

QUANTUM MECHANICS II EXAM

24 February 2021

Answers sheet

We consider a system of two non-identical spin 1/2 particles in three dimensions whose dynamics are described by the Hamiltonian

$$H_{tot} = H_1 + H_2, \quad (1)$$

$$H_1 = \frac{\vec{p}_1^2}{2m} + \frac{\vec{p}_2^2}{2m} - \frac{e^2}{|\vec{x}_1 - \vec{x}_2|}, \quad (2)$$

$$H_2 = -\frac{A}{\hbar^2} \vec{s}_1 \cdot \vec{s}_2, \quad (3)$$

where $\vec{x}_1, \vec{x}_2, \vec{p}_1, \vec{p}_2, \vec{s}_1, \vec{s}_2$ are respectively the position, momentum and spin operators of the two particles, and A and e are positive real constants.

Also consider the two following Hamiltonians:

$$H_3 = \frac{1}{\hbar^2} s_1^z, \quad (4)$$

$$H_4 = \frac{1}{\hbar^2} s_2^z, \quad (5)$$

$$H_5 = \frac{1}{\hbar^2} \vec{B} \cdot (\vec{s}_1 - \vec{s}_2), \quad (6)$$

$$H_6 = \frac{1}{\hbar^2} \vec{B} \cdot (\vec{s}_1 - \vec{s}_2) e^{i\omega t}, \quad (7)$$

where \vec{B} is a real vector and ω a positive real constant.

(1) The Hamiltonian H_1 can be separated into two commuting terms H_f and H_r :

$$H_1 = H_f + H_r. \quad (8)$$

To this end, let us define the relative coordinates

$$\vec{r} = \vec{x}_1 - \vec{x}_2. \quad (9)$$

With conjugate momenta given by

$$\vec{p} = \frac{\vec{p}_1 - \vec{p}_2}{2}, \quad (10)$$

$$\vec{P} = \vec{p}_1 + \vec{p}_2. \quad (11)$$

Define also the total mass M and reduced mass μ as

$$M = 2m, \quad (12)$$

$$\mu = \frac{m}{2}. \quad (13)$$

Using these definitions, the Hamiltonian H_1 can be written as

$$H_1 = H_f + H_r, \quad (14)$$

where

$$H_f = \frac{\vec{P}^2}{2M}, \quad (15)$$

$$H_r = \frac{\vec{p}^2}{2\mu} - \frac{e^2}{|\vec{r}|}. \quad (16)$$

- (2) The energy spectrum of the relative Hamiltonian is that of the hydrogen atom:

$$E_n^r = -\frac{\mu e^4}{2\hbar^2 n^2}. \quad (17)$$

For a given value for n all $l < n$ are permitted and for each value of l all $-l \leq l_z \leq l$ are permitted which corresponds to a degeneracy of n^2 .

- (3) In the absence of spin-orbit coupling, the spatial Hamiltonian H_1 and spin hamiltonian H_2 commute, so they can be diagonalized separately.

The spectrum of the relative Hamiltonian is given in the previous exercise, while the center of mass energy is simply

$$E_{cm} = \frac{(\vec{p}_1 + \vec{p}_2)^2}{2M} = \frac{\vec{P}^2}{2M}. \quad (18)$$

The energy corresponding to H_1 is thus

$$E_n^1 = \frac{\vec{P}^2}{2M} - \frac{\mu e^4}{2\hbar^2 n^2}. \quad (19)$$

Coming to H_2 , we note that it is diagonalized in the basis of eigenstates of the operators s^2 , s_1^2 and s_2^2 , where $\vec{s} = \vec{s}_1 + \vec{s}_2$:

$$H_2 = -\frac{A}{2\hbar^2} (\vec{s}^2 - \vec{s}_1^2 - \vec{s}_2^2). \quad (20)$$

For spin- $\frac{1}{2}$ particles the eigenvalues are

$$E_s^2 = -\frac{A}{2} \left(s(s+1) - \frac{3}{2} \right), \quad (21)$$

with $s \in \{0, 1\}$.

The energy spectrum of the Hamiltonian H_{tot} is thus

$$E_{n,s}^{tot} = \frac{P^2}{2M} - \frac{\mu e^4}{2\hbar^2 n^2} - \frac{A}{2} \left(s(s+1) - \frac{3}{2} \right). \quad (22)$$

The spectrum of the free (center-of-mass) hamiltonian is infinitely degenerate, with all vectors such that $|\vec{P}|$ is fixed corresponding to the same energy level. The relative hamiltonian has degeneracy n^2 as determined at point (2). Because it is given that the spacing of the levels of the Hamiltonian H_2 are smaller than that of the levels of the Hamiltonian H_1 there is no additional degeneracy as a result of different combinations of n and s returning the same energy. This leaves only the threefold degeneracy corresponding to the triplet state if $s = 1$, resulting in a total degeneracy of $3n^2$, and the degeneracy related to the spin singlet, which for $s = 0$ is n^2 .

- (4) As we have just seen the Hamiltonian H_1 can be separated into a free and a relative Hamiltonian. It follows that the wave function is the product of a free and a relative eigenfunction:

$$\psi(\vec{x}_1, \vec{x}_2) = \psi_f(\vec{R})\psi_r(\vec{r}), \quad (23)$$

where \vec{R} and \vec{r} are center-of-mass and relative coordinates respectively, ψ_f is an eigenstate of H_f and ψ_r an eigenstate of H_{+r} .

For the free Hamiltonian it has been shown in Eq. 6.11 and Eq. 6.12 of the textbook, that one can choose the eigenfunctions to be parity eigenstates. Hence the free wave function can always be chosen to be even or odd under parity:

$$\psi_f^\pm(-\vec{R}) = \pm\psi_f^\pm(\vec{R}), \quad (24)$$

where

$$\psi_f^\pm(\vec{R}) = \frac{1}{(2\pi)^{3/2}} \left(e^{i\vec{P}\cdot\vec{R}} \pm e^{-i\vec{P}\cdot\vec{R}} \right). \quad (25)$$

For the relative Hamiltonian the wavefunction can be written as a product of spherical harmonics and a radial function, see Eq. 11.213 for the general form. The radial wave function is parity invariant because r is parity invariant. Hence the parity transformation is entirely due to the angular part. The parity transformation in spherical coordinates is given in Eq. 9.117, which for spherical harmonics implies

$$\langle r\vartheta\phi|P|nlm\rangle = Y_{lm}(\pi - \vartheta, \varphi + \pi)\phi_{nl}(r) = (-1)^l Y_{lm}(\vartheta, \varphi)\phi_{nl}(r). \quad (26)$$

Hence the parity of the relative eigenfunction is entirely determined by the eigenvalue of the total relative orbital angular momentum l .

- (5) Let us define the radial distance $r = |\vec{x}_1 - \vec{x}_2|$, of which we want to calculate the mean value using:

$$\langle |\vec{x}_1 - \vec{x}_2| \rangle = \langle r \rangle = \int_0^\infty d\vec{x} \psi^*(r) r \psi(r). \quad (27)$$

The ground state wave function in spherical coordinates can be found in the textbook Eq. 11.226:

$$\psi(r, \theta, \varphi) = \frac{1}{\sqrt{\pi}} \frac{(e^2\mu)^{3/2}}{\hbar^3} e^{-e^2\mu r/\hbar^2} = \frac{1}{\sqrt{\pi}} \frac{1}{(a_0)^{3/2}} e^{-r/a_0}, \quad (28)$$

with $a_0 = \frac{\hbar^2}{e^2\mu}$. This we can plug into Eq. (27):

$$\langle r \rangle = \frac{4}{a_0^3} \int_0^\infty r^3 e^{-2r/a_0} = \frac{3}{2} a_0. \quad (29)$$

The mean value of the potential energy is

$$\langle E_{pot} \rangle = -e^2 \langle \frac{1}{r} \rangle = -e^2 \frac{4}{a_0} \int_0^\infty r e^{-2r/a_0} = -\frac{e^2}{a_0}. \quad (30)$$

- (6) The first order in the perturbation corresponds to the singlet state $|s = 0, s_z = 0\rangle$,

$$|s = 0, s_z = 0\rangle = \frac{1}{\sqrt{2}} (|+-\rangle - |-+\rangle), \quad (31)$$

and the triplet states

$$|1, 1\rangle = |++\rangle, \quad (32)$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}} (|+-\rangle + |-+\rangle), \quad (33)$$

$$|1, -1\rangle = |--\rangle. \quad (34)$$

The spin operator is $s_1^z = \frac{\hbar}{2}\sigma^z = \frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|)$, where the subscript 1 means that acts on the state corresponding to the first particle only.

The correction to the energy as a result of the perturbation in the singlet state is

$$E_{s=0,s_z=0}^3 = \left\langle s_z = 0, s = 0 \left| \frac{1}{\hbar^2} \lambda s_1^z \right| s = 0, s_z = 0 \right\rangle, \quad (35)$$

$$= \frac{1}{2} (\langle -+ | - \langle + - |) \left| \frac{1}{\hbar^2} \lambda s_1^z \right| (| + - \rangle - | - + \rangle), \quad (36)$$

$$= \frac{\lambda}{4\hbar} (\langle -+ | +- \rangle - \langle +- | -+ \rangle), \quad (37)$$

$$= 0. \quad (38)$$

For the triplet states we must compute the matrix of the perturbation in the degenerate subspace. We get, with a calculation similar to that for the singlet state (writing the bras as $\langle ss_z |$)

$$\langle H_3 \rangle = \begin{pmatrix} \langle 1-1 | H_3 | 1-1 \rangle & \langle 1-1 | H_3 | 10 \rangle & \langle 1-1 | H_3 | 11 \rangle \\ \langle 10 | H_3 | 1-1 \rangle & \langle 10 | H_3 | 10 \rangle & \langle 10 | H_3 | 11 \rangle \\ \langle 11 | H_3 | 1-1 \rangle & \langle 11 | H_3 | 10 \rangle & \langle 11 | H_3 | 11 \rangle \end{pmatrix} = \begin{pmatrix} -\frac{\lambda}{2\hbar} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\lambda}{2\hbar} \end{pmatrix}, \quad (39)$$

i.e. the matrix of the perturbation is diagonal. This happens despite the fact that the perturbation is not diagonal in the basis of eigenstates of H_{tot} , because the non-diagonal matrix element of the perturbation is between the triplet and the singlet, so it only contributes starting with the second perturbative order.

The correction to the three energy levels is thus

$$E_{s=1,s_z=-1}^3 = -\frac{\lambda}{2\hbar} \quad (40)$$

$$E_{s=1,s_z=0}^3 = 0 \quad (41)$$

$$E_{s=1,s_z=+1}^3 = \frac{\lambda}{2\hbar}. \quad (42)$$

It can now be observed that there is no longer any spin degeneracy.

- (7) The kinetic energy is made up of the sum of two parts: the part of the kinetic energy related to the free Hamiltonian, and the part related to the relative Hamiltonian.

The eigenstates of the free hamiltonian can be chose to be momentum eigenstates with eigenvalue \vec{P} . In such a state the kinetic energy is fixed and equal to

$$\langle E^{kin,f} \rangle = E^{kin,f} = \frac{\vec{P}^2}{2M}. \quad (43)$$

Coming to the relative hamiltonian, we note that for a Hamiltonian of the form $H = \frac{\vec{p}}{2\mu} + V(\vec{x})$ the kinetic energy can be determined using the virial theorem given by Eq. 11.134 in the textbook:

$$2\langle E^{kin} \rangle = \langle \vec{x} \cdot \vec{\nabla} V(\vec{x}) \rangle. \quad (44)$$

In our case, using the result Eq. (30) we get

$$\langle E^{kin,r} \rangle = -\frac{1}{2} e^2 \langle \vec{x} \cdot \vec{\nabla} r^{-1} \rangle = e^2 \frac{1}{2} \langle r^{-1} \rangle = -\frac{1}{2} E_{pot} = \frac{e^2}{2a_0}. \quad (45)$$

The expectation value of the total kinetic energy is thus

$$\langle E^{kin} \rangle = \langle (E^{kin,r} + E^{kin,f}) \rangle = \frac{\vec{P}^2}{2M} + \frac{1}{2} \frac{e^2}{a_0}. \quad (46)$$

Alternatively, one can write the momentum operator in terms of its derivatives in spherical coordinates. For this we can use the radial momentum as given in Eq 9.148 of the textbook:

$$p_r^2 = -\hbar^2 \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right). \quad (47)$$

Using this result, and noting that in the ground state $\bar{p}^2 = p_r^2$ because the ground state has vanishing angular momentum, we get

$$\langle E^{kin,r} \rangle = \frac{1}{2\mu} \langle \bar{p}^2 \rangle = \frac{1}{2\mu} \int d\vec{x} \psi^*(r, \theta, \varphi) p_r^2 \psi(r, \theta, \varphi), \quad (48)$$

$$= \frac{-\hbar^2}{2\mu} \int dr r^2 |\psi(r, \theta, \varphi)|^2 \left(\frac{1}{a_0^2} - \frac{2}{ra_0} \right), \quad (49)$$

$$= \frac{\hbar^2}{2\mu} \frac{1}{a_0^2} = \frac{e^2}{2a_0}, \quad (50)$$

here $\psi(r, \theta, \varphi)$ is again define as in Eq. (28).

A final possibility is to note that in an energy eigenstate with energy eigenvalue E $\langle E^{kin} + V \rangle = \langle H \rangle = E$. Hence in the ground state

$$\langle E^{kin,r} \rangle = E_0^{rel} - \langle E_{pot} \rangle = -\frac{e^2}{2a_0} + \frac{e^2}{a_0} = \frac{e^2}{2a_0}. \quad (51)$$

- (8) The time dependence of a state in a system described by the Hamiltonian $H = H_1 + H_5$, with $\vec{B} = |\vec{B}|\hat{x}$ is

$$|\psi, t\rangle = e^{-iHt/\hbar} |\psi\rangle. \quad (52)$$

Because there is no spin-orbit coupling, the spatial and spin wave functions evolve independently. Hence, the probability only depends on the spin wave function. This consideration will also hold for the subsequent questions (9) and (10).

Also, for this question one observes that the spin Hamiltonian H_5 does not couple the two spins. hence the spin wave function for the first and the second particle evolve independently. The probability then only depends on the time evolution of the spin wave function of the first particle, which is given by

$$|s_{z,1}, t\rangle = e^{-iHt/\hbar} |s_{z,1}\rangle. \quad (53)$$

If at time $t = 0$ the a measurement of the spin of the first particle is performed, and found to be $s_{1,z} = +\frac{\hbar}{2}$, the probability of a measurement returning $s_{1,z} = -\frac{\hbar}{2}$ at a time $t = T$ is then

$$P = \left| \langle - | e^{-i(H_1+H_5)T/\hbar} | + \rangle \right|^2, \quad (54)$$

$$= \left| \langle - | e^{-i|\vec{B}|\vec{s}_{1,x}T/\hbar^3} | + \rangle \right|^2, \quad (55)$$

$$= \left| \langle - | e^{-i|\vec{B}|\vec{\sigma}_{1,x}T/2\hbar^2} | + \rangle \right|^2, \quad (56)$$

$$= \left| \langle - | \cos(|\vec{B}|T/(2\hbar^2))\mathbb{I} - i \sin(|\vec{B}|T/(2\hbar^2))\sigma_{1,x} | + \rangle \right|^2, \quad (57)$$

$$= \sin^2(|\vec{B}|T/(2\hbar^2)). \quad (58)$$

- (9) At time $t = 0$ a spin measurement of the two particles is made, the result of the measurement on the first particle is $s_{1,z} = \frac{\hbar}{2}$. Here we are given a choice between performing the rest of this exercise

with the assumption that the measurement of the second particle returned either (a) $s_{2,z} = \frac{\hbar}{2}$ or (b) $s_{2,z} = -\frac{\hbar}{2}$.

In order to compute the given probability, we expand the two possible initial states and the final state on eigenfunctions of the Hamiltonian. The initial states are $|++\rangle = |1, 1\rangle$ for case (a) and $|+-\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle + |0, 0\rangle)$ for case (b). The final states that would result in measuring $s_{1,z} = -\frac{\hbar}{2}$, are $|--\rangle = |1, -1\rangle$ and $| - + \rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle - |0, 0\rangle)$.

Let us first consider option (a). In this case, the initial state is an eigenstate of the Hamiltonian, so this is a stationary state, and the probability is zero. More formally the probabilities, for the two possible final states, are

$$P_{--} = |\langle 1, -1 | 1, 1 \rangle|^2 = 0. \quad (59)$$

$$P_{-+} = \left| \frac{1}{\sqrt{2}} (\langle 0, 1 | - \langle 0, 0 |) | 1, 1 \rangle \right|^2 = 0. \quad (60)$$

$$(61)$$

Now for option (b) the probabilities for the two possible final states are

$$P_{--} = \left| \langle 1, -1 | \frac{1}{\sqrt{2}} \left(e^{-iE_1^2 T/\hbar} |1, 0\rangle + e^{-iE_0^2 T/\hbar} |0, 0\rangle \right) \right|^2 = 0; \quad (62)$$

$$P_{-+} = \left| \frac{1}{\sqrt{2}} (\langle 1, 0 | - \langle 0, 0 |) \frac{1}{\sqrt{2}} \left(e^{-iE_1^2 T/\hbar} |1, 0\rangle + e^{-iE_0^2 T/\hbar} |0, 0\rangle \right) \right|^2, \quad (63)$$

$$\begin{aligned} &= \frac{1}{4} \left| e^{-iE_1^2 T/\hbar} - e^{-iE_0^2 T/\hbar} \right|^2 = \frac{1}{4} \left| e^{-iAT/4\hbar} (e^{iAT/2\hbar} - e^{-iAT/2\hbar}) \right|^2, \\ &= \sin^2(AT/2\hbar). \end{aligned} \quad (64)$$

Hence, the probability in this case is

$$P = P_{-+} = \sin^2(AT/2\hbar). \quad (65)$$

- (10) Because the perturbation acts only on spin the spatial Hamiltonian only provides an overall phase which does not contribute to transition probabilities. The ground state of H_{tot} is the threefold degenerate triplet state $|n, s, s_z\rangle = |1, 1, s_z\rangle$, with $s_z \in -1, 0, 1$. The first excited state is $|n, s, s_z\rangle = |1, 0, 0\rangle$, which is the singlet state. Treating H_6 as a first order perturbation, the probability for a transition between any of the triplets states with different s_z and the singlet state is

$$P_{s_z}(t) = \left| \langle 1, 0, 0 | \frac{1}{i\hbar} \int_0^t dt' e^{iH_{tot}t'/\hbar} H_6 e^{-iH_{tot}t'/\hbar} | 1, 1, s_z \rangle \right|^2, \quad (66)$$

$$= \left| \frac{1}{\hbar} \int_0^t dt' e^{i(E_1^{tot} - E_0^{tot})t'/\hbar} \langle 1, 0, 0 | H_6 | 1, 1, s_z \rangle \right|^2, \quad (67)$$

$$= \left| \frac{1}{\hbar} \int_0^t dt' e^{i(\omega + A'/\hbar)t'} \langle 1, 0, 0 | \frac{1}{\hbar^2} \vec{B} \cdot (\vec{s}_1 - \vec{s}_2) | 1, 1, s_z \rangle \right|^2. \quad (68)$$

Without loss of generality we can now choose the magnetic field along the z axis, $\vec{B} = |\vec{B}|\hat{z}$, which gives

$$P_{s_z}(t) = \frac{1}{\hbar^6} \left| \int_0^t dt' \exp(i(\omega + A'/\hbar)t') |\vec{B}| \langle 1, 0, 0 | (\vec{s}_{1,z} - \vec{s}_{2,z}) | 1, 1, s_z \rangle \right|^2. \quad (69)$$

$$(70)$$

We now note that the Hamiltonian H_6 annihilates the $s_z = \pm 1$ states of the triplet, while it turns the $s_z = 0$ state of the triplet into the singlet:

$$\begin{aligned} H_6|n=1, s=1, s_z=0\rangle &= H_6 \frac{1}{\sqrt{2}} (|+-\rangle + |-+\rangle) \\ &= \frac{|\vec{B}|}{\hbar} \frac{1}{\sqrt{2}} (|+-\rangle - |-+\rangle) = \frac{|\vec{B}|}{\hbar} |n=1, s=1, s_z=0\rangle \end{aligned} \quad (71)$$

$$H_6|n=1, s=1, s_z=\pm 1\rangle = 0. \quad (72)$$

Using this, calculating the matrix element is relatively straightforward (as was just mentioned, acting on the singlet state with the Hamiltonian H_6 gives the $s_z = 0$ state of the triplet), and after doing so we find

$$P(t) = \frac{1}{\hbar^4} \left| \int_0^t dt' e^{i(\frac{A}{\hbar} + \omega)t'} |\vec{B}| \right|^2, \quad (73)$$

$$= \frac{4|\vec{B}|^2}{\hbar^4} \left[\left(\frac{A}{\hbar} + \omega \right) t \right]^{-2} \sin^2 \left[\left(\frac{A}{\hbar} + \omega \right) \frac{t}{2} \right] \quad (74)$$

- (11) In exercise (3) we found the energy spectrum of H_{tot} which was determined under the assumption that the two spin- $\frac{1}{2}$ particles of the system were non-identical. However, here we are asked to determine the spectrum for the case of identical particles and this affects the degeneracy. Because the particles are fermions, the wave function must be anti-symmetric.

Here we again consider the parity relation given in Eq. (26). Because r in that equation is a relative coordinate, parity corresponds to the interchange of the two particles. Hence, states with even l are even and states with odd l are odd.

Then, normally the degeneracy is found summing $0 \leq l \leq n-1$, with $2l+1$ states for each l . Here, one must distinguish n even and n odd.

For n odd and l even we have

$$\sum_{l \in \text{even}}^{n-1} (2l+1) = \sum_{l=0}^{(n-1)/2} (4l+1) = \frac{1}{2}n(n+1), \quad (75)$$

while for n odd and l odd we have

$$\sum_{l \in \text{odd}}^{n-1} (2l+1) = \sum_{l \in \text{odd}}^{n-2} (2l+1) = \sum_{l=0}^{(n-2)/2} (4l+1) = \frac{1}{2}n(n-1), \quad (76)$$

where we used

$$\sum_{l=0}^n = \frac{1}{2}n(n+1). \quad (77)$$

Now we still have to take into account the threefold degeneracy of the triplet state, which means that for l odd and n odd the degeneracy is $\frac{3}{2}n(n-1)$, while for l even and n odd the degeneracy is $\frac{1}{2}n(n+1)$.

Now we can repeat the above for n even. This time we find that for n even and l odd the degeneracy is $\frac{3}{2}n(n+1)$, while for the case with both n and l even the degeneracy is $\frac{1}{2}n(n-1)$.