1. Let's start with a problem about unitarity of integral operators. Specifically, consider the evolution operator $\hat{U}(t,t_0)$ of a quantum particle and its matrix elements — or rather its kernel —

$$U(\mathbf{x}_1,t_1;\mathbf{x}_0,t_0)\ =\ \langle\mathbf{x}_1|\,\hat{U}(t_1,t_0)\,|\mathbf{x}_0\rangle \tag{1}$$

in the position basis. This kernel is called the *evolution kernel* or the *propagation amplitude*: Physically, it's the amplitude of the particle which was located at point $\mathbf{x}_0$ at tome t_0 to be found at point $\mathbf{x}_1$ at a later time t_1; and it also describes the time evolution (in the Schrödinger picture) of the particle's wave-function in the time $t_1 - t_0$ according to

$$\psi(\mathbf{x}_1,t_1)\ =\int\!d^3\mathbf{x}_0\,U(\mathbf{x}_1,t_1;\mathbf{x}_0,t_0)\times\psi(\mathbf{x}_0,t_0). \tag{2}$$

For simplicity, consider the free non-relativistic spinless particle with Hamiltonian

$$\hat{H}\ =\ \frac{\hat{\mathbf{p}}^2}{2M}\,. \tag{3}$$

(a) The evolution operator for this free particle is diagonal in the momentum basis. Translate it to the position basis and show that

$$U(\mathbf{x}_1,t_1;\mathbf{x}_0,t_0)\ =\ \left(\frac{M}{2\pi i\hbar(t_1-t_0)}\right)^{3/2}\times\exp\left(\frac{i}{\hbar}\,\frac{m(\mathbf{x}_1-\mathbf{x}_0)^2}{2(t_1-t_0)}\right). \tag{4}$$

(b) Spell out the unitarity conditions $\hat{U}^\dagger\hat{U}=\hat{U}\hat{U}^\dagger=1$ in terms of the evolution kernel (1), specifically in terms of integrals of the form $\int d^3\mathbf{x}\,U^*(\cdots)U(\cdots)$.

(c) Now verify these conditions for the kernel (4) by explicit integration.

2. Next, a refresher of the undergraduate-level theory of the orbital angular momentum operator

$$\hat{\mathbf{L}} \stackrel{\text{def}}{=} \hat{\mathbf{x}} \times \hat{\mathbf{p}}, \qquad i.\ e.,\ \hat{L}_i \stackrel{\text{def}}{=} \epsilon_{ijk}\hat{x}_j\hat{p}_k\,. \tag{5}$$

It is also a good drill for the use of the canonical commutation relations

$$[\hat{x}_i, \hat{x}_j] = 0, \quad [\hat{p}_i, \hat{p}_j] = 0, \qquad [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij} \tag{6}$$

and in 3D index notations.

In this problem you should not use any wave-functions or the way the position and momentum operators act on them. Instead, threat the $\hat{x}_i$ and $\hat{p}_j$ as abstract Hermitian operators obeying the commutation relations (6), while the $\hat{L}_i$ operators are as defined in eq. (5). Show that eqs. (5) and (6) lead to:

(a) $[\hat{x}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{x}_k\,$;

(b) $[\hat{p}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{p}_k\,$;

(c) $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$ and therefore $\hat{\mathbf{L}} \times \hat{\mathbf{L}} = i\hbar\hat{\mathbf{L}}$;

(d) $[\hat{\mathbf{p}}^2, \hat{\mathbf{L}}] = 0 = [f(\hat{r}), \hat{\mathbf{L}}]$ for any function f of the radius $\hat{r} = (\hat{\mathbf{x}}^2)^{1/2}$;

(e) $[\hat{\mathbf{L}}, \hat{\mathbf{L}}^2] = 0$;

(f) $\hat{\mathbf{p}}^2 = \hat{p}_r^2 + \hat{r}^{-2}\hat{\mathbf{L}}^2$, where $\hat{p}_r \stackrel{\text{def}}{=} \frac{1}{2}\{\widehat{\frac{x_i}{r}}, \hat{p}_i\}$ (note: $\hat{p}_r$ so defined is hermitian).

3. Now, let's continue the story of the orbital angular momentum $\hat{\mathbf{L}}$ but switch to the wave-function formalism. In the Cartesian coordinate basis $|x, y, z\rangle$, the $\hat{\mathbf{x}}$ and the $\hat{\mathbf{p}}$ operators act in the usual way on the $\Psi(x, y, z)$. But for some of the operators you have seen in the previous problem, it's more convenient to use the spherical coordinate basis $|r, \theta, \phi\rangle$ and hence wave-functions $\Psi(r, \theta, \phi)$.

   (a) Show that in the spherical coordinate basis, the $\hat{p}_r$ operators from the problem 2(f) acts as

$$\hat{p}_r\Psi(r, \theta, \phi) \;=\; -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\Psi(r, \theta, \phi), \tag{7}$$

   and spell out the action of the $\hat{p}_r^2$ operator in the same basis.

(b) In the same basis, spell out the action of the $\hat{\mathbf{L}}^{\mathbf{2}}$ operator on the $\Psi(r,\theta,\phi)$.

Hint: in any coordinate basis $\hat{p}^2$ acts as $-\hbar^2\nabla^2$, and any E&M textbook will tell you how the Laplacian ∇^2 acts in the spherical coordinates. Then use the results of the parts 2(f) and 3(a).

Now let's apply this knowledge to a spinless particle moving in a central potential $V(r)$. Its Hamiltonian

$$\hat{H} \;=\; \frac{\hat{\mathbf{p}}^{\mathbf{2}}}{2M} \;+\; V(\hat{r}) \tag{8}$$

commutes with all 3 components $\hat{L}_i$ of the angular momentum, but the $\hat{L}_x, \hat{L}_y, \hat{L}_z$ operators do not commute with each other. As we saw in the previous homework set, this means the Hamiltonian (8) must have degenerate spectrum. Let's see how this works in more detail.

In the undergraduate school you should have learned that while you cannot simultaneously diagonalize all the angular momenta operators, you may simultaneously diagonalize the $\hat{\mathbf{L}}^2$ and the $\hat{L}_z$. The common eigenstates of these 2 operators have wave-functions of general form

$$\Psi(r,\theta,\phi) \;=\; \psi_r(r)\times Y_{\ell,m}(\theta,\phi) \tag{9}$$

where the radial wave function $\psi_r(r)$ may be any function of the radius while $Y_{\ell,m}(\theta,\phi)$ is a spherical harmonic; the corresponding eigenvalues are

$$\mathbf{L}^2 \;=\; \hbar^2\ell(\ell+1), \qquad L_z \;=\; \hbar m, \tag{10}$$

and their spectrum corresponds to integer $\ell = 0,1,2,3,\ldots$ and
integer $m = -\ell, (1-\ell), \ldots, (\ell-1), \ell$.

(c) Argue that the Hamiltonian (8) is block-diagonal in the $|r,\ell,m\rangle$ basis: it's diagonal WRT ℓ and m but not WRT r. On in the wave-function terms, when $\hat{H}$ act on the wave-function of the form (9), it yields

$$\hat{H}\Psi(r,\theta,\phi) \;=\; Y_{\ell,m}(\theta,\phi)\times \hat{H}_{\text{rad}}(\text{block } \ell, m)\psi_r(r). \tag{11}$$

Also, argue that that the radial Hamiltonian $\hat{H}_{\text{rad}}$ for a diagonal block of given ℓ and m depends on the ℓ but not on the m. Hint: use $[\hat{H},\hat{L}_x] = [\hat{H},\hat{L}_y] = 0$.

(d) Finally, show that

$$\hat{H}_{\text{rad}}(\ell)\psi_r(r) \;=\; -\frac{\hbar^2}{2M}\left(\frac{d^2\psi_r}{dr^2} + \frac{2}{r}\frac{d\psi_r}{dr}\right) + \left(\frac{\ell(\ell+1)\hbar^2}{2Mr^2} + V(r)\right)\psi_r(r). \tag{12}$$

4. In the next homework set#5 you shall learn how to apply the Harmonic oscillator formalism to the Landau levels of a charged particle moving in a magnetic field. But before we go that far, we need to learn about the quantum charged particles subject to magnetic fields, and maybe both magnetic and electric fields. That's what this problem is about.

A classical charged particle in a magnetic field has *canonical momentum*

$$\mathbf{p} \;=\; m\mathbf{v} + \frac{Q}{c}\mathbf{A}(\mathbf{x}_{\text{particle}}) \tag{13}$$

which is quite different from the usual *kinematic momentum* $\vec{\pi} = m\mathbf{v}$, and its classical Hamiltonian is

$$H(\mathbf{x},\mathbf{p}) \;=\; \frac{\vec{\pi}^2}{2m} \;=\; \frac{1}{2m}\left(\mathbf{p} - \frac{Q}{c}\mathbf{A}(\mathbf{x})\right)^2. \tag{14}$$

In quantum mechanics, it's the canonical momentum operators $\hat{p}_i$ $(i = x, y, z)$ which obeys the usual commutation relations

$$[\hat{x}_i, \hat{x}_j] \;=\; 0, \quad [\hat{p}_i, \hat{p}_j] \;=\; 0, \quad [\hat{x}_i, \hat{p}_j] \;=\; i\hbar\delta_{ij} \tag{15}$$

so in the coordinate basis they act as $\hat{p}_i\psi(\mathbf{x}) = -i\hbar(\partial/\partial x_i)\psi(\mathbf{x})$. On the other hand, the kinematic momenta

$$\hat{\pi}_i \;\stackrel{\text{def}}{=}\; \hat{p}_i - \frac{Q}{c}A_i(\hat{x},\hat{y},\hat{z}) \tag{16}$$

act in a more complicated fashion and obey more complicated commutation relations

$$[\hat{x}_i, \hat{x}_j] \;=\; 0, \quad [\hat{x}_i, \hat{\pi}_j] \;=\; i\hbar\delta_{ij}\,, \quad [\hat{\pi}_i, \hat{\pi}_j] \;=\; \frac{i\hbar Q}{c}\epsilon_{ijk}B_k(\hat{x},\hat{y},\hat{z}). \tag{17}$$

Finally, the Hamiltonian operator $\hat{H}$ follows from the classical Hamiltonian (14) as

$$\hat{H} \;=\; \frac{\hat{\vec{\pi}}^2}{2m} \;=\; \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{Q}{c}\mathbf{A}(\hat{\mathbf{x}})\right)^2. \tag{18}$$

(a) Unless you have attended my extra lecture on September 8, read the parts of my notes on classical mechanics and canonical quantization where I explain eqs. (13) through (18). Specifically, pages 5–7 where I explain the classical mechanics of a charged particle, and pages 8–9 where I explain the commutation relations.

(b) Use the commutation relations (17) to derive the Ehrenfest equations for the quantum charged particle. Specifically, show that

$$\frac{d}{dt}\langle\hat{\mathbf{x}}\rangle \;=\; \frac{1}{m}\left\langle\hat{\vec{\pi}}\right\rangle \quad\text{and}\quad \frac{d}{dt}\left\langle\hat{\vec{\pi}}\right\rangle \;=\; \frac{Q}{2mc}\left\langle\hat{\vec{\pi}}\times\hat{\mathbf{B}}-\hat{\mathbf{B}}\times\hat{\vec{\pi}}\right\rangle \tag{19}$$

where $\hat{\mathbf{B}} \stackrel{\text{def}}{=} \mathbf{B}(\hat{x},\hat{y},\hat{z})$.

(c) Now let's subject the particle to both electric and magnetic fields and allow both fields to be time-dependent, thus time-dependent Hamiltonian

$$\hat{H}(t) \;=\; Q\Phi(\hat{\mathbf{x}},t) \;+\; \frac{1}{2m}\left(\hat{\mathbf{p}}\;-\;\mathbf{A}(\hat{\mathbf{x}},t)\right)^2 \tag{20}$$

Show that in this case, the Ehrenfest equations become

$$\frac{d}{dt}\langle\hat{\mathbf{x}}\rangle \;=\; \frac{1}{m}\left\langle\hat{\vec{\pi}}\right\rangle \quad\text{and}\quad \frac{d}{dt}\left\langle\hat{\vec{\pi}}\right\rangle \;=\; Q\left\langle\hat{\mathbf{E}}\right\rangle \;+\; \frac{Q}{2mc}\left\langle\hat{\vec{\pi}}\times\hat{\mathbf{B}}-\hat{\mathbf{B}}\times\hat{\vec{\pi}}\right\rangle. \tag{21}$$

Hint: use Heisenberg–Dirac equations for the time-dependent operators, and remember that in a time-dependent vector potential $\mathbf{A}(\mathbf{x},t)$, the kinematic momentum operator (16) becomes *explicitly* time-dependent,

$$\frac{\partial}{\partial t}\hat{\vec{\pi}} \;=\; -\frac{Q}{c}\,\frac{\partial\mathbf{A}}{\partial t}(\hat{\mathbf{x}},t). \tag{22}$$