Electron-electron scattering implementation in DMD code

I. DENSITY MATRIX DYNAMICS WITH ELECTRON-ELECTRON SCATTERING

A. General master equaiton

According to Eq. (11.38), (11.51), (3.23) and (1.11) in thesis of R. Rosati, for electron-electron scattering (I also have derived it in another write-up Lindblad_ElecElec_derivation.pdf)

$$\begin{aligned}
\frac{\partial \rho_{12}}{\partial t}|_{ee} =& \frac{1}{2}\sum_{345}\left[(I-\rho)_{13}P_{32,45}\rho_{45} - (I-\rho_{45})P^{*}_{45,13}\rho_{32}\right] + H.C., \qquad (1)\\
P_{12,34} =& 2\sum_{56,78}(I-\rho)_{65}\mathscr{A}_{15,37}\mathscr{A}^{*}_{26,48}\rho_{78},\\
\mathscr{A}_{1234} =& \frac{1}{2}\left(A_{1234} - A_{1243}\right)\\
A_{1234} =& \frac{1}{2}\sqrt{\frac{2\pi}{\hbar}}\left(g_{1234}\delta^{1/2}_{1234} + g_{2143}\delta^{1/2}_{2143}\right),\\
g_{1234} =& \langle 1(r)|\langle 2(r')|V(r-r')|3(r)\rangle|4(r')\rangle\\
=& V(q_{13},\omega_{13})\delta_{k_1+k_2,k_3+k_4}\langle 1|3\rangle\langle 2|4\rangle,
\end{aligned}$$

where $\delta_{1234} = \delta^{G}(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$ is Gaussian function, $q_{13} = k_1 - k_3$ and $\omega_{13} = \epsilon_1 - \epsilon_3$. Moreover, since $V(q,\omega) = V(-q,-\omega)$, we have

$$A_{1234} = \sqrt{\frac{2\pi}{\hbar}}g_{1234}\delta^{1/2}_{1234}.$$

B. Direct and exchange parts

Expand the first term of Eq. 1,

$$\begin{aligned}
\sum_{345}(I-\rho)_{13}P_{32,45}\rho_{45} =& \frac{1}{2}\sum_{3456789}(I-\rho)_{13}(I-\rho)_{76}(A_{3648}-A_{3684})(A_{2759}-A_{2795})^{*}\rho_{89}\rho_{45}\\
=& \frac{1}{2}\sum_{3456789}(I-\rho)_{13}(I-\rho)_{76}\left[\begin{array}{c} A_{3648}A^{*}_{2759} + A_{3684}A^{*}_{2795}\\ -A_{3648}A^{*}_{2795} - A_{3684}A^{*}_{2759}\end{array}\right]\rho_{89}\rho_{45}.
\end{aligned}$$

By exchange the indices 8 and 4, and 9 and 5, we can easily find that

$$\begin{aligned}
\sum_{4589}A_{3648}A^{*}_{2759}\rho_{89}\rho_{45} &= \sum_{4589}A_{3684}A^{*}_{2795}\rho_{89}\rho_{45},\\
\sum_{4589}A_{3648}A^{*}_{2795}\rho_{89}\rho_{45} &= \sum_{4589}A_{3684}A^{*}_{2759}\rho_{89}\rho_{45}.
\end{aligned}$$

Therefore, we can define the direct and exchange parts of P as

$$\begin{aligned}
P^{d}_{1234} &= \sum_{56,78}(I-\rho)_{65}A_{1537}A^{*}_{2648}\rho_{78},\\
P^{ex}_{1234} &= \sum_{56,78}(I-\rho)_{65}A_{1537}A^{*}_{2684}\rho_{78}.
\end{aligned}$$

Obviously, the direct part is consistent with Eq. 99 of PRB 72, 125347 (2005) in semiclassical limit.

For two degenerate bands, energy will depends only on k point, so that (in static limit for screening)

$$A_{1234} = V\left(q_{13}\right)\delta_{k_1+k_2,k_3+k_4}\left\langle 1|3\right\rangle\left\langle 2|4\right\rangle\delta^{1/2}\left(\epsilon_{k_1}+\epsilon_{k_2}-\epsilon_{k_3}-\epsilon_{k_4}\right).$$

Suppose ρ is k-diagonal,

$$P^{d}_{12,34} = \left\{\begin{array}{c} V\left(q_{13}\right)^2\left\langle 1|3\right\rangle\left\langle 2|4\right\rangle\delta_{k_1+k_5,k_3+k_7}\left(\epsilon_{k_1}+\epsilon_{k_5}-\epsilon_{k_3}-\epsilon_{k_7}\right) \\ \times\mathrm{Tr}\left[\left\langle 8\delta_{k_8,k_7}|6\delta_{k_6,k_5}\right\rangle\left(I-\rho\right)^{k_5}_{65}\left\langle 5|7\right\rangle\rho^{k_7}_{n_7n_8}\right] \end{array}\right\}.$$

Therefore, our formula reduces to Eq. 9 in PRB 79, 125206 (2009) if neglecting the exchange contribution.

C. k-diagonal approximation

Approximate ρ is k-diagonal,

$$\begin{aligned}\frac{\partial\rho^{k_1}_{n_1n_2}}{\partial t}|_{ee} =& \frac{1}{2}\sum\left[\begin{array}{c}\left(I-\rho\right)^{k_1}_{n_1n_3}P^{k_1,k_4}_{n_1n_3,n_4n_5}\rho^{k_4}_{n_4n_5} \\ -\left(I-\rho\right)^{k_4}_{n_3n_4}P^{k_4,k_1,*}_{n_3n_4,n_1n_5}\rho^{k_1}_{n_5n_2}\end{array}\right]+H.C., \\ P^{k_1,k_3}_{n_1n_2,n_3n_4} =& \sum_{k_5n_5n_6n_7n_8}\left(I-\rho\right)^{k_5}_{n_6n_5}\mathscr{A}^{k_1k_5k_3k_7}_{n_1n_5n_3n_7}\mathscr{A}^{k_1k_5k_3k_7,*}_{n_2n_6n_4n_8}\rho^{k_7}_{n_7n_8}.\end{aligned}$$

Notice that $\mathscr{A}_{1234}=\mathscr{A}^{*}_{3412}$, we can define

$$\begin{aligned}Q^{k_1,k_3}_{n_1n_2,n_3n_4} =& P^{k_3,k_1,*}_{n_1n_2,n_3n_4} \\ =& \sum_{k_5n_5n_6n_7n_8}\left(I-\rho\right)^{k_5}_{n_5n_6}\mathscr{A}^{k_3k_5k_1k_7,*}_{n_1n_5n_3n_7}\mathscr{A}^{k_3k_5k_1k_7}_{n_2n_6n_4n_8}\rho^{k_7}_{n_8n_7} \\ =& \sum_{k_5n_5n_6n_7n_8}\left(I-\rho\right)^{k_5}_{n_5n_6}\mathscr{A}^{k_1k_7k_3k_5}_{n_3n_7n_1n_5}\mathscr{A}^{k_1k_7k_3k_5,*}_{n_4n_8n_2n_6}\rho^{k_7}_{n_8n_7} \\ =& 5\longleftrightarrow 7, 6\longleftrightarrow 8 \\ =& \sum_{k_7n_7n_8n_5n_6}\rho^{k_5}_{n_6n_5}\mathscr{A}^{k_1k_5k_3k_7}_{n_3n_5n_1n_7}\mathscr{A}^{k_1k_5k_3k_7,*}_{n_4n_6n_2n_8}\left(I-\rho\right)^{k_7}_{n_7n_8} \\ =& \sum_{k_5n_5n_6n_7n_8}\rho^{k_5}_{n_6n_5}\mathscr{A}^{k_1k_5k_3k_7}_{n_3n_5n_1n_7}\mathscr{A}^{k_1k_5k_3k_7,*}_{n_4n_6n_2n_8}\left(I-\rho\right)^{k_7}_{n_7n_8}.\end{aligned}$$

So $Q^{k_1,k_3}_{n_1n_2,n_3n_4} = P^{k_3,k_1,*}_{n_1n_2,n_3n_4} = P^{k_1,k_3}_{n_3n_4,n_1n_2}$ with ρ being replaced by $1-\rho$. The advantage of this definition is that we will only need matrices with $ik1 <= ik3$. Two additional things I want to mention are (i) in my implementation, I reordered the indices of matrices A or $\mathscr{A}$: $A_{1234}\rightarrow A_{1324}$ for doing matrix multiplications easier; (ii) matrix A is calculated without prefactor $\sqrt{2\pi/\hbar}$, I put this prefactor outside for $d\rho/dt$ instead.

II. SEMICLASSICAL LIMIT

A. Master equation

If $\rho=f$, we have

$$\frac{\partial f_1}{\partial t}|_{ee} = \sum_{2\neq 1}\left[\left(I-f_1\right)P_{11,22}f_2-\left(I-f_2\right)P_{22,11}f_1\right],$$

using the facts that $P_{11,22}$ is real and "2 = 1" term is zero. $P_{11,22}=2\sum_{34}\left(1-f_3\right)|\mathscr{A}_{1324}|^2f_4$. We can also separate P to two - the direct and exchange parts:

$$
\begin{aligned}
P^{d}_{1122} &= \sum_{34} (1-f_3)\,|A_{1324}|^2 f_4, \\
P^{ex}_{1122} &= \sum_{34} (1-f_3)\,A_{1324}A^{*}_{1342} f_4.
\end{aligned}
$$

Note that for two degenerate bands without spin-orbital coupling, for $P^{ex}_{1122} = \sum_{34} (1-f_3)\,A_{1324}A^{*}_{1342} f_4$, it is required that states 1, 2, 3 and 4 must have the same spin, while for $P^{d}_{1122} = \sum_{34} (1-f_3)\,|A_{1324}|^2 f_4$, it is require that 1 and 2 have the same spin and 3 and 4 have the same spin. Therefore, if sum does not run on spin, the prefactor of P^d will be double of the prefactor of P^{ex}.

B. ImΣ

Suppose the occupation of state "1" is perturbed from its equilibrium value by δf_1, i.e., $f_1 = f_1^{eq} + \delta f_1$, insert this into the above equation and linearize it,

$$
\frac{\partial f_1}{\partial t} = -\frac{2\pi}{N_k \hbar} \sum_{2\neq 1} \left[P_{11,22} f_2 + P_{22,11}(1-f_2)\right]\delta f_1.
$$

Notice that $\delta P_{11,22} = \frac{1}{N_k}\sum_3 (1-f_3)\,|\mathscr{A}_{1321}|^2 \delta f_1 - \frac{1}{N_k}\sum_3 |\mathscr{A}_{1123}|^2 f_3 \delta f_1$. Considering momentum concervation, k_3 will be fixed by k_1 and k_2, so that there will be only one k point contribute to $\delta P_{11,22}$. Therefore, $\delta P_{11,22}$ is actually zero if N_k goes to infinite. Therefore, $\delta P_{11,22}$ terms do not contribute to $\frac{\partial f_1}{\partial t}$.

Define carrier relaxation time τ_1 by $\frac{\partial f_1}{\partial t} = -\frac{\delta f_1}{\tau_1}$, we have

$$
\frac{1}{\tau_1} = \frac{2\pi}{N_k \hbar} \sum_{2\neq 1} \left[P_{11,22} f_2 + P_{22,11}(1-f_2)\right]. \tag{2}
$$

In my implementation, I have define $Q^{k_1 k_2}_{2211} = P^{k_2 k_1}_{2211}$ with f being replaced by $1-f$. Considering that the contribution of k pair (k_2, k_1) with $ik2 > ik1$ can be expressed by the quantities of (k_1, k_2),

$$
\begin{aligned}
\frac{1}{\tau_2} &= \frac{2\pi}{N_k \hbar} \sum_{ik1<ik2} \left[P^{k_2 k_1}_{2211} f_1 + Q^{k_2 k_1}_{1122}(1-f_1)\right] \\
&= \frac{2\pi}{N_k \hbar} \sum_{ik1<ik2} \left[Q^{k_1 k_2}_{2211} f_1 + P^{k_1 k_2}_{1122}(1-f_1)\right].
\end{aligned}
$$

C. Connection to ImΣ from finite temperature GW

Neglecting the exchange part, insert P^d into Eq. 2,

$$
\frac{1}{\tau_1} = \frac{2\pi}{N_k \hbar} \sum_{2\neq 1,34} |A_{1324}|^2 \left[f_2 f_4 (1-f_3) + (1-f_2) f_3 (1-f_4)\right].
$$

Considering the energy conservation $\omega = \epsilon_1 - \epsilon_2 = \epsilon_4 - \epsilon_3$, we have the relations $n(\omega) = \frac{f_1(1-f_2)}{f_2 - f_1}$ and

$$\begin{aligned}
f_2 f_4 (1-f_3) =& f_2 n(\omega)(f_3-f_4) \\
=& f_2 \frac{f_1(1-f_2)}{f_2-f_1}(f_3-f_4) \\
=& (n_1+1-f_2) f_1 (f_3-f_4), \\
(1-f_2) f_3 (1-f_4) =& (1-f_2) n(-\omega)(f_4-f_3) \\
=& (1-f_2) \frac{f_2(1-f_1)}{f_1-f_2}(f_4-f_3) \\
=& (n_1+1-f_2)(1-f_1)(f_3-f_4).
\end{aligned}$$

Therefore,

$$\frac{1}{\tau_1} = \frac{2\pi}{N_k \hbar} \sum_{2\neq 1,34} |A_{1324}|^2 (n_1+1-f_2)(f_3-f_4).$$

The above formula is equivalent to $\mathrm{Im}\Sigma$ given in Eq. 8 in PRB 66, 085116 (2002) based on finite-temperature GW at least in the limit $G = G' = 0$.