Kadanoff-Baym equations and approximate double occupancy in a Hubbard dimer.

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This brief note reports of preliminary results on the use of the Kadanoff-Baym Equations (KBE)\cite{Paper1} to compute double occupancies. The case discussed here is that of a Hubbard dimer, described by the time-dependent Hamiltonian:

\[
H = \sum_\sigma \left( -U^\gamma a_\sigma^\dagger a_\sigma^\dagger - U a_\sigma^\dagger a_\sigma + w(t) n_\sigma \right) + U \sum_{R=1,2} \hat{n}_R \hat{n}_{R^\dagger}, (1)
\]

where \(U\) is the on-site and interaction, \(\hat{n}_R = a_{R^\dagger} a_R\) and \(\sigma = \uparrow, \downarrow\). The term \(w(t)\) is a time-dependent, spin-independent field; in \(H\), all parameters are in units of the magnitude of the hopping term (the latter is taken \(= -1\)).

In the, \(t = 0\), initial state the dimer contains two electrons with opposite spin; this remains true at all times, since \(H\) has no spin-flip terms.

The study of this simple system reveals a shortcoming of the KBE when they are used together with many-body approximations (MBA:s). Following a route based on the equations of motion of the single-particle Green’s function, some conserving MBA:s (namely, the second Born approximation, BA, and the GW approximation, GWA) may give negative double occupancies \(\langle \hat{n}_R \hat{n}_{R^\dagger} \rangle\) which is clearly unphysical. The results obtained with the \(T\)-matrix approximation (TMA) are exempt from this problem. This is no accident, and in fact we provide an analytical proof of why, in the TMA, local double occupancies are intrinsically positive.

**Kadanoff-Baym equations.** - The KBE govern the time evolution of the non-equilibrium, two-time, single-particle Green’s function \(G(1,2) = -i\langle T_\gamma [\psi(1)\psi^\dagger(2)] \rangle\), where \(1\) denote single particle space/spin and time labels, \(\tau_1, \sigma_1, t_1\). Here, \(T_\gamma\) orders the times \(t_1, t_2\) on the Keldysh contour \(\gamma\) and the field operators are in the Heisenberg picture; the brackets \(\langle \rangle\) denote averaging over the initial state (or thermal equilibrium). Showing explicitly only the time labels (matrix notation/multiplication in space and spin indices is adopted), and specializing to time \(t_1\), we have \(\langle i\partial_{t_1} - h(t_1) \rangle G(t_1, t_2) = \delta(t_2 - t_1) + \int_\gamma \Sigma(t_1, t) G(t, t_2) dt\). Here \(h\) is the single particle Hamiltonian and \(\Sigma\), the kernel of the integral equation, is the self energy, which accounts for the interactions and is described within a given MBA, as discussed below. The initial state is the correlated ground state (we work at temperature, \(1/\beta \to 0\)), obtained by solving the Dyson equation \(G = G_0 + G_0 \Sigma[G] G\) self consistently, with \((\epsilon - h)G_0 = 1\). In practice we solve these equations using an algorithm discussed in\cite{Paper2}.

The MBA:s we consider are all conserving\cite{Paper3}, i.e. quantities such as the total energy, the number of particles and momentum are constant during the time evolution. The self energy in the BA includes all diagrams up to second order. The GWA amounts to add up all the bubble diagrams which give rise to the screened interaction, \(W = U + UFW\), where \(P(12) = G(12)G(21)\). In this case the self energy is \(\Sigma(12) = G(12)W(12)\). In the TMA one constructs the \(T\) by adding up all the ladder diagrams, \(T = \Phi - \Phi UT\), where \(\Phi(12) = G(12)G(12)\). The expression of the self energy then becomes \(\Sigma(12) = U^2G(21)T(12)\). For a detailed account of the different MBA:s see e.g.\cite{Paper4}.

**Double occupancy from the KBE.** - While in principle \(G\) gives access only to expectation values of one-body operators, its equations of motion (i.e., the KBE) permit to obtain also some quantities which involve expectation values of two-body operators, such as, e.g., the total energy. This route can be also used for the double occupancy \(d_R \geq 0\); for on-site \((U_R \neq 0)\) interactions,

\[
d_R = \langle \hat{n}_R \hat{n}_{R^\dagger} \rangle = -\frac{i}{U_R} \int_\gamma \Sigma(13) G(31^+) d\beta \]

Fig. 1 shows the time-dependent double occupancy on site 1 for \(U = 2\) and \(w(t) = w_0 \theta(t)\), where \(w_0 = 3\). We see that the ground state (\(t = 0\)) has positive double occupancies for all approximations while the BA and the GWA become negative after some time. This unphysical behavior is a drawback that these two MBA:s can have. According to Fig. the TMA, among the examined MBA:s, is the only one giving always positive correlation functions.

**Positiveness of the \(T\)-matrix.** - All the MBA:s used in this work are conserving. This, however, does not guarantee that other properties (e.g. spectral features or response functions) obtained with such MBA:s automatically satisfy further basic criteria. In fact, for our dimer, density correlations and pair correlations for GWA and BA may violate the positiveness condition: \(\langle \psi^\dagger(1)\psi^\dagger(2)\psi(2)\psi(1) \rangle \geq 0\). The pair correlation function is a rather sensitive measure of the quality of a MBA.
It has been known for a long time that the Random-Phase-Approximation (RPA) in the ground state gives pair correlations which, at metallic densities, are strongly negative at short distances. Later on, negative pair correlations at short distances were also found within the self-consistent GWA.

Would the situation improve if the response function was calculated self-consistently from changes in $\Sigma$ and thereby via the Bethe-Salpeter equation? Such response function fulfills all macroscopic conservation laws, but not necessarily yields pair correlation functions everywhere positive. For example, the RPA discussed above is the response function in the Kadanoff-Baym sense of the conserving Hartree approximation but it violates the positiveness condition.

We now turn specifically to the TMA, to show why this approximation the pair correlation is manifestly positive. In the ground state, for the TMA, the pair correlation is given by

$$\langle \hat{n}_{Rt} \hat{n}_{Rl} \rangle = -i T_{RR}(t, t^+) = -i T_{RR}(t, t^+),$$

(here $>$ ($<$) refers to the electron (hole) part) and its positiveness is a consequence of the positiveness of the T-matrix spectral function. The basic building block in the TMA is $\Phi_{RR'} = -i G_{RR'}(t - t') G_{RR'}(t - t')$. In Fourier space we have

$$\Phi_{RR'}(\epsilon) = \int \frac{C_{RR'}(\epsilon') \epsilon'}{\epsilon - \epsilon' + i\eta \text{sgn}(\epsilon' - 2\mu)},$$

where the spectral function $C_{RR'}$ is given by

$$C_{RR'}(\epsilon) = \int_{\epsilon-\mu}^{\epsilon+\mu} A_{RR'}(\epsilon') A_{RR'}(\epsilon - \epsilon') d\epsilon'.$$

Thus, $C_{RR'}(\epsilon)$ is positive (negative) definite for $\epsilon < 2\mu$ ($\epsilon > 2\mu$). The Dyson equation for the $T$-matrix is

$$\hat{T}(\epsilon) = \hat{\Phi}(\epsilon) - \hat{\Phi}(\epsilon) \hat{\Upsilon}(\epsilon) (\text{here } \hat{\Phi}, \hat{T}, \hat{\Upsilon} \text{ are matrices in site indices, and } \hat{U}_{RR'} = \hat{U}_{R} \delta_{RR'}).$$

This gives

$$\hat{T}^S = \hat{\Phi}^S - \hat{\Phi} \hat{\Upsilon}^a - \hat{\Phi}^\dagger \hat{\Upsilon}^S,$$

$$(1 + \hat{\Phi}^\dagger \hat{\Upsilon}) \hat{T}^S = \hat{\Phi}^S (1 - \hat{\Upsilon}^a),$$

and

$$\hat{T}(\epsilon) - \hat{T}^\dagger(\epsilon) = [1 - \hat{T}^r(\epsilon) \hat{\Upsilon}] [\hat{\Phi}(\epsilon) - \hat{\Phi}^\dagger(\epsilon)] [1 - \hat{\Upsilon}^a(\epsilon)],$$

where we have used the identity $(1 - \hat{\Upsilon}) (1 + \hat{\Phi} \hat{\Upsilon}) = 1$. The $T$-matrix has thus the spectral decomposition

$$\hat{T}(\epsilon) = \int \frac{\hat{D}(\epsilon') d\epsilon'}{\epsilon - \epsilon' + i\eta \text{sgn}(\epsilon' - 2\mu)},$$

where $\hat{D}(\epsilon) = [1 - \hat{T}^r(\epsilon) \hat{\Upsilon}] [\hat{C}(\epsilon) [1 - \hat{\Upsilon}^a(\epsilon)]]$. Consequently, $\hat{D}(\epsilon)$ is positive definite for $\epsilon < 2\mu$, and

$$\langle \hat{n}_{R} \hat{n}_{R} \rangle = -i T_{RR}(t, t^+) = \int_{-\infty}^{2\mu} D_{RR}(\epsilon') d\epsilon' \geq 0 . \quad (5)$$

The above result remains valid i) for a general two-body interaction $u(r_1 - r_2) \delta(t_1 - t_2)$, provided we use a symmetrized TMA which includes both direct and exchange ladder diagrams; ii) in the presence of an external field for $t > 0$. In this case, the proof is similar to the proof that manifestly positive $\mp i \Sigma^S$ give manifestly positive $\mp i G^S$ via the KBE.

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