Density Matrix Theory

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Sheet 9

1. Orthodox Theory of Coulomb Blockade

Consider a metallic island in tunnelling contact with source and drain leads and in capacitive interaction with a nearby metallic gate. The entire physical system is described by the Hamiltonian:

$$H = H_{\text{sys}} + H_{\text{ext}} + H_{\text{tun}} + H_{\text{leads}} \tag{1}$$

where

$$\begin{aligned} H_{\text{sys}} &= \sum_{i\,\sigma} \epsilon_i\, d^\dagger_{i\sigma} d_{i\sigma} + \frac{U}{2}\hat{N}(\hat{N}-1) \\ H_{\text{ext}} &= eV_{\text{g}}\hat{N} \\ H_{\text{tun}} &= \tau \sum_{\alpha\, i\, k\, \sigma} \left(c^\dagger_{\alpha k\sigma} d_{i\sigma} + d^\dagger_{i\sigma} c_{\alpha k\sigma} \right) \\ H_{\text{leads}} &= \sum_{\alpha k\sigma} \epsilon_k\, c^\dagger_{\alpha k\sigma} c_{\alpha k\sigma} \end{aligned} \tag{2}$$

and $\alpha = L, R$, k labels the momentum of the electron in the leads, while i the single particle eigenstates of the metallic island. The essential differences with the Anderson impurity model studied in the previous sheets is the continuity of the single particle spectrum of the metallic island with respect to the isolated energy level of the impurity. Finally, notice how the Coulomb interaction is treated in the constant interaction approximation ($\hat{N}$ is the total number of electrons on the metallic island).

1. Following the steps of the previous sheets, write the equation of motion for the reduced density matrix of the system in the Schrödinger picture.

2. Due to the continuous spectrum of the island and to the action of additional sources of dissipation, the island relaxes to equilibrium after each tunnelling event. Thus one can assume for the reduced density matrix the form $\hat{\rho}_{\text{red}} = \sum_N P_N(t)\hat{\rho}_{\text{th},N}$ where $\hat{\rho}_{\text{th},N}$ represents the system in the local thermal equilibrium:

$$\hat{\rho}_{\text{th},N} = \frac{1}{Z_N} \exp\left[-\beta(H_{\text{sys}} + H_{\text{ext}})\right] \mathcal{P}_N \tag{3}$$

   where $Z_N = \text{Tr}_{\text{sys}}\{\exp\left[-\beta(H_{\text{sys}} + H_{\text{ext}})\right]\mathcal{P}_N\}$ and $\mathcal{P}_N$ is the projector on the system states with N electrons. Which operations should one apply on $\hat{\rho}_{\text{red}}$ to obtain $P_N(t)$? What is the physical meaning of P_N? Moreover, prove that the interacting part of the system Hamiltonian and H_{ext} drop from the definition of $\hat{\rho}_{\text{th},N}$

3. Prove that the equation of motion for the variable $P_N(t)$ reads:

$$\dot{P}_N(t) = -\frac{1}{\hbar^2}\int_0^\infty \mathrm{d}t'\,\text{Tr}_{\text{sys}}\{\mathcal{P}_N \text{Tr}_{\text{B}}\{[H_{\text{tun}}, [H_{\text{tun}}(-t'), \sum_{N'} P_{N'}(t)\hat{\rho}_{\text{th},N'} \otimes \hat{\rho}_{\text{B}}]]\}\} \tag{4}$$

   and further simplify it by factorizing the bath and system traces.

4. Calculate explicitly the time evolution of the system operators by proving the relation:

$$d^\dagger_{i\sigma}(-t')\mathcal{P}_N = d^\dagger_{i\sigma}\exp\left[-\tfrac{i}{\hbar}\left(\epsilon_i + eV_{\rm g} + UN\right)\right]$$

5. In the limit of large particle number the canonical and the grand canonical ensembles coincide. Prove that the statement above implies the validity of the equation:

$$\mathrm{Tr}_{\rm sys}\{d^\dagger_{i\sigma}d_{i\sigma}\hat\rho_{{\rm th},N}\} \approx \mathrm{Tr}_{\rm sys}\{d^\dagger_{i\sigma}d_{i\sigma}\hat\rho_{{\rm th},\mu_N}\} \tag{5}$$

where

$$\hat\rho_{{\rm th},\mu_N} = \frac{\exp\{-\beta[\sum_{i\sigma}(\epsilon_i - \mu_N)\hat n_{i\sigma}]\}}{\mathrm{Tr}_{\rm sys}\{\exp\{-\beta[\sum_{i\sigma}(\epsilon_i - \mu_N)\hat n_{i\sigma}]\}\}} \tag{6}$$

and μ_N is defined by the relation $N = \mathrm{Tr}_{\rm sys}\{\hat N\hat\rho_{{\rm th},\mu_N}\}$.

6. Use the approximation introduced in the previous point to reduce the equation of motion of P_N to the form:

$$\begin{aligned}\dot P_N(t) = \sum_{\alpha\sigma}\frac{2\pi}{\hbar}D_{\rm sys}D_\alpha|\tau|^2\int {\rm d}\epsilon_i{\rm d}\epsilon_k\\
\big[-f^+_\alpha(\epsilon_k)f^-_{\rm sys}(\epsilon_i)\delta(\epsilon_i + eV_{\rm g} + UN - \epsilon_k)\,P_N(t)+\\
-\,f^-_\alpha(\epsilon_k)f^+_{\rm sys}(\epsilon_i)\delta(\epsilon_i + eV_{\rm g} + U(N-1) - \epsilon_k)\,P_N(t)+\\
+\,f^-_\alpha(\epsilon_k)f^+_{\rm sys}(\epsilon_i)\delta(\epsilon_i + eV_{\rm g} + UN - \epsilon_k)\,P_{N+1}(t)+\\
+f^+_\alpha(\epsilon_k)f^-_{\rm sys}(\epsilon_i)\delta(\epsilon_i + eV_{\rm g} + U(N-1) - \epsilon_k)\,P_{N-1}(t)\big]\end{aligned} \tag{7}$$

where $D_{\rm sys}$ and D_α are the α-lead and metallic island density of states respectively. Moreover δ is the Dirac distribution. Give a physical interpretation of the result in terms of Pauli exclusion principle and energy conservation.

7. Prove the following relations:

$$\begin{aligned}f^+(\epsilon_1)f^-(\epsilon_2) = n_B(\epsilon_1-\epsilon_2)[f^+(\epsilon_2) - f^+(\epsilon_1)]\\
\int_{-\infty}^{+\infty}{\rm d}\epsilon[f^+(\epsilon) - f^+(\epsilon+\omega)] = \omega\end{aligned} \tag{8}$$

and apply them to solve the eneergy integrsls in the equation of motion for $P_N(t)$ obtained at point 6. The result is the central equation for the orthodox theory of Coulomb blockade for metallic islands developed in 1986 by Averin and Likharev *i.e.*.

$$\dot P_N = -(\Gamma_{N\to N+1} + \Gamma_{N\to N-1})P_N + \Gamma_{N+1\to N}P_{N+1} + \Gamma_{N-1\to N}P_{N-1} \tag{9}$$

where

$$\begin{aligned}\Gamma_{N\to N+1} = \sum_{\alpha\sigma}\gamma_\alpha f(E(N+1) - E(N) - \mu_\alpha)\\
\Gamma_{N\to N-1} = \sum_{\alpha\sigma}\gamma_\alpha f(E(N-1) - E(N) + \mu_\alpha)\end{aligned} \tag{10}$$

are the tunnelling rates and $f(E) = En_B(E)$. Moreover $\gamma_\alpha = 2\pi/\hbar D_\alpha D_{\rm sys}|\tau|^2$ and $E(N)$ is the energy of the N-particle manybody ground state of the metallic island.

Frohes Schaffen!