Second Year Theory Option

QUANTUM MECHANICS

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Problem Set 3

G Two spin-$\frac{1}{2}$ systems

G1. As we have seen, a standard basis for a single spin-$\frac{1}{2}$ particle is $\{|\ \frac{1}{2},\frac{1}{2}\rangle, |\ \frac{1}{2},-\frac{1}{2}\rangle\}$, and these are represented in this basis by the column vectors $\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. For two particles of spin$-\frac{1}{2}$, a possible basis set is the four "product states" $\left\{|\ \frac{1}{2},\frac{1}{2}\rangle_1\ |\ \frac{1}{2},\frac{1}{2}\rangle_2, |\ \frac{1}{2},\frac{1}{2}\rangle_1\ |\ \frac{1}{2},-\frac{1}{2}\rangle_2, |\ \frac{1}{2},-\frac{1}{2}\rangle_1\ |\ \frac{1}{2},\frac{1}{2}\rangle_2, |\ \frac{1}{2},-\frac{1}{2}\rangle_1\ |\ \frac{1}{2},-\frac{1}{2}\rangle_2\right\}$ where the subscripts 1 and 2 refer to the different particles.This is often written as $\{\uparrow\uparrow,\uparrow\downarrow,\downarrow\uparrow,\downarrow\downarrow\}$ for short. These are represented by the corresponding "product wavefunctions" $\alpha_1\alpha_2,\ \alpha_1\beta_2,\ \beta_1\alpha_2,\ \beta_1\beta_2$.

The total spin operator for the two-spin system is defined by $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 = \frac{\hbar}{2}(\underline{\sigma}_1 + \underline{\sigma}_2)$; note that the matrices $\underline{\sigma}_1$ act **only** on α_1 and β_1, while the matrices $\underline{\sigma}_2$ act **only** on α_2 and β_2.

(i) Show that

$$S_z\alpha_1\alpha_2 = \hbar\alpha_1\alpha_2,\ S_z\alpha_1\beta_2 = S_z\alpha_2\beta_1 = 0,\ S_z\beta_1\beta_2 = -\hbar\beta_1\beta_2.$$

So these four states are all eigenstates of the z-component of the total spin.

(ii) It is frequently convenient to classify the states by the eigenvalue of the square of the total spin, $\mathbf{S}^2$. Eigenstates of $\mathbf{S}^2$ can be found as follows:-

$$\text{Note that } \mathbf{S}^2 = \frac{\hbar^2}{4}(\underline{\sigma}_1^2 + \underline{\sigma}_2^2 + 2\underline{\sigma}_1.\underline{\sigma}_2),$$

and that

$$\underline{\sigma}_1^2 = 3I = \underline{\sigma}_2^2.\text{ So } \mathbf{S}^2 = \frac{3\hbar^2}{2}I + \frac{\hbar^2}{2}\underline{\sigma}_1.\underline{\sigma}_2.$$

Consider now $\underline{\sigma}_1.\underline{\sigma}_2 = \sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}$.

Show that

$$\sigma_{1x}\alpha_1 = \beta_1, \sigma_{1x}\beta_1 = \alpha_1$$

$$\sigma_{1y}\alpha_1 = i\beta_1, \sigma_{1y}\beta_1 = -i\alpha_1$$

and hence that

$$\sigma_{1x}\sigma_{2x}\alpha_1\alpha_2 = \beta_1\beta_2, \sigma_{1y}\sigma_{2y}\alpha_1\alpha_2 = -\beta_1\beta_2, \sigma_{1z}\sigma_{2z}\alpha_1\alpha_2 = \alpha_1\alpha_2,$$

so that $\mathbf{S}^2\alpha_1\alpha_2 = 2\hbar^2\alpha_1\alpha_2$.

Verify similarly that

$$\mathbf{S}^2\beta_1\beta_2 = 2\hbar^2\beta_1\beta_2.$$

We know from E1 that **any** angular momentum $\mathbf{J}$ must have an eigenvalue $j(j+1)\hbar^2$ of $\mathbf{J}^2$, where $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ so the above eigenvalues of $\mathbf{S}^2$ correspond to "$\mathbf{S}^2 = S(S+1)\hbar^2$" with $S = 1$ i.e. these are states with $S = 1, S_z = +\hbar; S = 1, S_z = -\hbar$.

What about α_1, β_2 and $\alpha_2\beta_1$?

Show that

$$\begin{aligned} \underline{\sigma}_1.\underline{\sigma}_2\alpha_1\beta_2 &= 2\beta_1\alpha_2 - \alpha_1\beta_2 \\ \underline{\sigma}_1.\underline{\sigma}_2\beta_1\alpha_2 &= 2\alpha_1\beta_2 - \beta_1\alpha_2 \end{aligned}$$

So these two $\alpha_1\beta_2$ and $\beta_1\alpha_2$ **are not eigenfunctions of $\mathbf{S}^2$ even though they are eigenfunctions of** S_z. However, simple linear combinations of them are eigenfunctions of $\mathbf{S}^2$: show that

$$\mathbf{S}^2(\alpha_1\beta_2 + \beta_1\alpha_2) = 2\hbar^2(\alpha_1\beta_2 + \beta_1\alpha_2)$$

$$\mathbf{S}^2(\alpha_1\beta_2 - \beta_1\alpha_2) = 0.$$

Thus finally we have arrived at the re-classification according to the eigenvalues of $\mathbf{S}^2$ and S_z:-

$S = 1$	$S_z = \hbar$	$\alpha_1\alpha_2$
"triplet"	$S_z = 0$	$\frac{1}{\sqrt{2}}(\alpha_1\beta_2 + \beta_1\alpha_2)$ (normalised)
	$S_z = -\hbar$	$\beta_1\beta_2$
$S = 0$	$S_z = 0$	$\frac{1}{\sqrt{2}}(\alpha_1\beta_2 - \beta_1\alpha_2)$.
"singlet"		

Note that there are always just four states,however they are classified.

G2. A typical "hyperfine" term in a Hamiltonian for two spin-$\frac{1}{2}$ particles is

$$H_S = A\mathbf{S}_1.\mathbf{S}_2;$$

what are (i) the eigenstates of H_S? (ii) their multiplicities? (iii) the splitting (energy separation) between them?

G3. Positronium is a bound state of an electron and a positron. The Zeeman effect on the hyperfine structure of the ground state can be modelled by the Hamiltonian

$$H = A\underline{\sigma}_1.\underline{\sigma}_2 + C(\underline{\sigma}_1 - \underline{\sigma}_2).\mathbf{B}$$

where 1 refers to the e^- and 2 to the e^+, $\mathbf{B}$ is the magnetic field, and A and C are constants.

(i) Motivate this form for H.

(ii) Taking $\mathbf{B} = (0, 0, B)$, find the eigenvalues of H. Draw a diagram showing how the eigenvalues depend on B.

G4. Two spin-$\frac{1}{2}$ particles are created in an overall spin singlet state, and they recoil in opposite directions out of the production region. A detector is set up to measure the spin component of one of the particles along a direction $\mathbf{a}$, and a second detector records the spin component of the other particle along a direction $\mathbf{b}$, where $\mathbf{a}$, $\mathbf{b}$ are unit vectors. [Note: In the following, you can take the z-axis of the coordinate system to be along $\mathbf{a}$, to make the calculations simpler; why is this OK?]

(i) What is the probability that the first detector will record spin 'up' (i.e. spin component $+\frac{1}{2}$, in units of $\hbar$) along $\mathbf{a}$?

(ii) Show that if the first detector has given the result 'up' along $\mathbf{a}$, then the probability that the second detector will record 'up' along $\mathbf{b}$ is equal to $\frac{1}{2}(1 - \mathbf{a}.\mathbf{b})$.

(iii) Show that the expectation value of the product of the two measured spin components (in units of $\hbar^2$) along $\mathbf{a}$ and $\mathbf{b}$ is $-\frac{1}{4}\ \mathbf{a}.\mathbf{b}$. Let us call this quantity $C(\theta)$, where θ is the angle between $\mathbf{a}$ and $\mathbf{b}$.

(iv) Bell's theorem states that in any theory in which the behaviour of the spins of the two particles is governed by (local) 'hidden variables', the quantity $C(\theta)$ must satisfy the inequality

$$| 1 - 8C(\theta) + 4C(2\theta) | \leq 2.$$

Taking the quantum mechanical result for $C(\theta)$ obtained in part (iii), plot the function $f(\theta) = 1 - 8C(\theta) + 4C(2\theta)$ for θ between 0 and π. Is the inequality satisfied for all values of θ?

H. Identical particles of spin 0 and of spin-$\frac{1}{2}$

H1. Two identical spinless particles with coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ are subject to the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + V(| \mathbf{r} |)$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, and ∇_1 refers to $\mathbf{r}_1$, and ∇_2 to $\mathbf{r}_2$. Explain why the wavefunction (for stationary states) $\psi(\mathbf{r}_1, \mathbf{r}_2)$ can be written in factorised form as

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \phi(\mathbf{r})\Phi(\mathbf{R})$$

where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$. What is the form of $\Phi(\mathbf{R})$? What is the general form of the angular dependence of $\phi(\mathbf{r})$?

Show that only states in which the relative orbital angular momentum quantum number, ℓ, is <u>even</u> are allowed.

H2. A spin-independent Hamiltonian H has single particle states $\mid 0\rangle, \mid 1\rangle, \mid 2\rangle \ldots\ldots$ where $H \mid n\rangle = E_n \mid n\rangle$. Suppose a system of two identical such particles has Hamiltonian $H_1 + H_2$ and eigenstates $(H_1 + H_2) \mid n, m\rangle = (E_n + E_m) \mid n, m\rangle$.

(i) If the particles are spinless, what is the degeneracy of (a) the ground state (b) the first excited state?

(ii) If the particles have spin-$\frac{1}{2}$, what is the degeneracy of (a) the ground state (b) the first excited state?

I <u>Time-independent perturbation theory</u>

I1. A system is described by an unperturbed Hamiltonian

$$H_0 = p^2/2m + \frac{1}{2}m\omega^2 x^2,$$

where $H_0 \mid n\rangle = E_n^{(0)} \mid n\rangle$.

A perturbation $V = -\alpha x$ is applied.

(i) Show that the first order energy shift for every unperturbed state is zero.

(ii) Evaluate the second order energy shift

$$\Delta E_n^{(2)} = \sum_{k \neq n} \mid \langle k \mid V \mid n\rangle \mid^2 / (E_n^{(0)} - E_k^{(0)})$$

(the matrix elements of x are given in C1(vi)).

(iii) Solve the problem exactly (i.e. find the exact eigenvalues of $H_0 + V$; hint: it is helpful to re-express the Hamiltonian $H_0 + V$ in terms of $x' = x - b$ where b is a suitably chosen constant).

Comment on your result in relation to (i) and (ii). What physical situation might such a perturbation describe?

I2. The Hamiltonian for a certain two-state system in a given representation has the form

$$\begin{pmatrix} A_1 + B_1\epsilon & B_2\epsilon \\ B_2\epsilon & A_2 \end{pmatrix}$$

where all the quantities are real,and ϵ is a small parameter.

State what result perturbation theory would give for the energy eigenvalues to order ϵ in the cases (i) $A_1 \neq A_2$ (ii) $A_1 = A_2$. Obtain the exact eigenvalues and recover the results of perturbation theory by expanding in powers of ϵ up to first order.

I3. An isotropic two-dimensional harmonic oscillator is described by the Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}\, m\omega^2(x^2 + y^2).$$

(i) What are the energy levels of H?

(ii) Write down the ground state and first excited state wavefunctions.

A perturbation λxy is applied.

(iii) Calculate the first order energy shift of the ground state.

(iv) Calculate the first order energy shifts of the first excited states, and find the associated eigenstates to zeroth order in λ.

(v) Solve the problem exactly to check your answer.

I4. A hydrogen atom in a uniform electric field $\mathcal{E}$ along the z-axis is described by the Hamiltonian

$$-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} - ez\mathcal{E}$$

where the term in $\mathcal{E}$ is to be treated as a perturbation.

(i) Show that to first order in $\mathcal{E}$ the ground state energy is unchanged.

(ii) The unperturbed $n = 2$ state is 4-fold degenerate ($\{\mid n\ell m\rangle\} = \mid 211\rangle, \mid 210\rangle, \mid 21-1\rangle, \mid 200\rangle$). Applying first order degenerate perturbation theory in this four-dimensional state space, show that

(a) the states $\mid 211\rangle$ and $\mid 21-1\rangle$ remain eigenstates to this order.

(b) the remaining two eigenstates are $\frac{1}{\sqrt{2}}(\mid 210\rangle \pm \mid 200\rangle)$ with energies $E_{n=2} \pm 3a_0 e\mathcal{E}$ respectively, where a_0 is the Bohr radius.

Are these two states eigenstates of $\mathbf{L}^2$? of L_z? Discuss.

I5 .Consider the two-particle problem of H2, and introduce a perturbation V which depends on the coordinates of both particles, so that

$$H = H_1 + H_2 + V_{12}.$$

(i) Apply degenerate perturbation theory in the two-dimensional subspace with unperturbed energy $E_1 + E_0$ to show that, to first order in the matrix elements of V_{12}, the degeneracy is lifted and the new energies are

$$E_\pm = E_1 + E_0 + J \pm K$$

where $\langle 10 \mid V_{12} \mid 10\rangle = \langle 01 \mid V_{12} \mid 01\rangle = J$, and $\langle 10 \mid V_{12} \mid 01\rangle = \langle 01 \mid V_{12} \mid 10\rangle = K$.

If $K > 0$, what is the eigenstate belonging to E_-,to zeroth order in V_{12}?

(ii) Suppose the particles are identical and have spin-$\frac{1}{2}$ (but none of H_1, H_2 or V_{12} depend on spins). What spin wave function(s) should be associated with the E_- state in the case $K > 0$?

Show that the splitting between the E_+ and E_- states can be modelled by an effective Hamiltonian $H_{eff} = -\frac{2K}{\hbar^2}\,\mathbf{S}_1.\mathbf{S}_2$, acting in the spin space of the two particles.

J Time-dependent perturbation theory

J1. A two state system has wavefunction

$$\psi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} \quad \text{where} \quad \begin{aligned} i\hbar\dot{a} &= E_1 a + Vb \\ i\hbar\dot{b} &= E_2 b + Va \end{aligned}$$

where V is a real constant in time except that it is zero for $t \le 0$. Suppose that at $t = 0$ the system is such that $a(0) = 1$, $b(0) = 0$.

(i) Show that if we define c_1 and c_2 by

$$c_1 = e^{iE_1 t/\hbar} a, \quad c_2 = e^{iE_2 t/\hbar} b$$

then $i\hbar\dot{c}_1 = Vc_2 e^{i\omega_{12}t}$, $i\hbar\dot{c}_2 = Vc_1 e^{-i\omega_{12}t}$, where $\omega_{12} = (E_1 - E_2)/\hbar$, and $c_1(0) = 1$, $c_2(0) = 0$.

(ii) Show that to first order in V, and for small times $t > 0$,

$$\begin{aligned} c_2 &\approx \frac{V}{E_1 - E_2}[e^{-i\omega_{12}t} - 1] \\ c_1 &\approx 1. \end{aligned}$$

Hence show that the probability that the system will be found in the state represented by the vector $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ at $t > 0$ is, in this approximation,

$$\frac{V^2}{\hbar^2}\left\{\frac{\sin^2(\omega_{12}t/2)}{(\omega_{12}/2)^2}\right\}.$$

(iii) By differentiating the equation for c_2 given in (i), obtain a second order equation for c_2, and solve it subject to the initial conditions $c_2(0) = 0, \dot{c}_2(0) = Vc_1(0)/i\hbar = V/i\hbar$. Expand your result to lowest order in V to recover the result of (ii).

J2. A hydrogen atom in its ground state is placed in a uniform electric field E where

$$\begin{aligned} E &= 0 \quad t < 0 \\ E &= E_0 \exp(-\alpha t) \quad t \ge 0 \end{aligned}$$

where α is a positive real constant. Find the probability correct to second order in E_0 that the atom will have made a transition to a 2p state after a long time.

The normalised wavefunctions and energy levels for the hydrogen atom are

$$\begin{aligned}
\phi_{100} &= (\pi a_0^3)^{-\frac{1}{2}} \exp(-r/a_0), \quad E_1 = -e^2/8\pi\epsilon_0 a_0 \\
\phi_{210} &= \frac{1}{4}(2\pi a_0^5)^{-\frac{1}{2}} r \exp(-r/2a_0)\cos\theta, \quad E_2 = -e^2/32\pi\epsilon_0 a_0 \\
a_0 &= 4\pi\epsilon_0\hbar^2/me^2.
\end{aligned}$$

J3. Fermi's Golden Rule states that the transition probability per unit time $= \frac{2\pi}{\hbar} \mid V_{fi} \mid^2 \frac{dN}{dE}$ where $V_{fi} = \langle f \mid V \mid i \rangle$ is the matrix element of the perturbation, considered as causing transitions, and $\frac{dN}{dE}$ is the density of final states about the energy E.

Consider the application of this result to the scattering of a spinless particle by a potential $V(\mathbf{r})$. The states of the $V = 0$ problem are plane waves

$$\begin{aligned}
\phi_i(\mathbf{r}) &= \frac{1}{L^{3/2}} e^{i\mathbf{k}_i.\mathbf{r}} \\
\phi_f(\mathbf{r}) &= \frac{1}{L^{3/2}} e^{i\mathbf{k}_f.\mathbf{r}}
\end{aligned}$$

normalised in volume L^3.

(i) Prove that $\frac{dN}{dE} = \frac{mL^3}{8\pi^3\hbar^2} k \sin\theta d\theta d\phi$ where $k = \mid \mathbf{k}_i \mid = \mid \mathbf{k}_f \mid$ (elastic scattering) and θ, ϕ are the polar angles of $\mathbf{k}_f$.

(ii) Prove that the flux of incident particles is $\hbar\mathbf{k}_i/mL^3$, with magnitude $\hbar k/mL^3$.

(iii) The Golden Rule gives us the transition probability per unit time that, if we have one particle incident in a volume L^3, it will be scattered into a solid angle element $d\Omega = \sin\theta d\theta d\phi$. Call this $S(\theta)d\Omega$. The *differential cross section* is then defined as

$$\frac{d\sigma}{d\Omega} = S(\theta)/\text{incident flux}.$$

Consider the case $V(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0|\mathbf{r}|} e^{-|\mathbf{r}|/a}$ (a "screened Coulomb" or "Yukawa" potential). The matrix element $\langle f \mid V \mid i \rangle$ is

$$\begin{aligned}
\langle f \mid V \mid i \rangle &= \frac{1}{L^3} \int e^{-i\mathbf{k}_f.\mathbf{r}} \left(-\frac{e^2}{4\pi\epsilon_0} \frac{1}{\mid \mathbf{r} \mid} e^{-|\mathbf{r}|/a} \right) e^{i\mathbf{k}_i.\mathbf{r}} d^3\mathbf{r}, \\
&= -\frac{e^2}{4\pi\epsilon_0 L^3} \int e^{i\mathbf{q}.\mathbf{r}} \frac{e^{-r/a}}{r} d^3\mathbf{r}
\end{aligned}$$

where $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$ and $r = \mid \mathbf{r} \mid$. Do the integral as follows: change to polar coordinates with the z axis chosen along $\mathbf{q}$ (which is "external" to the integral). Do the integral over θ. Then do the integral over r. Show that

$$\langle f \mid V \mid i \rangle = -\frac{e^2}{\epsilon_0 L^3} \frac{1}{\mathbf{q}^2 + \frac{1}{a^2}}.$$

Now let $a \to \infty$ (the *Coulomb scattering case*) and show that

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{16\pi\epsilon_0 E} \right)^2 \frac{1}{\sin^4 \theta/2}$$

where θ is the angle between $\mathbf{k}_i$ and $\mathbf{k}_f$, and $E = \hbar^2 k^2/2m$. This is the *Rutherford Scattering Formula.*

Calculate $\frac{d\sigma}{d\Omega}$ (what are the *dimensions*?) for $E = 10keV$ and $\theta = 10^0$.