The derivation of the Lindblad equation for the electron-phonon 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

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

where

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

Therefore,

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

II. ELECTRON-PHONON

The electron-phonon Hamiltonian reads (see Eq. 4 in PHYSICAL REVIEW B 92, 235423 (2015))

$$\hat{H} = \sum_{12q\lambda}\left(g_{12}^{q\lambda+}\hat{c}_1^{\dagger}\hat{c}_2\hat{b}_q^{\dagger} + g_{12}^{q\lambda-}\hat{c}_1^{\dagger}\hat{c}_2\hat{b}_q\right).$$

Insert it in 1,

$$\begin{aligned}
\hat{A} =& \sum_{q\lambda}\left(\hat{G}^{q\lambda+}\hat{b}_{q\lambda}^{\dagger} + \hat{G}^{q\lambda-}\hat{b}_{q\lambda}\right),\\
\hat{G}^{q\lambda\pm} =& \sum_{12}G_{12}^{q\lambda\pm}\hat{c}_1^{\dagger}\hat{c}_2,\\
G_{12}^{q\lambda\pm} =& \sqrt{\frac{1}{\sqrt{2\pi}\bar{t}}}\int dt' e^{-\frac{\left(\epsilon_1-\epsilon_2\pm\omega_{q\lambda}\right)t'}{i\hbar}}g_{12}^{q\lambda\pm}e^{-\frac{1}{4}\left(\frac{t'}{\bar{t}}\right)^2}\\
=& \sqrt{\frac{2\pi}{\hbar}}g_{12}^{q\lambda\pm}\delta^{G,1/2}\left(\epsilon_1-\epsilon_2\pm\omega_{q\lambda}\right).
\end{aligned} \tag{3}$$

Since $\hat{G}^{q\lambda\pm,\dagger} = \sum_{34}G_{34}^{q\lambda\mp}\hat{c}_3^{\dagger}\hat{c}_4$,

$$\left[\hat{G}^{q\lambda\pm,\dagger}, \hat{c}_2^{\dagger}\hat{c}_1\right] = \sum_3\left(G_{32}^{q\lambda\mp}\hat{c}_3^{\dagger}\hat{c}_1 - G_{13}^{q\lambda\mp}\hat{c}_2^{\dagger}\hat{c}_3\right). \tag{4}$$

(The above equation is the same as Eq. A1 in PHYSICAL REVIEW B 90, 125140 (2014).)

To derive density matrix master equation of carrers, we assume $\hat{\rho} = \hat{\rho}^S \otimes \hat{\rho}^B$, where $\hat{\rho}^S$ is density matrix operator of carriers and $\hat{\rho}^B$ is that of phonons. For phonons, there are relations

$$\begin{aligned}
\mathrm{Tr_B}\left(\hat{\mathrm{b}}_{\mathrm{q}\lambda}\hat{\mathrm{b}}_{\mathrm{q'}\lambda'}\hat{\rho}^{\mathrm{B}}\right) =& \mathrm{Tr_B}\left(\hat{\mathrm{b}}^\dagger_{\mathrm{q}\lambda}\hat{\mathrm{b}}^\dagger_{\mathrm{q'}\lambda'}\hat{\rho}^{\mathrm{B}}\right) = 0,\\
Tr_B\left(\hat{b}_{q\lambda}\hat{b}^\dagger_{q'\lambda'}\hat{\rho}^B\right) =& \delta_{q,q'}\delta_{\lambda,\lambda'}n_{q\lambda},\\
Tr_B\left(\hat{b}^\dagger_{q\lambda}\hat{b}_{q'\lambda'}\hat{\rho}^B\right) =& \delta_{q,q'}\delta_{\lambda,\lambda'}\left(n_{q\lambda}+1\right),
\end{aligned}$$

Using the above relations, insert Eq. 3 and 4 into Eq. 2 and trace out phonon degrees of freedom,

$$\begin{aligned}
\frac{d\rho_{12}}{dt} =& \frac{1}{2}\mathrm{Tr}\mathrm{Tr}_B\left(\begin{array}{c}\sum_{q\lambda}\left(\left[\hat{G}^{q\lambda+,\dagger},\hat{c}^\dagger_2\hat{c}_1\right]\hat{b}_{q\lambda}+\left[\hat{G}^{q\lambda-,\dagger},\hat{c}^\dagger_2\hat{c}_1\right]\hat{b}^\dagger_{q\lambda}\right)\\ \times\sum_{q'\lambda'}\left(\hat{G}^{q\lambda+}\hat{b}^\dagger_{q'\lambda'}+\hat{G}^{q\lambda-}\hat{b}_{q'\lambda'}\right)\hat{\rho}^S\otimes\hat{\rho}^B\end{array}\right)+H.C.\\
=& \frac{1}{2}\mathrm{Tr}\sum_{q\lambda}\left(\begin{array}{c}\left[\hat{G}^{q\lambda+,\dagger},\hat{c}^\dagger_2\hat{c}_1\right]\hat{G}^{q\lambda+}\hat{\rho}^S\mathrm{Tr}_B\left(\hat{b}_{q\lambda}\hat{b}^\dagger_{q\lambda}\hat{\rho}^B\right)\\ +\left[\hat{G}^{q\lambda-,\dagger},\hat{c}^\dagger_2\hat{c}_1\right]\hat{G}^{q\lambda-}\hat{\rho}^S\mathrm{Tr}_B\left(\hat{b}^\dagger_{q\lambda}\hat{b}_{q'\lambda'}\hat{\rho}^B\right)\end{array}\right)+H.C.\\
=& \frac{1}{2}\mathrm{Tr}\sum_{q\lambda\pm}\left[\hat{G}^{q\lambda\pm,\dagger},\hat{c}^\dagger_2\hat{c}_1\right]\hat{G}^{q\lambda\pm}\hat{\rho}^S n^\pm_{q\lambda}+H.C.\\
=& \frac{1}{2}\mathrm{Tr}\sum_{345q\lambda\pm}\left(G^{q\lambda\mp}_{32}\hat{c}^\dagger_3\hat{c}_1-G^{q\lambda\mp}_{13}\hat{c}^\dagger_2\hat{c}_3\right)G^{q\lambda\pm}_{45}\hat{c}^\dagger_4\hat{c}_5\hat{\rho}^S n^\pm_{q\lambda}+H.C.\\
=& \frac{1}{2}\sum_{345q\lambda\pm}\left(G^{q\lambda\mp}_{32}h_{3145}-G^{q\lambda\mp}_{13}h_{2345}\right)G^{q\lambda\pm}_{45}n^\pm_{q\lambda}+H.C.,\\
h_{1234} =& \mathrm{Tr}\left(\hat{c}^\dagger_1\hat{c}_2\hat{c}^\dagger_3\hat{c}_4\hat{\rho}^S\right).
\end{aligned}$$

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

$$\begin{aligned}
h_{1234} \approx& \mathrm{Tr}\left(\hat{\rho}^S\hat{c}_2\hat{c}^\dagger_3\right)\mathrm{Tr}\left(\hat{\rho}^S\hat{c}^\dagger_1\hat{c}_4\right)\\
=& \mathrm{Tr}\left(\hat{\rho}^S\left(\delta_{23}-\hat{c}^\dagger_3\hat{c}_2\right)\right)\mathrm{Tr}\left(\hat{\rho}^S\hat{c}^\dagger_1\hat{c}_4\right)\\
=& \left(I-\rho\right)_{23}\rho_{41}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\frac{d\rho_{12}}{dt} =& \frac{1}{2}\sum_{345q\lambda\pm}\left(\left(I-\rho\right)_{14}G^{q\lambda\pm}_{45}\rho_{53}G^{q\lambda\mp}_{32}-G^{q\lambda\mp}_{13}\left(I-\rho\right)_{34}G^{q\lambda\pm}_{45}\rho_{52}\right)n^\pm_{q\lambda}+H.C.,\\
n^\pm_{q\lambda} =& n_{q\lambda}+0.5\pm0.5.
\end{aligned}$$

Define

$$\begin{aligned}
P_{1234} =& \sum_{q\lambda\pm}A^{q\lambda\pm}_{13}A^{q\lambda\pm,*}_{24},\\
A^{q\lambda\pm}_{13} =& G^{q\lambda\pm}_{13}\sqrt{n^\pm_{q\lambda}}.
\end{aligned}$$

We have

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

Indeed this is the same as Eq. 6 in PHYSICAL REVIEW B 92, 235423 (2015).