

Solutions to Tutorial Sheet 8

† denotes an online-only bonus question.

1. † *A helium atom has two electrons in states nlm and $n'l'm'$. Write down wavefunctions which are antisymmetric with respect to exchange, and calculate the degeneracy for all combinations with $n = 1$, $n' \leq 3$.*

We will expand the spatial wavefunctions in a basis of products of single particle states. We will expand the spin wavefunctions likewise, then the total wavefunction will be an antisymmetric product of spin and spatial. We will ignore normalisation.

Note that the exchange here is with respect to the particle labels, it should not be confused with the parity operator ($\mathbf{r} \rightarrow -\mathbf{r}$) despite each using the same symbol for the operator (\hat{P}_{12}).

Labelling the electron positions r_1, r_2 , using one-particle hydrogenic orbitals u_{nlm} as a basis, and ignoring electron-electron interactions, there are two degenerate spatial states $\Phi_1 = |u_{nlm}(r_1)u_{n'l'm'}(r_2)\rangle$ and $\Phi_2 = |u_{n'l'm'}(r_1)u_{nlm}(r_2)\rangle$. Under the exchange interaction we have

$$P_{12}\Phi_1 = \Phi_2; \quad P_{12}\Phi_2 = \Phi_1$$

So the appropriate linear combinations come from diagonalising the matrix:

$$\mathbf{P}_{12} = \begin{pmatrix} \langle \Phi_1 | P_{12} | \Phi_1 \rangle & \langle \Phi_1 | P_{12} | \Phi_2 \rangle \\ \langle \Phi_2 | P_{12} | \Phi_1 \rangle & \langle \Phi_2 | P_{12} | \Phi_2 \rangle \end{pmatrix}$$

To give spatial eigenfunctions $\Phi_1 + \Phi_2$ ($P_{12} = 1$) and $\Phi_1 - \Phi_2$. ($P_{12} = -1$)

For the spin, we have four possible products of one-particle states: $\uparrow\uparrow, \downarrow\uparrow, \uparrow\downarrow, \downarrow\downarrow$, which gives an matrix representation for the exchange operator:

$$\mathbf{P}_{12} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and exchange eigenstates: $\uparrow\uparrow, (\downarrow\uparrow + \uparrow\downarrow), \downarrow\downarrow$ with $P_{12} = 1$, $(\downarrow\uparrow - \uparrow\downarrow)$ with $P_{12} = -1$.

To get antisymmetric wavefunctions, we need $P_{12}^{space} P_{12}^{spin} = -1$. the allowed combinations are then:

$$\begin{aligned} &(\Phi_1 + \Phi_2)(\downarrow\uparrow - \uparrow\downarrow) \\ &(\Phi_1 - \Phi_2)\uparrow\uparrow \\ &(\Phi_1 - \Phi_2)(\downarrow\uparrow + \uparrow\downarrow) \\ &(\Phi_1 - \Phi_2)\downarrow\downarrow \end{aligned}$$

There are also four symmetric ($P_{12}^{space} P_{12}^{spin} = 1$) combinations which are not permitted for fermions.

Note further that if $nlm = n'l'm'$, then $(\Phi_1 - \Phi_2) = 0$, so only one state exists.

Degeneracy, ignoring electron-electron interactions: $n = 1$ and

$n' = 1$: $1 (u_{100}(r_1)u_{100}(r_2))(\downarrow\uparrow - \uparrow\downarrow)$

$n' = 2$: $4 \times 2 \times 4/2 = 16$: All (4) permutations above for u_{100} with each of u_{200} u_{210} u_{211} u_{21-1} , both (2) symmetric and antisymmetric cases, combined with any of the (4) spin wavefunctions, reduced by a factor of two since only the overall antisymmetric wavefunctions are allowed.

$n' = 3$: $9 \times 2 \times 4/2 = 36$ All (9) permutations above for u_{100} with each of u_{300} u_{310} u_{311} u_{31-1} u_{320} u_{321} u_{322} u_{32-1} u_{32-2} , then as above.

2. † *In muonic helium, one of the electrons is replaced by a muon. Write down the appropriate wavefunctions for states equivalent to those in question 1.*

In muonic helium, the muon and electron are distinguishable, so the wavefunction does not have to be an eigenstate of \hat{P}_{12} . Defining $\Phi_1 = |u_{nlm}(r_1)u_{n'l'm'}(r_2)\rangle$ and $\Phi_2 = |u_{n'l'm'}(r_1)u_{nlm}(r_2)\rangle$, with r_1 and r_2 the electron and muon positions respectively.

There are then eight possible wavefunctions

$$\begin{aligned} &(\Phi_1)(\downarrow\uparrow), \quad (\Phi_1)(\uparrow\uparrow), \quad (\Phi_1)(\uparrow\downarrow), \quad (\Phi_1)(\downarrow\downarrow), \\ &(\Phi_2)(\downarrow\uparrow), \quad (\Phi_2)(\uparrow\uparrow), \quad (\Phi_2)(\uparrow\downarrow), \quad (\Phi_2)(\downarrow\downarrow) \end{aligned}$$

For the ground state, each particle in $|u_{100}\rangle$, $\Phi_1 = \Phi_2$ and there are only four different states.

For excited states with electron in $|u_{nlm}\rangle$ and muon in $|u_{n'l'm'}\rangle$, we have always Φ_1 .

For $n = 1$, $n' = 2$ we have two degenerate states for the electron (from spin) and $4 \times 2 = 8$ for the muon. There is no restriction from exchange, so we have 16 degenerate states. $n = 2$, $n' = 1$ also has 16, by the same reasoning.

For $n = 1$, $n' = 3$ we have two degenerate states for the electron (from spin) and $9 \times 2 = 18$ for the muon. There is no restriction from exchange, so we have 36 degenerate states. $n = 2$, $n' = 1$ also has 36, by the same reasoning.

There are also similar numbers of states with the muon in nlm and the electron in $n'l'm'$, but these have different energy and are not degenerate with the states above.

3. *The isotropic harmonic oscillator in 3 dimensions is described by the Hamiltonian*

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{r}^2$$

where $\hat{p}^2 \equiv \underline{\hat{p}} \cdot \underline{\hat{p}}$ and $\hat{r}^2 \equiv \underline{\hat{r}} \cdot \underline{\hat{r}}$. By writing \hat{H} as

$$\hat{H} = \sum_i \left\{ \frac{\hat{p}_i^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_i^2 \right\} \quad i = 1, 2, 3$$

show that the eigenfunctions of \hat{H} are simply products of 1-dimensional oscillator eigenfunctions. Assuming the usual formula for the energy eigenvalues of a 1-dimensional harmonic oscillator, show that the eigenvalues of \hat{H} are given by

$$E_n = \left(n + \frac{3}{2}\right)\hbar\omega \quad n = 0, 1, 2, \dots$$

Writing $\hat{H} = \sum_i \hat{H}_i$ with

$$\hat{H}_i = \left\{ \frac{\hat{p}_i^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}_i^2 \right\}$$

it is easy to show that the eigenfunctions of \hat{H} are simply products of 1-dimensional oscillator eigenfunctions. Consider such a product. Let

$$U_n(x_1, x_2, x_3) \equiv u_{n_1}(x_1) u_{n_2}(x_2) u_{n_3}(x_3)$$

where the 1-dimensional eigenfunctions $u_{n_i}(x_i)$ satisfy the eigenvalue equations

$$\hat{H}_i u_{n_i}(x_i) = E_{n_i} u_{n_i}(x_i), \quad i = 1, 2, 3$$

and the eigenvalues are given by the usual formula for the 1-dimensional harmonic oscillator:

$$E_{n_i} = \hbar\omega \left(n_i + \frac{1}{2}\right), \quad n_i = 0, 1, 2, 3, \dots$$

Then

$$\begin{aligned} \hat{H}U_n &= \left(\hat{H}_1 + \hat{H}_2 + \hat{H}_3\right) u_{n_1}(x_1)u_{n_2}(x_2)u_{n_3}(x_3) \\ &= \left(E_{n_1} + E_{n_2} + E_{n_3}\right) u_{n_1}(x_1)u_{n_2}(x_2)u_{n_3}(x_3) \equiv E_n U_n \end{aligned}$$

where

$$E_n \equiv E_{n_1} + E_{n_2} + E_{n_3} = \hbar\omega \left(n_1 + n_2 + n_3 + \frac{3}{2}\right) \equiv \left(n + \frac{3}{2}\right) \hbar\omega$$

and we have defined

$$n \equiv n_1 + n_2 + n_3$$

Since each of n_1, n_2, n_3 takes integer values $0, 1, 2, \dots$ etc., the same is true of n . However, any given value of n can in general be obtained in several ways, giving rise to degeneracy as illustrated in the following table:

n	n_1	n_2	n_3	degeneracy, g_n
0	0	0	0	1
1	1	0	0	3
	0	1	0	
	0	0	1	
2	2	0	0	6
	0	2	0	
	0	0	2	
	1	1	0	
	1	0	1	
	0	1	1	

If two identical, spin 1/2, fermions are placed in the 3D-SHO potential, what is the degeneracy of the first excited state?

The ground state is non-degenerate. Both electrons are in the same $n=0$ state, so the spatial wavefunction is exchange-symmetric, which means the spin must be the antisymmetric singlet.

The first excited state has one electron in $n=0$ and one in $n=1$. There are six possible states, three symmetric and three antisymmetric. Combined with appropriate spin singlets or triplets this gives $(3 \times 1 + 3 \times 3) = 12$ states.

The second excited state may have one electron in $n=0$ and one in $n=2$. There are six possible states, 3 symmetric and 3 antisymmetric. Combined with appropriate spin singlets or triplets this gives $(3 \times 1 + 3 \times 3) = 12$ states.

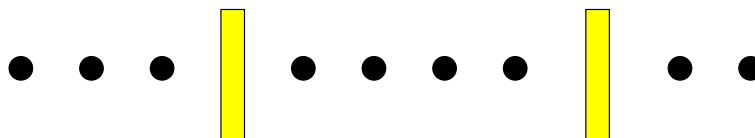
Or it may have two excitations with $n=1$, either both on the same electron, or one on each. This is a bit more complicated as there are 9 permutations. Of these, six have the electrons in different spatial states leading to $(6 \times 1 + 6 \times 3) = 24$ states. Three combinations have the electrons in the same spatial state: as with the ground state these must be singlets, so there are only three of them.

This gives a total of $12+24+12= 48$ possible second excited states for two electrons in a 3D-SHO.

* By considering the number of ways that a fixed integer, n , can be partitioned into three non-negative integers, show that the eigenvalues are $\frac{1}{2}(n+1)(n+2)$ -fold degenerate.

The degree of degeneracy, g_n , is the number of ways that the integer, n , can be partitioned into 3 integers, n_1, n_2, n_3 , all of which ≥ 0 .

Consider n objects on a line and two barriers which serve to partition the n objects into 3 sets:



The number of arrangements of the n objects + 2 barriers is $(n+2)!$ However, these are not all distinct since for a given arrangement of the n objects there are $2! = 2$ arrangements of the barriers (ie they can be swapped), whilst for fixed positions of the barriers, there are $n!$ equivalent arrangements of the n objects. Thus the number of distinct partitions of n is

$$g_n = \frac{(n+2)!}{2! n!} = \frac{1}{2}(n+1)(n+2)$$

4. The 3-dimensional isotropic harmonic oscillator can also be solved in spherical polar coordinates, since $V(r)$ is a central potential, with energy eigenstates labelled by n , ℓ and m_z , as for the hydrogen atom (except that, by convention, the ground state is labelled by $n = 0$ rather than $n = 1$). By using the parity properties of the eigenfunctions and the degree of degeneracy, try to find the angular momentum quantum number, ℓ , associated with the lowest three energy levels.

The ground state is straightforward. In Cartesian coordinates, in the notation of the previous question,

$$U_0(x_1, x_2, x_3) = u_0(x_1) u_0(x_2) u_0(x_3)$$

There is no degeneracy and the parity is *even*, since the 1-dimensional ground-state eigenfunction is even. This must correspond to $\ell = 0$ since the spherical harmonic Y_0^0 has even parity and there is no degeneracy with respect to m . Another way of saying this is that the wavefunction is spherically symmetric.

The first excited level is equally straightforward: the parity is odd and the degree of degeneracy is 3. In Cartesians, the energy eigenfunctions are

$$u_1(x_1) u_0(x_2) u_0(x_3), \quad u_0(x_1) u_1(x_2) u_0(x_3) \quad \text{and} \quad u_0(x_1) u_0(x_2) u_1(x_3)$$

and so must correspond to a solution in spherical polars with $\ell = 1$, which has parity $(-1)^\ell = -1$ and degeneracy $(2\ell + 1) = 3$: spherical harmonics Y_1^{-1} , Y_1^0 and Y_1^1 (i.e. $\sin\theta e^{-i\phi}$; $\cos\theta$; $\sin\theta e^{i\phi}$).

Note that the third of these corresponds to the wavefunction with $\ell = 1$ and $m = 0$. However, first two eigenfunctions do not correspond to states of definite m_z , but to linear combinations of states with $m_z = 1$ and $m_z = -1$.

At the second excited level, things are more complicated. The parity is again even and the degree of degeneracy is 6. The Cartesian eigenfunctions are

$$\begin{aligned} u_2(x_1) u_0(x_2) u_0(x_3), & \quad u_0(x_1) u_2(x_2) u_0(x_3), & \quad u_0(x_1) u_0(x_2) u_2(x_3), \\ u_1(x_1) u_1(x_2) u_0(x_3), & \quad u_1(x_1) u_0(x_2) u_1(x_3), & \quad u_0(x_1) u_1(x_2) u_1(x_3) \end{aligned}$$

Even parity implies even ℓ . The only way to get a total degeneracy of 6 is to take both $\ell = 0$ and $\ell = 2$, since

$$\sum_{\ell=0,2} (2\ell + 1) = 1 + 5 = 6$$

We are using the fact that the parity properties and the degree of degeneracy are physical properties of the system which cannot depend on our choice of coordinates.

The cartesian eigenfunctions are not necessarily eigenfunctions of the angular momenta. To obtain definite ℓ and m_z with well defined angular momenta would have to take linear combinations of these. These could be found by building a 6x6 matrix with elements such as $\langle u_2(x_1) u_0(x_2) u_0(x_3) | \hat{L}_z | u_0(x_1) u_2(x_2) u_0(x_3) \rangle$ and finding the eigenvectors. Presumably the eigenvalues would be -2,-1, 0,0,1, -1. The pair of states with $l_z = 0$ could then be separated by building a 2x2 matrix for \hat{L} . I didn't expect you to do this here!

The point of this question is to show that considering symmetry and degeneracy can simplify some aspects of solving the problem, and to illustrate that there may be more than one set of good quantum numbers, incompatible with other good sets (here N_x, N_y, N_z for the cartesian eigenstates, or E, ℓ, m_z for the spherical polar eigenstates)

5. A 1-d infinite square-well potential between 0 and $2a$ is occupied by two indistinguishable spin- $\frac{1}{2}$ fermions. Write down the possible degenerate states for the ground state and first two excited states.

The ground state has both fermions in the spatial ground state, and is therefore symmetric with exchange. For fermions, the spin state must be antisymmetric, i.e. singlet spin

$$\Phi(x_1, x_2) = |1, 1\rangle = (1/a) \sin(\pi x_1/2a) \sin(\pi x_2/2a) (\uparrow\downarrow - \downarrow\uparrow) / \sqrt{2}$$

If the particles repel one another via a delta function potential,

$$V(x_1, x_2) = 2aV_0\delta(x_1 - x_2)$$

use perturbation theory to evaluate the shift in energy of the ground state and show that if the fermions are non-interacting, the ground-state energy is the same as for distinguishable particles.

The potential does not involve the spin, hence we can write:

$$\Delta E = \langle 11|V|11\rangle = 2aV_0 \int \int \Phi^*(x_1, x_2) \delta(x_1 - x_2) \Phi(x_1, x_2) dx_1 dx_2$$

Using the property of the delta function that for any f :

$$\int \int \delta(x_1, x_2) f(x_1, x_2) dx_1 dx_2 = \int f(x, x) dx$$

$$\Delta E = 2aV_0 \int |\Phi(x, x)|^2 dx = 2V_0/a \int_0^{2a} \sin^4(\pi x/2a) dx = 4V_0 \int_0^1 \sin^4(\pi y) dy$$

The integral is $3/8$, so $\Delta E = 3V_0/2$. The wavefunction is a simple product, as it would be for distinguishable particles. Thus the energy shift is the same, although in the case of distinguishable particles the state would be fourfold degenerate.

Now evaluate the energy shift for the first excited state due to the interaction, comparing the case of indistinguishable particles with that for distinguishable ones.

The first excited state is $|1, 2\rangle$, but this does not obey exchange symmetry. We must make symmetric and antisymmetric combinations, and thus we have singlet and triplet combinations with the spatial states

$$\Phi^\pm(x_1, x_2) = (|1, 2\rangle \pm |2, 1\rangle) \sqrt{2}$$

This means the integrals required for the perturbation are

$$\Delta E = (\langle 1, 2|V|1, 2\rangle + \langle 2, 1|V|2, 1\rangle)/2 \pm (\langle 2, 1|V|1, 2\rangle + \langle 1, 2|V|2, 1\rangle)/2$$

By symmetry

$$\langle 1, 2|V|1, 2\rangle = \langle 2, 1|V|2, 1\rangle$$

$$\langle 2, 1|V|1, 2\rangle = \langle 1, 2|V|2, 1\rangle$$

And using the delta function property we find that

$$\langle 1, 2|V|1, 2\rangle = 2V_0/a \int \int \sin^2(\pi x/2a) \sin^2(\pi x/a) dx$$

$$\langle 1, 2|V|2, 1\rangle = 2V_0/a \int \int \sin^2(\pi x/2a) \sin^2(\pi x/a) dx$$

i.e. direct and exchange integrals are the same

Using the given integral $\Delta E = V_0 \pm V_0$

In the distinguishable case, we would have only the $\langle 1, 2|1, 2\rangle$ integral, i.e. $\Delta E = V_0$

Comment on the value of the triplet state.

The triplet state corresponds to the antisymmetric spatial state, i.e. the negative sign. An antisymmetric spatial wavefunction implies that the exclusion principle holds in space: the two particles cannot be in the same place. Since the delta function perturbation acts only when the two particles *are* in the same place, the energy is unshifted by this perturbation.