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### Problem 1: Continuity and unitarity (Written, 2 points)

**Learning objective**

This exercise verifies that the wave function gives rise to a consistent probability density. For one-dimensional scattering problems we can use the probability interpretation to proof a fundamental relation for the scattering parameters.

a) Show, that the probability density $\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$ obeys the continuity equation

$$\partial_t \rho(\mathbf{r}, t) = -\nabla \mathbf{j}(\mathbf{r}, t),$$

where $\mathbf{j}$ is the probability current

$$\mathbf{j}(\mathbf{r}, t) = -\frac{i\hbar}{2m}\left[\psi^*(\mathbf{r}, t)\nabla\psi(\mathbf{r}, t) - \psi(\mathbf{r}, t)\nabla\psi^*(\mathbf{r}, t)\right]. \tag{1}$$

Prove that the total probability, $\int d\mathbf{r}\, |\psi(\mathbf{r}, t)|^2$, is conserved.

b) Consider the scattering at a potential barrier with the reflection and transmission coefficients $r(k)$ and $t(k)$. Use the probability density current to show $|r(k)|^2 + |t(k)|^2 = 1$.

### Problem 2: Wave packet at a potential barrier (Oral)

**Learning objective**

In this exercise you will study a prototypical example of scattering in one dimension. Most scattering problems cannot be solved analytically, so you will learn how to find the solution numerically and derive an approximation which is valid in some parameter regimes.

Consider the following 1-dimensional potential

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \leq x \leq a \\ 0 & x > a \end{cases} \tag{2}$$

with $V_0 > 0$, and the solution of stationary Schrödinger equation

$$\psi_k(x) = \begin{cases} e^{ikx} + r(k)e^{-ikx} & x < 0 \\ B(k)e^{-\bar{k}x} + B'(k)e^{\bar{k}x} & 0 \leq x \leq a \\ t(k)e^{ikx} & x > a \end{cases} \tag{3}$$

with $k = \sqrt{2mE}/\hbar$, $\bar{k}^2 = 2mV_0/\hbar^2 - k^2$.

Suppose that at time $t_0$ one has a wave packet $\psi(x, t_0)$ centered at $-L$ and far from the barrier $L \gg a$ with $\sigma \ll L$

$$\psi(x, t_0) = \frac{1}{(2\pi\sigma)^{\frac{1}{4}}} e^{ik_0 x} e^{-\frac{(x+L)^2}{4\sigma}} \tag{4}$$

with $k_0 < \bar{k}$.

a) Determine the reflection and transmission coefficients $r(k)$ and $t(k)$.

b) Decompose the wave packet $\psi(x, t_0)$ into eigenstates of the Hamiltonian.

c) Suppose that the coefficients $t(k)$, $r(k)$, $B(k)$, $B'(k)$ are $k$-independent. Calculate the time evolution of the wave packet $\psi(x, t)$ and show that, after reaching the barrier, it splits into two wave packets: reflected and transmitted.

d) Numerically solve the time evolution of the wave packet in the general case with $t(k)$, $r(k)$, $B(k)$, $B'(k)$ explicitly $k$-dependent. Compare this exact solution to your approximations from task c).

### Problem 3: Kronig-Penney Model (Written, 6 points)

**Learning objective**

The Kronig-Penney model allows a simplified modelling of the electronic properties of crystals. An important property are the *energy bands*, narrowly spaced discrete energy levels that are separated from each other by "forbidden zones" where no stationary electronic states are allowed. With the help of this simple band structure model, solid state materials can be characterized as insulators, semimetals or metals. The origin for the appearance of energy bands lies on the one hand in the regular periodic arrangement of the atoms in a crystal and on the other hand is a consequence of quantum mechanical tunneling processes of electrons from one atom to the next.

To illustrate this concept we consider in the following a one-dimensional periodic comb of $\delta$-potentials

$$V(x) = g \sum_{n=-\infty}^{\infty} \delta(x - na) \tag{5}$$

where $g > 0$ is a coupling constant and $a$ denotes the lattice constant of the crystal.

a) First consider the potential $V(x) = g\delta(x)$. Show that for every solution $\psi(x)$ of the Schrödinger equation that $\psi'(x)$ is discontinuous at $x = 0$. Determine the difference $\Delta\psi' = \lim_{\varepsilon \searrow 0} \psi'(\varepsilon) - \lim_{\varepsilon \nearrow 0} \psi'(\varepsilon)$ as a function of the coupling strength $g$ and the particle mass $m$.

b) Show that this potential can be understood as a limiting case of a sequence of potential wells of depth $V_0$ and width $a$ which are separated by barriers of width $b$. Take the limit $b \to 0$ while keeping the coupling constant $g \equiv bV_0$ constant.

c) Find for the regions

$$na < x < (n+1)a, \quad n \in \mathbb{N}, \tag{6}$$

the solution of the Schrödinger equation and write down the continuity conditions at the boundary points $x = na$.

d) Use the symmetry properties of the Hamiltonian to show that the solutions of the Schrödinger equation are given by Bloch's Theorem

$$\psi_q(x) = u_q(x)e^{iqx} \qquad u_q(x+a) = u_q(x) \tag{7}$$

and determine the allowed $q$-values for a crystal of finite volume. This can be achieved by considering periodic boundary conditions in this one-dimensional model.

e) Use Bloch's Theorem to determine the coefficients of the general solution in the various regions between the $\delta$-potentials. Show that they can be reduced to two coefficients

$$\alpha_n = \alpha_0 e^{iqna} \qquad \beta_n = \beta_0 e^{iqna}. \tag{8}$$

Determine $\alpha_0$ and $\beta_0$ from the continuity conditions.

f) Use the results of task e) to determine the allowed and forbidden energy zones. Sketch the dispersion relation $E(q)$ for the Kronig-Penney model for $q = 0, 1, 2$ and discuss the influence of the coupling constant $g$ and the lattice constant $a$ on the band structure (i.e. the energy curves parametrized by q). Give a physical interpretation for the different cases.