PHYS457 - Honours Quantum Mechanics

Homework 6 - Solutions

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10.10. Cubic Potential

Determine the ground-state energy of a particle of mass μ in the *cubic* potential well

$$V(x_i) = \begin{cases} 0 & 0 < x_i < a, \\ \infty & \text{elsewhere} \end{cases} \qquad x_i = x, y, z.$$

Compare the volume of this infinite well with the spherical one eq. (10.64) and discuss in general terms whether the relative values of the ground-state energies for the two wells are consistent with the position-momentum uncertainty relation.

Solution. To solve this problem, we note that inside the well the particle is free. It thus suffices to solve the free-particle Hamiltonian (no potential) and impose boundary conditions. As the potential is the same in all directions x, y, z, the eigenfunctions can be written as

$$\psi(x, y, z) = \psi_x(x)\psi_y(y)\psi_z(z).$$

It thus suffices to solve the one-dimensional system—the so-called "particle in a box" model:

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2\psi_x}{\partial x^2} = E\psi_x \implies \frac{\partial^2\psi_x}{\partial x^2} = -\frac{2\mu E}{\hbar^2}\psi_x.$$

The solution is

$$\psi_x(x) = A\cos(k_x x) + B\sin(k_x x), \quad k_x = \sqrt{\frac{2\mu E}{\hbar^2}}.$$

The boundary conditions $\psi_x(0) = \psi_x(a) = 0$ give $A = 0$ and $k_x = \frac{\pi n_x}{a}$ for $n_x = 1, 2, \ldots$ The spectrum of the x component is hence

$$E_{n_x} = \frac{\hbar^2\pi^2 n_x^2}{2\mu a^2}.$$

Since the three-dimensional Schrödinger equation gives

$$\begin{aligned} E_{n_x,n_y,n_z}\psi &= -\frac{\hbar^2}{2\mu}\nabla^2\psi \\ &= -\frac{\hbar^2}{2\mu}\left[\left(\frac{\partial^2\psi_x}{\partial x^2}\right)\psi_y\psi_z + \psi_x\left(\frac{\partial^2\psi_y}{\partial y^2}\right)\psi_z + \psi_x\psi_y\left(\frac{\partial^2\psi_z}{\partial z^2}\right)\right] \\ &= (E_{n_x} + E_{n_y} + E_{n_z})\psi, \end{aligned}$$

the ground-state energy has $n_x = n_y = n_z = 1$ with $E_{1,1,1} = \frac{3\hbar^2\pi^2}{2\mu a^2}$. The volume of this infinite cubic well is a^3, whereas that of the spherical well of eq. (10.64) is $\frac{4\pi a^3}{3}$. While the numerical factors are different, the volume of both wells scales like $\sim a^3$. Via the position-momentum uncertainty principle, the momentum of the eigenstates in such potential wells should scale like

$$p \sim \frac{\hbar}{\sqrt[3]{V}} \sim \frac{\hbar}{a}$$

giving ground-state energies that have

$$E \sim \frac{p^2}{2\mu} \sim \frac{\hbar^2}{2\mu a^2}.$$

What we found—as well as $E_s = \frac{\hbar^2\pi^2}{2\mu a^2}$ (eq. 10.72) for the energies of the spherical potential—is thus consistent with the uncertainty relation. Additionally, we can look at the exact ratio E_c/E_s, where E_c and E_s are the ground-state energies of the free particle in the cubic and spherical well, respectively. Substituting exact expressions, we find

$$\frac{E_c}{E_s} = \frac{3\hbar^2\pi^2}{2\mu a^2}\left(\frac{\hbar^2\pi^2}{2\mu a^2}\right)^{-1} = 3.$$

That $E_c > E_s$ is to be expected from the position-momentum uncertainty relation, as the volume of a sphere of radius a is smaller than that of a cube of side length a (think of the sphere lying inside the cube). The uncertainty relation predicts

$$\frac{E_c}{E_s} \sim \frac{(V_s)^{2/3}}{(V_c)^{2/3}} = \left(\frac{4\pi}{3}\right)^{2/3} \simeq 2.6$$

which is again consistent.

9.23. Cylindrical Symmetry

The Hamiltonian for a three-dimensional system with *cylindrical* symmetry is given by

$$H = \frac{\boldsymbol{p}^2}{2\mu} + V(\rho)$$

where $\rho = \sqrt{x^2 + y^2}$.

(a) Use symmetry arguments to establish that both ρ_z, the generator of translations in the z direction, and L_z, the generator of rotations about the z axis, commute with H.

Solution. The translation operator in the z direction $T_z(a) = e^{-ip_z a/\hbar}$ obviously commutes with $V(\rho)$, as V does not depend on z. Therefore, $[p_z, V] = 0$. We also know that $[p_i, p_j] = 0$ for all i, j. In particular, $[p_z, p^2] = 0$. We conclude that $[p_z, H] = 0$. Furthermore, recall that $[L_z, p^2] = 0$. The fact that the potential $V = V(\rho)$ only depends on the radial distance from the z axis implies that $[L_z, V] = 0$, and hence also $[L_z, H] = 0$.

(b) Use the fact that H, p_z, and L_z have eigenstates in common to express the position-space eigenfunctions of the Hamiltonian in terms of those of p_z and L_z.

Solution. As p_z and L_z commute with H, there exists a common set of eigenstates $|E, p_z, m\rangle$. To find the position-space representation, we use the method of separation of variables:

$$\langle \rho, \phi, z | E, p_z, m\rangle = \psi(\rho, \phi, z) = R(\rho)\Phi(\phi)Z(z). \tag{1}$$

We first deal with Z. Since the eigenstates $|E, p_z, m\rangle$ have definite momentum p_z in the z, we must have

$$Z(z) = \langle z|p_z\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip_z z/\hbar}.$$

The angular part of the wavefunction Φ must be an eigenstate of $L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$ with angular momentum $m\hbar$, which we know is

$$\Phi(\phi) = e^{im\phi}.$$

(c) What is the radial equation? Note: The Laplacian in cylindrical coordinates is given by

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2}.$$

Solution. Using the wavefunction given in eq. (1) Schrödinger's equation $H\psi = E\psi$ yields

$$\begin{aligned} ER(\rho)\Phi(\phi)Z(z) &= \left[-\frac{h^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}\right) + V(\rho)\right] R(\rho)\Phi(\phi)Z(z) \\ &= -\frac{h^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R}{\partial\rho}\right)\Phi(\phi)Z(z) + \frac{1}{\rho^2}\frac{\partial^2\Phi}{\partial\phi^2}R(\rho)Z(z) + \frac{\partial^2 Z}{\partial z^2}R(\rho)\Phi(\phi)\right) \\ &\quad + V(\rho)R(\rho)\Phi(\phi)Z(z). \end{aligned}$$

Dividing both sides by $Z(z)$, we find

$$ER(\rho)\Phi(\phi) = -\frac{h^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R}{\partial\rho}\right)\Phi(\phi) + \frac{1}{\rho^2}\frac{\partial^2\Phi}{\partial\phi^2}R(\rho) + \frac{1}{Z(z)}\frac{\partial^2 Z}{\partial z^2}R(\rho)\Phi(\phi)\right) + V(\rho)R(\rho)\Phi(\phi).$$

Since this must be true for all (ρ, ϕ, z), we find the two equations

$$\frac{1}{Z(z)}\frac{\partial^2 Z}{\partial z^2} = k$$

and

$$ER(\rho)\Phi(\phi) = -\frac{h^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R}{\partial\rho}\right)\Phi(\phi) + \frac{1}{\rho^2}\frac{\partial^2\Phi}{\partial\phi^2}R(\rho) + kR(\rho)\Phi(\phi)\right) + V(\rho)R(\rho)\Phi(\phi) \tag{2}$$

for some constant k. From (b), we know that $k = p_z$. Since we want to find the radial equation, we focus on eq. (2). Dividing both sides by $R(\rho)\Phi(\phi)$,

$$E = -\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho R(\rho)}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R}{\partial\rho}\right) + \frac{1}{\rho^2}\left(\frac{1}{\Phi(\phi)}\frac{\partial^2\Phi}{\partial\phi^2}\right) + p_z\right) + V(\rho).$$

As this must be true for all (ρ, ϕ), we obtain the two equations

$$\frac{1}{\Phi(\phi)} \frac{\partial^2 \Phi}{\partial \phi^2} = k'$$

and

$$E = -\frac{\hbar^2}{2\mu} \left(\frac{1}{\rho R(\rho)} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial R}{\partial \rho} \right) + \frac{k'}{\rho^2} + p_z \right) + V(\rho)$$

for some constant k'. Again from (b), we know that $k' = -m^2$. Rearranging the last expression we find the radial equation

$$\frac{\partial^2 R}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial R}{\partial \rho} + \frac{2\mu R(\rho)}{\hbar^2} \left(E - V(\rho) + \frac{\hbar^2}{2\mu} \left(p_z - \frac{m^2}{\rho^2} \right) \right) = 0.$$

10.11. Cylindrical Potential

A particle of mass μ is in the *cylindrical* potential well

$$V(\rho) = \begin{cases} 0 & \rho < a \\ \infty & \rho > a \end{cases} \qquad \rho = \sqrt{x^2 + y^2}.$$

(a) Determine the three lowest energy eigenvalues for states that also have p_z and L_z equal to zero.

Solution. For states that have p_z and L_z equal to zero, the radial equation inside the well becomes

$$\frac{\partial^2 R}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial R}{\partial \rho} + \frac{2\mu E}{\hbar^2} R(\rho) = 0.$$

Multiplying both sides by ρ^2 (we are trying to recognize it as Bessel's equation), we obtain

$$\rho^2 \frac{\partial^2 R}{\partial \rho^2} + \rho \frac{\partial R}{\partial \rho} + \frac{2\mu E}{\hbar^2} \rho^2 R(\rho) = 0. \tag{3}$$

Writing

$$\tilde{\rho} = \sqrt{\frac{2\mu E}{\hbar^2}} \rho$$

and expressing eq. (3) in terms of $\tilde{\rho}$, we find

$$\frac{\hbar^2}{2\mu E} \tilde{\rho}^2 \frac{\partial^2 R}{\partial \tilde{\rho}^2} \left(\frac{\partial \tilde{\rho}}{\partial \rho} \right)^2 + \sqrt{\frac{\hbar^2}{2\mu E}} \tilde{\rho} \frac{\partial R}{\partial \tilde{\rho}} \frac{\partial \tilde{\rho}}{\partial \rho} + \tilde{\rho}^2 R(\tilde{\rho}) = 0$$

or

$$\tilde{\rho}^2 \frac{\partial^2 R}{\partial \tilde{\rho}^2} + \tilde{\rho} \frac{\partial R}{\partial \tilde{\rho}} + \tilde{\rho}^2 R(\tilde{\rho}) = 0,$$

which is Bessel's equation of order zero. The solution that is regular at the origin is the Bessel function of the first kind $J_0(\tilde{\rho})$. Now, the energies are determined by applying the boundary conditions. Let $k = \sqrt{2\mu E/\hbar^2}$ so that $J_0(\tilde{\rho}) = J_0(k\rho)$. The boundary condition gives $J_0(ka) = 0$. Thus, if $\{r_n\}_{n=1}^{\infty}$ are the zeros of the Bessel function, the energies are

$$E_n = \frac{\hbar^2}{2\mu a^2} r_n^2.$$

Unfortunately, it is unfeasible to find an analytic expression for the zeros r_n of the Bessel functions. Nonetheless, we can use numerical solutions (e.g., see here). The first three are

$$r_1 = 2.4 \quad r_2 = 5.5 \quad r_3 = 8.7$$

Corresponding to

$$E_1 = 5.8\frac{\hbar^2}{2\mu a^2} \quad E_2 = 30\frac{\hbar^2}{2\mu a^2} \quad E_3 = 75\frac{\hbar^2}{2\mu a^2}.$$

(b) Determine the three lowest energy eigenvalues for states with p_z equal to zero. The states may have nonzero L_z.

Solution. For $p_z = 0$, the radial equation inside the well becomes

$$\frac{\partial^2 R}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial R}{\partial \rho} + R(\rho)\left(\frac{2\mu E}{\hbar^2} - \frac{m^2}{\rho^2}\right) = 0.$$

Multiplying both sides by ρ^2 and writing the equation in terms of $\tilde{\rho} = \rho\sqrt{2\mu E/\hbar^2}$, we have

$$\tilde{\rho}^2\frac{\partial^2 R}{\partial \tilde{\rho}^2} + \tilde{\rho}\frac{\partial R}{\partial \tilde{\rho}} + R(\tilde{\rho})\left(\tilde{\rho}^2 - m^2\right) = 0,$$

which is the Bessel equation of order m. Again, there are solutions of the first and second kind, but only the first are regular at the origin, $J_m(\tilde{\rho})$. Letting $k = \sqrt{2\mu E/\hbar^2}$ and applying boundary conditions, we find $J_m(ka) = 0$. Again, the (ordered) energies are given by

$$E_n = \frac{\hbar^2}{2\mu a^2} r_n^2$$

where $\{r_n\}_{n=1}^{\infty}$ corresponds to the (ordered) set of zeroes, which are again found approximately (again, see here). The first three are

$$r_1 = 2.4 \quad r_2 = 3.8 \quad r_3 = 5.1,$$

which correspond to the first zeros of J_0, J_1 and J_2, respectively. The three lowest energies are thus

$$E_1 = 5.8\frac{\hbar^2}{2\mu a^2} \quad E_2 = 14\frac{\hbar^2}{2\mu a^2} \quad E_3 = 26\frac{\hbar^2}{2\mu a^2}.$$

The energy levels thus grow more slowly when the angular momentum may be nonzero.