Condensation of hard rods under gravity: Exact results in one dimension

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We present exact results for the density profile of a one dimensional array of N hard rods of diameter D and mass m under gravity g. For a strictly one dimensional system, the liquid-solid transition occurs at zero temperature, because the close-packed density ϕ_c is 1. However, if we relax this condition slightly such that $\phi_c=1-\delta$, we find a series of critical temperatures $T_c^{(i)}=mgD(N+1-i)/\mu_0$ with $\mu_0=1/\delta-1$, at which the ith particle undergoes the liquid-solid transition. The functional form of the onset temperature, $T_c^{(1)}=mgDN/\mu_0$, is consistent with the previous result [Physica A **271**, 192 (1999)] obtained by the Enskog equation. We also show that the increase in the center of mass is linear in T before the transition, but it becomes quadratic in T after the transition because of the formation of solid near the bottom.

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I. INTRODUCTION

In a previous paper [1], the author proposed that a hard sphere gas undergoes a condensation transition under gravity g, and identified the transition temperature T_c as the point at which the Enskog equation [2] fails to conserve the total number of particles. Based on the fact that hard spheres cannot be compressed beyond the close-packed density, it was suggested [1] and confirmed [3] that the missing particles should condense from the bottom and form a solid below T_c, and the fraction in the solid regime at a temperature $T<T_c$ was predicted to be $1-T/T_c$. The transition temperature T_c was determined as

$$T_c=mgD\mu/\mu_0, \tag{1}$$

where m and D are the mass and diameter of the hard sphere, μ is the layer number of the system, and μ_0 is a constant that depends on the level of approximation in truncating the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy [4], or perhaps in employing the density functional theory [5]. Hence, the value obtained by the Enskog theory [1], or more precisely by the Enskog pressure, may be close to the real value, but not precise. For example, if one uses the pressure form suggested by Percus and Yevick [6], this constant will be slightly different. For a one dimensional lattice gas [7,8], it can be shown that $\mu_0=-\ln[\alpha/(1-\alpha)]$ with $\alpha=\exp(-14)$. The crucial point, however, is that the scaling form of the transition temperature [Eq. (1)] should survive in all approximations. The purpose of this paper is to demonstrate this point by exactly solving the one dimensional hard sphere problem under gravity. For a strictly one dimensional (1D) system, the condensation transition occurs at zero temperature, because the close-packed density ϕ_c is 1. However, some useful information may be extracted from 1D results if we relax this condition slightly such that $\phi_c=1-\delta$. This may represent the case where the rods are compressible, or, as we discuss later, if we may model the weakly interacting high dimensional system by the coarse grained one dimensional system. Then the transition occurs at a finite temperature. Even though the fluctuations in three dimensions (3D) are very different from those in the 1D system, we will show in this paper that results obtained in this way appear to be relevant to real physical systems. Perhaps one may view such a 1D system as a coarse grained mean field approximation of the real three dimensional hard sphere system. We will obtain the exact transition temperature T_c and check its functional form against Eq. (1). We also determine the series of transition temperatures $T_c^{(i)}$ at which the ith layer undergoes the condensation transition. We further show how a sharp change in the center of mass statistics shows up before and after the transition. Before the transition, the increase in the center of mass is *linear* in T, while after the transtion it is *quadratic* in T, because of the formation of solid near the bottom, which is a characteristic of Fermi systems [9,10].

II. CONDENSATION OF ONE DIMENSIONAL HARD SPHERE GAS UNDER GRAVITY

Consider a collection of hard spheres of finite radius R (or diameter $D=2R$) in a one dimensional tube with the top open. Let the mass of the ith particle be m_i. We assume that each hard sphere is in thermal equilibrium with a heat reservoir at a temperature T. The system we have in mind is the one used in the usual molecular dynamics simulations, where each particle is kicked periodically by Gaussian noise so that the average kinetic energy of each particle $m\langle v^2\rangle/2=T$. We ignore the pressure due to the reservoir. In such a case, since the kinetics is separated out, we consider only the configurational integral in computing the partition function Z_N of the N particle assembly:

$$Z_N=\int_R^\infty dz_1\int_{z_1+2R}^\infty\cdots\int_{z_{N-1}+2R}^\infty dz_N \times\exp[-\beta' g(m_1z_1+\cdots+m_Nz_N)] \tag{2}$$

with $\beta'=1/T$. The hard sphere gas without gravity has been studied and is known as the Tonk gas [11]. The integral in Eq. (2) involves exponential functions and thus can be carried out exactly to yield

$$Z_N = \frac{1}{(\beta' g)^N} \frac{e^{-2\beta' g m_N R}}{m_N} \frac{e^{-2\beta' g(m_N+m_{N-1})R}}{(m_N+m_{N-1})} \times \cdots \times \frac{e^{-\beta' g(m_1+m_2+\cdots+m_N)R}}{(m_1+m_2+\cdots+m_N)}. \tag{3}$$

We now compute average quantities. First, the average position of the ith particle $\langle z_i(T)\rangle$ is given by

$$\langle z_i(T)\rangle = -\frac{1}{\beta' g}\frac{\partial \ln Z_N}{\partial m_i} = (2i-1)R + \frac{T}{g}\overline{z}_i, \tag{4}$$

where

$$\overline{z}_i = \sum_{j=1}^{i}\left(\frac{1}{\sum_{k=j}^{N} m_k}\right). \tag{5}$$

If all the masses are the same, i.e., $m_i = m$, then this reduces to

$$\langle z_i(T)\rangle/D = (i-1/2) + \frac{T}{mgD}\sum_{j=1}^{i}\frac{1}{N+1-j}. \tag{6}$$

Note that the first term, $\langle z_i(0)\rangle/D = i-1/2$, results from the close packing in the ground state $T=0$ and the second term represents the thermal expansion. Note also that $\Sigma_i^N\langle z_i(T)\rangle/D = N^2/2 + TN/mgD$. The dimensionless thermal expansion defined as $\overline{z}_i = (\langle\Delta z_i\rangle/D)(mgD/T)$ with $\langle\Delta z_i(T)\rangle = \langle z_i(T)\rangle - z_i(0)$ is independent of the temperature. For example,

$$\overline{z}_1 = 1/N, \quad \overline{z}_2 = 1/N + 1/(N-1),$$

$$\overline{z}_N = 1/N + 1/(N-1) + \cdots + 1/2 + 1.$$

The dimensionless mean expansion per particle is precisely given by the thermal energy injected into the system:

$$\langle\overline{z(T)}\rangle = \frac{1}{N}\left[\sum_i^N \langle\Delta z_i\rangle\right]\frac{mg}{T} = \frac{1}{N}\sum_i^N \langle z_i(t) - z_i(0)\rangle\frac{mg}{T} = \sum_{i=1}^{N}\overline{z}_i(T) = 1. \tag{7a}$$

The change in the center of mass due to the thermal expansion is *linear* in T:

$$\langle z(T)\rangle = \frac{1}{N}\sum_{j=1}^{N}[\langle z_i(T)\rangle - z_i(0)] = T/mg. \tag{7b}$$

We now compute the density profile $\rho(z_i)$ as a function of position z_i. Define the dimensionless density $\phi(z_i) = \rho(z_i)/\rho_c$ with $\rho_c = 1/D$. Then, since $\rho(z_i)\Delta z_i = \Delta i$, we find $\phi(z_i) = (\Delta i/\Delta z_i)/\rho_c$ and its discrete version becomes

$$\phi(z_i) = 1\Bigg/\left[1 + \frac{1}{\beta}\frac{1}{N+1-i}\right], \tag{8}$$

where we have used the relation

$$1/N + 1/(N-1) + \cdots + 1/(N-i+1) \approx -\int_{x=N}^{x=N-i+1} dx/x = -\ln[1-(i-1)/N] \tag{9}$$

and we have redefined the dimensionless temperature $\beta = mgD/T$ and the dimensionless coordinate $y_i = \langle z_i\rangle/D$:

$$y_i = (i-1/2) + \frac{1}{\beta}\sum_{j=1}^{i}\frac{1}{N-j+1}. \tag{10}$$

Note that $\int\rho(z_i)dz_i = \int\phi(y_i)dy_i = N\,\phi_c$ with ϕ_c the close-packed density. The density at the bottom layer, ϕ_0, is given by Eq. (8) with $i=1$, i.e., $\phi_0 = 1/[1+1/\beta N]$. For a strictly one dimensional system, the close-packed density $\phi_c = 1$, and thus by setting $\phi_0 = \phi_c = 1$ we find that the crystallization occurs at zero temperature in one dimension.

In order to extract some useful information from one dimensional results, and make them relevant to higher dimensions, we assume that the close-packed density is below 1 by a small amount, $0 < \delta \neq 0 \ll 1$, i.e., $\phi_c = 1-\delta$. What we have in mind is a coarse grained three dimensional system, or a system of spheres or rods that are slightly deformed under pressure, for which each column may interact weakly. In fact, we have found that such a system can be realized in molecular dynamics simulations if the system is initially arranged in a two dimensional square lattice with a little space between the columns. In such a case, the particles in each column do not mix, and the square structure is maintained [18]. Such a model can be understood as a coarse grained mean field model in the spirit of Ref. [7]. Certainly, the fluctuations in three dimensions (3D) are very different from those in 1D, and thus it may be objectionable to extend the results of 1D to 3D. Nevertheless, the results for 1D obtained in this way with regard to the existence of the condensation temperature, and perhaps the existence of the discrete jump in the condensation process, may survive in high dimension, as will be shown shortly.

Now, if we let $\phi_c = 1-\delta$, we can easily find the onset of the condensation temperature T_c at which the first layer becomes crystallized:

$$T_c = mgD\mu/\mu_0, \tag{11}$$

where $\mu = N$ is the initial layer number (or the Fermi energy [10]), and the constant μ_0 is given by

$$\mu_0 = \frac{1}{\delta} - 1. \tag{12}$$

Note that Eq. (11) has the same funtional form as Eq. (1). One may relate δ to the critical pressure $P_cD^2 = \mu_0 T_c/D$ at which the crystallization occurs. From the force balance equation, we find the pressure at the bottom:

$$P(0)D^2 = mg\int_0^\infty dz\,\phi(z) = mgN\phi_c. \qquad (13)$$

The factor D^2 was introduced to effectively model the three dimensional system. By equating $P(0)$ to the critical pressure P_c, we again find the transition temperature $T_c = mgD\mu/\mu_0(\phi_c)$. Reference [7] identifies the critical pressure as $P_c = 14T_c/D^3$. Hence, we find $\mu_0 = 14 = 1/\delta - 1$, and $\delta = 1/15 = 0.0667$. After the first layer becomes crystallized at T_c, the density profile above the second layer is given by Eq. (8) with N replaced by $N-1$ and $i = 1, \ldots, N-1$. This is effectively equivalent to shifting the origin from the first to the second layer. The second layer, which has now become the origin, becomes crystallized at the second critical temperature $T_c^{(2)}$: $\phi_0(T_c^{(2)}) = 1-\delta$. The process continues, and we can find a series of critical temperatures $T_c^{(i)}$ at which the ith layer in the original labeling becomes crystallized:

$$T_c^{(i)} = \frac{mgD(N+1-i)}{\mu_0}. \qquad (14)$$

So all the particles are crystallized at $T = T_c^{(N)} = mgD/\mu_0$, which is *not* the absolute zero, because $\delta \neq 0$. Note also that the crystallization of each layer proceeds with a discrete temperature jump $\Delta T = T_c^{(i+1)} - T_c^{(i)} = mgD/\mu_0$. Hence, the heat release or the latent heat Q resulting from the formation of one solid layer is $Q = \Delta T = mgD/\mu_0$. Biben *et al.* [12] investigated the density profile of a hard sphere suspension in a gravitational field using Monte Carlo simulations, and reported that for $\overline{\Delta} = mgD/T \leq 2.5$ the system is a strongly perturbed fluid, while at $\overline{\Delta} \approx 2.75$ the first two layers form a crystal, and the formation of third and fourth layer crystals occurs in a *discontinuous* manner between $\overline{\Delta} = 2.5$ and $\overline{\Delta} = 2.75$. Setting $mgD/T_c = 2.5$ and $T_c = mgDN/\mu_0$, we find $\mu_0 = 2.5N$ and $\delta \approx 1/(2.5N+1) \approx 0.038\,46$, if N is of order 10 [12]. Such findings do not seem to be inconsistent with the results presented above.

We now examine the center of mass statistics below the condensation point $T_c = T_c^{(1)}$. At a given temperature $T_c^{(i+1)} < T < T_c^{(i)}$, what is the fraction of particles in a condensed regime? At this temperature, particles up to the ith layer are condensed. Then, the fraction of particles in the condensed regime, $\zeta_F \equiv i/N$, which is termed the Fermi surface [1], is given by a simple manipulation of identities:

$$\zeta_F = i/N = 1 - \left[\frac{N-i}{N}\right] = 1 - T/T_c, \qquad (15)$$

where we used $T_c^{(i+1)}/T_c = [mgD(N-i)/\mu_0]/mgDN/\mu_0 = (N-i)/N \equiv T/T_c$.

Now, the dimensionless center of mass $\langle y(T)\rangle \equiv \langle z(T)\rangle/D$ is given by

$$\langle y(T)\rangle = \int_0^\infty dy\, y\,\phi(y) \Big/ \int_0^\infty dy\,\phi(y) \equiv I_2/I_1, \qquad (16)$$

where the integral now splits into two due to the formation of a solid below ζ_F. More precisely,

$$I_1 = \int_0^{\zeta_F} \phi_c\, dy + \int_{\zeta_F}^\infty \phi(y-\zeta_F)dy = \phi_c\zeta_F + (N-\zeta_F)\phi_c = N\phi_c. \qquad (17)$$

We need some manipulation in computing the denominator I_2. To this end, we again split I_2 into two integrals: one for the solid regime, which is essentially a rectangle, and the other for the fluid regime, where the density profile is given by Eq. (8) but with N replaced by $N' = N - \zeta_F$. Hence,

$$I_2 = \int_0^{\zeta_F} y\,\phi_c\, dy + \int_{\zeta_F}^\infty y\,\phi(y-\zeta_F)dy = \phi_c\zeta_F^2/2 + \zeta_F\phi_c(N-\zeta_F) + J, \qquad (18)$$

where

$$J \equiv \int_0^\infty dy\, y\,\phi(y) = \sum_{j=1}^{N-\zeta_F} y_j\phi_j\left(\frac{\Delta y_i}{\Delta i}\right)_{i=j} = \sum_{j=1}^{N-\zeta_F} z_j/D. \qquad (19)$$

But $\Sigma_j^{N'} z_j = D[N'^2/2 + TN'/mgD]$ [Eq. (6)]. Hence, with $N' = N - \zeta_F = NT/T_c$, we find

$$J = [N^2T^2/2T_c^2 + (N^2T^2/\mu_0T_c^2)] = N^2\Lambda(T/T_c)^2, \qquad (20)$$

where $\Lambda = [1/2 + 1/\mu_0]$. Note that the increase in the center of mass is quadratic in T, namely

$$\langle \Delta z(T)\rangle = \langle z(T)\rangle - ND/2 = \alpha ND(T/T_c)^2 \qquad (21)$$

with $\alpha = [2+\delta(1-\delta)]/[2(1-\delta)^2]$, which is a characteristic of Fermi systems [10].

In passing, we make the following remarks. In Ref. [7], an attempt was made to derive the condensation point for the lattice gas, which is again consistent with the form given by Eq. (1). While the lattice gas may capture some of the essence of hard sphere systems, it is important to recognize that the logarithmic singularity in the pressure of the lattice gas [7,13] is far different from the power law singularity of a real hard sphere gas [14]. Finally, the relevance of the present study to granular materials [15]: Granular materials are macroscopic particles, and the parameter $\overline{\Delta} = mgD/T \approx 10^{13}$ is an astronomical number, if one uses a usual temperature. Hence, the temperature T of the hard sphere gas should be interpreted differently. One way to relate this temperature to the vibrational strength of the granular bed is to compare the kinetic expansion of the granular bed to the thermal expansion of hard spheres, as was done in Ref. [10]. If we denote by $\overline{h}(\Gamma)$ the jump height of a single ball in a vibrating bed of vibrational strength $\Gamma = A\omega^2/g$ with A and ω the amplitude and frequency of the vibration, then we may set

$$\langle \Delta z(T)\rangle = \alpha ND(T/T_c)^2 = \overline{h}(\Gamma), \qquad (22)$$

from which we can find the relation between the thermal temperature T of the hard spheres and the vibrational strength Γ:

$$\frac{T}{T_c}=(1-\delta)\sqrt{\frac{\bar{h}}{D}\frac{1}{N}\frac{2}{2+\delta(1-\delta)}}, \tag{23}$$

or, equivalently,

$$\frac{T}{mg}=\delta\sqrt{\frac{2\bar{h}DN}{2+\delta(1-\delta)}}. \tag{24}$$

We point out that for granular materials excited by vibration in a two dimensional container, $\bar{\Delta}=mgD/T_c$ was determined by fitting the density profile of Ref. [9] by the Enskog profile. The estimated value was $\bar{\Delta}\approx 4.926$ [3], and the dimensioness temperature of the vibrating bed was $T/T_c=0.663$. However, we point out that we have not taken into account (a) the internal degrees of freedom [16] of the macroscopic particles, such as rotation, and (b) the inelastic collisions, which may lead to an interesting clustering instability [17]. Hence, one has to be somewhat careful in extending the results of elastic hard spheres to granular materials.

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