PC5203 Advanced Solid State Physics

Weeks 7-9, due Monday 18 Oct 2021

[main concepts to cover: definitions of Green's functions, fluctuation-dissipation theorem, contour ordered Green's functions, Langreth rule, Caroli/Landauer formula]

1. (a) If the Hamiltonian is a single quantum dot of electron with $\hat{H} = \epsilon c^+ c$ in thermal equilibrium, show that the fluctuation-dissipation theorem is trivially true, i.e., the Green's functions in energy space E satisfy $g^<(E) = -f(E)\big(g^r(E) - g^a(E)\big)$, here $f(E) = 1/(e^{\beta(E-\mu)} + 1)$ is the Fermi function. (b) Using the technique of diagonalizing an N-site Hamiltonian $\hat{H} = c^+ H c$, here the single particle H without the hat is an $N \times N$ Hermitian matrix, c is a column vector of N fermi annihilation operators, and c^+ is a row vector of Hermitian conjugate of c, show that the fluctuation-dissipation theorem still holds, i.e.,
$$G^< = -f(G^r - G^a)$$
here the Green's functions are matrices defined in the site space and in time domain t and Fourier transformed into energy domain E. (c) Using the Lehmann representation, show that the fluctuation-dissipation theorem holds in thermal equilibrium, for any Hamiltonian $\hat{H}$ (with interaction or without) for the electron Green's functions.

2. Consider the time ordering operator T. (a) Define the precise meaning of time ordering operator on the product of the Hamiltonian operators: $T(H(t_1)H(t_2))$. (b) Use your definition to show that the following equation is true:
$$\frac{1}{2!}\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 T\big(H(t_1)H(t_2)\big) = \int_{t'}^{t} dt_1 H(t_1) \int_{t'}^{t_1} dt_2 H(t_2)$$
where we assume $t > t'$. Note that the domain of integration on the left is on a square while the domain of the integral on the right-hand side is on a triangle. Draw illustrative pictures of the integration domains on the left and right side of the equal sign. (c) How would you modify the above equation if time order T is replaced by anti-time order $\bar{T}$?

3. One form of the Langreth theorem says, if the convolution in contour time is $C(\tau,\tau') = \int A(\tau,\tau'')B(\tau'',\tau')d\tau''$, then, for time-translationally invariant system in energy domain it is
$$C^<(E) = A^r(E)B^<(E) + A^<(E)B^a(E).$$

Here A, B, C are matrices. Time-translationally invariant system means, e.g., $A(t, t') = A(t - t')$. Show this explicitly by elementary means, i.e., use the fact that $C^{<}(t) = C^{+-}(t, 0)$, $A^r = A^{++} - A^{+-}$, etc, and the meaning of contour integral in τ in relation to real time t, and the convolution theorem for Fourier transform.

4. Consider the electron transport in a single quantum dot with the center Hamiltonian $H_c = \epsilon c^{\dagger} c$, weakly coupled to two leads called left and right bath, as shown below in the figure. The interaction of the quantum dot with lead will be approximated by a retarded self energy (through the Dyson equation) which is constant and purely imaginary, such that the left lead $\Gamma_L = i(\Sigma_L^r - \Sigma_L^a) = -2 \,\mathrm{Im}\, \Sigma_{\mathrm{L}}^{\mathrm{r}}$ is a constant independent of energy E, and similarly for the right lead. This is known as a wide-band approximation. (a) Determine the full Green's function $G^r(E)$, (b) Use the Caroli formula $\mathrm{Tr}(G^r \Gamma_L G^a \Gamma_R)$ together with the Landauer formula to show that the current is given by the formula

$$I_L = \frac{-e}{\hbar} \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \left(f_L(\epsilon) - f_R(\epsilon)\right),$$

in the weak coupling limit, that is, you can assume Γ_L and Γ_R are small (thus a peak can be approximated as a delta function, and the integration in energy E can be performed approximately). Here f is the Fermi function for the left lead at β_L, μ_L or similarly the right lead at β_R, μ_R evaluated at the energy level ϵ of the quantum dot.