

Statistical Physics & Condensed Matter Theory I: Exercise

Tunneling spectroscopy

Consider two systems described respectively by Hamiltonians H_1 and H_2 . Each system is described by second-quantized fermionic operators $a_{i,k}$ ($i = 1, 2$, k being *e.g.* a momentum-like index) obeying the anti-commutation relations

$$\{a_{i,k}, a_{i',k'}^\dagger\} = \delta_{ii'} \delta_{kk'}.$$

We now bring the systems in close contact with each other. Tunneling of particles between one system and the other then becomes possible. This is represented by the perturbation term

$$H_t = \sum_{kk'} \left(t_{kk'} a_{1,k}^\dagger a_{2,k'} + t_{kk'}^* a_{2,k'}^\dagger a_{1,k} \right) \equiv T + T^\dagger.$$

Our expectation is that if we were to put both sides at different chemical potentials (namely: at different voltages), there would be a current flowing from one side to the other because of the tunneling term. This current can be defined for example as the rate of change of the charge in system 2:

$$I = \frac{d}{dt} N_2, \quad N_i = \sum_k a_{i,k}^\dagger a_{i,k}.$$

a) Using $dA/dt = i[H, A]$, show that

$$I = J + J^\dagger, \quad J \equiv i \sum_{kk'} t_{kk'} a_{1,k}^\dagger a_{2,k'}.$$

b) We now apply linear response theory. According to the Kubo formula, the current through the junction as a function of time is given by

$$\bar{I}(t) = \int_{-\infty}^{\infty} dt' \mathcal{C}_{ret}^{I, H_t}(t-t'), \quad \mathcal{C}_{ret}^{I, H_t}(t-t') = -i\theta(t-t') \langle [I^I(t), H_t^I(t')] \rangle$$

in which the expectation value is the thermal, grand-canonical expectation value using the unperturbed theory. Assuming that correlations are purely diagonal in momentum index, and using Wick's theorem, show that this can be written in terms of the 'lesser' and 'greater' functions as

$$\bar{I}(t) = 2 \operatorname{Re} \int_{-\infty}^0 dt' \sum_{k_1 k_2} |t_{k_1 k_2}|^2 \left(\mathcal{C}_{\beta, \mu_1; k_1}^>(t') \mathcal{C}_{\beta, \mu_2; k_2}^<(-t') - \mathcal{C}_{\beta, \mu_1; k_1}^<(t') \mathcal{C}_{\beta, \mu_2; k_2}^>(-t') \right)$$

(note that this result becomes *time independent*: we are thus calculating a *static current*, which makes sense because our perturbation is also time-independent).

c) Fourier transforming the correlators according to

$$\mathcal{C}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \mathcal{C}(\omega),$$

making use of the Dirac identity in the form (P means the principal part under the integral sign)

$$\int_0^{\infty} dt e^{i\omega t} = \pi\delta(\omega) + iP\frac{1}{\omega},$$

and using the relations between the greater/lesser functions and the spectral function

$$\mathcal{C}_{\beta,\mu;k}^>(\omega) = -i(1 - n_F(\omega - \mu; \beta))A_{\beta,\mu;k}(\omega), \quad \mathcal{C}_{\beta,\mu;k}^<(\omega) = in_F(\omega - \mu; \beta)A_{\beta,\mu;k}(\omega),$$

show that the current is expressed as

$$\bar{I} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_{k_1 k_2} |t_{k_1 k_2}|^2 (n_F(\omega - \mu_2; \beta) - n_F(\omega - \mu_1; \beta)) A_{\beta,\mu_1;k_1}(\omega) A_{\beta,\mu_2;k_2}(\omega).$$

What happens to the current if we set $\mu_1 = \mu_2$? Interpret this result.

d) Let us now assume that system 1 is being ‘probed’ by system 2 (the latter is then *e.g.* a scanning tunneling tip). We make the assumption that this tip is metallic, so its density of states is more or less constant, and that we can approximate

$$\sum_{k_2} |t_{k_1 k_2}|^2 A_{\beta,\mu_2;k_2}(\omega) \simeq 2\pi t_{k_1} \nu_2$$

as being ω -independent (t_{k_1} is some real positive function of k_1 ; ν_2 is the density of states in the probe). Interpreting the chemical potential difference $\mu_2 - \mu_1 = V$ as a potential difference, show that the zero-temperature limit of the differential current (derivative of the current with respect to V at fixed μ_1) is a direct measure of the spectral function,

$$\lim_{\beta \rightarrow \infty} \frac{d\bar{I}}{dV} = \nu_2 \sum_{k_1} t_{k_1} A_{\beta,\mu_1;k_1}(\mu_1 + V).$$

This is a fundamental equation in the multi-faceted field of spectroscopy.