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Formation of binary correlations in strongly coupled plasmas

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Abstract

Employing quantum kinetic equations we study the formation of binary correlations in plasma at short time scales. It is shown that this formation is much faster than dissipation due to collisions, and in hot (dense) plasma the correlations form on the timescale of inverse plasma frequency (Fermi energy). This hierarchy of characteristic times is used to derive analytical formulae for the time dependence of the potential energy of binary interactions which measures the extent of correlations. We discuss the dynamical formation of screening and compare this with the static screened result. Comparisons are made with molecular dynamic simulations. In the low temperature limit we find an analytical expression for the formation of correlation which is general for any binary interaction. It can be applied in nuclear situations as well as for dense metals.
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Recent lasers allow one to create a high density plasma within a few femtoseconds and observe its time evolution on a comparable scale [1,2]. Naturally, this plasma is highly excited at the beginning and relaxes towards equilibrium by various mechanisms that might be dominant at some stage and subdominant in another one. The best known regimes are the fast local equilibration of electron and hole distributions due to binary collisions, and the slow global relaxation via diffusion, recombination, dissipation of energy into the host crystal, etc. There are, however, even faster processes than the local equilibration. These processes dominate during the very first stage of the relaxation, the so-called transient regime. In this Letter we discuss the transient regime in terms of the energy balance.

The transient regime has been already discussed from many different angles and for various systems (classical–quantum, nondegenerate–degenerate). Let us briefly review some of these approaches. We will show that they are equivalent, at least with respect to the energy balance.

Conceptually the simplest is the molecular dynamics. One takes N particles, distributes them randomly into a box and let them classically move under Coulomb forces due to their own charges. Those particles which are very close will be expelled from each other. Their first movement thus forms correlations which lower the Coulomb energy $V_C = e^2/r$. This buildup of screening stops when the effective Debye potential $V_D = e^2 e^{-\kappa r}/r$ is reached. An important question is whether the long-range or the short-range charge fluctuations dominate in

this process. In the former case, the characteristic time of the transient period should be the inverse plasma frequency $\tau_c = 1/\omega_p$. In the latter case we do not know.

If one “measures” all states of the systems by their distance from equilibrium, instead of *formation* of correlations one has to talk about their *decay*. Our presumption that the transient period is appreciably shorter than the local relaxation is thus just Bogolyubov’s principle of decay of correlations. The decay of correlations is linked with an alternative approach to the transient period, the formation of quasi-particles which has been numerically studied within Green functions [3]. We note that a very similar transient behavior has been observed for the nuclear matter [4,5], i.e., the formation/decay of correlation is a rather general phenomenon.

The first concept is based on the two-particle space correlations while the second one is based on the single-particle excitations. The quantity which allows us to follow both pictures in a unified manner is the energy of the system. It is composed from the kinetic energy $\langle k^2/2m \rangle$ and the correlation energy $E_{\text{corr}} = \frac{1}{2} \langle V_D \rangle - \langle V_C \rangle$, where $\langle V_C \rangle$ subtracts the background. In lowest order interaction and classical limit the correlation energy takes the Debye–Hückel form

$$E_{\text{corr}} = \frac{1}{2} \lim_{r \rightarrow 0} [V_D(r) - V_C(r)] = -\frac{\kappa e^2}{2}. \quad (1)$$

Of course, the total energy is conserved,

$$E_{\text{corr}} = \left\langle \frac{k^2}{2m} \right\rangle_0 - \left\langle \frac{k^2}{2m} \right\rangle, \quad (2)$$

where $\langle k^2/2m \rangle_0$ is the initial value of the kinetic energy. We will monitor the time dependence of the transfer of the correlation energy into the kinetic energy.

It is more convenient to calculate the kinetic energy than the correlation energy because the kinetic energy is a single-particle observable. To this end we can use the kinetic equation, of course, an equation which leads to the total energy conservation (2). It is immediately obvious that the ordinary Boltzmann equation cannot be appropriate for this purpose because the kinetic energy is an invariant of its collision integral and thus constant in time. We have to consider non-Markovian kinetic equations of Levinson type [1],

$$\begin{aligned} \frac{\partial}{\partial t} f_a(t) &= \frac{2}{\hbar^2} \sum_b \int \frac{dp dq}{(2\pi\hbar)^6} V_D^2(q) \int_0^t d\bar{t} \exp\left(-\frac{t-\bar{t}}{\tau}\right) \cos\left(\frac{1}{\hbar}(t-\bar{t})\Delta_E\right) \\ &\times [f'_a f'_b (1-\bar{f}_a)(1-\bar{f}_b) - \bar{f}_a \bar{f}_b (1-f'_a)(1-f'_b)], \end{aligned} \quad (3)$$

where $\Delta_E = k^2/2m_a + p^2/2m_b - (k-q)^2/2m_a - (p+q)^2/2m_b$ denotes the energy difference between initial and final states. The retardation of distributions, $\bar{f}_a(k, \bar{t})$, $\bar{f}'_a(k-q, \bar{t})$, etc., is balanced by the lifetime τ . The total energy conservation (2) for Levinson’s equation has been proved in Ref. [6].

The full solution of Levinson’s equation on the long time scale is a difficult problem, however, its solution in the short-time region $t \ll \tau$ can be written down analytically. In this time domain we can neglect the time evolution of distributions, $\bar{f}_a(\bar{t}) = f_a(0)$, and the life-time factor, $\exp[-(t-\bar{t})/\tau] = 1$. Eq. (3) can be integrated with respect to the time and the internal time integration can be done. The resulting equation for $f(t)$ represents the deviation of Wigner’s distribution from its initial value, $f_a(t) = f_a(0) + \delta f_a(t)$, and reads

$$\delta f_a(t) = 2 \sum_b \int \frac{dp dq}{(2\pi\hbar)^6} V_D^2(q) \frac{1 - \cos(t\Delta_E/\hbar)}{\Delta_E^2} [f'_a f'_b (1-f_a)(1-f_b) - f_a f_b (1-f'_a)(1-f'_b)]. \quad (4)$$

This formula shows how the two-particle and the single-particle concept of the transient behavior meet in the kinetic equation. The right-hand side describes how two particles correlate their motion to avoid the strong interaction regions. Since the process is very fast, the on-shell contribution to δf_a , proportional to t/τ , can be

neglected in the assumed time domain and δf has a pure off-shell character as can be seen from the off-shell factor $\Delta_E^{-2} [1 - \cos(t\Delta_E/\hbar)]$. The off-shell character of the mutual two-particle correlation is thus reflected in the single particle Wigner’s distribution.

The very fast formation of the off-shell contribution to Wigner’s distribution has been found in numerical treatments of Green functions [4,5]. Once formed, the off-shell contributions change in time with the characteristic time τ , i.e., following the relaxation (on-shell) processes in the system. Accordingly, the formation of the off-shell contribution signals that the system has reached the state the evolution of which can be described by the Boltzmann equation, i.e., the transient period has been accomplished.

From Wigner’s distribution one can readily evaluate the increase of kinetic energy,

$$\left\langle \frac{k^2}{2m} \right\rangle - \left\langle \frac{k^2}{2m} \right\rangle_0 = \sum_a \int \frac{dk}{(2\pi\hbar)^3} \frac{k^2}{2m_a} \delta f_a. \tag{5}$$

After substitution for δf_a from (4), we symmetrize in k and p and anti-symmetrize in the initial and final states which yields the correlation energy (2) as

$$E_{\text{corr}}^{\text{static}}(t) = - \sum_{ab} \int \frac{dk dp dq}{(2\pi\hbar)^9} V_D^2(q) \frac{1 - \cos(t\Delta_E/\hbar)}{\Delta_E} f'_a f'_b (1 - f_a)(1 - f_b). \tag{6}$$

This expression holds for general distributions f_a .

Of course, starting with a sudden switching approximation we have a Coulomb interaction and during the first transient time period the screening is formed. This can be described by the non-Markovian Lenard–Balescu equation [7] instead of the static screened equation (3). With the same discussion as above we end up instead of (6) with the dynamical expression of the correlation energy,

$$E_{\text{corr}}^{\text{dynam}}(t) = - \sum_{ab} \int \frac{dk dp dq}{(2\pi\hbar)^9} \frac{V_C^2(q)}{|\epsilon(q, (p+q)^2/2m_b - p^2/2m_b)|^2} \left(\frac{(k-q)^2}{2m_a} - \frac{k^2}{2m_a} \right) \times \frac{1 - \cos(t\Delta_E/\hbar)}{\Delta_E^2} f'_a f'_b (1 - f_a)(1 - f_b). \tag{7}$$

One sees that the bare Coulomb interaction V_C is renormalized by the dielectric function

$$\epsilon(q, \hbar\omega) = 1 - \sum_b V_C(q) \int \frac{dp}{(2\pi\hbar)^3} \frac{f_b(p + \frac{1}{2}q) - f_b(p - \frac{1}{2}q)}{pq/m_b - \hbar\omega + i\eta}. \tag{8}$$

All internal time integrals are bound to the time dependence of $f(t)$ and in the spirit of the above discussion can be carried out.

To demonstrate its results and limitations, we discuss (6) and (7) for special cases that allow for analytical treatment. To this end we use equilibrium initial distributions. As the first test, let us evaluate the correlation energy in equilibrium which is approached for large times $t \rightarrow \infty$. The off-shell factor $(1/\Delta_E) [1 - \cos(t\Delta_E/\hbar)]$ then turns into the principal value $\wp/\Delta E$. The equilibrium distributions f_a are natural for this case.

In the high temperature limit, where the distributions are nondegenerate,

$$f_a = n_a \hbar^3 \left(\frac{2\pi}{m_a T} \right)^{3/2} \exp\left(-\frac{k^2}{2m_a T}\right), \tag{9}$$

one can evaluate (6) and (7) for the mixture of particles. We assume the plasma consisting of two different types of particles a, b with different masses m_a, m_b . Performing a series of integrals we obtain the correlation energies

$$E_{\text{corr}}^{\text{static}}(\infty) = -\pi \sum_{ab} \left(\frac{4m_a m_b}{(m_a + m_b)^2} \right)^2 \frac{e_a^2 e_b^2 n_a n_b}{\kappa T} [1 - \sqrt{\pi} b \exp(b^2) \text{erfc}(b)],$$

$$E_{\text{corr}}^{\text{dynam}}(\infty) = -\pi^{3/2} \sum_{ab} \left(\frac{4m_a m_b}{(m_a + m_b)^2} \right)^2 \frac{2e_a^2 e_b^2 n_a n_b}{b \kappa T} [1 - \exp(b^2) \text{erfc}(b)]. \quad (10)$$

The parameter $b^2 = (\hbar\kappa)^2(m_a + m_b)/8m_a m_b T$ controls quantum corrections. Formula (10) is the correlation energy in the second Born approximation of the statically screened Debye potential as well as the dynamically screened one. The latter corresponds to the known Montroll result in plasma physics [8,9].

For identical particles in the classical limit $b \rightarrow 0$, we see that the static approximation (6) or (10) underestimates the known value of the correlation energy [8,9] while the dynamical result (7) or (10) agrees with this Ward result,

$$E_{\text{corr}}^{\text{static}}(\infty) = -\frac{e^2 \kappa}{4} [1 - \sqrt{\pi} \text{erfc}(b)] = -\frac{1}{4} e^2 n \kappa + o(b),$$

$$E_{\text{corr}}^{\text{dynam}}(\infty) = -\frac{e^2 \kappa}{2} \frac{\sqrt{\pi}}{b} [1 - e^{b^2} \text{erfc}(b)] = -\frac{1}{2} e^2 n \kappa + o(b). \quad (11)$$

One can see that in the classical limit the static result is just one half of the correct Debye–Hückel one (1). The dynamical result yields the correct correlation energy. This difference can be understood in analogy to the field energy of a dipole in an external electric field. If the dipole is already present but has just to be ordered, we obtain half of the correlation energy we would have if the dipole is formed itself by the field. In our case the static result assumes that we have a Debye screening from the beginning before the interaction is switched on. The dynamical result counts properly for the fact that the screening has to be formed itself which results into twice the correlation energy.

In order to compare the time dependence of the correlation energy from (6) with molecular dynamical simulations [10], we assume a one component plasma which possesses a Maxwellian velocity distribution (9) during this formation time. From (6) and (7), we find

$$\frac{\partial}{\partial t} \frac{E_{\text{corr}}^{\text{static}}(t)}{n} = -\frac{e^2 \kappa T}{2\hbar} \text{Im} \left((1 + 2z^2) e^{z^2} [1 - \text{erf}(z)] - \frac{2z}{\sqrt{\pi}} \right),$$

$$\frac{\partial}{\partial t} \frac{E_{\text{corr}}^{\text{dynam}}(t)}{n} = -\frac{e^2 \kappa T}{\hbar} \text{Im} \{ e^{z_1^2} [1 - \text{erf}(z_1)] \}, \quad (12)$$

where we used $z = \omega_p \sqrt{t^2 - it\hbar/T}$ and $z_1 = \omega_p \sqrt{2t^2 - it\hbar/T}$. This is the analytical quantum result of the time derivative of the formation of correlation for statically as well as dynamically screened potentials. For the classical limit $\hbar \rightarrow 0$, it is easy to integrate expression (12) with respect to times and arrive at

$$E_{\text{corr}}^{\text{static}}(t) = -\frac{1}{4} e^2 n \kappa \left(1 + \frac{2\omega_p t}{\sqrt{\pi}} - (1 + 2\omega_p^2 t^2) \exp(\omega_p^2 t^2) [1 - \text{erf}(\omega_p t)] \right),$$

$$E_{\text{corr}}^{\text{dynam}}(t) = -\frac{1}{2} e^2 n \kappa \left\{ 1 - \exp \left(\frac{\omega_p^2}{2} t^2 \right) \left[1 - \text{erf} \left(\frac{\omega_p}{\sqrt{2}} t \right) \right] \right\}. \quad (13)$$

In Figs. 1 and 2, these formulae are compared with molecular dynamic simulations [10] for different values of the plasma parameter Γ . The parameter $\Gamma = e^2/a_e T$, where $a_e = (3/4\pi n)^{1/3}$ is the interparticle distance or Wigner–Seitz radius, measures the strength of the Coulomb coupling. Ideal plasmas are found for $\Gamma \ll 1$. In this region the static formula (13) well follows the major trend of the numerical result, see Fig. 1. The agreement is in fact surprising, because we saw that the static result underestimates the dynamical long time Debye–Hückel result (1) $\frac{1}{2} \kappa e^2 = \sqrt{3}/2\Gamma^{3/2}$ by a factor of two.

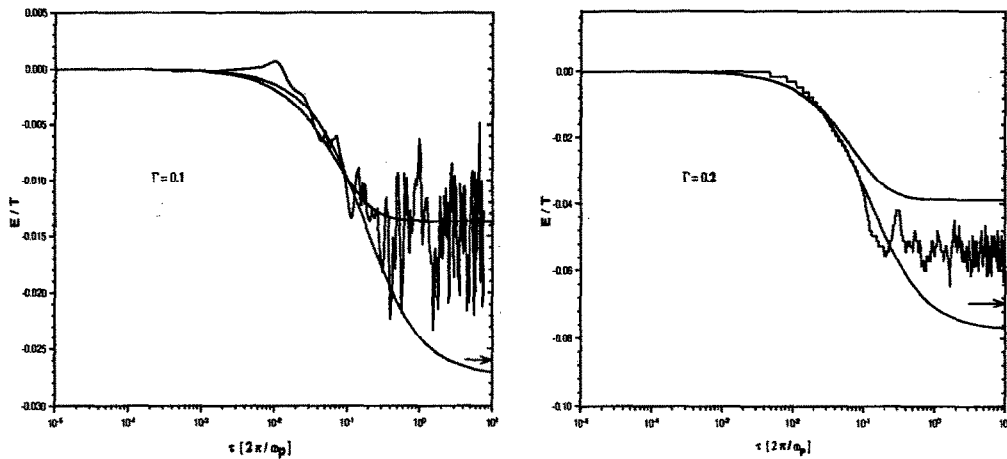


Fig. 1. The formation of the correlation energy due to molecular dynamic simulations [10] together with the analytical result of (13) for a plasma parameter $\Gamma = 0.1$ (left) and $\Gamma = 0.2$ (right). The upper curve is the static and the lower the dynamical calculation. The latter one approaches the Debye–Hückel result. The exact equilibrium correlation energy of MC simulations [11] are indicated by the arrow.

The explanation for this fact is that we can prepare the initial configuration within our kinetic theory such that sudden switching of interaction is fulfilled. However, in the simulation experiment we have initial correlations which are due to the setup within the quasiperiodic boundary condition and Ewald summations. This obviously results into an effective statically screened Debye potential, or at least the simulation results allow for this interpretation.

If we go to higher densities of $\gamma = 0.2$ in Fig. 1 (right), we see that the Debye–Hückel result is far off the correct equilibrium correlation energy. Nevertheless, the time scale is still appropriately described by the dynamical result. At still higher densities, like $\Gamma = 0.5$ and $\Gamma = 1$, see Fig. 2, non-ideal effects become important and the formation time is underestimated within (13). Of course, for higher plasma parameter the Born approximation fails. Nevertheless, formula (13) can still almost reproduce the formation time but slightly shorter than compared with the simulation. This is due to non-ideality which was found to be an expression of memory effects [12] and leads to a later relaxation. For strongly coupled plasma the Born approximation fails, of course, to reproduce the correct equilibrium value, but reproduces the formation time fairly good. The equilibrium value, of course, differs and takes smaller values than the Debye–Hückel result [11,13]. This regime is clearly out of the scope for our theory.

The characteristic time of formation of correlations in the high temperature limit is given by the time where (13) shows a saturation. This is reached at about the inverse plasma frequency,

$$\tau_c \approx \frac{1}{\omega_p} = \frac{\sqrt{2}}{v_{th}\kappa}. \tag{14}$$

The inverse plasma frequency indicates that the dominant role is played by long-range fluctuation. On the other hand, we also see that the correlation time is found to be given by the time a particle needs to travel through the range of the potential with a thermal velocity v_{th} . This confirms the numerical finding of Ref. [3] that the correlation or memory time is proportional to the range of interaction, i.e. rather of short-range character.

In the low temperature region, i.e., in a highly degenerate system $\mu \gg T$, one finds a different picture. From (6) follows [14]

$$E_{corr}^{low}(t) - E_{corr}^{low}(0) = E_{corr}^{low} \frac{1 - (1/x) \sin(x) + (2\mu/\pi T)^2 \{ \frac{1}{3} + [(1/x) \sin(x)]'' \}}{1 + \frac{1}{3} (2\mu/\pi T)^2}, \tag{15}$$

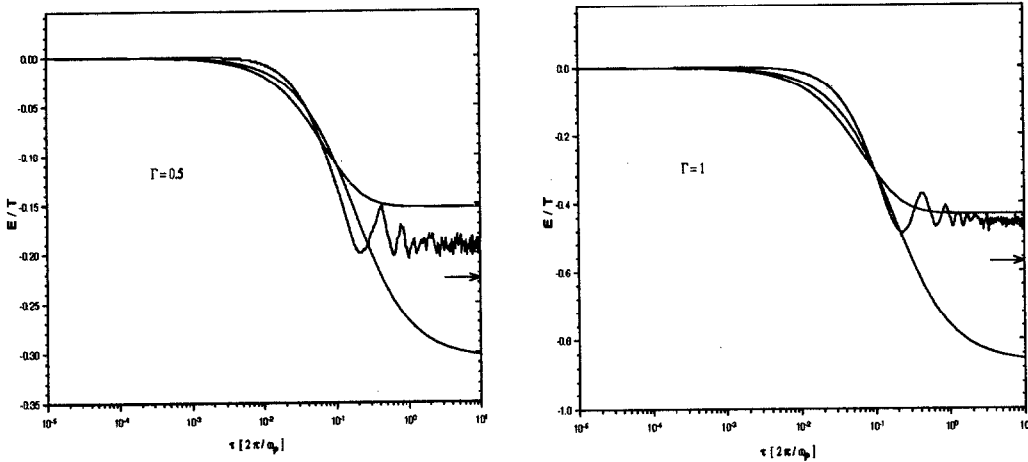


Fig. 2. The formation of the correlation energy due to molecular dynamic simulations [10] together with the result of (13) for a plasma parameter $\Gamma = 0.5$ (left) and $\Gamma = 1$ (right). The upper curve is the static and the lower the dynamical calculation. The latter one approaches the Debye–Hückel result. The simulation approaches the exact correlation energy [11] with higher densities indicated by the arrow.

with $x = (4\mu/\hbar)t$ and the equilibrium correlation energy

$$E_{\text{corr}} = \frac{\mu e^2}{12\kappa^3 \pi^2} \left[T^2 + \frac{1}{3} \left(\frac{2\mu}{\pi} \right)^2 \right] \left(\frac{m}{\hbar^2} \right)^4 \left(\arctan \frac{1}{b_l} + \frac{b_l}{1 + b_l^2} \right), \quad (16)$$

where $b_l = \hbar\kappa/2p_F$. We would like to point out that formula (15) is generally valid for any binary interaction and applicable in dense metal as well as nuclear situations. The only difference lies in the actual value of the equilibrium correlation energy which is dependent on the potential, of course. Indeed, (15) follows from the standard procedure of separating angular from energy integrals for low temperatures. The time dependence is carried exclusively by the energy integrals while the angular averaged interaction results in its factor.

Unlike in the classical case, the equilibrium limit of the degenerate case (15) is not reached monotonically but with oscillations that are damped with a power law t^{-1} in time. In other words, the correlation energy is rapidly built up and then oscillates around the equilibrium value (16). We can define the buildup time τ_c as the time where the correlation energy reaches its first maximum,

$$\tau_c = 1.05 \frac{\hbar}{\mu}, \quad (17)$$

with μ the Fermi energy. Note that τ_c is in agreement with the quasiparticle formation time known as Landau's criterion. Indeed, as argued above, the quasiparticle formation and the buildup of correlations are two alternative views of the same phenomenon.

The formation of binary correlations is very fast on the time scale of the dissipative process. With respect to dissipative regimes, the binary correlations can be treated as instant functionals of the single-particle distribution and thus included into the Boltzmann equation via various renormalizations of its ingredients, the screened Coulomb potential in the scattering rate or the quasiparticle corrections. Under extremely fast external perturbations, like the massive femtosecond laser pulses, the dynamics of binary correlations will hopefully become experimentally accessible. Even if a related measurement will not reveal any unexpected features, the experimental justification of basic concepts of the non-equilibrium many-body physics is very desirable. The theoretical support to such experiments is mostly based on the non-equilibrium Green functions or the molecular dynamics which both demand expensive numerical treatments. Unlike these two approaches, the presented

theory fails for special systems where the characteristic time of formation of correlations becomes longer or comparable with other time scales. For normal systems, it provides a simple tool for theoretical predictions.

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