PHY522; Quantum Mechanics II, Problem Set 5

Due Wed. 21 Feb 2007 at the beginning of class.

1. Attractive spherical well and Levinson's theorem.

Consider S-wave scattering of particles of mass m and incident energy $E > 0$ from an attractive 3D spherical well, with potential energy $V(r) = +V_0 < 0$ for $r < R$ and $V(r) = 0$ for $r > R$.

a) (*5 pts*) Plot the S-wave phase shift δ_0 as a function of dimensionless momentum $\chi = kR$ over the range $0 < \chi < 100$ for a series of values of the well depth parameter $\xi = mV_0R^2/\hbar^2$ from 0. to -40.0, in steps of -1.0. For this plot, require that the phase shift $\delta_0(\chi)$ be a continuous function of χ (no quadrant jumps), which approaches zero at large incident energy. (The algebra for this problem was done in the previous homework set.)

b) (*2 pts*) Note that the low-energy limit of the phase shift $\delta_0(k = 0)$ depends on the depth of the potential discontinuously, and approaches certain fixed values for this range of ξ. Determine the critical values of ξ where the limit $\delta_0(k = 0)$ "jumps" to three place accuracy using numerical experiments.

c) (*3 pts*) Now look up Levinson's Theorem, and explain the behavior of the phase shifts noted in part b). Determine what the exact values of the critical ξ should be according to this theorem, and compare them with your "experimental" values found in part b).

2. Momentum space wavefunctions.

In class we noted that one may define a momentum-space wavefunction $\phi(\vec{p}\,)$ by taking the overlap of a state of definite momentum $|\,\vec{p}\,\rangle$ with a general state vector $|\psi(t)\rangle$,

$$\phi(\vec{p}\,) = \langle\vec{p}\,|\psi(t)\rangle \ , \tag{1}$$

which is analogous to the more familiar position-space wavefunction

$$\psi(\vec{x}\,) = \langle\vec{x}\,|\psi(t)\rangle \ . \tag{2}$$

These wavefunctions are a Fourier transform pair,

$$\phi(\vec{p}\,) = \int\frac{d\vec{x}}{(2\pi\hbar)^{D/2}}\ e^{-i\vec{p}\cdot\vec{x}/\hbar}\ \psi(\vec{x}\,) \tag{3}$$

(in D space dimensions).

a) (*3 pts*) Show that the norm is preserved for this pair of wavefunctions,

$$\int d\vec{x}\ |\psi(\vec{x}\,)|^2 = \int d\vec{p}\ |\phi(\vec{p}\,)|^2 \ . \tag{4}$$

b) (*3 pts*) The normalized ground-state wavefunction for a particle of mass m moving in a Coulomb potential $V(r) = -\alpha\hbar c/r$ in three dimensions is given by

$$\psi_0(r) = \frac{1}{(\pi a_0^3)^{1/2}}\ e^{-r/a_0} \ . \tag{5}$$

($a_0 = \hbar/mc\alpha$, as you recall, is the Bohr radius.) Determine the corresponding momentum-space ground state wavefunction $\phi_0(\vec{p}\,)$ (as a function of $\vec{p}$, a_0 and $\hbar$).

c) (*2 pts*) There is a singularity in the momentum space wavefunction $\phi_0(\vec{p}\,)$ at a certain value of $\vec{p}\,^2$. Give this value, and explain what aspect of the large-r behavior of the real-space wavefunction $\psi_0(\vec{x}\,)$ is determined by this singularity.

d) (*2 pts*) Calculate the expected value of the kinetic energy $\vec{p}\,^2/2m$ for this ground state, first using the spatial wavefunction $\psi_0(r)$ and explicit gradients, and second using the momentum space wavefunction $\phi_0(\vec{p})$. (Express the result in terms of $\hbar, m$ and a_0 only.) The results of the two calculations should of course be identical.

3. Heisenberg picture matrix elements.

One may distribute the time evolution of a quantum mechnaical matrix element between the wavefunctions (states) and the operators in an infinite number of different ways, which is known as the choice of "picture". Introductory quantum mechanics assumes the Schrödinger picture, in which operators are fixed in time, and all the time evolution is in the states, which satisfy

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle \ , \tag{6}$$

with the solution

$$|\psi(t)\rangle = U(t,0)|\psi(0)\rangle \tag{7}$$

where $U(t,0)$ is the time evolution operator

$$U(t,0) = \exp\Big\{ -iHt/\hbar\Big\} \ . \tag{8}$$

One alternative is the Heisenberg picture, in which the state vectors are fixed and all the time dependence is in the operators, which satisfy the differential evolution

$$-i\hbar\frac{\partial}{\partial t}\mathcal{O}(t) = [H,\mathcal{O}(t)] \ , \tag{9}$$

which has the solution

$$\mathcal{O}(t) = U^\dagger(t,0)\ \mathcal{O}(0)\ U(t,0) \ . \tag{10}$$

Now we will consider the application of the choice of picture to a specific problem. Assume that a single spin-1/2 ion is in a magnetic field directed along the x-axis, described by the Hamiltonian

$$H = -\mu_B B\,\sigma_x \tag{11}$$

and that the spin initially lies along the z-axis, so that it is described by the Pauli spinor

$$|\psi(t=0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \ . \tag{12}$$

a) (*5 pts*) Find the subsequent behavior of the expected spin vector

$$\langle\vec{S}\,\rangle(t) \equiv \langle\psi(t)|\,\vec{S}\,|\psi(t)\rangle \tag{13}$$

using the Schrödinger picture, with the fixed spin operator $\vec{S} = \hbar\vec{\sigma}/2$.

b) (*5 pts*) Now repeat this exercise in the Heisenberg picture, with the state fixed at

$$|\psi(t)\rangle \equiv |\psi(0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{14}$$

but with the spin operator evolving as

$$\vec{S}(t) = U^\dagger(t,0)\ \hbar\vec{\sigma}/2\ U(t,0) \ . \tag{15}$$

You should find the same matrix element $\langle\vec{S}\,\rangle(t)$ as in part a).