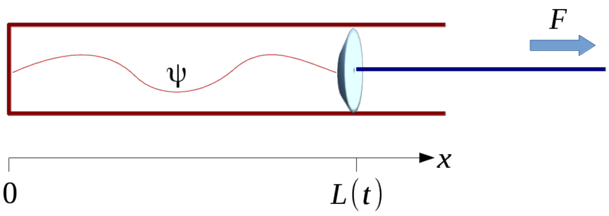
Sample Solutions Exercise 10

Exercise 10.1: Adiabatic expansion of a quantum state (12P)



Let us consider a single quantum-mechanical particle in a cylinder with a movable piston. The system is modeled as a one-dimensional quantum system with the potential

$$V(x,t) = \begin{cases} 0 & 0 < x < L(t) \\ \infty & \text{otherwise.} \end{cases}$$

The piston is first at rest, then moves with velocity v, and finally stops again:

$$L(t) = \begin{cases} L_0 & t \le 0 \\ L_0 + vt & 0 < t < T \\ L_1 = L_0 + vT & t \ge T \end{cases}$$

The particle evolves according to the Schrödinger equation $i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x,t)$ subjected to the boundary conditions $\psi(0,t) = \psi(L(t),t) = 0$.

(a) Determine the eigenenergies E_n and eigenfunctions $\psi_n(x,t)$ for $t < 0$. (1P)

(b) Verify that

$$\phi_n(x,t) = \sqrt{\frac{2}{L(t)}} \exp\left(\frac{i\alpha x^2}{L_0 L(t)} - \frac{in^2\pi^2(L(t)-L_0)}{4\alpha L(t)}\right) \sin\left(\frac{n\pi x}{L(t)}\right)$$

for $n = 1, 2, \ldots$ and with $\alpha = \frac{mL_0 v}{2\hbar}$ solves the time-dependent Schrödinger equation in the moving phase. (2P)

(c) Prove that for $t = 0$ the non-moving states $\psi_n(x,0)$ provide an orthonormal basis. Prove the same for the moving states $\phi_n(x,0)$ as well. (2P)

(d) Consider the moving eigenfunction $\phi_n(x,0)$ at $t = 0$ and expand it to first order in the velocity v. Let us refer to this approximated wave function as $\tilde{\phi}_n(x,0)$. (2P)

(e) Suppose that for $t < 0$ the particle is in its ground state $\psi_1(x,t)$. When the piston suddenly begins to move, the particle is no longer in its ground state, i.e., the coefficients c_n in the expansion

$$|\psi_1\rangle = \sum_{n=1}^{\infty} \underbrace{\langle\tilde{\phi}_n|\psi_1\rangle}_{c_n} |\phi_n\rangle$$

do not vanish for $n > 1$. This means that the particle is now in a nontrivial linear combination of all eigenmodes. To see this, compute the scalar products $\langle\tilde{\phi}_1|\psi_1\rangle$ and $\langle\tilde{\phi}_2|\psi_1\rangle$ to lowest order in v at $t = 0$. (2P)

(f) In the adiabatic limit of very very small velocities the particle remains practically in its ground state ($c_1 \approx 1$ and $c_n \approx 0$ for $n > 1$). Assuming that the particle is actually in the state ϕ_1 during expansion, compute the expectation value of the energy as a function of time. (2P)

(g) Calculate the energy loss $\Delta E = \langle E \rangle_{t=0} - \langle E \rangle_{t=T}$ during expansion and use it to calculate the force F that the particle exerts on the piston as well as the mechanical work ΔW performed by the piston. (1P)

Sample Solution

(a) The eigenfunctions and eigenenergies read:

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2L_0^2 m}\,, \qquad \psi_n(x,t) = \sqrt{\frac{2}{L_0}} e^{-\frac{i}{\hbar}E_n t} \sin\left(\frac{\pi n x}{L_0}\right)$$

(b) Both the left and the right hand side of the Schrödinger equation give

$$\frac{i\left(\frac{1}{L_0+tv}\right)^{5/2} \exp\left(-\frac{i\pi^2 h^2 n^2 t - iL_0 m^2 v x^2}{2hL_0^2 m + 2hL_0 m t v}\right)}{\sqrt{2}m}\left[2\pi h m n v x \cos\left(\frac{\pi n x}{L_0+tv}\right) + \right.$$
$$\left. + \sin\left(\frac{\pi n x}{L_0+tv}\right)\left(i\pi^2 h^2 n^2 + hmv(L_0+tv) + im^2 v^2 x^2\right)\right]$$

(c) At $t = 0$ the non-moving eigenfunctions are given by

$$\psi_n(x,0) = \sqrt{\frac{2}{L_0}} \sin\frac{n\pi x}{L_0}.$$

As we can find in any quantum mechanics textbook, these wave functions are mutually orthonormal

$$\langle \psi_n | \psi_{n'} \rangle_{t=0} = \int_0^{L_0} \mathrm{d}x\, \psi_n^*(x,0)\psi_{n'}(x,0) = \frac{2}{L_0}\int_0^{L_0} \mathrm{d}x \sin\frac{n\pi x}{L_0} \sin\frac{n'\pi x}{L_0} = \delta_{n,n'}\,.$$

where $n, n' \in \mathbb{N}$. In the same way we investigate the moving wave function at $t = 0$ which is given by:

$$\phi_n(x,0) = \sqrt{\frac{2}{L_0}} \exp\left(\frac{imvx^2}{2\hbar L_0}\right) \sin\frac{n\pi x}{L_0}.$$

Forming the scalar product, the additional exponential cancels with its complex conjugate, hence we arrive at exactly the same integral:

$$\langle \phi_n | \phi_{n'} \rangle_{t=0} = \int_0^{L_0} \mathrm{d}x\, \phi_n^*(x,0)\phi_{n'}(x,0) = \delta_{n,n'}\,.$$

(d) Expanding $\phi_n(x,0)$ to first order in v we obtain $\phi_n(x,0) = \tilde{\phi}_n(x,0) + O\left(v^2\right)$ with

$$\tilde{\phi}_n(x,0) \;=\; \sqrt{\frac{2}{L_0}} \sin\left(\frac{\pi n x}{L_0}\right) + \frac{i\left(\frac{1}{L_0}\right)^{3/2} m v x^2 \sin\left(\frac{\pi n x}{L_0}\right)}{\sqrt{2}\hbar}$$

(e) The scalar products are give by

$$\langle\tilde{\phi}_1|\psi_1\rangle \;=\; \int_0^{L_0} \mathrm{d}x\,\tilde{\phi}_1^*(x,0)\psi_1(x,0) \;=\; 1 - \frac{i\left(2-\frac{3}{\pi^2}\right)L_0 mv}{12h} \approx 1$$

$$\langle\tilde{\phi}_2|\psi_1\rangle \;=\; \int_0^{L_0} \mathrm{d}x\,\tilde{\phi}_2^*(x,0)\psi_1(x,0) \;=\; \frac{8iL_0 mv}{9\pi^2 h} \approx 0$$

(f) Compute the standard expectation value of the energy:

$$\bar{E}(t) \;=\; \langle\phi_1(t)|\mathbf{H}|\phi_1(t)\rangle \;=\; \int_0^{L(t)} \mathrm{d}x\,\phi_1^*(x,t)\Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial_x^2}\Big)\phi_1(x,t)$$

Inserting the wave functions this integral evaluates to:

$$\bar{E}(t) \;=\; \frac{\pi^2 h^2}{2mL^2(t)} - \frac{\left(3-2\pi^2\right)mv^2}{12\pi^2}\,.$$

The second term vanishes to first order in v. Hence the energy decreases in the adiabatic limit as $1/L^2(t)$.

(g) The force is the negative gradient of the energy, i.e.

$$F = -\frac{\mathrm{d}}{\mathrm{d}x}E(x) = -\frac{1}{v}\,\frac{\mathrm{d}}{\mathrm{d}t}E(t) = \frac{\hbar^2\pi^2}{mL(t)^3}$$

The work done by the system is the integral over 'force times distance':

$$W = \int_{L_0}^{L_0+vT} F(x)\cdot\mathrm{d}x \;=\; \int_{L_0}^{L_0+vT}\mathrm{d}x \;=\; \frac{\pi^2\hbar^2}{2m}\left(\frac{1}{L_0^2} - \frac{1}{(L_0+vT)^2}\right)$$

(Σ = 12P)