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Exercise 1: Decay of Metastable States (Written, 4 points + 3 bonus points ($\star$))

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. In the following we restrict ourselves to symmetric wave functions, which are described by the ansatz:

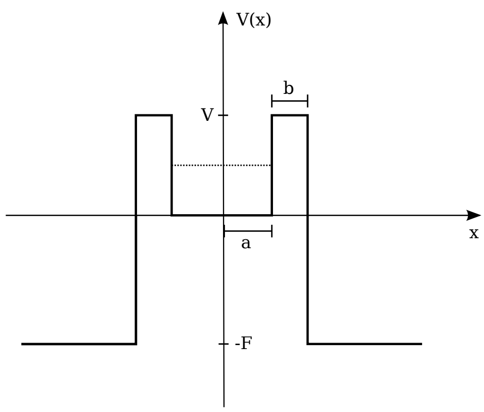
$$\begin{aligned} |x| < a: &\qquad \psi(x) = \cos(qx) \\ a < |x| < a+b: &\qquad \psi(x) = A\exp\left[-\kappa(|x|-a)\right] + B\exp\left[\kappa(|x|-a)\right] \\ |x| > a+b: &\qquad \psi(x) = C\exp\left[ik(|x|-a-b)\right] \end{aligned} \tag{1}$$

with $q = \sqrt{2mE}/\hbar$, $\kappa = \sqrt{2m(V-E)}/\hbar$ and $k = \sqrt{2m(E+F)}/\hbar$. 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*.

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. Expand in the small parameter κ/k.

$$q\sin(qa) = \kappa(A-B) = \kappa\cos(qa)\left[\coth(\kappa b) + \frac{\kappa}{ik\sinh(\kappa b)^2} + \mathcal{O}\left((\kappa/k)^2\right)\right] \tag{2}$$

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



b) To zeroth order in $\exp(-2\kappa b)$ the eigenenergies correspond to those of the potential well. Show that the lowest eigenergy E_0 for $q/\kappa \ll 1$ has the following form

$$E_0 = \frac{\hbar^2 q_0^2}{2m} \quad \text{with} \quad q_0 = \frac{\pi/2}{a + 1/\kappa}. \tag{3}$$

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

$$E_{\text{ms}} = E_0 + \Delta - i\Gamma/2. \tag{4}$$

Determine Δ and Γ. Show that the imaginary part of the energy can be interpreted as a decay rate

$$|\langle\psi(t)|\psi(t)\rangle|^2 \sim \exp(-\Gamma t). \tag{5}$$

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

$$j(x = a + b, t = 0) = \frac{\hbar k}{m}|\psi(a + b, 0)|^2/N = \frac{\Gamma}{2\hbar}. \tag{6}$$

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 δ_0 and δ_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 $\sigma = |f(1)|^2 + |f(-1)|^2 = \sigma_0 + \sigma_1$, where the partial scattering cross sections σ_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

$$\sigma_i = \frac{1}{(\tan \delta_i)^2 + 1}. \tag{7}$$

Prove that the partial scattering cross section exhibits poles at the complex energies E_{ms} and $E^\star_{\text{ms}}$.

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

$$\sigma_0(E) \sim \frac{1}{(E - E_0 + \Delta)^2 + \Gamma^2/4}. \tag{8}$$

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

Exercise 2: Kronig-Penney Model (Oral, 5 points)

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 δ-potentials

$$V(x) = g \sum_{n=-\infty}^{\infty} \delta(x - na) \tag{9}$$

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

a) 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.

b) Find for the regions

$$na < x < (n+1)a, \quad n \in \mathbb{N}, \tag{10}$$

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

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

$$\psi_q(x) = u_q(x)e^{iqx} \qquad u_q(x+a) = u_q(x) \tag{11}$$

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.

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

$$\alpha_n = \alpha_0 e^{iqna} \qquad \beta_n = \beta_0 e^{iqna}. \tag{12}$$

Determine a_0 and β_0 from the continuity conditions.

e) Use the results of task d) 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.