Effects of Quantum Fluctuations on Contact Probabilities of a Tunneling Pair in Dense Coulomb Liquids

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Path-integral Monte Carlo calculations for a tunneling pair in dense Coulomb liquids are performed to investigate effects of quantum fluctuations of the surrounding particles on its contact probability. We thereby find that the probabilities are enhanced significantly by the quantum fluctuations at low temperatures. By calculating various correlation functions and effective potentials for the tunneling pair, we demonstrate that the enhancement is associated with magnified and coherent quantum fluctuations of the surrounding particles near the tunneling pair. [S0031-9007(96)01254-9]

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Nuclear reaction is an elementary process of major importance in ultrahigh-pressure liquids [1] such as those realized in shock-compression experiments [2] and those predicted in the interiors of dense stars including white dwarfs and neutron stars [3]. Theoretical prediction for abundances of nuclear elements synthesized in the supernova process of a white dwarf may change sensitively depending on the rates of nuclear reactions adopted for the stellar interior [4]. Possible realization of nuclear fusion has been pointed out [5] for shock-compressed liquid metals. Nuclear reaction rates [5] are, in general, proportional to the contact probability of a pair of nuclei which tunnel through the repulsive Coulomb potential at short distances. In a dense liquid, the contact probability may be enhanced significantly in sensitive ways by the screening action of the surrounding nuclei due to internuclear many-particle correlations [5,6]. First-principles calculations for the contact probability of a tunneling pair are indispensable for accurate evaluations of the reaction rate in such liquids.

Much effort has been devoted to evaluation of the contact probability of two particles in the Coulomb liquid [5], i.e., an assembly of charged particles with same sign. In the existing theories for that problem, quantum fluctuations of the surrounding particles in the liquid were ignored or assumed to be negligible, and the contact probability was calculated by exploiting the effective pair potential derived from the radial-distribution function for corresponding *classical* systems [6–9]. Through model calculation for the tunneling probability of a physical variable coupled to a macroscopic system, however, Caldeira and Leggett [10] demonstrated significance of quantum fluctuations in the macroscopic system at the tunneling process. It is therefore expected for the Coulomb liquid at low temperatures, where the thermal de Broglie wavelength of a particle is comparable to the tunneling distance, that the effective pair potential and hence the contact probability of the tunneling pair are affected substantially by the quantum fluctuations of the surrounding particles.

In this Letter, we perform path-integral Monte Carlo (PIMC) calculations for a tunneling pair in dense Coulomb liquids at various conditions and show that the contact probabilities of the tunneling pair are enhanced significantly by inclusion of the quantum fluctuations of the surrounding particles. Mechanisms for such enhancement are investigated by considering effective potentials for the tunneling pair and various correlation functions for the quantum fluctuations.

We consider a one-component plasma (OCP) [5,11] consisting of N point particles (charge Ze, mass M) in volume V, whose positions are denoted as $\mathbf{r}_i$ for $i \in \{1, 2, \ldots, N\}$; uniform background charges with density $-ZeN/V$ are assumed to satisfy the charge neutrality condition. The Coulomb coupling parameter [5,11]

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

with the ion-sphere (or Wigner-Seitz) radius $a \equiv (4\pi N/3V)^{-1/3}$ and the inverse temperature in energy units $\beta \equiv 1/k_B T$. It has been shown through Monte Carlo calculations for the internal energies that the classical OCP solidifies at $\Gamma = 172$–180 [12–14]. The wave-mechanical nature of a particle may be characterized by [15]

$$\zeta^{3/2} \equiv \Lambda(\sqrt{\Gamma}/a)\,, \tag{2}$$

with the thermal de Broglie wavelength $\Lambda \equiv (2\hbar/\pi)\sqrt{\beta/M}$. For strongly coupled (i.e., $\Gamma \gg 1$) OCP's with $\zeta > 1$, the fluctuation volume of a particle may be dominated by its quantum spread since the characteristic width for the short-time thermal vibration of a particle is $a/\sqrt{\Gamma}$ as exemplified in the ion-sphere model [11].

The normalized radial-distribution function at zero separation, i.e., the contact probability, is defined in the Feynman path-integrals as [6,16]

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$$g(0) = V\frac{[\Pi_{i=1}^{N}\int_{\mathbf{r}_i(0)=\mathbf{r}_i(\beta\hbar)}\mathcal{D}\mathbf{r}_i(s)\exp[(-1/\hbar)\int_0^{\beta\hbar}ds\mathcal{H}(s)]]_{r_{12}(s_0)=0}}{\Pi_{i=1}^{N}\int_{\mathbf{r}_i(0)=\mathbf{r}_i(\beta\hbar)}\mathcal{D}\mathbf{r}_i(s)\exp[(-1/\hbar)\int_0^{\beta\hbar}ds\mathcal{H}(s)]} \quad (3)$$

at any imaginary time s_0; for simplicity we take $s_0 = 0$. Here $r_{ij}(s) \equiv |\mathbf{r}_i(s) - \mathbf{r}_j(s)|$,

$$\mathcal{H}(s) = \sum_{i=1}^{N}\frac{M}{2}\left|\frac{d}{ds}\mathbf{r}_i(s)\right|^2 + U(s), \quad (4)$$

and $U(s) = u(\mathbf{r}_1(s), \mathbf{r}_2(s), \ldots, \mathbf{r}_N(s))$, where $u(\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N)$ denotes the total Coulomb energy for the OCP with the particles located at $\mathbf{y}_i$ $(i \in \{1, 2, \ldots, N\})$. We assume the periodic boundary condition for the system and calculate values of u by using the Ewald's method. Exchange processes are ignored in Eq. (3), the validity of which will be discussed in a preceding paragraph. In Eq. (3), each quantum particle is represented as a loop in the interval of the imaginary time $s = [0, \beta\hbar]$. The characteristic width of a loop corresponds to the quantum spread of a corresponding particle. In the present formulation [Eq. (3)], the value of $g(0)$ is related to the contact probability of two loops $(i = \{1, 2\})$ at $s = s_0$.

In the semiclassical (SC) approximation to $g(0)$, we regard the surrounding particles $(i \in \{3, 4, \ldots, N\})$ as classical particles. The corresponding quantity $g_{\mathrm{SC}}(0)$ in the SC approximation is defined by the right hand side of Eq. (3) by assuming $U(s) = U_{\mathrm{SC}}(s) \equiv u(\mathbf{r}_1(s), \mathbf{r}_2(s), \mathbf{x}_3, \ldots, \mathbf{x}_N)$ where $\mathbf{x}_i \equiv \overline{\mathbf{r}_i(s)}$ is the time-averaged position with $\overline{A(s)} \equiv (1/\beta\hbar)\int_0^{\beta\hbar}dsA(s)$ for any function A. In former calculations for the contact probability [7–9], quantum fluctuations of the surrounding particles were ignored as in the SC approximation. The ratio $g(0)/g_{\mathrm{SC}}(0)$ defines the enhancement factor for the contact probability of a pair in a OCP due to quantum fluctuations of the surrounding particles. In the limit of low densities, both $g(0)$ and $g_{\mathrm{SC}}(0)$ reduce to $g_{\mathrm{Coul}}(0)$, which is defined by the right hand side of Eq. (3) with $N = 2$; a semianalytical formula for $g_{\mathrm{Coul}}(0)$ is known [17]. In the limit of low temperatures, the average of $r_{12}(s)$ in the numerator of Eq. (3) with $N = 2$ increases from $r_{12}(s) = 0$ at $s = 0$ to $r_{12}(s) = a\zeta$ at $s = \beta\hbar/2$ and then decreases to $r_{12}(s) = 0$ at $s = \beta\hbar$ as a function of s [6,7].

By transforming Eq. (3), we obtain the following formula for the enhancement factor:

$$\frac{g(0)}{g_{\mathrm{SC}}(0)} = \frac{\langle\exp[\beta\overline{U(s)} - \beta\overline{U_{\mathrm{SC}}(s)}]\rangle}{\langle\exp[\beta\overline{U(s)} - \beta\overline{U_{\mathrm{SC}}(s)}]\rangle_0} \quad (5)$$

where the averages $\langle\cdots\rangle_{(0)}$, i.e., $\langle\cdots\rangle$ and $\langle\cdots\rangle_0$, are defined as

$$\langle A(s')\rangle_{(0)} = \frac{[\Pi_{i=1}^{N}\int_{\mathbf{r}_i(0)=\mathbf{r}_i(\beta\hbar)}\mathcal{D}\mathbf{r}_i(s)A(s')\exp[-(1/\hbar)\int_0^{\beta\hbar}ds\mathcal{H}(s)]]_{(r_{12}(0)=0)}}{[\Pi_{i=1}^{N}\int_{\mathbf{r}_i(0)=\mathbf{r}_i(\beta\hbar)}\mathcal{D}\mathbf{r}_i(s)\exp[-(1/\hbar)\int_0^{\beta\hbar}ds\mathcal{H}(s)]]_{(r_{12}(0)=0)}} \quad (6)$$

for any function A. In the derivation of Eq. (5), we have used the equality $\exp(-(1/\hbar)\int_0^{\beta\hbar}ds\{\mathcal{H}(s) - U(s) + U_{\mathrm{SC}}(s)\}) = \exp[-(1/\hbar)\int_0^{\beta\hbar}ds\mathcal{H}(s)]\exp\{(1/\hbar)\int_0^{\beta\hbar}ds[U(s) - U_{\mathrm{SC}}(s)]\}$ in the kernels of path integrals [Eq. (3)]. A value of $g_{\mathrm{SC}}(0)$ is likewise obtained as

$$g_{\mathrm{SC}}(0) = \frac{\langle\exp[\beta\overline{U_{\mathrm{SC}}(s)} - \beta\overline{U_{12}(s)}]\rangle^{\mathrm{SC}}}{\langle\exp[\beta\overline{U_{\mathrm{SC}}(s)} - \beta\overline{U_{12}(s)}]\rangle_0^{\mathrm{SC}}}\, g_{\mathrm{Coul}}(0). \quad (7)$$

Here the averages $\langle\cdots\rangle^{\mathrm{SC}}$ and $\langle\cdots\rangle_0^{\mathrm{SC}}$ are defined in similar ways by Eq. (6) but with $U(s) = U_{SC}(s)$; $U_{12}(s) \equiv (Ze)^2/r_{12}(s)$.

We perform PIMC calculations for the liquid OCP's to obtain $g(0)/g_{\mathrm{SC}}(0)$ and $g_{\mathrm{SC}}(0)/g_{\mathrm{Coul}}(0)$ following the Metropolis algorithm [18]. A polynomial fitting formula [13] for the Ewald potential is used to accelerate computation speed. The imaginary-time interval $[0, \beta\hbar]$ is divided into ν slices [19] with equal spacings: $s_\alpha = \beta\hbar\alpha/\nu$ with $\alpha = \{0, 1, \ldots, \nu\}$. We adopt the primitive approximation [19] to calculate the action in Eq. (6); that is,

$$\prod_{i=1}^{N}\int_{\mathbf{r}_i(0)=\mathbf{r}_i(\beta\hbar)}\mathcal{D}\mathbf{r}_i(s)\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar}\mathcal{H}(s)\right] \approx C\left[\prod_{i=1}^{N}\prod_{\alpha=0}^{\nu-1}\int d\mathbf{r}_i(s_\alpha)\right]\exp\left[-\frac{M\nu}{2\beta\hbar^2}\sum_{\alpha=0}^{\nu-1}\Delta R_{\alpha,\alpha+1}^2 - \frac{\beta}{\nu}\sum_{\alpha=0}^{\nu-1}U(s_\alpha)\right], \quad (8)$$

where $\Delta R_{\alpha,\alpha+1}^2 \equiv \sum_{i=1}^{N}|\mathbf{r}_i(s_\alpha) - \mathbf{r}_i(s_{\alpha+1})|^2$ and C is a constant. At $r_{12}(s) \approx 0$, the action is dominated by the term $(Ze)^2/r_{12}(s)$. Because of its singularity at $r_{12}(s) = 0$, correct behaviors of $g(0)$ at $r \approx 0$, i.e., the cusp condition [11,17], may not be satisfied in the PIMC calculations with finite values of ν. To reproduce the correct formula [17] for the action at $r_{12}(s) \approx 0$, we modify the term $(Ze)^2/r_{12}(s)$ at $s = \{0, s_1, s_{\nu-1}\}$ contained in $U(s)$ [Eq. (8)] as $(Ze)^2 f/r_{12}(s)$ with $f = 1 - \exp[-\sqrt{8\Gamma\nu/\pi^2}r_{12}(s)/a\zeta^{3/2}]$. Values of $g_{\mathrm{SC}}(0)/g_{\mathrm{Coul}}(0)$ [Eq. (7)] are calculated by using $N = 100$ and $\nu = \{20, 50\}$ at $\Gamma = \{10, 30, 50, 90, 170\}$ and $\zeta = \{0.5, 1, 2\}$; 5×10^7 configurations are used to calculate each average. The difference in $g_{\mathrm{SC}}(0)/g_{\mathrm{Coul}}(0)$ between the cases with $\nu = 20$ and 50 is smaller than the error bars $\sim$0.2–

0.3; that is, no substantial ν dependence is observed. All the values of $g_{\rm SC}(0)/g_{\rm Coul}(0)$ are fitted to within errors of ± 0.3 by the formula $\ln[g_{\rm SC}(0)/g_{\rm Coul}(0)]_{\rm fit} = 1.132\Gamma - 0.0094\Gamma\ln\Gamma - \frac{5}{32}\Gamma\zeta^2(1 + a_1\zeta + a_2\zeta^2 + a_3\zeta^3)$ with $(a_1, a_2, a_3) = (-0.0348, -0.1388, 0.0222)$. Here the ζ^0 term is taken from Ref. [20]; the ζ^2 term, from Ref. [6].

Table I lists values of the enhancement factor $g(0)/g_{\rm SC}(0)$ in Eq. (5) calculated by using $N = \{50, 100\}$ and $\nu = 20$ at $\Gamma = \{30, 90, 170\}$ and $\zeta = \{1, 2\}$. Both averages in the numerator and denominator of Eq. (5) are obtained by using 3.2×10^9 ($N = 100$) and 2.0×10^8 ($N = 50$) configurations. Since both $U(s)$ and $U_{\rm SC}(s)$ in Eq. (5) are macroscopic quantities in proportion to N, fluctuations of $U_{(\rm SC)}(s)$ make relatively large error bars for $g(0)/g_{\rm SC}(0)$ in spite of such long runs. We find in Table I that (i) the enhancement is significant at $\Gamma \geq 90$ and $\zeta = 2$ and (ii) the value of $\ln[g(0)/g^{\rm SC}(0)]$ increases as ζ^3 while it is linear in Γ. Since quantum spread of a surrounding particle in the PIMC run at $(\Gamma, \zeta) = (170, 2)$ is $\sim 0.3a$ in radius, which is much smaller than the mean interparticle distance $\sim 1.8a$, we expect that further inclusion of the exchange processes will alter the value of $g(0)/g_{\rm SC}(0)$ to a negligible amount.

It is useful in the investigation of the mechanisms for such significant enhancement, $g(0)/g_{\rm SC}(0)$, to derive effective potential $w(r)$ experienced by the tunneling pair at $r_{12} = r$ and to compare it with the corresponding potential $w_{\rm SC}(r)$ in the SC approximation. We first calculate the different $\Delta w(r)$ of the potentials between the tunneling pairs at $r_{12} = r$ and $r_{12} = 0$:

$$\Delta w(r) \equiv \left\langle \frac{\overline{[U(s) - U(0)]\delta(\mathbf{r} - \mathbf{r}_{12}(s))}}{\overline{\delta(\mathbf{r} - \mathbf{r}_{12}(s))}} \right\rangle_0 . \quad (9)$$

Then $w(r) \equiv w(0) + \Delta w(r)$ is obtained by determining $w(0)$ to satisfy $g(0) = g_w(0)$ where $g_w(0)$ is defined by the right hand side of Eq. (3) but with $U(s) = w(r_{12}(s))$ in $\mathcal{H}(s)$. The potential $w_{\rm SC}(r)$ is obtained in the PIMC runs for the SC approximation through a similar procedure.

Figure 1 (bottom) depicts the ζ dependence of $\beta w_{\rm SC}(r) - \beta(Ze)^2/r$ calculated in the PIMC runs with $(N, \nu) = (100, 200)$ at $\Gamma = 170$. We find in Fig. 1 (bottom) that the screening action of the surrounding particles

TABLE I. Values of $g(0)/g_{\rm SC}(0)$ [Eq. (5)] calculated in the PIMC runs with $\nu = 20$. c denotes the sequential number of configurations used to calculate each average in Eq. (5).

Γ	ζ	N	c	$g(0)/g_{\rm SC}(0)$
170	2	100	3.2×10^9	7.4 ± 1.4
170	2	50	2.0×10^8	7.7 ± 2.8
90	2	100	3.2×10^9	3.0 ± 0.5
30	2	100	3.2×10^9	1.3 ± 0.3
170	1	100	3.2×10^9	1.3 ± 0.3
90	1	100	3.2×10^9	1.1 ± 0.2
30	1	100	3.2×10^9	1.0 ± 0.2

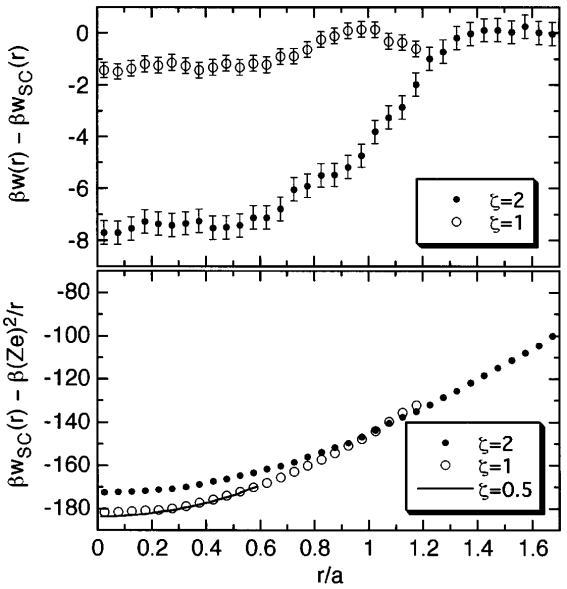

FIG. 1. Values of the effective potentials $w(r)$ and $w_{\rm SC}(r)$ calculated in the PIMC runs with $(N, \nu) = (100, 20)$ at $\Gamma = 170$: (top) $\beta w(r) - \beta w_{\rm SC}(r)$ at $\zeta = \{1, 2\}$; (bottom) $\beta w_{\rm SC}(r) - \beta(Ze)^2/r$ at $\zeta = \{0.5, 1, 2\}$.

becomes weaker as ζ increases in the SC approximation. At the tunneling process in the SC approximation, the surrounding particles located at $\mathbf{x}_i (i \in \{3, 4, \ldots, N\})$ arrange themselves to lower $\beta w_{\rm SC}(r)$ as a result of their interactions with the tunneling pair. The increase in $\beta w_{\rm SC}(r)$ at larger ζ may be attributed to the magnified fluctuations of $r_{12}(s)$ in the interval of time $s = [0, \beta\hbar]$. The differentials $\beta w(r) - \beta w_{\rm SC}(r)$ at $\Gamma = 170$ and $\zeta = \{1, 2\}$ are shown in Fig. 1 (top). Here we observe substantial lowering of the effective potential at $\zeta = 2$, which is in accordance with the significant enhancement of $g(0)/g_{\rm SC}(0)$ at $\zeta = 2$ [cf., Table I].

We investigate mechanisms for such lowering of $w(r)$ as compared to $w_{\rm SC}(r)$, by considering interparticle correlations of the quantum fluctuations $\delta\mathbf{r}_i(s) \equiv \mathbf{r}_i(s) - \overline{\mathbf{r}_i(s)}$ ($i \in \{1, 2, \ldots, N\}$). We introduce correlation functions defined as

$$D(z) \equiv \langle \overline{|\delta\mathbf{r}_i(s)|^2}\delta(z - z_{ij})\rangle_0 , \quad (10a)$$

$$F(z) \equiv \left\langle \frac{\overline{|\delta\mathbf{r}_i(s) \cdot \delta\mathbf{r}_j(s)|^2}\delta(z - z_{ij})}{\overline{|\delta\mathbf{r}_i(s)|^2}\,\overline{|\delta\mathbf{r}_j(s)|^2}} \right\rangle_0 - \frac{1}{3} , \quad (10b)$$

with $z_{ij} \equiv |\overline{\mathbf{r}_i(s)} - \overline{\mathbf{r}_j(s)}|$ for any pair of $i \in \{3, 4, \ldots, N\}$ and $j \in \{1, 2\}$. Function $D(z)$ measures magnitude of the fluctuations at distance z from the averaged position of a tunneling particle; $F(z)$, their interparticle coherence. As references for $D(z)$ and $F(z)$, corresponding functions $D_h(z)$ and $F_h(z)$ for the homogeneous OCP in which no tunneling processes are assumed, are defined by Eqs. (10) but with the average $\langle\cdots\rangle_0$ replaced by $\langle\cdots\rangle$ for any pair of $i, j \in \{1, 2, \ldots, N\}$. Values of $D(z)$ and $D_h(z)$ calculated in the PIMC runs

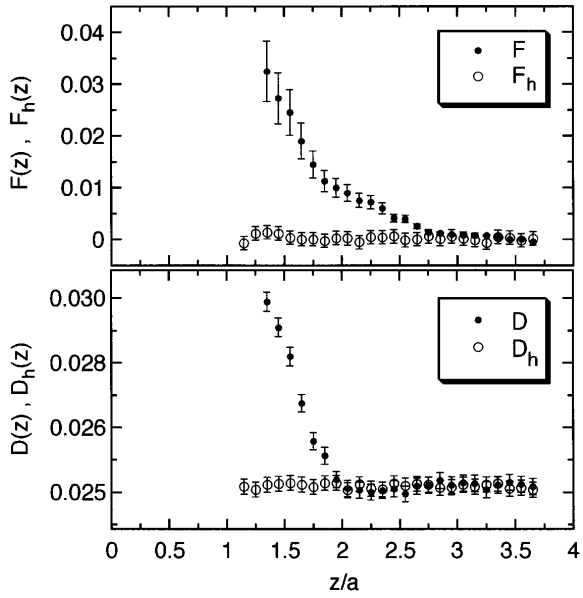

FIG. 2. Values of the correlation functions $F(z)$, $F_h(z)$, $D(z)$, and $D_h(z)$ [Eqs. (10)] calculated in the PIMC runs with $(N, \nu) = (100, 20)$ at $(\Gamma, \zeta) = (170, 2)$: (top) $F(z)$ at the tunneling, $F_h(z)$ for the homogeneous OCP; (bottom) $D(z)$ at the tunneling, $D_h(z)$ for the homogeneous OCP.

with $(N, \nu) = (100, 20)$ at $(\Gamma, \zeta) = (170, 2)$ are displayed in Fig. 2 (bottom); $F(z)$ and $F_h(z)$ at the same (Γ, ζ), In Fig. 2 (top). We observe in Fig. 2 (bottom) that $D(z) \sim D_h(z) \approx 0.025$ for $z > 1.8a$ and that the value of $D(z)$ increases linearly as z decreases for $z \leq 1.8a$. Through comparison between $F(z)$ and $F_h(z)$ in Fig. 2 (top), we find coherent quantum fluctuations of the surrounding particles for $z \leq 2.7a$ in the tunneling process, while no quantum coherence is observed for the homogeneous OCP.

Such magnified and coherent quantum fluctuations of the surrounding particles may act to compress the tunneling pair. Figure 3 depicts the normalized radial-

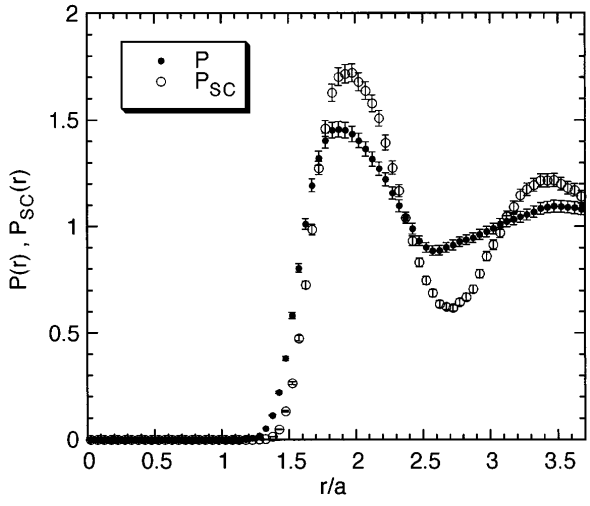

FIG. 3. Values of $P(r)$ [Eq. (11)] and $P_{\rm SC}(r)$ calculated in the PIMC runs with $(N, \nu) = (100, 20)$ at $(\Gamma, \zeta) = (170, 2)$.

distribution function for the surrounding particles at $s = 0$ defined as

$$P(r) \equiv \frac{V}{N} \sum_{i=3}^{N} \langle \delta(\mathbf{r}_1(0) - \mathbf{r}_i(0) - \mathbf{r}) \rangle_0 \qquad (11)$$

and the corresponding function $P_{\rm SC}(r)$ in the SC approximation, both of which are calculated in the PIMC runs with $(N, \nu) = (100, 20)$ at $(\Gamma, \zeta) = (170, 2)$. We find in Fig. 3 that the surrounding particles in $P(r)$, in fact, approach closer on the average to the tunneling pair at $r \leq 1.6a$ than in $P_{\rm SC}(r)$. Hence the repulsive forces of the surrounding particles toward the tunneling pair are stronger in $P(r)$ as compared to in $P_{\rm SC}(r)$, resulting in enhancement of the contact probability.

In summary, we have performed PIMC calculations for the contact probability of a tunneling pair in dense OCP's. We have found that the enhancement factor due to wave-mechanical nature of the surrounding particles takes on significant values at $\Gamma \geq 90$ and $\zeta = 2$. We have demonstrated that the enhancement is associated with magnified and coherent quantum fluctuations of the surrounding particles near the tunneling pair.

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