University of Illinois at Chicago
Department of Physics

Quantum Mechanics
Qualifying Examination

January 4, 2010.
9:00 am – 12:00 pm

Full credit can be achieved from completely correct answers to 4 questions. If the student attempts all 5 questions, all of the answers will be graded, and the top 4 scores will be counted toward the exam's total score.

Various equations, standard integrals, etc. are provided on the last page of the exam.

Question 1

In heavy (large Z) hydrogen-like atoms, where to a very good approximation the reduced mass μ is equal to the electron mass m_e, relativistic corrections to the electron's kinetic energy need to be taken into account due to its large orbital velocity.

a) Show that the first-order correction to the Hamiltonian due to the electron's relativistic kinetic energy is given by $\hat{H}_1 = -\frac{1}{2m_e c^2}\left(\frac{\mathbf{p}^2}{2m_e}\right)^2$.

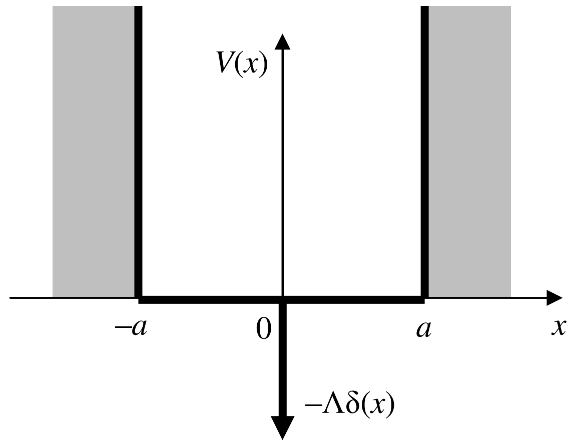
b) Verify that $\left\langle \frac{1}{r} \right\rangle = \frac{Z}{a_0}$ for the 1s state of the hydrogen-like atom.

c) Similarly, evaluate $\left\langle \frac{1}{r^2} \right\rangle$ for the 1s state of the hydrogen-like atom.

d) Use the fact that the unperturbed Hamiltonian is $\hat{H}_0 = \frac{\mathbf{p}^2}{2m_e} - \frac{Ze^2}{4\pi\varepsilon_0 r}$, and the results from parts (a), (b) and (c), to evaluate the first-order perturbation to the electron's kinetic energy due to the relativistic correction.

Question 2

Consider an *attractive* delta-function potential $-\Lambda\delta(x)$, where the parameter Λ characterizes the strength of the delta-function, positioned at the center of an infinite square well of width $2a$; that is, a potential given by



$V(x \le -a) = \infty$
$V(-a < x < 0) = 0$
$V(x = 0) = -\Lambda\delta(x)$
$V(0 < x < a) = 0$
$V(x \ge a) = \infty$

a) Show that the equation determining the energy E of the eigenstate bound to the delta-function is given by

$$\tanh(\kappa a) = \frac{\hbar^2\kappa}{m\Lambda},$$

where $\hbar\kappa = \sqrt{2m|E|}$ and m is the mass of the particle.

b) What is the minimum strength of the delta-function for which a state with $E < 0$ exists?

Question 3

Quantum dots are important material systems in nanoscience.

Consider an electron of charge e and mass m_e confined in an idealized quantum dot with $V(r) = 0$ for $r < a$ and $V(r) = \infty$ for $r > a$; that is, an infinite spherical well of radius a. The eigenstates of this potential are given by

$$\langle \mathbf{r} | \psi_{nlm} \rangle = C_{nl}\, j_l\left(\frac{s_{nl} r}{a}\right) Y_{lm}(\theta, \phi),$$

where $Y_{lm}(\theta,\phi)$ is the spherical harmonic associated with the usual angular momentum quantum numbers l and m, and C_{nl} is the normalization constant for the l^{th} spherical Bessel function j_l with roots s_{nl}. The first three spherical Bessel functions with $\rho = s_{nl} r/a$ are

$$j_0(\rho) = \frac{\sin\rho}{\rho} \qquad j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho} \qquad j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3}{\rho^2}\cos\rho$$

and the first few roots are given below:

s_{nl}	$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$
$n = 1$	π	4.49	5.76	6.99	9.36
$n = 2$	2π	7.73	9.10	10.42	
$n = 3$	3π				

The spherical Bessel functions also satisfy the relation

$$\int_0^a r^2 dr\, j_l\left(\frac{s_{nl} r}{a}\right) j_l\left(\frac{s_{n'l} r}{a}\right) = \frac{a^3}{2}\left[j_{l-1}(s_{nl})\right]^2 \delta_{nn'} .$$

a) What are the energies of the lowest four eigenstates?

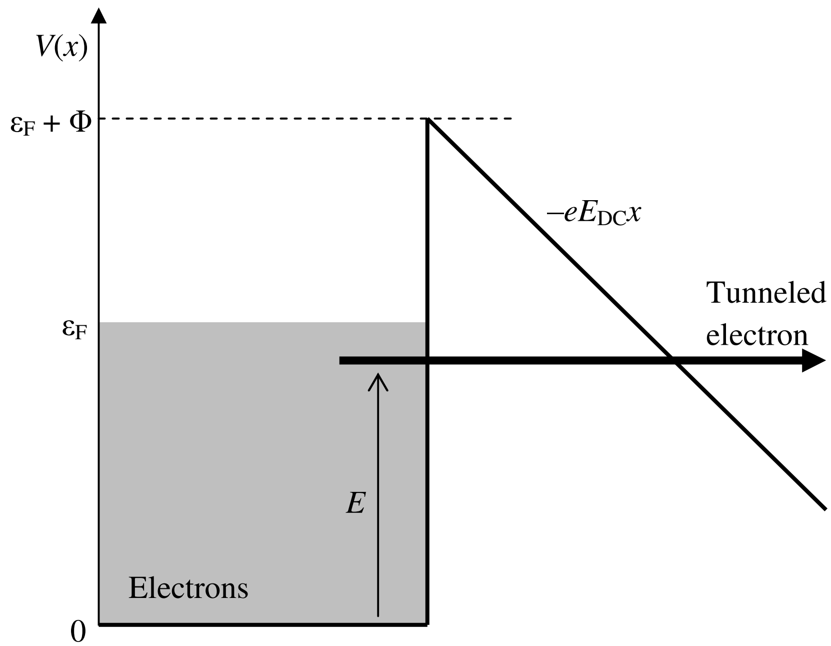
b) Evaluate the normalization constants C_{10} and C_{11}.

c) Consider the state $\langle \mathbf{r} | \psi \rangle = A\left[\left(\frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}\right)\sin\theta\cos\phi + \frac{\sin\rho}{\rho}\right]$, where A is a constant. With what probability is the ground state energy measured? And what is the probability of measuring a z-component of the angular momentum with a value $+\hbar$?

d) In the presence of a strong homogeneous magnetic field $\mathbf{B}$, the energy states split – the Zeeman effect. Neglecting spin (the normal Zeeman effect), the additional contribution to the Hamiltonian can be written as $H_1 = \frac{e}{2m_e}\mathbf{L}\bullet\mathbf{B}$. Amongst the four lowest states identified in part (a), at what magnetic field strength will states originating from one energy level overlap energetically with those from another?

Question 4

Field emission, a quantum tunneling phenomenon, occurs when a DC electric field E_{DC} applied perpendicular to a material surface becomes sufficiently strong to allow electrons in the material to tunnel out into the vacuum.



In materials like metals, the zero-point energy E of the electrons in the metal is usually defined in terms of the Fermi energy ε_F (the energy of the last filled electronic state at zero Kelvin), which is located at an energy Φ (the material work function) below the vacuum energy.

a) Using the approximation for the one-dimensional tunneling probability through a 'thick' barrier,

$$|T|^2 \approx \exp\left[-2\int_a^b dx\sqrt{\frac{2m}{\hbar^2}\left(V(x)-E\right)}\right],$$

of thickness $b-a$, determine the transmission probability for an electron at an arbitrary energy E; that is, at an energy $E' = \varepsilon_F + \Phi - E$ below the top of the barrier.

b) In a real material at non-zero temperature T, the energy distribution of electrons is given by the Fermi function

$$f(E) = \frac{1}{1+\exp\left(-\frac{\varepsilon_F - E}{k_B T}\right)},$$

where k_B is Boltzmann's constant. For $\exp\left[(\Phi - E')/k_B T\right] >> 1$, determine the energy below the top of the barrier for which electron field emission is most probable.

Question 5

Consider the following *spatial-coordinate-independent* two-particle Hamiltonian for a spin system consisting of two *identical* spin ½ particles:

$$\hat{H} = A + B\mathbf{S}_1 \bullet \mathbf{S}_2$$

where A and B are constants.

a) Find the 4×4 matrix representation of $\hat{H}$ in the uncoupled basis set

$$\left|\uparrow\uparrow\right\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix},\ \left|\uparrow\downarrow\right\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix},\ \left|\downarrow\uparrow\right\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix},\ \text{and}\ \left|\downarrow\downarrow\right\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix},$$

where $\left|\uparrow\right\rangle$ represents a spin-up particle with $S_z = \frac{1}{2}\hbar$ and a spin-down particle with $S_z = -\frac{1}{2}\hbar$ is $\left|\downarrow\right\rangle$.

b) Calculate the eigenvalues of $\hat{H}$.

c) What are the eigenstates of the diagonalized Hamiltonian?

d) Verify your results by finding the eigenvalues of the four states in the coupled basis $\left|S, M\right\rangle$ representing the total spin S and its z-component M.

Equation Sheet

$$Y_{00}(\theta,\phi)=\frac{1}{\sqrt{4\pi}} \qquad Y_{10}(\theta,\phi)=\sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_{1\pm1}(\theta,\phi)=\mp\sqrt{\frac{3}{8\pi}}\,e^{\pm i\phi}\sin\theta$$

$$Y_{20}(\theta,\phi)=\sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta-1\right) \qquad Y_{2\pm1}(\theta,\phi)=\mp\sqrt{\frac{15}{8\pi}}\,e^{\pm i\phi}\sin\theta\cos\theta$$

$$Y_{2\pm2}(\theta,\phi)=\sqrt{\frac{15}{32\pi}}\,e^{\pm 2i\phi}\sin^2\theta$$

$$E_n=-\left[\frac{\mu}{2\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2}=-13.6\frac{Z}{n^2}\text{ eV} \qquad a_0=\frac{4\pi\varepsilon_0\hbar^2}{\mu e^2} \qquad \frac{1}{\mu}=\frac{1}{m_e}+\frac{1}{M_{nucleus}}$$

$$R_{10}(r)=2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\exp\left[-\frac{Zr}{a_0}\right] \qquad R_{20}(r)=2\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(1-\frac{Zr}{2a_0}\right)\exp\left[-\frac{Zr}{2a_0}\right]$$

$$R_{21}(r)=\frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\frac{Zr}{a_0}\exp\left[-\frac{Zr}{2a_0}\right]$$

$$\int_0^\infty dx\,x^m\exp\left(-ax^2\right)=\frac{\Gamma\left(\frac{m+1}{2}\right)}{2a^{(m+1)/2}} \quad ; \quad \Gamma(n+1)=n\Gamma(n)\,,\ \Gamma(n+1)=n!\,,\ \Gamma\left(\tfrac{1}{2}\right)=\sqrt{\pi}$$

so that $$\int_0^\infty dx\,x^{2n}\exp\left(-\lambda^2x^2\right)=\frac{1.3.5\ldots(2n+1)\sqrt{\pi}}{2^n\lambda^{2n+1}}$$

$$\int_0^\infty dx\,x^n e^{-\lambda x}=\frac{n!}{\lambda^{n+1}}$$

$$\int dx\sqrt{A+Bx}=\frac{2}{3B}(A+Bx)^{\frac{3}{2}} \qquad \int dx\,x\sqrt{A+Bx}=-\frac{2(2A-3Bx)(A+Bx)^{3/2}}{15B^2}$$