Supplementary material for manuscript "Achieving the Scaling Limit for Nonequilibrium Green Functions Simulations"

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This supplement contains additional information on 1.) the time-evolution operators $\mathcal{U}(t,t')$, and 2.) the derivation of the G1–G2 formulas in GW approximation.

1 Time-evolution operators

The two-particle time-evolution operator appearing in Eq. (8) of the manuscript is defined as

$$\mathcal{U}^{(2)}_{npab}(t,t') \quad := \quad \mathcal{U}_{na}(t,t')\mathcal{U}_{pb}(t,t')\,, \tag{S1}$$

where $\mathcal{U}(t,t')$ obeys a Schrödinger equation,

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}_{na}(t,t') - \sum_b h^{\mathrm{HF}}_{nb}(t)\mathcal{U}_{ba}(t,t') = 0\,, \tag{S2}$$
$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t'}\mathcal{U}_{na}(t,t') + \sum_b \mathcal{U}_{nb}(t,t')h^{\mathrm{HF}}_{ba}(t') = 0\,.$$

Note that the retarded/advanced propagators of Eq. (6) of the main text are related to $\mathcal{U}$ via

$$\mathcal{U}_{ij}(t,t') = G^{\mathrm{R}}_{ij}(t,t') - G^{\mathrm{A}}_{ij}(t,t')\,. \tag{S3}$$

2 Derivation of the G1–G2 scheme for GW selfenergies

In the GW approximation, the selfenergy has the form [1],

$$\Sigma^{\gtrless}_{ij}(t,t') = \mathrm{i}\hbar\sum_{kl} W^{\gtrless}_{ilkj}(t,t')G^{\gtrless}_{kl}(t,t')\,, \tag{S4}$$

where, W is the dynamically screened interaction, which can be expressed in terms of the inverse dielectric function [2],

$$W^{\gtrless}_{ijkl}(t,t') = \sum_{mn} w_{imkn}(t)\varepsilon^{-1,\gtrless}_{mjnl}(t,t')\,. \tag{S5}$$

The collision integral in Eq. (2) of the manuscript then becomes,

$$I_{ij}(t) = \sum_k \int_{t_0}^t \mathrm{d}\bar{t}\left[\Sigma^{>}_{ik}(t,\bar{t})G^{<}_{kj}(\bar{t},t) - \Sigma^{<}_{ik}(t,\bar{t})G^{>}_{kj}(\bar{t},t)\right] \tag{S6}$$
$$= \mathrm{i}\hbar\sum_{klmnp} w_{imkn}(t)\int_{t_0}^t \mathrm{d}\bar{t}\left[\varepsilon^{-1,>}_{mlnp}(t,\bar{t})G^{>}_{kl}(t,\bar{t})G^{<}_{pj}(\bar{t},t) - \varepsilon^{-1,<}_{mlnp}(t,\bar{t})G^{<}_{kl}(t,\bar{t})G^{>}_{pj}(\bar{t},t)\right]. \tag{S7}$$

With Eq. (4) of the main text one finds the following expression for the time-diagonal element of the two-particle Green function,

$$\mathcal{G}_{npjm}(t) = \pm\sum_{kl}\int_{t_0}^t \mathrm{d}\bar{t}\left[\varepsilon^{-1,>}_{mkpl}(t,\bar{t})G^{>}_{nk}(t,\bar{t})G^{<}_{lj}(\bar{t},t) - \varepsilon^{-1,<}_{mkpl}(t,\bar{t})G^{<}_{nk}(t,\bar{t})G^{>}_{lj}(\bar{t},t)\right]. \tag{S8}$$

By construction, the interaction tensors obey the following symmetries [2],

$$w_{ijkl}(t) = w_{jilk}(t)\,, \tag{S9}$$

$$W^{\gtrless}_{ijkl}(t,t') = W^{\lessgtr}_{jilk}(t',t)\,. \tag{S10}$$

Using that, the dynamical screening is included in ε^{-1} via the recursive equation,

$$\begin{aligned}\varepsilon^{-1,\gtrless}_{ijkl}(t,t') =& \pm \mathrm{i}\hbar \sum_{mn} w_{mjnl}(t') G^{\gtrless}_{km}(t,t') G^{\lessgtr}_{ni}(t',t) \\ &\pm \mathrm{i}\hbar \sum_{mnpq} w_{jplq}(t') \Bigg[\int_{t_0}^{t} \mathrm{d}\bar{t} \left(G^{>}_{km}(t,\bar{t}) G^{<}_{ni}(\bar{t},t) - G^{<}_{km}(t,\bar{t}) G^{>}_{ni}(\bar{t},t) \right) \varepsilon^{-1,\lessgtr}_{pmqn}(t',\bar{t}) \\ &+ \int_{t_0}^{t'} \mathrm{d}\bar{t}\, G^{\gtrless}_{km}(t,\bar{t}) G^{\lessgtr}_{ni}(\bar{t},t) \left(\varepsilon^{-1,>}_{pmqn}(t',\bar{t}) - \varepsilon^{-1,<}_{pmqn}(t',\bar{t}) \right) \Bigg]\,.\end{aligned} \tag{S11}$$

Applying the HF-GKBA [cf. Eq. (6) and (7) of the main text] leads to the following expressions for $\mathcal{G}^{\mathrm{GKBA}}$,

$$\mathcal{G}^{\mathrm{GKBA}}_{npjm}(t) = \pm \sum_{klrs} \int_{t_0}^{t} \mathrm{d}\bar{t}\, \mathcal{U}_{nr}(t,\bar{t}) \left[\varepsilon^{-1,>}_{mkpl}(t,\bar{t}) n^{>}_{rk}(\bar{t}) n^{<}_{ls}(\bar{t}) - \varepsilon^{-1,<}_{mkpl}(t,\bar{t}) n^{<}_{rk}(\bar{t}) n^{>}_{ls}(\bar{t}) \right] \mathcal{U}_{sj}(\bar{t},t)\,, \tag{S12}$$

as well as for $\varepsilon^{-1}_{\mathrm{GKBA}} \to \varepsilon^{-1}$,

$$\begin{aligned}&\varepsilon^{-1,\gtrless}_{ijkl}(t \geq t') \\ &= \pm \mathrm{i}\hbar \sum_{mnpq} w_{mjnl}(t') \mathcal{U}_{kp}(t,t') n^{\gtrless}_{pm}(t') n^{\lessgtr}_{nq}(t') \mathcal{U}_{qi}(t',t) \\ &\pm \mathrm{i}\hbar \sum_{mnpqab} w_{jalb}(t') \Bigg[\int_{t_0}^{t} \mathrm{d}\bar{t}\, \mathcal{U}_{kp}(t,\bar{t}) \left(n^{>}_{pm}(\bar{t}) n^{<}_{nq}(\bar{t}) - n^{<}_{pm}(\bar{t}) n^{>}_{nq}(\bar{t}) \right) \mathcal{U}_{qi}(\bar{t},t) \varepsilon^{-1,\lessgtr}_{ambn}(t',\bar{t}) \\ &+ \int_{t_0}^{t'} \mathrm{d}\bar{t}\, \mathcal{U}_{kp}(t,\bar{t}) n^{\gtrless}_{pm}(\bar{t}) n^{\lessgtr}_{nq}(\bar{t}) \mathcal{U}_{qi}(\bar{t},t) \left(\varepsilon^{-1,>}_{ambn}(t',\bar{t}) - \varepsilon^{-1,<}_{ambn}(t',\bar{t}) \right) \Bigg]\,,\end{aligned} \tag{S13}$$

where $\mathcal{U}$ is given by Eq. (S2). With Eq. (S13), also the derivative of ε^{-1} is readily found,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} \varepsilon^{-1,\gtrless}_{ijkl}(t \geq t') =& \frac{1}{\mathrm{i}\hbar} \sum_{m} h^{\mathrm{HF}}_{km}(t) \varepsilon^{-1,\gtrless}_{ijml}(t \geq t') - \frac{1}{\mathrm{i}\hbar} \sum_{m} \varepsilon^{-1,\gtrless}_{mjkl}(t \geq t') h^{\mathrm{HF}}_{mi}(t) \\ &\pm \frac{1}{\mathrm{i}\hbar} \sum_{mnab} w_{manb}(t) \left[n^{>}_{km}(t) n^{<}_{ni}(t) - n^{<}_{km}(t) n^{>}_{ni}(t) \right] \varepsilon^{-1,\gtrless}_{ajbl}(t \geq t')\,.\end{aligned} \tag{S14}$$

Finally, the derivative of $\mathcal{G}^{\mathrm{GKBA}}$ can be set up,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{G}^{\mathrm{GKBA}}_{npjm}(t) =& \pm \frac{1}{(\mathrm{i}\hbar)^2} \sum_{kl} \left[\varepsilon^{-1,>}_{mkpl}(t,t) n^{>}_{nk}(t) n^{<}_{lj}(t) - \varepsilon^{-1,<}_{mkpl}(t,t) n^{<}_{nk}(t) n^{>}_{lj}(t) \right] \\ &\pm \sum_{klrs} \int_{t_0}^{t} \mathrm{d}\bar{t} \left(\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{U}_{nr}(t,\bar{t}) \right) \left[\varepsilon^{-1,>}_{mkpl}(t,\bar{t}) n^{>}_{rk}(\bar{t}) n^{<}_{ls}(\bar{t}) - \varepsilon^{-1,<}_{mkpl}(t,\bar{t}) n^{<}_{rk}(\bar{t}) n^{>}_{ls}(\bar{t}) \right] \mathcal{U}_{sj}(\bar{t},t) \\ &\pm \sum_{klrs} \int_{t_0}^{t} \mathrm{d}\bar{t}\, \mathcal{U}_{nr}(t,\bar{t}) \left[\left(\frac{\mathrm{d}}{\mathrm{d}t} \varepsilon^{-1,>}_{mkpl}(t,\bar{t}) \right) n^{>}_{rk}(\bar{t}) n^{<}_{ls}(\bar{t}) - \left(\frac{\mathrm{d}}{\mathrm{d}t} \varepsilon^{-1,<}_{mkpl}(t,\bar{t}) \right) n^{<}_{rk}(\bar{t}) n^{>}_{ls}(\bar{t}) \right] \mathcal{U}_{sj}(\bar{t},t) \\ &\pm \sum_{klrs} \int_{t_0}^{t} \mathrm{d}\bar{t}\, \mathcal{U}_{nr}(t,\bar{t}) \left[\varepsilon^{-1,>}_{mkpl}(t,\bar{t}) n^{>}_{rk}(\bar{t}) n^{<}_{ls}(\bar{t}) - \varepsilon^{-1,<}_{mkpl}(t,\bar{t}) n^{<}_{rk}(\bar{t}) n^{>}_{ls}(\bar{t}) \right] \left(\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{U}_{sj}(\bar{t},t) \right)\,.\end{aligned} \tag{S15}$$

With the introduction of the following auxiliary function [3],

$$P_{npjm}(t) = \pm \sum_{cd} \left[n^{>}_{pd}(t) n^{<}_{cm}(t) - n^{<}_{pd}(t) n^{>}_{cm}(t) \right] \sum_{rs} w_{drcs}(t) \mathcal{G}^{\mathrm{GKBA}}_{nsjr}(t)\,, \tag{S16}$$

Eq. (S15) can eventually be exactly brought to the following time-local form that is used in the G1–G2 scheme,

$$\begin{aligned}&\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{G}^{\mathrm{GKBA}}_{npjm}(t) - \left[h^{(2),\mathrm{HF}}, \mathcal{G}^{\mathrm{GKBA}} \right]_{npjm}(t) \\ &= \frac{1}{(\mathrm{i}\hbar)^2} \sum_{kqrs} w_{qrsk}(t) \left[n^{>}_{nq}(t) n^{>}_{pr}(t) n^{<}_{sj}(t) n^{<}_{km}(t) - n^{<}_{nq}(t) n^{<}_{pr}(t) n^{>}_{sj}(t) n^{>}_{km}(t) \right] \\ &+ P_{npjm}(t) + P_{pnmj}(t)\,.\end{aligned} \tag{S17}$$

References

[1] N. Schlünzen, S. Hermanns, M. Scharnke, and M. Bonitz, Ultrafast dynamics of strongly correlated fermions – Nonequilibrium Green functions and selfenergy approximations, J. Phys. Condens. Matter **32** (10), 103001 (2020)

[2] G. Stefanucci and R. van Leeuwen, *Nonequilibrium Many-Body Theory of Quantum Systems*, (Cambridge University Press, Cambridge, 2013)

[3] M. Bonitz, *Quantum Kinetic Theory*, 2nd ed. (Springer, Cham, 2016)