Prelim and Course Exam: Quantum Mechanics, Friday December 18 2020. 8:00am-12:00pm

- This exam paper is in two parts: **PART A** (QMII material) with **FOUR** questions and **PART B** (QMI material) with **TWO** questions.
- If you are taking this exam for prelim credit alone or for both course and prelim credit you have **FOUR** hours to answer the same **THREE** of the **PART A** questions and the same **ONE** of the **PART B** questions. The course credit component will only be based on the three problems from **Part A**.
- If you are taking this exam for QMII course credit alone you have **THREE** hours to answer **THREE** questions from **PART A**.

If a student submits solutions to more than three problems from part A or more than one problem from part B, only the first three problems from part A or the first problem from part B as listed on the exam will be graded. Students should write their solutions on blank 8.5 by 11 paper or in a blue book, putting their name on each page, the number of the problem and the number of the page in their solution on each page (i.e. 2-1 means first page of problem 2). Also each problem solution should be on a separate set of pages (i.e. not putting parts of two different problems on the same page). At the end of the exam students should scan in their solutions in sequence using a cell phone or a scanner and email them in a file or files (ideally pdf) to the prelim committee chair philip.mannheim@uconn.edu no later than 15 minutes after the end time of the exam. (It might be easier to transfer the files to a laptop first.) Label both the email header and the file or files with your name and the name of the exam. In the email state which problems you have attempted, which are prelim and which are course, and state how many pages there are for each of the problems. The chair will immediately check if the emailing is readable or if a resend is required.

Some possibly useful information

$$\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}+\frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta}+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$= \frac{\partial^2}{\partial \rho^2}+\frac{1}{\rho}\frac{\partial}{\partial \rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2}+\frac{\partial^2}{\partial z^2}$$

$$\boldsymbol{\nabla}\psi = \mathbf{e}_x\frac{\partial\psi}{\partial x}+\mathbf{e}_y\frac{\partial\psi}{\partial y}+\mathbf{e}_z\frac{\partial\psi}{\partial z} = \mathbf{e}_r\frac{\partial\psi}{\partial r}+\mathbf{e}_\theta\frac{1}{r}\frac{\partial\psi}{\partial\theta}+\mathbf{e}_\phi\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi} = \mathbf{e}_\rho\frac{\partial\psi}{\partial\rho}+\mathbf{e}_\phi\frac{1}{\rho}\frac{\partial\psi}{\partial\phi}+\mathbf{e}_z\frac{\partial\psi}{\partial z}.$$

$$\text{Hermite polynomial} = H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2} \quad , \quad H_0(x)=1 \quad , \quad H_1(x)=2x \quad , \quad H_2(x)=4x^2-2$$

$$\text{Laguerre} = L_n(r) = e^r\frac{d^n}{dr^n}\left(r^n e^{-r}\right) \quad , \quad \text{associated Laguerre} = L^q_{n+q}(r) = (-1)^q\frac{d^q}{dr^q}L_{n+q}(r) \quad .$$

$$\text{Legendre polynomial} = P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l \quad , \quad P_0(x)=1 \quad , \quad P_1(x)=x \quad , \quad P_2(x)=\frac{1}{2}(3x^2-1) \quad ,$$

$$\int_{-1}^{+1} dw P_\ell(w)P_{\ell'}(w) = \frac{2}{(2\ell+1)}\delta_{\ell\ell'}$$

$$\text{associated Legendre polynomial} = P_l^m(x) = (1-x^2)^{|m|/2}\frac{d^{|m|}}{dx^{|m|}}P_l(x)$$

$$\text{spherical harmonic} = Y_l^m(\theta,\ \phi) = (-1)^m\left[\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}\right]^{1/2} P_l^m(\cos\theta)e^{im\phi} \quad ,$$

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2} \quad , \quad Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta \quad , \quad Y_1^{\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1) \;,\; Y_2^{\pm 1} = \mp \left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{\pm i\phi} \;,\; Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$$

spherical Bessels : $$j_l(r) = (-1)^\ell r^\ell \left(\frac{1}{r}\frac{d}{dr}\right)^\ell \left(\frac{\sin r}{r}\right) \quad , \quad n_l(r) = (-1)^{(\ell+1)} r^\ell \left(\frac{1}{r}\frac{d}{dr}\right)^\ell \left(\frac{\cos r}{r}\right) \quad ,$$

with asymptotic behavior $$j_\ell(r) \to \frac{\cos(r - \ell\pi/2 - \pi/2)}{r} \quad , \quad n_\ell(r) \to \frac{\sin(r - \ell\pi/2 - \pi/2)}{r} \quad .$$

$$j_0(r) = \frac{\sin r}{r} \quad , \quad n_0(r) = -\frac{\cos r}{r} \quad , \quad j_1(r) = \frac{\sin r}{r^2} - \frac{\cos r}{r} \quad , \quad n_1(r) = -\frac{\cos r}{r^2} - \frac{\sin r}{r} \quad ,$$

$$j_2(r) = \frac{3\sin r}{r^3} - \frac{\sin r}{r} - \frac{3\cos r}{r^2} \quad , \quad n_2(r) = -\frac{3\cos r}{r^3} + \frac{\cos r}{r} - \frac{3\sin r}{r^2} \quad .$$

$$e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell j_\ell(kr) P_\ell(\cos\theta).$$

Some Gaussian integrals:

$$\int_0^\infty dx e^{-ax^2} = \frac{1}{2}\sqrt{\frac{\pi}{a}}, \quad \int_0^\infty dx x^2 e^{-ax^2} = \frac{1}{4}\sqrt{\frac{\pi}{a^3}}, \quad \int_0^\infty dx x^4 e^{-ax^2} = \frac{3}{8}\sqrt{\frac{\pi}{a^5}}.$$

For Harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$ the raising and lowering operators are defined as

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2} x + i\left(\frac{1}{2\hbar m\omega}\right)^{1/2} p; \qquad a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2} x - i\left(\frac{1}{2\hbar m\omega}\right)^{1/2} p.$$

Kinetic term in a fixed angular momentum sector

$$\frac{\mathbf{p}^2}{2m}[R(r)Y_l^m(\theta,\phi)] = \left[-\frac{1}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right] R(r)\right] Y_l^m(\theta,\phi).$$

Angular momentum raising and lowering operators

$$j_\pm |j,m\rangle = \sqrt{(j \mp m)(j \pm m + 1)}\ \ |j, m \pm 1\rangle.$$

PART A

1. Consider a hydrogen atom in an anisotropic harmonic potential. The Hamiltonian of the system is

$$H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r} + \frac{1}{2}m\omega^2[x^2 + y^2 + Cz^2].$$

Suppose ω is large enough so that the harmonic potential cannot be treated as a perturbation. We want to set up a variational calculation to estimate the ground state energy. When the anisotropy is significant ($C \gg 1$ or $C \ll 1$), we do not expect the ground state to be even approximately rotationally invariant. Let us instead consider a set of variational states with angular momentum one:

$$\Psi_\alpha^m(\mathbf{r}) = NY_1^m(\theta, \phi)\exp\{-\frac{\alpha}{2}r^2\},$$

where N is the normalization constant, and α is the only variational parameter.

(a) This Hamiltonian has a discrete symmetry $\phi \to -\phi$ where ϕ as usual is the azimuthal angle in polar coordinates (this transformation is a combination of parity $x_i \to -x_i$ and a rotation by π around the y axis, although this is not important for the purpose of this problem). By using this symmetry show that $\langle\Psi_\alpha^1|H|\Psi_\alpha^1\rangle = \langle\Psi_\alpha^{-1}|H|\Psi_\alpha^{-1}\rangle$.

(b) Suppose $C \ll 1$. Which value of the magnetic quantum number m (0, 1 or -1) would you choose to get a better variational estimate of the energy?

Hint: Think of the shape of Y_1^m for different m, and ask yourself which ones prefer larger/smaller values of z.

(c) For a variational function Ψ_α^0 (with zero magnetic quantum number) derive the variational equation for the ground state energy.

(d) For large frequency ω, find α approximately by neglecting the Coulomb interaction.

2. A particle is in the ground state of the harmonic oscillator potential with frequency ω:

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{x}^2.$$

At $t = 0$ an additional time dependent potential is turned on. The form of this potential is

$$V_2 = (1 - e^{-\lambda^2 t^2})\frac{1}{2}m\left(\Omega^2 - \omega^2\right)\mathbf{x}^2.$$

Suppose Ω is of the same order of magnitude as ω, so that V_2 is **not small**.

(a) First consider the case $\lambda \gg \omega$. What is the probability that at time $t \to \infty$ the particle is in the ground state of harmonic oscillator with frequency Ω?

(b) The same question but for $\lambda \ll \omega$.

(c) For this part V_2 is absent. Consider a different perturbation to H (for positive as well as negative times)

$$\delta V_1 = e^{-\lambda^2 t^2}\frac{1}{2}m\left(\Omega^2 - \omega^2\right)\mathbf{x}^2,$$

with $\Omega^2 - \omega^2 \ll \omega^2$. The potential δV_1 is switched on at $t = -\infty$. Calculate to lowest order in δV_1 the probability that the particle that at $t \to -\infty$ was in the ground state of the oscillator H, at $t \to \infty$ is found in the second excited state ($n = 2$) of the same oscillator.

3. Consider the scattering of a particle of mass m on a static potential $V(\mathbf{r})$. In the Born approximation the scattering amplitude is given by

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{-i\mathbf{q}\cdot\mathbf{r}'} V(\mathbf{r}') d^3\mathbf{r}',$$

where $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$ is the momentum transferred to the particle in the scattering.

(a) Calculate the scattering amplitude for a Yukawa potential $V(r) = \frac{g}{r}e^{-\mu r}$ as the function of the scattering angle θ.

(b) The scattering amplitude is given in terms of the phase shifts by

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\sin\delta_\ell P_\ell(\cos\theta),$$

where $P_\ell(\cos\theta)$ are Legendre polynomials. Using the scattering amplitude calculated in part (a), calculate the phase shift δ_0.

Hint: You can use the orthogonality of Legendre polynomials

$$\int_{-1}^{1} d(\cos\theta) P_\ell(\cos\theta) P_{\ell'}(\cos\theta) = \frac{2}{2\ell+1}\delta_{\ell\ell'}.$$

Also remember that in the Born approximation you should assume that the δ_ℓ are small, i.e. $\delta_\ell \ll 1$.

4. Consider a spin 1/2 electron moving in a Coulomb potential $V(r) = -e^2/r$. The electron has the spin-orbit interaction $\delta_{LS}H = \alpha\mathbf{S}\cdot\mathbf{L}$ (assume α is a constant for simplicity). The system is also put in an external constant magnetic field $\mathbf{B} = B\hat{z}$, and interacts with it via $\delta_B H = -g(L_z + 2S_z)B$ (g is a constant). The complete Hamiltonian is therefore

$$H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r} + \alpha\mathbf{S}\cdot\mathbf{L} - g(L_z + 2S_z)B.$$

Let us consider only the energy levels with the principal quantum number $n = 2$, i.e. the states $\ell = 0, 1$ - that is we assume that the electron can only occupy these states (you can disregard the radial part of the wave function in this calculation).

(a) Show that $\mathbf{L}^2$, $J_z = L_z + S_z$ and parity P commute with the Hamiltonian. Does L_z or S_z separately commute with H?

(b) Starting with the basis of product states $|\ell, \ell_z\rangle \otimes |s_z\rangle$ with $\ell = 0, 1$, construct the basis $|\ell, j, j_z\rangle$. Give explicit construction only for the sates $|\ell = 0, j = 1/2, j_z = 1/2\rangle$, $|\ell = 1, j = 3/2, j_z = 3/2\rangle$ and $|\ell = 1, j = 1/2, j_z = 1/2\rangle$ and then infer the rest of the states by symmetry.

(c) Show that the Hamiltonian $\delta_{LS}H = \alpha\mathbf{S}\cdot\mathbf{L}$ is diagonal in this basis, and calculate its eigenvalues. Is $\delta_B H = -g(L_z + 2S_z)$ also diagonal? For which values of ℓ, j, j_z and ℓ', j', j'_z do the matrix elements $\langle \ell, j, j_z|\delta_B H|\ell', j', j'_z\rangle$ not vanish? (Do not calculate the matrix elements themselves: use the symmetries to justify your answer.)

PART B

5. Consider a one-dimensional quantum-mechanical harmonic oscillator with Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}.$$

A convenient rewriting of the harmonic oscillator Hamiltonian may be obtained by setting

$$q = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (a + a^\dagger) \;\;,\;\; p = i\left(\frac{\hbar m\omega}{2}\right)^{1/2} (a^\dagger - a).$$

(a) The state $|0\rangle$ is defined by the condition $a|0\rangle = 0$. Show that the state $|0\rangle$ is the ground state of the harmonic oscillator.

(b) Using the fact that $a|0\rangle = 0$, and the fact that $p = -i\hbar\partial/\partial q$, construct $< q|0 >$ and show that it is the wave function of the ground state of the harmonic oscillator.

(c) Again using the fact that $a|0\rangle = 0$ construct the q dependence of the wave function of the first excited state of the harmonic oscillator, and check your answer by inserting it into the Schrodinger equation associated with H to get its eigenvalue.

6. The expectation value of an operator $\Omega(\mathbf{r}, \mathbf{p}, t)$ in a state $\psi(\mathbf{r}, t)$ is given as $< \Omega >= \int d^3r\psi^*(\mathbf{r}, t)\Omega\psi(\mathbf{r}, t)$.

(a) Show that $< \Omega >$ obeys Ehrenfast's theorem, viz.

$$i\hbar\frac{d}{dt} < \Omega >=< [\Omega, H] > + i\hbar < \frac{\partial\Omega}{\partial t} > .$$

(b) Then show for any $\psi(\mathbf{r}, t)$ which obeys the Schrodinger equation associated with the Hamiltonian $H = \mathbf{p}^2/2m + V(\mathbf{r})$ with real $V(\mathbf{r})$ that:

$$\frac{d}{dt} < \mathbf{r} >= \frac{< \mathbf{p} >}{m}, \quad \frac{d}{dt} < \mathbf{p} >= - < \frac{dV}{d\mathbf{r}} > \quad .$$

(c) In the presence of electromagnetism an appropriate Hamiltonian is

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

where $\mathbf{A}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$ are vector and scalar electromagnetic potentials. With the E and B fields being given by

$$\vec{E} = -\vec{\nabla}\phi - \frac{\partial\vec{A}}{\partial t}, \quad \vec{B} = \vec{\nabla} \times \vec{A}$$

Derive the appropriate Ehrenfest's theorem in this case to explicitly obtain the appropriate quantum-mechanical Lorentz force law:

$$m\frac{d < \vec{v} >}{dt} = q < \vec{v} \times \vec{B} > + q < E > \text{ where } < \vec{v} >= \frac{d < \vec{r} >}{dt}.$$

Hint: consider applying Ehrenfest's theorem twice, once to get $d < \vec{r} > /dt$ and a second time to get $d^2 < \vec{r} > /dt^2$.