QUANTUM MECHANICS II EXAM

19 July 2021

Answers sheet

We consider a system formed by three particles of spin $\frac{1}{2}$ and of equal mass m in three dimensions, confined within a parallelepiped. The particles are to be considered in general not identical. The dynamics are described by the Hamiltonian

$$H = \frac{\vec{p}_1^2}{2m} + \frac{\vec{p}_2^2}{2m} + \frac{\vec{p}_3^2}{2m} + V(\vec{x}_1) + V(\vec{x}_2) + V(\vec{x}_3) - \frac{\lambda}{\hbar^2}\vec{s}_1 \cdot \vec{s}_2 + \frac{1}{\hbar}\vec{B} \cdot (\vec{s}_1 + \vec{s}_2) - \frac{\mu}{\hbar^2}(\vec{s}_2 \cdot \vec{s}_3 + \vec{s}_3 \cdot \vec{s}_1), \quad (1)$$

where $\vec{x}_i$, $\vec{p}_i$ and $\vec{s}_i$ are the position, momentum and spin operators for the two particles, respectively, μ and λ are real positive constants and $\vec{B}$ is a three-dimensional vector with real components. The potential $V(\vec{x}_i)$ has the form

$$V(x_i) = \begin{cases} 0 \text{ if } \left|x_i^{(j)}\right| \leq a \\ \infty \text{ if } \left|x_i^{(j)}\right| > a \end{cases} \quad (2)$$

where $x_i^{(j)}$ is the j-th component of the position operator for the i-th particle and a is a positive real constant.

(1) If we set $\mu = \lambda = 0$, and $B_i = 0$ for each i, the Hamitlonian Eq. (1) becomes

$$H_V = \frac{\vec{p}_1^2}{2m} + \frac{\vec{p}_2^2}{2m} + \frac{\vec{p}_3^2}{2m} + V(\vec{x}_1) + V(\vec{x}_2) + V(\vec{x}_3), \quad (3)$$

which can be separated into three one-dimensional Hamiltonians describing a 'particle in a box' for each particle. Thus the eigenvalues spectrum is

$$E_V = E_{l_1,l_2,l_3} + E_{m_1,m_2,m_3} + E_{n_1,n_2,n_3}, \quad (4)$$

with with l_i, m_i and n_i positive integers, and

$$E_{i,j,k} = \frac{\pi^2\hbar^2}{8ma^2}\left(i^2 + j^2 + k^2\right). \quad (5)$$

(2) The wave function of the system described question (1) can be written as

$$\psi = \phi_{l_1,l_2,l_3}(\vec{x}_1)\,\phi_{m_1,m_2,m_3}(\vec{x}_2)\,\phi_{n_1,n_2,n_3}(\vec{x}_3)\,\chi_{s_1^2,s_1^z,s_2^2,s_2^z,s_3^2,s_3^z}, \quad (6)$$

where

$$\phi_{i,j,k}(\vec{x}) = \phi_i(x)\phi_j(y)\phi_k(z), \quad (7)$$

with

$$\phi_n(x) = \begin{cases} \sqrt{\frac{1}{a}}\cos\frac{n\pi}{2a}x, & \text{if } n \text{ is odd} \\ \sqrt{\frac{1}{a}}\sin\frac{n\pi}{2a}x, & \text{if } n \text{ is even} \end{cases} \quad (8)$$

and χ denotes the spin-dependant part of the wave function.

(3) If we again consider the system as described in exercise (1), the degeneracy of the ground state is $deg = 8$. This is because the spatial part of the ground state is non-degenerate, but each particle can be in one of two spin states, and thus the spin degeneracy is $deg = 2^3 = 8$.

For the first excited state the spatial part has $deg = 9$, leading to a total degeneracy of $deg = 9\times 8 = 72$.

(4) Here we are interested in the eigenvalues of the Hamiltonian Eq. (1) in case $\lambda \neq 0$, but $\mu = 0$, $B_i = 0$ for each i.

Let us consider

$$H_\lambda = -\frac{\lambda}{\hbar^2}\vec{s}_1 \cdot \vec{s}_2 \tag{9}$$

which can be written in a basis of the eigenstates of the operators s_{12}^2, s_{12}^z, s_1^2 and s_2^2, where $\vec{s}_{12} = \vec{s}_1 + \vec{s}_2$. In this basis the Hamiltonian is

$$H_\lambda = -\frac{\lambda}{2\hbar^2}\left(s_{12}^2 - s_1^2 - s_2^2\right), \tag{10}$$

and the corresponding eigenvalues are

$$E^\lambda_{s_{12}} = \frac{\lambda}{2}\left(s_{12}(s_{12}+1) - \frac{3}{2}\right), \tag{11}$$

for $s_{12} \in \{0, 1\}$.

(5) The degeneracy correspondig to the eigenvalues $E^\lambda_{s_{12}}$, is $deg = 2s_{12} + 1$. Since the third particle can be in one of two states for each value of $E^\lambda_{s_{12}}$, the total spin degeneracy is $deg = 2(2s_{12} + 1)$.

(6) Let us consider two angular momenta $\vec{L}_1$ and $\vec{L}_2$, and a total angular momentum $\vec{L}_{tot} = \vec{L}_1 + \vec{L}_2$. The Clebsch-Gordan coefficients $\langle m_1 m_2 | lm\rangle$ are only non-zero if $m = m_1 + m_2$. This can be shown using the identity for the third component of the angular momentum $\vec{L}^z_{tot} = \vec{L}^z_1 + \vec{L}^z_2$. Namely, we have

$$\vec{L}^z_{\text{tot}}|lm\rangle = \hbar m|lm\rangle, \qquad \left(\vec{L}^z_1 + \vec{L}^z_2\right)|m_1 m_2\rangle = \hbar(m_1 + m_2)|m_1 m_2\rangle, \tag{12}$$

from which it follows that

$$\langle m_1 m_2|\vec{L}^z_{\text{tot}} - \vec{L}^z_1 - \vec{L}^z_2|ml\rangle = \hbar(m - m_1 - m_2)\langle m_1 m_2|lm\rangle = 0. \tag{13}$$

Here it is clear that the Clebsch-Gordan coefficients can only be non-zero if $m = m_1 + m_2$.

(7) Here we wish to determine the Heisenberg equations of motion for the operator $\vec{s}_1$ in the case where λ, μ and $\vec{B}$ are all non-zero. The equations of motion for $\vec{s}_1$ are

$$\frac{d\vec{s}_1}{dt} = -\frac{i}{\hbar}[\vec{s}_1, H]. \tag{14}$$

To write out the left hand side, we use the components of $\vec{s}_1$ satisfy the commutation relations

$$[s_1^i, s_1^j] = i\hbar\epsilon^{ijk}s_1^k. \tag{15}$$

Working out the equation of motion for each component of $\vec{s}_1$ takes a bit of work, and the final answer is

$$\frac{d\vec{s}_1}{dt} = -\frac{\lambda}{\hbar^2}\vec{s}_2 \times \vec{s}_1 + \frac{1}{\hbar}\vec{B} \times \vec{s}_1 - \frac{\mu}{\hbar^2}\vec{s}_3 \times \vec{s}_1. \tag{16}$$

(8) Let us consider the Hamiltonian of question 4 (i.e. $\lambda \neq 0$, $\mu = 0$ and $B_i = 0$ for each i) as an unperturbed Hamiltonian. Now we suppose that $\vec{B} \neq 0$, and treat the term proportional to $\vec{B}$ as a perturbation. Without loss of generality we can assume that $\vec{B}$ is directed along the z-axis, and we can again write the Hamiltonian in a diagonal basis:

$$H_8 = H_V - \frac{\lambda}{\hbar^2}\vec{s}_1 \cdot \vec{s}_2 + \frac{1}{\hbar}|\vec{B}|s_{12}^z, \tag{17}$$

$$= H_V - \frac{\lambda}{2\hbar^2}(\vec{s}_{12}^{\,2} - \vec{s}_1^{\,2} - \vec{s}_2^{\,2}) + \frac{1}{\hbar}|\vec{B}|s_{12}^z, \tag{18}$$

In such case the first-order perturbation for the singlet state is given by

$$\Delta E_{s_{12}=0,s_{12}^z=0} = \langle s_{12}^z = 0, s_{12} = 0|\frac{1}{\hbar}|\vec{B}|s_{12}^z|s_{12} = 0, s_{12}^z = 0\rangle = 0, \tag{19}$$

and for the triplet state, in the basis

$$|s_{12} = 1, s_{12}^z\rangle = \begin{pmatrix} |1,1\rangle \\ |1,0\rangle \\ |1,-1\rangle \end{pmatrix} \tag{20}$$

it is given by

$$\Delta E_{s_{12}=1,s_{12}^z} = \langle s_{12}^z, s_{12} = 1|\frac{1}{\hbar}|\vec{B}|s_{12}^z|s_{12} = 1, s_{12}^z\rangle = |\vec{B}| \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{21}$$

The perturbation removes the spin degeneracy of particles 1 and 2.

(9) In the case where $B_i = 0$ for each i, but $\lambda = \mu \neq 0$, the Hamiltonian Eq. (1) can be written as

$$H_9 = H_V + H_\mu, \tag{22}$$

where

$$H_\mu = -\frac{\mu}{\hbar^2}\left(\vec{s}_1 \cdot \vec{s}_2 + \vec{s}_2 \cdot \vec{s}_3 + \vec{s}_3 \cdot \vec{s}_1\right), \tag{23}$$

$$= -\frac{\mu}{2\hbar^2}\left(\vec{s}_{123}^{\,2} - \vec{s}_1^{\,2} - \vec{s}_2^{\,2} - \vec{s}_3^{\,2}\right), \tag{24}$$

where we defined $\vec{s}_{123} = \vec{s}_1 + \vec{s}_2 + \vec{s}_3$. The eigenvalue spectrum of H_μ is

$$E^\mu_{s_{123}} = -\frac{\mu}{2}\left(s_{123}(s_{123}+1) - \frac{9}{4}\right), \tag{25}$$

with $s_{123} \in \{\frac{1}{2}, \frac{3}{2}\}$.
In order to compute the degeneracy consider the eight states of the basis $s_1^2, s_2^{;}s_3^3, s_1^z, s_2^z, s_3^z$:

$$|\frac{1}{2} \pm \frac{1}{2}\rangle_1|\frac{1}{2} \pm \frac{1}{2}\rangle_2|\frac{1}{2} \pm \frac{1}{2}\rangle_3. \tag{26}$$

We can combine the first two spins, thus getting a singlet and triplet $|1m\rangle_{12}|\frac{1}{2} \pm \frac{1}{2}\rangle_3$, $|00\rangle_{12}|\frac{1}{2} \pm \frac{1}{2}\rangle_3$. Combining now the result with the third particle we get states $|ss_zs_{12}\rangle$ corresponding to

$$|\frac{3}{2}, s_z, 1\rangle, \quad |\frac{1}{2}, s_z, 1\rangle, \quad |\frac{1}{2}, s_z, 0\rangle. \tag{27}$$

Hence the state with $s_{123} = \frac{3}{2}$ is four times degenerate (four possible values of s_z) and the state with $s_{123} = \frac{1}{2}$ is also four time degenerate (two possible values of s_z when $s_{12} = 1$ and two possible values of s_z when $s_{12} = 0$).

(10) Considering again a system described by the Hamiltonian of the previous question, H_9, we now assume the case in which the particles are identical. Furthermore, we also assume that $\mu = \lambda \gg \frac{1}{ma^2}$. This inequality means that ground state corresponds to a state in which the term proportional to μ in E_9 is minimized, and thus $s_{123} = \frac{3}{2}$. For $s_{123} = \frac{3}{2}$, the spin wave function is completely symmetric,

and thus we need a spatial wave function that is completely anti-symmetric. This means that any two particles cannot be in the same state, and thus ground state is

$$E_0 = E_{1,1,1} + E_{1,2,1} + E_{1,1,2} + E^{\mu}_{3/2}. \tag{28}$$

Because the wave function is completely antisymmetrized, it is not degenerate for each choice of quantum numbers of the three particles. However, there are three different ways of choosing these sets of quantum numbers for the spatial part: namely by having the two different particles in the first excited state to have their sets of quantum numbers equal to $((1,2,1);\,(1,1,2))$, or $((2,1,1);\,(1,1,2))$, or $((2,1,1);\,(1,2,1))$. This leads to a threefold degeneracy of the spatial wave function. Furthermore, there are four possible choices for s^z_{123}, the third component of the total spin, all asscoiated to a fully symmetric spin wave function, leading to a fourfold degeneracy of the spatial wave function. Hence there are 12 degenerate distinct fully antysimmetrized wave function, leading to $d = 12$.

(11) Let us consider a case similar to the previous question but this time assuming $\mu = \lambda \ll \frac{1}{ma^2}$. In this case the ground state is the state for which the spatial part of the eigenvalue is minimized. As an initial thought, one might think the spatial part of the eigenvalue thus becomes $E_{1,1,1}$, however this corresponds to a wave function where the spatial part is fully symmetric while we do not have a fully anti-symmetric spin wave function. For $s_{123} = \frac{1}{2}$ the spin part is anti-symmetric with respect to two particles, thus in this case the ground state is

$$E_0 = E_{1,1,1} + E_{1,1,1} + E_{1,1,2} + E^{\mu}_{1/2} \tag{29}$$