Phys. 506 Final Exam

1/28/71

1/28/71 ① "In a certain QM system, it is found that the eigenfcn $\psi(x)$ of energy E is translationally invariant, i.e. if $\psi(x)$ is a solution to $H\psi = E\psi$, then so is $\psi(x+\Delta x)$, where Δx is an arbitrary translation of the coordinate origin. Show, as a result of this, that the system momentum (operator) p must commute with the Hamiltonian H, i.e. $[H,p]=0$, so that p is a constant of the motion, which in turn means ψ describes a free particle."

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Have: $H\psi(x) = E\psi(x)$ and $H\psi(x+\Delta x) = E\psi(x+\Delta x)$.

Suppose Δx is small. Then by Taylor series expansion...

$$\psi(x+\Delta x) \simeq \psi(x) + \Delta x\left(\frac{\partial\psi}{\partial x}\right)_{\Delta x=0} = \psi(x) + \frac{i}{\hbar}\Delta x\, p\,\psi(x), \quad p = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\therefore\ 2^{\text{ND}} \text{ eq.} \Rightarrow \quad H\psi(x) + \frac{i}{\hbar}\Delta x\, Hp\,\psi(x) = E\psi(x) + \frac{i}{\hbar}\Delta x\, p\,\underbrace{E\psi(x)}_{=H\psi(x)}$$

cancel

or, $Hp\,\psi(x) = pH\psi(x)$, i.e. $[H,p]\,\psi(x) = 0$

Since this is true for general ψ, must have $[H,p]=0$. QED

2/3/71 ② "The wavefcn describing the motion of a free particle starting out at (x,t) and moving to (x',t') obviously depends only on the differences between initial and final coordinates. Consequently, the free particle propagator G_0 is at most a fcn of $x'-x$ and $t'-t$. A full Fourier integral representation of G_0 must then be of the form (in 1D)

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$$G_0(x'-x,t'-t) = \frac{1}{(2\pi)^2}\int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} d\omega\, g(k,\omega)\, e^{ik(x'-x)}\, e^{-i\omega(t'-t)}.$$

$g(k,\omega)$ is known as the free particle propagator in momentum space. Derive an expression for g, by taking into account the fact that G_0 obeys the point-source Schrödinger eqtn

$$\left(i\hbar \frac{\partial}{\partial t'} - \frac{p'^2}{2m}\right) G_0 = \hbar\, \delta(x'-x)\, \delta(t'-t).$$

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Operating through the Fourier integral by $\left(i\hbar\frac{\partial}{\partial t'} - \frac{p'^2}{2m}\right)$, we have

$$\frac{1}{(2\pi)^2}\int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} d\omega \left[\left(\hbar\omega - \frac{\hbar^2 k^2}{2m}\right) g(k,\omega)\right] e^{ik(x'-x)}\, e^{-i\omega(t'-t)} =$$

$$= \hbar\, \delta(x'-x)\, \delta(t'-t) = \frac{\hbar}{(2\pi)^2}\int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} d\omega\, e^{ik(x'-x)}\, e^{-i\omega(t'-t)}$$

The latter integral is the std rep$^{\underline{n}}$ of $\delta(x'-x)\,\delta(t'-t)$. The only way the integrals can be identical is if $[\ ] \equiv \hbar$. So

$$g(k,\omega) = 1\Big/\left(\omega - \frac{\hbar k^2}{2m}\right) \qquad \underline{\underline{QED}}$$

N.B. In order to complete the defn of $g(k,\omega)$, we have to decide how to go around the pole at $\omega = \hbar k^2/2m$. This is done by letting $\omega \to \omega + i\epsilon$. $\epsilon \to 0_+$ gives $\theta(t'-t)$, and the standard (retarded) propagator, while $\epsilon \to 0_-$ generates the advanced G_0.

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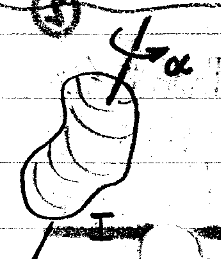

3 a) A "plane rotator" is a rigid body constrained to rotate (with arbitrary angular momentum) about a <u>fixed</u> axis in space. The rotation can be specified by choosing a point on the body and giving its azimuthal ∡ α w.r.t. the rotation axis. Suppose the body has moment of inertia I about the rotation axis. For the QM plane rotator, solve the time-independent

Schrödinger eqtn for the allowed energies E_m and normalized eigenfcns $\psi_m(\alpha)$ of the rotation. What is the degeneracy of the state with energy E_m?

b) Suppose, at time $t=0$, the rotator is in a state specified by a wave-fcn $\Psi(\alpha,0) = C\sin^2\alpha$, where C is a normalizing constant. What is the wavefcn $\Psi(\alpha,t)$ for $t>0$?

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a) Pick rotation axis to be z-axis of rect. cd. system. Rotational energy is

$$H = L_z^2/2I, \quad L_z = z\text{-comp. of } \measuredangle \text{ momentum}$$

QMly : $L_z = -i\hbar\frac{\partial}{\partial\alpha}$, so $H = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\alpha^2}$,

S. eqtn : $H\psi = E\psi \Rightarrow -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\alpha^2}\psi(\alpha) = E\psi(\alpha)$

or// $\left(\frac{\partial^2}{\partial\alpha^2} + m^2\right)\psi(\alpha) = 0$, $m = \sqrt{2IE/\hbar^2}$

Soln is : $\psi(\alpha) = C\,e^{-im\alpha}$

For $\psi(\alpha)$ single-valued over $0 \leq \alpha \leq 2\pi$, need $m = 0, \pm1, \pm2, \ldots$

$\therefore$ allowed energies are : $E_m = (\hbar^2/2I)m^2$, $m = 0, \pm1, \pm2, \ldots$

Degeneracy of level E_m is 2 for any $m \neq 0$.

Normalized eigenfcns are $\psi_m(\alpha) = \frac{1}{\sqrt{2\pi}}e^{-im\alpha}$ (A)

b) Can now expand any $\Psi(\alpha,t)$ in terms of $\psi_m(\alpha)$ by

$$\Psi(\alpha,t) = \sum_{m=-\infty}^{+\infty} c_m\,\psi_m(\alpha)\,e^{-\frac{i}{\hbar}E_m t}$$

By orthogonality of $\psi_m(\alpha)$, i.e. $\int_0^{2\pi} \psi_m^*(\alpha)\,\psi_n(\alpha)\,d\alpha = \delta_{mn}$, have

$$\Psi(\alpha,0) = \sum_m C_m \psi_m(\alpha) \implies C_m = \int \psi_m^*(\alpha)\,\Psi(\alpha,0)$$

Now if $\Psi(\alpha,0) = C\sin^2\alpha$, we have

$$C_m = \frac{C}{\sqrt{2\pi}} \int_0^{2\pi} e^{+im\alpha} \sin^2\alpha\, d\alpha$$

Write: $\sin^2\alpha = \left(\frac{1}{2i}\left(e^{+i\alpha} - e^{-i\alpha}\right)\right)^2 = \frac{1}{2} - \frac{1}{4}\left(e^{+2i\alpha} - e^{-2i\alpha}\right)$

$$\therefore\ C_m = \frac{C}{\sqrt{2\pi}} \int_0^{2\pi} \left[\frac{1}{2} e^{+im\alpha} - \frac{1}{4}\left(e^{i(m+2)\alpha} + e^{i(m-2)\alpha}\right)\right] d\alpha$$

But $\displaystyle\int_0^{2\pi} e^{ik\alpha}\, d\alpha = \frac{1}{ik}\left(e^{2\pi i k} - 1\right) = \begin{cases} \text{with } k \text{ an integer...} \\ 0 \text{ for } k \neq 0 \\ 2\pi \text{ for } k = 0 \end{cases}$

$\Rightarrow$ we have C_m values only for $m = 0$ & $m = \pm 2$, i.e.

$$c_0 = \frac{1}{2} C\sqrt{2\pi}, \quad C_{+2} = -\frac{1}{4} C\sqrt{2\pi}, \quad C_{-2} = -\frac{1}{4} C\sqrt{2\pi}$$

So the desired $\Psi(\alpha,t)$ is

$E_2 = 2\hbar^2/I$

$$\Psi(\alpha,t) = C\sqrt{2\pi}\left\{\frac{1}{2}\frac{1}{\sqrt{2\pi}} - \frac{1}{4}\frac{1}{\sqrt{2\pi}}\left[e^{2i\alpha} e^{-\frac{i}{\hbar}E_2 t} + e^{-2i\alpha} e^{-\frac{i}{\hbar}E_2 t}\right]\right\}$$

$$= \frac{C}{2}\left\{1 - \cos 2\alpha \times e^{-i(2\hbar/I)t}\right\} \leftarrow$$ Agrees with Ter Haar p. 103, prob. (1.34)

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④ "The expectation value of $1/r^2$ in the state $|nlm\rangle$ of a hydrogen-like atom (potential: $V(r) = -Ze^2/r$) is calculated to be

Prob. #④ ϕ507 Final (May 1992).

$$\langle 1/r^2 \rangle = \langle nlm|\frac{1}{r^2}|nlm\rangle = \left(\frac{Z}{a_0}\right)^2 / n^3\left(l+\tfrac{1}{2}\right), \quad a_0 = \hbar^2/me^2.$$

Use this to show that $\langle 1/r^3\rangle$ in the same state is given by

$$\langle 1/r^3\rangle = \langle nlm|\tfrac{1}{r^3}|nlm\rangle = \left(\frac{Z}{a_0}\right)^3 \Big/ n^3 l(l+\tfrac{1}{2})(l+1).$$

Hint: do not use explicit wavefunctions. Instead, look at the equation of motion for an electron in orbit.

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Eqtn of motion is : $mv^2/r = Ze^2/r^2 \Rightarrow L^2/r^3 = Zme^2/r^2$

Where $L = mvr$ is the orbital ∡ momentum. QMly, the eqtn of motion must be the same, in an expectation value sense, so we can write...

$$\langle L^2/r^3\rangle = Zme^2\langle 1/r^2\rangle$$

But $L^2 = l(l+1)\hbar^2$ w.r.t. state $|nlm\rangle$. So we have...

$$l(l+1)\hbar^2\langle 1/r^3\rangle = Zme^2\langle 1/r^2\rangle$$

or, $$\langle 1/r^3\rangle = \frac{(Z/a_0)}{l(l+1)}\langle 1/r^2\rangle, \quad a_0 = \hbar^2/me^2$$

$$= \left(\frac{Z}{a_0}\right)^3 \Big/ n^3 l(l+1)(l+\tfrac{1}{2}) \qquad \text{QED}$$

5 "Let $\vec{A} = (A_x, A_y, A_z)$ be a QM vector operator, and consider the quantity $\vec{I} = \psi^\dagger \vec{A}\psi$, which is the integrand of the expectation value of $\vec{A}$ in state ψ. Under a rotation of the coordinate system by an infinitesimal angle about any one of the coordinate axes, there are two equivalent ways to describe how $\vec{I}$, and hence $\vec{A}$, transforms. One either transforms ψ, leaving $\vec{A}$

unchanged (i.e. $\psi \to \psi'$, so that $\vec{I} \to \vec{I}' = \psi'^{\dagger} \vec{A} \psi'$), or one transforms $\vec{A}$, leaving ψ unchanged (i.e. $\vec{A} \to \vec{A}'$, so that $\vec{I} \to \vec{I}' = \psi^{\dagger} \vec{A}' \psi$). By equating the two equivalent forms for the transformed $\vec{I}$, derive a commutation for $\vec{A}$ and $\vec{J}$, where $\vec{J}$ is the total system angular momentum.

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It is sufficient to consider rotation by $\delta\varphi$ about z-axis. The results for rotations about the x & y axes will follow by the usual cyclic permutation of x, y & z. The transf^{n} of ψ is

$$\psi \to \psi' = (1 - i\delta\varphi J_z)\psi \,, \quad J_z \text{ in units of } \hbar$$

Only A_x & A_y are affected by a z-axis rotation. Since we ultimately will end up relating A_x & A_y to J_z, it is sufficient to consider one at a time, i.e. we shall look at I_x only. A_x transforms as

$$A_x \to A_x' = A_x - \delta\varphi A_y$$

Setting the two alternate expressions for I_x' equal, we find

$$\psi'^{\dagger} A_x \psi' = \psi^{\dagger} A_x' \psi$$

the two [ ] must be identical

or $\quad \psi^{\dagger}\left[(1 + i\delta\varphi J_z) A_x (1 - i\delta\varphi J_z)\right]\psi = \psi^{\dagger}\left[(A_x - \delta\varphi A_y)\right]\psi$

i.e. $\quad (A_x + i\delta\varphi J_z A_x)(1 - i\delta\varphi J_z) = A_x - \delta\varphi A_y$, neglect $O(\delta\varphi)^2$ on LHS

or $\quad -i\delta\varphi(A_x J_z - J_z A_x) = -\delta\varphi A_y$, cancel $\delta\varphi$ and mult. by $-i$

$$[J_z, A_x] = i A_y \implies \text{generalization } [J_\alpha, A_\beta] = i A_\gamma, \ \alpha\beta\gamma = \overrightarrow{123}$$

Had we used I_y, we would have gotten same thing. Generalization is "obvious".

(6) "A hydrogen-like atom (potential: $V(r) = -Ze^2/r$) is in its ground state $|100\rangle$, with total energy E_1 given by the usual Bohr formula. Calculate the probability that the electron will be found at a distance from the nucleus greater than its energy would permit from a classical standpoint."

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Bohr ground state energy is: $E_1 = -Z^2e^2/2a_0$

Classically: $\frac{mv^2}{r} = \frac{Ze^2}{r^2}$, and total energy $= \frac{1}{2}mv^2 - \frac{Ze^2}{r} = -\frac{Ze^2}{2r}$

Classical total energy $= E_1 \Rightarrow r = a_0/Z = r_0$

Normalized gnd state wavefcn is: $\psi_{100}(r) = \left(\frac{Z^3}{\pi a_0^3}\right)^{\frac{1}{2}} e^{-Zr/a_0}$

Probability that e found at $r \geq r_0$ is

$$P = \int_{r_0}^{\infty} |\psi_{100}(r)|^2 \times 4\pi r^2 dr = \frac{1}{2}\left(\frac{2Z}{a_0}\right)^3 \int_{r_0}^{\infty} r^2 e^{-\left(\frac{2Z}{a_0}\right)r} dr$$

or/ $P(x_0) = \frac{1}{2}\int_{x_0}^{\infty} x^2 e^{-x} dx$, with $x_0 = \frac{2Z}{a_0} r_0 = 2$

The integral can be done by partial integrations...

$$\int_{x_0}^{\infty} x^2 e^{-x} dx = -x^2 e^{-x}\Big|_{x_0}^{\infty} + 2\int_{x_0}^{\infty} x e^{-x} dx = x_0^2 e^{-x_0} - 2\left[x e^{-x}\Big|_{x_0}^{\infty} - \int_{x_0}^{\infty} e^{-x} dx\right]$$

$$= (x_0^2 + 2x_0 + 2)e^{-x_0}$$ ← Checks with Dwight, p.127

$\therefore P(x_0) = \frac{1}{2}(x_0^2 + 2x_0 + 2)e^{-x_0}$ ← Note $P(0) = 1$, as expected

Desired: $P(2) = 5e^{-2} = 0.6767$

⑦ "An operator F depends on the position vector $\vec{x}$ and particle momentum $\vec{p}$ only through the combinations $\vec{x}^2$, $\vec{p}^2$ and $\vec{x}\cdot\vec{p}$; that is, considered as a function of $\vec{x}$ and $\vec{p}$, $F = F(\vec{x}^2, \vec{p}^2, \vec{x}\cdot\vec{p})$ only. Let $\vec{L}$ be the system orbital angular momentum operator, and denote the eigenstates of $\vec{L}^2$ and L_z by $Y_{lm}(\vartheta,\varphi) = |lm\rangle$.

a) Calculate the commutator bracket $[\vec{L}, F]$.

b) State all that can be said about the matrix elements $\langle l'm'|F|lm\rangle$.

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$[\vec{L}, \vec{x}^2] = 0$ since $\vec{L}$ commutes with all sph. symmetric fcns

$[\vec{L}, \vec{p}^2] = 0$ as has been shown (e.g. Merzbacher, p. 176).

So we must worry about $[\vec{L}, \vec{x}\cdot\vec{p}]$. Taking 1^{ST} comp...

$$[\vec{L}_1, \vec{x}\cdot\vec{p}] = \sum_\alpha [L_1, x_\alpha p_\alpha] = \sum_\alpha \{ x_\alpha [L_1, p_\alpha] + [L_1, x_\alpha] p_\alpha \}$$

Recall $[L_i, p_j] = i\hbar p_k$, $ijk = \widehat{123}$, and sim'ly for comps of $\vec{x}$ (This was prob. ⑮ in PHYS. 505). Then we have...

$$[L_1, \vec{x}\cdot\vec{p}] = \{x_2 \underbrace{[L_1, p_2]}_{+i\hbar p_3} + \underbrace{[L_1, x_2]}_{+i\hbar x_3} p_2\} + \{x_3 \underbrace{[L_1, p_3]}_{-i\hbar p_2} + \underbrace{[L_1, x_3]}_{-i\hbar x_2} p_3\}$$

$$= i\hbar\{x_2 p_3 + x_3 p_2\} - i\hbar\{x_3 p_2 + x_2 p_3\} = 0$$

So $\vec{L}$ commutes with F, i.e. $[\vec{L}, F]$.

This means $\vec{L}$ & F have the eigenfcns $|lm\rangle$ in common. So

$$\langle l'm'|F|lm\rangle = F_{lm}\,\delta_{ll'}\,\delta_{mm'}$$

where F_{lm} is the average value of F in the state lm.