Reply to "Short-range screening potentials for classical Coulomb fluids: Reanalysis of Monte Carlo sampling and cluster model studies"

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The model reanalyses on the screening potential (SP) for the classical one-component plasmas, presented by Rosenfeld [preceding paper, Phys. Rev. E **52**, 2000 (1995)] have been re-examined in light of the Monte Carlo (MC) simulation data currently available. With due consideration of statistical uncertainties in the MC data, it is shown that these approximation schemes individually may not corroborate some of the MC data. The assessed value ($h_2/\Gamma = 0.00 \pm 0.01$) [Ichimaru *et al.*, Phys. Rev. E **50**, 2977 (1994)] of the quartic coefficient in the short-range expansion of the SP is consistent with all the data obtained by the first-principles direct MC samplings of h_2 and can reproduce MC values of the radial distribution function and SP uniformly for $10 \leq \Gamma \leq 160$.

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I. INTRODUCTION

The screening potential (SP), the balance between the bare Coulomb repulsion and the logarithm of the radial distribution function for a charged liquid, plays an essential role in the theoretical estimation of enhancement for the nuclear reaction rates in dense stellar matter [1]. The short-range correlations in a classical one-component plasma (OCP), which are not directly accessible in a Monte Carlo (MC) sampling of the radial distribution functions, have been approached through the first-principles analyses combining the short-range Widom [2] expansion of the SP and direct MC samplings of the potential-field distributions at properly constructed test charges [3,4].

In the preceding paper [5], Rosenfeld presents a reanalysis of the SP through sets of approximate model calculations. Each calculation is correct as far as we can see. In particular, Rosenfeld points out an error in another approximate cluster model calculation presented in Ref. [4]; an erratum for this correction has been published [6]. The principal conclusion in Ref. [4] with respect to the SP, however, is not affected by the correction, as reasoned in Sec. VI below.

In this paper we re-examine the model reanalyses on the SP presented in Ref. [5] in light of MC samplings for the coefficients of the Widom expansion and for the radial distribution functions [3,4,7]. It is thereby shown that the results of the approximate modeling schemes in Ref. [5], such as the extrapolation method and the so-called AJ(i) fits, individually may not be able to corroborate some of those MC indications. We point out, on the other hand, that the principal conclusion in Ref. [4], namely, its Eq. (20) or Eq. (5) below, is consistent with all the first-principles MC samplings [3,4] of the quartic coefficient in the short-range expansion of the SP; moreover, it leads to an extraction scheme [7] for the bridge functions, that reproduces the MC values of the radial distribution functions and hence the SPs uniformly for $10 \leq \Gamma \leq 160$ with the best accuracy hitherto attained. Thus, contrary to some of the criticisms offered in Ref. [5], Ref. [7] has shown already that Eqs. (20) and (33) in Ref. [4] are accurately consistent with all the current MC indications over $10 \leq \Gamma \leq 160$. Other criticisms in Ref. [5], related to Eqs. (25) and (31) in Ref. [4], have been answered in Ref. [8].

II. SHORT-RANGE SCREENING POTENTIAL

We consider a classical OCP [1] that consists of N identical particles of electric charge Ze in a volume V with a uniform compensating charge; $n = N/V$ is the average number density. The physical nature of such a plasma is characterized by a single dimensionless plasma parameter

$$\Gamma \equiv \frac{\beta(Ze)^2}{a} , \tag{1}$$

which measures the ratio between the average Coulomb energy and the average kinetic energy; β denotes the inverse temperature in energy units, and

$$a \equiv \left[\frac{3}{4\pi n} \right]^{1/3} \tag{2}$$

refers to the ion-sphere radius. Hereafter we shall measure all the radial distances such as r in units of a.

The SP, $H(r)$, is defined as

$$\beta H(r) = \frac{\Gamma}{r} + \ln[g(r)] . \tag{3}$$

It is the difference between the bare potential, the first term on the right-hand side, and the logarithm of the radial distribution function $g(r)$, and is closely related to the bridge function [1,7] in the theory of liquids.

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The principal issue under present debate is the *short-range expansion* [2] of the SP in a power series of r^2,

$$\beta H(r)=h_0+h_1r^2+h_2r^4+h_3r^6+\ldots , \quad (4)$$

around $r=0$, and in particular the theoretical assessment of the coefficients, h_0 and h_2, defined by the expansion above. The coefficient h_1, on the other hand, has been shown [9] exactly to take on the value $-\Gamma/4$.

III. MONTE CARLO SAMPLINGS FOR h_2

The quartic coefficient h_2 of the Widom expansion (4) has been expressed exactly in terms of a certain statistical average as Eq. (17) in Ref. [4]. This exact expression has been evaluated directly through the technique of MC sampling for the eight cases in OCP [3,4]. Table I summarizes the findings. We remark that these results are the outcomes from mutually independent cases of MC samplings; the statistical quality of each simulation has been reflected in the associated error bar. With the combined entry of central value and statistical uncertainty, each of these eight cases thus constitutes an elementary MC datum for h_2 currently available.

On the basis of these data, it has been concluded in Ref. [4] that the assessment

$$h_2/\Gamma=0.00\pm0.01 \quad (5)$$

is consistent with all the entries listed in Table I. We remark that such a procedure of assessment is sound and can stand by itself; no extra "support" from any *approximate* model considerations would be needed. Since we are well aware of the extent of various statistical uncertainties involved, as well as the limits in the MC sampling procedures as described in Ref. [4], we did not find it justifiable to explore a possible Γ dependence out of those data, however. To answer a point raised in the criticism in Sec. IV A of Ref. [5], the assessment proposed therein, $h_2/\Gamma=0.02\pm0.01$, is inconsistent with the evaluation in Table I for the cases $B2$, $C2$, $D1$, and $D2$.

IV. EXTRAPOLATION SCHEMES

Ogata, Iyetomi, and Ichimaru [3] carried out separate sets of MC sampling calculations for $g(r)$ and thereby determined a representation $f(r;\Gamma)$ for $\beta H(r)$ over an intermediate domain $r_{\min}<r<2$. In this expression, $r_{\min}$ refers to a minimum distance at which the value of $\beta H(r)$ may be meaningfully sampled. The intermediate function $f(r;\Gamma)$ was then extrapolated into the short-range domain by the use of Eq. (5), resulting in an assessment for h_0 as given by

$$h_0/\Gamma=1.356-0.0213\ln\Gamma-(0.456-0.0130\ln\Gamma)^2 . \quad (6)$$

Subsequently, Iyetomi, Ogata, and Ichimaru [7] used evaluations (5) and (6) to build an extraction scheme of the OCP bridge function that was successful in reproducing the MC values of the radial distribution function (cf. Fig. 7 in Ref. [7]) and the SP (cf. Fig. 5 in Ref. [7] and Figs. 7 and 8 in Ref. [4]) uniformly over $10\le\Gamma\le160$ to a high accuracy. This clearly constitutes the evidence for the consistency of Eqs. (5) and (6) with the MC distribution functions, including the SP, to answer the criticisms in Secs. IV C–IV F in Ref. [5]; the schemes suggested in Ref. [5] individually have not shown such a consistency, however.

Rosenfeld [10] employed a different extrapolation scheme, where he set three unknown parameters, h_0, h_2, and r_0, to be determined from the requirement that the function and its first two derivatives were continuous at r_0 between the short-range function (4) and the intermediate function $f(r;\Gamma)$; and obtained

$$h_2/\Gamma=[24(1.368-0.039\ln\Gamma)^2]^{-1} . \quad (7)$$

This formula yields $h_2/\Gamma=0.030$, 0.029, 0.028, 0.026 at $\Gamma=160$, 80, 40, 10, respectively. These values are inconsistent with the cases of MC sampling: $B2$, $C1$, $C2$, $D1$, and $D2$, in Table I.

In Sec. IV B of Ref. [5], as well as in Ref. [10], Rosenfeld makes a certain remark related to the relative magnitude between the connection point r_0 and $r_{\min}$, the minimum distance at which $H(r)$ can be sampled meaningfully by an MC method. It follows from these definitions that $r_0>r_{\min}$ is *not* a necessary condition for such an extrapolation, if the intermediate fitting function can extend itself below $r_{\min}$ to r_0 when $r_0<r_{\min}$, as Fig. 7 in Ref. [4] may exemplify. It would be good, of course, if $r_0>r_{\min}$ is realized, since the validity of a given extrapolation scheme could then be tested through a *direct comparison* with the MC data below r_0. In fact, such a case has already been exhibited in Fig. 8 of Ref. [4], where it is seen that the extrapolation scheme in Refs. [5] and [10] *fails* in such a test.

The extrapolation scheme in Ref. [10] for the coefficient h_2, as expressed in Eq. (7), depends on the derivatives of $f(r;\Gamma)$ at r_0. Since this function is derived from the MC samplings of $g(r)$, it may contain considerable statistical uncertainties, especially around $r=r_{\min}$ ($\approx r_0$) (cf. Figs. 7 and 8 in Ref. [4]); its derivatives are the quantities of further questionable accuracy. On the other hand, as shown earlier, the assessment (5) depends neither on the intermediate function $f(r;\Gamma)$ nor on an extrapolation procedure therefrom.

TABLE I. The values of the quartic coefficient h_2/Γ, calculated by the direct MC samplings in Refs. [3] and [4].

Case	Γ	h_2/Γ	Reference
$A1$	160	-0.0007 ± 0.034	[4]
$A2$	160	0.06 ± 0.13	[3]
$B1$	80	0.021 ± 0.022	[4]
$B2$	80	-0.07 ± 0.07	[3]
$C1$	40	0.011 ± 0.015	[4]
$C2$	40	-0.03 ± 0.04	[3]
$D1$	10	0.004 ± 0.012	[4]
$D2$	10	0.0006 ± 0.009	[3]

V. AJ(i) FITS

Alastuey and Jancovici [11] derived an overall approximate fit of $\beta H(r)$ over the whole interval, $0\le r\le1.6$, in a

polynomial,

$$\beta H(r)=h_0'+h_1'r^2+h_2'r^4+h_3'r^6 . \quad (8)$$

It should be noted that these authors have correctly termed this expression "an overall approximate fit ... over the whole interval $0\le r\le 1.6$" and that Eq. (8) is a polynomial fit, whereas Eq. (4) in the present study represents the *short-range expansion* around $r=0$. The set of the coefficients $\{h_i\}$ in Eq. (4) should therefore be different, both by definition and in practice, from $\{h_i'\}$ in Eq. (8). In Ref. [11], the coefficient h_0' was computed through a binary-ionic-mixture equation of state expressed approximately as a linear superposition of an OCP equation of state obtained by Hansen, Torrie, and Vieillefosse [12], and h_1' was assessed at $-\Gamma/4$. The remaining coefficients, h_2' and h_3', were the fitting parameters for an intermediate function such as $f(r;\Gamma)$ and were given the following values:

$$h_2'/\Gamma=0.039 , \quad h_3'/\Gamma=-0.0043 . \quad (9)$$

We have not misidentified this h_2' with the h_2 defined in Eq. (4), to answer a remark made in Sec. IV A of Ref. [5].

In Ref. [5], Rosenfeld then extended the Alastuey and Jancovici approach and set the so-called "AJ(i) fits," where i seems to denote the number of terms in a polynomial such as Eq. (8). Although no descriptions have been given in Ref. [5] as to the numerical procedures for the determination of $\{h_i'\}$ and the extent of the errors in the resultant fits, it is obvious that Rosenfeld has misidentified the h_2' so obtained with the h_2 defined in Eq. (4). Furthermore, his best estimate, AJ(5), in Fig. 1 of Ref. [5], disagrees with the MC indications in Table I for the cases $A1$, $B2$, and $C2$.

VI. OTHER MODEL CALCULATIONS

A number of approximate cluster model calculations assisted by the so-called "Onsager-molecules" concept have been described in Ref. [5]. There have been no complete pictures of the radial distribution function and SP, however, presented in these calculations in such a way as to exhibit consistency with the MC indications, such as those summarized in Refs. [1] and [4]; the same is true with the approximate cluster models in Ref. [4] as corrected in Ref. [6]. We recall, however, that the combination of Eqs. (5) and (6) has led to such a complete picture in Ref. [7].

In these connections, we may add a reservation with regard to the dependence of the model calculations in Ref. [5] on the Onsager-molecules concept, in order to assess an asymptotic behavior of h_2' in the limit of $\Gamma\to\infty$. It is well known [1] that the classical OCP in the limit of $\Gamma\to\infty$ is a bcc array of point charges, where the distribution functions, such as the radial distribution function, are expressed as superpositions of the three-dimensional δ functions located at the bcc-lattice points. The distribution functions thus exhibit extremely singular behaviors, so that one finds both $\{h_i\}$ in Eq. (4) and $\{h_i'\}$ in Eq. (8) to be ill-defined quantities in these circumstances.

Finally, some comments in Sec. IV of Ref. [5], concerning Eqs. (25) and (31) in Ref. [4], are related to the issues involving the binary-ionic-mixture equations of state, which have been adequately answered in Ref. [8].

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