The non-equilibrium Green function approach to inhomogeneous quantum many-body systems using the generalized Kadanoff–Baym ansatz

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Abstract
In the non-equilibrium Green function calculations, the use of the generalized Kadanoff–Baym ansatz (GKBA) allows for a simple approximate reconstruction of the two-time Green function from its time-diagonal value. With this, a drastic reduction of the computational needs is achieved in time-dependent calculations, making longer time propagation possible and more complex systems accessible. This paper gives credit to the GKBA that was introduced 25 years ago. After a detailed derivation of the GKBA, we recall its application to homogeneous systems and show how to extend it to strongly correlated, inhomogeneous systems. As a proof of concept, we present the results for a two-electron quantum well, where the correct treatment of the correlated electron dynamics is crucial for a correct description of the equilibrium and dynamic properties.

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(Some figures may appear in color only in the online journal)

1. Introduction
For the time-dependent description of non-equilibrium processes, the method of the non-equilibrium Green functions (NEGF) has been widely used, since it allows for a self-consistent treatment of electron–electron correlations, non-perturbative inclusion of external fields and systematic approximations via Feynman diagrams. The central quantity is the one-particle, two-time Green function, \( G(t, t') \), the time evolution of which is governed by the Keldysh–Kadanoff–Baym equations (KBE) [1]. To numerically solve these equations, a self-energy is introduced, which can be determined by many-body perturbation theory and which leads to a closed equation for \( G \). As a great advantage, it reduces the amount of needed memory to a quadratic scaling with propagation length, since for the determination of \( G(T, T') \) for time arguments \( T \leq T' \) only a knowledge of \( G(t = t') \) for all \( t \leq T \) is sufficient. This simplification has made numerous applications to spatially homogeneous systems possible. Here, we demonstrate that the GKBA may be equally successful in computing the behavior of finite inhomogeneous systems.

This restriction can be drastically alleviated by the introduction of a further approximation, the generalized Kadanoff–Baym ansatz (GKBA), which was introduced by Lipavsky et al some 25 years ago [3]. With the GKBA, for each time propagation step, the two-time Green function is reconstructed from its time-diagonal value: \( G(t, t') = F_{\text{GKBA}}[G(t = t')] \). As a great advantage, it reduces the amount of needed memory to a quadratic scaling with propagation length, since for the determination of \( G(T, T') \) for time arguments \( T \leq T' \) only a knowledge of \( G(t = t') \) for all \( t \leq T \) is sufficient. This simplification has made numerous applications to spatially homogeneous systems possible. Here, we demonstrate that the GKBA may be equally successful in computing the behavior of finite inhomogeneous systems.

This paper is organized as follows. After briefly recalling the basics of the NEGF formalism, we derive and list in detail the properties of the GKBA. Thereafter, we give a brief overview of its application to homogeneous systems in...
different fields of physics. In a third part, we extend the GKBA to inhomogeneous systems, using the technique of adiabatic switching [4] to correctly obtain the associated correlated initial state. Finally, the applicability of the GKBA to the spectrum of a two-electron quantum well is tested at different coupling strengths.

2. Theory

2.1. The non-equilibrium Green functions

To describe correlation effects and excitations in quantum many-particle systems, we chose the NEGF approach, as it allows for a systematic inclusion of correlations by diagrammatic expansions. In contrast to density matrix-based schemes, the Green functions method additionally easily offers direct access to dynamical spectral information as well as particle removal and addition energies. The main quantity is the one-particle Green function, defined as (we set $\hbar = 1$)

$$G(t, t') = -i\langle \tau_c (\Psi(t)\Psi^\dagger(t')) \rangle,$$

(1)

where the brackets denote thermodynamic averaging and $\tau_c$ is the time ordering operator on the Schwinger–Keldysh contour $C$ [5], on which $t$ and $t'$ are defined. $\Psi^{(i)}$ denotes a one-particle annihilation (creation) operator in a one-particle basis in second quantization. The equations of motion for $G$ are the KBE

$$[i\partial_t - h(t)] G(t, t') = \delta(t - t') + \int_C d\tau W(t, \tau) G^{(2)}(\tau; t, t'),$$

$$[-i\partial_{t'} - h(t')] G(t, t') = \delta(t - t') + \int_C d\tau W(t', \tau) G^{(2)}(\tau; t', t'),$$

(2)

where $h$ denotes the one-particle Hamiltonian, $G^{(2)}(\tau; t', t'') = -\langle \tau_c [\Psi(t)\Psi(t')\Psi^\dagger(t'')\Psi^\dagger(t'')] \rangle$ is the two-particle Green function and $W$ is an arbitrary interaction potential. The KBE are the first equations of the Martin–Schwinger hierarchy [6], which describes the coupling of the evolution of the one-particle Green function to the two-particle Green function, which itself is coupled to the three-particle Green function by a similar equation. To decouple this hierarchy and to make the KBE numerically tractable, a self-energy $\Sigma(t, t') = \Sigma[G(t, t')]$ is introduced. This self-energy can be found from a diagrammatic expansion in terms of Feynman diagrams, where only some classes of diagrams are chosen according to the properties of the examined system. With this, the KBE attain a formally closed form:

$$[i\partial_t - h(t)] G(t, t') = \delta(t - t') + \int_C d\tau \Sigma[G(t, \tau)] G(\tau, t'),$$

$$[-i\partial_{t'} - h(t')] G(t, t') = \delta(t - t') + \int_C d\tau G(t, \tau) \Sigma[G(\tau, t')].$$

(3)

2.2. Reconstruction problem

2.2.1. The Keldysh representation and the Dyson equation.

The two-time structure of the time contour $C$ suggests the use of a matrix representation for $G$ according to the different time orderings. There exist different representations, which are connected by a Keldysh rotation [7]. Here, we use the set involving less, retarded and advanced Green functions ($G^<$, $G^R$ and $G^A$) according to Langreth and Wilkins [8],

$$G = \begin{pmatrix} G^R & G^< \\ 0 & G^A \end{pmatrix}.$$ 

(4)

Note that this representation implies a two-time dependence of each component and is overcomplete as the conjugation relation $\left(G^R(t, t')\right)^\dagger = G^A(t', t)$ holds. To simplify the notation, we will make use of the greater Green function $G^\triangleright$, which relates to the other components as

$$G^\triangleright(t, t') = G^R(t, t') - G^A(t, t') + G^<(t, t').$$

(5)

With these definitions, we arrive at a formal solution for $G$ by time integration of equation (3), yielding the non-equilibrium version of the Dyson equation,

$$G = G_0 + G_0 \Sigma G.$$ 

(6)

Here $G_0$ denotes the non-interacting or Hartree–Fock (HF) Green function, whose inverse is given by $G_0^{-1}$:

$$G_0^{-1} = G_0^{-1} \cdot I = \begin{pmatrix} G_0^{-1} & 0 \\ 0 & G_0^{-1} \end{pmatrix},$$

(7)

where $(G_0)^{-1}$, the common inverse of the components $G^R$ and $G^A$, reads

$$(G_0^{-1})^{-1}(t, t') = \delta(t, t') [i\partial_t - h(t)].$$

(8)

The matrix multiplication in equation (6) is to be understood also including a time integration on the contour over intermediate time coordinates, so that, for example,

$$(G_0 \Sigma G)(t, t') = \int_C d\tau G_0(t, \tau) \Sigma(\tilde{\tau}, \tilde{\tau}) G(\tilde{\tau}, t').$$

(9)

2.2.2. Equation of motion for $G^<$ in terms of the density matrix.

Following Spicka et al [9], an intermediate step towards the GKBA is to express the equation of motion of $G^<$ in terms of the density matrix $\rho(t) = -i G^< \dot{G}(t, t)$. To start with, we provide some useful relations between $G^R$ and the respective self-energies $\Sigma^R$, $\Sigma^<$, $\Sigma^A$.

By right-multiplication of equation (6) with $G_0^{-1}$ and left-multiplication with $(G_0^{-1})^{-1}$, we obtain, taking the retarded/advanced component, the following:

$$G_0^{-1} = G^{-1, R/A} + \Sigma^{R/A}.$$ 

(10)

Now taking the less-component of equation (6), after left-multiplication with $(G_0^{-1})^{-1}$, we find that

$$\left(G_0^{-1}\right)^{-1} G^< = I^< + (\Sigma G)^< = (\Sigma G)^<.$$ 

(11)

Using the Langreth–Wilkins rules [8], it follows that

$$(G_0^{-1})^{-1, R} G^< + (G_0^{-1})^{-1, A} G^A = \Sigma^R G^< + \Sigma^< G^A.$$ 

(12)
Note that the multiplication is to be understood in the same manner as in equation (9), including contour time integration. Since $(G_0)^{-1,c} \equiv 0$, equation (12) simplifies to

$$
(G_0)^{-1}G^c = \Sigma^R G^c + \Sigma G^A,
$$

and the use of equation (10) yields

$$
(G^{-1.R} + \Sigma^R) G^c = \Sigma^R G^c + \Sigma G^A.
$$

Analogously, we find the conjugate equation, resulting in two final differential equations:

$$
G^{-1.R} G^c = \Sigma^c G^A,
$$

$$
G^c G^{-1.A} = G^R \Sigma^c.
$$

Now it is convenient to also split $G^c$ into two parts corresponding to the time arguments $t > \tilde{t}$ and $t < \tilde{t}$:

$$
G^c(t,t') = G^c_R(t,t') - G^c_A(t,t'),
$$

$$
G^c_R(t,t') \equiv \Theta(t - \tilde{t}) G^c(t,t'),
$$

$$
G^c_A(t,t') \equiv -\Theta(t' - \tilde{t}) G^c(t,t').
$$

This allows us to separately derive an equation for $G^c_R$ and $G^c_A$ from which equation (17) allows us to recover the equation for $G^c$. For $G^c_R$, one calculates:

$$
\begin{aligned}
[G^{-1.R}G^c_R](t,t') &= \left[(G_0)^{-1} - \Sigma^R \right]G^c_R(t,t') \\
&= \int_\mathcal{C} d\bar{t} \left[\delta(t-\bar{t}) \left(i\delta_\Sigma-h(\bar{t})\right) \Theta(\bar{t}-t') G^c(\bar{t},t') \right] \\
&\quad - \int_\mathcal{C} d\bar{t} \Sigma^R(t,\bar{t}) G^c_R(\bar{t},t') \\
&= \int_\mathcal{C} d\bar{t} \left[\delta(t-\bar{t}) \left(i\delta(\bar{t},t')G^c(\bar{t},t') + i\Theta(\bar{t}-t')\delta_\Sigma G^c(\bar{t},t') \right) \\
&\quad - h(\bar{t})\Theta(\bar{t}-t')G^c(\bar{t},t') \right] - \int_\mathcal{C} d\bar{t} \Sigma^R(t,\bar{t}) G^c_R(\bar{t},t') \\
&= \delta(t-t') i G^c(t,t') \\
&\quad + \Theta(t-t') \int_\mathcal{C} d\bar{t} \Theta(\bar{t}-t') (G_0)^{-1}(t,\bar{t}) G^c(\bar{t},t') \\
&\quad - \int_\mathcal{C} d\bar{t} \Sigma^R(t,\bar{t}) G^c_R(\bar{t},t') \\
&= \delta(t-t') i G^c(t,t') \\
&\quad + \Theta(t-t') \int_\mathcal{C} d\bar{t} \Theta(\bar{t}-t') (G_0)^{-1}(t,\bar{t}) G^c(\bar{t},t') \\
&\quad - \int_\mathcal{C} d\bar{t} \Sigma^R(t,\bar{t}) G^c_R(\bar{t},t') \\
&= \delta(t-t') i G^c(t,t') \\
&\quad + \Theta(t-t') \int_\mathcal{C} d\bar{t} \Theta(\bar{t}-t') G^{-1.R}(t,\bar{t}) G^c(\bar{t},t') \\
&\quad + \int_\mathcal{C} d\bar{t} \Sigma^R(t,\bar{t}) G^c_R(\bar{t},t') - \int_\mathcal{C} d\bar{t} \Sigma^R(t,\bar{t}) G^c_R(\bar{t},t'),
\end{aligned}
$$

where the inclusion of the last term under the $\Theta$-function is justified, since the contour product of two retarded functions is again a retarded function. The two last terms cancel and one finds, employing equation (15),

$$
\delta(t-t') i G^c(t,t') + \Theta(t-t') \int_\mathcal{C} d\bar{t} \Theta(\bar{t}-t') G^{-1.R}(t,\bar{t}) G^c(\bar{t},t') = \delta(t-t') i G^c(t,t') \\
+ \Theta(t-t') \int_\mathcal{C} d\bar{t} \Sigma^c(t,\bar{t}) G^A(\bar{t},t') \\
- \Theta(t-t') \int_\mathcal{C} d\bar{t} \Theta(\bar{t}-\tilde{t}) G^{-1.R}(t,\bar{t}) G^c(\bar{t},t').
$$

Here, the last term compensates for the step function in the second term. With equation (10) and noting that

$$
\int_\mathcal{C} d\bar{t} \Theta(\bar{t}-\tilde{t}) (G_0)^{-1}(t,\bar{t}) G^c(\bar{t},t') \equiv 0,
$$

it follows that

$$
\begin{aligned}
\delta(t-t') i G^c(t,t') + \Theta(t-t') \int_\mathcal{C} d\bar{t} \Sigma^c(t,\bar{t}) G^A(\bar{t},t') \\
- \Theta(t-t') \int_\mathcal{C} d\bar{t} \Theta(\bar{t}-\tilde{t}) G^{-1.R}(t,\bar{t}) G^c(\bar{t},t') \\
= \delta(t-t') i G^c(t,t') \\
+ \Theta(t-t') \int_\mathcal{C} d\bar{t} \Theta(\bar{t}-\tilde{t}) G^c(\bar{t},t') \\
+ \Theta(t-t') \int_\mathcal{C} d\bar{t} \Theta(\bar{t}-\tilde{t}) \Sigma^c(\bar{t},\tilde{t}) G^A(\tilde{t},t'),
\end{aligned}
$$

where, in the second term, the fact was used that $G^A$ includes a step function by definition. Left-multiplying by $G^R$ and explicitly writing out the integrals, one arrives at the equation for $G^c_R(t,t') = G^c(t,t')$, valid for times $t > \tilde{t} > t_0$:

$$
G^c(t,t') = -G^R(t,t') \rho(t') \\
+ \int_{t_0}^t d\tilde{t} \int_{t_0}^{\tilde{t}} d\bar{t} G^R(t,\bar{t}) \Sigma^c(\bar{t},\tilde{t}) G^A(\tilde{t},t') \\
+ \int_{t_0}^t d\tilde{t} \int_{t_0}^{\tilde{t}} d\bar{t} G^R(t,\bar{t}) \Sigma^A(\bar{t},\tilde{t}) G^A(\tilde{t},t').
$$

In a similar manner, one can derive the equation for $G^c_A(t,t') = -G^A_A(t,t')$ in the time domain $t_0 < t < \tilde{t}$, which reads

$$
G^c(t,t') = \rho(t) G^A(t,t') \\
+ \int_{t_0}^t d\tilde{t} \int_{t_0}^{\tilde{t}} d\bar{t} G^R(t,\bar{t}) \Sigma^c(\bar{t},\tilde{t}) G^A(\tilde{t},t') \\
+ \int_{t_0}^t d\tilde{t} \int_{t_0}^{\tilde{t}} d\bar{t} G^c(t,\bar{t}) \Sigma^A(\bar{t},\tilde{t}) G^A(\tilde{t},t').
$$

Note that by exchanging all less with greater quantities and replacing the density matrix $\rho := f^c$ by $f^c = 1 - f^c$ in equations (23) and (24), the analogous expression for $G^c$ is easily obtained.
2.3. The generalized Kadanoff–Baym ansatz (GKBA)

Combining equations (23) and (24), retaining only the terms without the integrals, the GKBA [3] is recovered:

\[ G_{\text{GKBA}}^R(t, t') = -G^R(t, t') f^R(t') + f^R(t) G^A(t, t'). \]  

(25)

With this equation, a means of reconstructing the off-diagonal Green function from the density matrix is found, which obeys particle number conservation, has a per se causal structure and does not depend on assumptions about near equilibrium; for a recent discussion, see, e.g., [9].

2.3.1. Choice of propagators \( G^{R/A} \).

When looking at equation (25), it should be noted that the GKBA is only formally closed in terms of \( \rho \), since it depends on the knowledge of the retarded (advanced) propagators \( G^R (G^A) \), which themselves obey non-Markovian two-time equations of motion of a similar complexity. This can be overcome by the use of propagators, which obey a Markovian evolution. In this paper, we chose HF propagators, as they incorporate the interaction at mean-field level in contrast to, e.g., ideal propagators. The HF propagators \( G^{R/A}_{\text{HF}} \) are given by

\[ G^{R/A}_{\text{HF}}(t, t') = \frac{i}{\hbar} [\pm (t - t')] \exp \left( -i \int_{t'}^t d\tilde{t} H(\tilde{t}) \right), \]  

(26)

where \( H \) denotes the mean-field HF Hamiltonian, which is governed by the time-dependent density matrix.

2.3.2. Choice of self-energy.

To show the advantages of the GKBA, we exemplarily apply the second-order Born approximation, leading to a self-energy \( \Sigma_2(t, t') \), the less component of which is given by

\[ \Sigma_2^R(t, t') = \delta(t - t') \Sigma_{\text{HF}}(t) + G^R(t, t') W(t) W(t') G^A(t', t) G^R(t', t) - G^R(t, t') W(t) G^A(t', t) G^R(t', t) W(t'). \]  

(27)

The evaluation of the collision integral \( I = \int_{t'}^t \Sigma G \), the right-hand side of the KBE, equation (3), is twofold simplified by the GKBA as we can use the reconstructed \( G(t, t') \) in \( I \) as well as in \( \Sigma \). For instance, the less-part of \( \Sigma_{2B} \) for \( t > t' \) now reads

\[ \Sigma_{2B}^R(t, t') = \delta(t - t') \Sigma_{\text{HF}}(t) + G^R(t, t') f^R(t') \times \left[ W(t) W(t') f^R(t') G^A(t', t) G^R(t', t) f^R(t') - W(t) f^R(t') G^A(t', t) G^R(t', t) f^R(t') W(t') \right]. \]  

(28)

So, only the single-time quantity \( f^R \) has to be stored in memory, as the HF propagators \( G^{R/A}(t, t') \) can be computed each time step, and the demand scales linearly with propagation length. That way, in total three approximations were taken:

1. The self-energy was introduced to decouple the Martin–Schwinger hierarchy.
2. The two-time Green function was reconstructed within the GKBA according to equation (25), neglecting the integral terms in equations (23) and (24).

3. The propagators \( G^{R/A} \) were approximated by HF propagators, which can be explicitly calculated for each \( (t, t') \).

3. The application to homogeneous systems: an overview

The GKBA has been applied to spatially homogeneous charged particle systems already in the mid-1990s and has allowed for many numerical studies of ultrafast carrier relaxation. Electron–phonon scattering in semiconductors was investigated, e.g., in [10, 11]. Electron–electron interactions in plasmas and semiconductors were studied with the GKBA and the results tested against full two-time calculations in [12–14]. The use of correlated spectral functions (beyond HF propagators) was analyzed in [15]. For an overview of the GKBA and applications to electron–hole plasmas in semiconductors, see the textbook [16]. The second type of applications was devoted to dense plasmas, in particular laser plasmas. To capture strong field effects in the Coulomb scattering process (such as harmonics generation and inverse bremsstrahlung), a gauge-invariant generalization of the GKBA was derived in [17] and used in [18, 19].

Since the application of the GKBA transforms the NEGF approach into a single-time theory, there should exist close connections to the purely single-time approach of reduced density operators (quantum Bogoliubov–Born–Green–Kirkwood–Yvon hierarchy). In fact, this has been studied in detail in [20], and a one to one correspondence can be established in the limit of free or HF propagators. There, it was also shown that the GKBA does not destroy the conserving properties of the underlying NEGF approximation as long as no approximations to the time structure of the propagators are introduced. In particular, in the relevant case of free or HF propagators, the conservation laws and sum rules are preserved [21]. For a recent overview of the GKBA and its relation to quantum transport and density functional theory, see [22].

4. The application to inhomogeneous systems

4.1. Initial state preparation under the GKBA

In order to solve the KBE equation (3), one has to supply an initial value for \( G(0, 0) \). For large, homogeneous systems described in section 3, the initial state is reached from an arbitrary state after a characteristic equilibration time. For small, strongly correlated systems, no equilibration takes place and the preparation of the correlated initial state has to be performed differently to avoid strong artifacts, such as unphysical oscillations. For full two-time calculations, the initial state can be found by means of the extended Matsubara–Schwinger–Keldysh time-contour (containing an additional imaginary time branch) and solution of the Dyson equation (6) on its imaginary branch, e.g. [23], using the same self-energy (for details and implementation, see, e.g., [24]). Here, however, the application of the GKBA poses a problem, since no corresponding equilibrium approximation is known so far. This can be remedied by using adiabatic switching as discussed below.
In general, according to the adiabatic theorem [25], the ground state of an interacting system can be found by taking the ideal system, for which the ground state is assumed to be known, and adiabatically switching on the interaction. If this procedure is performed slowly enough, the system is undergoing a transition through successive eigenstates of the respective Hamiltonians with gradually higher interaction strength. Finally, the fully interacting ground state is reached. Here, we use this method of generating the initial state that is consistent with the GKBA. We use a monotonic switching function \( f \), which has the following properties:

\[
\begin{align*}
  f(t_0) &= 0, \quad f(t_1) = 1, \quad 0 \leq f(0 < t < t_1) \leq 1, \quad (29)
\end{align*}
\]

where \( t_1 \) is the end of the switching process and the start of the time-dependent calculation. It is important that, with this method, the interaction that normally is time independent becomes inherently time dependent. This especially should be kept in mind when dealing with quantities involving interaction terms. For example, the HF propagators now include \( W(t) \) and the self-energy contains \( W(t) \) and \( W(t') \). In the calculations below, we use a Fermi-like switching function \( f^*_{\lambda}(t) \) (see figure 1):

\[
f^*_{\lambda}(t) = 1 - \frac{1}{1 + \exp \left( \frac{t - t_0}{\tau} \right)},
\]

where \( f^*_{\lambda}(t_0) = \frac{1}{2} \) and the smoothness of the switching increases with the value of the time constant \( \tau \).

4.2. The application to electrons in quantum wells

To test the ability of the GKBA to describe correlation effects in an inhomogeneous system, we study two electrons in a quantum well potential. After preparing the system in the correlated initial state via adiabatic switching, the system is disturbed by a short dipole kick [26] with a sufficiently small amplitude, and the time-dependent dipole moment is computed. Fourier transformation then yields the correlated dipole excitation spectrum in linear response with the relevant vertex corrections, thereby fully preserving conservation laws and sum rules [26]. All calculations are performed in the context of a finite-element discrete variable representation (FEDVR) basis, which drastically reduces the numerical complexity; for details, see [2, 27].

We consider \( N = 2 \) electrons in a quantum well potential, which is effectively a one-dimensional (1D) system, if the lateral electronic motion is neglected. We assume that the system is in singlet configuration \( |S, M_S\rangle = |0, 0\rangle \). The confinement energy is given by \( E^*_0 = \hbar^2/(m^* L^2) \), where \( m^* \) is the effective mass of the electrons within the quantum well potential of width \( L \). The two-particle Hamiltonian in units of \( E^*_0 \) reads

\[
H_2(t) = \sum_{i=1}^{2} \left( -\frac{1}{2} \nabla_i^2 + f_0 \cdot \delta(t - t_0) \right) + \lambda^*[ (x_1 - x_2)^2 + \kappa^2 ]^{-1/2},
\]

where \( x_j \) are the particle positions. The first term denotes the single-particle contributions, involving the potential energy and the dipole delta-kick with amplitude \( f_0 \ll 1 \).

The second term describes the two-particle Coulomb interaction. A cut-off parameter \( \kappa \) has been inserted to regularize the 1D Coulomb potential, which is set to a value of 1 throughout the calculations. The relative interaction strength between the electrons is given by the dimensionless coupling parameter \( \lambda^* = L/a_0^* \equiv e^2 m^* L / (4 \pi \epsilon_0 \epsilon^* \hbar^2) \), where \( \epsilon^* \) denotes the material’s dielectric constant that enters the effective Bohr radius \( a_0^* \).

4.3. Numerical results

In figure 2, the ground-state dipole excitation spectrum of the two-electron quantum well is presented for different values of the coupling parameter \( \lambda \). In grayscale, the results of GKBA calculations using second-order Born self-energy are shown. The white dashed lines represent the excitation energies from exact diagonalization (ED). Exemplarily for \( \lambda^* = 1 \), the respective time-dependent dipole moment \( d(t) \) can be seen in the figure above the spectrum. The first 50 a.u. of the propagation, where the dipole moment is zero, account for the adiabatic switching (denoted by ‘AS’ in the figure). While \( d(t) \) appears to be monochromatic, in fact, it contains numerous additional frequencies which can only be resolved using a sufficiently long time propagation. The present GKBA calculation makes this possible. It has a total duration of \( T = 40 \times 00 \) time steps and is readily performed within 24 h for a few tens of basis functions.

Let us first discuss the general structure of the excitation spectrum that is obtained from the ED calculations. The excitations can be classified according to the number of electrons involved in the transitions, leading for the two-electron quantum well to the distinction between single (SE) and double excitations (DE). In particular, the DEs are of great interest in the dynamics of correlated electronic systems. Obviously, they cannot be captured by mean-field-type approaches such as HF. For \( \lambda^* = 1 \), the lowest excitation from the ground state, denoted by ‘a’, is a SE of energy \( \omega^*_{\text{ED}} = 0.61 E^*_0 \). It is followed by a DE (‘1’), with \( \omega^*_{\text{ED}} = 2.17 E^*_0 \), another SE (‘b’), at \( \omega^*_{\text{ED}} = 2.95 E^*_0 \), two DEs, (‘2’) at \( \omega^*_{\text{ED}} = 4.54 E^*_0 \) and (‘3’) at \( \omega^*_{\text{ED}} = 5.31 E^*_0 \), respectively, and another SE (‘c’) with energy \( \omega^*_{\text{ED}} = 6.89 E^*_0 \).

Consider now the results of the GKBA calculations. It can be clearly seen from figure 2 that it shows SEs as well as DEs, although the quality of their description differs significantly. While the SEs are very well described and are practically

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**Figure 1.** Fermi function for adiabatic switching. The half-time is \( t_0 = 25 \) and the switching time constant is chosen to be \( \tau = 3 \).

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**Figure 2.** Ground-state dipole excitation spectrum of two electrons in a quantum well potential. In grayscale, the results of GKBA calculations using second-order Born self-energy are shown. The white dashed lines represent the excitation energies from exact diagonalization (ED). Exemplarily for \( \lambda^* = 1 \), the respective time-dependent dipole moment \( d(t) \) can be seen in the figure above the spectrum. The first 50 a.u. of the propagation, where the dipole moment is zero, account for the adiabatic switching (denoted by ‘AS’ in the figure). While \( d(t) \) appears to be monochromatic, in fact, it contains numerous additional frequencies which can only be resolved using a sufficiently long time propagation. The present GKBA calculation makes this possible. It has a total duration of \( T = 40 \times 00 \) time steps and is readily performed within 24 h for a few tens of basis functions.
identical to the exact results over the whole range of coupling parameters $\lambda^*$, the DE energies only coincide in the limit $\lambda^* \rightarrow 0$, and the deviations from the exact result increase approximately linearly with $\lambda^*$, leading to a relative error of the order of 20% at $\lambda^* = 2.5$ for the lowest DE (‘1’). Thus, the primary conclusion is that our NEGF approach within the GKBA is indeed able to reproduce the DEs in the spectrum. At the same time, their energy appears with an incorrect $\lambda^*$-dependence in the present second Born approximation for the self-energy, suggesting that not all processes leading to these excitations are captured. For completeness, we note that, for coupling strengths $\lambda^* > 1$, additional excitations appear in the spectrum that cannot be attributed to real excitations in the system (cf., e.g., ‘E’).

To analyze the numerical performance of the GKBA, we tested it against full two-time calculations, both using the same second-order Born self-energy. Figure 3 shows the scaling of the computation time with the propagation time $T$ on a single standard CPU. From the graph, it can be seen that the full propagation scales with $T$ to a power of more than 3; we expect that it will converge to a scaling of $O(T^3)$ for longer time propagation. The GKBA, in contrast, scales only as $O(T^2)$. The figure shows that the GKBA allows us to increase the propagation duration $T$ by three or more orders of magnitude compared to two-time calculations. This, in addition to the significant reduction of memory consumption, paves the way for much longer propagation times in the future.

In this paper, we have recalled the idea and previous applications of the GKBA and demonstrated how to extend it to inhomogeneous, finite systems. The key to an efficient and consistent simulation was to correctly provide a correlated initial state via adiabatic switching of the interaction. For a first test of the accuracy of the approximations, we have applied the formalism to a two-electron quantum well model system and studied the ground state dipole excitation spectrum for different coupling parameters. While our approach is easily applicable to systems containing more particles, the two-electron case allows for a benchmark against exact diagonalization results.

Our numerical results confirmed that the GKBA correctly recovers, in addition to single-particle excitations, DEs as well. These are currently of great interest for many applications in semiconductor optics and transport but cannot be obtained by standard tools such as time-dependent HF. At the same time, we found that, while SEs are reproduced with high accuracy, the DEs are correctly captured only at small coupling. Inherent to the GKBA in second Born approximation is an incorrect coupling parameter dependence of the DE energies of order $\propto (\lambda^*)^{-1}$, in contrast to the correct scaling of $\propto (\lambda^*)^{-2}$. This is in good agreement with our similar findings for the four-electron quantum well case [28]. Since a similar scaling is observed for the full two-time propagation within the second-order Born self-energy, we conclude that this behavior of the DE energies is not a
deficiency of the GKBA but indicates the limitations of the involved (weak coupling) second Born approximation for the self-energy. Evidently, higher terms in the Born series are required in order to restore the correct scaling. Therefore, in future work we will study higher order approximations for the self-energy such as $T$-matrix or GW approximation. It will be interesting to see whether the GKBA performs similarly well, allowing again to omit the complicated integral terms in the full equations (23) and (24).

Our results based on the GKBA open up a broad variety of new many-body applications of inhomogeneous finite systems. In our recent work [2, 27], we demonstrated that these systems become tractable by using the FEDVR representation. Still there were essential limitations of full two-time calculations in terms of computation time and memory requirements. These limitations can now be mitigated to a large extent with the help of GKBA by increasing the duration of time propagation by more than three orders of magnitude. Not only does this allow for a much more accurate computation of electronic spectra, including DEs. At the same time, true non-equilibrium problems such as nonlinear excitation and relaxation dynamics or pump–probe problems in inhomogeneous systems are now within the reach of NEGF simulations.

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