Reply to "Comment on 'Direct linear term in the equation of state of plasmas' "

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The long-standing discrepancy in the equation of state of charge neutral plasmas, the occurrence of an e^2 direct term in the second virial coefficient, is dealt with. We state that such a contribution should not appear for a pure Coulomb interaction.

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I. INTRODUCTION

The introduction to the field is outlined in Ref. [1] and will not be given here. We mention that the Comment [2] is not focused on the essential points of Ref. [1]. A large part of the Comment [2] includes historical remarks which might be subject to a separate work, but is not directly related to Ref. [1]. Also, solutions for the $n^{5/2}$ terms are a separate topic and are not the focus of Ref. [1]. Especially, the question of the existence of a linear direct term has to be answered prior to the determination of terms of the order $n^{5/2}$ and of higher orders for the equation of state (EOS). See Sec. IV.

II. THE Q FUNCTION

The Q function is a well-defined physical quantity. It occurs in the density (n_a) expansion of thermodynamic variables, for instance, the pressure or the free energy, of a single- or multicomponent system (species $a,b,\dots$). For a pure Coulomb system, the second virial coefficient can be expanded in a series of powers of $\xi_{ab} = e_a e_b/(4\pi\epsilon_0\lambda_{ab}k_BT)$ (in SI units) where the thermal wavelengths are given by $\lambda_{ab} = \hbar/(2m_{ab}k_BT)^{1/2}$, and $m_{ab} = m_a m_b/(m_a+m_b)$ is the reduced mass (see Ref. [3]). It is a peculiarity of the long-range Coulomb interaction that the lowest order terms $\propto\xi_{ab},\xi_{ab}^2$ are divergent and are treated separately. For charge-neutral plasmas, after a partial summation, the Debye term $\propto n^{3/2}$ is obtained. Thus, up to all exchange contributions and two terms of order e^6, $Q_{ab}(T)$ represents the full direct part of the second virial coefficient. Thus, $Q_{ab}(T)$ is a physical quantity defined by Eqs. (1) and (2) of Ref. [1] [see also Eqs. (1), (2), (4), and (7) of Ref. [4] and Eqs. (6.216) and (6.217) in Ref. [5]].

III. RESULTS FOR THE Q FUNCTION

The evaluation of $Q_{ab}(T)$ is a matter of a clearly defined mathematical task, and there is only one result for the pure Coulomb system, namely, the expression *without* the linear direct term.

In the literature, three different results are given for $Q_{ab}(T)$. To avoid confusion, we will denote them by (a) $Q_{ab}^{\rm KKR}(T)$, (b) $Q_{ab}^{\rm Eb}(T)$, and (c) $Q_{ab}^{\rm AP}(T)$. It is a question of rigor to prove which is the correct result for the well-defined $Q_{ab}(T)$.

(a) $Q_{ab}^{\rm KKR}(T)$ (Q in Ref. [1]) is obtained for a pure Coulomb interaction, summing up all ladder diagrams in a Green's functions approach [see Eq. (3) of Ref. [1] and Eq. (6.218) in Ref. [5]]. It contains no linear term $\propto\xi_{ab}$.

(b) $Q_{ab}^{\rm Eb}(T) = Q_{ab}^{\rm KKR}(T) + \xi_{ab}/6$ can be obtained if the average of the potential modified by a short-range contribution (Kelbg) is considered. $Q_{ab}^{\rm Eb}(T)$ as a result for the Q function has been taken, e.g., in Eq. (6.4) in Ref. [6] and Eq. (2.53) in Ref. [7]. For the problem in this context, see Sec. IV. It was shown in the Appendix of Ref. [1] that the $\xi_{ab}/6$ arises because the Coulomb interaction was modified at short distances by quantum terms, in order to allow for classical calculations. The appearance of the linear term must be considered as an artifact which does not appear in the strict treatment of a pure Coulomb system. The proof of the origin of the $\xi_{ab}/6$ term, given in the Appendix of Ref. [1], was not commented on in Ref. [2].

(c) Alastuey and Perez [8] derived an expression, Eq. (6.15), from a path-integral representation for the virial expansion. The corresponding result $Q_{ab}^{\rm AP}(T)$ is compared to (see Ref. [8]) "*the so-called quantum second-virial coefficient $Q_{ab}^{\rm Eb}(T)$ introduced by Ebeling*." The result, Eq. (7.3) of Ref. [8], can be written as

$$Q_{ab}^{\rm AP}(T) = Q_{ab}^{\rm KKR}(T) + \xi_{ab}/6 + \Delta Q_{ab}^{\rm AP}(T). \qquad (1)$$

More directly, this decomposition for $a=b$ is shown in Eq. (7.4) of Ref. [8]. Alastuey and Perez continue in [8]: *"As already mentioned in Ref. [16], all the terms in the expansion (7.3) coincide with those calculated by Ebeling and co-workers [20]* (presently Ref. [7]) *via the effective-potential method, except the diffraction term of order $\rho^{5/2}$ proportional to $\hbar^2$ which is missing in their expressions."*

A diffraction term of the order n^2 appears already in Eq. (7.4) of Ref. [8] for the one-component plasma. Expressions for the quantum diffraction term $\Delta Q_{ab}^{\rm AP}(T)$ are obtained from Eqs. (7.6) and (7.7b) of Ref. [8]. According to Ref. [1], the term $\Delta Q_{ab}^{\rm AP}(T)$ introduced by Alastuey and Perez [8] is, in first order of ξ_{ab}, exactly $-\xi_{ab}/6$ to eliminate the unjustified $\xi_{ab}/6$ term in Eq. (1). This was also shown in Ref. [8], Sec. VII B. There, the diffraction term is discussed, and this is also outlined in Ref. [2]. Consequently, we have to admit more precisely, in contrast to a remark in Ref. [1], that Alastuey and Perez [8] also did not obtain the e^2 linear direct term in the second virial coefficient.

However, let us now look at the paper by Alastuey and Ballenegger [9]. There is a statement, in response to Refs. [5,10] and in contrast to Ref. [8], that there is a linear direct term in the EOS. This can be seen from Eqs. (13), (16), and (40) in Ref. [9], where the function $Q_{ab}^{\rm Eb}(T)$ is used. Here, the appearance of the linear direct term is in contradiction to the former work, Ref. [8].

IV. CONSEQUENCES

We discuss the consequences for the thermodynamic properties of Coulomb systems if $\xi_{ab}/6$ arises as an additional contribution in the direct term of the second virial coefficient. We give three examples:

(a) The second virial coefficient of the two-component plasma (TCP): We have to perform the summation over the constituents a,b. Because of charge neutrality, the contributions $\xi_{ab}/6$ compensate each other, and the different expressions $Q_{ab}^{\mathrm{KKR}}(T), Q_{ab}^{\mathrm{Eb}}(T), Q_{ab}^{\mathrm{AP}}(T)$ give the same result. This was also emphasized in the Comment [2].

(b) The second virial coefficient of the one-component plasma (OCP) is influenced by the choice of different Q functions. In papers on the OCP, Refs. [11,12], there is no linear term in the EOS. In Ref. [8], it is shown, e.g., in Eq. (7.4), how the linear contribution, arising from $Q_{ab}^{\mathrm{Eb}}(T)$, is compensated by a diffraction term.

(c) We consider terms of the order $n^{5/2}$. The existence or nonexistence of the direct linear term produce discrepancies in the order beyond n^2 in the EOS. We give examples in which the (unjustified) "choice" of different functions Q (with or without a linear term) produces different results: Eq. (2.52) in Ref. [7] and Eqs. (2) and (6) in Ref. [4]. These different results cannot be simultaneously "correct" for different Q functions.

The situation in Eqs. (7.3) and (7.4) in Ref. [8] is different. In Ref. [8], the unjustified terms of order $n^{5/2}$, arising from a linear term in $Q_{ab}^{\mathrm{Eb}}(T)$, are eliminated by diffraction terms. The correct result $Q_{ab}^{\mathrm{KKR}}(T)$ without the linear term would avoid the introduction of diffraction terms.

V. PURE COULOMB SYSTEM VERSUS COULOMB POTENTIAL PLUS ADDITIONAL SHORT-RANGE POTENTIAL

We have shown that for a pure Coulomb system, there is no linear direct term. The term in question appears if the mean value of the potential energy is taken for a system whose particles interact via the Coulomb potential *plus an additional short-range potential*, i.e., via the Kelbg potential. This was outlined in the Appendix of Ref. [1].

VI. SUMMARY

In conclusion, we find that the Comment [2] does not answer the essential questions raised in Ref. [1]. For a pure Coulomb system, the mean value of the potential energy has to be taken for the Coulomb potential and does not give a linear direct term in the second virial coefficient and in the relevant $Q_{ab}(T)$ function. In contrast, a linear direct term $\xi/6$ appears in the second virial coefficient and in the relevant $Q_{ab}(T)$ function from taking the mean value of the Kelbg potential instead of that of the Coulomb one. For pure Coulomb systems, the existence of a linear direct term leads to unjustified higher orders in the EOS beyond n^2.

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