Artificial damping in the Kadanoff-Baym dynamics of small Hubbard chains

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Abstract. We perform a comparative study of exact and approximate time-evolved densities in small Hubbard chains. The approximate densities are obtained via many-body perturbation theory (Hartree-Fock, 2nd Born, GW and T-matrix approximations) within the framework of the time-dependent Kadanoff-Baym equations. Benchmarking approximate results against exact ones allows us to address two rather fundamental issues in the non equilibrium dynamics of strongly correlated systems. I) A characterisation of the performance of several standard MBAs in the non-equilibrium regime. Having a definite notion of how good a specific MBA can be is highly relevant to its application to cases (typically, infinite systems) where exact solutions are not available. Our results show that the T-matrix approximation is overall superior to the other MBAs, at all electron densities. II) A scrutiny of the whole idea of Many Body Perturbation Theory in the Kadanoff-Baym sense, when applied to finite systems. The surprising outcome of our study is that during the time evolution, the KBE develop an unphysical steady state solution. This is a genuinely novel feature of the time-dependent KBE, i.e. is not inherited from possible limitations/approximations in the calculation of the initial state. Our extensive numerical characterisation gives robust evidence that the problem occurs in general, whenever MBPT is applied to finite systems, and approximate self energies based upon infinite partial summations are used. We also offer some more conceptual and general consideration on the dependence of this behaviour on the number of particles and system size. This is followed by our conclusions and glimpses of future work.

1. Introduction
The Kadanoff-Baym equations (KBE) [1, 2] are one of the main frameworks to describe quantum systems out of equilibrium [3, 5]. Recently, the KBE have received renewed attention due to the increased capability of solving them numerically [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. A main advantage of the KBE is their direct connection to Many Body Perturbation Theory (MBPT): One can build, in a systematic way, approximations for the one-particle Greens function, $G$, the key quantity in the KBE. The range of validity of the Many Body Approximations (MBAs) can be studied by comparing the approximate results with exact numerical ones for finite strongly correlated systems. Naturally, in finite closed systems one cannot address some important issues such as the onset of the steady state regime, or the role of dissipation, as they for example occur in quantum transport geometries [14]. This approach has, however, a second fundamental advantage, i.e. it unravels the role of finite size effects in the KBE.

In addition, the study of small clusters with strong interactions in a time dependent (TD) environment is interesting of its own: in recent years, the topic has grown in importance, boosted
by various technological advances such as coupled quantum dots [17] in nanoscale devices and the emerging field of atomtronics [18] in optical lattices. In reality, nanosystems often contain hundreds or thousands of atoms; such sizes are very difficult to treat, especially if we wish to describe their dynamics and excitations. Typically, one then represents the real system by a Hubbard-like model with much fewer degrees of freedom (core electrons eliminated by pseudopotential techniques, perhaps the host material in a quantum dot system is taken into account via effective-mass approximations, etc.) which account only for the active orbitals.

Small clusters in non equilibrium attached to leads have been studied in the stationary limit [12] as well in real-time [14]. In this paper we do not consider the role of reservoirs, and focus on the real-time evolution of small clusters (more specifically, open-ended Hubbard chains), through full CI calculations as well as within MBAs by propagation of the KBE. We consider the Hartree-Fock approximation (HFA), the 2nd Born approximation (BA), the GW-approximation (GWA) [19] and the T-matrix approximation (TMA) [20, 21] all of which, a part from HFA, have self energies which are non local in space and time. These four approximations are all conserving [1], which is a central requirement of the KBE approach. We make a spin-dependent treatment of the GW [12, 22], which among other things mitigates the problem of self screening as discussed in [23, 24]. Another common approach to microscopic TD phenomena is Time Dependent Density Functional Theory (TDDFT) [25]. A well established connection exists between TDDFT and MBPT on the Keldysh contour [26]. Here, to highlight this link, we will obtain MBPT-based exchange-correlation (xc) potentials via TD reverse engineering [27], using the TD densities from MBAs we used (Section 4). The TDDFT approach is summarised in Section 5; in Sections 6 and 7, we present ground state and TD results, respectively; Section 8 describes in more detail specific features of the TD densities; in Section 9, we briefly address the significance of long-range interactions, i.e. beyond the onsite term $U$. Finally, our conclusions and outlook are presented in Section 10.

2. Model system

The systems we investigate are open-ended Hubbard chains, described by the following Hamiltonian:

$$H = \sum_{R\sigma} \epsilon_R \hat{n}_{R\sigma} - V \sum_{\langle RR' \rangle \sigma} a_{R\sigma}^{\dagger} a_{R'\sigma}^{\dagger} + U \sum_{R} \hat{n}_{R\uparrow} \hat{n}_{R\downarrow} + \sum_{R \sigma} w_R(t) \hat{n}_{R\sigma}$$

(1)

Here $\hat{n}_{R\sigma} = a_{R\sigma}^{\dagger} a_{R\sigma}$, $\sigma = \uparrow, \downarrow$, $\langle RR' \rangle$ denotes nearest neighbour sites, $\epsilon_R$ are the onsite energies. The $V = 1$ is the hopping parameter, $U$ is the interaction energy and $w_R(t)$ is a local external field which can be of any shape in time $t$ and space. $U$ and $w_R(t)$ are given in units of $V$.

We consider chains of lengths $L = 2, 4, 6$ and $N_e = 2, 4, 6$ number of electrons (1/6 and half filling); we take spin-up and -down electrons equal in number, $N_\uparrow = N_\downarrow$; this will hold under time evolution since $H$ has no spin-flip terms. In the rest of the paper, the filling will be assigned by $n = N_\uparrow / L$. Our exact solution are obtained via short iterative Lanczos propagation.

3. Kadanoff-Baym equations

To describe the system out of equilibrium, we determine the one-particle Greens function $G(t_1, t_2)$ by solving its equation of motion [1, 26]

$$(i\partial_{t_1} - h(t_1)) G(t_1, t_2) = \delta(t_1, t_2) + \int_{\gamma} \Sigma(t_1, t) G(t, t_2) dt$$

(2)
and the adjoint one corresponding to $t_2$. Here $h$ is the single particle Hamiltonian, $\gamma$ represents the Keldysh contour [2] and $\Sigma$ is the self energy, whose functional dependence on $G$ is established by the approximation used. Instead of using the more conventional contour in Fig. (1i), we use the equivalent contour in Fig. (1ii) [5] which is numerically more favourable and has an analytical limit when $T \to 0$. On this contour the $G$ and $\Sigma$ decay exponentially at $t_1, t_2 \to \pm i\beta/2$ and therefore we only need dense meshpoints close to zero. This is in contrast to the traditional contour Fig. (1ii) where one needs many meshpoints close to zero as well as close to $-i\beta$ due to the periodicity properties of $G$ and $\Sigma$ [4].

The KBE specialised to the lesser component and $t_1$ for this contour become

$$
(i\partial_{t_1} - h (t_1)) G^< (t_1, t_2) = \int_0^{t_1} d\tau \left[ \Sigma^R (t_1, \tau) G^< (\tau, t_2) + \Sigma^< (t_1, \tau) G^A (\tau, t_2) \right] + \frac{1}{i} \int_0^{\beta/2} d\tau \left[ \Sigma^< (t_1, -i\tau) G^> (-i\tau, t_2) + \Sigma^> (t_1, i\tau) G^< (i\tau, t_2) \right].
$$

(3)

Here the superscripts $<, >, R, A$ have their usual meaning [1, 2]. In this paper we will work at zero temperature, $T \to 0$. We obtain the correlated ground state by solving, by simple iteration, the Dyson’s equation

$$
G = G_0 + G_0 \Sigma [G] G
$$

self-consistently, with $(\epsilon - h)G_0 = 1$. We then use this as the initial state [3] for the time evolution. Eq. (3) is solved by propagation using a predictor-corrector method similar to that presented in [28]. The conservation laws as well as the time reversal symmetry are obeyed up to arbitrary accuracy. We use a meromorphic representation for the spectral functions as the system is finite [29]. As an example, the Green’s function can be written as $G_{RR} (\epsilon) = \sum_j A^j_{RR} (\epsilon - a_j)^{-1}$, where $A^j_{RR}$ are residue matrices and $a_j$ are pole positions in the single particle orbital representation. This representation is very convenient as convolutions
become simple matrix products [30] and are obtained analytically: Given two functions

\[ B_{RR'}(\epsilon) = \sum_j B_{RR'}^j(\epsilon - b_j), \quad D_{RR'}(\epsilon) = \sum_k D_{RR'}^k(\epsilon - d_k) \]  

(4)

then, for the convolution \( C_{RR'}(\epsilon) \), we get

\[ C_{RR'}(\epsilon) = \int B_{RR'}(\epsilon') D_{RR'}(\epsilon - \epsilon') \frac{d\epsilon'}{2\pi i} = \sum_{j,k} B_{R'R}^j D_{R'R}^k \frac{1}{\epsilon - b_j - d_k} \]  

(5)

The number of poles increases rapidly at every iteration. To keep this under control in a numerically manageable way, we merge small and close poles according to some importance threshold criteria, by replacing two poles by an effective one. The residue matrix of the effective pole is the sum of the two old residue matrices and the pole position is the center of gravity of the poles being replaced. Here the “mass” of a pole is the trace of the corresponding residue matrix.

4. Many-body approximations (MBAs)

In a one-band Hubbard model, the interaction can be treated either spin-dependent, \( U \sum_R n_{R\uparrow} n_{R\downarrow} \) or spin-independent, \( \frac{1}{2} U \sum_R a_R^\dagger a_R^\dagger a_R a_R \). These treatments are evidently equivalent in any order by order expansion such as the HFA or BA (Fig. (1)) as the diagrams suffering from self interaction are exactly compensated by corresponding exchange diagrams. In approximations based upon partial summations, however, this equivalence is in general lost. To illustrate this point we consider the GWA, \( \Sigma(12) = G(12) W(12) \) both spin-independent (GWA), which gives \( W = UPU + (UP)^2W \) and spin-dependent (SGWA), which results in \( W = UPW \) and \( (UP)^2W \), where \( P(12) = G(12) G(21) \) in both treatments. In this paper, the TMA, \( \Sigma(12) = U^2 G(21) T(12) \), is treated only spin-dependent and \( T = \phi - \phi UT \) where \( \phi(12) = G(12) G(12) \).

The computational cost increases considerably with increasing complexity of the self energy, along the sequence HFA, BA, GWA and TMA. The main difference is that in the GWA and TMA, in addition to propagating \( G \), we also need, in parallel, to solve the integral equations for \( W \) or \( T \). As an example, the equation for \( T^< \) is

\[ T^<(t_1, t_2) = \Phi^<(t_1, t_2) - U \int_0^{t_1} d\tau [\Phi^R(t_1, \tau) T^<(\tau, t_2) + \Phi^<(t_1, \tau) T^A(\tau, t_2)] + \frac{U}{\pi} \int d\tau \left[ \Phi^<(t_1, -i\tau) T^>(-i\tau, t_2) + \Phi^>(t_1, i\tau) T^<(i\tau, t_2) \right], \]  

(6)

which is solved iteratively. The solution of the coupled integral equations (3, 6) for the \( G \) and the \( W \) or \( T \) is done self-consistently at every time step.

5. TDDFT from MBPT and the effective potential

Our KBE results for the TD densities also provide insight for TDDFT approaches to strongly correlated systems (e.g., to the Hubbard model). Given a specific MBA, from the resulting TD density we obtain the corresponding effective potential \( v_{eff} = v_H + w + v_{xc} \), where \( v_H \) is the Hartree potential and \( v_{xc} \) the exchange correlation potential. In practice, this is done via a numerical reverse engineering procedure [27], by minimising \( |n(t) - n_{KS}(t)| \) at each time-step, where \( n_{KS} = \sum_\nu |\psi^K S_\nu|^2 \) is the Kohn-Sham density, found by solving \( i\psi^K S_\nu = (\hat{t} + v_{eff}) \psi^K S_\nu \) and with the kinetic energy given by \( \hat{t} = -V \sum_{\langle RR'\rangle \sigma} a_{R\sigma}^\dagger a_{R'\sigma} \).

\[ \]
6. The initial, ground state spectral function

We start by solving the Dyson’s equation self-consistently to obtain the initial $G$ for propagating the KBE.

![Graph showing spectral functions for different U values](image)

**Figure 2.** Ground state spectral functions for $L=6$ at half filling and different interaction strengths $U$. The curves correspond to exact (black), TMA (red), BA (green), GWA (blue) and HFA (orange). The curves are shifted for clearer comparison and we have used a Lorentzian broadening $\Gamma = 0.2$.

In Figs. (2, 3), we present results for the hole and electron contributions to the spectral density for different particle concentrations and interaction strengths. The performance of MBAs generally deteriorates with increasing $U$. The cases we display are the same to be considered for the TD results. Already the ground state results reveal some basic and generic features of the different many-body approximations we employ to evolve our clusters in time. Such features, discussed in Figs. (2, 3), are common to other clusters with different size, fillings and interactions strengths, whose results we do not show here.

The case of half filling is shown in Fig. 2. We note that all curves exhibit electron-hole symmetry, and that, on increasing $U$, a correlation gap opens. This feature is reproduced at different extent by the approximate schemes. The BA gives the best description, yet it largely underestimates the gap. We note that our non-magnetic HFA solutions reproduce, albeit shifted in energy, the non-interacting spectral density. At large $U$, the exact solution displays satellite structures which mimic the upper and lower Hubbard bands in extended systems. Such behaviour is however incorrectly described by all the approximations, which (especially in the case of the BA and the GWA) also introduce spurious satellites further away from the band.
Figure 3. Ground state spectral functions for $L=6$ at $n = 1/6$ and different interaction strengths $U$. The curves correspond to exact (black), TMA (red), BA (green), GWA (blue) and HFA (orange). The curves are shifted for clearer comparison and we have used a Lorentzian broadening $\Gamma = 0.2$.

Results for the low density regime are presented in Fig. (3). For $U=1$, the main effect of the interaction is an increased asymmetry in the band region; the overall agreement between exact and approximate results is rather good, especially for the BA and the TMA (both the BA and the GWA slightly overestimate the shoulder on the high end of the band region). For $U=4$, the most notable feature in the exact solution is a satellite feature at high energy (about 6.5 at the bottom of panel 3b; in an extended system, for $U=4$ this would be a two-electron anti-bound state and it would lie outside the band continuum). Such satellite is well reproduced by the TMA (although its distance from the band region is overestimated). In contrast, the satellite is smeared out in the BA and GWA, and obviously absent in the HFA (in the HFA, there are no correlation effects). In the band region, for $U=4$, there is a moderate agreement between exact and approximate results.

We also compared GWA against SGWA results: with the latter we noted a slight improvement, which is expected, as the SGWA includes fewer faulty diagrams; yet, the SGWA is still worse than the BA or the TMA. Since the improvement is marginal, results are not shown here (however, some SGWA results will presented for the TD densities below). It is worth noting that, using a MBA expansion in terms of non-magnetic propagators, the SGWA has a magnetic instability as a function of $U$. In the dimer, where the poles of $W[G_0]$ are $\epsilon = \pm \sqrt{4V^2 \pm 2VU}$, this occurs for $U \geq 2V$ (such symmetry breaking is absent in the dimer exact solution).
We note that the spectral functions are better at first iteration, see Fig. (4); this corresponds to the known fact that self-consistent partial diagrammatic summations often deteriorate the spectral properties compared to non self-consistent ones [31, 32]. Self consistency is required for dynamically conserving approximations, and for total energy calculations; but different partial summation criteria should be specifically adopted for spectral densities [31]. For example, in some cases, vertex corrections are required to remove artefacts introduced by self consistency [30].

We conclude this section by remarking that all MBAs based on partial summations involve infinitely many diagrams, and this results in infinitely many, but discrete, number of poles in the ground state spectral functions [33]. This is in contrast to the exact solution which, as a consequence of the finiteness of phase space of the system, has only a finite number of poles.

7. Time dependence
For $t < 0$, the system is in its ground (initial) state, as discussed in the previous section. At $t > 0$, an external field is applied. In our calculations, we have employed different kinds of external fields, but in this paper we present results only for the form $w_R(t) = w_0 \delta_{R,1} \Theta(t)$, i.e. we let the (stepwise) perturbation to act only on the leftmost, $R = 1$, site. The time is given in units of the inverse hopping parameter $(1/V)$. 

![Figure 4. First iteration and self-consistent TMA spectral function versus exact one. $L=6$ and in a): $n = 1/6$ and in b): $n = 1/2$. The curves correspond to exact (black), first iteration TMA (green) and self-consistent TMA (blue). The curves are shifted for clearer comparison and we have used a Lorentzian broadening $\Gamma = 0.2$.](image)
In Fig. (5), panels a-e), we show time-dependent densities corresponding to the initial states shown in Fig. (3). In panel f), we present results for $v_{eff}$ in a selected case. All curves represent the dynamics on site 1. In the panels a) and b), $n = 1/2$ while in panels c) to f), $n = 1/6$. In panel a) we show the simplest case ($U = 1, w_0 = 1$) for which all MBAs give a good description of the density. In panel b), the interaction as well as the external field are increased and we see clearly that the HFA performance is poor while the other MBAs are very similar and closer to the exact density. In panel c) we see that the HFA and TMA are on top of the exact density while the BA and GWA start to deviate after some time (with BA being the slowest). This implies that even if the ground states are not too different, the BA and GWA fail to describe the non-linear response. In panel d) we see that none of the MBAs give a satisfactory description. We attribute this to the fact that the ground state spectral function is not well described in the band region, which is important when the external field is weak. In panel e), however, the TMA is seen to perform very well (contrary to the other MBAs which either lack or completely misplaces the satellite) as the influence of the satellite becomes essential. It is also clearly seen that similarly as in panel c) the BA and GWA fail in the non-linear regime. In panel f) we show the corresponding $v_{eff}$ for the different MBAs. The comparison of exact versus MBPT-based xc-potentials for TDDFT shows trends similar to those for the densities: in particular, the $v_{eff}$
of the TMA is superior to those of the other MBAs.

**Figure 6.** Time dependent densities for $L = 4$, $U = 1$, $w_0 = 5$ and $n = 1/2$. The curves correspond to exact (black), GWA (thick orange) and SGWA (thick blue).

In Fig. (6) we compare GWA, SGWA and TMA. Because of the magnetic instability in the SGWA, we can compare only for weak interaction, $U < 2$. We see that the SGWA is slightly better than its spin-independent counterpart but inferior to the TMA.

As general comment to our findings, the GWA is known to provide a good screening of the Coulomb interaction, while the TMA gives a better description if the interaction is short ranged, especially in the low density regime. The overall good performance (both for the ground state as well as for the time evolution) of the TMA for the short-ranged Hubbard Hamiltonian is in agreement with previous studies of ground state properties of clusters [30, 34]. In other words, the performance of the different approximations in the ground state has non negligible relevance to the TD behaviour of the system. In particular, an external perturbation redistributes the electrons also in the unoccupied energy levels, and two basic spectral features, the band-gap and the satellite, play a key role in the TD evolution.

8. Damping

When we propagate our system under the action of a strong external field we reach an artificial steady state, see Fig. (7). (By a steady state we mean a state where the single-particle properties are independent of time, and where the one-particle Green’s function depends only on the time difference). Hints of this behaviour are already present in Fig. (5), but here we wish discuss this feature in greater detail.

The damping is not a numerical artefact, Fig. (8). Particle and energy conservation are strictly obeyed within our numerical accuracy. When we reverse the direction of time in the
Figure 7. Densities for $L = 2, n = 1/2, U = 1, w_0 = 5$, exact (thick orange) and GWA (black). Damping of GWA density versus exact solution.

Figure 8. Conservation laws (left) and time reversal (right) for $L = 2, n = 1/2, U = 1, w_0 = 5$. propagation, the system goes back to the initial state and remains there. The damping rate increases with the strength of the external field and is absent in the regime where linear response applies. In this limit the dynamics is described by the Bethe-Salpeter equation, with a kernel
The latter would have a discrete spectrum in our MBAs, and so would the resulting density response. This leads to a non-damped dynamics.

\[ \delta \Sigma / \delta G \]

\( \frac{\delta \Sigma}{\delta G} \). The latter would have a discrete spectrum in our MBAs, and so would the resulting density response. This leads to a non-damped dynamics.

\[ A(T, \omega) = -Tr \text{Im} \int_{-2T}^{2T} e^{i\omega \tau} \left[ G^> - G^< \right] \left( T + \frac{\tau}{2}, T - \frac{\tau}{2} \right) d\tau, \]

where \( T = (t_1 + t_2)/2 \) and \( \tau = (t_1 - t_2) \), and its counterpart in time space. At the steady state, the spectral function gets broadened in energy space, Fig. (9a), and damped in time space, Fig. (9b). Note that, for our dimer, the exact instantaneous spectral function would continue to oscillate.

To study the non-linear response behaviour, a convenient quantity is the instantaneous spectral function

\[ A(T, \omega) = -Tr \text{Im} \int_{-2T}^{2T} e^{i\omega \tau} \left[ G^> - G^< \right] \left( T + \frac{\tau}{2}, T - \frac{\tau}{2} \right) d\tau, \]

where \( T = (t_1 + t_2)/2 \) and \( \tau = (t_1 - t_2) \), and its counterpart in time space. At the steady state, the spectral function gets broadened in energy space, Fig. (9a), and damped in time space, Fig. (9b). Note that, for our dimer, the exact instantaneous spectral function would continue to oscillate.

The damping rate depends on the MBA used - in general the TMA is slowest - and it acts strongest on the perturbed site. Further numerical investigations, not reported here, indicate that the entity of this artificial damping generally decreases with system size. No similar trend was seen for the dependence on the number of particles. Of course, our present results do not give a complete picture of how the large size limit is gradually obtained; nevertheless, we would like to present the reader with some general remarks. In an exact dynamics, a finite system will never fully relax to a stationary steady state. Due to decoherence, a finite but large system will, however, reach a quasi-steady state. As the system grows in size this damping becomes more and more complete. Thus, after long time the system, in an exact time dynamics, would exhibit noise-like fluctuations which never die but which decrease in amplitude with system size, whereas an approximate KBE treatment would lead to a fully stationary state. The difference between exact and approximate time dynamics is therefore expected to become less and less important as the system size grows.

The steady state is not unique for a given final external field, \textit{i.e.} it depends on how the perturbation is switched on. With an adiabatic turn-on we reach the ground state of system with an onsite energy corresponding to the final external final, in accordance with the adiabatic theorem. If the perturbation is switched on suddenly we reach a non-physical steady state with the same energy as at \( t = 0^+ \). The non uniqueness of the steady state is of great importance.
as it implies multiple solutions of the stationary KBE. In other words, given a final external potential, we have in principle infinitely many solutions to the stationary KBE.

The MBAs used here are entirely defined by a generating functionals $\Phi[G]$ and the corresponding set of self-consistent KBE for $G$: thus, strictly speaking, there is no direct connection to underlying wave-functions. Therefore, there is no built-in guarantee that for instance systems in a finite phase space only can have a finite number of excited states, and that they do not exhibit spurious stationary states in time dynamics.

In finite systems, all self-consistent MBAs, which include partial infinite-order summations, will include diagrams for the self energy which annihilate more holes/particles than those which can be accommodated. In an “exact” theory, all these unphysical contributions will give no net contribution, but this perfect cancellation will in general not occur in approximate schemes like the GWA or the TMA. We saw above that these self-consistent infinite summations give spectral functions with incorrect pole structure, with discrete but infinitely many poles. In the time dynamics these unphysical aspects of our MBAs manifest themselves as a reservoir to which our system becomes attached, and this leads to damping.

![Figure 10](image.png)

**Figure 10.** Time dependent densities for Born approximations with different levels of self consistency for $L = 2, n = 1/2, U = 1, w_0 = 5$: $\text{BA}_0$ (black), $\text{BA}_{\text{HFA}}$ (thick orange) and $\text{BA}$ (thick blue).

To show the effect of an increasing level of self consistency on the dynamical behaviour, we discuss in Fig. (10) three particle-conserving versions of the BA [35]. If, in the BA (or GWA), we evaluate the polarisation with ground-state propagators ($\text{BA}_0$), the density does not damp. If we now instead evaluate the polarisation with propagators in the time-dependent HFA approximation ($\text{BA}_{\text{HFA}}$), we obtain a partially damped solution. If we allow for full self consistency (BA), finally, the solution damps. In conclusion we see that if all $G$s that build up the self energy move consistently with the external field we reach a steady state [36].

The damping mechanism is inherent to the time propagation scheme and is not consequence of the infinite number of poles in the initial state. To unambiguously illustrate this point, we performed a calculation initialised with the non-interacting propagator $G_0$, which has a finite
number of poles (this calculation corresponds to a sudden switch-on of the interaction as well as of the external field). In Fig. (11) we clearly see that the non-interacting initial state gives rise to a very similar damped density profile. It is worth noting that the curves in Fig. (11), which closely resemble each other, indicate a robustness of the KBE evolution against the initial conditions.

9. Beyond the Hubbard $U$: long range interactions

An obvious extension of the simple Hamiltonian of Eq. (1) is the inclusion of long range model interactions. These can modify the behaviour of the system in a non trivial way, for example altering/inducing a charge/spin order, affecting the screening response, etc. Most of the features induced by these additional interactions depend considerably on specific details, such as the lattice coordination number, the actual range of the interaction, its functional dependence on the inter-particle distance, etc. However, other aspects of the long range interactions can be rather general in character. For example, let us consider an additional term of the form $\frac{1}{2} \sum_{RR',\sigma\sigma'} v_{RR'} a^\dagger_{R\sigma} a_{R'\sigma'} a_{R'\sigma'} a^\dagger_{R\sigma}$, where $R \neq R'$. If we examine the effects of this term for a Hubbard dimer with two particles with opposite spin, where $R, R' = 1, 2$, the off-site interaction energy $v_{12}$ leads exactly to an energy shift of $v_{12}/2$ and a renormalisation $U \rightarrow |U - v_{12}|$. One can also consider an infinite system with an infinite-range, constant interaction $v_{R \neq R'} = v_\infty$ (compensated by a similar uniform jellium-like background). In this case too, the system reduces to one where the non trivial part of the interaction is entirely local, with strength $|U - v_\infty|$. Those just discussed are two rather extreme examples; however, some support to the notion that long range interactions may somewhat diminish the role of the local term $\hat{U}$ comes also from an exact solution for two particles on a lattice with long-range (but not constant) interactions [37]. Results in [37] showed that, in the presence of a local interaction $\hat{U}$ plus offsite terms, the two particle spectral function can be fairly described by another Hamiltonian with purely on-site

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**Figure 11.** Time dependent densities for the GWA, initialised with the self-consistent GWA ground state (black) and the non-interacting $G_0$ (thick orange).
interaction $U' < U$. Another result emerging from such a study was that, in the presence of strong enough offsite interaction (schematically, when $v$/bandwidth $\gg 1$), two-particle repulsive bound states are formed, which are not purely local in character. Thus, we would expect that in the low density regime, if $v$/bandwidth $\gg 1$, the TMA would produce a satellite structure in the one-particle spectral density which would correspond to a two-body resonance delocalised in space. This should also affect the non-equilibrium behaviour. We argue that the latter two features (reduction of the onsite interaction, and delocalised bound states) could be quite general effects induced by offsite interactions; nevertheless, their detailed analysis is beyond the scope of this paper, and thus deferred to future work.

10. Conclusions and outlook
In this paper, we have studied the non-equilibrium KBE dynamics of clusters with strong correlation within the HFA, the BA, the GWA and the TMA and compared with an exact treatment. We have shown that the TMA performs very well for low fillings and is in general superior to the GWA and the BA. We have also discussed the limitations of conventional MBAs for finite systems. In particular, we observed an unphysical steady state solution of the KBE with approximate self-consistent schemes based upon partial summations. We argue that this is a general result when applying infinite order perturbation theory to finite systems. We have found that the artificial damping is inherent to the self-consistent MBA’s time dynamics and that it is insensitive to the initial Green’s function, i.e., to the initial correlations. The approximations which damp most strongly are generally those which are also poor in describing the short-time dynamics.

The present work may be extended in several different directions. A first direction is to try to cure the KBE dynamics from the artificial damping without breaking the link with MBPT and the possibility of systematic expansions. A way to do this could be to use the variational properties of the underlying $\Phi$ functional and determine the corresponding TDDFT potentials via the Sham-Schlüter equation. At full self-consistency nothing has been gained - the TDDFT dynamics would reproduce the damped KBE dynamics. However, by relaxing the full self-consistency and use optimised one-particle $G$ when constructing the exchange correlation potential, $v_{xc}$ [38, 39] we expect that the artificial damping will be reduced or removed without seriously deteriorating the short-time dynamics. In the BA approximation, this corresponds essentially to use a (time-) optimised independent-particle $G$ for constructing the self-energy and $v_{xc}$; we saw in section 8 that the damping is indeed reduced. The idea to construct approximate TDDFT potentials from variational MBPT may also be very useful on its own and makes it possible to treat larger and more complex systems.

A second direction is to benchmark approximate TD dynamics also for systems attached to external leads by comparing approximate KBE results with those of time-dependent density-matrix renormalisation group calculations, [40], or other non-perturbative schemes. Work along these lines is currently under way.

As a third line of investigation we note that, at present, time-dependent KBE numerical calculations are relatively heavy. In this work we have used higher order formulae for time propagation and integration in order to speed up the calculations. To treat realistic systems, however, much further work on algorithms is required to make the calculations feasible.

Finally, the KBE are equally suitable for bosonic degrees of freedom. In transport phenomena vibrations often play an crucial role, and it would be interesting to study vibronic coupling (on the model level in the initial phase) to shed more light on these problems.

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