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Relaxation of a quantum many-body system from a correlated initial state. A general and consistent approach

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Various approaches to a theoretical treatment of the dynamics of quantum many-body systems starting from a correlated initial state are discussed. In particular, we compare the concept of the BBGKY–hierarchy (single-time reduced density operators) and that of nonequilibrium Green's functions (two-time correlation functions). Conditions for physically meaningful initial correlations are established.

1 Introduction

In recent years the interest in strongly correlated many-body systems and their dynamics has increased substantially triggered by the experimental progress in producing Bose condensates, Wigner crystals, dusty and colloidal plasmas etc. Most theoretical work so far has been able to explain equilibrium or linear response properties, e.g. [1, 2], leaving the treatment of nonequilibrium dynamics and short-time phenomena open.

Though most traditional treatments of quantum many-body systems neglect the influence of initial correlations on the time evolution, the importance of this problem has been realized from the very beginning, e.g. [3]. Formally this question is almost trivial in kinetic theories for single-time statistical quantities based on the BBGKY-hierarchy, e.g. [4, 5]. However, in nonequilibrium Green's functions, the non-trivial time structure renders this problem essentially more difficult. In the 1970s and 1980s remarkable progress has been made by Hall [6], Tikhodeev [7], Danielewicz [8] and others who discussed how to convert the initial correlation information into additional selfenergy contributions acting as new driving terms in the dynamics of the two-time correlation functions. Most of these considerations, however, concentrated on the effect of ground state or equilibrium correlations. In recent papers [9, 10, 11] we have further developed this idea and presented a novel completely general derivation on the basis of the Martin–Schwinger hierarchy which is valid for arbitrary initial states.

Nevertheless, a variety of questions is still open as recently noted by Martin [12] and Keldysh [13]. This includes the problem of how to distinguish physically relevant from unphysical initial states and how about the equivalence of the single-time and two-time theories. In this paper we address these two questions and critically assess previous works.

2 Initial correlations in single-time kinetic theory

As noted above, the problem of initial correlations is readily handled in the framework of the BBGKY hierarchy and all physical questions are most easily discussed here. Decoupling this hierarchy at any level n leads to a system of n first order[1] differential equations for the single-particle statistical operator F_1 and the correlation coperators g_{12}, g_{123},..., $g_{1\ldots n}$. This system requires as a boundary condition n conditions for the n functions. As the special case of interest to us we may limit ourselves to given values for each function at a certain time t_0:

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[1] Only the time-dependence is of relevance for the present discussion.

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$F_1(t_0), ..., g_{1...n}(t_0)$. Moreover, all problems are understood already on the level of binary correlations where either $g_{123} = ... = g_{1...n} \equiv 0$ or all three-particle and higher order operators are known functionals of F_1 and g_{12} (the actual functional form is defined by the actual decoupling approximation).

Then the dynamical problem is formulated according to (for the inclusion of spin statistics effects, see [5, 14])

$$i\hbar\frac{\partial}{\partial t}F_1 - \left[\bar{H}_1, F_1\right] = n\mathrm{Tr}_2\left[V_{12}, g_{12}\right], \qquad F_1(t_0) = F_1^0, \tag{1}$$

$$i\hbar\frac{\partial}{\partial t}g_{12} - \left[\bar{H}_{12}, g_{12}\right] = [V_{12}, F_1F_2] + n\mathrm{Tr}_3\left\{[V_{13}, F_1g_{23}] + [V_{23}, F_2g_{13}] + [V_{13}+V_{23}, g_{123}]\right\}, \tag{2}$$

with $g_{12}(t_0) = c_0$ describing correlations existing in the system at time $t = t_0$ and the effective Hamiltonians (U_1^H denotes the Hartree (mean field) potential)

$$\bar{H}_1 = H_1 + U_1^H, \qquad \bar{H}_{12} = \bar{H}_1 + \bar{H}_2 + V_{12}. \tag{3}$$

The equation for g_{12} can be solved formally . The solution reads e.g. in second Born approximation, i.e. neglecting three-particle correlations, g_{123}, ladder terms [V_{12} in $\bar{H}_{12}$] and polarization terms [second and third term on the r.h.s. of Eq. (2), for solutions beyond the Born approximation see [5, 14]] , for $t \geq t_0$,

$$g_{12}(t) = U_{12}^{0\mathrm{R}}(tt_0)\, c_0\, U_{12}^{0\mathrm{A}}(t_0t) + \frac{1}{i\hbar}\int_{t_0}^{\infty} d\bar{t}\, U_{12}^{0\mathrm{R}}(t\bar{t})\left\{\hat{V}_{12}F_1F_2 - F_1F_2\hat{V}_{12}^{\dagger}\right\}\Big|_{\bar{t}} U_{12}^{0\mathrm{A}}(\bar{t}t), \tag{4}$$

where the propagators are two-time functions (mathematical Green's functions) obeying a simpler equation of motion with a delta inhomogeneity[2], and $\hat{V}_{12}$ is the shielded potential, $\hat{V}_{12} = (1 \pm nF_1 \pm nF_2)V_{12}$, [5, 14]. Solution (4) contains a (rapidly decaying) initial correlation term and a contribution describing correlation build up due to collisions, e.g. [4, 5]. Inserting this solution into Eq. (1) yields a closed kinetic equation for F_1 with the traditional (non-Markovian) collision integral I plus an additional collision term I^{IC} containing c_0 [5],

$$i\hbar\frac{\partial}{\partial t}F_1(t) - \left[\bar{H}_1, F_1(t)\right] = I(t) + I^{\mathrm{IC}}(t). \tag{5}$$

In these equations, so far, the initial moment t_0 and the shape of c_0 are completely arbitrary. The simplest case is that of thermodynamic equilibrium (or ground state) correlations c^{EQ} which arise in a many-body system in the absence of external perturbations after a sufficiently long time (practically, this time is rather short and given by the correlation time τ_{cor}). In most cases c^{EQ} is known or can be computed from simpler equilibrium theories. Alternatively, it is always possible to design a real physical process (or a "gedankenexperiment") which produces the state c^{EQ} beginning from uncorrelated particles. For example, in a semiconductor this real process is optical excitation or electrical injection of electrons (holes) which are produced mutually uncorrelated (although this is not always the case, see below) and build up their correlations due to collisions within the correlation time. In general we can always think of an initial state where all particles are so far apart that all interactions are negligible and then bring them together by some external (real or ficticious) force which has vanished by the time t_0.

From these considerations we conclude that, to be physically meaningful, an initial correlation $c_0 = g_{12}(t_0)$ must include the possibility to be produced by an earlier evolution which starts from an uncorrelated state[3] at $t = t_-$ in the remote past, or as early as $t_0 - \tau_{\mathrm{cor}}$, see Fig. 1. The only requirement is that this physical process is included into the theoretical model. This consideration is, of course, not limited to equilibrium initial correlations. We may equally choose any nonequilibrium state existing in the system between $t = t_-$ and t_0. Then we can create the many-particle state at any time $t > t_0$ by many ways, for example, (a) by starting from an uncorrelated state at $t = t_-$, $g_{12}^a(t_-) = 0$ or, (b) by starting at $t = t_0$ using the correlations formed earlier, during the time

[2] $U^{0\mathrm{R(A)}}(t,t')$ is a retarded (advanced) propagator which is identically zero for $t < t'$ ($t > t'$) related by $[U^{0\mathrm{A}}(t,t)]^* = U^{0\mathrm{R}}(t,t')$

[3] Here we do not consider long-living correlations, but our discussion is readily generalized to this case.

interval $[t_-, t_0]$, as "initial" correlations:

$$g_{12}^{(a)}(t) = \frac{1}{i\hbar}\int_{t_-}^{\infty} d\bar{t}\, U_{12}^{0\mathrm{R}}(t\bar{t})\left\{\hat{V}_{12}F_1F_2 - F_1F_2\hat{V}_{12}^{\dagger}\right\}\Big|_{\bar{t}} U_{12}^{0\mathrm{A}}(\bar{t}t), \tag{6}$$

$$g_{12}^{(b)}(t) = U_{12}^{0\mathrm{R}}(tt_0)\, c_0\, U_{12}^{0\mathrm{A}}(t_0t) + \frac{1}{i\hbar}\int_{t_0}^{\infty} d\bar{t}\, U_{12}^{0\mathrm{R}}(t\bar{t})\left\{\hat{V}_{12}F_1F_2 - F_1F_2\hat{V}_{12}^{\dagger}\right\}\Big|_{\bar{t}} U_{12}^{0\mathrm{A}}(\bar{t}t). \tag{7}$$

The initial value c_0 in Eq. (7), i.e. the correlations built up at time t_0, is given by

$$g_{12}(t_0) = \frac{1}{i\hbar}\int_{t_-}^{\infty} d\bar{t}\, U_{12}^{0\mathrm{R}}(t_0\bar{t})\left\{\hat{V}_{12}F_1F_2 - F_1F_2\hat{V}_{12}^{\dagger}\right\}\Big|_{\bar{t}} U_{12}^{0\mathrm{A}}(\bar{t}t_0). \tag{8}$$

Inserting this result into Eq. (7), we immediately recognize that $g_{12}^{(a)}(t) = g_{12}^{(b)}(t)$ for any $t \geq t_0$ under the only condition that the propagators possess a semi-group property, i.e. for any three times $t_{i+2} > t_{i+1} > t_i > t_-$, $U^{0\mathrm{R}}(t_{i+2}, t_i) = U^{0\mathrm{R}}(t_{i+2}, t_{i+1})U^{0\mathrm{R}}(t_{i+1}, t_i)$, and similarly for $U^{0\mathrm{A}}$.

3 Initial correlations in the nonequilibrium Green's functions approach

Let us now consider the same problem in the framework of nonequilibrium Green's functions. The strength of this approach – the formal closure of the Martin–Schwinger hierarchy on the single-particle level by introduction of the selfenergy,

$$\int d2\, V(1-2)\, g_{12}(12, 1'2^+) = \int d\bar{1}\, \Sigma(1,\bar{1})\, g(\bar{1}, 1'), \qquad 1 \equiv \mathbf{r}_1, t, \tag{9}$$

unfortunately, makes the physical understanding of initial correlations less obvious than in the case of the BBGKY hierarchy. In fact, the whole dynamical problem is now reduced to finding the two correlation functions $g^{\gtrless}$ as a function of two times by solving the Kadanoff–Baym/Keldysh equations (KBE) [3, 15, 9, 10]

$$\left(i\hbar\frac{\partial}{\partial t} - \frac{p_1^2}{2m_1}\right) g^{\gtrless}(\mathbf{p}_1; t, t') = \int_{t_0}^{\infty} d\bar{t}\, \left[\Sigma^{\mathrm{R}}(\mathbf{p}_1; t, \bar{t}) g^{\gtrless}(\mathbf{p}_1; \bar{t}, t') + \Sigma^{\gtrless}(\mathbf{p}_1; t, \bar{t}) g^{\mathrm{A}}(\mathbf{p}_1; \bar{t}, t')\right] + I^{\mathrm{IC}}(\mathbf{p}_1; t, t'), \tag{10}$$

$$\left(-i\hbar\frac{\partial}{\partial t'} - \frac{p_1^2}{2m_1}\right) g^{\gtrless}(\mathbf{p}_1; t, t') = \int_{t_0}^{\infty} d\bar{t}\, \left[g^{\mathrm{R}}(\mathbf{p}_1; t, \bar{t}) \Sigma^{\gtrless}(\mathbf{p}_1; \bar{t}, t') + g^{\gtrless}(\mathbf{p}_1; t, \bar{t}) \Sigma^{\mathrm{A}}(\mathbf{p}_1; \bar{t}, t')\right] + I^{\mathrm{IC}^*}(\mathbf{p}_1; t', t), \tag{11}$$

generalized to include an initial correlation term I^{IC}. In Born approximation it is given by [9, 10] (for generalizations beyond the Born approximation, see [11])

$$I^{\mathrm{IC}}(\mathbf{p}_1; t, t') = -2i\hbar^5\mathcal{V}\int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\frac{d\mathbf{q}}{(2\pi\hbar)^3} V(\mathbf{q}) \times g^{\mathrm{R}}(\mathbf{p}_1 + \mathbf{q}; t, t_0) g^{\mathrm{R}}(\mathbf{p}_2 - \mathbf{q}; t, t_0)\, c(\mathbf{p}_1 + \mathbf{q}, \mathbf{p}_2 - \mathbf{q}, \mathbf{p}_1, \mathbf{p}_2; t_0)\, g^{\mathrm{A}}(\mathbf{p}_2; t_0, t) g^{\mathrm{A}}(\mathbf{p}_1; t_0, t'), \tag{12}$$

and $g^{\mathrm{R/A}}$ are the standard retarded/advanced Green's functions, cf. footnote 2. Alternatively, the initial correlation contribution can be expressed as an additional term in the selfenergy [9, 10]. Due to the inclusion of initial correlations, the equations are valid for an arbitrary finite initial time t_0. This is far more general than the commonly used Bogolyubov condition of weakening of initial correlations, where $\lim_{t_0 \to -\infty} c(t_0) = 0$ and, at the same time, the lower limit of the time integration of the collision integrals is set to $-\infty$.

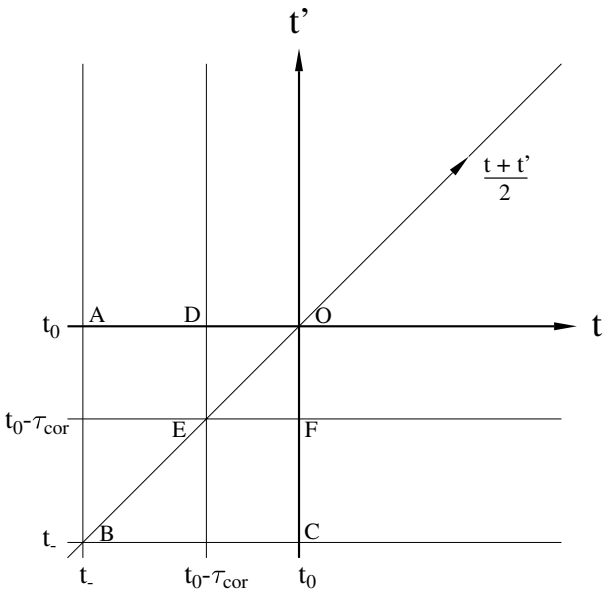

Fig. 1 Two-time plane in which the KBE (10–12) are solved. To start the evolution at the point O (t_0, t_0), in the general correlated initial state the knowledge of $g^{\gtrless}$ in the square $OABC$ is necessary. Equivalently, one can start at B (t_-, t_-) with an uncorrelated initial state and include the correlation buildup in the dynamics. The single-time dynamics, Eq. (5) is analogous, but proceeds along the time diagonal, line through B and O.

The structure of the KBE is analogous to Eq. (5). The main difference is that the evolution proceeds not only along a single-time axis but in a two-time plane, the diagonal of which corresponds to the time in Eq. (5). Now, what about the initial conditions which have to be provided to solve these equations? The mathematical answer is clear: to calculate $g^{\gtrless}$ in the quadrant $t, t' \geq t_0$ we need the one-particle correlation functions at $t = t' = t_0$, $g^{\gtrless}(t_0, t_0)$, and, in addition, the initial value of the two-particle correlation function, $c(t_0)$. But what is the connection between these two quantities? Can they be chosen independently and arbitrarily, or are there restrictions of physical nature as in the single-time case above?

In order to answer these questions, let us imagine to start a calculation at a time t_- in the remote past, i.e. at least with $t_- \leq t_0 - \tau_{\rm cor}$ (see Fig. 1, point B, and discussion in Sec. 2). At that time, the system is uncorrelated, i.e. $c(t_-) = 0$, and starts to evolve in time under the action of scattering and a possible excitation process. Imagine that the evolution is interrupted at $t = t' = t_0$ (point O). At this stage, $g^{\gtrless}$ are known in the whole square $OABC$. Now, there exist (at least) two possibilities to resume the evolution at t_0 (see the discussion in Sec. 2): (a) to continue the previous calculation as if it would not have been interrupted, or (b) to condense the information obtained so far in an "initial" correlation $c(t_0)$ and start at $t = t' = t_0$ a new calculation including the additional collision integral $I^{\rm IC}$.

If we require the two ways to be consistent with each other, we get from the system (10–12) the condition

$$
\begin{aligned}
&-2i\hbar\mathcal{V}\int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\frac{d\mathbf{q}}{(2\pi\hbar)^3}V(\mathbf{q})c(\mathbf{p}_1+\mathbf{q},\mathbf{p}_2-\mathbf{q},\mathbf{p}_1,\mathbf{p}_2;t_0) = \\
&= \int_{t_-}^{t_0} d\bar{t}\,\left[\Sigma^{>}(\mathbf{p}_1;t_0,\bar{t})g^{<}(\mathbf{p}_1;\bar{t},t_0) - \Sigma^{<}(\mathbf{p}_1;t_0,\bar{t})g^{>}(\mathbf{p}_1;\bar{t},t_0)\right]. \qquad (13)
\end{aligned}
$$

This is our main result which allows us to construct the function $c(t_0)$ from the information obtained from an arbitrary evolution preceding t_0. Further, Eq. (13) shows which single-time information is required: we need $g^{\gtrless}$ and $\Sigma^{\gtrless}$ on the two lines $\overline{OA}$ and $\overline{OC}$[4]. Furthermore, keeping in mind the fact that the memory depth of the

[4] In fact, due to the symmetry $g^{\gtrless}(t,t') = -\left[g^{\gtrless}(t',t)\right]^*$, $\Sigma^{\gtrless}(t,t') = -\left[\Sigma^{\gtrless}(t',t)\right]^*$, one of these lines is sufficient.

system is limited by the correlation time $\tau_{\rm cor}$, the span of the time integration in (13) is reduceed and one needs to know the quantities only on the lines $\overline{OD}$ and $\overline{OF}$.

The problem is simplified if we consider the selfenergies in second Born approximation,

$$\Sigma^{\gtrless}(\mathbf{p}_1,t,t') = 2\hbar^2 \int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\frac{d\mathbf{q}}{(2\pi\hbar)^3}\,|V(\mathbf{q})|^2\, g^{\gtrless}(\mathbf{p}_1+\mathbf{q};t,t')g^{\gtrless}(\mathbf{p}_2-\mathbf{q};t,t')g^{\lessgtr}(\mathbf{p}_2;t',t). \quad (14)$$

In that case, the initial correlation $c(t_0)$ can be obtained explicitly from (13):

$$c(\mathbf{p}_1+\mathbf{q},\mathbf{p}_2-\mathbf{q},\mathbf{p}_1,\mathbf{p}_2;t_0) = \frac{i\hbar}{\mathcal{V}}\int_{t_-}^{t_0} d\bar{t}\,V(\mathbf{q})\,\big[g^{>}(\mathbf{p}_1+\mathbf{q},t_0,\bar{t})g^{>}(\mathbf{p}_2-\mathbf{q},t_0,\bar{t})g^{<}(\mathbf{p}_2;\bar{t},t_0)g^{<}(\mathbf{p}_1;\bar{t},t_0)$$
$$-g^{<}(\mathbf{p}_1+\mathbf{q},t_0,\bar{t})g^{<}(\mathbf{p}_2-\mathbf{q},t_0,\bar{t})g^{>}(\mathbf{p}_2;\bar{t},t_0)g^{>}(\mathbf{p}_1;\bar{t},t_0)\big]\,. \quad (15)$$

Thus, in Born approximation the knowledge of $g^{\gtrless}$ on the two lines $\overline{OA}$ and $\overline{OC}$ (or $\overline{OD}$ and $\overline{OF}$) is sufficient.[5] Our approach equally applies to a variety of other scattering processes including carrier–phonon and electron–impurity scattering. More details will be given in [16].

In summary, there exist two alternative approaches to describe the influence of initial correlations on the dynamic evolution: (a) to explicitly include the build-up of correlations into the calculations (this was done e.g. for an electron gas in [17] and for electron-hole plasmas in [18, 19]). However, in cases where this explicit description of the excitation process is not required because its result may be well-known [case (b)], one can use the latter to construct the initial correlation $c(t_0)$, allowing for a significantly more efficient calculation. This approach has been used for example in the short-time evolution of ultracold laser produced plasmas [20].

In this paper we have clearified the relation of the two concepts. We have shown that a correlated initial state can be characterized equivalently by one-particle quantities (correlation functions $g^{\gtrless}$ in a time square of length $\tau_{\rm cor}$ before t_0) or a two-particle quantity [pair correlation function c in a single time point (t_0,t_0)]. We have motivated the physical restrictions on the initial binary correlation $c(t_0)$: only those which can be produced from an uncorrelated state by a physical process are meaningful. This may be a real process (experiment), or a ficticous but physically reasonable procedure ("gedankenexperiment").

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[5] We note that for more general approximations for $\Sigma^{\gtrless}$, $g^{\gtrless}$ may be needed in the whole square $OABC$, or $ODEF$, respectively.