Physics 501: Mathematical Methods Final Exam, Spring 2007

May 3, 2007

Exam instructions This may be taken any time between April 29, 2007 and May 5, 2007; though the exam has been designed to occupy three hours, there is no specified time constraint beyond the one week interval specified above.

If you have questions about the wording of problems on this exam, please send me email at djpriour@glue.umd.edu; I should be able to respond at least within 24 hours, though likely sooner. In addition, you are welcome to stop by my office at any time during the week of the exam.

Materials permitted: The course text, *Mathematical Methods for Physicists* by Arfken and Weber is permitted, as are any notes handed out or taken during class. Worked homework problems may also be consulted. However, collaboration with classmates on this exam is strictly forbidden.

1 Ordinary Bessel Functions and the quantum mechanical infinite circular well. (35 *points*)

- Consider a particle of mass m in a circular well of radius a with an infinite confining potential $V(r)$ such that

$$V(r) = \left\{ \begin{array}{c} 0, \ r \leq a \\ \infty, \ r > a \end{array} \right\}; \tag{1}$$

practically speaking, this corresponds to the boundary condition $\psi(a,\theta) = 0$, where θ is the angle in the polar coordinate system. Within the circular well, the potential is zero, so the only contribution to $\mathcal{H}$ will be the kinetic energy term.

Thus, the wave equation which we wish to examine (and ultimately obtain the ground state energy for) is

$$\mathcal{H}\psi_0 = -\frac{\hbar^2}{2m}\nabla^2\psi_0 = E_0\psi_0 \tag{2}$$

Expressed in polar coordinates, our Schroedinger equation has the form

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi_0}{\partial r^2} + r^{-1}\frac{\partial\psi_0}{\partial r} + r^{-2}\frac{\partial^2\psi_0}{\partial\theta^2}\right) = E_0\psi_0 \tag{3}$$

- Let us proceed with the solution of the wave equation for the infinite circular well. We begin by multiplying both sides of the Schroedinger equation by $\hbar^2/2m$ and using the notation $\epsilon \equiv 2mE\ /\hbar^2$. This leads to

$$-\left(\frac{\partial^2\psi_0}{\partial r^2} + r^{-1}\frac{\partial\psi_0}{\partial r} + r^{-2}\frac{\partial^2\psi_0}{\partial\theta^2}\right) = \epsilon\psi_0 \tag{4}$$

  Separating the variables would yield $\psi_0(r,\theta) = \phi_0(r)\Theta_0(\theta)$; since our interest is in the ground state, we have $\Theta_0(\theta) = 1$, leaving only dependence on the radial coordinate r. To simplify matters further, we rescale the coordinates with $\rho \equiv \alpha r$ and choose $\alpha = \sqrt{\epsilon}$, and we obtain

$$\frac{\partial^2\phi_0}{\partial\rho^2} + \rho^{-1}\frac{\partial\phi_0}{\partial\rho} + \phi_0 = 0, \tag{5}$$

  which we recognize as Bessel's differential equation of order zero. We demand that $\phi_0(r)$ be well behaved for $\rho = 0$, so the ordinary Bessel function of the first kind $J_0(\rho)$ is the appropriate solution. In terms of the proper coordinate r, the ground state wave function is $J_0(\sqrt{\epsilon}r)$.

- We will now fix the energy eigenvalue E_0 by appealing to the boundary condition $\phi_0(r = a) = 0$ (set up by the infinite potential). Hence, we must find ϵ such that $\epsilon = (\rho_1/a)^2$, where ρ_1 is the first zero of $J_0(\rho)$. Keeping in mind that $\epsilon = 2mE/\hbar^2$, one finds‘

$$E_0 = \frac{\hbar^2 \rho_1^2}{2ma^2} \tag{6}$$

- (b) Show that the Taylor expansion for $J_0(\rho)$ (up to the first four nonzero terms) is

$$J_0(\rho) = 1 - \frac{1}{4}\rho^2 + \frac{1}{64}\rho^4 - \frac{1}{2304}\rho^6 + \ldots \tag{7}$$

- (c) The approximate condition for the first zero ρ_1 is

$$1 - \frac{1}{4}\rho_1^2 + \frac{1}{64}\rho_1^4 - \frac{1}{2304}\rho_1^6 \approx 0. \tag{8}$$

  The goal of this part of the problem is to solve for ρ_1 using the *Newton-Raphson* technique, an iterative method for finding roots of nonlinear equations.

  In what follows, we describe Newton's technique for calculating roots in the general single variable case. Consider the nonlinear equation $f(x) = 0$ for the root x, and suppose a reasonable initial guess x_0 has been supplied. The *improved* estimate is given by $x_1 = x_0 - f(x_0)/f'(x_0)$ (where $f'(x) = df/dx$). To refine x_1 further, we use x_1 as the starting value for a new iteration, and we calculate $x_2 = x_1 - f(x_1)/f'(x_1)$; the Newton iterations continue in this manner until the desired level of convergence is achieved.

  Our goal is to apply the Newton-Raphson technique to the problem at hand to recover the smallest value of ρ_1 such that $1 - \rho_1^2/4 + \rho_1^4/64 - \rho_1^6/2304 = 0$. $\rho_1 = 2$, a solution to $1 - \rho_1^2/4 = 0$, is suggested as an initial value for ρ_1. Beginning with this value, carry out three Newton iterations. Using the result, write down an estimate for the ground state energy in terms of $\hbar^2/(2ma^2)$ and compare with $E_0 = 5.7832\hbar^2/(2ma^2)$.

- (d) Consider the approximate solution $\phi^{\text{trial}} = \cos(\pi r/2a)$, which vanishes at the boundary as required; calculate the energy expectation value within this state with

$$\langle E \rangle = \frac{\langle \phi^{\rm trial} | \mathcal{H} | \phi^{\rm trial} \rangle}{\langle \phi^{\rm trial} | \phi^{\rm trial} \rangle}; \tag{9}$$

compare this estimate for the ground state energy with $E_0 = 5.7832\hbar^2/(2ma^2)$.

2 The isotropic harmonic oscillator and spherical harmonics (35 *points*)

- Here, we will examine the three dimensional isotropic harmonic oscillator (in reduced units), where

$$\mathcal{H}\psi = -\frac{1}{2}(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}) + \frac{1}{2}(x^2 + y^2 + z^2)\psi = E\psi \tag{10}$$

- (a) Separate the variables with the Ansatz

$$\psi = \phi_x(x)\phi_y(y)\phi_z(z); \tag{11}$$

show that this permits the reduction of the three dimensional problem to three single variable decoupled equations in x, y, z. Hence, show that ϕ_x, ϕ_y, and ϕ_z are determined by

$$-\frac{1}{2}\frac{d^2\phi_x}{dx^2} + \frac{1}{2}x^2\phi_x = E_x\phi_x \tag{12}$$

$$-\frac{1}{2}\frac{d^2\phi_y}{dy^2} + \frac{1}{2}y^2\phi_y = E_y\phi_y \tag{13}$$

$$-\frac{1}{2}\frac{d^2\phi_z}{dz^2} + \frac{1}{2}z^2\phi_z = E_z\phi_z \tag{14}$$

Thus, the problem has been reduced to three separate one dimensional harmonic oscillator equations. Note that the eigenstates $\psi_{n_x n_y n_z}$ will have the form

$$\psi_{n_x n_y n_z}(x, y, z) \equiv \phi_{n_x}\phi_{n_y}\phi_{n_z}, \tag{15}$$

with energies given by

$$E_{n_x n_y n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right) \tag{16}$$

- (b) Obtain the first several eigenstates and eigen-energies; show that

$$\psi_{000} = \pi^{-3/4} e^{-\frac{1}{2}(x^2+y^2+z^2)};\ E_{000} = 3/2 \quad (17)$$

$$\psi_{100} = (4\pi)^{-3/4} x e^{-\frac{1}{2}(x^2+y^2+z^2)};\ E_{100} = 5/2 \quad (18)$$

$$\psi_{010} = (4\pi)^{-3/4} y e^{-\frac{1}{2}(x^2+y^2+z^2)};\ E_{010} = 5/2 \quad (19)$$

$$\psi_{001} = (4\pi)^{-3/4} z e^{-\frac{1}{2}(x^2+y^2+z^2)}\ ; E_{001} = 5/2 \quad (20)$$

$$\psi_{011} = 2\pi^{-3/4} yz e^{-\frac{1}{2}(x^2+y^2+z^2)}\ ; E_{011} = 7/2 \quad (21)$$

$$\psi_{101} = 2\pi^{-3/4} xz e^{-\frac{1}{2}(x^2+y^2+z^2)}\ ; E_{101} = 7/2 \quad (22)$$

$$\psi_{110} = 2\pi^{-3/4} xy e^{-\frac{1}{2}(x^2+y^2+z^2)}\ ; E_{011} = 7/2 \quad (23)$$

$$\psi_{002} = (4\pi)^{-3/4}(1/2 + z^2) e^{-\frac{1}{2}(x^2+y^2+z^2)}\ ; E_{002} = 7/2 \quad (24)$$

$$\psi_{020} = (4\pi)^{-3/4}(1/2 + y^2) e^{-\frac{1}{2}(x^2+y^2+z^2)}\ ; E_{020} = 7/2 \quad (25)$$

$$\psi_{200} = (4\pi)^{-3/4}(1/2 + x^2) e^{-\frac{1}{2}(x^2+y^2+z^2)}\ ; E_{200} = 7/2 \quad (26)$$

- (c) We have successfully solved the isotropic harmonic oscillator in the rectangular Cartesian coordinate stystem. Due to the spherical symmetry of the isotropic oscillator Hamiltonian, the states $\psi_{n_x n_y n_z}$ can be expressed in terms of *spherical harmonics* and radial wave functions. By forming the appropriate linear combinations, express the wave functions in terms of the spherical harmonics and the radial functions; the pertinent spherical harmonics are listed below. **Note**: don't spend a great deal of time worrying about specific normalization constants. I'm really only interested in the correct r,θ, and ϕ dependences.

  As a further hint, note that each of the spherical harmonics $\left\{Y_0^0, Y_1^1, Y_1^0, Y_1^{-1}, Y_2^2, Y_2^1, Y_2^0, Y_2^{-1}, Y_2^{-2}\right\}$ will be represented at least once, and Y_0^0 will appear twice.

  It will be useful to write the Cartesian coordinates x, y, z in terms of spherical polar coordinates with

$$x = r\sin(\theta)\cos(\phi) \quad (27)$$

$$y = r\sin(\theta)\sin(\phi) \quad (28)$$

$$z = r\cos(\theta) \quad (29)$$

In addition, it is advised that the states written above be combined (via linear combination) to yield a new set of wave functions for which the z component of the angular momentum $m\hbar$ is well defined. In this vein, it may be useful to keep in mind that $\cos(\phi) = (e^{i\phi} + e^{-i\phi})/2$ and $\sin(\phi) = (e^{i\phi} - e^{-i\phi})/2i$ Spherical harmonics which may be needed are

$$
\begin{aligned}
Y_0^0 &= 1/\sqrt{4\pi} && (30)\\
Y_1^1 &= -\sqrt{3/8\pi}\sin(\theta)e^{i\phi} && (31)\\
Y_{10} &= \sqrt{3/4\pi}\cos(\theta) && (32)\\
Y_1^{-1} &= \sqrt{3/8\pi}\sin(\theta)e^{-i\phi} && (33)\\
Y_2^2 &= 3\sqrt{5/96\pi}\sin^2(\theta)e^{2i\phi} && (34)\\
Y_2^1 &= -3\sqrt{5/24\pi}\sin(\theta)\cos(\theta)e^{i\phi} && (35)\\
Y_2^0 &= \sqrt{5/4\pi}\left(\frac{3}{2}\cos^2(\theta) - \frac{1}{2}\right) && (36)\\
Y_2^{-1} &= 3\sqrt{5/24\pi}\sin(\theta)\cos(\theta)e^{-i\phi} && (37)\\
Y_2^{-2} &= 3\sqrt{5/96\pi}\sin^2(\theta)e^{-2i\phi} && (38)
\end{aligned}
$$

3 Perturbation theory (30 *points*)

- Consider the eigen-equation

$$\mathcal{H}_0\psi_n = E_n, \tag{39}$$

where $\mathcal{H}_0$ is given by

$$\mathcal{H}_0 = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 16 & 0 \\ 0 & 0 & 0 & 32 \end{bmatrix}, \tag{40}$$

so our eigen-equation will have the form

$$\begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 16 & 0 \\ 0 & 0 & 0 & 32 \end{bmatrix} \begin{bmatrix} \psi_{n1}^{(o)} \\ \psi_{n2}^{(0)} \\ \psi_{n3}^{(0)} \\ \psi_{n4}^{(0)} \end{bmatrix} = E_n^{(0)} \begin{bmatrix} \psi_{n1}^{(o)} \\ \psi_{n2}^{(0)} \\ \psi_{n3}^{(0)} \\ \psi_{n4}^{(0)} \end{bmatrix} \tag{41}$$

- (a) Obtain the eigenvalues $E_n^{(0)}$ and normalized eigenvectors for $\mathcal{H}_0\psi_n = E_n$ (this can be done by inspection).
- (b) Consider the perturbation $\hat{h}$, given by

$$\hat{h} = \lambda \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{42}$$

- (c) Calculate the first order shift $\lambda\Delta E_n^{(1)}$ for each energy eigenvalue; recall that in general, the first order shift is given by

$$\lambda\Delta E_n^{(1)} = \lambda\langle\psi_n^{(0)}|\hat{h}|\psi_n^{(0)}\rangle \tag{43}$$

- (d) Calculate the second order shift $\lambda^2\Delta E_n^{(2)}$ and the first order corrections $\lambda\phi_n^{(1)}$ to each of the 4 eigenstates. Possibly useful formulae are

$$\lambda\phi_n^{(1)} = \lambda \sum_{m\neq m} \left(\frac{\langle\psi_m^{(0)}|\hat{h}|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \right) \psi_m^{(0)} \tag{44}$$

and

$$\Delta E_n^{(2)} = \sum_{m\neq n} \frac{|\langle\psi_n^{(0)}|\hat{h}|\psi_m^{(0)}\rangle|^2}{(E_n^{(0)} - E_m^{(0)})} \tag{45}$$