8.513: Coherent and collective phenomena in quantum transport Problem Set # 2 Due: 09/18/08

Scattering theory of transport, II

1. Quantum point contact.

One can model quantum point contact (QPC) in a two-dimensional electron gas [see van Wees, et al, Phys. Rev. Lett. 60, 848 (1988)] by a quadratic saddle-like potential:

$$U(x,y) = -\frac{1}{2}ax^2 + \frac{1}{2}by^2 + U_0 \tag{1}$$

The x dependence describes potential along conduction direction, the y dependence describes confinement in transverse direction. The parameters a and b depend on the geometry of the split gate used to create QPC; the energy U_0 is proportional to gate voltage V_g and can be varied.

(i) Identify scattering channels by separating variables in the 2d Schrödinger equation and discuss the two-terminal conductance G dependence on U_0 treating electrons as an ideal degenerate Fermi gas. Use the result for transmission coefficient, $T(\epsilon) = |t|^2 = e^{2\pi\epsilon/\hbar\omega}/(e^{2\pi\epsilon/\hbar\omega} + 1)$, derived for 1d inverted parabolic potential $U(x) = -\frac{1}{2}m\omega^2 x^2$.

(ii) Find the thermopower coefficient of the QPC. Consider the situation when a small temperature difference $\delta T = T_L - T_R$ exists between the reservoirs, whereas no voltage is applied, $V = \mu_L - \mu_R = 0$. Find the electric current induced by temperature difference, $I = A\delta T$, and determine the thermo-electric coefficients (see Lecture 2, page 7).

2. Breit-Wigner resonances.

Consider a general scattering matrix S. Being unitary, S can be brought to a diagonal form:

$$S = \sum_{\alpha=1\dots N} e^{2i\theta_{\alpha}} |\alpha\rangle \langle \alpha|, \qquad (2)$$

where $|\alpha\rangle$ and $\langle\alpha|$ are in- and out-states, and N is the number of scattering channels.

As a function of energy, the scattering matrix $S(\epsilon)$ is analytic in the upper half-plane of complex ϵ . This condition expresses causality requirement. (Think of the relation $\psi_{out} = S\psi_{in}$ from the cause-effect point of view and compare to Kramers-Kronig properties of susceptibility.)

Since $S(\epsilon)$ is analytic in the upper complex half-plane, $\operatorname{Im} \epsilon > 0$, the phase factors in Eq.(2) may have zeros in this half-plane, but no poles or other singularities (such as branch cuts, etc.). Show that each zero $\epsilon = z_j$ must be accompanied by a pole at $\epsilon = z_j^*$ in the lower half-plane $\operatorname{Im} \epsilon < 0$.

(i) Suppose now that one of the zeros $z_j = \epsilon_0 + \frac{i}{2}\Gamma$ is much closer to the real axis than other zeros. For ϵ values close enough to ϵ_0 the S-matrix can be approximated by Breit-Wigner (BW) model

$$S = e^{2i\theta_n^{(reg)}} \frac{\epsilon - \epsilon_0 - \frac{i}{2}\Gamma}{\epsilon - \epsilon_0 + \frac{i}{2}\Gamma} |n\rangle \langle n| + S^{(reg)}$$
(3)

where $S^{(reg)}$ and $e^{2i\theta_n^{(reg)}}$ describe the "regular" parts of the S-matrix which have no singularity at $\epsilon = z_j^*$.

(ii) Transport through a quantum dot can be schematically described by a 1D Schroedinger equation with potential that confines particle between two barriers. As a simple model, we consider $U(x) = \lambda \delta(x - a/2) + \lambda \delta(x + a/2)$. In this potential, the resonances $\epsilon_{1,2,3...}$ are described by the

standing wave condition $k_n a \approx \pi n$. Consider the limit of strong barriers (large λ) and find the Breit-Wigner form of the S-matrix for near a resonance ϵ_n .

Find the transmission and reflection coefficients, $T(\epsilon) = |t|^2$ and $R(\epsilon) = |r|^2$, and analyze their energy dependence near a resonance.

3. Quasi-bound states and scattering for inverted parabola. (This is a hard one)

In this problem we analyze scattering on an inverted parabola, used in Problem 1 to model quantum point contact. Consider a 1d Schrödinger equation

$$\epsilon\psi = -\frac{1}{2}\psi'' - \frac{1}{2}x^2\psi \tag{4}$$

We learned in Problem 2 that complex poles and zeros are related to quasi-bound states which have only the "out" but no "in" component. Here we demonstrate how one can reconstruct the S matrix by analyzing these states.

(i) Show that the state $\psi_0(x) = e^{ix^2/2}$ represents a quasi-bound state for complex energy $\epsilon_0 = -i/2$ which has only outgoing but no incoming component at infinity.

Write the Hamiltonian in the form $H = -a^{\dagger}a - i/2$, where

$$a = 2^{-1/2}(x + id/dx), \quad a^{\dagger} = 2^{-1/2}(x - id/dx)$$

are analogs of the ladder (lowering and raising) operators for this problem. From the commutators of these operators and H, treating a, a^{\dagger} by analogy with harmonic oscillator problem, show that there are quasi-energy states with energies

$$\epsilon_n = -i\left(n + \frac{1}{2}\right), \quad n \ge 0,\tag{5}$$

where even and odd values of n correspond to even and odd states $\psi_n(x)$.

(ii) Show that the 2×2 scattering matrix for this problem can be diagonalized in the channel space in the even and odd basis:

$$S = e^{2i\theta_+} |+\rangle \langle +| + e^{2i\theta_-} |-\rangle \langle -|, \quad \text{where} \quad |+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix}, \quad |-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix}, \tag{6}$$

and θ_{\pm} are energy-dependent scattering phases for the even and odd channels. From this representation, find the ratio of the transmission and reflection amplitudes,

$$f(\epsilon) = t(\epsilon)/r(\epsilon) \tag{7}$$

in terms of the phase factors $e^{2i\theta_{\pm}}$.

(iii) Use the information obtained in part (i), combined with the result of Problem 1, to show that the quantities $e^{2i\theta_+}$ ($e^{2i\theta_-}$) as a function of complex energy, have zeros at $\epsilon = -\epsilon_n$ and poles at $\epsilon = \epsilon_n$, where $n \ge 0$ is an even (odd) integer. Use this result to evaluate the function $f(\epsilon)$ at the points $\epsilon = \pm i(n + 1/2)$ of the complex ϵ plane.

Having this information, reconstruct the function $f(\epsilon)$ and to find the transmission and reflection coefficients for inverted parabola $U(x) = -\frac{1}{2}m\omega^2 x^2$.

Hint: Two analytic functions of complex variable which coincide on a set of points z_n with a limiting point somehere in the complex plane or at infinity, coincide in the entire plane.