Lattice plasma in infinitely many dimensions

Michael Schulz and Harry L. Frisch
Department of Chemistry, University at Albany, State University of New York, Albany, New York 12222
(Received 31 May 1994; revised manuscript received 14 February 1995)

The equation of state of a neutral plasma in infinitely many dimensions has been obtained exactly. Only the second-order virial coefficient is nonvanishing. The present method can also be used as an approximation for lower dimensions.

PACS number(s): 05.20.−y, 64.30.+t, 64.70.−p

I. INTRODUCTION

Recently, it has pointed out that considerable simplifications arise in many-body problems in the limit of infinite space dimensions, both for equilibrium properties [1–3] and for dynamical problems (thermodynamic kinetic theory) [4]. The effects of high spatial dimensionality on the qualitative properties lead to dramatic structural simplifications of a hard core continuum fluid in infinite dimensions [5–8] and also for lattice gases [9]. Therefore, we expect such simplifications also for the high-dimensionality limit of a neutral plasma. The Coulomb interaction between two charged particles at a distance r is determined by the characteristic long range potential

$$\phi(\mathbf{r}) = \frac{1}{\varepsilon_0} \frac{1}{K_d d(d-2)} \frac{e_1 e_2}{r^{d-2}}, \tag{1}$$

where K_d is the volume of the unit shell

$$K_d = \frac{\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d+2}{2}\right)}. \tag{2}$$

This potential guarantees the validity of the Maxwell law $\int \mathbf{E} d\mathbf{A} = e\varepsilon_0^{-1}$. The Fourier representation of this potential has the well known structure

$$\phi(\mathbf{q}) = \frac{1}{\varepsilon_0} \frac{e_1 e_2}{q^2}, \tag{3}$$

which is independent of dimension. In finite dimensions, this potential leads to a complicated diagrammatic representations, which allows only a perturbation theory-like approximation (ring graph summation [10], mean field approximation [11]). The consideration of the short range hard core interaction leads to additional complications. Therefore, we introduce a simple cubic lattice in which each lattice site can be occupied by only one particle. This lattice model, called a lattice plasma, realizes therefore the short range excluded volume effect and we must determine only the contribution of the long range interaction. However, as we will show in this paper, considerable simplifications occur for a plasma on a regular lattice in the limit of infinitely many space dimensions and we are able to give an equation of state for the thermodynamic properties of such a plasma.

II. LATTICE PLASMA IN HIGH DIMENSION

We introduce a d-dimensional cubic lattice of the unit length a with $G = N_0^d$ lattice sites, i.e., a volume $V = Ga^d$. The plasma can be described by three states e_i for each lattice site i, given by

$$e_i = \begin{cases} +e_0 & \text{with probability} \quad \frac{\rho}{2} \\ 0 & \text{with probability} \quad 1-\rho \\ -e_0 & \text{with probability} \quad \frac{\rho}{2}. \end{cases}$$

In addition, we can define an important thermodynamic energy scale as the energy of two neighboring particles

$$\phi_0 = \frac{1}{\varepsilon_0} \frac{\Gamma\left(\frac{d+2}{2}\right)}{d(d-2)\pi^{\frac{d}{2}}} \frac{e_0^2}{a^{d-2}} \tag{4}$$

and the ratio

$$\zeta = \frac{\phi_0}{k_B T}. \tag{5}$$

At this point we can start the important discussion about the thermodynamic existence of a plasma. An essential question is the energy that is necessary to separate a larger neutral particle into two separated charged particles. Without all quantum mechanics effects and internal energy barriers, we need at least an energy of the order ϕ_0 for the separation of two neighboring particles. This energy can be obtained only from the kinetic energy of the particles. The average kinetic energy of a particle is given by the equal distribution theorem $\bar{E} = \frac{d}{2} k_B T$. Therefore, we can expect that a plasma occurs if the ratio between ϕ_0 and $\bar{E}$ becomes of order 1, i.e., we have the plasma criterion $1 > \phi_0/\bar{E} \sim \zeta d^{-1}$ and therefore for large dimensions the condition $\zeta \leq d$ for the existence of a plasma.

Very important is the connection between the real space lattice (given by the lattice sites i with position $\mathbf{r}_i$) and the lattice in q space (Fourier space) with sites at the position $\mathbf{q}$. Note that the number of q vectors is equal to the number G of lattice sites in real space and that each q vector occupies a volume $(2\pi)^d/V$ in q space. Thus we get the lattice representation of the long range Coulomb potential

$$\phi(\mathbf{r}) = \frac{1}{\varepsilon_0 V} \sum_q \frac{e_1 e_2}{q^2}. \tag{6}$$

1063-651X/95/52(1)/442(4)/$06.00

Note that the sum runs over all q vectors of q space without $q = 0$. This vector corresponds to a total integral (or sum) over the full real space and can separated by a constant energy.

Using the conservation conditions

$$\sum_{i=1}^{G} e_i^2 = \rho G e_0^2, \tag{7}$$

$$\sum_{i=1}^{G} e_i = 0, \tag{8}$$

we get the canonical partition function

$$Z = \sum_{\{\mathbf{e}\}} \exp\left\{-\frac{\beta}{2}\sum_{i,j}{}' \frac{e_i e_j}{e^2}\phi_0\left(\frac{a}{\mid \mathbf{r}_i - \mathbf{r}_j \mid}\right)^{d-2}\right\}. \tag{9}$$

(The sum $\sum'$ mean the summation over all pairs of different sites.) The partition function is realized as a sum over all configurations $\{\mathbf{e}\}$ of charge distributions on the lattice. Using $s_i = e_i e^{-1}$ with the states $0,\pm1$ we get

$$\begin{aligned} Z &= \sum_{\{\mathbf{s}\}} \exp\left\{-\frac{\beta e^2}{2\varepsilon_0 V}\sum_{i,j} s_i s_j (1-\delta_{ij}) \sum_q e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}\frac{1}{q^2}\right\} \\ &= \sum_{\{s\}} \exp\left\{-\frac{\beta e^2}{2\varepsilon_0 V}\left[\sum_{i,j} s_i s_j \sum_q e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}\frac{1}{q^2} - G\rho\sum_q \frac{1}{q^2}\right]\right\} \\ &= \left(\prod_q e^{\frac{\beta G \rho e^2}{2\varepsilon_0 V q^2}}\right)\sum_{\{s\}} \exp\left\{-\frac{\beta e^2}{2\varepsilon_0 V}\sum_q q^{-2}\left|\sum_j s_j e^{i\mathbf{q}\cdot\mathbf{r}_j}\right|^2\right\}. \end{aligned} \tag{10}$$

The quadratic term is now transformed into a linear term by introducing a functional integration over an additional complex field ψ_q. Hence we get, with $\tilde{\beta} = \beta e_0^2/(2\varepsilon_0 V)$,

$$\begin{aligned} Z = &\left(\prod_q e^{\frac{\beta G \rho e_0^2}{2\varepsilon_0 V q^2}}\right)\sum_{\{s\}}\int D\psi \prod_q\left(\frac{q^2}{\tilde{\beta}\pi}\right) \\ &\times \exp\left\{\sum_q\left(-\frac{q^2}{\tilde{\beta}}\psi_q\psi_q^* - i\left[\psi_q^*\sum_j s_j e^{i\mathbf{q}\cdot\mathbf{r}_j}\right.\right.\right. \\ &\left.\left.\left. + \psi_q \sum_j s_j e^{-i\mathbf{q}\cdot\mathbf{r}_j}\right]\right)\right\}, \end{aligned} \tag{11}$$

or by defining

$$Z_0 = \prod_q \exp\left\{\frac{\beta G \rho e_0^2}{2\varepsilon_0 V q^2}\right\} \tag{12}$$

and using the Fourier representation of the field ψ

$$\psi_j = \psi(\mathbf{r}_j) = \sum_q \psi_q e^{-i\mathbf{q}\cdot\mathbf{r}_j}, \tag{13}$$

we obtain

$$\begin{aligned} Z = Z_0 &\int D\psi \prod_q\left(\frac{q^2}{\tilde{\beta}\pi}\right)\exp\left\{-\sum_q \frac{q^2\psi_q\psi_q^*}{\tilde{\beta}}\right\} \\ &\times \prod_j\left[1-\rho+\frac{\rho}{2}\left(e^{-i(\psi_j^*+\psi_j)} + e^{i(\psi_j^*+\psi_j)}\right)\right]. \end{aligned} \tag{14}$$

The potential part of this partition function is determined by the real part of ψ. Therefore, we can separate

$$\psi_j = \phi_j + i\chi_j \tag{15}$$

and realize the integration over χ. Hence

$$\begin{aligned} Z = Z_0 &\int D\psi \prod_q\left(\frac{q^2}{\tilde{\beta}\pi}\right)^{\frac{1}{2}}\exp\left\{-\sum_j \frac{1}{\tilde{\beta}G}(\nabla\phi_j)^2\right\} \\ &\times \exp\left\{\sum_j \ln[1-\rho+\rho\cos(2\phi_j)]\right\}, \end{aligned} \tag{16}$$

where $\nabla\phi_j$ is the discrete representation of the gradient. The prefactor of $(\nabla\phi)^2$ is given by

$$\tilde{\beta}G = \frac{\beta e^2 G}{2\varepsilon_0 V} = \frac{1}{2}\left(\frac{\phi_0}{k_B T}\right)\frac{d(d-2)K_d}{a^2} = \frac{1}{2}\zeta\sigma_d a^{-2} \tag{17}$$

with $\sigma_d = d(d-2)K_d$. Therefore, with decreasing ζ or increasing dimension d, the value $\tilde{\beta}G$ increases rapidly of order $\sim d^{d/2}$. On the other hand, a reasonable ζ is at least of order d, i.e., the prefactor of $(\nabla\phi)^2$ becomes very large in the case of a high-dimensional lattice plasma. This means that the thermodynamic fluctuations are of order $\overline{\mid \nabla\phi \mid} \sim \sigma_d^{1/2}\zeta^{1/2}$; we found no essential change of the field ϕ (given by $\Delta\phi \sim 1$), at least over a large distance $L_\phi \sim \sigma_d^{-1/2}\zeta^{-1/2}$. Consequently, for sufficiently large d we have always the case that a finite volume $V = L_0^d$ is small in comparison to the volume $V_\phi = L_\phi^d$ of a relative constant field ϕ. Therefore, we expect in the volume V only small fluctuations around the average value of ϕ. As a result of this discussion, we can use the saddle point method for the determination of the partition function Z and because the fluctuations are sufficiently small, this methods becomes an exact solution for high dimensions. The saddle point is given by $\phi_0 = 0$ and all other multiples of 2π. Because of the above discussion we can neglect all field configurations, which changes their value by as much as 2π. Thus each relevant field configuration shows fluctuations only around one multiple of 2π. Therefore, we can restrict ourself to the case

$\phi_0 = 0$ and expand the potential in powers of the fluctuations ξ ($\phi = \phi_0 + \xi$) to second (harmonic) order. We get, up to an irrelevant (but infinite) multiplicable constant (which follows from the consideration off all other multiples of 2π)

$$Z = Z_0 \int D\psi \prod_q \left(\frac{q^2}{\tilde{\beta}\pi}\right)^{\frac{1}{2}} \times \exp\left\{-\int \frac{d^d r}{a^d}\left[\frac{2a^2}{\zeta\sigma_d}(\nabla\xi)^2 + 2\rho\xi^2\right]\right\}. \quad (18)$$

On integration

$$Z = Z_0 \prod_q \left(\frac{q^2}{\tilde{\beta}}\frac{1}{G\left[\frac{2a^2q^2}{\zeta\sigma_d} + 2\rho\right]}\right)^{\frac{1}{2}} = Z_0 \prod_q \left(\frac{q^2}{q^2 + \frac{\zeta\sigma_d\rho}{2a^2}}\right)^{\frac{1}{2}}. \quad (19)$$

Subject to (12) it follows that

$$F = \frac{k_B T}{2}\sum_q \left[\ln\left(1 + \frac{\zeta\sigma_d\rho}{2a^2q^2}\right) - \frac{\zeta\sigma_d\rho}{2a^2q^2}\right]. \quad (20)$$

Note that the integration over q is restricted by the finite number of q vectors. The usual method is to define the cutoff by the Debye radius Λ, which is given by the relation

$$G = \sum_q 1 = \frac{V}{2\pi^d}\int d^d q = \frac{V}{2\pi^d}K_d\Lambda^d, \quad (21)$$

i.e., we get for the UV cutoff

$$\Lambda = \frac{2\pi}{K_d^{\frac{1}{d}} a} \rightarrow \sqrt{\frac{2\pi}{e}}\frac{\sqrt{d}}{a}. \quad (22)$$

The high-dimensionally limit follows by using Stirgling's representation of the Γ function ($e = 2.73\ldots$ is the Euler number). From (20) we can define a screening length $l_d = \kappa_d^{-1}$

$$\kappa_d^2 = \frac{\sigma_d\zeta\rho}{a^2}. \quad (23)$$

This κ_d can interpreted as an upper cutoff (IR cutoff). Note that κ_d becomes very small in the high-dimension limit, i.e., the screening effect remains relevant for such a length that is as large as the volume length L_0 (see also the discussion above). However, we get for the free energy of the lattice plasma

$$\begin{aligned} F &= \frac{k_B T V}{2(2\pi)^d}\int d^d q\left[\ln\left(1 + \frac{\kappa_d^2}{q^2}\right) - \frac{\kappa_d^2}{q^2}\right] \\ &= \frac{k_B T V}{2(2\pi)^d} d K_d \kappa_d^d \int_0^{\frac{\Lambda}{\kappa}} x^{d-1}dx\left[\ln(1 + x^{-2}) - x^{-2}\right] \\ &= -N k_B T\frac{dK_d}{2(2\pi)^d n}\kappa_d^d I_d\left(\frac{\Lambda}{\kappa}\right) \end{aligned} \quad (24)$$

with $n = \rho a^{-d}$ the particle density. The integral I_d has the structure

$$I_d(z) = -\int_0^z x^{d-1}dx\left[\ln(1 + x^{-2}) - x^{-2}\right] \quad (25)$$

and can be solved exactly. For small dimensions d, particular for $d < 4$, $I(z)$ converges for $z \rightarrow \infty$. Therefore, we can approximate $I(\Lambda/\kappa_d) \approx I_d(\infty)$. [For $d = 3$, $I_3(\infty) = 1/3$.] Therefore, we can give an interpretation of the saddle point approximation in the low-dimensional case: The transformation in the representation of the field ϕ is closed to a resummation of the original ring graphs of the plasma [10]. Moreover, we can say that this approximation becomes exactly in the high-dimensional limit $d \rightarrow \infty$.

It is very important for the interpretation of the effects of a long range Coulomb potential ($d < 4$) on the free energy

$$\frac{F}{Nk_BT} = -\frac{dK_d}{2(2\pi)^d}\left(\frac{e_0^2}{k_BT\varepsilon_0}\right)^{\frac{d}{2}} n^{\frac{d}{2}-1} I_d(\infty) \quad (26)$$

that F does not depend on the length scale of the lattice units a. For large d and large ratios Λ/κ_d it is sufficient to replace the integral (25) by $\int x^{d-1}dx[x^{-4}/2 - x^{-6}/3 + \cdots]$ (first two nonvanishing terms of the Taylor expansion) and we get

$$I(z) = \frac{z^{d-4}}{2(d-4)} - \frac{z^{d-6}}{3(d-6)} + \cdots \quad (27)$$

and therefore

$$\begin{aligned} \frac{F}{Nk_BT} &= -\frac{dK_d}{4(d-4)(2\pi)^d n}\Lambda^d\left(\frac{\kappa_d}{\Lambda}\right)^4 \times\left[1 - \frac{4(d-4)}{6(d-6)}\left(\frac{\kappa_d}{\Lambda}\right)^2 + \cdots\right] \\ &= -\frac{d}{4(d-4)a^d n}\left(\frac{\kappa_d}{\Lambda}\right)^4 \times\left[1 - \frac{4(d-4)}{6(d-6)}\left(\frac{\kappa_d}{\Lambda}\right)^2 + \cdots\right], \end{aligned} \quad (28)$$

or by using (4), (5), and

$$\left(\frac{\kappa}{\Lambda}\right)^2 = \left(\frac{e_0^2}{\varepsilon_0 k_B T}\right)\left(\frac{e}{2\pi d}\right) n a^2 \quad (29)$$

we get

$$\frac{F}{Nk_BT} = -\frac{d}{4(d-4)}\left(\frac{e_0^2}{\varepsilon_0 k_B T}\right)^2\left(\frac{e}{2\pi d}\right)^2 \times n a^{4-d}[1 - o(d^{-1})]. \quad (30)$$

This free energy depends now on the length scale of a unit lattice site, i.e., the volume of the lattice particle $v_0 = a^d$ controls, for dimensions $d > 4$, the free energy. This is a very important effect. Whereas for low dimensions $d < 4$ the infrared (long range) divergences $\sim r^{2-d}$ are dominant, we have the inverse situation for high dimensions $d > 4$, i.e., the (ultraviolet) short range divergences of the same power low $\sim r^{2-d}$ remain relevant. Because of the finite distance between neighboring lattice sites, the diameter a and therefore the volume v_0 of the lattice particles control the free energy

$$\frac{F}{Nk_BT} = -\frac{d}{4(d-4)}\left(\frac{e_0^2}{\varepsilon_0 k_B T}\right)^2\left(\frac{e}{2\pi d}\right)^2 n v_0^{\frac{4-d}{d}}. \quad (31)$$

Finally, we get from (31) the pressure

$$\frac{p}{nk_BT} = 1-\frac{d}{4(d-4)}\left(\frac{e_0^2}{\varepsilon_0 k_B T}\right)^2\left(\frac{e}{2\pi d}\right)^2 n v_0^{\frac{4-d}{d}}. \quad (32)$$

The lattice spacing dependence raises the question of which scaling should be used in the continuum case. In general, the lattice unit corresponds to the minimal distance of two particles. Therefore, the lattice plasma should have the same properties as a hard core system with Coulomb interaction with a hard core diameter of the length a; only the prefactors should be changed because the lattice plasma has cubiclike particles, whereas in the continuous case usually hard spheres are used. Therefore, an exact prediction for the continuum hard sphere case is very difficult by using only the present results, but the general scaling $F \sim a^{4-d}$ can also be predicted for the continuous case. Therefore, we get an extremely strong divergence for $d \to \infty$ and simultaneously $a \to 0$. A detailed analysis for the plasma in continuous space is in preparation.

ACKNOWLEDGMENTS

This work has been supported by the National Science Foundation, Grant No. DMR9023541, the Deutsche Forschungsgemeinschaft, Grant No. schu 934/1-2, and the Alexander von Humboldt Foundation (Germany).

[1] H.O. Carmesin, H.L. Frisch, and J.K. Percus, Phys. Rev. B **40**, 9416 (1989).
[2] H.L. Frisch, N. Rivier, and D. Wyler, Phys. Rev. Lett. **54**, 2061 (1985).
[3] T.R. Kirkpatrick, J. Chem. Phys. **85**, 3515 (1986).
[4] Y. Elskens and H.L. Frisch, Phys. Rev. A **37**, 4351 (1988).
[5] H.L. Frisch and J.K. Percus, Phys. Rev. A **35**, 4696 (1987).
[6] D. Wyler, N. Rivier, and H.L. Frisch, Phys. Rev. A **36**, 2422 (1987).
[7] J.K. Percus, in *Studies in Statistical Mechanics*, edited by J.L. Lebowitz (North-Holland, Amsterdam, 1987).
[8] J.L. Lebowitz and J.K Percus, Phys. Rev. **144**, 251 (1966).
[9] H.E. Stanley, Phys. Rev. **176**, 718 (1968).
[10] J. Mayer, J. Chem. Phys. **18**, 1426 (1950).
[11] P. Debye and E. Hückel, Phys. Z. **24**, 185 (1923).