Rutgers - Physics Graduate Qualifying Exam Quantum Mechanics: September 1, 2006

$\mathbf{Q}\mathbf{A}$

J is an angular momentum vector with components J_x, J_y , and J_z . A quantum mechanical state is an eigenfunction of J^2 and J_z with eigenvalues $15/4 \hbar^2$ and $1/2\hbar$ respectively.

- 1. Evaluate the expectation values $\langle J_x \rangle$ and $\langle J_y \rangle$ in this state.
- 2. Find the expectation values $\langle J_x^2 \rangle$ and $\langle J_y^2 \rangle$ in this state.

Show and justify any intermediate steps in your calculations.

AngMom Solution

- 1. Using the commutator $[J_y, J_z] = i\hbar J_x$ one finds $i\hbar < J_x > = < J_y J_z > - < J_z J_y > = (\hbar/2)(< J_y > - < J_y >) = 0$, and similarly for $< J_y >$.
- First one can show that the two expectation values are equal. Perhaps the simplest way to do this is to note that J²_x and J²_y transform into one another under a rotation R = exp(iπJ_z/(2ħ)) and this operator and its inverse become unity when applied to the eigenstate:
 < J²_y >=< RJ²_xR⁻¹ >= exp(iπ/4) < J²_y > exp(-iπ/4) =< J²_y >.
 (Another approach is to expand < J²_x > in intermediate states and then use the commutator to show i < m'|J_x|m >= (m m') < m'|J_y|m >, together with the fact that only states with |m m'| = 1 contribute.) Then the relation J² = J² + J² + J² immediately gives

$$\langle J_x^2 \rangle = \langle J_y^2 \rangle = ((15/4)\hbar^2 - (\hbar/2)^2)/2 = (7/4)\hbar^2.$$

Students can also adopt a simpler approach: by symmetry or rotational invariance, $\langle J_x^2 \rangle = \langle J_y^2 \rangle = (J^2 - J_z^2)/2$.

QB

Consider the Schrödinger equation with a one-dimensional quartic potential: $V(x) = \lambda x^4$.

- 1. Find the lowest upper limit for the ground state energy of a particle of mass m using a Gaussian trial wave function of the form $\psi_t(x) = N \exp(-ax^2)$, where N is a normalizing constant and a is a parameter which can be varied.
- 2. Give a trial function which will give an upper limit for the energy of the first excited state in this potential. You do not need to carry out the calculation of the energy limit, but you should justify your choice of trial function.

You may find the following definite integrals useful:

 $I_0 = \int_0^\infty exp(-px^2)dx = \frac{1}{2}\sqrt{\frac{\pi}{p}}$ and, for positive integers n, $I_n = \int_0^\infty x^{2n}exp(-px^2)dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^n p^n}I_0$

VarQuartic Solution

1. Using the integrals provided it is easy to show that

$$\begin{split} N^2 \sqrt{\pi/(2a)} &= 1\\ \text{and then that}\\ &< \psi_t |V| \psi_t >= 3\lambda/(16a^2)\\ \text{and} \end{split}$$

 $\langle \psi_t | K | \psi_t \rangle = \hbar^2 a / (2m)$. The expectation value of the total Hamiltonian in the trial wave function can then be written as

 $\alpha a + \beta/a^2$ where $\alpha = \hbar^2/(2m)$ and

 $\beta = 3\lambda/16.$

This has its minimum value of $3(\alpha/2)^{2/3}\beta^{1/3}$ when $a = (2\beta/\alpha)^{1/3}$. The upper limit for the ground state energy is, therefore $(3/4)^{4/3}(\lambda\hbar^4/m^2)^{1/3} = 0.6814\cdots(\lambda\hbar^4/m^2)^{1/3}$. (This is indeed greater than the exact value, found numerically, of $0.667886\cdots(\lambda\hbar^4/m^2)^{1/3}$.)

2. For a one-dimensional even potential the eigenstates are alternately even and odd, so an odd trial wave function of the form, say, $Nx \exp(-bx^2)$ would be orthogonal to the exact ground state wave function and therefore the expectation value would have to be greater than the energy of (odd-parity) first excited state.

A proof would expand the trial wave function in terms of the exact wave functions, with coefficients c_i , so that the expectation value of the Hamiltonian would be

$$\sum_i |c_i|^2 E_i,$$

which is clearly greater than or equal to E_1 if c_0 vanishes.

QC1

The wave function of the bound state of a particle of mass m in the one-dimensional attractive deltafunction potential $V(x) = -\lambda \delta(x)$ can be written as $\psi(x) = Nexp(-a|x|)$, where N is the normalization constant.

- 1. Find a and the energy eigenvalue E in terms of λ and m.
- 2. Find the uncertainties in momentum and position Δp and Δx in terms of λ and m. Verify that the uncertainty relation is satisfied.

DeltaPot Solution

1. The wavefunction has a discontinuous slope at x = 0 and therefore $d^2\psi/dx^2 = a^2\psi - 2a\delta(x)\psi$. Inserting this in the Schrödinger equation $-(\hbar^2/2m)d^2\psi/dx^2 - V(x)\psi = E\psi$, gives $a = \lambda m/\hbar^2$ and

 $E = -\hbar^2 a^2 / 2m = -(m/2)(\lambda/\hbar)^2.$

2. The normalization condition requires $N^2 = a$. Straightforward integration gives $\langle x^2 \rangle = 1/(2a^2)$. To find $\langle p^2 \rangle$ one can use the expression for $d^2\psi/dx^2$ in (1) to show $\langle p^2 \rangle = a^2\hbar^2$.

Using the expression for *a* found in (1) then gives $\Delta x = \hbar^2/(\sqrt{2}\lambda m)$ and $\Delta p = \lambda m/\hbar$, so that $\Delta x \Delta p = \hbar/\sqrt{2} > \hbar/2$, consistent with the uncertainty relation $\Delta x \Delta p \ge \hbar/2$.

QC2

The eigenstates of the three-dimensional isotropic harmonic oscillator with potential $V(r) = \frac{1}{2}kr^2$ can be labelled either by the cartesian indices (n_x, n_y, n_z) or by the angular momentum indices (n, ℓ, m) , with $n = n_x + n_y + n_z$.

- 1. What is the degeneracy of the nth energy level?
- 2. For n = 0, 1, and 2 list all of the degenerate states in both representations.
- 3. The wavefunctions in the angular momentum representation can be written $\psi_{n,\ell,m} = (u_{n,\ell}(r)/r)Y_{\ell,m}(\theta,\phi)$, where $u_{n,\ell}(r)$ is the radial wave function. Among the states in angular momentum representation you listed in (2) two have the same ℓ but different energies. Sketch the radial wave functions $u_{n,\ell}(r)$ for these two states, making clear how they differ.
- 4. Which of the n = 1 states in the cartesian representation listed in (2) is identical to a state in the angular momentum representation? Explain why.

3dOsc Solution

- 1. The number of states D_n for a given n equals the number of ways one can choose 3 non-negative integers adding to n. This can be found, for example, using $D_n = \sum_{n_x=0}^n \sum_{n_y=0}^{n-n_x} 1 = (1/2)(n+1)(n+2).$
- 2. For n = 0 the cartesian state is (0,0,0) and the angular momentum state is (0,0,0). For n = 1 the 3 cartesian states are (1,0,0), (0,1,0), and (0,0,1) while the angular momentum states are (1,1,1),(1,1,0), and (1,1,-1). For n = 2 the 6 cartesian states are (2,0,0), (0,2,0), (0,0,2), (0,1,1),(1,0,1), and (1,1,0) while the angular momentum states are (2,0,0), (2,2,2), (2,2,1), (2,2,0), (2,2,-2).
- 3. The angular momentum states (0,0,0) and (2,0,0) both have zero angular momentum. Their radial wave functions satisfy the same radial equation, but with different energies, so they must be orthogonal. The first must have no nodes, the 2nd one node between r = 0 and $r = \infty$.
- 4. The cartesian state (0,0,1) and the angular momentum state (1,1,0) are both proportional to $z = r \cos(\theta)$ times a Gaussian and therefore must be identical up to a phase.

QD1

The integral form of the Schrödinger equation for the scattering of a particle of mass m from a potential $V(\mathbf{r})$ is $\psi(\mathbf{r}) = exp(i\mathbf{k_i} \cdot \mathbf{r}) - (m/(2\pi\hbar^2)) \int \frac{exp(i\mathbf{k}|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') \psi(\mathbf{r}') d^3r'.$

- 1. Use the large r limit of this expression to get an expression for the scattering amplitude f in terms of an integral involving the wave function ψ .
- 2. Use this expression to find the Rutherford cross section in the Born approximation, i.e find f to first order in V for $V = q_1 q_2/(4\pi\epsilon_0 r)$ and use it to calculate the differential cross section. In the Born approximation $\psi(\mathbf{r}')$ is replaced by the initial plane wave, $f(\mathbf{k_f}, \mathbf{k_i}) = -(m/(2\pi\hbar^2)) \int e^{-i\mathbf{q}\cdot\mathbf{r}'} V(\mathbf{r}') d^3r'$, where $\mathbf{q} = \mathbf{k_f} \mathbf{k_i}$ is the momentum transfer.

RuthScatt Solution

1. For $r \gg r'$ one has the expansion $|\mathbf{r} - \mathbf{r}'| = r - \mathbf{r} \cdot \mathbf{r}'/r + \cdots$. Using this in the exponential in the integrand, and just the r in the denominator, one finds $\psi(\mathbf{r}) = exp(i\mathbf{k_i} \cdot \mathbf{r}) + f(\mathbf{k_f}, \mathbf{k_i})e^{ikr}/r$, where $f(\mathbf{k_f}, \mathbf{k_i}) = -(m/(2\pi\hbar^2)) \int e^{-i\mathbf{k_f} \cdot \mathbf{r}'} V(\mathbf{r}')\psi(\mathbf{r}')d^3r'$, is the scattering amplitude with $bfk_f = k\mathbf{r}/r$ the final momentum $\mathbf{p_f}$ divided by \hbar .

2. To avoid complications due to the somewhat poorly defined integral we consider first the case of a Yukawa potential where the integral is

 $\int e^{-i\mathbf{q}\cdot\mathbf{r}} \frac{e^{-ar}}{r} d^3r = 4\pi/(q^2 + a^2).$ Taking the limit $a \to 0$ then give for Rutherford scattering $f_B = -(m/(2\pi\hbar^2)) \times (q_1q_2/(4\pi\epsilon_0)) \times 4\pi/q^2.$ Since $q = 2k\sin(\theta/2)$, the square of this gives the standard Rutherford cross section $d\sigma/d\Omega = (mq_1q_2/(4\pi\epsilon_0))^2/(2p\sin(\theta/2))^4.$ (A possibly more familiar form uses cgs units and the fact that $E = p^2/(2m).$)

QD2

The energy eigenvalues of the one-dimensional harmonic oscillator increase linearly with the quantum number n, while those for the one-dimensional infinite square well increase quadratically with n.

Consider a particle of mass m in the one-dimensional "V" potential, $V(x) = \lambda |x|$.

- 1. Use the Bohr-Sommerfeld condition or the WKB approximation to find the approximate dependence of the energy levels of this system on the quantum number n for large n. Give the estimates for the first four energy levels in terms of $\epsilon \equiv (\frac{\hbar^2 \lambda^2}{2m})^{1/3}$.
- 2. Draw a graph showing the potential and the first four energy levels as horizontal lines. On each of these lines sketch the corresponding wave function. (You will probably want to make this graph as large as possible so that everything fits without overlap.)
- 3. Discuss the related problem (the quantum mechanics of the "bouncing ball") where $V(x) = \infty$ for x < 0, while $V(x) = \lambda x$ for x > 0. How are the energy levels and wave functions here related to those for the V potential?

Vpotential Solution

1. The condition for the *n*th energy level is $\oint p(x)dx = (n - 1/2)h,$ where

 $p(x) = \sqrt{2m(E_n - V(x))}$

is the classical momentum at position x and $n = 1, 2, 3, \cdots$.

(The Bohr-Sommerfeld condition usually does not include the -1/2 on the right-hand side which comes from the connection formulae in the WKB approximation.)

For the V potential this condition becomes

 $4\sqrt{2m\lambda}\int_0^{x_t}\sqrt{x_t-x}dx = (n-1/2)h,$

where $x_t = E_n/\lambda$ is the classical turning point. Evaluating the integral and re-arranging gives $E_n = (n - 1/2)^{2/3} (3\pi/4)^{2/3} \epsilon$.

Thus for large *n* the energy increase as $n^{2/3}$. The estimates for E_n/ϵ for the first four levels are 1.1155, 2.3203, 3.2616, and 4.0818, which are fairly close to the exact numbers 1.01879297, 2.3381074, 3.24819758, and 4.08794944 obtained from the zeroes of the Airy function and its derivative.

- 2. See the figure below. Note that the nth wave function has n-1 nodes between $\pm \infty$ and that the curvature changes from negative to positive at the turning points where the energy levels cross the potential.
- 3. In this case the wave function must satisfy the same differential equation for positive x but must vanish at x = 0. The odd-parity wave functions $(n = 2, 4, 6, \cdots)$ satisfy this condition and thus are the eigenfunctions in this case, with the lowest exact eigenvalues of 2.3381074ϵ and 4.08794944ϵ .

