Preliminary Exam: Quantum Mechanics, Friday August 23, 2019. 9:00-1:00

Answer a total of any **FOUR** out of the five questions. Put the solution to each problem in a **separate** blue book and put the number of the problem and your name on the front of each book. If you submit solutions to more than four problems, only the first four problems as listed on the exam will be graded.

Some possibly useful information

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

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

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

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

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

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

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

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

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

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2} \quad , \quad Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta \quad , \quad Y_1^{\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{\pm i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1) \ , \ Y_2^{\pm1} = \mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta e^{\pm i\phi} \ , \ Y_2^{\pm2} = \left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta e^{\pm 2i\phi}$$

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

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

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

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

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

1. **(a)** Eigenstates of the hydrogen atom obey the Schrodinger equation

$$\begin{aligned} H\psi(r,\theta,\phi) &= -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}+\frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta}+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(r,\theta,\phi)-\frac{e^2}{r}\psi(r,\theta,\phi) \\ &= E\psi(r,\theta,\phi). \end{aligned}$$

The wave functions can be written as $\psi(r,\theta,\phi)=R_{n,\ell}(r)Y_\ell^m(\theta,\phi)$ where $R_{n\ell}(r)$ is the radial wave function and n is the principle quantum number, and can also be written as eigenkets of the form $|n,\ell,m\rangle$. The first few radial functions are of the form

$$R_{10}(r)=2(a_0)^{-3/2}e^{-r/a_0},\quad R_{20}(r)=\left(2-\frac{r}{a_0}\right)(2a_0)^{-3/2}e^{-r/2a_0},\quad R_{21}(r)=(2a_0)^{-3/2}\frac{r}{a_0\sqrt{3}}e^{-r/2a_0},$$

where $a_0=\hbar^2/me^2$. Determine the energies of all of the $\psi(r,\theta,\phi)$ wave functions that have these three radial functions, and determine the degeneracy of all energy levels with $n=1$ and all energy levels with $n=2$.

(b) The atom is now perturbed by a constant electric field E_0 pointing in the z direction so that the interaction is of the form

$$V=eE_0r\cos\theta.$$

Determine the change in the ground state energy up to second order in V. Should your calculation involve a summation over states you do not need to actually perform the summation, but you do need to indicate which terms in the summation are non-zero. You may neglect contributions from continuum states.

(c) Consider all energy levels with $n=2$, and consider matrix elements $V_{ij}=\langle i|V|j\rangle$ where $|i\rangle$ and $|j\rangle$ are any of the $n=2$ wave functions. For which (i,j) combinations are these matrix elements non-zero? Calculate the change in energy of each of the $n=2$ eigenstates to first order in V.

Hint: You may find it easier to do parts **(b)** and **(c)** in the $|n,\ell,m\rangle$ basis.

2. Suppose the particle creation and annihilation operators $a_i^\dagger$ and a_i that obey

$$[a_i,a_j]=\left[a_i^\dagger,a_j^\dagger\right]=0,\qquad \left[a_i,a_j^\dagger\right]=\delta_{ij}$$

can be algebraically expressed in terms of a new set of operators $b_i^\dagger$ and b_i that obey the same canonical commutation relations:

$$[b_i,b_j]=\left[b_i^\dagger,b_j^\dagger\right]=0,\qquad \left[b_i,b_j^\dagger\right]=\delta_{ij}. \tag{1}$$

(The operators $b_i^\dagger$ and b_i are often said to "create/annihilate quasiparticles.") The commutation relations above imply that there is a unique state $|0_b\rangle$ that is annihilated by all b_i; this state is usually referred to as the quasiparticle vacuum, the so-called Fock space states of the form $b_i^\dagger|0_b\rangle$ are the one-quasiparticle states, $b_i^\dagger b_j^\dagger|0_b\rangle$ are the two-quasiparticle states, etc. It is convenient to make a unitary operator transform:

$$b_i=Ua_iU^\dagger,\quad b_i^\dagger=Ua_i^\dagger U^\dagger, \tag{2}$$

where U is a unitary operator in the Fock space, usually of the form e^X for some anti-Hermitian polynomial X in a_i and $a_i^\dagger$.

(a) Show that the unitarity of U automatically guarantees that b_i and $b_i^\dagger$ satisfy (1), and that the quasiparticle state $|0_b\rangle=U|0_a\rangle$ is the quasiparticle vacuum where $|0_a\rangle$ is the original vacuum state that the a_i annihilate.

(b) Verify that for $X=\sum_n\left(c_na_n^\dagger-c_n^*a_n\right)$, one gets the c-number shift $e^Xa_ne^{-X}=a_n-c_n$.

(c) Now let $X=\sum_n\frac{1}{2}\eta_n\left(e^{i\lambda_n}(a_n^\dagger)^2-e^{-i\lambda_n}(a_n)^2\right)$ (with real η_n and λ_n). Show that for $U=e^X$, (2) defines a so-called Bogoliubov transformation:

$$b_i=a_i\cosh\eta_i-e^{i\lambda_i}a_i^\dagger\sinh\eta_i,\qquad b_i^\dagger=a_i^\dagger\cosh\eta_i-e^{-i\lambda_i}a_i\sinh\eta_i.$$

(d) In order to see the utility of the Bogoliubov transformation, consider the simple case of one creation/annihilation operator pair with $\lambda=\pi$. This gives $b=a\cosh\eta+a^\dagger\sinh\eta$. Use this transformation to obtain the eigenvalues of the following Hamiltonian:

$$H=\hbar\omega a^\dagger a+\frac{1}{2}V\left(a^2+a^{\dagger 2}\right),$$

where V is constant. Also give the upper limit on V for which this can be done.
Hint: write H in terms of the $b,b^\dagger$ operators, and find a value for η that gives H the form of a simple harmonic oscillator

3. **(a)** In quantum mechanics there is a parity operator P that effects $P^{-1}\vec{x}P = -\vec{x}$ where $\vec{x}$ is the 3-dimensional position operator, while leaving time unchanged. Under the parity operator how do the following operators transform: the momentum $\vec{p}$, the angular momentum $\vec{L}$, the spin operator $\vec{S}$ of a spin one-half electron, the electric field $\vec{E}$, and the magnetic field $\vec{B}$. Consider the Hamiltonian $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})$ where $V(\vec{x})$ is even under parity. What does this imply for the behavior of the eigenstates of H under parity?

   (b) Also in quantum mechanics there exists a time reversal operator T that effects the transformation $T : t \to t' = -t$. Assuming the validity of the Schrödinger equation and the symmetry of the Hamiltonian $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})$ under time reversal, show that for the time reversal operator, the following property has to be valid:

$$T^{-1}(-i)T = i.$$

   (c) If T preserves the norm of the states it acts on, show that a general way to write this operator is $T = UK$, where U is unitary and K is the complex conjugation operator. What is U for spinless, nondegenerate particles? What is thus the value of T^2 for those particles?

   (d) Consider a non-relativistic spin-$\frac{1}{2}$ particle at rest with spin operator $\vec{S}$. Explain (without calculation) why we need to get $T^{-1}\vec{S}T = -\vec{S}$.

   (e) With $\vec{S} \propto \vec{\sigma}$, where $\vec{\sigma}$ is the vector of Pauli matrices, show that $T^{-1}\vec{S}T = -\vec{S}$ does indeed hold if we set $U = \sigma_y$.

4. **(a)** Consider rotations through an angle φ about an axis $\hat{\mathbf{n}}$, and denote $\boldsymbol{\varphi} = \varphi\,\hat{\mathbf{n}}$. Given the total angular momentum $\mathbf{J}$ that generates infinitesimal rotations, upon an active rotation an arbitrary state $|\psi\rangle$ transforms to $|\psi'\rangle = e^{-i\boldsymbol{\varphi}\cdot\mathbf{J}/\hbar}|\psi\rangle$, and operators remain unchanged. Show that when the rotation angle φ is "infinitesimal", the expectation value of an arbitrary operator A changes upon the rotation of the system by

$$\delta\langle A\rangle = -\frac{i}{\hbar}\langle\psi|[A, \boldsymbol{\varphi}\cdot\mathbf{J}]|\psi\rangle\,. \tag{3}$$

Note: the classical notion of vector $\mathbf{V}$ entails certain transformation properties under infinitesimal rotations, namely

$$\delta V_k = \epsilon_{ijk}\,\varphi_i V_j, \tag{4}$$

where ϵ_{ijk} are the standard Levi-Civita symbols and the summation convention is implied. For a three-component operator $\mathbf{V}$ to be a vector operator, we require that its expectation value transforms under rotations like a classical vector. A combination of (3) and (4) then shows that the expectation value of a vector operator in an arbitrary state and arbitrary rotation must satisfy

$$\epsilon_{ijk}\,\varphi_i\langle V_j\rangle = -\frac{i}{\hbar}\langle[V_k, \boldsymbol{\varphi}\cdot\mathbf{J}]\rangle. \tag{5}$$

Also bear in mind that the expectation values of two operators are the same in an arbitrary state precisely when the operators are the same.

   (b) Show that if the commutators of a three-component operator $\mathbf{V}$ with the angular momentum $\mathbf{J}$ satisfy

$$[V_i, J_j] = i\hbar\,\epsilon_{ijk}\,V_k\,, \tag{6}$$

   then (5) is valid.

   (c) Conversely, (6) is also a necessary condition for (5). Show this, for instance, by studying equation (5) in the special cases when $\boldsymbol{\varphi}$ is a unit vector in each coordinate direction.

Equation (6) is the practical criterion for vector operators in quantum mechanics.

5. **(a)** Using relativistic kinematics, show that the leading relativistic correction to the kinetic energy of an electron is

$$E_k = \ldots - \frac{p^4}{8m_e^3c^2} + \ldots.$$

   (b) Find the leading correction to the energy of the ground state of hydrogen due to relativistic kinematics.
   Hint: $(\psi, p^4\psi) = (p^2\psi, p^2\psi)$. Formally $p^2\psi$ has a delta function singularity, but the delta function does not contribute in this problem. The ground state wave function is proportional to e^{-r/a_0}.