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Short-time dynamics with initial correlations

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The short-time dynamics of correlated systems is strongly influenced by initial correlations, giving rise to an additional collision integral in the non-Markovian kinetic equation. Exact cancellation of the two integrals is found if the initial state is thermal equilibrium, which is an important consistency criterion. Analytical results are given for the time evolution of the correlation energy, which are confirmed by comparisons with molecular dynamics simulations.

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Although the Boltzmann kinetic equation is successfully applied to many problems in transport theory, it has some serious shortcomings [1]. Among these, the Boltzmann equation cannot be used on short-time scales, where memory effects are important [2,3]. In such situations, a frequently used non-Markovian kinetic equation is the so-called Levinson equation [4,5]. One remarkable feature of this equation is that it describes the formation of correlations in good agreement with molecular dynamics simulations [6]. Nevertheless, the Levinson equation is incomplete for two reasons: (i) It does not include correlated initial states, and (ii) when the evolution of the system starts from the equilibrium state, the collision integral does not vanish, but gives rise to spurious time evolution. The latter point has been addressed by Lee *et al.* [7], who clearly show that from initial correlations there must appear terms in the kinetic equation which ensure that the collision integral vanishes in thermal equilibrium.

The aim of this Rapid Communication is to derive the contributions from initial correlations to the non-Markovian Levinson equation within perturbation theory. We will restrict ourselves to the Born approximation, which allows us to present the most straightforward derivation. The inclusion of higher order correlations can be found in Refs. [3,8–10]. The effect of initial correlations becomes particularly transparent from our analytical results, which may also serve as a benchmark for numerical simulations.

The outline of this paper is as follows. First we give the general scheme of inclusion of initial correlations into the Kadanoff and Baym equations in terms of the density fluctuation function. We show that initial correlations enter the kinetic equation as self-energy corrections and mean-field-like contributions in terms of the initial two-particle correlation function. An analytical expression for the time dependent correlation energy of a high temperature plasma is presented and then compared with molecular dynamics simulations.

To describe density fluctuations we start with the causal density-density correlation function [11]

$$L(121'2')=G_2(121'2')-G(11')G(22'), \tag{1}$$

where 1 denotes cumulative variables $(x_1,t_1,\ldots)$. $G(1,2)=1/i\langle T\Psi(1)\Psi(2)^+\rangle$ and $G_2(121'2')$ are the one- and two-particle causal Green's functions. Their dynamics follows the Martin-Schwinger hierarchy

$$\begin{aligned}\left[i\hbar\frac{\partial}{\partial t_1}+\frac{\left(\frac{\hbar}{i}\nabla_1\right)^2}{2m}-\Sigma_H(1)\right]G(1,1')&=\delta(1-1')+\int d3V(1,3)L(1,3,1',3^+),\\ \left[i\hbar\frac{\partial}{\partial t_1}+\frac{\left(\frac{\hbar}{i}\nabla_1\right)^2}{2m}\right]G_2(121'2')&=\delta(1-1')G(2,2')-\delta(1-2')G(2,1')\\ &\quad+\int d3V(1,3)G_3(1,2,3,1',2',3^+),\end{aligned} \tag{2}$$

where $V(1,2)$ is the interaction amplitude and $\Sigma_H(1)=\int d2V(1,2)G(2,2^+)$ is the Hartree self-energy.

Using for G_3 the polarization approximation

$$\begin{aligned}G_3(1231'2'3')=&G(11')G(22')G(33')\\&+G(11')L(232'3')+G(22')L(131'3')\\&+G(33')L(121'2'),\end{aligned} \tag{3}$$

leads to a closed equation for L, which is conveniently rewritten as integral equation

$$\begin{aligned}L(1,2,1',2')=&L_0(1,2,1',2')-G_H(1,2')G(2,1')\\&+\int d4G_H(1,4)G(4,1')\\&\times\int d3V(4,3)L(2,3,2',3^+),\end{aligned} \tag{4}$$

where $(G_H^R)^{-1}$ denotes the left-hand side of the first equation (2) and we have taken into account the boundary condition

$$(G_H^R)^{-1}L_0=0. \tag{5}$$

In the case that all times in Eq. (4) approach t_0, the right-hand side vanishes except L_0 which represents, therefore, the contribution from initial correlations. They propagate in time according to the solution of Eq. (5) [9],

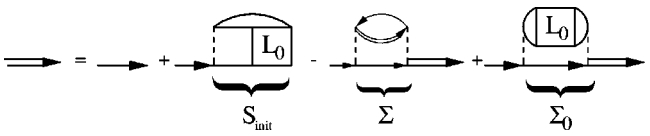

FIG. 1. Dyson equation including density fluctuation up to second Born approximation. Besides the initial correlation term $\mathcal{S}_{\rm init}$ discussed in [8,9], a new type of self energy Σ_0 appears which is induced by initial correlations. Since the latter one contains interaction by itself, this term is of next order Born approximation.

$$L_0(121'2') = \int dx_1 dx_2 dx_1' dx_2' G_H^R(1,x_1t_0) \times G_H^R(2,x_2t_0) L_{00}(x_1,x_2,x_1',x_2',t_0) \times G_H^A(1',x_1't_0) G_H^A(2',x_2't_0). \quad (6)$$

Here L_{00} is the initial two-particle correlation function.

Inserting Eq. (4) into the first equation of (2) and restricting to the Born approximation we obtain for the causal function $[G_{HF}^{-1}(1,2) = G_H^{-1}(1,2) + V(1,2)G^<(1,2)]$,

$$G_{HF}^{-1}(1,3)G(3,2) = \delta(1-2) + \mathcal{S}_{\rm init}(1,2) + \int_{\mathcal{C}} d4\{\Sigma_0(1,4) + \Sigma(1,4)\}G(4,2), \quad (7)$$

where the integration is performed along the Keldysh contour $\mathcal{C}$ with the self-energy in Born approximation

$$\Sigma(1,2) = \int d3d5 V(1,3) G_H(1,2) V(2,5) \times G_H(3,5^{++}) G(5,3^+). \quad (8)$$

Two new terms appear due to initial correlations,

$$\Sigma_0(1,2) = \int d3d5 V(1,3) G_H(1,2) V(2,5) L_0(3,5,3^+,5^{++}), \quad (9)$$

$$\mathcal{S}_{\rm init}(1,2) = \int d3 V(1,3) L_0(1,3,2,3^+).$$

The integral form of Eq. (7) is given in Fig. 1 from which definitions (9) are obvious.

The equation for the retarded Green's function $G^R(1,2) = -i\Theta(t_1-t_2)[G^>(1,2) + G^<(1,2)]$, where $G^<(1,2) = \langle \Psi^+(2)\Psi(1)\rangle$ and $G^>(1,2) = \langle \Psi(1)\Psi^+(2)\rangle$, is derived from Eq. (7) as

$$(G_{HF}^{-1} - \Sigma_0^R - \Sigma^R) G^R = \delta(1-2) + \mathcal{S}_{\rm init}^R(1,2) \quad (10)$$

and leads to the Kadanoff-Baym equation

$$(G_{HF}^{-1} - \Sigma^R)G^< - G^<(G_{HF}^{-1} - \Sigma^A) = (\Sigma + \Sigma_0)^< G^A - G^R(\Sigma + \Sigma_0)^< + \mathcal{S}_{\rm init} - \mathcal{S}_{\rm init}^*. \quad (11)$$

Using the generalized Kadanoff-Baym ansatz [12]

$$G^<(t_1,t_2) = iG^R(t_1,t_2)\rho(t_2) - i\rho(t_1)G^A(t_1,t_2), \quad (12)$$

we obtain the kinetic equation for the reduced density matrix $\rho(t) = G^<(t,t)$

$$\frac{\partial}{\partial t}\rho(k,t) = \mathcal{I}(k,t) + \mathcal{I}_0(k,t) + \mathcal{I}_1(k,t), \quad (13)$$

with

$$\mathcal{I}(k,t) = \frac{2}{\hbar^2}{\rm Re}\int_{t_0}^t dt_1 \int \frac{dqdp}{(2\pi\hbar)^6} V^2(q) G^R(t,t_1,k-q) \times G^A(t_1,t,k) G^R(t,t_1,p+q) G^A(t_1,t,p) \times [\rho(t_1,k-q)\rho(t_1,p+q)[1-\rho(t_1,p)] \times [1-\rho(t_1,k)] - \rho(t_1,k)\rho(t_1,p) \times \{1-\rho(t_1,p+q))[1-\rho(t_1,k-q)]\}, \quad (14)$$

$$\mathcal{I}_0(k,t) = \frac{2}{\hbar}{\rm Im}\int \frac{dqdp}{(2\pi\hbar)^6} V(q) G^R(t,t_0,k-q) \times G^A(t,t_0,k) G^R(t,t_0,p+q) G^A(t,t_0,p) \times \left\langle \frac{p-k}{2} + q | L_{00}(p+k,t_0) | \frac{p-k}{2} \right\rangle, \quad (15)$$

$$\mathcal{I}_1(k,t) = \frac{2}{\hbar^2}{\rm Re}\int_{t_0}^t dt_1 \int \frac{dq}{(2\pi\hbar)^3} \mathcal{L}_0(q,t,t_1) V^2(q) \times G^R(t,t_1,k-q) G^A(t_1,t,k) \times [\rho(t_1,k-q) - \rho(t_1,k)], \quad (16)$$

where $L_{00}(x_1,x_2,x_3,x_4) = \langle x_1 - x_2 | L_{00}[(x_1+x_2/2) - (x_3 + x_4/2)] | x_3 - x_4\rangle$ and $\mathcal{L}_0(q,t,t') = \int dx e^{-iqx}\langle x/2 | L_0(0) | x/2\rangle$. We like to note that Eq. (13) is valid up to second-order gradient expansion in the spatial coordinate. This variable has to be added simply in all functions and on the left-hand side of Eq. (13) the standard mean-field drift appears.

The first part [Eq. (14)] is just the precursor of the Levinson equation in second Born approximation $\sim V^2$. The term (16) coming from Σ_0 leads to corrections to the third Born approximation, since it is $\sim V^2\mathcal{L}_0$. A discussion of higher-order correlation contribution within the *T*-matrix approximation can be found in Refs. [2,10] and of general initial conditions in Ref. [13]. The second part [Eq. (15)] following from $\mathcal{S}$ gives just the correction to the Levinson equation, which will guarantee the cancellation of the collision integral for an equilibrium initial state. Recently, the analogous term in the collision integral has been derived by other means [9].

Multiplying the kinetic equations (13)–(15) with a momentum function $\phi(k)$ and integrating over k, one derives the balance equations

$$\langle \dot{\phi}(k)\rangle = \int \frac{dk}{(2\pi\hbar)^3}\phi(k)\mathcal{I} + \int \frac{dk}{(2\pi\hbar)^3}\phi(k)\mathcal{I}_0. \quad (17)$$

For the standard collision integral follows

$$\langle \phi(k)\mathcal{I}\rangle = \frac{1}{\hbar^2}\mathrm{Re}\int \frac{dkdqdp}{(2\pi\hbar)^9}\int_{t_0}^{t} dt_1 V^2(q) G^R(t,t_1,k-q) \times G^A(t_1,t,k) G^R(t,t_1,p+q) G^A(t_1,t,p) \times \rho(t_1,k-q)\rho(t_1,p+q)[1-\rho(t_1,p)] \times [1-\rho(t_1,k)]\{\phi(k)+\phi(p)-\phi(k-q) - \phi(p+q)\}, \quad (18)$$

from which it is obvious that density and momentum ($\phi = 1,k$) are conserved, while a change of kinetic energy $\phi = k^2/2m$ is induced which exactly compensates the two-particle correlation energy and, therefore, assures total energy conservation of a correlated plasma [14]. Initial correlations, Eq. (15), give rise to additional contributions to the balance equations [3,9]. We get

$$\langle \phi(k)\mathcal{I}_0\rangle = \frac{1}{4\hbar}\int \frac{dkdqdp}{(2\pi\hbar)^9} V(q) \times \left(\left\langle \frac{p-k}{2}+q \middle| L_0(p+k) \middle| \frac{p-k}{2} \right\rangle - \text{c.c.} \right) \times \{\phi(k)+\phi(p)-\phi(k-q)-\phi(p+q)\}, \quad (19)$$

which keeps the density and momentum also unchanged and only a correlated energy is induced. The self-energy corrections from initial correlations which correct the next Born approximation, (16), would lead to

$$\langle \phi(k)\mathcal{I}_1\rangle = \frac{2}{\hbar^2}\mathrm{Re}\int \frac{dkdq}{(2\pi\hbar)^6}\int_{t_0}^{t} dt_1 V^2(q) \times \mathcal{L}_0(q,t,t_1)\rho(t_1,k) G^R(t,t_1,k-q) G^A(t_1,t,k) \times \{\phi(k-q)-\phi(k)\}, \quad (20)$$

which shows that the initial correlations induce a flux besides an energy in order to equilibrate the correlations imposed initially towards the correlations developed during dynamical evolution if higher than $\sim V^2$ correlations are considered.

We will consider in the following only second Born approximation $\sim V^2$ and have therefore to use from Eq. (10)

$$G^R(t_1,t_2,k) \approx -i\Theta(t_1-t_2)\mathrm{e}^{i(k^2/2m\hbar)(t_2-t_1)}, \quad (21)$$

and for L_{00} the first Born approximation

$$\left\langle \frac{k-p}{2} \middle| L_{00}(k+p) \middle| \frac{k-p}{2}-q \right\rangle = -\frac{\mathcal{P}}{\Delta\epsilon} V_0(q)\{\rho_0(k)\rho_0(p)[1-\rho_0(k-q)] \times [1-\rho_0(p+q)] - [1-\rho_0(k)][1-\rho_0(p)] \times [\rho_0(k-q)\rho_0(p+q)]\}, \quad (22)$$

where $\mathcal{P}$ denotes the principal value, $\Delta\epsilon = k^2/2m + p^2/2m - (k-q)^2/2m - (p+q)^2/2m$ and ρ_0 the initial Wigner distribution. Then the explicit collision integral (14) reads

$$\mathcal{I}(k,t) = \frac{2}{\hbar^2}\int_{t_0}^{t} dt_1 \int \frac{dqdp}{(2\pi\hbar)^6} V^2(q)\cos\left[\left(\frac{k^2}{2m}+\frac{p^2}{2m} - \frac{(k-q)^2}{2m} - \frac{(p+q)^2}{2m} \right) \frac{(t-t_1)}{\hbar} \right] \times \{\rho(t_1,k-q)\rho(t_1,p+q)[1-\rho(t_1,p)-\rho(t_1,k)] - \rho(t_1,k)\rho(t_1,p)(1-\rho(t_1,p+q)-\rho[(t_1,k-q)]\} \quad (23)$$

and the new term due to initial correlations (15) is

$$\mathcal{I}_0(k,t) = -\frac{2}{\hbar^2}\int_{t_0}^{t} dt_1 \int \frac{dqdp}{(2\pi\hbar)^6} V(q)V_0(q)\cos\left[\left(\frac{k^2}{2m}+\frac{p^2}{2m} - \frac{(k-q)^2}{2m} - \frac{(p+q)^2}{2m} \right) \frac{(t-t_1)}{\hbar} \right] \{\rho_0(k-q) \times \rho_0(p+q)[1-\rho_0(p)-\rho_0(k)] - \rho_0(k)\rho_0(p) \times [1-\rho_0(p+q)-\rho_0(k-q)]\}. \quad (24)$$

To show the interplay between collisions and correlations, we have calculated the initial two-particle correlation function in the ensemble, where the dynamical interaction $V(q)$ is replaced by some arbitrary function $V_0(q)$. Therefore, the initial state deviates from thermal equilibrium except when $V(q) = V_0(q)$ and $\varrho(t_0) = \varrho_0$.

The additional collision term, $\mathcal{I}_0$, cancels exactly the Levinson collision term in the case that we have initially the same interaction as during the dynamical evolution ($V_0 = V$) and if the system starts from the equilibrium $\rho(t) \equiv \rho_0$. Therefore, we have completed our task and derived a correction of the Levinson equation that ensures the cancellation of the collision integral in thermal equilibrium [15].

On very short-time scales we can neglect the change in the distribution function. Assuming a Maxwellian initial distribution with temperature T and neglecting degeneracy, we can calculate explicitly the collision integrals and obtain analytical results. We choose as a model interaction a Debye potential $V_i(q) = 4\pi e^2\hbar^2/[q^2+\hbar^2\kappa_i^2]$ with fixed parameter $\kappa_i = \kappa_D$ and for the initial correlations $\kappa_i = \kappa_0$. We obtain for the change of kinetic energy on short times from Eqs. (18) and (19)

$$\frac{\partial}{\partial t}E_{\mathrm{kin}}(t) = \mathcal{E}[V(q)^2](t) - \mathcal{E}[V_0(q)V(q)](t), \quad (25)$$

which can be integrated [6] to yield

$$E_{\mathrm{kin}}(t) = E_{\mathrm{total}} - E_{\mathrm{init}}(t) - E_{\mathrm{coll}}(t). \quad (26)$$

For the classical limit we obtain explicitly the time dependent kinetic energy

$$\frac{E_{\mathrm{coll}}(t)}{nT} = -\frac{\sqrt{3}\Gamma^{3/2}}{4x}\partial_y[y\mathcal{F}(y)]_{y=x\tau}, \quad (27)$$

where $\mathcal{F}(y) = 1 - \mathrm{e}^{y^2}\mathrm{erfc}(y)$, $\tau = t\omega_p/\sqrt{2}$, $x = \kappa_D/\kappa$, and $\kappa^2 = 4\pi e^2 n/T = \omega_p^2 T/m$. The plasma parameter is given as usually by $\Gamma = e^2/a_e T$, where $a_e = (3/4\pi n)^{1/3}$ is the Wigner-Seitz radius.

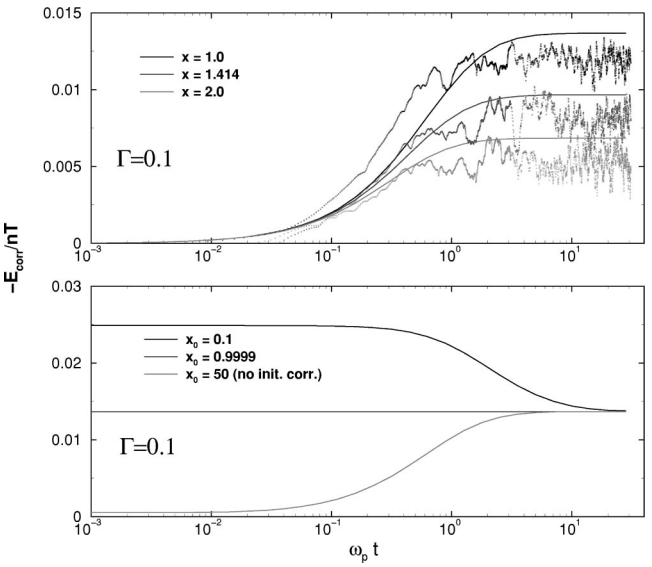

FIG. 2. Formation of correlation energy $-\mathcal{E}_{\rm corr}=\mathrm{E}_{\rm total}-\mathcal{E}_{\rm init}-\mathcal{E}_{\rm coll}=\mathcal{E}_{\rm kin}$ in a plasma with Debye interaction V_i. The upper panel compares analytical results (27) with MD simulations from [16] for three different ratios of κ_D to the inverse Debye length $x=\kappa_D/\kappa$. In the lower panel we compare theoretical predictions for the inclusion of Debye initial correlations characterized by $x_0=\kappa_0/\kappa$, where $x=\kappa_D/\kappa=1$.

In Fig. 2, upper panel, we compare the analytical results of Eq. (27) with MD simulations [16] using the Debye potential V_i as bare interaction. The evolution of kinetic energy is shown for three different ratios x. The agreement between theory and simulations is quite satisfactory; in particular, the short-time behavior for $x=2$. The stronger initial increase of kinetic energy observed in the simulations at $x=1$ may be due to the finite size of the simulation box, which could increasingly affect the results for increasing range of the interaction.

Now we include the initial correlations choosing the equilibrium expression (22), which leads to

$$\frac{E_{\rm init}(t)}{nT}=-\frac{\sqrt{3}\Gamma^{3/2}}{2(x_0^2-x^2)}[x\mathcal{F}(x\tau)-x_0\mathcal{F}(x_0\tau)], \qquad (28)$$

where $x_0=\kappa_0/\kappa$ characterizing the strength of the initial Debye correlations (22) with the Debye potential V_0 which contains κ_0 instead of κ_D. Besides the kinetic energy (28) from initial correlations, the total energy $E_{\rm total}$ (26) now includes the initial correlation energy, which can be calculated from the long-time limit of Eq. (27), leading to

$$\frac{E_{\rm total}}{nT}=\frac{\sqrt{3}\Gamma^{3/2}}{2(x+x_0)}. \qquad (29)$$

The result (26) is seen in Fig. 2, lower panel. We observe that if the initial correlation is characterized by a potential range larger than the Debye screening length, $x_0<1$, the initial state is overcorrelated, and the correlation energy starts at a higher absolute value than without initial correlations relaxing towards the correct equilibrium value. If, instead, $x_0=1$, no change of correlation energy is observed, as expected. Similar trends have been observed in numerical solutions [9].

In summary, in this Rapid Communication initial correlations are investigated within kinetic theory. Explicit correction terms appear on every level of perturbation theory correcting the non-Markovian kinetic equation properly in a way that the collision integral vanishes if the evolution starts from a correlated equilibrium state. Furthermore, the conservation laws of a correlated plasma are proven, including the contributions from initial correlations. It is shown that besides the appearance of correlation energy a correlated flux appears if correlations higher than Born are considered.

Deriving analytical formulas for high temperature plasmas allowed us to investigate the time dependent formation of the correlation energy and the decay of initial correlations. The comparison with molecular dynamics simulations is found to be satisfactory. Including initial correlations the cases of over- and undercorrelated initial states are discussed. While starting from equilibrium the correlation energy does not change; for over- and undercorrelated states the equilibrium value is approached after a time of the order of the inverse plasma frequency.

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[15] It is interesting to note that the corrections to the next Born approximation (16) due to initial correlations is of the type found in impurity scattering. Therefore, the initial correlations higher than $\sim V^2$ are governed by another type of dynamics than the buildup of correlations involved in $\mathcal{I}$ and $\mathcal{I}_0$.
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