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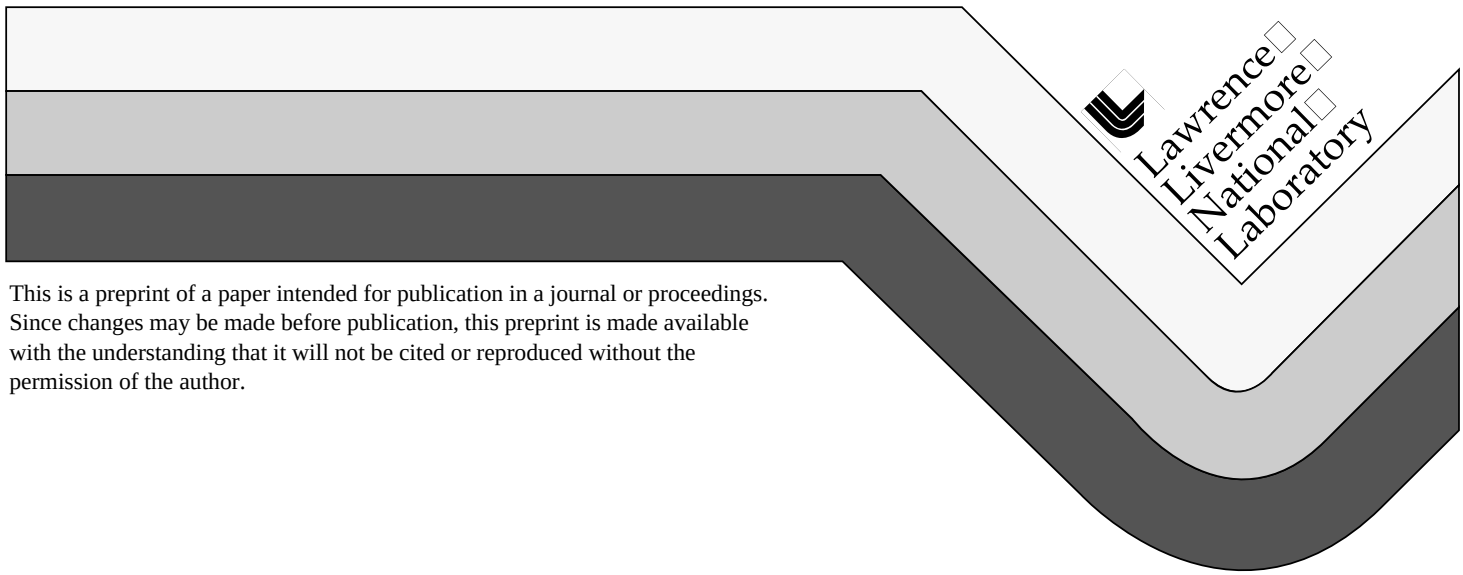

Screening Enhancement of Thermonuclear Reactions in High Density Stars

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ABSTRACT

The screening function for zero separation for two is reacting nuclei in a strongly coupled OCP plasma is obtained using new very accurate Monte Carlo OCP fluid simulation data by two methods. The first method obtains, H(0), the screening function at x =0, from the difference of free energies before and after the reaction. The second method is a direct fitting of the Widom expansion in powers of x^2 to the MC data for the pair distribution function, g(x). The two methods agree to .2%.

INTRODUCTION

Thermonuclear reaction rates in high density stars, such as the onset of C - C reactions in white dwarf stars, are governed by the probability that the two reacting nuclei get sufficiently close that they can tunnel through the Coulomb barrier. Screening by neighboring ions significantly reduces this barrier. The dominant effect in the fluid portion of the white dwarfs is governed by the screening function defined by the ion-ion pair distribution function:

$$g(x) = \exp\{-\Gamma/x + H(x)\} \qquad (1)$$

where $\Gamma = Z^2/akT$ is the usual OCP coupling parameter and distance is measured in units of the ion sphere radius, $a = \{(4\pi/3)N/V\}^{-1/3}$. The screening enhancement factor[1] is exp(H(0)). A complete calculation of H(0) requires inclusion of small electron polarization effects[2] and ion quantum effects[3,4]. The purpose of this report is to give up to date results for the classical calculation of H(0) from recent very long and accurate Monte Carlo simulations of the OCP internal energy, U/NkT, and the pair distribution function, g(x).

There are two general approaches to the problem of extracting an accurate value the screening function at r = 0:

i) H(0) is given by a thermodynamic relation, the difference of Helmholtz free energies before and after the reaction[5].

ii) Fitting the available MC data points to the Widom expansion which gives H(x) in powers[6] of x^2.

Both approaches were used by Rosenfeld[7] and found to give comparable accuracy using the data given by Ogata et al[8]. Recently Ogata[9] has presented a direct Monte Carlo sampling method to obtain H(0). Although his results partially bridge the gap between Refs. 7 and 8, we believe that some of his results are still inaccurate because of an inaccurate fitting function for the OCP energy equation of state. In this report we give results from more accurate very long MC OCP simulations with the two approaches. We find that the two approaches agree to about .2 %.

HELMHOLTZ FREE ENERGY

Our OCP fluid simulations use N = 1000 point ions in a uniform neutralizing background. We start from random positions, equilibrate over a few million configurations, and then average over approximately 500 million configurations to obtain u = U/NkT for each value of Γ; Helmholtz free energy, f = F/NkT, is obtained by integration from 0 to Γ. Our simulations are 10 to 20 times longer than those given by Ogata et al[8], and consequently our MC error, i.e. noise, is roughly ± 0.0001 to ±0.0007. Table 1 gives our current best data for the OCP internal energy:

Table 1
OCP Monte Carlo internal energy results

Γ	U/NkT	
1.	-0.57205 ±	0.00005
3.174802	-2.25491 ±	0.00010
5.	-3.75696 ±	0.00010
10.	-7.99837 ±	0.00014
15.	-12.31729 ±	0.00013
20.	-16.67327 ±	0.00016
31.74802	-26.98179 ±	0.00022
40.	-34.25940 ±	0.00026

62.40251	-54.09648 ±	0.00034
80.	-69.72742 ±	0.00041
100.	-87.52500 ±	0.00040
120.	-105.34679 ±	0.00050
140.	-123.18569 ±	0.00054
160.	-141.03963 ±	0.00069
180.	-158.90257 ±	0.00059
200.	-176.77350 ±	0.00071

Table 1 includes the data points previously published by DeWitt, Slattery, and Chabrier[10] and five additional values at Γ = 100, 120,140, and 180. The 16 data points in Table 1 are believed to be the current most accurate available values for the OCP U/NkT. As in Ref. 10 we have fitted these points to simple fitting function:

$$u = a\Gamma + b\Gamma^s + c \qquad (2)$$

with four fitting parameters, a, b, s, and c. Temperature integration from $\Gamma = 0$ to Γ gives the Helmholtz free energy as:

$$f = a\Gamma + (1/s)b\Gamma^s + c\ln\Gamma + d \qquad (3)$$

and the integraton constant d requires $F(\Gamma = 1)/NkT = -0.4368$. The fitting coefficients for the data in Table 1 are a = -0.899172, b = 0.602249, s = 0.323064, c = - 0.274823, d = -1.4018 with a standard deviation for the fit as $\sigma = \pm$ 0.00056. The five new data points in Table 1 result in only a small change from the fit given in Ref. 10. The value of σ is comparable to the Monte Carlo noise.

The value of H(0) is obtained from the difference of Helmholtz free energies before and after the reaction, and requires use of the linear mixing approximation[10] and a small correction to linear mixing the form of which was first derived by Ogata, et al[11]. Using the fit to the OCP data for f given above we obtain:

$$H(0) = \{1.056299\Gamma + 1.039957\Gamma^{.323064} - .274823\ln\Gamma - 1.084319\} - (.027\ln\Gamma + .048) \qquad (4)$$

Eq. 4 is a small improvement over Eq. 17 in Rosenfeld[7] because of the more accurate fit to the OCP data and the inclusion of the second term which gives the numerical value of the deviation from linear

mixing[10]. Note that this correction has the opposite sign from the Ogata et al[11] result, and is so small in magnitude that it can affect only the low Γ values of H(0).

WIDOM EXPANSION

An alternative method of obtaining H(0) is possible if the MC data for g(r) is sufficiently accurate. The Widom expansion in powers of x^2 around x = 0 may be written as:

$$h(x) = H(x)/\Gamma = h_o - (1/4)x^2 + h_2x^4 - h_3x^6 + ... \quad (5)$$

where all coefficients are slowly varying functions of Γ except for h_1 which is exactly 1/4 for the OCP[1]. An appropriate region for fitting h(x) numerical data from g(x) is the first peak region of g(x), namely $x_o < x < 2$ with x_o the smallest value of x for which g(x) can be obtained with desired accuracy. For Γ = 160 there are 21 MC values of g(x) in the range 1.1 to 2. The fit of these data points to Eq. 5 gives: h_o = 1.075108, h_1 =.248325, h_2 = .033637 and h_3 = .001851. Note how closely the fitted value of h_1 comes to the known exact value of .25. In Table 2 we give representative results for the two methods of obtaining h_o , Eqs. 4 and 5, the earlier work of Ogata et al[8], and the recent direct MC sampling of Ogata[9].

Table 2, Screening Function at x = 0

Γ	h_o (Eq. 4)	h_o (Eq. 5)	h_o (Ogata, et al[8])	h_o (Ogata[9])
160	1.0737	1.0751	1.096	1.083
80	1.0803	1.0824	1.104	1.090
40	1.0879	1.0898	1.110	1.098
20	1.0953	1.0980	1.116	
10	1.0994	1.0976	1.125	1.118
1	.9450	.9418		

CONCLUSION

It is clear from Table 2 that the two methods of obtaining H(0) discussed in the text are remarkably consistent, and agree to about .2%. The original Ogata et al[9] results are larger by about 2% than our

results. The direct Monte Carlo sampling method of Ogata[10] agrees with our results to within about 1%. From our results we think that the classical portion of the screening function is now known to a fraction of 1%. The next challenge will be to obtain the quantum corrections to similar accuracy.

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