

# 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  $\mu$  in the *cubic* potential well

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

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  $n_x = 1, 2, \dots$ . 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 larger than that of a cube of side length  $a$ . The larger the well, the more the ground-state wavefunction can “flatten out” to satisfy the boundary conditions (a steep wavefunction is associated with higher kinetic energy). 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

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

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

- (a) Use symmetry arguments to establish that both  $\rho_z$ , 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:

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

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  $\Phi$  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

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

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

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

Since this must be true for all  $(\rho, \phi, z)$ , we find the two equations

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

and

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

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

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

As this must be true for all  $(\rho, \phi)$ , we obtain the two equations

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

and

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

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

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

### 10.11. Cylindrical Potential

A particle of mass  $\mu$  is in the *cylindrical* potential well

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

- (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  $\rho^2$  (we are trying to recognize it as Bessel's equation), we obtain

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

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

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

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.