

The derivation of the Lindblad equation for the electron-impurity scattering

I. LINDBLAD DYNAMICS

According to Eq. 4 and 5 of PHYSICAL REVIEW B 90, 125140 (2014) or Eq. 3.20 and 3.21 of Rosati's thesis, the scattering term has the form

$$\frac{d\hat{\rho}}{dt} = \sum_s \left(\hat{A}^s \hat{\rho} \hat{A}^{s,\dagger} - \frac{1}{2} \left\{ \hat{A}^{s,\dagger} \hat{A}^s, \hat{\rho} \right\} \right),$$

where A^s is an operator of a scattering channel s , for electron-impurity scattering, s represents one impurity,

$$\hat{A}^s = \sqrt{\frac{1}{\sqrt{2\pi t}}} \int dt' e^{-\frac{H_0 t'}{i\hbar}} \hat{H}^s e^{\frac{H_0 t'}{i\hbar}} e^{-\frac{1}{4} \left(\frac{t'}{t} \right)^2}. \quad (1)$$

If all impurities are equivalent, we have $\sum_s = N_{i,cell} = n_i V_{cell}$, where $N_{i,cc}$ is number of impurities in unit cell and n_i is impurity density. To emphasize the scattering mechanism being the electron-impurity one, we will write s as i . Therefore,

$$\begin{aligned} \frac{d\rho_{12}}{dt} &= n_i V_{cell} \text{Tr} \left(\hat{c}_2^\dagger \hat{c}_1 \frac{d\hat{\rho}}{dt} \right) \\ &= \frac{1}{2} n_i V_{cell} \text{Tr} \left(\hat{c}_2^\dagger \hat{c}_1 \hat{A}^i \hat{\rho} \hat{A}^{i,\dagger} + \hat{A}^i \hat{\rho} \hat{A}^{i,\dagger} \hat{c}_2^\dagger \hat{c}_1 - \hat{c}_2^\dagger \hat{c}_1 \hat{A}^{i,\dagger} \hat{A}^i \hat{\rho} - \hat{\rho} \hat{A}^{i,\dagger} \hat{A}^i \hat{c}_2^\dagger \hat{c}_1 \right) \\ &= \frac{1}{2} n_i V_{cell} \text{Tr} \left(\left[\hat{A}^{i,\dagger}, \hat{c}_2^\dagger \hat{c}_1 \right] \hat{A}^i \hat{\rho} + \hat{\rho} \hat{A}^{i,\dagger} \left[\hat{c}_2^\dagger \hat{c}_1, \hat{A}^i \right] \right) \\ &= \frac{1}{2} n_i V_{cell} \text{Tr} \left(\left[\hat{A}^{i,\dagger}, \hat{c}_2^\dagger \hat{c}_1 \right] \hat{A}^i \hat{\rho} \right) + H.C.. \end{aligned} \quad (2)$$

II. ELECTRON-IMPURITY

The electron-impurity Hamiltonian for impurity i reads

$$\begin{aligned} \hat{H}^i &= \sum_{12} g_{12}^i c_1^\dagger c_2, \\ g_{12}^i &= \langle 1(r) | V^i(r) | 2(r) \rangle \\ &= V^i(q_{12}) \langle 1 | 3 \rangle, \\ V^i(q) &= \frac{-Ze^2}{V_{cell} \epsilon_r \epsilon_0 q^2}. \end{aligned}$$

where $q_{12} = k_1 - k_2$. $\epsilon_r = 1 + \frac{q_0^2}{q^2}$ in typical Debye model. Insert it in 1,

$$\begin{aligned} \hat{A}^i &= \sum_{12} A_{12}^i \hat{c}_1^\dagger \hat{c}_2, \\ A_{12}^i &= \sqrt{\frac{1}{\sqrt{2\pi t}}} \int dt' e^{-\frac{(\epsilon_1 - \epsilon_2)t'}{i\hbar}} g_{12}^i e^{-\frac{1}{4} \left(\frac{t'}{t} \right)^2} \\ &= \sqrt{\frac{2\pi}{\hbar}} g_{12}^i \delta^{G,1/2}(\epsilon_1 - \epsilon_2). \end{aligned} \quad (3)$$

Since $\hat{A}^{i,\dagger} = \hat{A}^i$,

$$\left[\hat{A}^{i,\dagger}, \hat{c}_2^\dagger \hat{c}_1 \right] = \sum_3 \left(A_{32}^i \hat{c}_3^\dagger \hat{c}_1 - A_{13}^i \hat{c}_2^\dagger \hat{c}_3 \right). \quad (4)$$

Insert Eq. 3 and 4 into Eq. 2,

$$\begin{aligned} \frac{d\rho_{12}}{dt} &= \frac{1}{2} n_i V_{cell} \text{Tr} \left(\sum_3 \left(A_{32}^i \hat{c}_3^\dagger \hat{c}_1 - A_{13}^i \hat{c}_2^\dagger \hat{c}_3 \right) \sum_{45} A_{45}^i \hat{c}_4^\dagger \hat{c}_5 \hat{\rho} \right) + H.C. \\ &= \frac{1}{2} n_i V_{cell} \sum_{345} \left(A_{32}^i h_{3145} - A_{13}^i h_{2345} \right) A_{45}^i + H.C., \\ h_{1234} &= \text{Tr} \left(\hat{c}_1^\dagger \hat{c}_2 \hat{c}_3^\dagger \hat{c}_4 \hat{\rho} \right). \end{aligned}$$

To close the equation, the mean-field approximation is introduced for h ,

$$\begin{aligned} h_{1234} &\approx \text{Tr} \left(\hat{\rho} \hat{c}_2 \hat{c}_3^\dagger \right) \text{Tr} \left(\hat{\rho} \hat{c}_1^\dagger \hat{c}_4 \right) \\ &= \text{Tr} \left(\hat{\rho} \left(\delta_{23} - \hat{c}_3^\dagger \hat{c}_2 \right) \right) \text{Tr} \left(\hat{\rho} \hat{c}_1^\dagger \hat{c}_4 \right) \\ &= (I - \rho)_{23} \rho_{41}. \end{aligned}$$

Therefore,

$$\frac{d\rho_{12}}{dt} = \frac{1}{2} n_i V_{cell} \sum_{345} \left((I - \rho)_{14} A_{45}^i \rho_{53} A_{32}^i - A_{13}^i (I - \rho)_{34} A_{45}^i \rho_{52} \right) + H.C.,$$

Define

$$\begin{aligned} P_{1234} &= A_{13}^i A_{24}^i, \\ A_{13}^i &= \sqrt{\frac{2\pi}{\hbar}} g_{13}^i \delta^{G,1/2} (\epsilon_1 - \epsilon_3). \end{aligned}$$

We have

$$\frac{d\rho_{12}}{dt} = \frac{1}{2} n_i V_{cell} \sum_{345} \left((I - \rho)_{14} P_{4253} \rho_{53} - (I - \rho)_{34} P_{3415}^* \rho_{52} \right) + H.C..$$

III. SEMI-CLASSICAL LIMIT

Obviously, in semiclassical limit,

$$\begin{aligned} \frac{df_1}{dt} &= \frac{1}{2} n_i V_{cell} \sum_2 \left((I - f_1) P_{1122} f_2 - (I - f_2) P_{2211} f_1 \right) + H.C. \\ &= n_i V_{cell} \sum_{2 \neq 1} (f_2 - f_1) P_{1122}, \\ P_{1122} &= \frac{2\pi}{\hbar} |g_{12}^i|^2 \delta^G (\epsilon_1 - \epsilon_2). \end{aligned}$$

Easily, we can define

$$\frac{1}{\tau_1} = \frac{2\pi}{\hbar} n_i V_{cell} \sum_2 |g_{12}^i|^2 \delta^G(\epsilon_1 - \epsilon_2),$$

The above equation is the same as Eq. 1, 8 and 9 of PHYSICAL REVIEW MATERIALS 3, 033804 (2019) and is consistent with Eq. 9.52 of Theory of Electron Transport in Semiconductors by Carlo Jacoboni and Eq. in Eq. 19 of Reviews of Modern Physics 53, 745 (1981).