Direct Monte Carlo sampling of the short-range screening potentials for classical Coulomb liquids

Shuji Ogata
Department of Applied Sciences, Yamaguchi University, 2557 Tokiwadai, Ube 755, Japan
(Received 31 August 1995)

A Monte Carlo (MC) simulation scheme to sample directly the screening potentials for Coulomb liquids at short interparticle distances is formulated on the basis of the importance sampling techniques. It is applied to the one-component plasmas at various degrees of the Coulomb coupling to obtain the screening potentials with high accuracy; a fitting formula for the MC values of the potentials is presented. The results for the screening potentials at zero separation are compared with those obtained in various approximation methods, and are utilized for the analyses of the excess free energy for binary-ionic-mixture plasmas through a thermodynamic self-consistency equation with respect to the screening potentials.

PACS number(s): 52.25.−b, 61.20.−p, 05.20.Gg

I. INTRODUCTION

Classical Coulomb liquid, a collection of charged particles with the same sign, is one of the fundamental systems in statistical plasma physics [1], and offers an accurate theoretical model for the interior materials of dense astrophysical objects such as white dwarfs [2,3]. The interparticle correlations and thermodynamic properties for the liquid have been studied by various kinds of theoretical methods including integral equation formalisms [2,4] and Monte Carlo (MC) simulation techniques [5,6].

The screening potential [7,8] is defined as the differential between the potential of mean force and the bare Coulomb potential in such a liquid. Accurate values of the potentials at short interparticle distances are essential in various phases of the theoretical calculations: The enhancement factor of the nuclear reaction rates in the liquid due to many-body correlations may depend sensitively on the short-range screening potentials [9]. The screening potentials at zero separation play important roles in the theoretical investigation of the equation of state for binary-ionic-mixture plasmas [10].

MC simulations for the Coulomb liquids have been performed to obtain the screening potentials from first principles [9,11]. Due to the strong Coulomb repulsion at short interparticle distances, however, the potentials could be sampled directly in the MC runs only for the distance $r \gtrsim a = (4\pi n/3)^{-1/3}$ (n denotes the mean density of plasma particles) in the strong coupling regime [9]. Various approximation schemes [8,9] which exploit the MC values at $r \gtrsim a$, as well as the short-range expansion [12] of the potential with respect to r^2, have been proposed to evaluate the potentials at $r < a$.

In this paper, we present a MC simulation scheme to sample the screening potential for such a Coulomb liquid at short distances, i.e., $r \lesssim a$. In the scheme, sampling probabilities at $r \lesssim a$ are enhanced by introducing an attractive interaction potential between two particles in the liquid in addition to the Coulomb potential. The present MC scheme is applied successfully to the one-component plasmas to obtain the short-range screening potentials with high accuracy at various values of the Coulomb coupling parameter. Values of the screening potentials at zero separation obtained in those MC runs are compared with those obtained in approximate theoretical methods, and are utilized to investigate the excess free energy for binary-ionic-mixture plasmas through a thermodynamic self-consistency equation with respect to the screening potentials.

II. DIRECT SAMPLING SCHEME FOR SCREENING POTENTIALS

For simplicity, we consider a one-component plasma (OCP) [2,13] consisting of N point particles with charge Ze embedded in the uniform background charges of volume V; the position of the particle $i \in \{1,2,\ldots,N\}$ is denoted as $\mathbf{r}_i$. The thermodynamic state of the OCP is characterized by the Coulomb coupling parameter

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

with the ion-sphere radius $a \equiv (4\pi N/3V)^{-1/3}$, and the inverse temperature in energy units $\beta \equiv 1/k_B T$.

The radial distribution function, i.e., joint probability of two particles at an interparticle separation $\mathbf{r}$, is defined as [4]

$$g(\mathbf{r}) = g(r) = V \frac{\prod_{i=1}^{N} \int d\mathbf{r}_i \delta(\mathbf{r}-\mathbf{r}_{12}) \exp(-\beta\Phi_N)}{\prod_{i=1}^{N} \int d\mathbf{r}_i \exp(-\beta\Phi_N)} . \tag{2}$$

Here $\mathbf{r}_{12} \equiv |\mathbf{r}_1 - \mathbf{r}_2|$ and Φ_N denotes the total interaction potential in the system calculated as

$$\Phi_N \equiv \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{(Ze)^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \rho_b \sum_{i=1}^{N} \int d\mathbf{r} \frac{Ze}{|\mathbf{r}_i - \mathbf{r}|} + \frac{\rho_b^2}{2} \int d\mathbf{r} \int d\mathbf{r}' \frac{1}{|\mathbf{r}-\mathbf{r}'|} , \tag{3}$$

with the charge density $\rho_b = -ZeN/V$ for background

charges.

The screening potential is defined in terms of $g(r)$ as [7]

$$H(r)=\frac{(Ze)^2}{r}+\frac{1}{\beta}\ln[g(r)] \ . \tag{4}$$

Accurate values of $H(r)$ at short distances are essential in the improvement of the liquid theory through analyses of the short-range bridge function [14], as well as in the calculation of the enhancement factors for the nuclear reaction rates due to many-body correlations [9].

In the usual MC simulations for the OCP's [5,6], one generates a series of particle configurations in proportion to the probability function $p(\{\mathbf{r}_i\})\propto\exp(-\beta\Phi_N)$. Sampling probabilities for $g(r)$ at $r\ll a$ are extremely small in number due to the largeness of $(Ze)^2/r_{12}$ in Φ_N at $r_{12}=r\ll a$. Ogata, Iyetomi, and Ichimaru (OII) [9] performed extra-long MC runs for the OCP's at $\Gamma=10$ and at 160 using $N=432$ MC particles to sample $H(r)$ at short distances. The minimum values of r_{12} sampled in their runs were $0.4a$ at $\Gamma=10$ and $1.1a$ at $\Gamma=160$. We note in this connection that their MC values of $H(r)$ at $\Gamma=10$ contained relatively large error bars for $0.4a\le r\le 0.5a$, as depicted by open circles with error bars in Fig. 6 (below).

We may enhance the sampling at $r\lesssim a$ by introducing a fictitious attractive potential $w(r_{12})$ between the two particles, $i=1$ and 2. This idea is realized by rewriting $g(r)$ in Eq. (2) as

$$g(r)=V\frac{\prod_{i=1}^{N}\int d\mathbf{r}_i\,\delta(\mathbf{r}-\mathbf{r}_{12})\exp[-\beta\Phi_N-\beta w(r_{12})]\exp[\beta w(r_{12})]}{\prod_{i=1}^{N}\int d\mathbf{r}_i\exp[-\beta\Phi_N-\beta w(r_{12})]\exp[\beta w(r_{12})]}$$
$$=\frac{G_w(r)\exp[\beta w(r)]}{G_w^{\rm norm}} \ , \tag{5}$$

with

$$G_w(r)=V\langle\delta(\mathbf{r}-\mathbf{r}_{12})\rangle_w \ , \tag{6a}$$

$$G_w^{\rm norm}=\langle\exp[\beta w(r_{12})]\rangle_w \ , \tag{6b}$$

where

$$\langle A\rangle_w\equiv\frac{\prod_{i=1}^{N}\int d\mathbf{r}_i\,A\exp[-\beta\Phi_N-\beta w(r_{12})]}{\prod_{i=1}^{N}\int d\mathbf{r}_i\exp[-\beta\Phi_N-\beta w(r_{12})]} \tag{7}$$

for any function A. We note that $g(r)$ in Eq. (5) is independent of the forms for $w(r_{12})$. Equation (5) signifies that $g(r)$ for the OCP may be obtained from MC simulations for a different system with the total interaction potential

$$\Phi_N'\equiv\Phi_N+w(r_{12}) \ . \tag{8}$$

In such simulation runs, the potential $w(r_{12})$ acts to enhance the sampling at short distances, since MC configurations are generated with the probability $p'(\{\mathbf{r}_i\})\propto\exp(-\beta\Phi_N')$.

An explicit formula for $w(r_{12})$ suitable for the direct MC sampling of the OCP $H(r)$ at $r\lesssim 2a$ may be determined by taking into account the following requirements: (i) $w(r_{12})\to-(Ze)^2/r_{12}$ at $r_{12}\to 0$, and (ii) $(\partial/\partial r_{12})[w(r_{12})+(Ze)^2/r_{12}]>0$ at $r_{12}\gtrsim 2a$. Requirement (i) acts to reduce the Coulomb potential between the two particles ($i=1$ and 2) at $r_{12}\approx 0$; and (ii) is effective to bound the two particles within $r_{12}\lesssim 2a$. We thereby adopt the following formula for $w(r_{12})$:

$$\beta w(r_{12})=-\Gamma\frac{\mathrm{erfc}(\alpha_1 r_{12}/a)}{r_{12}/a}+\alpha_2\left[\frac{r_{12}}{a}\right]^2 , \tag{9}$$

with the complementary error function defined as

$$\mathrm{erfc}(x)=\frac{2}{\sqrt{\pi}}\int_x^\infty\exp(-t^2)dt \ . \tag{10}$$

Values of α_1 and α_2 in Eq. (9) are chosen as

$$(\alpha_1,\alpha_2)=\begin{cases}(0.85,5.0) & \text{at } \Gamma=10 \ ,\\ (0.85,3.0) & \text{at } \Gamma=40 \ ,\\ (0.85,1.0) & \text{at } \Gamma=80 \ ,\\ (0.85,0.1) & \text{at } \Gamma=160 \ ,\end{cases} \tag{11}$$

for the purpose of importance sampling at $0\le r\lesssim 2a$.

III. MONTE CARLO SAMPLING RESULTS

A. Screening potentials for OCP's

We have performed MC simulation runs for the system with the total interaction potential Φ_N' in Eq. (8) at $\Gamma=\{10,40,80,160\}$ using $N=1000$ MC particles to obtain OCP $H(r)$ at short distances. Starting from a configuration in which $\mathbf{r}_2,\mathbf{r}_3,\ldots,\mathbf{r}_{1000}$ are distributed randomly and $\mathbf{r}_1=\mathbf{r}_2$, we have generated a series of MC configurations following the Metropolis algorithm [15]. The particle i to be displaced on trial in the algorithm was chosen with the probabilities 25% for $i=\{1,2\}$ and 0.05% for $i=\{3,4,\ldots,1000\}$. In each run, we waited for the initial interval of $c/N=0\to 16\times 10^3$, where c denotes the sequential number of MC configurations, until the system reached an equilibrium state.

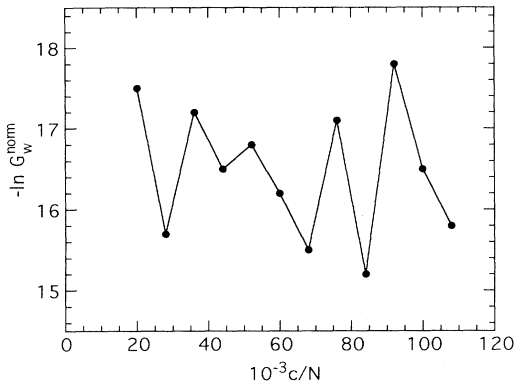

FIG. 1. Sequential evolution of $-\ln G_w^{\text{norm}}$ in the MC run at $\Gamma=160$. Values of the parameters in $w(r_{12})$ [Eq. (9)] are $(\alpha_1,\alpha_2)=(0.85,0.1)$. Each data point is obtained as the average over the period of $\Delta C/N=8\times10^3$.

Averages $G_w(r)$ and G_w^{norm} in Eqs. (6) were calculated from the sequential MC configurations in the period of $c/N=16\times10^3\rightarrow112\times10^3$ as follows: We first construct the histogram $\Delta N_V(k)$ of $r_{12}\in[d(k-1),d(k)]$ with $d(k)=0.04ak$ $(k=1,2,\ldots)$. Denoting the volume of the bin as $\Delta V(k)\equiv(4\pi/3)\{[d(k)]^3-[d(k-1)]^3\}$, we thereby evaluate the quantity $G_w(r)$ and G_w^{norm} as

$$G_w(d_{l-(1/2)})=\frac{\Delta N_V(l)}{\Delta V(l)}\frac{\sum_{k=1}^{k_{\max}}\Delta V(k)}{\sum_{k=1}^{k_{\max}}\Delta N_V(k)} \tag{12}$$

and

$$G_w^{\text{norm}}=\frac{\sum_{k=1}^{k_{\max}}\Delta N_V(k)\exp(\beta d_{k-(1/2)})}{\sum_{k=1}^{k_{\max}}\Delta N_V(k)}, \tag{13}$$

where $d_{k-(1/2)}\equiv[d(k-1)+d(k)]/2$, and $k_{\max}$ corresponds to the maximum number of k with $\Delta N_V(k)>0$.

Figure 1 shows the sequential evolution of G_w^{norm} [Eq. (13)] obtained in the MC run at $\Gamma=160$; each data point was obtained as the average over the short interval of $\Delta c/N=8\times10^3$. MC data for G_w^{norm} appear to be fluctuating uniformly as a function of c/N, which is a manifestation of the equilibrium state. We find from Fig. 1 that $\ln G_w^{\text{norm}}=-16.2\pm0.5$.

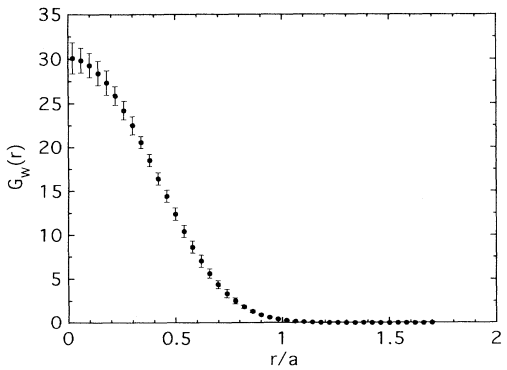

FIG. 2. Sampling results for $G_w(r)$ obtained in the MC run at $\Gamma=160$. Values of the parameters in $w(r_{12})$ [Eq. (9)] are $(\alpha_1,\alpha_2)=(0.85,0.1)$.

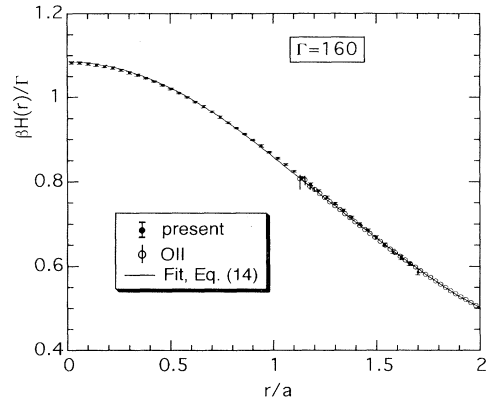

FIG. 3. MC results for $\beta H(r)/\Gamma$ at $\Gamma=160$. Solid circles represent present results, open circles the OII results in Ref. [9]. The solid curve represents the fitting formula [Eq. (14)].

MC values of $G_w(r)$ [Eq. (12)] at $\Gamma=160$ are depicted in Fig. 2. As was intended, MC samplings were well performed for $0\le r\le1.7a$. Relative uncertainty $|\delta G_w(r)/G_w(r)|$ at each value of r is about 0.07 for $0\le r\le1.5a$, which is much smaller than that of $|\delta G_w^{\text{norm}}/G_w^{\text{norm}}|\sim e^{-0.5}\approx0.6$. Hence the accuracy of $H(r)$ defined in Eq. (4) with Eq. (5) depends mainly on that of G_w^{norm} in the present sampling scheme.

Figure 3 displays the MC results for the normalized screening potential, $\beta H(r)/\Gamma$, in Eq. (4). The solid circles with error bars represent present MC results calculated through Eqs. (4) and (5) using values of G_w^{norm} and $G_w(r)$ presented in Figs. 1 and 2; the open circles with error bars, OII MC results in Ref. [9]. Present data agree with the OII data to within their error bars for $1.1a\le r\le1.7a$ where both data exist. For $r<1.1a$, while no OII data exist, the present MC scheme can predict $\beta H(r)/\Gamma$ with high accuracy.

Present MC data for $\beta H(r)/\Gamma$ at different values of Γ

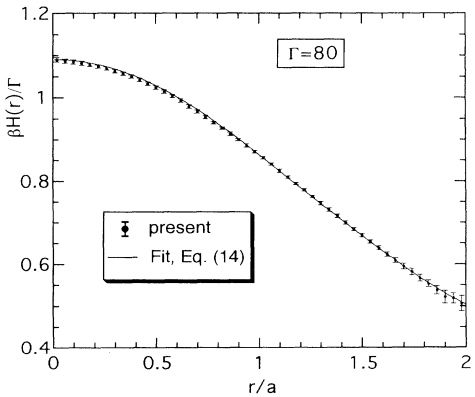

FIG. 4. MC results for $\beta H(r)/\Gamma$ at $\Gamma=80$. Solid circles represent present results, the solid curve the fitting formula [Eq. (14)].

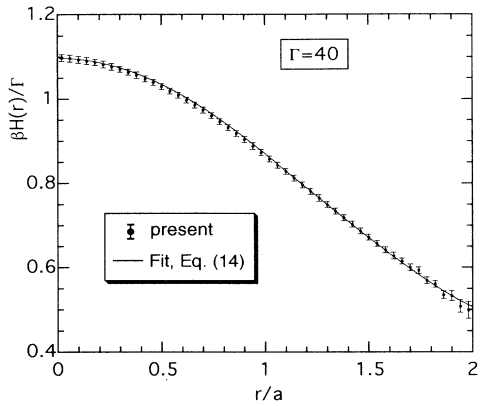

FIG. 5. Same as Fig. 4, but at $\Gamma=40$.

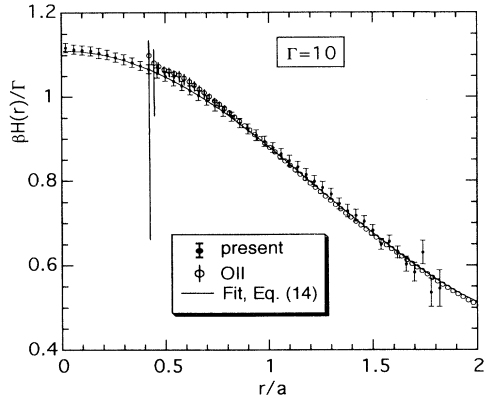

FIG. 6. Same as Fig. 3, but at $\Gamma=10$.

are depicted as solid circles with error bars in Figs. 4 ($\Gamma=80$), 5 ($\Gamma=40$), and 6 ($\Gamma=10$); they are accurate for $0\le r\lesssim 2.0a$ at $\Gamma=80$, for $0\le r\lesssim 2.0a$ at $\Gamma=40$, and for $0\le r\lesssim 1.8a$ at $\Gamma=10$. At $\Gamma=10$, present MC data agree with OII MC data to within their error bars for $0.4a\le r\lesssim 1.8a$ as seen in Fig. 6.

A useful fitting formula for the present MC values of $\beta H(r)/\Gamma$ applicable at $5<\Gamma\lesssim 180$ is obtained as

$$\beta H(r)/\Gamma=\begin{cases} A_1-\frac{1}{4}x^2[1-\exp(-A_2/x)] & \text{for } x\le A_3\ , \\ A_4-A_5x+\dfrac{1}{x}\exp(A_6\sqrt{x}-A_7) & \text{for } A_3<x\le 2 \end{cases} \tag{14}$$

with $x\equiv r/a$ and

$$\begin{aligned} &A_1=1.132-0.0094\ln\Gamma,\quad A_2=2.55-0.043\ln\Gamma\ , \\ &A_3=1.22-0.047\ln\Gamma,\quad A_4=1.356-0.0213\ln\Gamma\ , \\ &A_5=0.456-0.013\ln\Gamma,\quad A_6=9.29+0.79\ln\Gamma\ , \\ &A_7=14.83+1.31\ln\Gamma\ . \end{aligned} \tag{15}$$

Formula (14) is represented as solid curves in Figs. 3–6 to demonstrate its accuracy.

It is known that the short-range screening potential may be expanded as a power series of r^2 [8,12,16]:

$$\beta H(r)=h_0+h_1(r/a)^2+h_2(r/a)^4+O(r^6) \quad \text{at } r\approx 0\ . \tag{16}$$

The liquid theory gives the identity $h_1/\Gamma=-\frac{1}{4}$ [7,16]. On the basis of the direct MC calculation with respect to h_2, it has been concluded that $h_2/\Gamma=0.00\pm 0.01$ [8,9]. Present formula (14) for $\beta H(r)/\Gamma$ reduces to $\beta H(r)/\Gamma=A_1-(1/4)(r/a)^2+0(r/a)^4$ at $r\approx 0$ in accordance with these investigations.

B. Screening potentials at zero separation

Various approximation methods have been proposed for the evaluation of $H(0)$; a comprehensive review of the methods and their results are given in Ref. [8]. Here we compare values of $H(0)$ obtained in the present MC sampling scheme with those obtained in approximation theories.

Considering that the coefficients in the expansion (16) take on $h_1=-\Gamma/4$ and $h_2/\Gamma=0.00\pm 0.01$, OII adopted a polynomial formula $[\beta H(r)]_{\rm OII}=[\beta H(0)]_{\rm OII}-(\Gamma/4)(r/a)^2$ for $\beta H(r)$ at $r\le r_{\min}$. Values of $[\beta H(0)]_{\rm OII}$ and $r_{\min}$ were determined from the condition that $[\beta H(r)]_{\rm OII}$ connects smoothly at $r=r_{\min}$ with the OII MC data for $\beta H(r)$ obtained at intermediate distances. OII thereby found in Ref. [9] that

$$[\beta H(0)]_{\rm OII}=\Gamma(1.356-0.0213\ln\Gamma)-\Gamma(0.456-0.0130\ln\Gamma)^2\ . \tag{17}$$

Rosenfeld (R92) [17] extrapolated the OII MC data for $\beta H(r)$ from intermediate distances toward $r=0$ by using a polynomial formula $[\beta H(r)]_{R92}=[\beta H(0)]_{R92}-(1/4)(r/a)^2+h_2^R(r/a)^4$. The parameter h_2^R was determined by considering the higher order derivatives of OII MC data for $\beta H(r)$ with respect to r.

Table I compares present values of $\beta H(0)$ with $[\beta H(0)]_{\rm OII}$ and with $[\beta H(0)]_{R92}$ at various values of Γ.

TABLE I. Values of the screening potentials at zero separation. $\beta H(0)$ refers to the present MC result, $[\beta H(0)]_{\rm OII}$ to the OII evaluation [Eq. (17)], and $[\beta H(0)]_{R92}$ to Rosenfeld's evaluation in Ref. [17].

Γ	$\beta H(0)$	$[\beta H(0)]_{\rm OII}$	$[\beta H(0)]_{R92}$
10	11.18±0.11	11.25	11.01
40	43.92±0.32	44.44	43.56
80	87.20±0.40	88.28	86.64
160	173.28±0.48	175.33	172.16

Small but substantial deviations of $\beta H(0)$ are found from $[\beta H(0)]_{\rm OII}$ at $\Gamma \geq 40$ and from $[\beta H(0)]_{R92}$ at $\Gamma \geq 10$; it is a manifestation of approximate natures contained in the OII and $R92$ evaluations. Extent of such differentials enlarges as Γ increases for both cases; at $\Gamma=160$, $\beta H(0)-[\beta H(0)]_{\rm OII}=-2.05\pm0.48$ and $\beta H(0)-[\beta H(0)]_{R92}=1.12\pm0.48$.

It has been shown that $H(0)$ corresponds to the differential in the excess free energies before and after the nuclear fusion[16]. We consider a binary-ionic mixture (BIM) consisting of N_1 particles with $Z_1 e$ and N_2 particles with charge $Z_2 e$ in volume V. Let $f_{\rm ex}^{\rm BIM}(R_Z,x_2,\Gamma_1)$ denotes the excess free energy in units of N/β ($N=N_1+N_2$) for a BIM with charge ratio $R_Z=Z_2/Z_1$ and molar fraction $x_2=N_2/N$ at a Coulomb coupling parameter $\Gamma_1\equiv\beta(Z_1e)^2/a_1$ with $a_1=[(4\pi N/3V)(1-x_2+x_2R_Z)]^{-1/3}$; $f_{\rm ex}^{\rm OCP}(\Gamma)$, the excess free energy for the OCP. A thermodynamic self-consistency equation with respect to the deviation

$$\Delta f_{\rm ex}^{\rm BIM}(R_Z,x_2,\Gamma_1)\equiv f_{\rm ex}^{\rm BIM}(R_Z,x_2,\Gamma_1)-f_{\rm ex}^{\rm LM} \tag{18}$$

from the linear mixing (LM) evaluation

$$f_{\rm ex}^{\rm LM}\equiv(1-x_2)f_{\rm ex}^{\rm OCP}(\Gamma_1)+x_2 f_{\rm ex}^{\rm OCP}(R_Z^{5/3}\Gamma_1) \tag{19}$$

is thereby obtained as [7,8]

$$\left[\frac{\partial}{\partial x_2}\Delta f_{\rm ex}^{\rm BIM}(2,x_2,\Gamma)\right]_{x_2=0} = 2f_{\rm ex}^{\rm OCP}(\Gamma)-f_{\rm ex}^{\rm OCP}(2^{5/3}\Gamma)-\beta H(0)\ . \tag{20}$$

The LM evaluation $f_{\rm ex}^{\rm LM}$ corresponds to the energy for the state in which two species of particles contained in the BIM are demixed totally. The sign and magnitude of $[(\partial/\partial x_2)\Delta f_{\rm ex}^{\rm BIM}]_{x_2=0}$ play important parts in the analyses of the phase diagrams for BIM's [10].

Table II lists values of $[(\partial/\partial x_2)\Delta f_{\rm ex}^{\rm BIM}]_{x_2=0}$ calculated through Eq. (20) at various values of Γ. Here present MC values are used for $\beta H(0)$; values of $f_{\rm ex}^{\rm OCP}$ are calculated from the fitting formula [6]

$$f_{\rm ex}^{\rm OCP}(\Gamma)=-0.898\,004\Gamma+3.871\,44\Gamma^{1/4} -0.882\,812\Gamma^{-1/4} -0.860\,97\ln\Gamma-2.526\,92\ . \tag{21}$$

Possible errors contained in this formula [Eq. (21)] have been assessed to be ±0.004 at $5\lesssim\Gamma\leq180$ [18]. We find in Table II that (i) $[(\partial/\partial x_2)\Delta f_{\rm ex}^{\rm BIM}]_{x_2=0}$ takes on a negative value at $\Gamma=\{10,40,80,160\}$, and (ii) its magnitude enlarges as Γ increases. It should be noted that the finding (i) has been predicted by Ogata *et al.* [10] through MC simulation studies for the BIM excess internal energies.

TABLE II. Calculated values of $[(\partial/\partial x_2)\Delta f_{\rm ex}^{\rm BIM}]_{x_2=0}$ in Eq. (20) at various values of Γ.

Γ	$\left[\frac{\partial}{\partial x_2}\Delta f_{\rm ex}^{\rm BIM}(2,x_2,\Gamma)\right]_{x_2=0}$
10	-0.19 ± 0.11
40	-0.40 ± 0.32
80	-0.80 ± 0.40
160	-1.60 ± 0.48

IV. CONCLUDING REMARKS

We have formulated a direct MC sampling scheme for the short-range screening potential $H(r)$ in a Coulomb liquid. In the scheme, values of $H(r)$ are obtained from distribution of the interparticle distances between two particles ($i=1$ and 2), for which a fictitious attractive interparticle potential $w(r_{12})$ is introduced. The present scheme is applied to strongly coupled OCP's to obtain $H(r)$ with high accuracy at short distances. Values of $H(0)$ obtained in the present MC runs are compared with those in OII and $R92$ evaluations to find non-negligible deviations from both OII and $R92$ values. Through the self-consistency equation (20), with respect to $H(0)$, we find the inequality $[(\partial/\partial x_2)\Delta f_{\rm ex}^{\rm BIM}(2,x_2,\Gamma)]_{x_2=0}<0$ at $\Gamma=\{10,40,80,160\}$.

Present value of $\beta H(0)$ is smaller than $[\beta H(0)]_{\rm OII}$ by about 1% at $\Gamma=160$, as compared in Table II. The principal quantity controlling the thermal enhancement in the nuclear reaction rates due to many-body correlations is $E_0\equiv\exp[\beta H(0)]$ [7]. Such a small differential between $\beta H(0)$ and $[\beta H(0)]_{\rm OII}$, however, exerts significant influence on the evaluation of E_0. At $\Gamma=160$, we may obtain $E_0({\rm present})\sim0.3E_0({\rm OII})$.

The present scheme for the importance sampling of $g(r)$ and $H(r)$ at short distances can be applied straightforwardly to other systems with repulsive interparticle potentials, whose results should contribute much to the development of the liquid theory.

ACKNOWLEDGMENT

Most of the calculations were performed on the HITAC S-3800/480 supercomputer at the computer center, University of Tokyo.

[1] S. Ichimaru, *Statistical Plasma Physics, Vol. I: Basic Principles* (Addison-Wesley, Redwood City, CA, 1992).
[2] S. Ichimaru, *Statistical Plasma Physics, Vol. II: Condensed Plasmas* (Addison-Wesley, New York, 1994).
[3] H. M. Van Horn, in *Strongly Coupled Plasma Physics*, edited by S. Ichimaru (North-Holland/Yamada Science Foundation, Amsterdam/Osaka, 1990), p. 3; Science **252**, 384 (1991).
[4] J.-P. Hansen and I. R. McDonald, *Theory of Simple Liquids*, 2nd ed. (Academic, London, 1986).
[5] W. L. Slattery, G. D. Doolen, and H. E. DeWitt, Phys. Rev. A **21**, 2087 (1980); **26**, 2255 (1982).
[6] S. Ogata and S. Ichimaru, Phys. Rev. A **36**, 5451 (1987).
[7] S. Ichimaru, Rev. Mod. Phys. **65**, 255 (1993).

[8] S. Ichimaru, S. Ogata, and K. Tsuruta, Phys. Rev. E **50**, 2977 (1994); **51**, 3788(E) (1995).
[9] S. Ogata, H. Iyetomi, and S. Ichimaru, Astrophys. J. **372**, 259 (1991).
[10] S. Ogata, H. Iyetomi, S. Ichimaru, and H. M. Van Horn, Phys. Rev. E **48**, 1344 (1993).
[11] H. E. DeWitt, H. C. Graboske, and M. S. Cooper, Astrophys. J. **181**, 439 (1973).
[12] B. Widom, J. Chem. Phys. **39**, 2808 (1963).
[13] S. Ichimaru, Rev. Mod. Phys. **54**, 1017 (1982).
[14] H. Iyetomi, S. Ogata, and S. Ichimaru, Phys. Rev. A **46**, 1051 (1992).
[15] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
[16] B. Jancovici, J. Stat. Phys. **17**, 357 (1977).
[17] Y. Rosenfeld, Phys. Rev. A **46**, 1059 (1992).
[18] S. Ogata and S. Ichimaru, Phys. Rev. E **52**, 3297 (1995).