & -1 & 0 \\ & & & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \end{pmatrix} = -2 \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \end{pmatrix}. \qquad \text{(C.6.2.2.19)}$$

For the elements we obtain:
$a = -2a \rightarrow a = 0$,
$-b + c\sqrt{2} = -2b \rightarrow b = -c\sqrt{2}$,
$b\sqrt{2} = -2c \rightarrow b = -c\sqrt{2}$,
$e\sqrt{2} = -2d \rightarrow d = -e\sqrt{2}/2$,
$d\sqrt{2} - e = -2e \rightarrow d = -e\sqrt{2}/2$,
$f = -2f \rightarrow f = 0$.
So we have 4 elements of the state vectors: b, c, d and e. The 2 vectors should be orthogonal. A simple solution to choose:

$$\begin{pmatrix} 0 \\ b \\ c \\ 0 \\ 0 \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 \\ 0 \\ 0 \\ d \\ e \\ 0 \end{pmatrix}.$$

Applying normalization, $b^2 + c^2 = 1$, we find $b = \pm\frac{\sqrt{2}}{\sqrt{3}}$, and $c = \pm\frac{1}{\sqrt{3}}$.
With these elements we can construct 4 vectors of which only 2 are relevant. The other 2 vectors are the relevant ones multiplied by a phase vector $e^{i\pi}$. I choose one particular combination of b, c. On the basis of orthogonality. Then we have:

$$\begin{pmatrix} 0 \\ -\frac{\sqrt{2}}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{C.6.2.2.20}$$

Again applying normalization, $d^2 + e^2 = 1$, we find $d = \pm\frac{1}{\sqrt{3}}$, and $e = \pm\frac{\sqrt{2}}{\sqrt{3}}$.
I choose the combination which gives for the second state vector:

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{1}{\sqrt{3}} \\ -\frac{\sqrt{2}}{\sqrt{3}} \\ 0 \end{pmatrix}. \tag{C.6.2.2.21}$$

With some "backwards engineering" we can write both state vectors as tensor products of a spin 1 and a spin $\frac{1}{2}$.

Then we have for (C.6.2.2.20): $-\frac{\sqrt{2}}{\sqrt{3}}\begin{pmatrix}1\\0\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} + \frac{1}{\sqrt{3}}\begin{pmatrix}0\\1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix}$. (C.6.2.2.22)

For (C.6.2.2.21) we find: $\frac{1}{\sqrt{3}}\begin{pmatrix}0\\1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} - \frac{\sqrt{2}}{\sqrt{3}}\begin{pmatrix}0\\0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix}$. (C.6.2.2.23)

These are the same as we found with the Trick Method:
(C.6.2.2.22)↔(C.6.2.2.13) and (C.6.2.2.23)↔(C.6.2.2.15).

Now we look after the other eigenvalue $\lambda = A\hbar^2$ and see what the eigenvectors will look like.

$$\begin{pmatrix} 1 & 0 & 0 & & & \\ 0 & -1 & \sqrt{2} & & 0 & \\ 0 & \sqrt{2} & 0 & & & \\ & & & 0 & \sqrt{2} & 0 \\ & 0 & & \sqrt{2} & -1 & 0 \\ & & & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \end{pmatrix}. \tag{C.6.2.2.24}$$

From equating the elements of the matrix product on the left hand side with the elements of the vector on the right hand side, we find:

$a = a,$
$-b + c\sqrt{2} = b \rightarrow c\sqrt{2}/2,$
$b\sqrt{2} = c \rightarrow\ b \rightarrow c\sqrt{2}/2,$
$e\sqrt{2} = d \rightarrow d = e\sqrt{2},$
$d\sqrt{2} - e = e \rightarrow d = e\sqrt{2},$
$f = f.$

Now we have 6 elements to construct 4 state vectors. The leading principle is simplicity.

It comes as no surprise we will meet the factors $\frac{1}{\sqrt{3}}$ and $\frac{\sqrt{2}}{\sqrt{3}}$ again.
The most simple state vectors are, complying with orthogonality:

$$\begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix} \text{ and } \begin{pmatrix}0\\0\\0\\0\\0\\1\end{pmatrix}. \qquad \text{(C.6.2.2.25)}$$

These two state vectors can be constructed with the tensor product of spin 1 and spin ½.
Hence

$$\begin{pmatrix}1\\0\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} \qquad \text{(C.6.2.2.26)}$$

and

$$\begin{pmatrix}0\\0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}. \qquad \text{(C.6.2.2.27)}$$

These two state vectors we found with the Trick method: (C.6.2.2.3) and (C.6.2.2.8)
Still two state vectors to go.
We have, on the basis of simplicity and orthogonality(with (C.6.2.2.20) and (C.6.2.2.21), the combinations b, c and d, e.
These are the 2 column vectors we need:

$$\begin{pmatrix}0\\\frac{1}{\sqrt{3}}\\\frac{\sqrt{2}}{\sqrt{3}}\\0\\0\\0\end{pmatrix} \text{ and } \begin{pmatrix}0\\0\\0\\\frac{\sqrt{2}}{\sqrt{3}}\\\frac{1}{\sqrt{3}}\\0\end{pmatrix}. \qquad \text{(C.6.2.2.28)}$$

The tensor products are:

$$\frac{1}{\sqrt{3}}\begin{pmatrix}1\\0\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} + \frac{\sqrt{2}}{\sqrt{3}}\begin{pmatrix}0\\1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix}, \qquad \text{(C.6.2.2.29)}$$

and

$$\frac{\sqrt{2}}{\sqrt{3}}\begin{pmatrix}0\\1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} + \frac{1}{\sqrt{3}}\begin{pmatrix}0\\0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix}. \qquad \text{(C.6.2.2.30)}$$

These two are the same we found with the Trick method:
(C.6.2.2.29)↔(C.6.2.2.6) and (C.6.2.2.30)↔ $(C.6.2.2.11)$.
Alas, the evaluation is left with some ambiguity, since the signs of the elements of the column vectors derived with matrix method could be interchanged. However, then the signs of the constants in the resulting state vectors would differ from the signs of the vectors of the trick method.
To conclude, the matrix representation of a coupled spin $(\frac{1}{2}) \times (1)$ is presented The Clebsch Gordon coefficients are derived in Exercise 7, Chapter 4.
The Hamiltonian:

$$A\hbar^2\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & -1 & 0 & \sqrt{2} & 0 \\ 0 & \sqrt{2} & 0 & -1 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

We leave this exercise.
Quite an evaluation.

Exercise 3.
Find the eigenvalues of the Hamiltonian of three interacting spin-1/2 particles:
$H = A[\overrightarrow{s_1}.\overrightarrow{s_2} + \overrightarrow{s_1}.\overrightarrow{s_3} + \overrightarrow{s_3}.\overrightarrow{s_2}]$.
The Hamiltonian is a sequence of 3 pairs of spin$(\frac{1}{2}) \times (\frac{1}{2})$ couples. The matrices representing the couples are indistinguishable.
Hence the Hamiltonian reduces to: $H = 3A[\overrightarrow{s_1}.\overrightarrow{s_2}]$.
The results of the analysis of section 6.2.2 on Coupled Spins can be used for the Trick Method and the Matrix Method.
The eigenvalues found in section 6.2.2 are multiplied by the factor 3/2 or denoting the Hamiltonian of section 6.2.2 by H_1, we have $H = \frac{3}{2}H_1$.
So the eigenvalues for the 3 pairs of coupled spins are:
$E_0 = -\frac{9}{4}A\hbar^2$ with the spin singlet as eigenstate
and
$E_1 = \frac{3}{4}A\hbar^2$ with the spin triplet as the three eigenstates.

6.2.3 Tight-Binding Model

Feynman et al derived the states and eigenvalues by solving the recurrencyrelations as given in Vol III-chapter 13-1 and-2, Eq. 13.6. Like those given by Mahan, Eqs. (6.47)-(6.49).
This section is about electron eigenstates in solids and molecules. The Hamiltonian is:
$H = H_0 + V$,
where H_0 is a $N \times N$ diagonal matrix and Mahan illustrated this model for a one dimensional lattice and a circular lattice(carbon atoms in benzene). The eigen functions and eigenvalues are found. The eigenfunctions are expressed in the atomic orbital, Eq. (6.43). No further attention is paid to the atomic orbitals in this section.
Since the Hamiltonian is a $N \times N$ matrix operator we will have N column state vectors with N elements. So we have to find $N \times N$ vector elements. As mentioned by Feynman (Vol. III) determinants are fine when there are 2, 3, or 4 equations. So, for $N > 4$ it is not convenient to work with the matrix and the determinant. I suppose for this reason Mahan chooses the trial function given in Eq. (6.52) *as Feynman did, Eq. (13.10) Vol. III.*
In Eq. (6.52) Mahan presented the components of the eigenvectors. I suppose these have to be normalized separately. I will investigate this in some detail.
Let us start with an almost trivial case: a linear lattice with two atoms, $N = 2$. We will start with the Hamiltonian and compare the results with Eq. (6.52).
For $N = 2 : H = \begin{pmatrix} E_0 & V \\ V & E_0 \end{pmatrix}$. We denote the eigenvalue λ and the determinant to be

evaluated is $\begin{vmatrix} E_0-\lambda & V \\ V & E_0-\lambda \end{vmatrix} = 0.$
We obtain $E_0 - \lambda = \pm V$.
Hence the eigenvalues for this system are: $\lambda_1 = E_0 - V$ and $\lambda_2 = E_0 + V$.
Remark: These eigenvalues are found with Eq.(6.64).
With these eigenvalues we can construct the eigenvectors with components a_i, $i = 1{,}2$.
$\begin{pmatrix} E_0 & V \\ V & E_0 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \lambda_1 \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$.
This expression gives us 2 equations with the result $a_1 = -a_2$.
Normalization leads to: $a_1 = \frac{1}{2}\sqrt{2}$ and $a_2 = -\frac{1}{2}\sqrt{2}$.
The eigenvector is: $\psi_1 = \begin{pmatrix} \frac{1}{2}\sqrt{2} \\ -\frac{1}{2}\sqrt{2} \end{pmatrix}$. Remark: the other vector differs a phase shift factor $e^{i\pi}$ and is irrelevant.
The other eigenvector for $\lambda_2 = E_0 + V$ is found to be, in a similar way:
$\psi_2 = \begin{pmatrix} \frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{pmatrix}$.
Now let us work with the expressions given by Mahan: $a_j = \sin j\theta_\alpha$ and $\theta_\alpha = \frac{\pi\alpha}{N+1}$.
For $N = 2$ the 2×2 components of the eigenvectors are: $\sin\theta_1$, $\sin 2\theta_1$, and $\sin\theta_2$, $\sin 2\theta_2$. With the value of $\theta_\alpha = \frac{\pi\alpha}{N+1}$ the results for the eigenvectors are:
$\psi_1 = \begin{pmatrix} \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} \end{pmatrix}$ and $\psi_2 = \begin{pmatrix} \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} \end{pmatrix}$. Obviously, these vectors are not normalized.
Consequently we have to multiply the elements of the vectors by $\frac{1}{3}\sqrt{6}$ and obtain:
$\psi_1 = \begin{pmatrix} \frac{1}{2}\sqrt{2} \\ -\frac{1}{2}\sqrt{2} \end{pmatrix}$ and $\psi_2 = \begin{pmatrix} \frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{pmatrix}$.
The result is: two eigenvalues and two eigenvectors.
What could the atomic orbitals be in this $N = 2$ case?
The next case to analyse is the one dimensional lattice with $N = 3$.
For $N = 3$ the Hamiltonian is: $\begin{pmatrix} E_0 & V & 0 \\ V & E_0 & V \\ 0 & V & E_0 \end{pmatrix}$,
and the determinant for the eigenvalues λ to be evaluated is

$$\begin{vmatrix} E_0-\lambda & V & 0 \\ V & E_0-\lambda & V \\ 0 & V & E_0-\lambda \end{vmatrix} = 0.$$

The eigenvalues are $\lambda_1 = E_0 - V\sqrt{2}$, $\lambda_2 = E_0$, and $\lambda_3 = E_0 + V\sqrt{2}$.
Remark: these eigenvalues are also found with Eq. (6.64).
Similar to the $N = 2$ case, we find for $N = 3$ three eigenstates given as column vectors:

$$\psi_1 = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2}\sqrt{2} \\ \frac{1}{2} \end{pmatrix}, \psi_2 = \begin{pmatrix} \frac{1}{2}\sqrt{2} \\ 0 \\ -\frac{1}{2}\sqrt{2} \end{pmatrix} \text{ and } \psi_3 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2}\sqrt{2} \\ \frac{1}{2} \end{pmatrix}.$$

Using the approach by Mahan for the components a_j of the column vectors $a_j = \sin j\theta_\alpha$ and $\theta_\alpha = \frac{\pi\alpha}{N+1}$:

$$\psi_1 = \begin{pmatrix} \frac{1}{2}\sqrt{2} \\ -1 \\ \frac{1}{2}\sqrt{2} \end{pmatrix}, \psi_2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \text{ and } \psi_3 = \begin{pmatrix} \frac{1}{2}\sqrt{2} \\ 1 \\ \frac{1}{2}\sqrt{2} \end{pmatrix}.$$

As you will notice, these vectors are not normalized. All the components need to be divided by $\sqrt{2}$.

The result is: three eigenvalues and three eigenvectors.

Now we analyse the one-dimensional lattice with $N = 4$.

As can be expected this analysis, using the matrix and the determinant, becomes a bit more complicated.

For $N = 4$ the Hamiltonian is: $\begin{pmatrix} E_0 & V & 0 & 0 \\ V & E_0 & V & 0 \\ 0 & V & E_0 & V \\ 0 & 0 & V & E_0 \end{pmatrix}$.

The determinant for the eigenvalues λ to be evaluated has as diagonal elements again $E_0 - \lambda$. The remaining elements are the same as found in the Hamiltonian:

$$\begin{vmatrix} E_0 - \lambda & V & 0 & 0 \\ V & E_0 - \lambda & V & 0 \\ 0 & V & E_0 - \lambda & V \\ 0 & 0 & V & E_0 - \lambda \end{vmatrix} = 0 .$$

With pivotal condensation (Chisholm and Morris) and expanding by the fourth column, we obtain a polynomial resulting into 4 eigenvalues:

$$\lambda_1 = E_0 - V\sqrt{\left(\frac{3}{2} + \frac{1}{2}\sqrt{5}\right)} = E_0 + 2V\cos\frac{4\pi}{5},$$

$$\lambda_2 = E_0 - V\sqrt{\left(\frac{3}{2} - \frac{1}{2}\sqrt{5}\right)} = E_0 + 2V\cos\frac{3\pi}{5},$$

$$\lambda_3 = E_0 + V\sqrt{\left(\frac{3}{2} - \frac{1}{2}\sqrt{5}\right)} = E_0 + 2V\cos\frac{2\pi}{5} \text{ and}$$

$$\lambda_4 = E_0 + V\sqrt{\left(\frac{3}{2} + \frac{1}{2}\sqrt{5}\right)} = E_0 + 2V\cos\frac{\pi}{5}.$$

The right hand side of these expressions are found with Eq. (6.64).

Having found the four eigenvalues we can construct the four eigenstates with $H\psi = \lambda\psi$ in column vector representation.

Hence

$$\begin{pmatrix} E_0 & V & 0 & 0 \\ V & E_0 & V & 0 \\ 0 & V & E_0 & V \\ 0 & 0 & V & E_0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \lambda_i \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}.$$

From this expression four values of a , normalized, are derived:
$a = \pm \frac{1}{\sqrt{1+\frac{1}{8}(1\pm\sqrt{5})^3}}$.
b, c and d are expressed in a . In this way we find the four eigenstates ψ_i.
The other approach is by using Eq. (6.52), representing the components of the eigenstate, Mahan. Then, the components $a_j = \sin(j\theta_\alpha)$ and $\theta_\alpha = \frac{\pi\alpha}{5}$, $\alpha = 1,2,3,4$.
Let us analyse one particular state with $\alpha = 1$.
So the components of the eigenvector are: $\sin\theta_1$, $\sin 2\theta_1$, $\sin 3\theta_1$, $\sin 4\theta_1$ and $\theta_1 = \frac{\pi}{5}$.
For these components the vector is not normalized.
The normalization factor is: $\frac{1}{2(1+\sqrt{\left(\frac{3}{2}+\frac{1}{2}\sqrt{5}\right)}-\sqrt{\left(\frac{3}{2}-\frac{1}{2}\sqrt{5}\right)})}$.
The result is: four eigenvalues and four eigenvectors
$N \geq 5$, not convenient indeed.
I leave the analysis here. Most probably we will deal with the atomic orbital in the exercises.

Homework 4,5,6.

Exercise 4.
A benzene molecule (C_6H_6) has a ring of six carbon atoms. The $2p_z$ orbitals of carbon are perpendicular to the plane. They form a periodic system of six identical states for an electron. Use the first-neighbour tight binding model.
a. What are the six different eigenvalues and eigenvectors of this system?
b. Six electrons occupy these states in the neutral molecule. Including spin degeneracy, which states are occupied, assuming $V > 0$?
Feynman et al analysed the benzene molecule in section 15-4 of Vol. III.
$2p_z$ orbitals: I assume this to be the notation of section 5.4.3 of Chapter 5 Mahan and
p: $l = 1$,
$2p$: $n = 2, l = 1$,
$2p_z$: $n = 2, l = 1, m = 0$.
So $n = 1$ is the closed shell.
ad a. The six eigenvectors and eigenvalues of this system.
In section 6.2.3 Mahan dealt with the tight-binding model for the carbon atoms in benzene. Here I will present the results of this section.
The eigenvalues, with help of the trial function Eq. (6.66), are Eq. (6.68):
$E_\alpha = E_0 + 2V\cos[\frac{2\pi\alpha}{N}]$.
For $N = 6$ we have $\alpha = 0, \pm1, \pm2, \pm3$.
Hence there are four different eigenvalues.
We have the Hamiltonian as a matrix. The eigenfunctions are represented with column vectors. The elements of the eigenfunction are $a_j = e^{i(j\theta_\alpha)}$, Eq. (6.66). Then according to the periodicity: $\theta_\alpha = \frac{2\pi\alpha}{N}$, $\alpha = 0, \pm1, \pm2, \pm3$, Eq. (6.67).
As mentioned by Mahan $\alpha = \pm\frac{N}{2}$ gives the same eigenvalue.

The 6 eigenvectors are: $\psi_\alpha = \frac{1}{\sqrt{6}}\begin{pmatrix} e^{\frac{i\pi\alpha}{3}} \\ e^{\frac{i2\pi\alpha}{3}} \\ e^{\frac{i3\pi\alpha}{3}} \\ e^{\frac{i4\pi\alpha}{3}} \\ e^{\frac{i5\pi\alpha}{3}} \\ e^{\frac{i6\pi\alpha}{3}} \end{pmatrix}$,

the four eigenvalues:
$E_\alpha = E_0 + 2V\cos[\frac{\pi\alpha}{3}]$.
with $\alpha = 0, \pm 1, \pm 2, \pm 3$, Eq. (6.67).
So we have two states with the same energy for $\alpha = \pm 1, \pm 2$.
We assume V to be positive: the two lowest energy levels are:
$E_3 = E_0 - 2V$, and
$E_2 = E_0 - V$.
Feynman et al: These are possible states for one electron. If we have more than one electron , two-with opposite spins-can go into each state.
For the benzene molecule we have to put in six electrons. For the ground state they will go into the lowest possible energy states-two at $s = 0$($\alpha = 3$, Nz), two at $s = +1$($\alpha = 2$, Nz) and two at $s = -1$($\alpha = -2$,Nz).

ad b.
Which states are occupied with $V > 0$?
The answer to this question has been given by Feynman et al.
The six electrons are found in the two lowest energy levels. Including spin degeneracy , two electrons are in $E_3 = E_0 - 2V$ and four in $E_2 = E_0 - V$ (two at $\alpha = 2$ and two at $\alpha = -2$).
The energy E of the ground state is:
$E = 2(E_0 - 2V) + 4(E_0 - V) = 6E_0 - 8V$.

Exercise 5.
Assume a hypothetical molecule composed of six carbon atoms in a line. Use the same matrix elements as in exercise 4. What are the energies of the six orbital states for the $2p_z$ system. What is the total energy of six electrons in these states. Is it higher or lower than for the ring?
This case has been analysed by Mahan on page 164.
The eigenvalues are given by Eq. (6.54):
$E = E_0 + 2V\cos\theta$ or
$E_\alpha = E_0 + 2V\cos[\frac{\pi\alpha}{N+1}]$ Eq.(6.64)
$N = 6$ and $\alpha = 1,2,\ldots,5,6$.
For the six electrons, including spin degeneracy, the total energy E is :
$E = 6E_0 - 6.99V$.
Hence the energy for the six atoms in a line is larger than the energy of the six atoms in a ring: $E_{line} - E_{ring} \cong V$.

Exercise 6.
A tetrahedron is a polygon with vertices equidistant from each other(e.g., CH_4) An electron

on a vertex has a site energy E_0 and a matrix element V for hopping to any other vertex.
a. Write down the Hamiltonian for this problem.
b. Give its eigenvalues and eigenvectors.
ad. a. The tetrahedron, is it a linear chain, is it a ring? It is certainly not a linear chain.
Is it a ring? Let's have a look. The tetrahedron consists of 4 equilateral triangles. We number the vertices by 1, 2, 3 and 4. Open up the tetrahedron and you see the possibility to hop from 4 to 1, then to 2, 3, 4, 1, and so on. This resembles the character of a ring. So the Hamiltonian can be represented by a 4×4 matrix similar to Eq. (6.65):

$$H = \begin{pmatrix} E_0 & V & 0 & V \\ V & E_0 & V & 0 \\ 0 & V & E_0 & V \\ V & 0 & V & E_0 \end{pmatrix}.$$

ad. b. With this matrix we can find the eigenvalues with pivotal condensation and the eigenvectors.
Here, I will use the trial function given by Mahan, Eq. (6.66).

The 4 eigenvectors are: $\psi_\alpha = \frac{1}{2}\begin{pmatrix} e^{\frac{i\pi\alpha}{2}} \\ e^{i\pi\alpha} \\ e^{\frac{i3\pi\alpha}{2}} \\ e^{i2\pi\alpha} \end{pmatrix}$, with $\alpha = 0, \pm 1, \pm 2$, Eq. (6.67).

As mentioned by Mahan $\alpha = \pm 2$ gives the same eigenvalue.
The eigenvalues are, with Eq.(6.68):
$E = E_0 + 2V$, $\alpha = 0$,
$E = E_0$, $\alpha = \pm 1$ and
$E = E_0 - 2V$, $\alpha = 2$.
For the two states $\alpha = \pm 1$ we have 1 eigenvalue $E = E_0$.

6.3 The stark Effect

This section is about the linear splitting of energy levels in a constant electric field F in atomic hydrogen. The electric field is considered to be a perturbation of the Hamiltonian and $U = -eFr\cos\theta$, Eq (6.70).
Furthermore, the $n = 1$ state of atomic hydrogen does not have a Stark effect (Mahan). In exercise 5.24 we showed for the ground state, Eq. (5.346), $E = E_{Ry} - \frac{\alpha}{2}F^2 + O(F^4)$.
Mahan dealt with the $n = 2$ case, with a degeneracy of 4.
With these four states we have a matrix of 4×4.
Mahan writes on top of page 167 : " *The electric field causes nonzero matrix elements between two of these (four, Nz) states, and these two have a change in energy proportional to F* ". How come? Well, parity is key.
In section 6.2 on Matrix methods, Mahan presented the off diagonal matrix elements of the perturbed Hamiltonian V_{lm} .
(Nota bene: in the section on Stark Effect, Mahan uses U instead of V).
For the atomic hydrogen and $n = 2$ only $\langle 2s|U|2p_z\rangle$ contributes to the off-diagonal elements of the Hamiltonian operator. There are four orbital states: $2s, 2p_z, 2p_{+1}$ and $2p_{-1}$.
In section 5.4.3 on Hydrogen Eigenfunctions the functions for these four states can be found.
Evaluating the integrals involved, it appears only $\langle 2s|U|2p_z\rangle$ contributes. The other

"sandwiches" do not, since the integrals for the "sandwiches" involved contain a $\cos\theta$ (the electric field) and a $\sin\theta$ except for the $|2s\rangle$ state (see Griffiths). The parity.
Then Mahan obtained the expression for $\langle 2s|U|2p_z\rangle$ to be $M = 3ea_0F$, Eq. (6.75). The only expectation value contributing to the perturbed Hamiltonian.
The resulting 4×4 matrix is: $\begin{pmatrix} E_2 & M & 0 & 0 \\ M & E_2 & 0 & 0 \\ 0 & 0 & E_2 & 0 \\ 0 & 0 & 0 & E_2 \end{pmatrix}$.
Just below Eq. (6.76), Mahan presented the order of states. Here I present them in the following notation:
$|nlm\rangle$: $|200\rangle, |210\rangle, |211\rangle$, and $|21-1\rangle$. I can imagine this order to lead to the most diagonalized matrix as shown above.
Remark:
Styer presented a different sequence of the eigenstates:
$|nlm\rangle$: $|200\rangle, |211\rangle, |210\rangle$, and $|21-1\rangle$.
This order of appearance leads to te following perturbed Hamiltonian(Mahan notation):

$$\begin{pmatrix} E_2 & 0 & M & 0 \\ 0 & E_2 & 0 & 0 \\ M & 0 & E_2 & 0 \\ 0 & 0 & 0 & E_2 \end{pmatrix}.$$

To obtain this matrix, it makes sense to take notice of the possibility of $\int_0^{2\pi} d\phi e^{-im'\phi}e^{im\phi}$ to be zero for $m' \neq m$.
Then, Styer rearranged the sequence of eigenstates into the sequence presented by Mahan and Styer obtained the matrix as given by Mahan: the most diagonalized matrix. Again, a demonstration of the leading principle: make the matrix as simple as possible.
With the determinant Eq. (6.76), the eigenvalues λ_i are obtained. The eigenvectors can be found with:

$$\begin{pmatrix} E_2 & M & 0 & 0 \\ M & E_2 & 0 & 0 \\ 0 & 0 & E_2 & 0 \\ 0 & 0 & 0 & E_2 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \lambda_i \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}. \qquad \text{(C.6.3.1)}$$

Using the simplicity argument, normalization and orthogonality the four eigenvectors are:

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}\right] \text{ and } \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}\right]. \qquad \text{(C6.3.2)}$$

The order of the eigenstates with eigenvalues, using (C6.3.2), are given in Eqs. (6.77)-(6.79).
We have a degeneracy of 3.
To me, it is not as straightforward as presented by Mahan and Styer to distribute the eigenvalues among the various states.
Furthermore, Mahan explained the reason why most of the matrix elements are zero.

Homework 7.

Exercise 7.
Workout the first-order Stark effect for the $n = 3$ shell of atomic hydrogen.
On page 169 Mahan paid some attention to this $n = 3$ case. The degeneracy is 9.

We have nine degenerate orbital states. Let us sum then up:
I will use the notation $|nlm\rangle$ and indicate the radial quantum n_r number separately.
$|300\rangle$, $n_r = 2$.
The radial eigenfunction R_{3s} is, Eq. (5.131) and $\rho = r/a_0$,

$$R_{3s} = 2(\tfrac{1}{3})^{3/2} e^{-r/3a_0}\left[1-\frac{2r}{3a_0}+\frac{2}{27}\left(\frac{r}{a_0}\right)^2\right]. \tag{C.6.3.3}$$

The spherical harmonic is: $Y_0^0 = C_{00}P_0^0 = \frac{1}{\sqrt{4\pi}}$.

$$\text{Hence the eigenstate } |300\rangle = \frac{1}{\sqrt{\pi}}(\tfrac{1}{3})^{3/2} e^{-r/3a_0}\left[1-\frac{2r}{3a_0}+\frac{2}{27}\left(\frac{r}{a_0}\right)^2\right]. \tag{C.6.3.4}$$

$|310\rangle, n_r = 1$.
The radial eigenfunction R_{3p} is, Eq. (5.133) and $\rho = r/a_0$:

$$R_{3p} = \frac{1}{3}\left(\frac{2}{3}\right)^{\frac{5}{2}} \frac{r}{a_0} e^{-\frac{r}{3a_0}}\left(1-\frac{r}{6a_0}\right). \tag{C.6.3.5}$$

The spherical harmonic $Y_1^0 = C_{10}P_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$.

$$\text{The eigenstate } |310\rangle = \frac{1}{3}\sqrt{\frac{3}{4\pi}}\left(\frac{2}{3}\right)^{\frac{5}{2}} \frac{r}{a_0} e^{-\frac{r}{3a_0}}\left(1-\frac{r}{6a_0}\right)\cos\theta. \tag{C.6.3.6}$$

$|311\rangle, n_r = 0$.
The radial eigenfunction R_{3p+} , Eq. (5.133) and $\rho = r/a_0$, equals (C.6.3.5).
The spherical harmonic $Y_1^1 = C_{11}P_1^1 e^{i\phi} = \sqrt{\frac{3}{8\pi}}\sin\theta\ e^{i\phi}$.

$$\text{The eigenstate } |311\rangle = \frac{1}{3}\sqrt{\frac{3}{8\pi}}\left(\frac{2}{3}\right)^{\frac{5}{2}} \frac{r}{a_0} e^{-\frac{r}{3a_0}}\left(1-\frac{r}{6a_0}\right)\sin\theta\, e^{i\phi}. \tag{C.6.3.7}$$

$|31-1\rangle, n_r = 0$.
The radial eigenfunction R_{3p-} , Eq. (5.133) and $\rho = r/a_0$, equals (C.6.3.5).
Since the spherical eigenfunction has the absolute value of m in the superscript of the associated Legendre polynomial,
the spherical harmonic $Y_1^{-1} = C_{11}P_1^1 e^{-i\phi} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi}$.

$$\text{The eigenstate } |31-1\rangle = \frac{1}{3}\sqrt{\frac{3}{8\pi}}\left(\frac{2}{3}\right)^{\frac{5}{2}} \frac{r}{a_0} e^{-\frac{r}{3a_0}}\left(1-\frac{r}{6a_0}\right)\sin\theta\, e^{-i\phi}. \tag{C.6.3.8}$$

$|322\rangle, n_r = 0$.
The radial eigenfunction R_{3d} is, Eq. (5.134) and $\rho = r/a_0$:

$$R_{3d} = \frac{1}{81}\sqrt{\frac{8}{15}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}} . \tag{C.6.3.9}$$

The spherical harmonic $Y_2^2 = C_{22}P_2^2 e^{2i\phi} = \frac{3}{4}\sqrt{\frac{5}{6\pi}}\sin^2\theta\, e^{2i\phi}$.

$$\text{The eigenstate } |322\rangle = \frac{1}{54}\sqrt{\frac{1}{\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}}\sin^2\theta\, e^{2i\phi}. \tag{C.6.3.10}$$

$|32-2\rangle, n_r = 0$.
The radial eigenfunction is given in (C.3.6.9). The spherical harmonic equals the one given for the state $|322\rangle$, except for the sign of ϕ.

The eigenstate $|32-2\rangle = \frac{1}{54}\sqrt{\frac{1}{\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}}\sin^2\theta\, e^{-2i\phi}$. (C.6.3.11)

$|321\rangle, n_r = 0$.

The radial eigenfunction is given by (C.6.3.9).

The spherical harmonic $Y_2^1 = C_{21}P_2^1 e^{i\phi} = 3\sqrt{\frac{5}{24\pi}}\sin\theta\cos\theta\, e^{i\phi}$.

The eigenstate $|321\rangle = \frac{1}{81}\sqrt{\frac{1}{\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}}\sin\theta\cos\theta\, e^{i\phi}$. (C.6.3.12)

$|32-1\rangle, n_r = 0$.

The radial eigenfunction is given by (C.6.3.9). The spherical harmonic equals the one given for the state $|321\rangle$, except for the sign of ϕ.

The eigenstate $|32-1\rangle = \frac{1}{81}\sqrt{\frac{1}{\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}}\sin\theta\cos\theta\, e^{-i\phi}$. (C.6.3.13)

$|320\rangle, n_r = 0$.

The radial eigenfunction is given by (C.6.3.9).

The spherical harmonic $Y_2^0 = C_{20}P_2^0 = \frac{1}{4}\sqrt{\frac{5}{\pi}}[3(\cos\theta)^2 - 1]$.

The eigenstate $|320\rangle = \frac{1}{162}\sqrt{\frac{2}{3\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}}[3(\cos\theta)^2 - 1]$. (C.6.3.14)

Now we found the 9 degenerate eigenstates with the same eigenvalue $E_3 = -\frac{E_{Ry}}{9}$.

The next step to take to find out about the Stark effect on these degenerated states.

What does the matrix looks like?

As mentioned before, Mahan discussed this in some detail at the end of section 6.3 page 169.

We have a 9×9 matrix of which we have to analyse $(81-9)/2$ elements or $\binom{9}{2}$ elements, the binomial coefficient. Mahan indicated most of the matrix elements to be zero due to parity. The diagonal elements are: $E_3 = -\frac{E_{Ry}}{9}$, and $E_{Ry} = \frac{e^2}{2a_0}$.

For the off-diagonal elements we have to evaluate the integral given in Eq. (6.12):

$\int d\tau \psi_l^* V \psi_m = \langle l|V|m\rangle \equiv V_{lm}$.

We develop this integral in some detail: $\int_0^\infty r^2\, dr \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\, \psi_l^* V \psi_m$. (C.6.3.15)

ψ_m is the representative of the 9 degenerate states derived above and $V = -eFr\cos\theta$.

What is the order of appearance of the elements in the matrix in order to find a matrix as diagonalized as possible? This can be done by trial and error. Mahan discussed this on page 169. However, I learned from (Styer, *The Stark Effect,* Chapter 16[2,3]) this to be covered by general rules :

$\langle nlm|r\cos\theta\,|nlm\rangle = 0$, the diagonal elements of V_{lm}, and

$\langle nlm|r\cos\theta\,|n'l'm'\rangle = 0$, with $\int_0^{2\pi} e^{\pm ik\phi} = 0$, for $k \geq 1$ and $\{k \in \mathbb{N}\}$. Furthermore: $k = m + m'$.

The matrix elements vanish unless $l = l' \pm 1$. The selection rule……It follows that the matrix

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[2] Available as draft Textbook, Pdf.

[3] For the Stark effect, linear and non-linear see also Fitzpatrick.

elements vanishes by symmetry when $l = l' = 0$. It's about integrating $\int_0^{\pi} \cos\theta d\theta = 0$.
These rules indicates the order of appearance of the eigenstates in the matrix elements:
$|300\rangle, |310\rangle, |320\rangle, |311\rangle, |321\rangle, |31-1\rangle, |32-1\rangle, |322\rangle, |32-2\rangle$.
The first row of the matrix and its non-zero off-diagonal elements are found by multiplying $\langle 300|$ subsequently with $|310\rangle, |320\rangle, |311\rangle, |321\rangle, |31-1\rangle, |32-1\rangle, |322\rangle, |32-2\rangle$ and $r\cos\theta$ sandwiched in between.
The second row of the matrix and its non-zero off-diagonal elements are found by multiplying $\langle 310|$ subsequently with $|320\rangle, |311\rangle, |321\rangle, |31-1\rangle, |32-1\rangle, |322\rangle, |32-2\rangle$ and $r\cos\theta$ sandwiched in between. And so on. Then we find for the matrix representation of the Hamiltonian $H_0 + V$, the diagonal elements included:

$$\begin{pmatrix}
E_3 & A & 0 & & & & & & \\
A & E_3 & B & & 0 & & & 0 & \\
0 & B & E_3 & & & & & & \\
 & & & E_3 & 0 & 0 & 0 & 0 & 0 \\
 & 0 & & 0 & E_3 & C & 0 & 0 & 0 \\
 & & & 0 & C & E_3 & 0 & 0 & 0 \\
 & & & 0 & 0 & 0 & E_3 & 0 & 0 \\
 & 0 & & 0 & 0 & 0 & 0 & E_3 & 0 \\
 & & & 0 & 0 & 0 & 0 & 0 & E_3
\end{pmatrix}.$$

Now the evaluation of the matrix reduces to find the integrals A, B, and C.
The matrix displays the block structure.
The results for the other integrals are (Styer):
$A = 3\sqrt{6}eFa_0, B = 3\sqrt{3}eFa_0, C = \frac{9}{2}eFa_0$.
The eigenvalues of the above 9×9 matrix give the energy levels and eigenstates:
$\lambda = E_3 + 9eFa_0$, degeneracy 1, $\frac{1}{\sqrt{2}}(|300\rangle + |310\rangle)$,
$\lambda = E_3 + \frac{9}{2}eFa_0$, degeneracy 2, $\frac{1}{\sqrt{2}}(|311\rangle + |321\rangle)$ and $\frac{1}{\sqrt{2}}(|31-1\rangle + |32-1\rangle)$,
$\lambda = E_3$, degeneracy 3, $|322\rangle, |32-2\rangle$ and $|320\rangle$,
$\lambda = E_3 - \frac{9}{2}eFa_0$, degeneracy 2, $\frac{1}{\sqrt{2}}(|311\rangle - |321\rangle)$ and $\frac{1}{\sqrt{2}}(|31-1\rangle - |32-1\rangle)$,
$\lambda = E_3 - 9eFa_0$, degeneracy 1, $\frac{1}{\sqrt{2}}(|300\rangle - |310\rangle)$.

6.4 Perturbation Theory.

In this section another technique is presented to find out about the perturbed Hamiltonian.

6.4.1 General Formulas.

The basic equation we will deal with is Eq. (6.13).
I assume E_n^0 in Eq. (6.86) should be read as $E_l^{(0)}$.
The Hamiltonian at the bottom of page 171 is based on the assumptions given in section 6.2.1 below Eq. (6.19): $E_1 = E_2$ and $V_{11} = V_{22}$.
The Hamiltonian is used to deal with degenerate states. It is not clear to me where the results of the analysis of the degenerate states enter the perturbation process. In the equations (6.111) and (6.112)?

Homework 8, 11, 12, 14.

Exercise 8.

In the perturbation theory solution, derive the second-order correction $C_{lm}^{(2)}$ to the wave function.

At the bottom of page 173 Mahan presented the two equations for second-order perturbation:

$$0 = D_2 = \left(E_n^{(0)} - E_l^{(0)}\right)C_{nl}^{(2)} + E_n^{(1)}C_{nl}^{(1)} + E_n^{(2)}C_{nl}^{(0)} - \sum_m V_{lm}C_{nm}^{(1)} \qquad (6.90)$$

and

$$0 = \sum_m \Re[2\, C_{nm}^{(0)*}C_{nm}^{(2)} + |C_{nm}^{(1)}|^2]\,. \qquad (6.103)$$

$\Re$ is the real part of the complex function.

So we have to find out about $E_n^{(2)}$ and $C_{nl}^{(2)}$.

$E_n^{(1)} = V_{nn}$, Eq. (6.107).

$C_{nl}^{(1)} = \frac{V_{ln}}{E_n^{(0)}-E_l^{(0)}}$, Eq. (6.110).

Mahan furthermore derived $E_n^{(2)}$. With $C_{nl}^{(0)} = \delta_{nl}$, we have $\left(E_n^{(0)} - E_l^{(0)}\right)C_{nl}^{(2)} + E_n^{(1)}C_{nl}^{(1)} = 0$ and using Eq. (6.110)

$$E_n^{(2)} = \sum_m V_{nm}C_{nm}^{(1)} = \sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n^{(0)}-E_m^{(0)}}. \qquad (6.113)$$

The eigenvalue $E_n = E_n^{(0)} + V_{nn} + E_n^{(2)}$. (6.114)

Now we need to find $C_{nl}^{(2)}$. To this end we use Eq. (6.103).

We know $C_{nm}^{(0)} = \delta_{nm}$ (a real number). So Eq. (6.103) gives us: $2C_{nn}^{(2)} + |C_{nn}^{(1)}|^2 = 0$, and from first order perturbation we have $C_{nn}^{(1)} = 0$. Consequently $C_{nn}^{(2)} = 0$.

For $n \neq l$, Eq. (6.90) leads to :

$$0 = \left(E_n^{(0)} - E_l^{(0)}\right)C_{nl}^{(2)} + E_n^{(1)}C_{nl}^{(1)} - \sum_m V_{lm}C_{nm}^{(1)}. \qquad (C.6.4.1.1)$$

Substitute $E_n^{(1)} = V_{nn}$, Eq. (6.107) and $C_{nl}^{(1)} = \frac{V_{ln}}{E_n^{(0)}-E_l^{(0)}}$, Eq. (6.110) into (C.6.4.1.1) we obtain

$$C_{nl}^{(2)} = -\frac{V_{nn}\,V_{ln}}{(E_n^{(0)}-E_l^{(0)})^2} + \frac{1}{E_n^{(0)}-E_l^{(0)}}\sum_{m\neq n}\frac{V_{lm}V_{mn}}{E_n^{(0)}-E_m^{(0)}}. \qquad (C.6.4.1.2)$$

We have to find the second order correction to the wave function.

The wave function: $\psi_n = \sum_m C_{nm}\,\phi_m$, Eq. (6.84) and

to second order $C_{nm} = C_{nm}^{(0)} + C_{nm}^{(1)} + C_{nm}^{(2)}$ derived from Eq. (6.85).

With $C_{nm}^{(0)} = \delta_{nm}$ the wave function approximation is:

$$\psi_n = \sum_m (C_{nm}^{(0)} + C_{nm}^{(1)} + C_{nm}^{(2)})\phi_m. \qquad (C.6.4.1.3)$$

Now we have all the ingredients for the wave function. Take care of the subscripts.

$C_{nm}^{(0)} = \delta_{nm}$,

$C_{nm}^{(1)} = \frac{V_{mn}}{E_n^{(0)}-E_m^{(0)}}$ and using (C.6.4.1.2)

$$C_{nm}^{(2)} = -\frac{V_{nn}\,V_{mn}}{(E_n^{(0)}-E_l^{(0)})^2} + \frac{1}{E_n^{(0)}-E_m^{(0)}}\sum_{m\neq n}\frac{V_{mm}V_{mn}}{E_n^{(0)}-E_m^{(0)}}.$$

Substitute these expressions into (C.6.4.1.3):

$$\psi_n = \phi_n + \sum_{m\neq n}\frac{1}{E_n^{(0)}-E_m^{(0)}}\left[V_{mn} + \left(\sum_{m\neq n}\frac{V_{mm}V_{mn}}{E_n^{(0)}-E_m^{(0)}}\right) - \frac{V_{nn}V_{mn}}{E_n^{(0)}-E_m^{(0)}}\right]\phi_m\ . \qquad (C.6.4.1.4)$$

Exercise 11.

For the helium atom, write
$H_0 = -\frac{\hbar^2}{2m}[\nabla_1^2 + \nabla_1^2] - 2e^2\left[\frac{1}{r_1} + \frac{1}{r_2}\right]$
and
$V = \frac{e^2}{|\vec{r_1} - \vec{r_2}|}$.
Estimate the ground-state energy from first-order perturbation theory.
The potential V is assumed to be the perturbation.
In section 5.7.3 the ground state of the helium atom is evaluated by means of the variational theory.
There the energy is found to be
$E = -5.695\ E_{Ry}$. To translate this into a perturbed part and the part without electron-electron interaction V we have
$E_1 = E_1^{(0)} + E_1^{(1)} = -8E_{Ry} + 2.305E_{Ry} = -5.695\ E_{Ry}$.
Now perturbation theory:
We can use various results obtained in section 5.7.3.
Again , the energy without electron-electron interaction $E_1^{(0)} = -8E_{Ry}$.
The section on general formulas for perturbation theory gives us the matrix element for the perturbation of the ground state $E_1^{(1)}$:
$E_1^{(1)} = V_{11}$.
Eq. (6.12) is the general presentation for the matrix element.
In our case: $V_{11} = \int d\tau \phi_1^*(r_1, r_2) V \phi_1(r_1, r_2)$. (C.6.4.1.5)
$\phi_1(r_1, r_2)$ is given by Eq. (5.238) with $\alpha = Z$ and $V = \frac{e^2}{|\vec{r_1} - \vec{r_2}|}$.
Then $V_{11} = \int d\tau \phi_1^*(r_1, r_2) V \phi_1(r_1, r_2) = e^2 \int d^3r_1 \int d^3r_2 \frac{|\phi_1(r_1, r_2)|^2}{|\vec{r_1} - \vec{r_2}|}$. Eq.(5.252)
We have to evaluate the integral: $e^2 \int d^3r_1 \int d^3r_2 \frac{|\phi_1(r_1, r_2)|^2}{|\vec{r_1} - \vec{r_2}|}$.
For completeness I summarize the ingredients for $\phi_1(r_1, r_2)$:
$\phi_1(r_1, r_2) = \phi_1(r_1)\phi_1(r_2)$,
$\phi_1(r) = \phi_{1s}(r) = \frac{1}{\sqrt{4\pi a_0^3}} 2Z^{3/2} e^{-Zr/a_0}$. [Eq. (5.129) and Eq. (5.140)]
Keep in mind Eq.(5.140) to be given for the hydrogen atom: $Z = 1$.
The evaluation is presented by Mahan on page 140. The result is represented by Eq. (5.262).
Substitution of $Z = 2$ for α and the normalization integral $I = 1$ in Eq. (5.262) lead to
$V_{11} = \frac{5}{2} E_{Ry}$.
Now with $E_1^{(1)} = V_{11}$
$E_1 = E_1^{(0)} + E_1^{(1)} = -8E_{Ry} + \frac{5}{2} E_{Ry} = -5.5E_{Ry}$.
This result is even higher than that found by variational calculation: $-5.695\ E_{Ry}$. The latter result being less than 2% too high (Mahan).

Exercise 12.

Consider a hydrogen atom that has added a delta-function potential $V(r) = \lambda\delta(r)/r^2$. If λ is small, how does this perturb the energy levels of the atom? Are states with different angular momenta affected differently?

Remark: Although λ is small, is $V(r) = \lambda\delta(r)/r^2$ to be considered a strong potential in the core region at small values of r? See page 154 Mahan.

The hydrogen atom has a high degree of degeneracy.

So we have to find out how to deal with:

$\psi_n = \sum_m \phi_m$, where ϕ_m represents the m-th state of the unperturbed Hamiltonian and m is the principal quantum number and summation index.

Let us first look for the matrix elements resulting from the added delta-function potential.

Mahan used the subscripts l, m as summation indices. I will use the summation indices i and j to prevent confusion with the angular quantum numbers.

The matrix element $V_{ij} = \lambda \int d\tau \phi_i^* \frac{\delta(r)}{r^2} \phi_j$. (C.6.4.1.6)

ϕ_i is a product of the radial eigenfunction and the angular eigenfunction $F(\theta, \phi)$.

With the principal quantum number $i = l_i + n_{r_i} + 1$, l_i is the angular quantum number of state i and n_{r_i} is the radial quantum number of state i.

$\delta(r)$ "works" on functions dependent on r. In our case the radial eigenfunction. (See section 5.4.3 Hydrogen Eigenfunctions, Mahan). For the principal quantum number i the radial eigenfunction is:

$$R_i = N_i \left(\frac{r}{a_0}\right)^{l_i} e^{-\frac{r}{ia_0}} L_{n_{r_i}}^{(2l_i+1)} \left[\frac{2r}{ia_0}\right], \qquad \text{(C.6.4.1.7)}$$

and the associated Laguerre polynomial

$$L_{n_{r_i}}^{(2l_i+1)} = \sum_{k=0}^{n_{r_i}} \binom{n_{r_i} + 2l_i + 1}{n_{r_i} - k} \frac{\left(\frac{2r}{ia_0}\right)^k}{k!} \ . \qquad \text{(C.6.4.1.8)}$$

For the matrix element we have to evaluate (C.6.4.1.6),which can be written as:

$$V_{ij} = \lambda \int_0^{2\pi} d\phi \int_0^{\pi} d\theta F^*(\theta, \phi) F(\theta, \phi) \sin\theta \int_0^{\infty} dr r^2 R_i^* \frac{\delta(r)}{r^2} R_j, \qquad \text{(C.6.4.1.9)}$$

here ϕ in $F(\theta, \phi)$ represents the angle.

Due to the delta-function potential we have only a contribution at $r = 0$. Consequently, $l_i = 0$ in (C.6.4.1.7) and $k = 0$ contributes in (C.6.4.1.8).

So $i = l_i + n_{r_i} + 1$ gives $n_{r_i} + 1 = i$.

The contribution of the radial eigenfunction to the matrix element reduces into a number $R_i = N_i(n_{r_i} + 1) = iN_i$.

As mentioned by Mahan(page 123), N_i is a normalization constant. For the states with the angular quantum number $l_i = 0$ and $k = 0$ (in the Laguerre polynomial) we find for the normalization constant $N_i = 2(\frac{1}{i})^{3/2}$.

Now the angular eigenfunction $F(\theta, \phi)$. We know this to be a spherical harmonic.

Since $l_i = 0$, we have for the spherical harmonic $F(\theta, \phi) = Y_0^0 = \frac{1}{\sqrt{4\pi}}$.

Hence the matrix element $V_{ij} = \lambda ij N_i N_j / 2$, (C.6.4.1.10)

where $\int_0^{\infty} dr \delta(r)$ is set equal to ½.

Note: This is based on $\int_{-\infty}^{\infty} \delta(x) dx = 1$, and

$\int_{-\infty}^{\infty} \delta(x)\, dx = \int_{-\infty}^{0} \delta(x) dx + \int_{0}^{\infty} \delta(x) dx = -\int_{0}^{-\infty} \delta(x) dx + \int_{0}^{\infty} \delta(x) dx$.
With $\delta(-x) = \delta(x)$, $\int_{0}^{-\infty} \delta(-x) d(-x) + \int_{0}^{\infty} \delta(x) dx = 2 \int_{0}^{\infty} \delta(x) dx.$
ij represents the product of the principle quantum numbers i and j.

For example, $V_{11} = 2\lambda$. To find this, use have been made of the normalization of the radial eigenfunction with $i = 1$ and consequently $n_{r_i} = 0$; $i = l_i + n_{r_i} + 1$.
Then with help of the general formulas of section (6.4.1), we find for the perturbation of the ground state eigenvalue $E_1^{(1)} = V_{11} = 2\lambda$; Eq.(6.107). Hence, the lowest energy correction goes linear with the amplitude of the delta-function potential:
$E_1 = -E_{Ry} + 2\lambda$.
Is there a correction for the ground state ψ_1? According to the general formulas there is.
Eq. (6.112): $\psi_1^{(1)} = \phi_1 + \sum_{i \neq 1} \frac{\phi_i V_{i1}}{\frac{E_{Ry}}{i^2} - E_{Ry}}$. Well the problem arises with ϕ_i: an eigenfunction with the lowest degeneracy of $4 (i = 2)$.
Mahan: "*For degenerate states ………… just diagonalize the Hamiltonian matrix that contains all the degenerate states*";(page173). All degenerate states, all values of n? *„Da spricht Mahan ein grosses Wort gelassen aus (Goethe)*". Fitzpatrick dealt with this problem uses rules derived from the non-linear Stark effect. What to do? Mahan analysed the linear Stark effect in section 6.3. Let us deal with the simplest case $n = 2$ as Mahan did for the Stark effect.
For this case the degeneracy is 4.
The states are $\phi_{200}, \phi_{211}, \phi_{210}$, and ϕ_{21-1}. (C.6.4.1.11)
The 4×4 matrix has, besides the non-perturbed diagonal elements $E_2 = -E_{Ry}/4$, in addition due to the delta-function perturbation a non-zero contribution of the pair of elements ϕ_{200}.
Completely similar to the derivation of the matrix element V_{ij} given by (C.6.4.1.10), the additional matrix element $M = \lambda/2$ for $n = 2$.
To construct the 4×4 determinant the order of appearance of the states is given by (C.6.4.1.11). Then we find for the determinant with the eigenvalue α:

$$\begin{vmatrix} E_2 + M - \alpha & 0 & 0 & 0 \\ 0 & E_2 - \alpha & 0 & 0 \\ 0 & 0 & E_2 - \alpha & 0 \\ 0 & 0 & 0 & E_2 - \alpha \end{vmatrix} = 0.$$

The four eigenvalues are: $\alpha = E_2 + \lambda/2, E_2, E_2, E_2$.
The four eigenstates are: $\phi_{200}, \phi_{211}, \phi_{210}$, and ϕ_{21-1}. Now we have a degeneracy of 3.
What happens is, the energy level of ϕ_{200} is increased by $\lambda/2$. The states with angular momenta $\neq 0$ are not affected.
What about $n = 3$? In this case ϕ_{300} is affected. Then we have a 9×9 determinant. Instead of a degeneracy 9, the degeneracy becomes 8 and the energy level of ϕ_{300} is increased by $\frac{2\lambda}{3}$. The states with angular momenta $\neq 0$ are not affected.
Remark: the question of the ground state has not been answered. We found from perturbation theory a shift in the energy level of 2λ. What could happen to the ground state?

The general expression for the ground state is: $\psi_1 = R_1(r)Y_0^0(\theta, \phi)$.
The differential equation for the radial part is, with $l = 0$, $\chi_1(r) = rR_1(r)$ and Eq. (5.57),

$$\left[\frac{d^2}{dr^2} - \frac{\lambda\delta(r)}{r^2} + \frac{2me^2}{\hbar^2 r} + \frac{2mE_1}{\hbar^2}\right] \chi_1(r) = 0.$$

Hence, for the ground state we will find a radial eigenfunction $R_1(r)$ different from the unperturbed radial eigenfunction , Eq. (5.129), $R_{1s} = 2e^{-r/a_0}$.

Exercise 14.
A small charge $Q(Q \ll e)$ is placed a long distance $R(R \gg a_0)$ from a hydrogen atom. What is the leading term , in powers of $1/R$, of the energy change in the system. Compare this to the classical result.
We shall use the notation of **exercise 12.**
The radial wave function is given by the Eqs. (C.6.4.1.7) and (C.6.4.1.8). To prevent confusion with the radial eigenfunction, the long distance R is denoted by r_0 .
For the matrix element we have to evaluate (C.6.4.1.6), which can be written as:

$$V_{ij} = -Q^2 \int_0^{2\pi} d\phi \int_0^{\pi} d\theta F^*(\theta, \phi) F(\theta, \phi) \sin\theta \int_0^{\infty} dr r^2 R_i^* \frac{1}{|r - r_0|} R_j, \tag{C.6.4.1.12}$$

here ϕ in $F(\theta, \phi)$ represents the angle.
Let us start with the ground state energy .
The radial eigenfunction is $R_1 = 2e^{-r/a_0}$ (eq. (5.129)) and the angular eigenfunction $F = Y_0^0 = \frac{1}{\sqrt{4\pi}}$.
With respect to the perturbation, proportional to $\frac{1}{|r - r_0|}$, we know the perturbation to depend on r, both angles θ and ϕ; the spherical coordinates. As mentioned by Mahan(page 139 and 140), the angular part must be evaluated carefully.
In general $|r - r_0| = \sqrt{r^2 + r_0^2 - 2rr_0 \cos\theta \cos\phi}$.
I shall not present the details. However, I just mention here the angular part is not easily to be evaluated. I could not find exact solutions. The WolframAlpha app runs out of computing time. There is an elegant solution to this problem. By locating the charge Q at the z-axis, $|r - r_0|$ no longer depends on the angle ϕ. As a consequence, we can use the analysis of Mahan presented on page 140.
Hence, we first evaluate the θ part of the integral in (C.6.1.4.12).
We find with Eq. (5.256):

$$\int_0^{\pi} \frac{\sin\theta d\theta}{\sqrt{r^2 + r_0^2 - 2rr_0 \cos\theta}} = \frac{1}{rr_0}[r + r_0 - |r - r_0|] = \frac{1}{r_>} \ . \tag{C.6.4.1.13}$$

So (C.6.4.1.12) becomes:

$$V_{11} = -2Q^2 \int_0^{\infty} r^2 \, e^{-2r/a_0} \frac{1}{r_>} dr. \tag{C.6.4.1.14}$$

Now we have to look at the integration interval, since
for $r < r_0$, $\frac{1}{r_>} = \frac{2}{r_0}$,
and for $r > r_0$, $\frac{1}{r_>} = \frac{2}{r}$.
With these expressions for integration we have for the matrix element:

$$V_{11} = -4Q^2\{\int_0^{r_0} \frac{r^2}{r_0} e^{-\frac{2r}{a_0}} dr + \int_{r_0}^{\infty} r e^{-2r/a_0} dr\} ,$$

And this results into $V_{11} = -\frac{Qa_0^3}{r_0}(1 - \frac{r_0}{a_0} e^{-\frac{2r_0}{a_0}})$.

Hence the leading term in the energy change of the ground state for $\frac{r_0}{a_0} \gg 1$ is, $\frac{Qa_0^3}{r_0}$.

Now for the principal quantum number 2.

To find out about the energy change we have to evaluate a 4×4 matrix where it is not clear to me on beforehand which matrix elements are zero due to parity.

The states to be considered are:

$R_{2s} = \left(\frac{1}{2}\right)^{\frac{3}{2}} \left(1 - \frac{r}{a_0}\right) e^{-\frac{r}{a_0}}$, $Y_0^0 = \frac{1}{\sqrt{4\pi}}$,

$R_{2p} = \frac{1}{\sqrt{4!}} \frac{r}{a_0} e^{-\frac{r}{2a_0}}$, $Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\phi}$,

$R_{2p} = \frac{1}{\sqrt{4!}} \frac{r}{a_0} e^{-\frac{r}{2a_0}}$, $Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$ and

$R_{2p} = \frac{1}{\sqrt{4!}} \frac{r}{a_0} e^{-\frac{r}{2a_0}}$, $Y_1^{-1} = \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{-i\phi}$.

Analyses of the matrix elements results into 10 off-diagonal elements to be zero. For the resulting two off-diagonal elements and the four diagonal elements I could not find exact solutions. WolframAlpha did not produce results either: computing timed out.

The question to compare the result with the classical result I did not understand. Is there an energy shift in the classical result?

I leave this exercise.

6.4.2 Harmonic Oscillator in Electric Field.

In this section Mahan presented the classical solution and the exact quantum mechanical solution for the one-dimensional case.

The Hamiltonian for a charged particle is:

$H = \frac{p^2}{2m} + \frac{K}{2} x^2 + Fx$. This can be rewritten as:

$$H = \frac{p^2}{2m} + \frac{K}{2}(x + \frac{F}{K})^2 - \frac{F^2}{2K} \ . \qquad (6.119)$$

Choose the new $x' = x + \frac{F}{K}$.

Schrödinger's equation can be written as:

$\left[\frac{p^2}{2m} + \frac{K}{2}(x')^2\right] \psi(x') = E'\psi(x')'$,

where $E' = E + \frac{F^2}{2K}$.

Given these both equations and the analysis of section 2.3 the eigen values and eigen functions are found: Eqs. (6.120) and (6.121). For completeness I will present these :

The eigenfunctions $\psi_n = \phi_n\left(x + \frac{F}{K}\right)$,

and

The eigenvalues $E_n = \hbar\omega\left(1 + \frac{1}{2}\right) - \frac{F^2}{2K}$, $\omega^2 = \frac{K}{m}$.

Then Mahan solved the same problem with perturbation theory.

Second order perturbation theory gives the exact eigenvalue. However, all orders of perturbation theory are needed to give the exact eigenfunction, Mahan.

Homework 9, 10.

Exercise 9.

In the perturbation theory solution, derive the third order $E_n^{(3)}$. Verify that it gives zero for the perturbation $V = Fx$ on the harmonic oscillator.

In order to find out about $E_n^{(3)}$, we have to collect the expressions with $l = 3$ in Eq. (6.84). In this way the expression for $E_n^{(3)}$ is:

$$\left(E_n^{(0)} - E_l^{(0)}\right)C_{nl}^{(3)} + E_n^{(3)}C_{nl}^{(0)} + E_n^{(2)}C_{nl}^{(1)} + E_n^{(1)}C_{nl}^{(2)} - \sum_m V_{lm}C_{nm}^{(2)} = 0. \qquad \text{(C.6.4.2.1)}$$

We know $C_{nl}^{(0)}$ to be δ_{nl}. In order to find $E_n^{(3)}$ form (C.6.4.2.1) we must set $n = l$.

Eq. (6.108) gives us $C_{nn}^{(1)} = 0$.

As given by Mahan second-order perturbation gives for $C_{nn}^{(2)}$, see bottom of page 173:

$0 = \sum_m \Re[2\, C_{nn}^{(0)*}C_{nn}^{(2)} + |C_{nn}^{(1)}|^2]$, consequently $C_{nn}^{(2)} = 0$.

So the expression for $E_n^{(3)}$ reduces to:

$$E_n^{(3)} = \sum_m V_{nm}C_{nm}^{(2)}. \qquad \text{(C.6.4.2.2)}$$

To complete the expression for $E_n^{(3)}$ we have to obtain $C_{nm}^{(2)}$.

$C_{nm}^{(2)}$ is given by Eq. (6.90). Now we have all the ingredients. From Eq. (6.90) we have, keeping in mind $n \neq l$ or $n \neq m$,

$$\left(E_n^{(0)} - E_m^{(0)}\right)C_{nm}^{(2)} + E_n^{(1)}C_{nm}^{(1)} + E_n^{(2)}C_{nm}^{(0)} - \sum_m V_{mm}C_{nm}^{(1)} = 0. \qquad \text{(C.6.4.2.3)}$$

With $E_n^{(2)}C_{nm}^{(0)} = 0$ and $E_n^{(1)}C_{nm}^{(1)} = V_{nn}\frac{V_{mn}}{E_n^{(0)}-E_m^{(0)}}$, Eqs. (6.107) and (6.110),

$$C_{nm}^{(2)} = -V_{nn}\frac{V_{mn}}{\left(E_n^{(0)}-E_m^{(0)}\right)^2} + \frac{1}{E_n^{(0)}-E_m^{(0)}}\sum_m V_{mm}\frac{V_{mn}}{E_n^{(0)}-E_m^{(0)}} . \qquad \text{(C.6.4.2.4)}$$

(C.6.4.2.2) and (C.6.4.2.4) give the third order $E_n^{(3)}$.

The next question is to verify $E_n^{(3)} = 0$ for the perturbation $V = Fx$ on the harmonic oscillator.

In section 6.4.2 Mahan analysed the harmonic oscillator up to the second order perturbation. The result concerning this exercise is: $V_{nm} = 0$ for $m \neq n \pm 1$. So in (C.6.4.2.4) V_{mm} and V_{nn} equal zero.

Hence $C_{nm}^{(2)} = 0$ and $E_n^{(3)} = 0$, (C.6.4.2.2).

Exercise 10.

The exact eigenvalue spectrum in one dimension for the potential:

$\frac{M}{2}[\omega_0^2 + \Omega^2]x^2$,

is

$E_n = \hbar\sqrt{\omega_0^2 + \Omega^2}\left(n + \frac{1}{2}\right)$.

Divide the Hamiltonian according to

$H = H_0 + V$, with

$H_0 = \frac{p^2}{2M} + \frac{M}{2}\omega_0^2 x^2$, and $V = \frac{M}{2}\Omega^2 x^2$.

Treat V as a perturbation to H_0 . Find the contribution to the energy in first- and second-order perturbation theory. Successive term should correspond to expanding the exact result in a Taylor series:

$E_n = \hbar\sqrt{\omega_0^2 + \Omega^2}\left(n + \frac{1}{2}\right) = \hbar\omega_0\left(n + \frac{1}{2}\right)\left[1 + \frac{\Omega^2}{2\omega_0^2} + \cdots\right].$

We can use the analysis of the harmonic oscillator given in sections 2.3 and 6.4.2 .

So we have $E_n^{(0)} = \hbar\omega_0\left(n + \frac{1}{2}\right)$, Eq. (6.123), the unperturbed eigenvalue.

Furthermore, the perturbation contributes to the eigenvalue $E_n^{(1)}$, Eq. (6.107) and $E_n^{(2)}$, Eq(6.113). Given these expressions, we need to evaluate the matrix elements.

These are $V_{nm} = \frac{M}{2}\Omega^2\langle n|x^2|m\rangle$. (C.6.4.2.5)

In section 2.3 the matrix element is given in Eq. (2.132):

$\langle n|x^2|m\rangle = \frac{x_0^2}{2}[\sqrt{n(n-1)}\delta_{n,m+2} + \sqrt{(n+1)(n+2)}\delta_{n,m-2} + (2n+1)\delta_{n,m}]$. (C.6.4.2.6)

Where $x_0 = \sqrt{\frac{\hbar}{M\omega_0}}$. (C.6.4.2.7)

Then

$m = n-2, \langle n|x^2|m\rangle = \frac{x_0^2}{2}\sqrt{n(n-1)}$, (C.6.4.2.8)

$m = n+2, \langle n|x^2|m\rangle = \frac{x_0^2}{2}\sqrt{(n+1)(n+2)}$, (C.6.4.2.9)

and

$m = n, \langle n|x^2|m\rangle = \frac{x_0^2}{2}(2n+1).$ (C.6.4.2.10)

Otherwise $\langle n|x^2|m\rangle = 0$.

Let us start with first order.

$E_n^{(1)} = V_{nn}$, Eq. (6.107).

Hence, with (C.6.4.2.5) and (C.6.4.2.10),

$E_n^{(1)} = \frac{M}{2}\Omega^2\frac{x_0^2}{2}(2n+1).$

With (C.6.4.2.6), the preceding expression can be written as

$E_n^{(1)} = \frac{\hbar}{4}\frac{\Omega^2}{\omega_0}(2n+1).$ (C.6.4.2.11)

To first order

$E_n = E_n^{(0)} + E_n^{(1)}.$

This becomes, with the zeroth, Eq. (6.123), and first order, (C.6.4.2.11), of the eigenvalues:

$E_n = \hbar\omega_0\left(n + \frac{1}{2}\right) + \frac{\hbar}{4}\frac{\Omega^2}{\omega_0}(2n+1) = \hbar\omega_0\left(n + \frac{1}{2}\right)\left[1 + \frac{1}{2}\frac{\Omega^2}{\omega_0^2}\right].$ (C.6.4.2.12)

Now for the second order contribution to the perturbation: $E_n^{(2)}$, Eq(6.113).

$E_n^{(2)} = \sum_{m\neq N}\frac{|V_{nm}|^2}{E_n^{(0)} - E_m^{(0)}}$.

The two terms contributing to this summation are given by (C.6.4.2.8) and (C.6.4.2.9).

Hence $E_n^{(2)} = (\frac{M}{2}\Omega^2\frac{x_0^2}{2})^2\left[\frac{(n+1)(n+2)}{\hbar\omega_0(n-n-2)} + \frac{n(n-1)}{\hbar\omega_0(n-n+2)}\right]$. (C.6.4.2.13)

With (C.6.4.2.7), we have:

$E_n^{(2)} = -\frac{\hbar}{16}\frac{\Omega^4}{\omega_0{}^3}(2n+1).$ (C.6.4.2.14)

The contribution to the energy in first- and second-order:

$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)}$ becomes with the expressions found for $E_n^{(1)}$, (C.6.4.2.11), and $E_n^{(2)}$, (C.6.4.2.13):

$$E_n = \hbar\omega_0\left(n+\frac{1}{2}\right) + \frac{\hbar\,\Omega^2}{4\,\omega_0}(2n+1) - \frac{\hbar}{16}\frac{\Omega^4}{{\omega_0}^3}(2n+1).$$

This can be written as

$$E_n = \hbar\omega_0\left(n+\frac{1}{2}\right)\left[1+\frac{1}{2}\frac{\Omega^2}{\omega_0^2}-\frac{1}{8}\frac{\Omega^4}{\omega_0^4}\right].$$

The first three terms of the Taylor expansion of the exact result.

6.4.3 Continuum States.

Mahan presents in this section the procedure for continuum states. As an example, Mahan showed the results of perturbation theory for the Yukawa potential without bound states. The eigenvalues are not perturbed. The eigenstates are.

On page 179 Mahan gave the eigen function for the special case with wave number $\boldsymbol{k}$ equal to zero: Eqs. (6.148) and (6.149). Use has been made of: $E(Q) = \hbar^2Q^2/2m$.

Homework 13.

Exercise 13.

Consider the change in the continuum wave function using first order perturbation theory for the case that $V(r)$ is a repulsive square well($V(r) = V_0$ for $r < a$). Find $V(\vec{Q})$. Evaluate (6.147) when $\vec{k} = 0$.

Remark: in section 5.3.1 (Mahan) on Central Potentials this problem of a repulsive square well is dealt with for $E < V_0$. The solutions for the radial part of the eigenfunctions are considered. The angular solutions are spherical harmonics. Inside the square well is a decaying exponential function represented by a spherical Bessel function with imaginary argument. For $a < r$ the solution for the radial eigenfunction is presented by spherical Bessel functions, a phase shift included. In Exercise 4 of that chapter the s-wave is calculated.

Here we consider the continuum wave function: no bound states.

Mahan: “Then $\phi(\vec{k},\vec{r})$ =exp$(i\vec{k},\vec{r})$.”

The perturbation is the repulsive potential.

Mahan: “The first step, always, is to calculate the matrix elements. For plane waves eigenfunctions, the matrix element is just the Fourier transform of the potential.”

Like Mahan I will use the overbar to present the transform.

The transform of the perturbation potential is:

$$\bar{V}(\vec{k}-\vec{k'}) = \int d^3r\, e^{-i\vec{r}.(\vec{k}-\vec{k'})}V_0 \qquad \text{(C.6.4.3.1)}$$

Mahan: ”The integral is evaluated first by doing the angular integrals. Define $v = \cos\theta$, where θ is the angle between $\vec{r}$ and $\vec{Q} = \vec{k} - \vec{k'}$ “:

With (C.6.4.3.1) we have

$$\bar{V}(Q) = 2\pi\int_0^a r^2\,dr\int_{-1}^1 dv\, e^{-irQv}\,, \qquad \text{(C.6.4.3.2)}$$

using Eq. (6.142) , (C.6.4.3.2) becomes :

$$\bar{V}(Q) = \frac{4\pi V_0}{Q}\int_0^a r\sin(Qr)dr \qquad \text{(C.6.4.3.3)}$$

Integration of (C.6.4.3..3) gives us:

$$\bar{V}(Q) = \frac{4\pi V_0}{Q^3}[-Qa\cos(Qa) + \sin(Qa)]\,. \qquad \text{(C.6.4.3.4)}$$

So we found $\bar{V}(Q)$.

The next step is to evaluate Eq.(6.147) for $\vec{k} = 0$. With $\vec{k'} = \vec{k} - \vec{Q}$ and leaving out the symbol for the principal part of the denominator, Eq. (6.147) can be written as:

$$\psi(0,\vec{r}) = \frac{1}{\sqrt{\Omega}}\left\{1 - \int \frac{d^3Q}{(2\pi)^3}\frac{\bar{V}(Q)e^{-i\vec{Q}.\vec{r}}}{-E(-Q)}\right\}. \qquad \text{(C.6.4.3.5)}$$

Then with $E(Q) = \hbar^2 Q^2/2m$ and (C.6.4.3.4) we obtain:

$$\psi(0,\vec{r}) = \frac{1}{\sqrt{\Omega}}\{1 - \frac{4mV_0}{\pi\hbar^2 r}\int_0^\infty \frac{dQ}{Q^4}[Qa\cos(Qa) - \sin(Qa)]\sin(Qr)\} \qquad \text{(C.6.4.3.6)}$$

The angular integral in (C.6.4.3.5)is given by Eq. (6.142).

Well, as mentioned by Mahan, the integral in (C.6.4.3.6) can be evaluated by contour integration or by looking up the results in tables.

First I evaluated both function $Qa\cos(Qa)\sin(Qr)/Q^4$ and $\sin(Qa)\sin(Qr)/\,Q^4$ separately with the WolframAlpha app. Then you will find both integral do not converge. Together the WolframAlpha did not conclude the calculations in a reasonable time.

The possible next step is to rewrite (C.6.4.3.6):

$$\psi(0,\vec{r}) = \frac{1}{\sqrt{\Omega}}\{1 - \frac{4mV_0}{\pi\hbar^2 r}\int_0^\infty \frac{dQ}{2Q^4}[Qa\sin(Q(r-a)) + \mathrm{Qa}\sin\big(Q(r+a)\big) - \cos\big(Q(r-a)\big) - \cos(Q(r+a))]\}. \qquad \text{(C.6.4.3.7)}$$

Is this an improvement?

In tables you can find integrals like $\int x^n\cos(\,bx)dx$ expressed in gamma functions. I do not know whether this applies for $n < 0$.

Thinking about this I was wondering, keeping in mind the calculations with the WolframAlpha app, whether another way of representing the integral in (C.6.4.3.6) could be of some help reducing calculation time:

$$\int_0^\infty \frac{dQ}{Q^4}\Big[Qa\cos(Qa) - \sin(Qa)\Big]\sin(Qr) = \int_0^\infty dQ\Big[\frac{a^2r}{Q}\frac{\cos(Qa)}{Qa}\frac{\sin(Qr)}{Qr} - \frac{ar}{Q^2}\frac{\sin(Qa)}{Qa}\frac{\sin(Qr)}{Qr}\Big].$$

This integral can be rewritten with spherical Bessel functions

$j_0(Qa) = \frac{\sin(Qa)}{Qa}$, $j_0(Qr) = \frac{\sin(Qr)}{Qr}$ and $\frac{\cos(Qa)}{Qa} = \frac{j_{0(Qa)}}{Qa} - j_1(Qa)$.

Then we have for the above integral:

$$\int_0^\infty dQ\Big[\frac{a^2r}{Q}\left(\frac{j_{0(Qa)}}{Qa} - j_1(Qa)\right)j_0(Qr) - \frac{ar}{Q^2}j_0(Qa)j_0(Qr)\Big] \qquad \text{(C.6.4.3.8)}$$

Using again WolframAlpha, the integral becomes $-\pi a^3$ for $r > a$.

Hence with this result and (C.6.4.3.6) we have

$$\psi(0,\vec{r}) = \frac{1}{\sqrt{\Omega}}\left\{1 + \frac{4ma^3V_0}{\hbar^2 r}\right\}. \qquad \text{(C.6.4.3.9)}$$

Now the question is on the table: in what way does this result relates to the asymptotic expansion of Eq. (5.86). This equation represents the exact solution of the above problem for $\vec{k} \to 0$.

Using the result of exercise 4 of chapter 5 for the phase shift δ_0 and Eq. (5.86), the result for the radial part of the wave function with $\vec{k} \to 0$ is:

$R(r) = C[1 + \frac{a}{r} - \frac{1}{\alpha r}\tanh \alpha a]$ for $r > a$.
In this equation C is a constant. The $1/r$ behaviour is found.

6.4.4 Green's Function

In this section an alternative procedure to evaluate the first-order change in the eigenfunction of continuum states is presented. The procedure is based on Green's function. The first-order change in the eigenfunction is given by Eq. (6.153), equal to the third part of the right-hand side of Eq.(6.138). And eq. (6.154) is equal to Eq. (6.140), where $V(r')$ in Eq(6.140) is represented by the Yukawa potential.
Keep in mind Mahan, in the evaluation of Green's function, replaced $\vec{r} - \overrightarrow{r'}$ by r in the Eqs. (6.156) and (6.157). The first-order change in the eigenfunction is given by Eq. (6.158). This should be equal to the first-order change represented by the second term of the right hand side of Eq.(146).
Then, on page 181 Mahan writes: " *We evaluate this (Eq.(6.158) ,Nz) for the Yukawa potential. Again, the integral is hard to evaluate for general values of $\vec{k}$ and $\vec{r}$."* Hence Mahan did not evaluate Eq. (6.158). Instead he looked for a simple result: the behaviour at large r . The result is given in Eq. (6.162).

6.5 The Polarizability.

Mahan mentioned *the polarizability easily applied to objects that have no permanent dipole.* The relation between the induced dipole moment and the applied field F_ν is presented in Eq. (6.163). This equation describes the relation between the dipole moment and the applied electric field by means of the constant $\alpha_{\mu\nu}$. The subscript denotes the coordinates.
Note: usually $\mu\nu$ are used to describe four-vectors in special relativity(Susskind, 2).
$\alpha_{\mu\nu}$ is a tensor.

6.5.1 Quantum Definition

Mahan defined polarizability using the ground-state energy of the object in the external field F_ν .
Eq. (6.165):
$\Delta E = -\int \vec{P} \cdot d\vec{F} = -\int F_\mu \alpha_{\mu\nu} dF_\nu = -\frac{1}{2} F_\mu \alpha_{\mu\nu} F_\nu$,
with the Einstein summation convention.
Mahan presented, Eq. (6.166), the polarization for spherical symmetric systems. A polynomial in F^2.
In Eq. (6167) the effect of nonlinear terms in Eq. (6.163) are presented.
Using second order perturbation theory, the energy shift is presented in Eq. (6.168).
In Eq.(6.168) the first order result reflects the perturbation for molecules with a fixed dipole moment. As mentioned by Mahan, this agrees with the result of classical physics.
Eq. (6.169) gives the exact definition of polarizability.

In this section the polarizability of an electron in the ground state of hydrogen is discussed. The expression for the polarizability to be evaluated is presented by Eq. (6.173) page 184.

Mahan mentioned the popular approximation to be the replacement of the summation in Eq. (6.173) by the first term in the summation. Reference is made to chapter 5 page 124, the section on Hydrogen eigenfunctions, Eq. (5.142):

$\langle 2p_z|z|1s\rangle = a_0 \frac{2^{15/2}}{3^5} = 0.745 \cdot a_0,$

with a_0 the Bohr radius.

With this expression and the expression for the energy, the polarizability α ,Eq. (6.175), is obtained.

Up to the middle of page 185, Mahan dis cussed the approximations of the polarizability.

Fitzpatrick, Graduate Course presented an approximation in section 7.4 on the *Quadratic Stark Effect*:

- approximation Mahan : $\alpha = 4a_0^3$,
- approximation Fitzpatrick: $\alpha = 5.3a_0^3$.

For hydrogen, an exact solution can be obtained by solving Schrodinger's equation in parabolic coordinates.

As mentioned by Mahan, top of page 186, "*An exact result for the polarizability is obtained using the formula for the first order change in the eigenfunction",* Eq. (6.182).

I suppose, this is about the general formula in section 6.4.1 on *General Formulas*, Eq. (6.112).

On the pages 186-188 the exact result for the polarizability is obtained.

Homework 15

Exercise 15

Calculate the exact polarizability α of an electron bound to an alpha-particle.

Note: on page 185 Mahan writes "*Hydrogen is the only atom for which the polarizability can be derived exactly."* So?

The formula of the polarizability of a particle in state n is presented in Eq.(6.169).

6.6 van der Waals Potential

The van der Waals potential energy is presented in Eq. (6.211).

The van der Waals force is generally weak. For neutral objects that have no long range Coulomb interaction, the van der Waals interaction provides the longest-range force…… The van der Waals force exists beyond the range of chemical bonding.

The interaction Hamiltonian is presented in Eq. (6.213).

With the dipole interaction denoted by Eq. (6.214), the interaction Hamiltonian H_{AB} between the two objects A and B is expanded in Taylor series to second- order in the relative distances, Eq. (6.215). The resulting interaction Hamiltonian is presented in Eq.(6.216) and gives the van der Waals interaction.

Then, Mahan introduced perturbation theory, Eqs. (6.217) and (6.218).

It is assumed that the eigen functions for the separate objects exist and form a complete set, Eqs. (6.219)-(6.221).

A product eigenfunction is considered to be a valid representation and used in Eq.(6.225), the first order perturbation energy. This energy appeared to be zero.

The van der Waals potential energy is derived from second order perturbation theory, Eq.(6.226).

6.7 Spin-Orbit Interaction

The magnetic moment of a particle with spin is presented in Eq. (6.243).
The form of the interaction is given in Eq. (6.246). At the top of page 195 Mahan derived (6.246) in phenomenological way, so to speak. A classical field theory approach(Susskind, 2).

6.7.1 Spin-Orbit in Atoms

Spherical symmetric potentials are used.
Spin-orbit interaction is described by Eqs. (6.252) and (6.253).
Mahan used the technique of the coupling of spins for the coupling of spin and angular momentum.
It is a problem about the coupling of orbital angular momentum and spin angular momentum. Since, Mahan analysed electrons, it is about the coupling of angular momentum l and $s = \frac{1}{2}$.[4]
The relevant equations for the quantum numbers l and s are Eqs. (6.256)-(6.259).
The first order perturbation equation is presented in Eq. (6.260).
The possible states are presented in Eqs. (6.261) and (6.262).
The splitting of the energy level of the p-state is illustrated in Figure 6.5. There are two states, one with a degeneracy of 4 and one with a degeneracy of 2. The six states are given by Eqs. (6.266) and (6.267). Use has been made of Table 4.1 page 105., the Glebsch-Gordon coefficients for $j = \frac{3}{2}$ and $j = \frac{1}{2}$. These quantum numbers represent the summation of spin angular- and orbital momentum.
On page 198 another way to determine the influence of the spin-orbit interaction is to diagonalize the matrix, The Matrix Method section 6.2, similar to the coupled spin problem in section 6.2.2. Mahan concludes the matrix method to present the correct result.

6.7.2 Alkali Valence electron in Electric Field

In this section a more complicated and realistic example of the role of electric fields is discussed. The application of an electric field for the outer electron in an alkali atom is analysed. It is about one electron, since the closed shell is considered to be harmless. Eight states are included: the ground state and the first exited state.
On page 200, the 8×8 matrix is obtained and analysed. The results are presented in Figure 6.6 page 202.

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[4] The subject matter is also dealt with by Fitzpatrick in The Graduate Course Chapter 6 *Addition of Angular Momentum,* and in The Undergraduate Course in Chapter 11 of the same title. In chapter 12, of the same Course about time independent perturbation theory, the perturbation dealt with is due to relativistic effects. The splitting of the unperturbed energy levels are presented: the fine structure of Hydrogen. Presented by Mahan on page 168, The Stark Effect.

This section concludes with the remark the alkali atom in an electric field to be typical for the response to external perturbations.

6.8 Bound Particles in Magnetic Fields.

The magnetic field has only a small influence on the energy states. Consequently, perturbation theory is an adequate instrument to evaluate this influence.
The magnetic field can be treated as a constant over the space to be considered: the space of the atom.
The unperturbed Hamiltonian and the perturbation are presented in the Eqs.(6.290)-(6.292).
The magnetic field enters the Hamiltonian as a vector potential, see Chapter 5. The symmetric gauge is used.
The result for the perturbation potential is given in Eq.(6.296).
The perturbation potential consists of three expressions, Eq.(2.9.7).
They are the starting point for perturbation theory.

6.8.1 Magnetic Susceptibility

The magnetic susceptibility χ plays the role for the magnetic field that is analogous to the electron polarizability α for electric field.
The energy shifts of first an second order are presented in Eqs. (6.300) and (6.302) respectively.

6.8.2 Alkali Atom in Magnetic Field

Mahan presented an example of magnetic phenomena for alkali atoms.
It is about one electron outside a closed shell. So, the single electron can be studied.
Three interactions are considered:
-spin-orbit,
-Pauli,
-Landau.
The interaction Hamiltonian is presented in Eq. (304).
The resulting matrix, Eq.(305) is analysed.
The splitting is shown in Figure 6.7 .

6.8.3 Zeeman Effect

The weak field response is called the Zeeman effect. The modification of the Hamiltonian is due to the external magnetic field.
The expectation value of the interaction Hamiltonian is given in Eq.(6.315).
With this expectation value, the various energy shifts are calculated and presented at the top of page 209).

6.8.4 Paschen-Back Effect.

This is about very large magnetic fields. The magnetic interaction is the dominant term: the mirror reverse of the procedure for the Zeeman effect.

Homework.

After reading Exercise 15, I leave Mahan

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