Exact Algebraic Tails of Static Correlations in Quantum Plasmas at Low Density

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We give the exact low-density coefficients of the large-distance algebraic tails of static correlations in quantum plasmas. Quantum statistics is taken into account, and the interaction is the pure Coulomb potential without any regularization. The low-density expansions, valid in regimes of weak coupling and low degeneracy, are obtained by using a path-integral formalism at finite temperature. Applications to the hydrogen plasma in the Sun and to the charge-carrier gas in germanium are given. The interplay with classical Debye screening is discussed. [S0031-9007(97)02472-1]

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In astrophysics or in laboratory physics, matter can often be considered as a fluid of nonrelativistic quantum point charges (for instance, nuclei and electrons) with Coulomb interaction $e_\alpha e_\gamma/r$ between two charges e_α and e_γ separated by a distance r (α and γ are species indices). Contrary to the common belief according to which Coulomb screening always leads to exponential clustering — as it is the case in the classical regime, in the semiclassical Thomas-Fermi model or in the quantum random phase approximation (RPA) — the existence of algebraic tails in the static correlations of quantum plasmas has been gradually displayed. After the first doubts raised about exponential screening of external charges [1,2], a $\hbar$ expansion of the internal correlations about their classical values was produced for a multicomponent plasma [3,4] in the Maxwell-Boltzmann (MB) approximation and with a Coulomb potential regularized at short distances in order to prevent the classical collapse of charges with opposite signs. (The latter can be avoided only by taking into account the Fermi statistics for a system where all negative and/or positive charges are fermions [5].) The MB particle-particle correlations fall off as $1/r^6$ with a coefficient starting at the order $\hbar^4$. More recently, in the framework of a path-integral "loop" formalism, which takes into account the quantum statistics (Bose or Fermi) and deals with the pure $1/r$ Coulomb potential [6], without any regularization at short distances, it was shown that after exact resummation of the long-range tail of the Coulomb interaction the truncated two-body distribution function $\rho^T_{\alpha\gamma}(r)$ (called correlation in the following) decays as $A_{\alpha\gamma}/r^6$ in real matter [7]. In fact, the argument is perturbative in the sense that it relies on a term-by-term analysis of an expansion with respect to some auxiliary parameter "density of loop." (In the standard many-body perturbation theory using Feynman diagrams at finite temperature, such a general analysis seems not to be possible, as explained in Ref. [6]; hints that some corrections to the RPA diagrams induce algebraic tails in correlations have been exhibited only for the very special model of the one-component plasma with a neutralizing background [8].) However, as it will be accounted for in a future extended paper, low-density expansions for real multicomponent plasmas can be devised from the general loop formalism valid at any density. Thus the conclusions of Ref. [7] are strengthened by exact analytical results in the low-density regime — such results are not available in other quantum situations at the moment — and the existence of the algebraic tails of correlations is settled as follows.

In this Letter, we present the exact analytical low-density limit for the coefficients of the algebraic tails $A_{\alpha\gamma}/r^6$, B_α/r^8, and C/r^{10} for the particle-particle, particle-charge, and charge-charge correlations, $\rho^T_{\alpha\gamma}(r)$, $\sum_\alpha e_\alpha \rho^T_{\alpha\gamma}(r)$, and $\sum_{\alpha,\gamma} e_\alpha e_\gamma \rho^T_{\alpha\gamma}(r)$, respectively. The coefficient of the $1/r^8$ falloff of the induced charge density derived from the linear response theory is also given. These results hold for real plasmas, with quantum statistics and no modelization of the Coulomb interaction, in regimes of low degeneracy and weak coupling at finite temperature. By producing the above low-density coefficients, we settle the existence of the algebraic tails from the theoretical point of view. Numerical estimations are made for the core of the Sun and the charge carriers in an intrinsic semiconductor, because these systems meet the required conditions for the validity of the low-density limit. Though the effect is quantitatively small within a large range of distances in these situations, its existence is qualitatively important, in principle, because it determines the effective interactions between charges. The effect might turn out to be observable in some future, more refined experiments involving correlations, perhaps in plasmas in stronger quantum conditions, such as electrons in metals, but the calculation of the coefficients of the algebraic tails in these systems is far beyond the scope of the present paper.

Another point of the Letter is to exemplify how low-density expansions give a flavor of the subtle mechanisms at stake and their interplay with the fast classical screening usually taken for granted. The origin of the algebraic tails, namely, the absence of exponential screening for the quantum fluctuations of the dipolar interaction

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between charges surrounded by their polarization clouds, is sketched in the path-integral formalism. We exhibit how, at the first 2 orders in density, the above cascade of power laws (when summing over charges) is determined by the basic rules of classical screening in macroscopic electrostatics, which are themselves entirely enforced by the Debye contribution. (The mechanisms are similar but more complex at higher orders in density.)

The derivation of low-density expansions, which is based on a scaling analysis of resummed Mayer bonds, is similar to that used in Ref. [9]. We have checked that it allows one to retrieve the virial expansion of the pressure for a quantum multicomponent plasma up to order $\rho^{5/2}$ given in [10] and derived in [9,11]. ρ generically denotes the densities, and half-integer powers arise from the Debye scale κ_D^{-1}, where $\kappa_D^2 \equiv 4\pi\beta\sum_\alpha e_\alpha^2\rho_\alpha$. For particles with charge e_α (e_γ) and mass m_α (m_γ), the explicit values of the algebraic tails at the first order in density are

$$\rho_{\alpha\gamma}^T(r) \underset{r\to\infty}{\sim} \frac{1}{r^6}\frac{\beta^4\hbar^4}{240}\rho_\alpha\rho_\gamma \times \sum_{\alpha'}\frac{e_{\alpha'}^2}{m_{\alpha'}}\left[\delta_{\alpha,\alpha'} - \frac{4\pi\beta e_\alpha e_{\alpha'}\rho_{\alpha'}}{\kappa_D^2}\right] \times \sum_{\gamma'}\frac{e_{\gamma'}^2}{m_{\gamma'}}\left[\delta_{\gamma,\gamma'} - \frac{4\pi\beta e_\gamma e_{\gamma'}\rho_{\gamma'}}{\kappa_D^2}\right], \quad (1)$$

$$\sum_\gamma e_\gamma\rho_{\alpha\gamma}^T(r) \underset{r\to\infty}{\sim} -\frac{1}{r^8}\frac{\beta^4\hbar^4}{8}\frac{\rho_\alpha}{\kappa_D^2}\left[\sum_\gamma\frac{e_\gamma^3\rho_\gamma}{m_\gamma}\right] \times \sum_{\alpha'}\frac{e_{\alpha'}^2}{m_{\alpha'}}\left[\delta_{\alpha,\alpha'} - \frac{4\pi\beta e_\alpha e_{\alpha'}\rho_{\alpha'}}{\kappa_D^2}\right], \quad (2)$$

$$\sum_{\alpha,\gamma} e_\alpha e_\gamma\rho_{\alpha\gamma}^T(r) \underset{r\to\infty}{\sim} \frac{1}{r^{10}}7\beta^4\hbar^4\frac{1}{\kappa_D^4}\left[\sum_\gamma\frac{e_\gamma^3\rho_\gamma}{m_\gamma}\right]^2. \quad (3)$$

In the zero-density limit, the coefficient of the charge-charge correlation does not vanish. This reflects the fact that the results obtained in the limit of an infinitely dilute plasma do not coincide with the calculations performed for particles in the vacuum, where no screening effect takes place. Moreover, according to the linear response theory, the induced charge density $\sum_\gamma e_\gamma\rho_\gamma^{\rm ind}(r;\delta q)$ in the presence of an infinitesimal external charge δq decays as $1/r^8$ [7] as the particle-charge correlation. At the first order in density, we get

$$\frac{\sum_\gamma e_\gamma\rho_\gamma^{\rm ind}(r;\delta q)}{\delta q} \underset{r\to\infty}{\sim} \frac{1}{r^8}\frac{\pi\beta^5\hbar^4}{2}\frac{1}{\kappa_D^4}\left[\sum_\gamma\frac{e_\gamma^3\rho_\gamma}{m_\gamma}\right]^2. \quad (4)$$

Comparison of (4) with the linear term with respect to the given charge e_α in (2) shows that the algebraic tails satisfy the more general relation, valid at any distance and for any finite charge e_α,

$$\lim_{\rho_\alpha\to 0}\frac{\sum_\gamma e_\gamma\rho_{\alpha\gamma}^T(r)}{\rho_\alpha} = \sum_\gamma e_\gamma\rho_\gamma^{\rm ind}(r;e_\alpha)\bigg|_{\rho_\alpha=0}. \quad (5)$$

This relation states that in the limit where one species α becomes more and more dilute, so that it disappears from the plasma, the charge density induced by one charge e_α can be retrieved from the particle-charge correlation.

We notice that in the case of a two-component plasma of charges e_+ and e_-, with masses m_+ and m_-, the coefficients $A_{\alpha\gamma}^{(n)}$ of the $1/r^6$ tail of the particle-particle correlations at the order ρ^n, with $n = 2, 5/2$, are positive and the corresponding effective interaction is attractive whatever the signs of the charges. Moreover, these coefficients satisfy the relation

$$\frac{A_{++}^{(n)}}{\rho_+^2} = \frac{A_{--}^{(n)}}{\rho_-^2} = \frac{A_{+-}^{(n)}}{\rho_+\rho_-}. \quad (6)$$

The peculiar identity (6) is due to a classical contribution in the screening of every quantum charge by the surrounding plasma. It is no longer satisfied at higher orders in density, $n \geq 3$, because then quantum dynamical and statistical effects are involved and destroy the symmetry between the various species of particles. At the order ρ^2,

$$\rho_{\alpha\gamma}^T(r) \underset{r\to\infty}{\sim} \frac{\rho_\alpha\rho_\gamma}{r^6}\frac{\beta^4\hbar^4}{240}\left(\frac{e_+e_-}{e_+ + |e_-|}\right)^2\left[\frac{e_+}{m_+} + \frac{|e_-|}{m_-}\right]^2. \quad (7)$$

If $e_+ = -e_- \equiv e$, the local neutrality implies that $\rho_+ = \rho_- \equiv \rho$ and the tail (7) is equal to $\rho^2(\xi_D/r)^6$ times $(9/320)\Gamma^5(\lambda_-/a)^4[1 + (m_-/m_+)]^2$, where $\xi_D \equiv \kappa_D^{-1}$ is the Debye length, λ_- is the de Broglie thermal wavelength of the negative charges, $\lambda_- \equiv \sqrt{\beta\hbar^2/m_-}$, a is the mean interparticle distance and $\Gamma \equiv \beta e^2/a = (1/3)\,(a/\xi_D)^2$ is the coupling constant.

The formula (7) can be applied to the core of the Sun. As a first approximation, the latter can be seen as a hydrogen plasma almost fully ionized by pressure and temperature, with a mass density $\rho_m \sim 160$ g/cm^3 at temperature $T \sim 1.5\,10^7$ K. Thus $a \sim 0.1$ Å, the system is rather weakly degenerated, $\lambda_-/a \sim 0.7$, and weakly coupled, $\Gamma \sim 0.1$. The contribution from the algebraic tail (7) becomes as large as the classical Debye-Hückel contribution,

$$\rho_{\alpha\gamma}^{TD}(r) = -\rho_\alpha\rho_\gamma\beta e_\alpha e_\gamma\frac{e^{-r/\xi_D}}{r}, \quad (8)$$

at a crossover distance $r_* \sim 31\,\xi_D$. Thus the algebraic tail appears only at very large distances compared with the Debye screening length; at intermediate distances, the Debye approximation is valid, while at short distances, quantum contributions become predominant. (In particular, quantum dynamics prevents the collapse of two charges with opposite signs, while quantum statistics arises for particles of the same species.) In fact, both Debye and exchange effects in the correlations are important for the thermodynamics, and the low-density equation of state [10], also retrieved from the present formalism, describes successfully the core of the Sun [12]. Another class of systems to be investigated is that of solid state physics. The domain of applicability of the formulas given in the present Letter is that of intrinsic semiconductors, where the charge-carrier gas (electrons and holes) is indeed at finite temperature and weakly degenerated as well as weakly coupled. For instance, in germanium, where the mass of holes is equal to that of electrons, $a \sim 1530$ Å, $T \sim 300$ K, so that $\lambda_-/a \sim 0.01$, $\Gamma \sim 0.4$, and $r^* \sim 43\,\xi_D$. A clear experimental evidence of the static tails is still to be found, maybe in semiconductors with stronger degeneracy and stronger coupling, where r_* would be of the same order as ξ_D and the attractive effective interaction (6) might play a role.

At a more technical level, we briefly summarize how a path-integral formalism allows one to show the following two points. First, contrary to classical fluctuations which are exponentially screened, equilibrium quantum fluctuations induce algebraic tails in the static correlations. Second, at the first 2 orders in density, these tails reduce to the square of some kind of screened dipolar potential between quantum fluctuations of the charges surrounded by their polarization clouds. On one hand, thanks to the Feynman-Kac formula, the quantum Gibbs factor in position representation is given by a path integral and the quantum fluctuations of particles at the inverse temperature β can be described in terms of loops with random shapes. Indeed, a particle at position $\mathbf{r}$ that is not exchanged with any other one in a given density-matrix element is associated with one closed path $\mathbf{r} + \lambda_\alpha \boldsymbol{\xi}(s)$, where λ_α is the de Broglie thermal length of species α and $\boldsymbol{\xi}(s)$ (with $0 \le s \le 1$) is a dimensionless Brownian bridge, $\boldsymbol{\xi}(s=0) = \boldsymbol{\xi}(s=1) = \mathbf{0}$, with a normalized Gaussian measure. On the other hand, p particles that are exchanged with one another under a cyclic permutation correspond to open paths which can be collected into a closed loop. The internal degrees of freedom of the latter are the species α of the involved particles, the "exchange degeneracy" p, and the shape of the curve formed by the positions of the p particles and the Brownian paths that link them together. The grand partition function of the system of quantum point charges with quantum statistics, and which interact through the Coulomb potential, is equal to that of a gas of classical loops with Maxwell-Boltzmann statistics, and which interact via some two-body potential of Coulomb type [6,13]. (See also Ref. [14] for a brief account). The quantum Hamiltonian does not involve the spins, and the latter only contribute to degeneracy factors in the loop fugacities. The interaction between loops couples only curve elements with abscissas that are equal up to an integer, so that it does not coincide with the electrostatic potential between charged wires, except for its monopole-monopole and monopole-multipole parts. Thus, after exact resummations [6], the large-distance $1/r$ and $1/r^2$ tails of the loop interaction are exponentially screened, whereas there appears a partially (not exponentially) screened dipolar potential $v^{\rm dip}_{\alpha\gamma}$. As shown in Ref. [7], after integration over quantum fluctuations, rotational invariance and the harmonicity of the function $1/r$ eventually lead to an $1/r^6$ decay for the particle-particle correlations at any density. At the first order in density, only loops with exchange degeneracy p equal to 1 do contribute,

$$v^{\rm dip}_{\alpha\gamma}(\mathbf{r}, \boldsymbol{\xi}, \boldsymbol{\xi}') = -e_\alpha e_\gamma \int_0^1 ds \int_0^1 ds' [\delta(s-s') - 1] \times [\lambda_\alpha \boldsymbol{\xi}(s) \cdot \nabla][\lambda_\gamma \boldsymbol{\xi}'(s') \cdot \nabla]\left(\frac{1}{r}\right), \tag{9}$$

while the exact value of the tails $A_{\alpha\gamma}/r^6$, B_α/r^8, and C/r^{10} turn out to coincide, after proper summation over charges, with the algebraic tail of the convolution

$$\sum_{\alpha',\gamma'} \int d\mathbf{x} \int d\mathbf{y}\, S^D_{\alpha\alpha'}(\mathbf{x}) g_{\alpha'\gamma'}(\mathbf{r} + \mathbf{y} - \mathbf{x}) S^D_{\gamma'\gamma}(\mathbf{y}) . \tag{10}$$

In (10) α' and γ' run from 1 to the number of species, and

$$g_{\alpha'\gamma'}(\mathbf{r}) \equiv \int D(\boldsymbol{\xi}_1) \int D(\boldsymbol{\xi}_2) \frac{\beta^2}{2} [v^{\rm dip}_{\alpha'\gamma'}(\mathbf{r}, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2)]^2 \tag{11}$$

is an effective squared dipolar potential. The structure factor $S^D_{\alpha\gamma}(\mathbf{r} - \mathbf{r}') \equiv \rho_\alpha\, \delta_{\alpha,\gamma} \delta(\mathbf{r} - \mathbf{r}') + \rho^{TD}_{\alpha\gamma}(|\mathbf{r} - \mathbf{r}'|)$ involves the short-ranged classical Debye correlation (8). The latter correlation, calculated in a linearized approximation, is well defined for particles with pure Coulomb interaction, whereas the total classical correlation for point particles is not, because of the collapse between charges with opposite signs. We notice that, according to Eq. (5.12) of Ref. [4], where the quantum correlations are calculated with MB statistics and a Coulomb potential regularized at the origin, the term of order $\hbar^4$ in the large-distance behavior of the approximate MB correlation reduces to (10) when the classical correlations between particles with short-ranged repulsion in Eq. (5.12) are replaced by the Debye correlations (8). The systematic analysis of our diagrammatics shows that the exact algebraic tails at the next order in density behave, after adequate summation over charges, as the decay of the convolution (10) only renormalized by a factor of order $\rho^{1/2}$. The latter half-integer power arises from integrals scaled by the Debye length.

We stress that the algebraic decays of the correlations are compatible with the basic screening laws, according to which the polarization cloud around either an internal or an infinitesimal external charge exactly compensates this charge. In the classical case, multicomponent plasmas with a Coulomb potential regularized at the origin obey these laws, because the classical Debye correlation saturates the corresponding sum rules,

$$\int d\mathbf{r} \sum_\gamma e_\gamma S^D_{\alpha\gamma}(r) = 0 , \tag{12}$$

$$\int d\mathbf{r} \frac{r^2}{6} \sum_{\alpha,\gamma} e_\alpha e_\gamma S^D_{\alpha\gamma}(r) = -\frac{1}{4\pi\beta}, \tag{13}$$

where (13) is the so-called Stillinger-Lovett sum rule [15]. An argument, which involves a decomposition of the classical correlation into the sum of the Debye correlation and a convolution analogous to (10), with a fast decaying function in place of $g_{\alpha\gamma}$, is given in Sec. IV of Ref. [7] (where the repulsive core potential was omitted in the notations). At the quantum level, a generalization of this argument exists: there still exists some memory of the classical exponential screening of macroscopic electrostatics which ensures the basic screening laws [7].

Moreover, the above memory of classical screening is also responsible for the cascade of inverse power laws, $1/r^6$, $1/r^8$, $1/r^{10}$, in the decays of the particle-particle, particle-charge, and charge-charge correlations, at any order in density [7]. In fact, we show that at the first 2 orders in density the cascade is enforced only by the classical screening rules entirely satisfied by the Debye contribution. At the first 2 orders in density, the leading algebraic tails are given by the convolution (10), with a renormalized factor at the second order in density. Since $S^D_{\alpha\gamma}$ is short ranged, the falloff of the particle-particle correlation $\rho^T_{\alpha\gamma}(r)$ arises from

$$\sum_{\alpha',\gamma'} \left[\int d\mathbf{x}\, S^D_{\alpha\alpha'}(\mathbf{x})\right]\left[\int d\mathbf{y}\, S^D_{\gamma'\gamma}(\mathbf{y})\right] g_{\alpha'\gamma'}(r), \tag{14}$$

while, according to (12) and (13) and the identity $\int d\mathbf{r}\,\mathbf{r} \sum_\gamma e_\gamma S^D_{\alpha\gamma}(r) = \mathbf{0}$, the decay of the particle-charge correlation $\sum_\gamma e_\gamma \rho^T_{\alpha\gamma}(r)$ is given by

$$\sum_{\alpha',\gamma'} \left[\int d\mathbf{x}\, S^D_{\alpha\alpha'}(\mathbf{x})\right]\left[\int d\mathbf{y} \frac{|\mathbf{y}|^2}{6} \sum_\gamma e_\gamma S^D_{\gamma'\gamma}(\mathbf{y})\right] \times \Delta g_{\alpha'\gamma'}(r), \tag{15}$$

and the $1/r^{10}$ tail of the charge-charge correlation $\sum_{\alpha,\gamma} e_\alpha e_\gamma \rho^T_{\alpha\gamma}(r)$ results from

$$\sum_{\alpha',\gamma'} \left[\int d\mathbf{x} \frac{|\mathbf{x}|^2}{6} \sum_\alpha e_\alpha S^D_{\alpha\alpha'}(\mathbf{x})\right] \times \left[\int d\mathbf{y} \frac{|\mathbf{y}|^2}{6} \sum_\gamma e_\gamma S^D_{\gamma'\gamma}(\mathbf{y})\right] \Delta\Delta g_{\alpha'\gamma'}(r). \tag{16}$$

By taking into account $\Delta(1/r^6) = 30/r^8$ and $\Delta(1/r^8) = 56/r^{10}$, together with (8) and (13), we get the tails (1)–(3), which indeed satisfy $\sum_\gamma e_\gamma A_{\alpha\gamma} = 0$ and $\sum_\alpha e_\alpha B_\alpha = 0$, in accordance with the general cascade of power laws.

In conclusion, we briefly discuss the coefficient $A_{\alpha\gamma}$ of the algebraic decay of the particle-particle correlations at higher orders in density. Half-integer powers of the density appear, because the quantum contributions are partially screened by classical collective effects at large distances, and the latter are scaled by the Debye length. Contrary to the terms of order ρ^2 and $\rho^{5/2}$, which are purely proportional to $\hbar^4$, the term of order ρ^3 involves two kinds of terms. The terms of the first kind are proportional to $\hbar^4$ arising from one squared dipolar potential $[v^{\mathrm{dip}}_{\alpha\gamma}]^2$ times a function which has essential singularities when $\hbar$ goes to zero, because it involves the contributions from exchange phenomena and from quantum dynamical effects (bare — bound and scattering — two-body states). The terms of the second kind are proportional to $\hbar^6$ either because they involve one $[v^{\mathrm{dip}}_{\alpha\gamma}]^2$ multiplied by a screened "diffraction" $\hbar^2$ correction due to the long range of the Coulomb potential or because they result from the product of one $v^{\mathrm{dip}}_{\alpha\gamma}$ with a convolution of two $v^{\mathrm{dip}}_{\alpha\gamma}$'s. Eventually, at the order ρ^2 and $\rho^{5/2}$, the leading algebraic decays arise only from the squared fluctuations of one dipolar interaction, and the coefficients of these tails are entirely determined by free quantum dynamics, Maxwell-Boltzmann statistics, and classical screening; however, from the order ρ^3 on, the mechanisms are more intricate and contributions from quantum dynamics and statistics of interacting charges emerge in the coefficients of the algebraic decays.

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