

N dependence in the classical one-component plasma Monte Carlo calculations

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We calculate the internal energy of the classical one-component plasma using a Monte Carlo technique for 128, 250, 432, 686, and 1024 particles for $1 < \Gamma < 300$ in order to determine the effect of a differing number of particles on the thermodynamics. By fitting the internal energy to a function of Γ and N (the particle number), we find the free energy for both the liquid and solid for an infinite number of particles.

Earlier we reported¹ some accurate thermodynamic results for Monte Carlo calculations on the classical one-component plasma (OCP) for 128 ions (particles). The purpose of this report is to show the change in the thermodynamics when a larger number of particles are used in the Monte Carlo simulation.

The results of calculations on systems with 250, 432, 686, and 1024 particles are given along with some old and new results for 128 particles. We also discuss the N dependence of these results; we will derive a free energy for both the liquid and the solid phases.

The calculational procedure used here is the same as that used in Ref. 1. As before, the OCP system is characterized by the Coulomb coupling parameter Γ where $\Gamma = (Ze)^2/\bar{r}kT$, with the ion sphere radius

$\bar{r} = (4\pi N/3V)^{-1/3}$, N is the number of ions, and V is the volume of the system.

Table I gives the internal energies (U/NkT) corrected for center-of-mass motion for our calculation on the one-component plasma. Table I also gives Γ , the error, the number of ions, whether it was a liquid or a lattice start, and the number of Monte Carlo configurations beyond the relaxation run in units of 10^6 . To determine the error and at what point the system was relaxed, we fitted sequential 10^5 averages of U/NkT versus the number of such averages for each Γ (and number of particles) to a straight line in the least-squares sense. When the line had zero or nearly zero slope after a certain number of 10^5 averages at the beginning of the run had been discarded, we considered the system to be

TABLE I. Internal energies. U/NkT is the excess internal energy per ion divided by kT . The configurations are the number of configurations after a relaxation run.

Γ	U/NkT	Error $\pm\sigma$	Number of ions N	Type of start	Configuration (millions)
1.0	-0.574	0.000	128	liquid	1.4
1.0	-0.572	0.000	686	liquid	4.0
2.0	-1.321	0.000	128	liquid	1.0
2.0	-1.320	0.000	686	liquid	3.1
3.0	-2.113	0.001	128	liquid	2.2
3.0	-2.113	0.000	686	liquid	8.0
4.0	-2.928	0.001	128	liquid	2.3
4.0	-2.928	0.000	686	liquid	7.3
5.0	-3.754	0.001	128	liquid	1.5
5.0	-3.757	0.000	686	liquid	5.2
6.0	-4.593	0.001	128	liquid	1.0
6.0	-4.594	0.001	686	liquid	9.5
10.0	-7.993	0.001	128	liquid	1.6
10.0	-7.998	0.001	686	liquid	7.7
15.0	-12.309	0.003	128	liquid	1.0
15.0	-12.318	0.001	686	liquid	5.5
20.0	-16.670	0.003	128	liquid	1.0

TABLE I (Continued).

Γ	U/NkT	Error $\pm\sigma$	Number of ions N	Type of start	Configuration (millions)
20.0	-16.673	0.001	686	liquid	19.9
30.0	-25.437	0.001	128	liquid	12.8
30.0	-25.439	0.001	250	liquid	15.8
30.0	-25.441	0.001	686	liquid	13.9
40.0	-34.251	0.002	128	liquid	16.0
40.0	-34.255	0.001	250	liquid	18.0
40.0	-34.255	0.001	686	liquid	16.0
50.0	-43.102	0.001	686	liquid	19.7
60.0	-51.956	0.002	128	liquid	15.8
60.0	-51.956	0.002	250	liquid	12.0
60.0	-51.961	0.001	686	liquid	15.9
80.0	-69.715	0.002	128	liquid	9.0
80.0	-69.721	0.002	250	liquid	9.0
80.0	-69.725	0.001	686	liquid	30.8
100.0	-87.501	0.004	128	liquid	4.5
100.0	-87.498	0.005	250	liquid	2.0
100.0	-87.524	0.002	686	liquid	23.8
100.0	-87.522	0.001	1024	liquid	21.3
105.0	-91.963	0.005	128	liquid	4.4
110.0	-96.411	0.005	128	liquid	2.8
115.0	-100.860	0.005	128	liquid	3.9
115.0	-100.877	0.004	250	liquid	6.4
120.0	-105.323	0.005	128	liquid	5.8
120.0	-105.343	0.002	686	liquid	31.8
120.0	-105.345	0.002	1024	liquid	23.0
125.0	-109.780	0.004	128	liquid	5.1
125.0	-109.799	0.005	250	liquid	3.0
125.0	-109.796	0.004	432	liquid	3.8
130.0	-114.239	0.006	128	liquid	3.1
130.0	-114.264	0.002	1024	liquid	23.9
135.0	-118.693	0.005	128	liquid	4.8
135.0	-118.712	0.004	250	liquid	7.8
140.0	-123.148	0.003	128	liquid	15.8
140.0	-123.177	0.003	250	liquid	10.5
140.0	-123.181	0.005	432	liquid	3.0
140.0	-123.179	0.002	686	liquid	23.7
140.0	-123.188	0.002	1024	liquid	18.5
145.0	-127.609	0.003	128	liquid	24.8
145.0	-127.634	0.003	250	liquid	15.8
150.0	-132.061	0.003	128	liquid	15.3
150.0	-132.093	0.003	250	liquid	15.3
150.0	-132.115	0.002	432	liquid	26.4
150.0	-132.110	0.002	1024	liquid	23.6
155.0	-136.536	0.004	128	liquid	12.6
155.0	-136.571	0.003	250	liquid	23.3
160.0	-141.000	0.006	128	liquid	8.6
160.0	-141.031	0.007	250	liquid	4.6
160.0	-141.039	0.004	432	liquid	6.6
160.0	-141.036	0.002	686	liquid	38.6
160.0	-141.036	0.002	1024	liquid	27.2
160.0	-141.729	0.006	128	lattice	4.2
160.0	-141.716	0.009	250	lattice	2.0
165.0	-145.461	0.005	128	liquid	7.0
165.0	-145.505	0.004	432	liquid	7.4
170.0	-149.915	0.006	128	liquid	7.6
170.0	-149.958	0.005	250	liquid	6.8
170.0	-149.966	0.004	432	liquid	6.2

TABLE I (Continued).

Γ	U/NkT	Error $\pm\sigma$	Number of ions N	Type of start	Configuration (millions)
170.0	-149.967	0.003	686	liquid	10.1
170.0	-149.970	0.001	1024	liquid	35.0
170.0	-150.703	0.005	128	lattice	6.8
170.0	-150.699	0.002	250	lattice	23.0
170.0	-150.696	0.002	432	lattice	28.0
170.0	-150.697	0.002	686	lattice	25.0
180.0	-159.672	0.002	128	lattice	18.0
180.0	-159.674	0.002	250	lattice	19.4
180.0	-159.667	0.002	432	lattice	28.8
200.0	-176.765	0.002	686	liquid	28.8
200.0	-177.605	0.003	128	lattice	9.9
200.0	-177.603	0.002	250	lattice	22.0
200.0	-177.605	0.002	432	lattice	26.0
200.0	-177.603	0.001	686	lattice	23.0
220.0	-195.539	0.003	128	lattice	6.0
220.0	-195.533	0.002	250	lattice	18.0
220.0	-195.536	0.002	432	lattice	16.8
240.0	-213.469	0.003	128	lattice	9.9
240.0	-213.460	0.002	250	lattice	18.9
240.0	-213.459	0.001	432	lattice	30.0
240.0	-213.463	0.001	686	lattice	31.9
300.0	-267.239	0.002	128	lattice	17.8
300.0	-267.233	0.001	432	lattice	25.0
300.0	-267.233	0.001	686	lattice	31.9

relaxed. The average and the standard deviation of the means (the error) were then computed in this zero-slope region.

In Fig. 1 we have plotted the thermal fraction of the internal energy for all of the data. The thermal fraction is defined as $(U - U_0)/NkT$ where U_0 is the energy of a bcc lattice ($U_0 = -0.895929\Gamma$). On this scale the error bars are hardly visible.

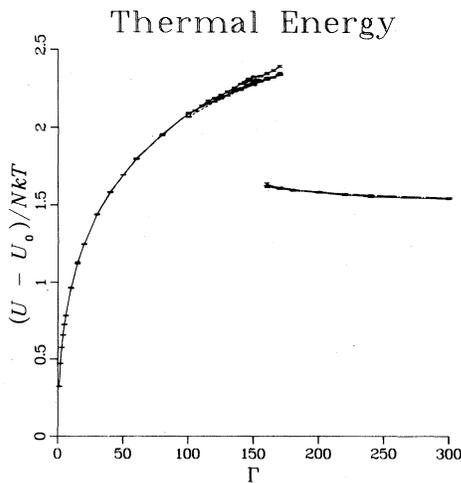


FIG. 1. Thermal energy for both the liquid and solid OCP phases. The error bars are hardly visible at this scale.

Figure 2 shows the thermal energy for 100 $\leq \Gamma \leq 170$. The N dependence is apparent and is systematic. The "humps" in the region $140 < \Gamma < 155$ appear to be a boundary effect since the size of the hump decreases substantially when the

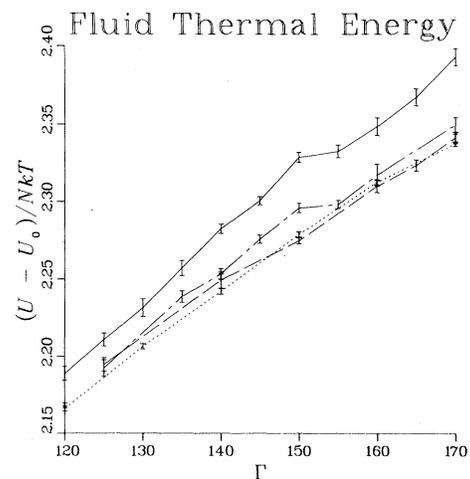


FIG. 2. Thermal energy for the fluid OCP phase. Error bars are $\pm\sigma$ (σ is the standard deviations of the means of 100 000 configuration averages). Solid curve, 128 particles; chain-dashed curve, 250 particles; chain-dotted curve, 432 particles; dotted curve, 686 particles; dashed curve, 1024 particles.

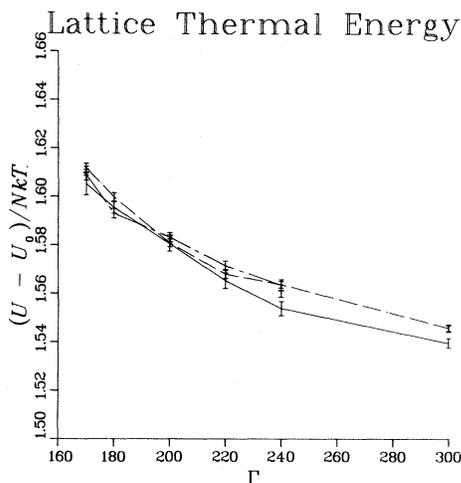


FIG. 3. Thermal energy for the solid OCP phase. Error bars are $\pm\sigma$ (σ is the standard deviations of the means of 100 000 configuration averages). Solid curve, 128 particles; chain-dashed curve, 250 particles; chain-dotted curve, 432 particles; dotted curve, 686 particles.

number of particles increases. The calculations in this region for $N = 128$ and 250 also seemed to depend upon the initial random positions. This anomaly did not appear at lower or higher Γ . The humps also appeared when we ran Hansen's² lower-precision OCP code although they were shifted in Γ .

Figure 3 shows the thermal fraction of the energy for the lattice runs ($170 < \Gamma < 300$). The N dependence is smaller than the liquid case. It also is not as systematic since some of the curves cross.

We fitted the liquid-phase data with the form³

$$U/NkT = a\Gamma + b\Gamma^{1/4} + c/\Gamma^{1/4} + d + e\Gamma/N,$$

where

$$\begin{aligned} a &= -0.897744, & b &= 0.95043, & c &= 0.18956, \\ d &= -0.81487, & e &= 0.009656. \end{aligned} \quad (1)$$

Obvious humps were excluded for the fit. The solid data were likewise fitted to the form

$$U/NkT = \frac{3}{2} + U_0 + h/\Gamma^2 + m\Gamma/N, \quad (2)$$

where $h = 3225$ and $m = -0.0006587$. We tried a

variety of expressions for the N -dependence terms, e.g., $(\ln N)/N$ and $\Gamma(\ln N)/N$. The term shown seemed to fit the best.

Letting N go to infinity we recover the expressions given in Ref. 1 for the Helmholtz free energy of a liquid and a solid, viz.,

$$\begin{aligned} F(\Gamma)/NkT &= a\Gamma + 4(b\Gamma^{1/4} - c/\Gamma^{1/4}) + (d+3)\ln\Gamma \\ &\quad - [a + 4(b-c) + 1.1516] \end{aligned} \quad (3)$$

for the liquid, and

$$F(\Gamma)/NkT = -0.895929\Gamma + 9\ln\Gamma/2 - 1.8856 - h/2\Gamma^2 \quad (4)$$

for the solid [our earlier paper¹ was in error for the number 1.1516 in Eq. (3) due to incorrect integration].

The intersection of Eqs. (3) and (4) gives the Γ at the fluid-solid transition. We find that $\Gamma_m = 178 \pm 1$. The error ± 1 corresponds to the maximum and minimum intersection points of the three liquid free-energy curves (obtained by fitting $U/NkT - \sigma$, U/NkT , and $U/NkT + \sigma$) with the corresponding three solid free-energy curves. (σ is the standard deviation of the relaxed means.) In Ref. 1 we derived the result that $\Gamma_m = 168 \pm 4$. This was based on data from 128-particle runs. Consequently, we see that Γ_m is very sensitive to the number of particles and that some attempt must be made (as we have done here) to remove the N dependence from Monte Carlo data.

We conclude by stating two questions that have arisen as a result of this work for which we do not have answers. The first is, "What causes the humps in the data for $140 < \Gamma < 155$?" Since the size of the hump decreases as the number of particles increases, we expect this phenomenon to be a boundary effect. The second question is, "What is the exact form of the N -dependence?" The term given earlier ($\text{const} \times \Gamma/N$) gives the best fit to our data, but there is no rigorous theory to guide us.

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²J. P. Hansen, Phys. Rev. A **8**, 3096 (1973).

³H. E. DeWitt and Y. Rosenfield, Phys. Lett. **75A**, 79 (1979).