Achieving the Scaling Limit for Nonequilibrium Green Functions Simulations

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The dynamics of strongly correlated fermions following an external excitation reveals extremely rich collective quantum effects. Examples are fermionic atoms in optical lattices, electrons in correlated materials, and dense quantum plasmas. Presently, the only quantum-dynamics approach that rigorously describes these processes in two and three dimensions is the nonequilibrium Green functions (NEGF) method. However, NEGF simulations are computationally expensive due to their $T^3$ scaling with the simulation duration $T$. Recently, $T^2$ scaling was achieved with the generalized Kadanoff-Baym ansatz (GKBA), for second-order Born (SOA) selfenergies, which has substantially extended the scope of NEGF simulations. Here we demonstrate that GKBA-NEGF simulations can be performed with order $T^1$ scaling, both for SOA and GW selfenergies, and point out the remarkable capabilities of this approach.

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Strongly correlated fermion systems are attracting increasing interest in many fields including dense plasmas [1,2], warm dense matter [3,4], strongly correlated materials [5,6], ultracold atoms [7,8], and atoms and molecules in strong radiation fields [9,10]. Of particular relevance are the relaxation phenomena that occur following an external excitation such as a rapid change ("quench") of the confinement or the interaction strength, the impact of charged particles [11,12], or the photoionization of atoms by lasers or free-electron lasers [13,14]. Many theoretical approaches to the dynamics of strongly correlated fermions are limited either to one-dimensional systems (density-matrix renormalization-group simulations, DMRG) or short times (quantum Monte Carlo). The first quantum simulations of the expansion of correlated fermions in two and three dimensions were recently achieved using nonequilibrium Green functions (NEGF) [8] and exhibited very good agreement with experiments. The high accuracy of NEGF simulations was also demonstrated by comparison to DMRG [15]. However, these NEGF simulations are hampered by an unfavorable scaling with the simulation duration according to $T^3$ resulting from the two-time structure of the NEGF and the memory effects in the collision integral (see below).

This behavior can be relieved by applying the generalized Kadanoff-Baym ansatz (GKBA) [16,17], which reduces the dynamics of the NEGF $G(t, t')$ to propagation along the time diagonal $t = t'$. It could be demonstrated that, indeed, the expected improvement of the scaling, $N_t^3 \rightarrow N_t^2$ (in the following we will use the number of discretization time steps $N_t = T/\Delta t$, can be achieved in practice for the selfenergy in the second-order Born approximation (SOA) [18,19] where initial correlation effects can be treated even more efficiently [20,21]. It could further be shown that this approximation, in many cases, does not lead to a loss of accuracy [10,15,22]. For these reasons, NEGF simulations using the GKBA with Hartree-Fock propagators (HF-GKBA) [cf. Eqs. (6) and (7) below] have become a powerful tool for studying the quantum dynamics in many fields, including optically excited semiconductors [23–25], excitonic insulators [26], quantum transport and molecular junctions [27,28], laser-excited plasmas [29,30] and atoms [10,13], strongly correlated electrons [22], and fermionic atoms in optical lattices [15,31]. In recent years, significant effort was devoted to improve the GKBA, see, e.g., Refs. [17,20–22,27,32–34]. Nevertheless, the quadratic scaling with $N_t$ still makes the approach much less efficient than competing methods that scale linearly with $N_t$, such as molecular dynamics, fluid theory, time-dependent density-functional theory within the adiabatic approximation, or Boltzmann-type (Markovian) kinetic equations.

In this Letter we demonstrate that the same linear scaling with $N_t$, which is the ultimate limit in time-dependent simulations, can be achieved for NEGF simulations within the HF-GKBA. This allows for unprecedented long simulations as well as for high-quality energy spectra that are computed via Fourier transformation of time-dependent quantities, see, e.g., Refs. [35–37]. We demonstrate this efficiency gain, compared to the original HF-GKBA, for finite Hubbard clusters and predict an even stronger gain for a basis in which the Green function and selfenergy are diagonal, such as for spatially homogeneous systems. Moreover, our approach allows one to compute additional quantities that are not directly accessible in standard NEGF schemes, such as the time-dependent pair-distribution function, the static and dynamic structure factor, and various correlation functions. Finally, we prove that linear scaling can be achieved also for more advanced
selfenergies, such as GW, where all existing schemes scale as $N^4$.

Theory.—We consider a general many-particle system with the Hamiltonian

$$H(t) = \sum_{ij} h_{ij}(t) \hat{c}_i^\dagger \hat{c}_j + \frac{1}{2} \sum_{ijkl} w_{ijkl}(t) \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l,$$

where the replacement $k \leftrightarrow s$ is used to match Eq. (3). Comparing Eq. (4) with the first equation of the Martin-Schwinger hierarchy for the many-particle Green functions [39] reveals that $\mathcal{G}(t)$ is nothing but the time-diagonal element of the two-particle Green function, and Eq. (5) is its explicit form in the second-Born approximation [40]. Next, we introduce the GKBA [16,19] (summation over initial correlations, by supplementing Eq. (10) with an

containing a single-particle contribution $\hat{h}$ and a pair interaction $\hat{w}$. The matrix elements are computed with an orthonormal system of single-particle orbitals $|i\rangle$. The creation ($\hat{c}_i^\dagger$) and annihilation ($\hat{c}_i$) operators of particles in state $|i\rangle$ define the one-body nonequilibrium Green functions (correlation functions; here and below “$\pm$” refers to bosons and fermions) $G_{ij}^\pm(t, t') = \pm (i/\hbar) \langle \hat{c}_i^\dagger(t') \hat{c}_j(t) \rangle$ and $G_{ij}^\mp(t, t') = (i/\hbar) \langle \hat{c}_j(t') \hat{c}_i(t) \rangle$, where the averaging is performed with the correlated unperturbed density operator of the system. The response of the system (1) to an external excitation is described by the Keldysh-Kadanoff-Baym equations (KBE) on the time diagonal [16,19] where the Green function reduces to the single-particle density matrix, $\pm i \hbar \mathcal{G}_{ij}^\pm(t, t) = n_{ij}(t)$,

$$\frac{\partial n_{ij}(t)}{\partial t} - \frac{1}{\hbar} \sum_k \mathcal{H}_{ik}(t) n_{kj}(t) = \pm [I + I^\dagger] n_{ij}(t),$$

with a mean-field Hamiltonian $\mathcal{H}$. Here $I$ is the collision integral that takes into account interaction effects beyond Hartree-Fock, including scattering and dissipation, which we will treat in leading order, i.e., within the SOA [19,38]:

$$I_{ij}(t) = (i\hbar)^2 \sum_{mnp} w_{mnp}(t) \int_0^t d\tau \mathcal{W}_{qrsk}(\tau)$$

$$\times \left[ G_{mq}^\pm(\tau, \bar{t}) G_{pr}^\pm(\bar{t}, \tau) G_{sk}^\pm(\bar{t}, t) G_{ij}^\pm(t, \tau) - (\leftrightarrow \leftrightarrow) \right],$$

where we defined $w_{qrsj}^\pm = w_{qrjs}^\pm = \pm w_{qrjs}^\pm$. Clearly, the computational effort to solve Eqs. (2) and (3) scales with the number of time steps as $N^3$.

We now demonstrate that, in the HF-GKBA approximation, Eqs. (2) and (3) can be reformulated such that the effort is reduced to $N^2$ scaling. First, we introduce an auxiliary four-index function $\mathcal{G}$,

$$I_{ij}(t) = \pm i \hbar \sum_{mnp} w_{mnp}(t) \mathcal{G}_{npjm}(t),$$

$$\mathcal{G}_{npjm}(t) = i \hbar \sum_{kqrs} \int_0^t d\tau \mathcal{W}_{qrsk}(\tau)$$

$$\times \left[ G_{mq}^\pm(\tau, \bar{t}) G_{pr}^\pm(\bar{t}, \tau) G_{sk}^\pm(\bar{t}, t) G_{ij}^\pm(t, \tau) - (\leftrightarrow \leftrightarrow) \right].$$

Finally, we remove the time integral in Eq. (8) by differentiating with respect to time which yields

$$i \hbar \frac{d}{dt} \mathcal{G}_{npjm}(t) - [h^{(2)}_{\text{HF}}, \mathcal{G}_{npjm}](t)$$

$$= \frac{i}{(i\hbar)^2} \sum_{qrs} \mathcal{W}_{qrsk}(\tau) \mathcal{G}_{npjm}(t),$$

where $h^{(2)}_{ijkl}(t) = \delta_{jk} h_{ik}(t) + \delta_{ij} h_{kl}(t)$. With this we have shown that NEGF theory within the HF-GKBA can be brought to a memory-less form (10) which, indeed, changes the scaling from quadratic to linear with $N$. This was achieved by introducing the two-particle Green function on the time diagonal $\mathcal{G}$ and by solving coupled time-local equations for $\mathcal{G}(t, t)$ and $\mathcal{G}(t)$. We, therefore, will refer to this as the “G1–G2” scheme. In fact, the one-to-one correspondence of NEGF theory within the HF-GKBA to time-local equations has been observed before [18,42]. In Ref. [42] it was also shown how to include arbitrary initial correlations, by supplementing Eq. (10) with an initial value, $\mathcal{G}_{\text{KBA}}(t_0) = \mathcal{G}_0$. In Eq. (8) this gives rise to an additional homogeneous solution that leads to an additional collision integral in the time-diagonal KBE (2), in agreement with recent results [20,21].
TABLE I. Scaling of the CPU time with the number of time steps $N_t$ and basis dimension $N_b$ of the traditional non-Markovian HF-GKBA and the present time-local scheme (G1–G2), for three relevant basis sets, for SOA and GW selfenergies.

| Basis and pair potential | SOA | GW |
|--------------------------|-----|-----|
| General: $w_{ij}$        | $O(N_b^3 N_t^2)$ | $O(N_b^3 N_t^2)$ |
| Hubbard: $U$             | $O(N_b^3 N_t^2)$ | $O(N_b^3 N_t^2)$ |
| Jellium: $v_{ij}$        | $O(N_b^5 N_t^2)$ | $O(N_b^5 N_t^2)$ |

In the following we analyze the G1–G2 scheme more in detail. One readily confirms that the CPU time required to solve Eq. (10), for a general basis of dimension $N_b$, scales as $O(N_b^3 N_t^2)$ [43]. In contrast, the original HF-GKBA scales as $O(N_b^5 N_t^2)$ and, thus, a dramatic speedup is expected, for any $N_b$ [45]. At the same time, for many practical applications optimized basis sets are being used for which the scaling of both schemes has to be established separately. We, therefore, consider below two representative examples—the Hubbard basis and the uniform electron gas. The scaling for all three cases is summarized in Table I.

Hubbard basis.—The (Fermi-)Hubbard model is a key system in the theory of strongly correlated electrons in solids, see, e.g., Refs. [46,47], and it is being directly realized with fermionic atoms in optical lattices, see, e.g., Refs. [7,48,49]. It is defined by the Hubbard Hamiltonian

$$\hat{H}(t) = -J \sum_{\langle i,j \rangle} \sum_{\alpha} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\alpha} + U(t) \sum_{i} \hat{\hat{n}}_i^\uparrow \hat{\hat{n}}_i^\downarrow,$$

which includes hopping processes between nearest-neighbor sites $(i,j)$ with amplitude $J$ and an on-site interaction $U$, and $\alpha$ labels the spin projection. The integral (4) reads,

$$I_{ij}^{(\uparrow)}(t) = -i\hbar U(t) G_{ij}^{(\uparrow)}(t),$$

and the equation of motion (10) for $G$ simplifies to [50]

$$i\hbar \frac{d}{dt} G_{npmj}^{(\uparrow)}(t) = \left[ \hat{h}_{nmj}^{(\uparrow)}(1)G_{ij}^{(\uparrow)}(t) - \left[ \hat{h}_{nmj}^{(\uparrow)}(t) \right]_{n'p'mj}(t) \right] = \left( i\hbar \right)^2 \sum_k U(t) \times \left[ \hat{G}_{nk}^{(\uparrow)}(t,t)G_{pk}^{(\uparrow)}(t,t)G_{kj}^{(\uparrow)}(t,t)G_{km}^{(\uparrow)}(t,t)\right] = \cdots.$$
The Hamiltonian of the UEG in second quantization reads [3]

\[ \hat{H}(t) = \sum_{\alpha} \frac{\hbar^2}{2m} \hat{\phi}_\alpha^\dagger \hat{\phi}_\alpha + \sum_{pq\alpha} v_{pq} \hat{\phi}_p^\dagger \hat{\phi}_q^\dagger \hat{\phi}_q \hat{\phi}_p, \]

with the Coulomb matrix element \( v_{pq} = (4\pi e^2/|q|^2) \). The integral (4) becomes

\[ i\hbar \frac{d}{dt} G_{pq}^{\sigma\sigma}(t) = G_{pq}^{\sigma\sigma}(t) (h_{pp}^{\text{HF}} + h_{pp+q,q+q}^{\text{HF}} - h_{pp}^{\text{HF}} - h_{pp+q,q+q}^{\text{HF}}) \]

\[ = (i\hbar)^2 \{ v_{pq}(t) \delta_{\sigma,\sigma} v_{q-p-q} \} \times \{ G_{pq}^{\sigma\sigma}(t,t) G_{p+q,q+q}^{\sigma\sigma}(t,t) G_{q+q+q,q}^{\sigma\sigma}(t,t) - (\leftrightarrow) \}. \]

Interestingly, Eq. (12) scales as \( O(N_3^3 N_1^2) \) vs \( O(N_3^4 N_1^2) \), for the standard HF-GKBA, cf. Table I, and the G1–G2 scheme brings about a dramatic acceleration, independent of basis size.

**Spectra and two-particle observables.**—In addition to accelerating the time evolution, the G1–G2 scheme gives also access to more accurate spectral information. While within the HF-GKBA spectral functions are treated on the Hartree-Fock level, correlation effects in energy spectra can be recovered by investigating the temporal response of the system to a short weak external excitation (linear response), see, e.g., Refs. [35–37]. This is demonstrated in Fig. 3 where the energy spectrum is retrieved via Fourier transform of the density evolution in a Hubbard system. Here the long propagation time enabled by the G1–G2 scheme allows us to resolve correlation effects in the spectra, in particular broadening and shift of peaks as well as the emergence of new states at high energies.

Furthermore, the G1–G2 scheme allows one to compute several quantities that are difficult or even impossible to access within standard NEGF schemes. This includes the nonequilibrium pair-correlation function (PDF) \( g(r_1, \sigma_1; r_2, \sigma_2; t) \) and its Fourier transform—the static structure factor. Moreover, dynamic quantities, such as the density- and spin-correlation functions or velocity-autocorrelation functions and the related transport coefficients—the dynamic structure factor, diffusion and absorption coefficients, and the dynamical conductivity within and beyond linear response—are becoming directly accessible. In Fig. 4, we show, as an example, the time evolution of the pair-correlation function (PCF, i.e., the correlated part or the PDF) relative to site 1, \( \delta g_{1,11}(t) \), for a spatially homogeneous spin-symmetric 20-site Hubbard chain following an interaction quench \( U/J = 0 \rightarrow 2 \) at \( t = 0 \). Sign-alternating correlations emerge rapidly and approach the correlated ground state (GS). Inset shows \( \delta g_{1,11}(t) \), for \( U/J = 2 \), computed via adiabatic switching. The dashed line corresponds to data in the main figure.
different basis sets in Table I (details are given in Ref. [41], and similar results are observed for $T$-matrix selfenergies). The huge computational advantage brought about by G1–G2-GW simulations becomes evident also in Fig. 2; even for Hubbard systems the G1–G2 scheme is advantageous, except for very short simulations. This indicates that a large class of problems is now becoming accessible for accurate NEGF simulations that had remained out of reach so far.

Summary and discussion.—We have implemented an alternative approach to NEGF simulations within the HF-GKBA that is memory-free and achieves the ultimate limit of linear scaling with the propagation duration $T$, as opposed to the common HF-GKBA approach with SOA (GW) selfenergies that is of order $T^2$ ($T^3$). This is achieved by solving coupled time-local equations for $G(t, t)$ and the time-diagonal two-particle Green function $G(t)$. With this G1–G2 scheme we also established a direct link to the independent reduced-density-matrix (RDM) approach that has become popular in recent years in many fields, see, e.g., Refs. [42,55–60]. Applying our derivation allows one to identify those RDM approximations that are equivalent to common selfenergies in NEGF theory what enables one to make use of the full power of Feynman diagrams in RDM theory. We expect that the demonstrated astonishing scaling of the G1–G2 scheme will make highly accurate NEGF simulations of many nonequilibrium processes such as in laser-excited correlated systems achievable.

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