Problem 5.1: Position space and momentum space representation

Learning objective

The difficulty of many problems in physics can be drastically reduced by choosing the appropriate basis. The representation of operators depends on that choice. In this exercise we study the position space and momentum space basis in detail.

Consider the position space basis \{\ket{x}\} which is an eigenbasis of the position operator \(\hat{x}\) with eigenvalues \(x\) and the momentum space basis \{\ket{p}\} which is an eigenbasis of the momentum operator \(\hat{p}\) with eigenvalues \(p\). The spectra of both operators are continuous such that the normalization condition and the completeness relation read

\[ \langle \lambda' | \lambda \rangle = \delta(\lambda' - \lambda), \quad I = \int d\lambda |\lambda\rangle \langle \lambda| \quad \lambda = x, p. \]  

a) Using the canonical commutation relation, show that \(e^{-i\hbar \hat{p}a} \hat{x} e^{i\hbar \hat{p}a} = \hat{x} + a I\). Show that \(e^{-i\hbar \hat{p}a} \ket{x}\) is an eigenstate of \(\hat{x}\) with eigenvalue \(x + a\), i.e. \(e^{-i\hbar \hat{p}a} \ket{x} = \ket{x + a}\).

b) Let \(\langle x | \phi \rangle = \phi(x)\) be the component of a physical state vector \(\ket{\phi}\) in the basis \(\ket{x}\). Calculate the matrix elements of the operators \(\hat{x}\) and \(e^{-i\hbar \hat{p}a}\) in the position space basis and deduce the representation of the momentum operator in position space.

c) Determine the wave functions \(\psi_p(x)\) of the eigenvectors \(\ket{p}\) in the position space representation. (Hint: Choose the normalization factor such that (1) is fulfilled.)

d) Let \(\langle p | \phi \rangle = \tilde{\phi}(p)\) be the component of a physical state vector \(\ket{\phi}\) in the basis \(\ket{p}\). Find the action of the operators \(\hat{x}\) and \(\hat{p}\) in the momentum space representation.

e) Show that \(e^{i\hbar \hat{p}a} f(\hat{x}) e^{-i\hbar \hat{p}a} = f(\hat{x} + a I)\).

Problem 5.2: Delta function potential

Learning objective

The \(\delta\)-function potential is another prime example of an exactly solvable potential in one dimension. In this exercise, we study the attractive case, and show that there is always exactly one bound state. This solution can also be understood as the limit of a potential well with narrow width.

We consider the following one-dimensional potential \(V(x) = g\delta(x)\) where \(g < 0\) is a coupling constant.
a) Show that for a general solution $\psi(x)$ of the Schrödinger equation, $\psi'(x)$ is discontinuous at $x = 0$. Determine the difference $\Delta \psi' = \lim_{\varepsilon \to 0^-} \psi'(\varepsilon) - \lim_{\varepsilon \to 0^+} \psi'(\varepsilon)$ as a function of the coupling strength $g$ and the particle mass $m$.

b) For $E < 0$ and $g < 0$, calculate the bound states of the delta potential. Derive the energy as a function of the coupling strength $g$ and the particle mass $m$.

c) Now we consider the case $E > 0$. Calculate the scattering states and deduce the reflection and transmission probabilities.

d) Show that the bound state of the $\delta$-Potential emerges also from the lowest state of a potential well in the limit where the width $w \to 0$ and the potential strength $V_0 \to -\infty$, but the product of the two is fixed.

Problem 5.3: Decay of Metastable States

Learning objective

Tunneling is an important quantum mechanical phenomenon with wide macroscopic implications, one example is radioactive decay. Double well potentials are often employed to model the decay of metastable states caused by tunneling. In this exercise you will study this phenomena employing a simple symmetric potential well with finite walls and depth (double well in one direction). You will find that there is a special time dependent solution, which exhibits an exponential decay in time.

We consider a particle in the potential $V(x)$ (see figure below). It can be expected that for $F \gg V$ and $V \gg E > 0$ the system possesses states that correspond to bound states, but which are not stable and can decay through quantum mechanical tunneling out of the central potential well. These solutions are a special superposition of eigenstates of the Hamiltonian. Remarkably, these solutions can be directly found by allowing for complex energies $E$ and the following Ansatz for the wave function:

$$
\begin{align*}
|x| < a : & \quad \psi(x) = \cos(qx) \\
|a < |x| < a + b : & \quad \psi(x) = A \exp[-\gamma(|x| - a)] + B \exp[\gamma(|x| - a)] \\
|x| > a + b : & \quad \psi(x) = C \exp[ik(|x| - a - b)]
\end{align*}
$$

(2)
with \( q = \sqrt{2mE/h} \), \( \gamma = \sqrt{2m(V - E)/h} \) and \( k = \sqrt{2m(E + F)/h} \). Note that this ansatz contains only an outgoing plane wave for \( |x| > a + b \). Such an ansatz introduces boundary conditions which violate the hermiticity of the Hamiltonian, i.e. a finite probability current is leaving the system and the norm of the wave function is no longer conserved. As a consequence the eigenenergies have an imaginary part. These wave functions are termed metastable states and are true time-dependent solutions of the Schrödinger equation.

a) Formulate the continuity conditions for the wave function \( \psi(x) \) and its derivative \( \psi'(x) \) at each potential step and show that the following implicit equation determines the eigenenergies \( E_n \).

\[
q \sin(qa) = \gamma(A - B) = \gamma(qa) \left[ \coth(\gamma b) + \frac{\gamma}{ik \sinh(\gamma b)^2} + O \left( \frac{(\gamma/k)^2}{\gamma} \right) \right]
\]  
(3)

We consider a large barrier, i.e. tunneling is exponentially suppressed by \( \exp(-2\gamma b) \). Therefore expand Eq. (3) in the small parameter \( \exp(-2\gamma b) \).

b) To zeroth order in \( \exp(-2\gamma b) \) the eigenenergies are those of a potential well of finite depth. Show that for \( q/\gamma \ll 1 \) the lowest eigenergy \( E_0 \) has the following form

\[
E_0 = \frac{\hbar^2 q_0^2}{2m} \quad \text{with} \quad q_0 = \frac{\pi/2}{a + 1/\gamma}.
\]  
(4)

c) To first order in \( \exp(-2\gamma b) \) the energy \( E_{ms} \) can be written as

\[
E_{ms} = E_0 + \Delta - i\Gamma/2.
\]  
(5)

Determine \( \Delta \) and \( \Gamma \). Show that the imaginary part of the energy can be interpreted as a decay rate

\[
\langle \psi(t)|\psi(t) \rangle \sim \exp(-\Gamma t).
\]  
(6)

Note that \( |\psi(t)\rangle \) is the wavefunction inside the well.

d) Show that the probability current density is given by the following relations

\[
j(x = a + b, t = 0) = \frac{\hbar k}{m} |\psi(a + b, 0)|^2/N = \frac{\Gamma}{2\hbar}.
\]  
(7)

What is a meaningful normalization \( N \) of the wavefunction?

e) Now we consider the true eigenenergies of the potential \( V(x) \) which respect the hermiticity of the Hamiltonian. Such solutions are characterized by an ingoing and outgoing wave for \( |x| > a + b \). The ground state and first excited state in a symmetric potential behave asymptotically (for \( |x| \to \infty \)) like

\[
\psi_0 \sim \cos(|x|k + \delta_0) \\
\psi_1 \sim \text{sgn}(x)i \sin(|x|k + \delta_1)
\]

where

\[
\text{sgn}(x) = \begin{cases} 
+1 & \text{if } x > 1 \\
0 & \text{if } x = 0 \\
-1 & \text{if } x < 1.
\end{cases}
\]
The phases $\delta_0$ and $\delta_1$ are the scattering phases of the symmetric and antisymmetric wave functions, respectively.

Write down the ansatz for the symmetric wavefunction for the potential $V(x)$ and formulate the continuity conditions, which determine the scattering phase $\delta_0(E)$ for the energy $E$. Compare the equations with the expressions from task a).

f) We define the scattering cross section $\sigma = \sigma_0 + \sigma_1$, where the partial scattering cross sections $\sigma_i$ describe scattering with the corresponding symmetry of the wavefunction. The optical theorem expresses the partial scattering cross sections in terms of the corresponding scattering phases

$$\sigma_i = \frac{1}{(\tan \delta_i)^2 + 1}. \quad (8)$$

Prove that the partial scattering cross section exhibits poles at the complex energies $E_{ms}$ and $E_{*ms}$.

g) Show that in the vicinity of the poles $\sigma_0(E)$ takes the following form

$$\sigma_0(E) \sim \frac{1}{(E - E_0 + \Delta)^2 + \Gamma^2/4}. \quad (9)$$

This shows that metastable states result in resonances in the partial scattering cross sections.