

Comment on “Direct linear term in the equation of state of plasmas”

A. Alastuey

Laboratoire de Physique, ENS Lyon, UMR CNRS 5672, 46 allée d’Italie, 69364 Lyon Cedex 07, France

V. Ballenegger

Institut UTINAM, Université de Bourgogne-Franche-Comté, UMR CNRS 6213, 16 route de Gray, 25030 Besançon Cedex, France

W. Ebeling

Institut für Physik, Humboldt Universität Berlin, Newtonstrasse 15, 12489 Berlin, Germany

(Received 1 April 2015; published 8 October 2015)

In a recent paper [Phys. Rev. E **91**, 013108 (2015)], Kraeft *et al.* criticize known exact results on the equation of state of quantum plasmas, which have been obtained independently by several authors. They argue about a difference in the definition of the direct two-body function $Q(x)$, which appears in virial expansions of thermodynamical quantities, but $Q(x)$ is not a measurable quantity in itself. Differences in definitions of intermediate quantities are irrelevant, and only differences in physical quantities are meaningful. Beyond Kraeft *et al.*’s broad statement that there is no agreement at order $\rho^{5/2}$ in the virial equation for the pressure, we show that their published results for this quantity are in fact in perfect agreement with previous existing expressions.

DOI: [10.1103/PhysRevE.92.047101](https://doi.org/10.1103/PhysRevE.92.047101)

PACS number(s): 52.25.Kn, 05.30.Fk, 52.27.Gr

Virial expansions of pressure in powers of density ρ for quantum plasmas have been studied for many years by several authors using different methods. The first expressions for virial coefficients at order $\rho^{5/2}$ included were obtained by Ebeling using Morita’s effective potential method in Refs. [1,2]. These results were recovered by several authors of the Rostock school, using various methods, including, in particular, thermal Green’s functions, as summarized in the book by Kraeft *et al.* [3]. Alastuey and Perez [4] computed such virial coefficients starting from the Feynman-Kac path integral representation. They found agreement up to order ρ^2 and established that previous expressions were missing a quantum-diffraction contribution at order $\rho^{5/2}$. Kahlbaum [5] recovered this diffraction term within the Morita-Kelbg effective potential method. Brown and Yaffe published a detailed calculation of the virial coefficients, once more using a completely different method, namely, an effective field theory [6]. In their thorough, 164-pages-long report, they recover exactly the known results for the virial coefficients up to order $\rho^{5/2}$ included. Notice that formulas for the virial coefficients in the presence of a magnetic field have been also derived by Cornu [7], and at zero field, they do coincide, up to order $\rho^{5/2}$ included, with the results obtained by previous authors [4–6].

Despite the above remarkable agreement, Kraeft, Kremp, and Röpke (KKR) claim in a recent article [8] that the results obtained by the previous authors, as well as their own ones in some previous works, in particular, those described in Ref. [3], contain unjustified contributions at order $\rho^{5/2}$. To pinpoint the source of the alleged problem in the aforementioned works, Kraeft, Kremp, and Röpke argue about the subtleties in the so-called charging procedure, in particular, in relation to the introduction of short-range effective potentials. It must be stressed that such ingredients do not intervene at all in most of the works [4,6,7,9,10] qualified by KKR to contain questionable results. In those articles, thermodynamical properties are calculated for a quantum multicomponent plasma, i.e., a mixture of particles of different species a , each characterized by its charge e_a , mass m_a , and spin σ_a , in which the particles

interact via the pure $1/r$ Coulomb potential without an additional short-range potential.

Beyond their above arguments, which anyway do not apply to the derivations in Refs. [4,6,7,9,10], Kraeft, Kremp, and Röpke also state that those papers contain an unjustified use of the Ebeling’s function $Q(x)$ introduced in Refs. [1,2], or, in other words, that the presence of the linear term $-x/6$ in $Q(x)$ is assumed. We stress that, in fact, the authors of such papers do not make any *a priori* assumption about the emergence of Ebeling’s $Q(x)$ function. The corresponding calculations are performed following independent routes, all different from the method introduced by Ebeling. The final results are rewritten in terms of $Q(x)$ only to compare with Ebeling’s formulas, as mentioned explicitly, for instance, at the beginning of Sec. VII of Ref. [9]. It is obvious that any expression, say, S , can be written as $Q(x)$ plus a difference $S - Q(x)$. The only meaningful quantity to compare is the *full* expression at a given order, which does not reduce to the sole contribution of $Q(x)$, neither at order ρ^2 nor at order $\rho^{5/2}$. The full contribution could of course also be expressed in terms of another function than the genuine $Q(x)$ of Ebeling.

For instance, we can introduce the function $Q_{\text{KKR}}(x) = Q(x) + x/6$ defined in Ref. [8] into formula (7.3) of Ref. [9] for the virial expansion of the free energy of a quantum plasma. At order ρ^2 , both $Q(x)$ and $Q_{\text{KKR}}(x)$ eventually lead to the same contribution because the sum of the linear terms in the Born parameters $x_{ab} = -\sqrt{2}\beta e_a e_b / \lambda_{ab}$, with $\lambda_{ab} = (\beta \hbar^2 / m_{ab})^{1/2}$ and $m_{ab} = m_a m_b / (m_a + m_b)$, vanish owing to the neutrality condition $\sum_a e_a \rho_a = 0$, where ρ_a is the density of species a . At order $\rho^{5/2}$, the contribution of the Q ’s can be rewritten as that of the Q_{KKR} ’s plus a diffraction term proportional to \hbar^2 , which then has to be added to the genuine diffraction term in formula (7.3). In terms of Q_{KKR} , the formulas thus keep the same form with a diffraction term at order $\rho^{5/2}$ modified to reflect the change in the definition of Q .

In Ref. [8], KKR emphasize that the calculation of direct contributions, within their formalism, leads to the more natural introduction of Q_{KKR} rather than Q . We stress that this is

specific to the methodology described in Ref. [8], but it does not intervene at all in other calculations [4,6,7,9,10], while the corresponding final results can be expressed equivalently in terms of Q_{KKR} or Q or other truncated traces [11], as explained above. Neither the isolated contribution of Q_{KKR} , nor that of Q or of a truncated trace Z , are measurable quantities. Only the full virial coefficients in thermodynamic functions, such as the pressure or the free energy, make an unambiguous physical sense. At a given order in ρ , each virial coefficient only depends on the temperature, and on the fundamental constants, namely, the charges, masses, spins of particles, and Planck's constant. The corresponding expression is of course independent of any definition of auxiliary quantities which may arise in the calculations, such as Q_{KKR} , Q , or Z . The crucial point is to compare the virial coefficients computed within the formalism exposed in Ref. [8] to those derived in Refs. [4,6,7,9].

At order ρ^2 , there is no difference between the virial coefficients given Refs. [8,9], as remarked by KKR. The two formulas are written in a slightly different form, but they agree owing to the charge neutrality. Notice that both expressions establish that there is no direct linear contribution of order $\rho^2 e^2$ in the thermodynamical properties of quantum plasmas.

At order $\rho^{5/2}$, the complete expression of the virial coefficient, including all contributions from the function $Q(x)$ [or $Q_{\text{KKR}}(x)$], is not given in Ref. [8]. In this article, KKR give instead the expansion of the pressure in terms of the fugacities z and, at order $z^{5/2}$, they give only the e^2 expansion of the fugacity-virial coefficient up to order e^5 . Additional calculations are therefore required to compare the computed coefficients. Kraeft, Kremp, and Röpke expect a discrepancy at order $\rho^{5/2}$ because the final formula for this coefficient published in Refs. [4–7] happens to be written in terms of $Q(x)$ instead of $Q_{\text{KKR}}(x)$. We underline that $Q(x)$ was not an *a priori* ingredient in the calculations in those works and repeat that $Q(x)$ appears in the final formula only because the authors wanted to confront their expression with Ebeling's formula. To compare KKR's result given by Eq. (26) in Ref. [8] with the one of Refs. [4–7], one has, on one side, to derive from Eq. (26) the corresponding density-virial coefficient at order $\rho^{5/2}$ (and order e^5 at most) by using thermodynamic identities. On the other side, one has to expand the full virial coefficient of order $\rho^{5/2}$ with respect to e^2 up to the required order, a calculation already performed in Ref. [9], which presents in detail the results obtained in Ref. [4].

The terms of order $\rho^{5/2}$ and e^5 at most in the virial expansion of the free energy f (in units of $k_B T$) are given in formula (7.13) of Ref. [9]. The corresponding terms in the expansion of the pressure follow from identity $\beta p = \sum_a \rho_a \partial f / \partial \rho_a - f$. They reduce to the sum of three terms, namely, a direct contribution of order $\rho^{5/2} e^5$,

$$-\frac{\pi}{8} \sum_{a,b} \beta^2 e_a^2 e_b^2 \frac{\beta \hbar^2 (m_a + m_b)}{m_a m_b} \rho_a \rho_b \kappa, \quad (1)$$

plus an exchange contribution of order $\rho^{5/2} e^3$,

$$\frac{3\pi^{3/2}}{4} \sum_a \frac{(-1)^{2\sigma_a+1}}{2\sigma_a+1} \beta e_a^2 \left(\frac{\beta \hbar^2}{m_a} \right)^{3/2} \rho_a^2 \kappa, \quad (2)$$

plus an exchange contribution of order $\rho^{5/2} e^5$,

$$-\frac{3\pi}{2} \sum_a \frac{(-1)^{2\sigma_a+1}}{2\sigma_a+1} \beta^2 e_a^4 \frac{\beta \hbar^2}{m_a} \rho_a^2 \kappa, \quad (3)$$

where $\kappa = (4\pi\beta \sum_a e_a^2 \rho_a)^{1/2}$ is the Debye wave number. We emphasize that the direct term (1) arises from both the contribution of the Q 's and from the diffraction term in formula (7.3) of Ref. [9]. In Ref. [8], the terms of order $z^{5/2}$ and e^5 at most in the pressure βp are given in formula (26). Using the identity $\rho_a = z_a \partial \beta p / \partial z_a$ where z_a is the fugacity of species a , we infer from formula (26) that the corresponding terms of order $\rho^{5/2}$ and e^5 at most in the virial expansion of βp reduce to the sum of a direct contribution plus two exchange contributions. The direct contribution and the exchange contribution of order $\rho^{5/2} e^3$ are identical to, respectively, formulas (1) and (2) computed from Ref. [9], while the exchange contribution of order $\rho^{5/2} e^5$ is twice the expression (3). However, it is known, for the reasons exposed below, that the term of order $z^{5/2} e^5$ in formula (26) of Ref. [8] should be divided by 2: This restores a perfect agreement for the exchange contribution (3). There is thus no discrepancy in the literature since the virial coefficient at order $\rho^{5/2}$ and orders e^n with $n \leq 5$ given in Ref. [8] agree with the results published in Refs. [4–7,9].

Let us compare also the formula for the virial equation of state in the instructive case of the one-component plasma (OCP), made with a single mobile species, namely, point particles with charge e , mass m , spin σ , and interacting via the pure $1/r$ Coulomb potential, immersed in a uniform rigid neutralizing background with charge density $-\epsilon\rho$. The correct result according to KKR is derived in Ref. [12]. We have to compare formula (15) of Ref. [12] for the virial expansion of the pressure with the more general (i.e., nonperturbative in e^2) result (7.4) given in Ref. [9] for the *free energy* of this system, a result which was first computed in Ref. [4]. Notice that the virial coefficient at order ρ^2 written in Ref. [9] involves a contribution of $Q(x)$ with $x = -\beta e^2 / \lambda$ and $\lambda = (\beta \hbar^2 / m)^{1/2}$ plus a diffraction term proportional to \hbar^2 . The sum of these two terms can be rewritten exactly as a contribution due to $Q_{\text{KKR}}(x)$ only. There is thus no direct linear contribution of order $\rho^2 e^2$ in the thermodynamical properties of the OCP, similarly to the absence of a direct $O(\rho^2 e^2)$ contribution in the multicomponent plasma. The formula for the pressure, when expanded at high temperatures in powers of e^2 , is given by Eq. (7.15) of Ref. [9] (see also Ref. [13]). The method used in Ref. [12] is based on standard many-body perturbative expansions in e^2 of thermal Green's functions, and it first provides the pressure in terms of the fugacity z , namely, formula (14) for $p(z)$. The expression of $p(\rho)$ then follows through the straightforward elimination of the fugacity in favor of the density, owing to the identity $\rho = z \partial \beta p / \partial z$. We have checked that the corresponding expression of $p(\rho)$ does exactly reduce to formula (7.15) of Ref. [9] [beware the missing factor 1/2 in Eq. (15) of Ref. [12]; see Ref. [14]]. Thus, there is a perfect agreement between the results derived in Ref. [9] and in Ref. [12].

In summary, as far as one considers the various expressions given in or cited in Ref. [8], there is a perfect agreement with Refs. [4–7,9] for the full virial coefficient of order

ρ^2 , where direct linear terms of order $\rho^2 e^2$ cancel out both for the multicomponent mixture and for the OCP. The direct contribution to pressure at order $\rho^{5/2}$ and e^5 given by Eq. (1) agrees in all recent papers [4–10,12]. In the older papers [1–3], the coefficient differs by a factor of 2 due to missing three-body effects which were detected only in the 90's. The exchange contributions to pressure at order $\rho^{5/2}$ and orders e^3 and e^5 given by Eqs. (2) and (3), respectively, agree in all cited papers, as expected, since there is no controversy about them. Therefore, no discrepancy exists at the considered orders, and all available results are identical. Contributions of order $\rho^{5/2}$

and orders higher than e^5 currently have only been computed in Refs. [4–7], which all agree.

The fact that an important result can be proved by following different routes is very satisfactory. Any alternative derivation is always enriching. The above comments and detailed comparison of the results show that the arguments in Ref. [8] do not shed any doubt on the current well-established results for the virial equation of state of quantum plasmas. We hope that the present discussion stimulated by KKR contributed to a clarification of some intricate technical points in the quantum statistical theory of Coulomb systems.

-
- [1] W. Ebeling, The exact free energy of low density quantum plasmas, *Physica* **40**, 290 (1968).
- [2] W. Ebeling, Zur Quantenstatistik der Bindungszustände in Plasmen 2, *Ann. Phys.* **22**, 392 (1969).
- [3] W. D. Kraeft, D. Kremp, W. Ebeling, and G. Röpke, *Quantum Statistics of Charged Particle Systems* (Plenum, New York, 1986).
- [4] A. Alastuey and A. Perez, Virial expansion of the equation of state of a quantum plasma, *Europhys. Lett.* **20**, 19 (1992).
- [5] T. Kahlbaum, The quantum-diffraction term in the free energy for Coulomb plasma and the effective-potential approach, *J. Phys. IV* **10**, 455 (2000).
- [6] L. S. Brown and L. G. Yaffe, Effective field theory for highly ionized plasmas, *Phys. Rep.* **340**, 1 (2001).
- [7] F. Cornu, Quantum plasma with or without uniform magnetic field. II. Exact low-density free energy, *Phys. Rev. E* **58**, 5293 (1998).
- [8] W. D. Kraeft, D. Kremp, and G. Röpke, Direct linear term in the equation of state of plasmas, *Phys. Rev. E* **91**, 013108 (2015).
- [9] A. Alastuey and A. Perez, Virial expansions for quantum plasmas: Fermi-Bose statistics, *Phys. Rev. E* **53**, 5714 (1996).
- [10] A. Alastuey and V. Ballenegger, Thermodynamics of atomic and ionized hydrogen: Analytical results versus equation-of-state tables and Monte Carlo data, *Phys. Rev. E* **86**, 066402 (2012).
- [11] D. Wendland, V. Ballenegger, and A. Alastuey, Quantum partition functions of composite particles in a hydrogen-helium plasma via path integral Monte Carlo, *J. Chem. Phys.* **141**, 184109 (2014).
- [12] H. E. DeWitt, M. Schlanges, A. Y. Sakakura, and W. D. Kraeft, Low density expansion of the equation of state for a quantum electron gas, *Phys. Lett. A* **197**, 326 (1995).
- [13] The high-temperature result (7.15) of Ref. [9] for the OCP coincides with expressions (1)–(3) when they are restricted to a single particle species by suppressing the sums. However, we underline that the ρ^2 term in the finite-temperature result (7.4) for the OCP cannot be obtained by restricting the sums over species to a single one in formula (7.3) for the multicomponent mixture. That subtlety can be understood by considering the OCP as the limit of a two-component mixture, where the first species a is fixed once for all, namely, we set $\rho_a = \rho$, $e_a = e$, $m_a = m$, $\sigma_a = \sigma$, while the second species b becomes infinitely heavy, $m_b \rightarrow \infty$, infinitely dense, $\rho_b \rightarrow \infty$, and infinitely weakly charged, $e_b \rightarrow 0$, with $e_b \rho_b = -e\rho$ fixed. The species b is then expected to play the role of a classical uniform and rigid background in that limit. If we take the corresponding limit of formula (7.3), we see that all contributions of $Q(x_{bb})$ vanish, but the contribution of $Q(x_{ab})$ at order ρ^2 does not vanish and exactly reduces to the diffraction term proportional to \hbar^2 present in formula (7.4), which can be obtained independently by a direct calculation within the OCP model.
- [14] In Ref. [12], formula (15) (with n instead of ρ) contains either a mistake or a misprint in the exchange term of order $n^{5/2} e^3$, which has to be divided by 2, as already quoted by Brown and Yaffe [6]. Notice that the computation of that term requires some care because both the classical Debye term of order $z^{3/2} e^3$ and the ideal exchange term of order z^2 in $p(z)$ contribute through the elimination of z in favor of $n = \rho$.