Sakurai Ch.6 Problems 1-7

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1 Sakurai 6.1

A. N identical spin $1/2$ *particles are subjected to a one-dimensional simple harmonics oscillator potential. What is the ground-state energy? What is the Fermi energy?*

The particles are spin $1/2$ and only fermions have half-integer spin. Fermions also obey the Pauli exclusion principle, which states that no two fermions can occupy the same state. Thus, not all the particles will occupy the ground state energy of the 1D harmonic oscillator. They end up piling up on each other until they are pushed up to higher and higher energy states. If you begin counting at $n = 0$ for the 1st particle, and $n = 1$ for the 2nd particle, then both occupy the lowest energy($(1/2)\hbar\omega$), one particle having spin up, and one having spin down. Therefore, it is best to say you have a total of $N/2$ particles and sum up only the spin up(or spin down) and multiply the sum by 2. Then you will have the total sum of energies for all the particles, where the nth energy level is:

$$E_n = (n + 1/2)\hbar\omega$$

First I will sssume I have an even total number of particles, 2 for each energy state. I will start summing at $n = 0$ and the sum will go to $N/2-1$. So, summing up the energies of the particles for $N/2$ particles and multiplying by 2 yeilds:

$$E_{grdEven} = 2\sum_{n=0}^{N/2-1}(n + 1/2)\hbar\omega = 2\hbar\omega\frac{N}{2}[\frac{(1/2) + (N/2 - 1) + 1/2)}{2}] = \frac{N^2}{4}\hbar\omega$$

If you assume that we have an odd number of total particles, then sum will go to $N/2 - 1/2$ because there is only one in the top energy state. It is the last fermion that is the odd one out in the most energetic state.

$$E_{grdOdd} = 2\sum_{n=0}^{N/2-1/2}(n+1/2)\hbar\omega = 2\hbar\omega\frac{N}{2}[\frac{1/2 + N/2 - 1/2 + 1/2}{2}] = \frac{N^2 + N}{4}\hbar\omega$$

What is the Fermi energy?

The Fermi energy is the maximum or highest state of energy that is occupied. Cohen-Tannoudji [p.1398] defines the Fermi energy as the highest individual energy found in the ground state. The unluckiest fermion with the highest energy is the last one marked $N/2 - 1$. Its energy is found using E_n.

$$E_{FermiEven} = (N/2 - 1 + 1/2)\hbar\omega = (N-1)\frac{\hbar\omega}{2}$$

For an odd number of particles, the highest individual energy found is held by the fermion marked $N/2 - 1/2$. Its energy can also be plugged into E_n.

$$E_{FermiOdd} = (N/2 - 1/2 + 1/2)\hbar\omega = \frac{N}{2}\hbar\omega$$

B. What are the ground state and Fermi energies if we ignore the mutual interactions and assume N to be very large?

If N is very large, then it doesn't really matter whether we have an even or an odd number of particles. One extra particle isn't going to make much difference when we are talking about such a huge energy. Thus, the ground state energies (as well as the Fermi energies) for both an odd and even amount of particles can be approximated to be the same:

$$\text{As } N \to \infty \text{ then } \; E_{Fermi} = \frac{N}{2}\hbar\omega \; \text{ and } \; E_{ground} = \frac{N^2}{4}\hbar\omega$$

2 Sakurai 6.2

It is obvious that two nonidentical spin 1 particles with no orbital angular momenta (that is, s-states for both) can form j=0, j=1, and j=2. Suppose, however, that the two particles are identical. What restrictions do we get?

It is not obvious to the novice quantum mechanics student that j=0, j=1, and j=2 for total angular momentum formed for two nonidentical spin 1 particles with l=0. A careful derivation of:

$$J = j_1 + j_2, j_1 + j_2 - 1, j_1 + j_2 - 2, ..., |j_1 - j_2|$$

is given in Cohen-Tannoudji 1977, p. 1017, that explains the pattern and why the total angular momentum ranges from $J = s_1 + s_2 = 0$ (if one particle is spin -1 and the other is spin +1) to $J = s_1 + s_2 = 2$ (if both particles are spin +1). Thus leading to the values, 0, 1, and 2. A more simple walk-through is given by Griffiths p. 167, but he also refers to the proof of Cohen-Tannoudji.

Spin 1 particles are bosons. Empirically, a system of N identical particles that are totally symmetrical under the interchange of any pair are called bosons. Thus, the total wavefunctions we are dealing with are symmetric under interchange. The l=0 requirement dictates that the spatial wavefunction is symmetric. Thus we need to impose the restriction that only symmetric Clebsch-Gordon combinations are allowed, i.e. that only symmetric spin wave functions are allowed.

For the values of j=0, 1, and 2, the following expression for changing the order of the two particles is useful:

$$\langle j_2, j_1; m_2, m_1 | j, m \rangle = (-1)^{j_1+j_2-j} \langle j_1, j_2; m_1, m_2 | j, m \rangle$$

This symmetry relation is found in Cohen-Tannoudji p. 1041. Here the sign is of most concern. If the sign is positive, then the interchange is symmetric. If the sign is negative, then the interchange is antisymmetric and should be disregarded. In our case, both particles are spin 1, $j_1 = j_2 = s = 1$ therefore the sign term is $(-1)^{2-j}$. For various values of j only even values will create a symmetric interchange of particles. Therefore only the states with j=0, and j=2 are allowed.

3 Sakurai 6.3

Discuss what would happen to the energy levels of a helium atom if the electron were a spinless boson. Be as quantitative as you can.

This problem illustrates a quantuum mechanical effect due to particle identity. Assuming that the electron has a symmetric wave function under interchange, i.e. is a boson, and that its spin happens to be zero, we have a situation very similiar to the spin singlet state for the helium atom. The spin singlet state has total spin zero, $-1/2 + 1/2 = 0$ and a symmetric space function. For the spin singlet case, the electrons have a tendency to come close to each other resulting in appreciable electrostatic repulsion and more excitation (higher energy levels). As for a quantitative description, the spatial wave function is always symmetrical(thus $I + J$ and not $I - J$), and the energy of state (1s)(nl) is:

$$E = E_{100} + E_{nlm} + \Delta E$$

with

$$\Delta E = \langle \frac{e^2}{r_{12}} \rangle = I + J$$

where both I and J are positive defined in Sakurai (6.4.19):

$$I = \int d^2x_1 \int d^3x_2 |\psi_{100}(x_1)|^2 |\psi_{nlm}(x_2)|^2 \frac{e^2}{r_{12}}$$

$$J = \int d^2x_1 \int d^3x_2 \psi_{100}(x_1)\psi_{nlm}(x_2) \frac{e^2}{r_{12}} \psi^*_{100}(x_2)\psi^*_{nlm}(x_1)$$

This should push the energy levels higher for the helium atom, leaving the ground state the same.

4 Sakurai 6.4

Three spin 0 particles are situated at the corners of an equilateral triangle. Let us define the z-axis to go through the center and in the direction normal to the plane of the triangle. The whole system is free to rotate about the z-axis. Using statistics considerations, obtain restrictions on the magnetic quantum numbers corresponding to J_z.

In this problem the wave function is symmetric under the interchange of any two particles, because we are dealing with bosons. So, if you rotate the triangle to interchange the particles positions, say particle 1 goes to 2's position, particle 2 goes to 3's position and particle 3 goes to 1's position, then you have rotated the triangle 120°. This rotation is represented by the rotation operator given by Sakurai (3.1.16):

$$\mathcal{D}_z(\phi) = exp(\frac{-iJ_z\phi}{\hbar}) \text{ where } J_z = m_z\hbar$$

thus the operator becomes

$$\mathcal{D}_z(120^\circ) = exp(-im_z\frac{2\pi}{3})$$

The wavefunction of the system will be unchanged after this rotation because you can't tell the particles apart from each other, they are identical!

$$exp(-im_z\frac{2\pi}{3})|\psi\rangle = |\psi\rangle$$

This happens when

$$exp(-m_z\frac{2\pi}{3}) = 1$$

therefore; because of Euler's relation $e^{-i2\pi n} = cos(2\pi n) - isin(2\pi n) = 1$;

$$m_z = \text{ any multiple of 3}$$

5 Sakurai 6.5

Consider three weakly interacting, identical spin 1 particles.
a. Suppose the space part of the state vector is known to be symmetric under interchange of any pair. Using notatin $|+\rangle|0\rangle|+\rangle$ *for particle 1 in* $m_s = +1$, *particle 2 in* $m_s = 0$, *particle 3 in* $m_s = +1$, *and so on, construct the normalized spin states in the following three cases:*
(i) All three of them in $|+\rangle$
(ii) Two of them in $|+\rangle$, *one in* $|0\rangle$.
(iii) All three in differenet spin states.
What is the total spin in each case?
b. Attempt to do the same problem when the space part is antisymmetric under

interchange of any pair.

The spin wave function must be symmetric in these cases. If all three particles are in the $|+\rangle$ state, the ket is aleady symmetric and normalized, with total spin 3:

$$X_1 = |+\rangle|+\rangle|+\rangle$$

If two are in $|+\rangle$ and one in $|0\rangle$, the total spin is 2, with notation:

$$X_2 = \frac{1}{\sqrt{3}}(|+\rangle|+\rangle|0\rangle + |+\rangle|0\rangle|+\rangle + |0\rangle|+\rangle|+\rangle)$$

If all three are in different states, then the notation is:

$$X_3 = \frac{1}{\sqrt{6}}(|+\rangle|-\rangle|0\rangle + |+\rangle|0\rangle|-\rangle + |0\rangle|+\rangle|-\rangle + |0\rangle|-\rangle|+\rangle + |-\rangle|+\rangle|0\rangle + |-\rangle|0\rangle|+\rangle)$$

This is essentially equation (6.5.23) in Sakurai. From Sakurai p. 373, there are 10 dimensions for symmetry in the 3 primitive object group, or 10 symmetrical states:

$$\begin{array}{|c|c|c|}\hline 1&1&1\\\hline\end{array}\quad\begin{array}{|c|c|c|}\hline 1&1&2\\\hline\end{array}\quad\begin{array}{|c|c|c|}\hline 1&1&3\\\hline\end{array}\quad\begin{array}{|c|c|c|}\hline 1&2&2\\\hline\end{array}\quad\begin{array}{|c|c|c|}\hline 1&2&3\\\hline\end{array}$$

$$\begin{array}{|c|c|c|}\hline 1&3&3\\\hline\end{array}\quad\begin{array}{|c|c|c|}\hline 2&2&2\\\hline\end{array}\quad\begin{array}{|c|c|c|}\hline 2&2&3\\\hline\end{array}\quad\begin{array}{|c|c|c|}\hline 2&3&3\\\hline\end{array}\quad\begin{array}{|c|c|c|}\hline 3&3&3\\\hline\end{array}$$

Where only the $\begin{array}{|c|c|c|}\hline 1&2&3\\\hline\end{array}$ and $\begin{array}{|c|c|c|}\hline 2&2&2\\\hline\end{array}$ states have $m_J = 0$, because $+1+0+-1 = 0$ and $0+0+0 = 0$. Sakurai mentions that $\begin{array}{|c|c|c|}\hline \ & \ & \ \\\hline\end{array}$ contains both $j = 3$(seven states) and $j = 1$(three states). Therefore X_3 is a mixed j=3 and j=1 state.

For part B., the space part is antisymmetric and that means that (i) and (ii) are not possible because:

$$\begin{array}{|c|}\hline 1\\\hline 1\\\hline 1\\\hline\end{array}\ \text{and}\ \begin{array}{|c|}\hline 1\\\hline 1\\\hline 2\\\hline\end{array}$$

do not increase as you go down, violating the rules of Young's Tableaux.

For the case of all three being in different states (iii) is the singlet J = 0 state. The best way to get this is from a convenient trick used for constructing completely antisymmetric wave functions, the Slater determinant, which in this case is:

$$\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array} = \frac{1}{\sqrt{3!}}\begin{vmatrix} |+\rangle_1 & |0\rangle_1 & |-\rangle_1 \\ |+\rangle_2 & |0\rangle_2 & |-\rangle_2 \\ |+\rangle_3 & |0\rangle_3 & |-\rangle_3 \end{vmatrix}.$$

This yeilds the antisymmetric spin function:

$$\begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline 3 \\ \hline \end{array} = \frac{1}{\sqrt{6}}(|+\rangle|0\rangle|-\rangle - |+\rangle|-\rangle|0\rangle + |0\rangle|-\rangle|+\rangle - |0\rangle|+\rangle|-\rangle + |-\rangle|+\rangle|0\rangle - |-\rangle|0\rangle|+\rangle)$$

6 Sakurai 6.6

Suppose the electron were a spin $\frac{3}{2}$ particle obeying Fermi-Dirac statistics. Write the configuration of a hypothetical Ne (Z = 10) atom made up of such 'electrons' [that is, the analog of $(1s)^2(2s)^2(2p)^6$]. Show that the configuration is highly degenerate. What is the ground state (the lowest term) of the hypothetical Ne atom in spectroscopic notation($^{2S+1}L_j$, where S, L, and J stand for the total spin, the total orbital angular momentum, and the total angular momentum, respectively) when exchange splitting and spin-orbit splitting are taken into account?

Sakurai states on p. 251 that for an atomic electron, each level should be expected to have a $2j + 1$ fold rotational degeneracy as long as there is no external electric or magnetic field. So for a fixed l=0, such as in the s orbital, $s+l = 3/2+0 = j$. When $j = 3/2$, there is a $2j+1 = 2(3/2)+1 = 4$ multiplicity. To find out how many of these crazy electrons can be held in each s,p,d,f etc orbital the formula $4n^2$ works, as opposed to $2n^2$ for when the electrons are not crazy. For instance:

$$\begin{aligned}
(2s+1)(2l+1) &= (2(1/2)+1)(2(0)+1) &&= 2 \text{ electrons in s orbital} \\
(2s+1)(2l+1) &= (2(1/2)+1)(2(1)+1) &&= 6 \text{ electrons in p orbital} \\
(2s+1)(2l+1) &= (2(1/2)+1)(2(2)+1) &&= 10 \text{ electrons in d orbital} \\
(2s+1)(2l+1) &= (2(1/2)+1)(2(3)+1) &&= 14 \text{ electrons in f orbital}
\end{aligned}$$

$2n^2$ = number of electrons held at energy level, $2+6+10+14 = 2n^2 = 2(4)^2 = 32$

This is not the whole story, as Griffiths puts it,[p.190] because electron-electron repulsion throws the counting off, but its good enough for our purposes. So, in the case of dealing with crazy electrons that have 3/2 spin, the counting will go differently:

$$\begin{aligned}
(2s+1)(2l+1) &= (2(3/2)+1)(2(0)+1) &&= 4 \text{ electrons in s orbital} \\
(2s+1)(2l+1) &= (2(3/2)+1)(2(1)+1) &&= 12 \text{ electrons in p orbital} \\
(2s+1)(2l+1) &= (2(3/2)+1)(2(2)+1) &&= 20 \text{ electrons in d orbital} \\
(2s+1)(2l+1) &= (2(3/2)+1)(2(3)+1) &&= 28 \text{ electrons in f orbital}
\end{aligned}$$

$4n^2$ = number of electrons held at energy level, $4+12+20+28 = 4n^2 = 4(4)^2 = 64$

So for a hypothetical Ne with 10 hypothetical 3/2 spin electrons, the analog of $(1s)^2(2s)^2(2p)^6$ is:

$$(1s)^4(2s)^4(2p)^2$$

This configuration is highly degenerate because there are so many possible states of spin and orbital angular momentum available. This follows from $C(12, 2) = 12!/((12 - 2)!2!) = 66$, where we have 4 different values of S, 3 different values of L, and 2 electrons. Because there are 2 valence electrons, each with spin 3/2, the possible total spin follows:

$$S = s_1 + s_2, s_1 + s_2 - 1, s_1 + s_2 - 2, ..., |s_1 - s_2| = 3, 2, 1, 0$$

The total orbital angular momentum also follows:

$$L = l_1 + l_2, l_1 + l_2 - 1, l_1 + l_2 - 2, ..., |l_1 - l_2| = 2, 1, 0$$

There is a restriction on the possible states because the electrons we are dealing with are still fermions and are subject to the Pauli exclusion principle. The angular momentum and spin configurations must be antisymmetric under particle exchange, leading to spin and spatial functions having opposite parity. With L_{even} symmetric, L_{odd} antisymmetric, S_{even} antisymmetric, and S_{odd} symmetric the possible states are only:

$$|S, L\rangle = \begin{array}{lll} |3,1\rangle & = (2*3+1)(2*1+1) & = 21 \quad \text{states} \\ |2,2\rangle & = (2*2+1)(2*2+1) & = 25 \quad \text{states} \\ |2,0\rangle & = (2*2+1)(2*0+1) & = 5 \quad \text{states} \\ |1,1\rangle & = (2*1+1)(2*1+1) & = 9 \quad \text{states} \\ |0,2\rangle & = (2*0+1)(2*2+1) & = 5 \quad \text{states} \\ |0,0\rangle & = (2*0+1)(2*0+1) & = 1 \quad \text{state} \end{array}$$

Which adds up to 66 states, (very highly degenerate). Hund's rule says that the state with the largest possible value of S is the most stable state, and stability decreases with decreasing S. So the state with $S = 3$ has the lowest energy and thus will be used for the ground state. The orbital angular momentum and spin will be in opposite directions. The lowest J lies in the lowest energy, thus $J = |L - S| = 2$. With L=1, S=3, and J=2, the formula for spectroscopic notation becomes:

$$^{2S+1}L_j \quad = \quad ^{2(3)+1}1_2 \quad = \quad ^7P_2$$

7 Sakurai 6.7

Two identical spin $\frac{1}{2}$ fermions move in one dimension under the influence of the infinite-wall potenital $V = \infty$ for $x < 0$, $x > L$, and V=0 for $0 \leq x \leq L$.
a. Write the ground-state wave function and the ground-state energy when the two particles are constrained to a triplet spin state(ortho state).
b. Repeat (a) when they are in a singlet spin state (para state).
c. Let us no suppose that the two particles interact mutually via a very short-range attractive potential that can be approximated by

$$V = -\lambda\delta(x_1 - x_2) \quad (\lambda > 0)$$

Assuming that perturbation theory is valid even with such a singular potential, discuss semiquantitatively what happens to the energy levels obtained in (a) and (b).

The ortho state or triplet spin state is symmetrical [as explained on p.363], thus the space part of the wave function will be antisymmetrical to agree with Fermi-Dirac statistics (6.3.6). We are after the ground state wavefunction which by the way, for a single particle in the infinite well potential is:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x)$$

with ground state energy:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

with $n = 1$ for the ground state. For two fermions though, the antisymmetrical ground state wave function is:

$$\psi_{grd} = \frac{1}{\sqrt{2}}[\omega_1(x_1)\omega_2(x_2) - \omega_1(x_2)\omega_2(x_1)]$$

Plugging in for the values of the ω's

$$\textbf{Triplet}: \quad \psi_{grd} = \frac{\sqrt{2}}{L}[\sin\frac{\pi x_1}{L}\sin\frac{2\pi x_2}{L} - \sin\frac{\pi x_2}{L}\sin\frac{2\pi x_1}{L}]$$

with ground state energy:

$$E_{grd} = E_1 + E_2 = \frac{\pi^2\hbar^2}{2mL^2} + \frac{2^2\pi^2\hbar^2}{2mL^2} = \frac{5\pi^2\hbar^2}{2mL^2}$$

For the para state, or singlet spin state, we have an antisymmetrical spin function. Therefore, using the same Fermi-Dirac statistics, we need a symmetrical space part of the wave function:

$$\psi_{grd} = \frac{1}{\sqrt{2}}[\omega_1(x_1)\omega_1(x_2) + \omega_1(x_2)\omega_1(x_1)] = \frac{2}{\sqrt{2}}[\omega_1(x_1)\omega_1(x_2)]$$

after normalization (because there is only 1 term!)

$$\textbf{Singlet}: \quad \psi_{grd} = \omega_1(x_1)\omega_1(x_2) = \frac{2}{L}\sin\frac{\pi x_1}{L}\sin\frac{\pi x_2}{L}$$

with ground state energy:

$$E_{grd} = E_1 + E_1 = \frac{\pi^2\hbar^2}{mL^2}$$

As for the interaction via a perturbation $V = -\lambda\delta(x_1 - x_2)$ the energy level changes can be explored using first order perturbation theory: $E' = \langle\psi_0|V|\psi_0\rangle$.

The triplet state has a shift:

$$E'_{triplet} = \int dx_1 dx_2 \frac{-\lambda}{2}[\omega_1(x_1)\omega_2(x_2) - \omega_1(x_2)\omega_2(x_1)]^2 \delta(x_1 - x_2)$$

This is going to be zero no matter what, because for the particles to actually interact, they must be at the same position, to avoid the delta function being zero, but if they are at the same position, then $\omega_1(x_1)\omega_2(x_2) - \omega_1(x_2)\omega_2(x_1)$ becomes $\omega_1(x)\omega_2(x) - \omega_1(x)\omega_2(x) = 0$. Therefore, semiquantitatively,

$$E'_{triplet} = 0$$

The singlet state has a shift:

$$E'_{singlet} = -\int dx_1 dx_2 |\omega_1(x_1)\omega_1(x_2)|^2 \lambda\delta(x_1 - x_2)$$

This will actually have an answer because to interact the particles need to be at the same place, and when that happens the symmetric space function doesnt go to zero, it follows

$$\begin{aligned} E'_{singlet} &= -\int dx_1 dx_2 \frac{4}{L^2}[\sin\frac{\pi x_1}{L}\sin\frac{\pi x_2}{L}]^2 \lambda\delta(x_1 - x_2) \\ &= -4\frac{\lambda}{L^2}\int dx \sin^4\frac{\pi x}{L} \\ &= -4\frac{\lambda}{L^2}\int_0^L dx \sin^4\frac{\pi x}{L} \end{aligned}$$

and because

$$\int_0^L dx \sin^4\frac{\pi x}{L} = \frac{3}{8}L - \frac{\sin 2\frac{\pi}{L}L}{4\frac{\pi}{L}} + \frac{\sin 4\frac{\pi}{L}L}{32\frac{\pi}{L}} = \frac{3}{8}L$$

the shift in energy is finally,

$$E'_{singlet} = -4\frac{\lambda}{L^2}(\frac{3}{8}L) = -\frac{12\lambda}{8L} = -\frac{3\lambda}{2L}$$