First-principles quantum simulation study of the enhancement factors of the thermonuclear reaction rates in dense stellar matter

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Abstract. The rate of nuclear fusion reaction, which is proportional to the tunnel-contact probability of a reacting pair of nuclei, is enhanced significantly in dense stellar matter by the many-body correlations of the surrounding nuclei. Path-integral Monte Carlo calculations for the contact probabilities of a tunnelling pair in a dense Coulomb liquid of nuclei, an accurate model for the matter in the interiors and on the surfaces of white dwarfs and neutron stars, are performed to investigate quantum effects of the surrounding nuclei. We show that the probabilities are enhanced significantly by the wave-mechanical spreading of the surrounding nuclei. Exchange of the Bose nuclei alters the probability by negligible amounts for conditions of astrophysical interest.

1. Introduction

Rates of nuclear fusion reactions are key quantities as regards determining the internal structures and time evolution of dense stars such as white dwarfs and neutron stars [1]. Theoretical predictions for the abundances of nuclear elements synthesized in the supernova process of a white dwarf may also depend sensitively on the rates of nuclear reactions adopted for the stellar interior [2]. The nuclear reaction rate [3] is, 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 [3–5]. First-principles calculations for the contact probability of a tunnelling pair in such liquids offer invaluable information for accurate evaluations of the reaction rates.

Much effort has been devoted to evaluation of the contact probability of two particles in the Coulomb liquid [3–5], i.e., an assembly of charged particles with same sign. In the existing theories relating to that problem, quantum fluctuations of the surrounding particles in the liquid were ignored, and the contact probability was calculated by exploiting the effective pair potential derived from the radial-distribution function for corresponding *classical* systems [3–8]. However, for the Coulomb liquid at low temperatures, where the thermal de Broglie wavelength of a particle is comparable to the tunnel distance, the effective pair potential and hence the contact probability of the tunnelling pair are expected to be affected substantially by the quantum fluctuations of the particles.

We report on path-integral Monte Carlo (PIMC) calculations for a tunnelling pair in a dense Coulomb liquid under various conditions, to show that the contact probabilities of

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the tunnelling pair are enhanced significantly by inclusion of the quantum fluctuations of the surrounding particles.

2. Formulation

We consider a one-component plasma (OCP) [3, 9] consisting of N point particles (charge Ze and mass $M = Am_u$ with $m_u \approx 1.66 \times 10^{-27}$ kg) in volume V, whose positions are denoted as 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 [3, 9] is

$$\Gamma \equiv \frac{\beta(Ze)^2}{a} \approx 35.8 \left(\frac{Z}{6}\right)^2 \left(\frac{12}{A}\right)^{1/3} \left(\frac{\rho_m}{10^9 \text{ g cm}^{-3}}\right)^{1/3} \left(\frac{10^8 \text{ K}}{T}\right) \tag{1}$$

with the ion-sphere (or Wigner–Seitz) radius $a \equiv (4\pi N/3V)^{-1/3}$ and the inverse temperature given in energy units, $\beta \equiv 1/k_B T$. The classical OCP solidifies at $\Gamma = \Gamma_s \sim 178$–$180$ [3, 9, 10]. The extent of the wave-mechanical nature of a particle may be measured using [11, 12]

$$\zeta^{3/2} \equiv \Lambda \frac{\sqrt{\Gamma}}{a} \approx 0.592 \left(\frac{Z}{6}\right)^{2/3} \left(\frac{12}{A}\right)^{2/3} \left(\frac{\rho_m}{10^9 \text{ g cm}^{-3}}\right)^{1/3} \left(\frac{10^8 \text{ K}}{T}\right)^{2/3} \tag{2}$$

with the thermal de Broglie wavelength $\Lambda \equiv (2\hbar/\pi)\sqrt{\beta/M}$. The characteristic width for short-time thermal vibration of a particle is $a/\sqrt{\Gamma}$ for a strongly coupled OCP (i.e., $\Gamma \gg 1$) as exemplified in the ion-sphere model [9]. We may regard strongly coupled OCPs with $\zeta > 1$ as quantum liquids.

The normalized radial-distribution function at zero separation, i.e., the contact probability, is defined in terms of the Feynman path integrals as [5, 13]

$$g(0) = V \left[\prod_{i=1}^{N} \int_{r_i(0)=r_i(\beta\hbar)} \mathcal{D}r_i(s) \exp\left[-\frac{1}{\hbar} \int_0^{\beta\hbar} ds \ \mathcal{H}(s)\right] \right]_{r_{12}(0)=0}$$

$$\times \left(\prod_{i=1}^{N} \int_{r_i(0)=r_i(\beta\hbar)} \mathcal{D}r_i(s) \exp\left[-\frac{1}{\hbar} \int_0^{\beta\hbar} ds \ \mathcal{H}(s)\right] \right)^{-1}. \tag{3}$$

Here

$$\mathcal{H}(s) = \sum_{i=1}^{N} (M/2)[\dot{r}_i(s)]^2 + U(s)$$

and $r_{ij}(s) \equiv |r_i(s) - r_j(s)|$; $U(s) = u(r_1(s), r_2(s), \ldots, r_N(s))$ where $u(y_1, y_2, \ldots, y_N)$ denotes the total Coulomb energy for the OCP with the particles located at y_i ($i \in \{1, 2, \ldots, N\}$). The effects of particle exchange are ignored in equation (3), which will be considered in section 3. A periodic boundary condition is assumed for the system. In equation (3), each particle is represented as a loop in the interval of imaginary time $s \in [0, \beta\hbar]$. The characteristic width of a loop corresponds to the quantum spread of the particle. In the present formulation (equation (3)), the values of $g(0)$ are related to the contact probabilities of two loops ($i = \{1, 2\}$) at $s = 0$.

In the semi-classical (SC) approximation to $g(0)$, we regard the surrounding particles ($i \in \{3, 4, \ldots, N\}$) as classical particles. The corresponding quantity $g_{SC}(0)$ in the SC approximation is defined by the right-hand side of equation (3), but assuming that

$U(s) = U_{SC}(s) \equiv u(\boldsymbol{r}_1(s), \boldsymbol{r}_2(s), \boldsymbol{x}_3, \ldots, \boldsymbol{x}_N)$ where $\boldsymbol{x}_i \equiv \overline{\boldsymbol{r}_i(s)}$ is the time-averaged position with

$$\overline{A(s)} \equiv (1/\beta\hbar) \int_0^{\beta\hbar} \mathrm{d}s \; A(s)$$

for any function A. The ratio $g(0)/g_{SC}(0)$ 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 $g_{SC}(0)$ reduce to $g_{Coul}(0)$ which is defined by the right-hand side of equation (3) with $N = 2$; a semi-analytical formula for $g_{Coul}(0)$ is known [14].

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

$$\frac{g(0)}{g_{SC}(0)} = \frac{\langle \exp[\beta\overline{U(s)} - \beta\overline{U_{SC}(s)}] \rangle}{\langle \exp[\beta\overline{U(s)} - \beta\overline{U_{SC}(s)}] \rangle_0} \tag{4}$$

where $\langle \cdots \rangle_0$ and $\langle \cdots \rangle$ denote PIMC averages using the Hamiltonian $\mathcal{H}(s)$ with and without the constraint $r_{12}(0) = 0$, respectively. The values of $g_{SC}(0)$ are likewise obtained as

$$g_{SC}(0) = \frac{\langle \exp[\beta\overline{U_{SC}(s)} - \beta\overline{U_{12}(s)}] \rangle^{SC}}{\langle \exp[\beta\overline{U_{SC}(s)} - \beta\overline{U_{12}(s)}] \rangle_0^{SC}} g_{Coul}(0). \tag{5}$$

Here the PIMC averages $\langle \cdots \rangle_{(0)}^{SC}$ are defined similarly to $\langle \cdots \rangle_{(0)}$, but by using $U(s) = U_{SC}(s)$ in $\mathcal{H}(s)$; also, $U_{12}(s) \equiv (Ze)^2/r_{12}(s)$.

3. PIMC results

We perform PIMC calculations for the liquid OCPs to obtain values of $g(0)/g_{SC}(0)$ and $g_{SC}(0)/g_{Coul}(0)$ following the Metropolis algorithm. The imaginary-time interval $[0, \beta\hbar]$ is divided into ν slices [15] with equal spacings: $s_\alpha = \beta\hbar\alpha/\nu$ with $\alpha = \{0, 1, \ldots, \nu\}$. We adopt the primitive approximation [15] to calculate the action for each $[s_\alpha, s_{\alpha+1}]$; its formula for $r_{12}(s) \approx 0$ is modified to satisfy the cusp condition [9, 14] with finite values of ν.

Values of $g_{SC}(0)/g_{Coul}(0)$ are calculated for $N = 100$ and $\nu = \{20, 50\}$ at $\Gamma = \{10, 30, 50, 90, 170\}$ and $\zeta = \{0.5, 1, 2\}$. They are fitted to within errors of ± 0.3 by the formula

$$\ln[g_{SC}(0)/g_{Coul}(0)]_{fit} = 1.132\,\Gamma - 0.0094\,\Gamma\ln\Gamma - \frac{5}{32}\,\Gamma\zeta^2(1 + a_1\zeta + a_2\zeta^2 + a_3\zeta^3)$$

with $(a_1, a_2, a_3) = (-0.0348, -0.1388, 0.0222)$. Here the ζ^0-term is taken from reference [16], while the ζ^2-term is taken from reference [5].

Table 1 lists values of the enhancement factor, $g(0)/g_{SC}(0)$, in equation (4) calculated for $N = \{50, 100\}$ and $\nu = 20$ at $\Gamma = \{30, 90, 170\}$ and $\zeta = \{1, 2\}$. The averages in the numerator and denominator of equation (4) are both obtained by using 3.2×10^9 ($N = 100$) and 2.0×10^8 ($N = 50$) configurations. Since both $U(s)$ and $U_{SC}(s)$ in equation (4) are macroscopic quantities proportional to N, fluctuations of $U_{(SC)}(s)$ lead to relatively large error bars for $g(0)/g_{SC}(0)$ in spite of such long runs. We find in table 1 that (i) the enhancement is significant at $\Gamma \geqslant 90$ and $\zeta = 2$ and (ii) the value of $\ln[g(0)/g^{SC}(0)]$ increases in proportion to ζ^3 while it is linear in Γ.

We have investigated in references [11, 12] mechanisms of such enhancement in $g(0)/g_{SC}(0)$ at $\Gamma \geqslant 90$ and $\zeta = 2$. The surrounding particles quantum fluctuate *coherently* near the tunnelling pair at larger values of Γ. As we increase ζ, such coherent fluctuations

Table 1. Values of $g(0)/g_{SC}(0)$ (equation (4)) calculated in the PIMC runs. c denotes the number of sequential configurations used to calculate each average in equation (4).

Γ	ζ	N	c	$g(0)/g_{SC}(0)$
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

increase in magnitude and act to enhance the fluctuations of the distances, $r_{12}(s)$, between the tunnelling pair. Correspondingly, the probabilities of finding the pair at $r_{12} \ll a$ increase; in other words, the effective pair potential for the tunnelling pair is reduced for $r_{12} \ll a$. The contact probabilities for the tunnelling pair increase as a result of such reduction of the potential.

Nuclei are Bose particles in many astrophysical applications [1, 2, 12], including that of $C^{6+} + C^{6+}$ reactions in carbon matter in a white dwarf. By performing separate PIMC runs in which the exchange of Bose nuclei is taken into account explicitly, we have found in reference [12] that the exchange processes alter the probabilities by negligible amounts for conditions of astrophysical interest.

Acknowledgments

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