Second Year Theory Option

QUANTUM MECHANICS

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Problem Set 2

C. The Harmonic Oscillator

C1. A one-dimensional harmonic oscillator has the Hamiltonian $H = p^2/2m + \frac{1}{2}m\omega^2x^2$ where $[x,p] = i\hbar$. Define the operators a and $a^\dagger$ by

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right).$$

(i) Show that $[a, a^\dagger] = 1$ and, by induction or otherwise, that $[a, (a^\dagger)^n] = n(a^\dagger)^{n-1}$.

(ii) Show that $H = \hbar\omega(a^\dagger a + \frac{1}{2}) = \hbar\omega(aa^\dagger - \frac{1}{2})$. Deduce that $[a^\dagger, H] = -\hbar\omega a^\dagger$, and use this result to prove that if $H \mid n\rangle = E_n \mid n\rangle$, then $Ha^\dagger \mid n\rangle = (E_n + \hbar\omega)a^\dagger \mid n\rangle$. State and prove a similar result for $a \mid n\rangle$.

(iii) Explain why there must be a state $\mid 0\rangle$ such that $a \mid 0\rangle = 0$. What is the energy eigenvalue for $\mid 0\rangle$? Deduce the energy spectrum of the oscillator.

(iv) By considering $\langle x \mid a \mid 0\rangle$, obtain the (unnormalised) ground state wavefunction $\langle x \mid 0\rangle$. Find the (unnormalised) first excited state wavefunction.

(v) Show that the normalised energy eigenstates $\mid n\rangle$ satisfy

$$a \mid n\rangle = \sqrt{n} \mid n-1\rangle, a^\dagger \mid n\rangle = \sqrt{n+1} \mid n+1\rangle$$

and that

$$\mid n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} \mid 0\rangle$$

where $\langle 0 \mid 0\rangle = 1$.

(vi) Show that $\sqrt{\frac{2m\omega}{\hbar}}x \mid n\rangle = \sqrt{n} \mid n-1\rangle + \sqrt{n+1} \mid n+1\rangle$ and hence that

$$\langle n \mid \frac{1}{2}m\omega^2x^2 \mid n\rangle = \frac{1}{2}(n + \frac{1}{2})\hbar\omega.$$

What is $\langle n \mid p^2/2m \mid n\rangle$?

(vii) Using just the states $\mid 0\rangle, \mid 1\rangle, \mid 2\rangle$ and $\mid 3\rangle$, calculate the 4×4 matrix $\mathbf{x}$ representing x in this (truncated) basis. Also calculate the matrix $\mathbf{p}$ representing p. Calculate $\mathbf{xp} - \mathbf{px}$ and comment on the result.

(viii) Defining the exponential of an operator A by

$$\exp A = \sum_{n=0}^{\infty}\frac{A^n}{n!},$$

show that the (un-normalised) state $\mid \alpha\rangle$ defined by $\mid \alpha\rangle = \exp(\alpha a^\dagger) \mid 0\rangle$ (where α is a complex number and $a \mid 0\rangle = 0$) satisfies

$$a \mid \alpha\rangle = \alpha \mid \alpha\rangle.$$

By considering the matrix element $\langle x \mid a \mid \alpha\rangle$, show that

$$\langle x \mid \alpha\rangle = N \exp\left[-\frac{m\omega x^2}{2\hbar} + \sqrt{\frac{2m\omega}{\hbar}}\alpha x\right]$$

where N is a normalisation constant which need not be determined.

D Particle in an electromagnetic field

D1. The Hamiltonian for a particle of mass m and charge Q that moves in a magnetic field $\mathbf{B}$ with vector potential $\mathbf{A}$ is

$$H = \frac{1}{2m}(\mathbf{p} - Q\mathbf{A})^2.$$

Show that when $\mathbf{B} = (0, 0, B)$, with B a constant, H may be written

$$H = H_{xy} + \frac{p_z^2}{2m} \text{ where } H_{xy} \equiv \frac{1}{2m}\left\{(p_x + \frac{1}{2}QBy)^2 + (p_y - \frac{1}{2}QBx)^2\right\}.$$

Show that H_{xy} may be written

$$H_{xy} = \frac{1}{4m}(aa^\dagger + a^\dagger a),$$

where

$$a \equiv \pi_x + i\pi_y \text{ with } \begin{cases} \pi_x \equiv p_x + \frac{1}{2}QBy, \\ \pi_y \equiv p_y - \frac{1}{2}QBx. \end{cases}$$

Evaluate the commutators $[\pi_x, \pi_y]$ and $[a, a^\dagger]$ and determine the energy spectrum of H_{xy}.

Show that the ground-state wavefunction is a function $\psi(x, y)$ that satisfies the equation

$$\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\psi = -\frac{QB}{2\hbar}(x + iy)\psi.$$

By introducing new coordinates $u \equiv x + iy$ and $v \equiv x - iy$, or otherwise, obtain a suitable wavefunction ψ.

D2. **Note:** this question is about *gauge invariance* which is not in the Part A Theoretical Physics syllabus.

The Hamiltonian describing a particle of charge e and mass m in an electromagnetic field is

$$H(\mathbf{A}, \phi) = \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi$$

where the vector and scalar potentials $\mathbf{A}$ and ϕ are related to the electric and magnetic fields in the usual way, and $\mathbf{p} = -i\hbar\bigtriangledown$.

Consider the gauge transformation

$$\begin{aligned} \mathbf{A} &\Rightarrow \mathbf{A}' = \mathbf{A} + \bigtriangledown \wedge \\ \phi &\Rightarrow \phi' = \phi - \frac{\partial \wedge}{\partial t} \\ \psi &\Rightarrow \psi' = \psi \, \exp(ie \wedge /\hbar) \end{aligned}$$

(i) Show that

$$(\mathbf{p} - e\mathbf{A}')\psi' = \exp(ie \wedge /\hbar)[(\mathbf{p} - e\mathbf{A})\psi].$$

(ii) Show that

$$\left(i\hbar\frac{\partial}{\partial t} - e\phi'\right)\psi' = \exp(ie \wedge /\hbar)\left[\left(i\hbar\frac{\partial}{\partial t} - e\phi\right)\psi\right].$$

(iii) Hence show that if

$$i\hbar\frac{\partial\psi}{\partial t} = H(\mathbf{A}, \phi)\psi$$

then

$$i\hbar\frac{\partial\psi'}{\partial t} = H(\mathbf{A}', \phi')\psi'.$$

What is the significance of this result?

(iv) In the absence of the eletromagnetic field, the probability current density $\mathbf{j}$ is defined by

$$\mathbf{j} = \frac{\hbar}{2mi}(\psi^* \bigtriangledown \psi - \psi(\bigtriangledown\psi)^*). \qquad (*)$$

Writing $\psi = \mid \psi \mid \exp(i\theta)$, show that

$$\mathbf{j} = \frac{\hbar}{m} \mid \psi \mid^2 \bigtriangledown\theta. \qquad (1)$$

Is this $\mathbf{j}$ invariant under a gauge transformation? Show that if $\bigtriangledown$ in the above definition $(*)$ of $\mathbf{j}$ is replaced by $\bigtriangledown - ie\mathbf{A}/\hbar$, a gauge invariant probability current density is obtained; give the expression for it analogous to (1).

(v) In certain physical situations (notably inside a superconductor) ψ may be taken to be real, and constant. Interpreting $e\mathbf{j}$ as the electromagnetic current (in the gauge-invariant case) show that, for the special case $\mathbf{A} = (0, 0, A(x))$ solutions of the Maxwell equation for $\mathbf{B}$ exist of the form

$$\mathbf{B} = (0, B_0 \exp(-x/\lambda), 0)$$

where

$$\lambda = (m/\mu_0 e^2 \mid \psi \mid^2)^{\frac{1}{2}}.$$

E. Angular momentum

E1. The angular momentum operators (J_x, J_y, J_z) are Hermitian and satisfy $[J_x, J_y] = i\hbar J_z$. Define $J_+ = J_x + iJ_y$, $J_- = J_x - iJ_y$.

(i) Show that

$[J_z, J_+] = \hbar J_+, [J_z, J_-] = -\hbar J_-,$

$[\mathbf{J}^2, J_+] = [\mathbf{J}^2, J_-] = 0,$

$[J_+, J_-] = 2\hbar J_z,$

and that

$$\begin{aligned} \mathbf{J}^2 = J_z^2 + \tfrac{1}{2}(J_+J_- + J_-J_+) &= J_z{}^2 + J_+J_- - \hbar J_z \\ &= J_z^2 + J_-J_+ + \hbar J_z \end{aligned}$$

(here $\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2$).

(ii)From these results show that if $\mid j, m\rangle$ is an eigenstate of $\mathbf{J}^2$ and of J_z with eigenvalues $j(j+1)\hbar^2$ and $m\hbar$ respectively,then $J_+ \mid j, m\rangle$ is an eigenstate of $\mathbf{J}^2$ and J_z belonging to the eigenvalues $j(j+1)\hbar^2$ and $(m+1)\hbar$; state and prove a corresponding result for $J_- \mid j, m\rangle$.

(iii) Consider

$$\langle j, m \mid J_x^2 \mid j, m\rangle = \sum_{j', m'} \mid \langle j, m \mid J_x \mid j', m'\rangle \mid^2 \geq 0 \;;$$

Similarly $\langle j, m \mid J_y^2 \mid j, m\rangle \geq 0$. Hence $\langle j, m \mid J_x^2 + J_y^2 \mid j, m\rangle \geq 0$, from which it follows that $\langle j, m \mid \mathbf{J}^2 - J_z^2 \mid j, m\rangle = \langle j, m \mid J_x^2 + J_y^2 \mid j, m\rangle \geq 0$. So $m^2 \leq j(j+1)$.

Hence for a given eigenvalue of $\mathbf{J}^2$, the possible eigenvalues of J_z are bounded above and below. Since J_+ acting on an eigenstate raises its J_z eigenvalue by $\hbar$ (see (ii)), the eigenstate for the maximum allowed value of m must be such that J_+ "kills" it: $J_+ \mid j, m_{\max}\rangle = 0$.

Using the relation

$$\begin{aligned} 0 &= J_-J_+ \mid j, m_{\max}\rangle \\ &= (\mathbf{J}^2 - J_z^2 - \hbar J_z) \mid j, m_{\max}\rangle \quad \text{(see (i))} \end{aligned}$$

deduce that if $\mid j, m_{\max}\rangle$ is an eigenstate of $\mathbf{J}^2$ with eigenvalue $j(j+1)\hbar^2$ then the value of $m_{\max}$ is j. Similarly show that there is a lowest possible m value, which is

$m_{\min} = -j$. Deduce further that there are, in all, $2j+1$ states with this value of $\mathbf{J}^2$ and with J_z values $j\hbar$, $(j-1)\hbar, \ldots -j\hbar$, from which it follows that j is either an integer or half an odd integer.

(iv) We have seen that $J_+ \mid j, m\rangle = C \mid j, m+1\rangle$ where C is an as yet unknown constant. By considering the scalar product of this state with itself, and assuming that the states $\mid j, m\rangle$ are normalised, show that

$$\mid C \mid^2 = [j(j+1) - m(m+1)]\hbar^2.$$

The standard **convention** is to define C to be real and then

$$J_+ \mid j, m\rangle = [j(j+1) - m(m+1)]^{\frac{1}{2}}\hbar \mid j, m+1\rangle.$$

Note that the RHS is zero when $m = j$. By considering $J_- J_+ \mid j, m\rangle = C J_- \mid j, m+1\rangle$, show that

$$J_- \mid j, m\rangle = [j(j+1) - m(m-1)]^{\frac{1}{2}}\hbar \mid j, m-1\rangle,$$

which vanishes when $m = -j$.

(v) Show that for $j = \frac{1}{2}$, the matrices representing J_x, J_y and J_z are

$$J_x^{(\frac{1}{2})} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, J_y^{(\frac{1}{2})} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, J_z^{(\frac{1}{2})} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

in the basis $\{\mid \frac{1}{2}, \frac{1}{2}\rangle, \mid \frac{1}{2}, -\frac{1}{2}\rangle\}$. These are usually written as

$$S_i \equiv J_i^{(\frac{1}{2})} = \frac{\hbar}{2}\sigma_i \quad (\text{or } \mathbf{S} = \frac{1}{2}\hbar\underline{\sigma})$$

where the σ_i are the Pauli matrices , and $\underline{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. What are the column vectors representing the basis states, in this basis?

(vi) Find the matrices $J_x^{(1)}, J_y^{(1)}, J_z^{(1)}$ for the case $j = 1$, in a similar basis.

F Spin-$\frac{1}{2}$ systems

F1. Let $\hat{\mathbf{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ be a unit vector in 3-D space with polar angles θ, ϕ. Define $S_n = S_x n_x + S_y n_y + S_z n_z$ where $\mathbf{S}$ is as in E1(v). Check that

$$S_n = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}.$$

Check that the eigenvalues of S_n are $\pm\frac{1}{2}\hbar$, and that the corresponding normalised eigenvectors can be written as

$$u_1 = \begin{pmatrix} \cos(\theta/2)\ e^{-i\phi/2} \\ \sin(\theta/2)\ e^{i\phi/2} \end{pmatrix}, u_2 = \begin{pmatrix} -\sin(\theta/2)\ e^{-i\phi/2} \\ \cos(\theta/2)\ e^{i\phi/2} \end{pmatrix}.$$

Verify that $u_1^\dagger u_2 = 0, u_2^\dagger u_2 = 1$.

Express $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ as a linear combination of u_1 and u_2. A spin-$\frac{1}{2}$ particle is in a state such that its z-component of spin has the value $+\frac{1}{2}\hbar$. What is the probability that, if its spin component along the $\hat{\mathbf{n}}$ axis were measured, the result would be $+\frac{1}{2}\hbar$?

F2. (i) Verify that $u_{x+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is a normalised eigenvector of S_x of E1(v), with eigenvalue $\frac{\hbar}{2}$. Express u_{x+} as a linear combination of eigenvectors of S_z. If particles in this spin state are passed through a Stern-Gerlach apparatus with the magnetic field along the z-direction, what will be observed?

(ii) Suppose now that we consider particles in an "*unpolarised*" spin state i.e. in a state which is itself unknown, but which is equally likely to correspond to "$S_z = +\frac{1}{2}\hbar$" as to "$S_z = -\frac{1}{2}\hbar$" (or any other direction) . So the particles in such a state are in $u_{z+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ with 50 % probability, and in $u_{z-} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ with 50 % probability. What will be observed if such particles are passed through the S-G apparatus of part (i)?

(iii) How could the difference between particles in the state u_{x+} and particles in the unpolarised state be distinguished experimentally?

F3 The time variation of the 'spin wave function' of spin-half particle of mass m and charge q in a magnetic field $\mathbf{B}$ is given by

$$i\hbar\frac{d\psi}{dt} = H\psi,$$

where

$$\psi = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$$

and

$$H = -\frac{gq}{2m}\mathbf{S}.\mathbf{B};$$

ψ_a and ψ_b are time-dependent complex numbers.

(i) Show that H is Hermitian and find its eigenvalues.

(ii) By substituting $\psi = u\ exp(-iEt/\hbar)$, where u is a complex 2-component column vector, show how the two possible energies of stationary states are related to the eigenvalues of H. For the case where $\mathbf{B} = B(\sin\theta, 0, \cos\theta)$, write down the normalized eigenvectors of H. Express the general solution of the Schrödinger equation above in terms of the eigenvectors of H and the energies E_1 and E_2 of the stationary states.

(iii) At $t = 0$, a spin-$\frac{1}{2}$ particle has spin projection $+\frac{1}{2}\hbar$ along the x-axis. At that moment, it enters some apparatus that has a constant magnetic field along the z-axis, i.e. $\mathbf{B} = (0, 0, B)$. At time t, it emerges from the apparatus, and a measurement of its spin component along the x-axis is made. What is the spin wavefunction of the particle at time t? Show that the probability of obtaining the result $+\frac{1}{2}\hbar$ at time t is $\cos^2 \frac{1}{2}\omega t$ where $\omega = \frac{E_1 - E_2}{\hbar}$.

F4. The average value of $\mathbf{S}$ is defined as $\langle \mathbf{S} \rangle = \psi^\dagger \mathbf{S} \psi$, where $\mathbf{S}$ and ψ are as in F3. Show that

$$\frac{d}{dt}\langle \mathbf{S} \rangle = \frac{gq}{2m}\langle \mathbf{S} \rangle \times \mathbf{B}$$

and describe the motion of $\langle \mathbf{S} \rangle$ in space.