Quantum theory of condensed matter II

Mesoscopic physics

Prof. Milena Grifoni	Tue	8:00 - 10:00	9.2.01
	Fri	10:00 - 12:00	H33
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Sheet 6

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1. Double square barrier

Consider the one dimensional problem of a wave packet impinging a double square barrier. Assume for the scattering region the following parametrization of the potential:

$$U(x) = \begin{cases} U_1 & 0 \leq x \leq W_1 \\ U_2 & W_1 + d \leq x \leq W_1 + d + W_2 \\ 0 & \text{else} \end{cases} \tag{1}$$

where U_1, U_2, W_1, W_2 and d are all positive. You should use the method of finite differences and the Fisher-Lee relations to calculate numerically the transmission through the system. In particular: Remember that the second derivative of the wavefunction has to be discretized as

$$\begin{aligned} \psi(x) &\to \psi(x_i) \equiv \psi_i \\ \psi''(x) \to \psi''(x_i) &= \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{a^2} \end{aligned} \tag{2}$$

being a the discretization lattice spacing . This leads to the discrete Schrödinger equation $H_{ij}\psi_j = E\psi_i$ with

$$H_{ij} = (2t + U_i)\delta_{ij} - t\delta_{i+1,j} - t\delta_{i-1,j}\,. \tag{3}$$

$t = \hbar^2/2ma^2$ is the hopping parameter and $U_i \equiv U(x_i)$.

1. In the lecture it was shown that the problem of inverting the full (infinite) matrix $E - H$ can be avoided by using the finite sized Hamiltonian of the scattering region H_S and taking the leads into account by adding the so-called self energy $\Sigma^{R/A} = \Sigma^{R/A}_{L,\,ij} + \Sigma^{R/A}_{R,\,ij}$ with

$$\Sigma^R_{L,\,ij} = -te^{ika}\delta_{i1}\delta_{1j}, \quad \text{and} \quad \Sigma^R_{R\,ij} = -te^{ika}\delta_{iN}\delta_{Nj}. \tag{4}$$

   Moreover it holds $\Sigma^A_{\alpha,\,ij} = (\Sigma^R_{\alpha,\,ji})^*$. "1" and "$N$" in Eq. (4) are the first and the last point in the scattering region respectively. The retarded/advanced Green function of the scattering region is then

$$G^{R/A}_S = \left(E - H_S - \Sigma^{R/A}\right)^{-1}. \tag{5}$$

   Set up H_S and calculate $G^{R/A}_S$ numerically. You can use for example Matlab to invert the matrix.

   (3 Points)

2. Relate the Green function to the transmission using the Fisher-Lee relation derived in class

$$T = \mathrm{Tr}\left[\Gamma_R\, G^R_S\, \Gamma_L\, G^A_S\right] \quad \Gamma_\alpha = i[\Sigma^R_\alpha - \Sigma^A_\alpha]\,. \tag{6}$$

   (2 Points)

3. Plot the transmission as a function $E > 0$ for different parameters of the barriers and lattice spacings. Compare the numerical result to the analytical one:

$$T(E) = |\frac{t_1 t_2}{1 - r_1 r_2 e^{2ik_E d}}|^2 \tag{7}$$

where

$$\begin{aligned} t_i &= \frac{e^{ik_E W_i}}{\cosh(\kappa_{i,E} W_i) + i\frac{\epsilon_{i,E}}{2}\sinh(\kappa_{i,E} W_i)} \\ r_i &= -i\frac{\eta_{i,E}}{2}\frac{\sinh(\kappa_{i,E} W_i)}{\cosh(\kappa_{i,E} W_i) + i\frac{\epsilon_{i,E}}{2}\sinh(\kappa_{i,E} W_i)} \end{aligned} \tag{8}$$

and $k_E = \sqrt{2mE}/\hbar$, $\kappa_{i,E} = \sqrt{2m(U_i - E)}/\hbar$, $\epsilon_{i,E} = \kappa_{i,E}/k_E - k_E/\kappa_{i,E}$ and $\eta_{i,E} = \kappa_{i,E}/k_E + k_E/\kappa_{i,E}$. Give a physical interpretation of the results.

(3 Points)

Frohes Schaffen!