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A Hard Core Bose Gas

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We study a one-dimensional gas of Bosons interacting through Neumann hard cores of diameter a. Attractive boundary conditions are imposed on the system, so that when $a = 0$ the model exhibits Bose–Einstein condensation and singular thermodynamic functions. In the presence of a hard core ($a > 0$), the free energy density retains its singularity, but Bose–Einstein condensation does not persist, even in the generalized sense.

KEY WORDS: Bose–Einstein condensation; Onsager–Penrose criterion; generalized condensation; Neumann hard core; reduced density matrices.

1. INTRODUCTION

Sixty years after the discovery of Bose–Einstein condensation in the free Bose gas,[1] the following problem remains largely unsolved: Is this phenomenon stable with respect to the introduction of a two-body interaction? This is one of the basic questions of quantum statistical mechanics, and the importance of the issue for our understanding of the structure of the theory can hardly be denied, not to mention applications to superfluidity.

The following partial results have been obtained in special cases:

(i) A mean-field repulsive interaction does not destroy the condensation phenomenon.[2–4]

(ii) If the Hamiltonian of the free gas has a gap in its spectrum, then Bose–Einstein condensation is stable under perturbation by any integrable two-body potential of positive type.[5]

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On the other hand, there is a class of results which can be viewed as *stability of the absence of condensation*:

(a) Using Bogoliubov's inequality, one can show[6,7] that in a situation in which the *free* Bose gas does not show any condensation, neither does a gas with superstable interaction.

(b) Lenard,[8,9] and Schultz[10] have proved that there is no condensation (even in a generalized sense; see (1)) in a model of one-dimensional Bosons with point hard core and periodic boundary conditions.

This last group of studies were prompted by the claim by Girardeau[11] that the model described in (b) exhibited *generalized condensation* in the sense that

$$\lim_{\varepsilon \to 0} \lim_{V \to \infty} V^{-1} \sum_{j: E_j^V \leqslant \varepsilon} \langle N_j^V \rangle > 0 \tag{1}$$

instead of the usual

$$\lim_{V \to \infty} V^{-1} \langle N_0^V \rangle > 0 \tag{2}$$

where $E_0^V < E_1^V \leqslant \cdots$ denote the eigenvalues of the one-particle kinetic energy in a box of volume V and N_j^V are the occupation numbers of the corresponding eigenstates. Lenard's work disproving Girardeau's conjecture is an elegant piece of mathematical physics, but it must be said that the result itself is hardly a surprise. Indeed there is *no* generalized condensation in model (b) in the *free* case, so that if the result of Ref. 11 were true, it would mean that a *repulsive* interaction has created a (generalized) condensate, a very unlikely event indeed. Another argument against Girardeau's prediction is that the Hamiltonian of model (b) is unitarily equivalent to that of a free Fermi gas, and so the thermodynamic functions do not show any singularity.

The manner in which model (b) should be modified in order to become relevant to the problem of stability of Bose–Einstein condensation is now clear:

(α) first of all, one should start from a situation in which the *free* gas exhibits condensation.

(β) next, the interaction should be such that it does not destroy the Bose statistics.

That condition (α) can be met in one dimension through a choice of attractive boundary conditions was first demonstrated by Robinson[12]; see also Ref. 13. As for condition (β), we show in Section 2.1 that it holds for suitably defined hard cores involving Neumann conditions at the contact between the particles.

A consequence of the choice of a Neumann hard core is that the interaction Hamiltonian is now related to that of a free Bose gas [instead of a Fermi gas for model (b)]; this gives an easy access to the thermodynamics of the system, which exhibits a singularity at a critical value of the density (see Section 3). Hence our model seems to be a very strong candidate for showing Bose–Einstein condensation. Note also that our choice of boundary conditions (mixed attractive and repulsive) has the effect of creating a gap in the spectrum of the one-particle kinetic energy operator [see (55)], so that by extrapolation of (ii) one could expect that the interacting gas retains the condensation property of the free gas.

However, there is no *a priori* evidence for this, because the equivalence between our model and a free gas does not go beyond the thermodynamical level: indeed the correspondence between Hamiltonians [see (29)], does *not* extend to occupation numbers or creation operators. Hence, correlations or averages (and in particular condensation properties) of our model cannot be deduced from those of the free gas. In fact it turns out that our model does *not* show Bose–Einstein condensation, even at zero temperature, a rather unexpected result (see Theorem 3).

The next possibility is that the system could display generalized condensation [see (1)]. Indeed, for noninteracting systems, this has been shown to be equivalent to the presence of a singularity in the thermodynamic functions.[14] However this phenomenon is also absent from our model at zero temperature (see Corollary 2). Hence, the model studied in this paper illustrates how unstable the phenomenon of Bose–Einstein condensation can be: it can be destroyed even by a perturbation which is gentle enough to preserve the singularity in the thermodynamic functions. It is also worth stressing that the discovery of a singularity in the thermodynamic functions of an interacting Bose gas is no evidence for Bose–Einstein condensation, even in the generalized sense [see remark (i) in Section 4.2].

We conclude this introduction with some general remarks on Bose–Einstein condensation. It is sometimes stated that for an interacting system, the very concept of macroscopic occupation of a one-particle kinetic energy eigenstate is not appropriate, and that a new formulation of the problem is required. We wish to point out that this is not so. We work for simplicity at zero temperature, but everything can be extended to strictly positive temperatures.

Consider N interacting bosons in a rectangular box Ω of volume L^ν, and suppose that $\Phi(x_1,..., x_N) \in \mathscr{S}_N(L^2(\Omega^N))$ is the real-valued ground state wave function of the system. The one-body reduced density matrix at $T=0$ is

$$\rho_L(x, y) = N \int_\Omega d^\nu z_1 \cdots \int_\Omega d^\nu z_{N-1} \Phi(x, z_1,..., z_{N-1}) \times \Phi(y, z_1,..., z_{N-1}) \tag{3}$$

We denote by

$$R^L_\Phi : L^2(\Omega) \mapsto L^2(\Omega) \tag{4}$$

the integral operator with kernel $\rho_L(x, y)$.

Let $f \in L^2(\Omega)$ be a normalized one-particle wave function. The average number of particles in the state f is $(\Phi, N^L_f \Phi)$, where the operator N^L_f on $\mathscr{S}_N(L^2(\Omega^N))$ is

$$N^L_f = P_f \otimes I \otimes \cdots \otimes I + I \otimes P_f \otimes I \otimes \cdots \otimes I + \cdots + I \otimes \cdots \otimes I \otimes P_f \tag{5}$$

$P_f : L^2(\Omega) \mapsto L^2(\Omega)$ being the orthogonal projection onto f. Now, by virtue of the symmetry (or, for that matter, skew symmetry) of Φ, we have for arbitrary f in $L^2(\Omega)$:

$$(\Phi, N^L_f \Phi) = N \int_\Omega d^\nu x_0 \cdots \int_\Omega d^\nu x_N f(x_0) f(x_N)\, \Phi(x_0, x_1,..., x_{N-1}) \times \Phi(x_1,..., x_N) = (f, R^L_\Phi f) \tag{6}$$

The condition

$$\lim_{L \to \infty} L^{-\nu} \sup_{f \in L^2(\Omega), \|f\| = 1} (f, R^L_\Phi f) > 0 \tag{7}$$

is usually called the *Onsager–Penrose criterion* for existence of Bose–Einstein condensation.[15] In view of the identity (6), we see that this is essentially the usual criterion. The only difference is that one does not look at the occupation of a one-particle state prescribed in advance (say the ground state of the one-particle kinetic energy); instead one looks for the occupation of whatever one-particle level is most populated, and (6) shows that this must be the eigenvector of R^L_Φ with the highest eigenvalue (note that for finite L, R^L_Φ is trace-class and self-adjoint, so that the supremum in formula (7) is actually attained for some f^L_0 in $L^2(\Omega)$).

2. THE MODEL

2.1. Neumann Hard Cores

Consider N bosons in $[0, L]$ interacting through a hard core of diameter a. Formally, the Hamiltonian of this system is the operator on $\mathscr{S}_N(L^2([0, L]^N))$ given by

$$\frac{-1}{2} \sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} + \sum_{1 \leq i < j \leq N} V(x_i - x_j) \tag{8}$$

where

$$V(y)=\begin{cases}0, & \text{if } |y|>a \\ \infty, & \text{if } |y|\leqslant a\end{cases} \tag{9}$$

The best way to make sense of such an expression is to take care of the hard core condition through a restriction of the configuration space. The *accessible region* $\Omega^a_{L,N}$ is defined as

$$\Omega^a_{L,N}=\{(x_1,..., x_N)\in[0, L]^N: |x_i-x_j|>a, i\neq j=1, 2,...N\} \tag{10}$$

The suitable Hilbert space for the description of hard core systems is

$$\mathscr{H}^a_{L,N}=\mathscr{S}_N(L^2(\Omega^a_{L,N})) \tag{11}$$

and the formal expression (8), (9) is replaced by the Hamiltonian

$$H^a_{L,N}=\frac{-1}{2}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} \qquad \text{on} \quad \mathscr{H}^a_{L,N} \tag{12}$$

In order for (12) to determine unambigously a self-adjoint operator, one has to choose a set of boundary conditions. The boundary of the accessible region is made of two parts: the *outer boundary*

$$B_{\text{out}}=\{(x_1,..., x_N)\in\Omega^a_{L,N}: x_i=0 \text{ or } x_i=L \text{ for some } i\} \tag{13}$$

and the *inner boundary*

$$B_{\text{in}}=\{(x_1,..., x_N)\in\Omega^a_{L,N}: |x_i-x_j|=a \text{ for some } i\neq j\} \tag{14}$$

Obviously, the choice of the inner boundary conditions completes the specification of the interaction. Throughout this paper we work with *Neumann boundary conditions* on B_{in}:

$$\left(\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_j}\right)\Psi(x_1,..., x_N)\,|_{x_i-x_j=a}=0 \tag{15}$$

The operator (12), supplemented with (15) and a suitable boundary condition on B_{out} (see Section 2.3), defines the Hamiltonian of the Bose gas with *Neumann hard cores.*

A special feature of hard cores in one dimension is that $H^a_{L,N}$ is unitarily equivalent to a Hamiltonian with zero-radius hard core and modified L. This is a well known property,[16] but recall its derivation for the reader's convenience; first note that $\Omega^a_{L,N}$ can be decomposed as follows:

$$\Omega^a_{L,N}=\cup_{\pi\in S_N}R_\pi \tag{16}$$

where the disjoint regions R_π are defined by

$$\begin{aligned} 0 \leqslant x_{\pi(1)} &< x_{\pi(2)} - a \\ a < x_{\pi(2)} &< x_{\pi(3)} - a \\ 2a < x_{\pi(3)} &< x_{\pi(4)} - a \\ &\cdots\cdots \\ &\cdots\cdots \\ (N-1)\, a < x_{\pi(N)} &\leqslant L \end{aligned} \tag{17}$$

Define then the mapping

$$D_N : \Omega^a_{L,N} \mapsto [0, L-(N-1)\, a]^N \tag{18}$$

by means of its action on each region R_π:

$$\begin{aligned} (y_1,..., y_j,..., y_N) &\equiv D_N(x_1,..., x_j,..., x_N) \\ &= [x_1 + a - a\pi^{-1}(1),..., x_j + a - a\pi^{-1}(j),..., x_N \\ &\quad + a - a\pi^{-1}(N)] \qquad \text{in} \quad R_\pi \end{aligned} \tag{19}$$

or equivalently

$$y_{\pi(j)} = x_{\pi(j)} - a(j-1), \qquad j = 1, 2,..., N \tag{20}$$

Note that D_N maps R_π onto the region

$$0 \leqslant y_{\pi(1)} < y_{\pi(2)} < \cdots < y_{\pi(N)} \leqslant L - a(N-1) \tag{21}$$

Define finally [with the same notation as before; see (11)]

$$\mathscr{D}_N : \mathscr{H}^a_{L,N} \mapsto \mathscr{H}^0_{L-a(N-1),N} \tag{22}$$

$$\mathscr{D}_N \Psi = \Psi \circ D_N^{-1} \tag{23}$$

To any operator A on $\mathscr{H}^a_{L,N}$ we can associate a unitarily equivalent operator $\hat{A}$ on $\mathscr{H}^0_{L-a(N-1),N}$ by the formula

$$\hat{A} = \mathscr{D}_N A \mathscr{D}_N^{-1} \tag{24}$$

In particular, for the Hamiltonian (12):

$$\hat{H}^a_{L,N} = \frac{-1}{2} \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} \qquad \text{on} \quad \mathscr{H}^0_{L-a(N-1),N} \tag{25}$$

and the boundary conditions are now required to hold on $\hat{B}_{\text{out}}$ and $\hat{B}_{\text{in}}$ where

$$\hat{B}_{\text{out}} = \{(x_1, ..., x_N) \in [0, L - a(N-1)]^N : x_i = 0 \quad \text{or} \quad x_i = L - a(N-1) \text{ for some } i\} \tag{26}$$

$$\hat{B}_{\text{in}} = \{(x_1, ..., x_N) \in [0, L - a(N-1)]^N : x_i = x_j \text{ for some } i \neq j\} \tag{27}$$

The above discussion is classical (see Ref. 16)] and its validity does not depend on the nature of the boundary condition on B_{in}. But if we specialize to Neumann hard cores, we see that (15) becomes [using (23), (19), (27)]

$$\left(\frac{\partial}{\partial x_i} - \frac{\partial}{\partial x_j}\right) \Phi(x_1, ..., x_N) \,|_{x_i = x_j} = 0 \tag{28}$$

But since every Φ in $\mathscr{H}^0_{L-a(N-1),N}$ is symmetric, (28) is automatically satisfied. This means that the inner boundary $\hat{B}_{\text{in}}$ can be completely overlooked, and thus

$$\hat{H}^a_{L,N} \equiv \mathscr{D}_N H^a_{L,N} \mathscr{D}_N^{-1} = H^{\text{free}}_{L-a(N-1),N} \tag{29}$$

where $H^{\text{free}}_{L,a(N-1),N}$ is the operator on

$$\mathscr{H}^{\text{free}}_{L,a(N-1),N} = \mathscr{S}_N(L^2[0, L - a(N-1)]^N) = \mathscr{S}_N(\{L^2[0, L - a(N-1)]\}^{\otimes N}) \tag{30}$$

describing N free bosons in $[0, L - a(N-1)]$ with appropriate boundary conditions on $\hat{B}_{\text{out}}$. In other words, the transformation (24) is an exact diagonalization of our interacting Hamiltonian.

Remarks. (i) For Dirichlet hard cores, one finds that $H^a_{L,N}$ is unitarily equivalent to the Hamiltonian of a gas of free *fermions* in $[0, L - a(N-1)]$; see Refs. 7–10 and 15.

(ii) In view of the close connection of $H^a_{L,N}$ and $H^{\text{free}}_{L-a(N-1),N}$, the reader might be tempted to conclude that the Bose gas with Neumann hard cores is merely a disguised version of the free Bose gas. We emphasize that this is not so, because the unitary transformation (24) *does not preserve occupation numbers*. By this we mean that, upon applying the transformation $\mathscr{D}_N \cdot \mathscr{D}_N^{-1}$ to a number operator N_f of the original model, one does *not* obtain a number operator of the transformed system; nor is N_f easily expressible in terms of creation and annihilation operators of the new model. Hence there is no simple transformation which would allow us to predict averages occupation numbers (or more general correlation functions) of the hard core gas in terms of those of the associated free gas.

2.2. Reduced Density Matrix at Zero Temperature

In this section, we obtain the explicit form of the one-body reduced density matrix of a Bose gas with Neumann hard cores at zero temperature. From now on we work for simplicity with $N+1$ particles in $[0, L]$, and we put

$$L' = L - aN \tag{31}$$

Let $\Psi(x_1,..., x_{N+1})$ be the ground state wave function of $H^a_{L,N+1}$. Then [see (23), (24), and (29)]

$$\Psi = (\varphi^{\otimes(N+1)}) \circ D_{N+1} \tag{32}$$

where $\varphi(x)$ is the (real-valued) ground state of the one-particle operator

$$-\frac{1}{2}\frac{d^2}{dx^2} \quad \text{on} \quad L^2([0, L']) \tag{33}$$

with a boundary condition to be specified later.

Theorem 1. Let $\rho_L(x, y)$ be the one-body reduced density matrix describing $(N+1)$ bosons in $[0, L]$ with Neumann hard cores at zero temperature. Then for $x \leqslant y$

$$\rho_L(x, y) = \sum_{0 \leqslant j < k \leqslant N}{}' I_L^{(j,k)}(x, y) + \sum_{0 \leqslant j \leqslant N}{}'' I_L^{(j,j)}(x, y) \tag{34}$$

where

$$I_L^{(j,k)}(x, y) = \frac{(N+1)!\, \varphi(x-ja)\, \varphi(y-ka)}{j!(k-j)!(N-k)!} \times \left[\int_0^{x-ja} dz \varphi^2(z)\right]^j \left[\int_{x-(j-1)a}^{y-ka} dz \varphi(z-a)\, \varphi(z)\right]^{k-j} \times \left[\int_{y-ka}^{L'} dz \varphi^2(z)\right]^{N-k} \tag{35}$$

with φ as in (32). In (34), $\sum'$ denotes the sum restricted to

$$ja \leqslant x, \qquad (k-j)\, a \leqslant y-x-a, \qquad (N-k)\, a \leqslant L-y \tag{36}$$

and $\sum''$ the sum restricted to

$$ja \leqslant x, \qquad (N-j)\,a \leqslant L-y \tag{37}$$

Proof. By definition of $\rho_L(x, y)$ [see (3)]:

$$\rho_L(x, y) = (N+1) \int_0^L dz_1 \cdots \int_0^L dz_N\, \Psi(x, z_1,..., z_N)\, \Psi(y, z_1,..., z_N) \tag{38}$$

$$= (N+1)! \int_{0 \leqslant z_1 < z_2 ...} dz_1 \cdots \int_{< z_N \leqslant L} dz_N\, \Psi(x, z_1,..., z_N) \times \Psi(y, z_1,..., z_N) \tag{39}$$

Supposing that $x \leqslant y$, this can be written as

$$\begin{aligned}
&(N+1)! \sum_{0 \leqslant j < k \leqslant N}{}' \int_{0 \leqslant z_1 < \cdots < z_j < x < z_{j+1} < \cdots} dz_1 \cdots \int_{z_k < y < z_{k+1} < \cdots z_N \leqslant L} dz_N \\
&\quad \times \Psi(z_1,..., z_j, x, z_{j+1},..., z_N)\, \Psi(z_1,..., z_k, y, z_{k+1},..., z_N) \\
&\quad + (N+1)! \sum_{0 \leqslant j \leqslant N}{}'' \int_{0 \leqslant z_1 < \cdots} dz_1 \int_{< z_j < x \leqslant y < z_{j+1} < \cdots z_N \leqslant L} dz_N \\
&\quad \times \Psi(z_1,..., z_j, x, z_{j+1},..., z_N)\, \Psi(z_1,..., z_j, y, z_{j+1},..., z_N)
\end{aligned} \tag{40}$$

where $\sum'$ and $\sum''$ are as in (36), (37), and we have put $z_0 \equiv 0$, $z_{N+1} \equiv L$. Using (32) and (19), the integrand of the first and second terms read, respectively,

$$\begin{aligned}
&\varphi(x-aj)\, \varphi(y-ak) \prod_{m=1}^{j} \varphi^2(z_m - a(m-1)) \\
&\qquad \times \prod_{p=j+1}^{k} \varphi(z_p - ap)\, \varphi(z_p - a(p-1)) \prod_{q=k+1}^{N} \varphi^2(z_q - aq)
\end{aligned} \tag{41}$$

and

$$\varphi(x-aj)\, \varphi(y-aj) \prod_{m=1}^{j} \varphi^2(z_m - a(m-1)) \prod_{p=j+1}^{N} \varphi^2(z_p - ap) \tag{42}$$

so that the result (34) follows by changing the variables of integration. ∎

Note in particular the form of the local density [when $x = y$, the sum $\sum'$ does not contribute; see (36)]:

$$\rho_L(x) \equiv \rho_L(x, x) = (N+1) \sum_{j=0}^{N}{}^{*} \binom{N}{j} \varphi^2(x - ja) \times \left[\int_0^{x-ja} dz\varphi^2(z)\right]^j \left[\int_{x-ja}^{L'} dz\varphi^2(z)\right]^{N-j} \tag{43}$$

where $\sum^*$ denotes the sum restricted to

$$x - L' \leqslant ja \leqslant x \tag{44}$$

Remark. We do not distinguish between $\Psi(x_1,..., x_{N+1})$, defined in principle on $\Omega^a_{L,N+1}$ only, and its extension to $[0, L]^{N+1}$ obtained by putting the function equal to zero on the inaccessible region $[0, L]^{N+1} \backslash \Omega^a_{L,N+1}$.

2.3. Outer Boundary Conditions

So far we have not specified the outer boundary conditions. Since our main purpose is to test the stability of Bose–Einstein condensation with respect to the introduction of a Neumann hard core, we shall select boundary conditions for which the one-dimensional *free* Bose gas shows macroscopic occupation of its ground state. It was first proved by Robinson[12] that *attractive boundary conditions* have the required property (see also Ref. 13). It turns out that in our model, the following boundary conditions (repulsive at 0 and attractive at L) are easier to handle:

$$\begin{aligned} \frac{\partial}{\partial x_i} \Psi(x_1,..., x_{N+1}) \big|_{x_i=0} &= \sigma\Psi(x_1,..., x_{N+1} \big|_{x_i=0} \\ \frac{\partial}{\partial x_i} \Psi(x_1,..., x_{N+1}) \big|_{x_i=L} &= \sigma\Psi(x_1,..., x_{N+1}) \big|_{x_i=L} \end{aligned} \tag{45}$$

where $\sigma > 0$ is a fixed parameter. When translated in terms of

$$\Phi = \Psi \circ D^{-1}_{N+1} = \varphi^{\otimes (N+1)} \tag{46}$$

these become simply

$$\varphi'(0) = \sigma\varphi(0), \qquad \varphi'(L') = \sigma\varphi(L') \tag{47}$$

The one-particle Schrödinger problem

$$-\tfrac{1}{2}\varphi'' = E\varphi, \qquad \varphi \in L^2[0, L'] \tag{48}$$

with boundary conditions (47) has the following normalized solutions:

First a set of eigenvectors with positive energy

$$E_n^{L'}=\frac{n^2\pi^2}{2L'^2}, \qquad n=1,2,... \tag{49}$$

$$\varphi_n^{L'}(x)=\left(\frac{2}{L'}\right)^{1/2}\sin\left(\frac{n\pi x}{L'}+\alpha_n^{L'}\right) \tag{50}$$

where

$$\tan\alpha_n^{L'}=\frac{n\pi}{\sigma L'} \tag{51}$$

But there is also an eigenvector with negative energy

$$E_0^{L'}=-\frac{\sigma^2}{2} \tag{52}$$

$$\varphi_0^{L'}(x)=Ce^{\sigma x} \tag{53}$$

$$C=\left(\frac{2\sigma}{\exp 2\sigma L'-1}\right)^{1/2} \tag{54}$$

This choice of boundary conditions completes the description of our model. The explicit form of the one-body reduced density matrix at zero temperature can be obtained by inserting (53) in (35).

3. THERMODYNAMIC FUNCTIONS

One of the physical consequences of the unitary equivalence (29) is that the thermodynamics of our model is closely related to that of the free Bose gas with boundary conditions (47). For this reason we shall first review the properties of this model.

3.1. Review of the Free Gas

Consider a gas of free Bosons in $[0, L]$ with boundary conditions of the type (47). The spectrum of the one-particle Hamiltonian is [see (49), (52)]

$$\left\{-\frac{\sigma^2}{2},\frac{n^2\pi^2}{2L^2}, \qquad n=1,2,...\right\} \tag{55}$$

This implies that, even after the thermodynamic limit, the grand canonical pressure $p_0(\mu)$ for this model is defined only for values of the chemical potential such that

$$\mu<-\frac{\sigma^2}{2} \tag{56}$$

or in terms of the activity

$$z < e^{-(1/2)\beta\sigma^2} \equiv z_0 \tag{57}$$

The equation of state

$$\pi_0 = \pi_0(\rho) \tag{58}$$

(we call π_0 the pressure as a function of the density and we omit systematically the β dependence) is given by

$$\pi_0(\rho) = \frac{1}{(2\pi)^{1/2}\beta^{3/2}} g_{3/2}(z_0) \qquad \text{for} \quad \rho \geqslant \rho_0^c \tag{59a}$$

and can be got for $\rho < \rho_0^c$ by elimination of μ between

$$p_0(\mu) = \frac{1}{(2\pi)^{1/2}\beta^{3/2}} g_{3/2}(e^{\beta\mu}) \tag{59b}$$

$$\rho_0(\mu) = \frac{1}{(2\pi\beta)^{1/2}} g_{1/2}(e^{\beta\mu}) \tag{59c}$$

The critical density ρ_0^c is given by

$$\rho_0^c = \frac{1}{(2\pi\beta)^{1/2}} g_{1/2}(z_0) \tag{60}$$

In (59), (60), the functions $g_{1/2}$, $g_{3/2}$ are defined as

$$g_\alpha(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^\alpha} \tag{61}$$

Since the equivalence between our interacting Hamiltonian and the free one is N dependent, the relation between the thermodynamics of the two systems is best studied on *canonical* quantities, such as the free energy density per unit volume $f_0(\rho)$.

Using the equation

$$\pi_0(\rho) = \rho f'_0(\rho) - f_0(\rho) \tag{62}$$

we obtain easily from (59a)

$$f_0(\rho) = -\frac{\sigma^2\rho}{2} - \frac{1}{(2\pi)^{1/2}\beta^{3/2}} g_{3/2}(z_0) \qquad \text{when} \quad \rho \geqslant \rho_0^c \tag{63}$$

In the regime $\rho < \rho_0^c$, it is difficult to get an explicit expression for f_0, but we can see that there is a jump in f_0'' at $\rho = \rho_c$:

$$f_0''(\rho_0^c+) - f_0''(\rho_0^c-) = \left(\frac{2\pi}{\beta}\right)^{1/2} \left(\frac{-1}{g_{-1/2}(z_0)}\right) \tag{64}$$

3.2. The Interacting Gas

We turn to our model of interacting gas. Its free energy density at finite volume is

$$f_a^L\left(\frac{N}{L}\right) \equiv -\frac{1}{\beta L} \log \operatorname{Tr} e^{-\beta H_{L,N}^a} \tag{65}$$

$$= -\frac{1}{\beta L} \log \operatorname{Tr} e^{-\beta H_{L-a(N-1),N}^{free}} \tag{66}$$

$$= \frac{L - a(N-1)}{L} f_0^{L-a(N-1)} \left[\frac{N}{L - a(N-1)}\right]$$

$$= \frac{L - a(N-1)}{L} f_0^{L-a(N-1)} \left[\frac{N}{L} \frac{L}{L - a(N-1)}\right] \tag{67}$$

so that in the limit $L \to \infty$:

$$f_a(\rho) = (1 - a\rho) f_0\left(\frac{\rho}{1 - a\rho}\right), \qquad \rho < \frac{1}{a} \tag{68}$$

Hence there is a critical density

$$\rho_a^c = \frac{\rho_0^c}{1 + a\rho_0^c} < \frac{1}{a} \tag{69}$$

such that [see (63)]:

$$f_a(\rho) = \rho\left[-\frac{\sigma^2}{2} + \frac{a}{(2\pi)^{1/2} \beta^{3/2}} g_{3/2}(z_0)\right] - \frac{1}{(2\pi)^{1/2} \beta^{3/2}} g_{3/2}(z_0), \ \rho \geq \rho_a^c \tag{70}$$

There is again a jump in f''_a at $\rho = \rho_a^c$:

$$f_a''(\rho_a^c+) - f_a''(\rho_a^c-) = -\left(\frac{2\pi}{\beta}\right)^{1/2} \frac{1}{g_{-1/2}(z_0)} \left[1 + \frac{a}{(2\pi\beta)^{1/2}} g_{1/2}(z_0)\right]^3 \tag{71}$$

The shape of $f_a(\rho)$ is similar to that of $f_0(\rho)$ (see Fig. 1), except for the fact that the slope of the linear segment $[\rho_a^c, a^{-1}]$ can be positive or negative depending on the value of the parameters a, σ.

Remarks. (i) It might be surprising that $f_a(\rho)$ does not tend to $+\infty$ as ρ approaches the closest packing density a^{-1}. In fact, this can be understood as follows: at finite colume the closest packing limit is $N \to La^{-1}+1$. But in this limit, all the positive eigenvalues of the one-particle kinetic energy in $[0, L-a(N-1)]$ tend to $+\infty$ [see (55)], so that in view of (66), $f_a^L(\rho) \to +\infty$ as $\rho \to a^{-1}+L^{-1}$. Hence the graph of the limiting function $f_a(\rho)$ should really be supplemented by the value $+\infty$ at the end point $\rho = a^{-1}$.

(ii) The presence of a straight segment in $f_a(\rho)$ indicates that the model may have abnormally large fluctuations of its number density,[17] a phenomenon which is usually believed to be a pathology of the free Bose gas.

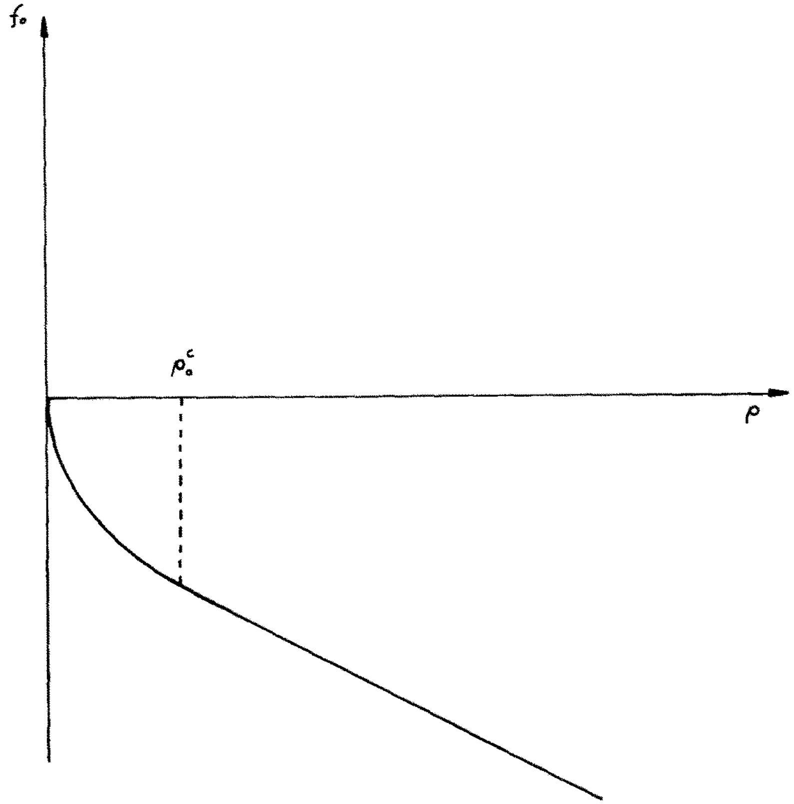

Fig. 1. The free energy density for the free gas.

4. ZERO-TEMPERATURE PROPERTIES

4.1. The Local Density

Our subsequent discussion of Bose–Einstein condensation depends crucially on the properties of the local density $\rho_L(x)$; see (43). Our first result is an upper bound.

Proposition 1. Let $\rho_L(x)$ be as in (43), with φ as in (53) and $\sigma > 0$. Then, for L and N large enough

$$\rho_L(x) \leqslant 4\sigma(N+1)^{3/2}[1+\log(N-1)] + 8\sigma(N+1) \tag{72}$$

Proof. Substituting (53) in (43), we get

$$\begin{aligned}\rho_L(x) = {} & \frac{(N+1)\, C^{2N+2}}{(2\sigma)^N} \sum_{j=0}^{N}{}^{*} \binom{N}{j} e^{2\sigma(x-ja)}\{e^{2\sigma(x-ja)}-1\}^j \\ & \times \{e^{2\sigma L'} - e^{2\sigma(x-ja)}\}^{N-j} \end{aligned} \tag{73}$$

$$\begin{aligned} = {} & (N+1)\, 2\sigma[1-e^{-2\sigma L'}]^{-(N+1)} \sum_{j=0}^{N}{}^{*} \binom{N}{j} e^{2\sigma(x-ja-L')} \\ & \times \{e^{2\sigma(x-ja-L')} - e^{-2aL'}\}^j\{1-e^{2\sigma(x-ja-L')}\}^{N-j} \end{aligned} \tag{74}$$

$$\begin{aligned} \leqslant {} & (N+1)\, 2\sigma[1-e^{-2\sigma L'}]^{-(N+1)} \sum_{j=0}^{N}{}^{*} \binom{N}{j} e^{2\sigma j(x-ja-L')} \\ & \times \{1-e^{2\sigma(x-ja-L')}\}^{N-j} \end{aligned} \tag{75}$$

Extracting from the sum the terms $j=0$ and N, and putting

$$B_N = [1-e^{-2\sigma L'}]^{-(N+1)} \tag{76}$$

we have

$$\begin{aligned} \rho_L(x) - 4\sigma(N+1)\, B_N \leqslant {} & 2\sigma(N+1)\, B_N \sum_{j=1}^{N-1}{}^{*} \binom{N}{j} e^{2\sigma j(x-ja-L')} \\ & \times \{1-e^{2\sigma(x-ja-L')}\}^{N-j} \end{aligned} \tag{77}$$

$$\leqslant 2\sigma(N+1)\, B_N \sum_{j=1}^{N-1}{}^{*} \binom{N}{j} \tag{78}$$

$$\times \max_{0 \leqslant y \leqslant L'} \{e^{2\sigma j y}(1-e^{2\sigma y})^{N-j}\} \tag{79}$$

$$= 2\sigma(N+1)\, B_N \sum_{j=1}^{N+1}{}^{*} \frac{N!}{N^N} \frac{j^j}{j!} \frac{(N-j)^{N-j}}{(N-j)!}$$

Now, the following version of Stirling's formula,[18]

$$e^{7/8} < \frac{k!}{k^k \sqrt{k} e^{-k}} < e \tag{80}$$

implies

$$\rho_L(x) - 4\sigma(N+1)\, B_N \leqslant 2\sigma(N+1)\, B_N e^{-3/4} N^{1/2} \sum_{j=1}^{N-1}{}^{*} \frac{1}{\sqrt{j}} \frac{1}{(N-j)^{1/2}} \tag{81}$$

$$\leqslant 2\sigma B_N (N+1)^{3/2} \sum_{j=1}^{N-1}{}^{*} \frac{1}{j} \tag{82}$$

$$\leqslant 2\sigma B_N (N+1)^{3/2} [1 + \log(N-1)] \tag{83}$$

This proves the result (72), because

$$B_N \to 1 \quad \text{as} \quad N \to \infty \quad \blacksquare \tag{84}$$

The reader might think that, because of the hard core interaction, the local density should be bounded by the close packing density a^{-1}; but in fact in the absence of translational invariance, the only restriction imposed on $\rho_L(x)$ by the presence of a hard core is the following one [see also remark (i) at the end of this section].

Proposition 2. For a one-dimensional system with arbitrary statistics and hard core diameter a, the local density $\rho_L(x)$ obeys the condition

$$\int_b^{b+a} dx \rho_L(x) \leqslant 1 \qquad \text{for} \quad \text{every } b \tag{85}$$

We omit the proof, which is independent of the nature of the hard core; see Section 2.

Proposition 3. $\rho_L(x)$ is a continuous function of x.

Proof. From the definition of $\rho_L(x) = \rho_L(x, x)$ [see (38)] we have

$$\rho_L(x) = (N+1) \int_{\Omega(x)} dz_1 \cdots dz_N\, \Psi^2(x, z_1, \dots, z_N) \tag{86}$$

$$= (N+1) \sum_{\pi \in S_{N+1}} \int_{\Omega_\pi(x)} dz_1 \cdots dz_N\, \Psi^2(x, z_1, \dots, z_n) \tag{87}$$

where

$$\Omega(x)=\{(z_1,\ldots,z_N):(x,z_1,\ldots,z_N)\in\Omega^a_{L,N+1}\} \tag{88}$$

$$\Omega_\pi(x)=\{(z_1,\ldots,z_N):(x,z_1,\ldots,z_N)\in R_\pi\} \tag{89}$$

with the same notation as before; see (10) and (17). Now, $\varphi(y)=Ce^{\sigma y}$ is continuous, and so Ψ is continuous in $\Omega^a_{L,N+1}$ [see (32)]. Moreover, the x dependence induced by $\Omega_\pi(x)$ is also continuous, because it comes through the limits of integration. For example the term $\pi=I$ in (87) reads explicitly:

$$\int_{x+a}^{L} dz_1 \int_{z_1+a}^{L} dz_2 \cdots \int_{z_{N-1}+a}^{L} dz_N\, \Psi^2(x,z_1,\ldots,z_N) \qquad \blacksquare \tag{90}$$

Remarks. (i) One can infer from propositions 1 and 3 that for any $y<1$, the scaled density $\rho_L(Ly)$ becomes asymptotically smaller than the closest packing density a^{-1}.

(ii) Proposition 3 (and its proof), can be extended in a straightforward manner to yield continuity of $\rho_L(x,y)$ in each variable.

4.2. Absence of Condensation

Let f be an arbitrary normalised function in $L^2[0,L]$. The average occupation number of the level f at zero temperature is [see (6), (38)]

$$\langle N_f^L\rangle=\int_0^L dx\int_0^L dy \bar{f}(x)\,f(y)\,\rho_L(x,y) \tag{91}$$

The key result of this section is an upper bound for the occupation of

$$h(x)=\frac{1}{\sqrt{L}} \tag{92}$$

Theorem 2. With the above notation

$$\langle N_h^L\rangle\leqslant\frac{1}{\sigma L}\{\log(2N+1)+\gamma\} \tag{93}$$

where γ depends only on σ and a [see (104)].

Proof. With φ given by (53), the explicit form of (35) is

$$I_L^{j,k}(x, y)=\frac{(N+1)!\, C^{2N+2}}{j!(k-j)!(N-k)!}\frac{e^{\sigma(x+y-ja-ka)}}{(2\sigma)^N}$$
$$\times\ [e^{2\sigma(x-ja)}-1]^j[e^{2\sigma(y-ka)}-e^{2\sigma(x-ja+a)}]^{k-j}$$
$$\times\ [e^{2\sigma L'}-e^{2\sigma(y-ka)}]^{N-k}e^{-\sigma a(k-j)} \tag{94}$$

And we have

$$\langle N_h^L\rangle=\frac{2}{L}\int_0^L dy\int_0^y dx\rho_L(x, y) \tag{95}$$

$$=\frac{2}{L}\sum_{0\leqslant j<k\leqslant N}\int_{(k+1)a}^{L'+ka} dy\int_{ja}^{y-(k-j+1)a} dxI_L^{(j,k)}(x, y)$$
$$+\frac{2}{L}\sum_{j=0}^{N}\int_{ja}^{L'+ja} dy\int_{ja}^{y} dxI_L^{(j,j)}(x, y) \tag{96}$$

Inserting (94) in (96) we find, after a few simple transformations:

$$\langle N_h^L\rangle=\frac{2}{L}\frac{C^{2N+2}}{L(2\sigma)^{N+2}}\sum_{0\leqslant j<k\leqslant N}\frac{(N+1)!}{j!(k-j)!(N-k)!}e^{\sigma a(2N+1-k-j)}$$
$$\times\int_1^A\frac{dv}{\sqrt{v}}\int_1^v\frac{du}{\sqrt{u}}(u-1)^j(v-u)^{k-j}(A-v)^{N-k}$$
$$+\frac{2}{L}\frac{C^{2N+2}}{(2\sigma)^{N+2}}\sum_{j=0}^{N}\frac{(N+1)!}{j!(N-j)!}$$
$$\times\int_1^B\frac{dv}{\sqrt{v}}\int_1^v\frac{du}{\sqrt{u}}(u-1)^j(B-v)^{N-j} \tag{97}$$

where we have set

$$A=\exp[2\sigma(L'-a)] \tag{98}$$

$$B=\exp[2\sigma L'] \tag{99}$$

By a repeated use of the inequality

$$\frac{1}{\sqrt{y}}\leqslant\frac{1}{(y-1)^{1/2}}\qquad y\geqslant 1 \tag{100}$$

and of the formula

$$\int_1^D dz(z-1)^\gamma(D-z)^l = \frac{l!(D-1)^{\gamma+l+1}}{(\gamma+1)\cdots(\gamma+l+1)} \tag{101}$$

(where $\gamma > -1$ need not be ar ·nteger) we deduce the following bound on (97):

$$\langle N_h^L\rangle \leqslant \frac{2}{L}\frac{C^{2N+2}}{(2\sigma)^{N+2}}\Bigg[(A-1)^{N+1}e^{(2N+1)\sigma a} \times \sum_{0\leqslant j<k\leqslant N}\frac{k!}{j!(j+1/2)\cdots(k+1/2)}e^{-\sigma a(k+j)} + (B-1)^{N+1}\sum_{j=0}^{N}\frac{1}{j+1/2}\Bigg] \tag{102}$$

$$\leqslant \frac{1}{\sigma L}\left\{2\sum_{0\leqslant j<k\leqslant N} e^{-\sigma a(k+j+1)} + [2+\log(2N+1)]\right\} \tag{103}$$

$$\leqslant \frac{2}{\sigma L}\left[\frac{e^{-\sigma a}}{(1-e^{-\sigma a})^2}+1\right] + \frac{\log(2N+1)}{\sigma L} \tag{104}$$

This completes the proof of Theorem 2. ∎

Corollary 1. Let $f \in L^2[0, L]$ be a normalized wave function obeying

$$|f(x)| \leqslant D_L \quad \text{on} \quad [0, L] \tag{105}$$

Then

$$\langle N_f\rangle \leqslant \frac{D_L^2}{\sigma}[\log(2N+1)+\gamma] \tag{106}$$

In particular if we put

$$N_j^L = N_{\varphi_j^L}, \qquad j = 0, 1, 2,... \tag{107}$$

where φ_j^L are the eigenvectors of the one-particle kinetic energy, we have

$$\langle N_0^L\rangle \leqslant \frac{2\sigma}{1-e^{-2\sigma L}}[\log(2N+1)+\gamma] \tag{108}$$

$$\langle N_j^L\rangle \leqslant \frac{2}{\sigma L}[\log(2N+1)+\gamma], \qquad j = 1, 2,... \tag{109}$$

Proof. The inequality (106) follows immediately from the proof of Theorem 2. The explicit form of the wave functions φ_j^L is the same as in (50), (53) with L' replaced by L. The estimates (108), (109) follow readily. ▮

The inequality (108) shows that φ_0^L (the ground state of the one-particle kinetic energy operator of the model) is not macroscopically occupied. This is in striking contrast with the free gas, where the condensation in the mode φ_0^L is complete at $T=0$. We obtain in Proposition 4 a better estimate of $\langle N_0^L \rangle$, but before doing that we exploit (109) to show that even the milder criterion (1) is not fulfilled.

Corollary 2. There is no generalized condensation in this model; more precisely, with the notation of (107):

$$L^{-1} \sum_{j: E_j^L < \varepsilon} \langle N_j^L \rangle \leqslant L^{-1}[\log(2N+1)+\gamma]\left[\frac{2\sigma}{1-e^{-\sigma L}}+\frac{2(2\varepsilon)^{1/2}}{\sigma\pi}\right] \tag{110}$$

Proof. Using (108), (109) we have

$$L^{-1} \sum_{j: E_j^L \leqslant \varepsilon} \langle N_j^L \rangle \leqslant L^{-1}[\log(2N+1)+\gamma]\left[\frac{2\sigma}{1-e^{-\sigma L}}+\frac{2}{\sigma L} N_\varepsilon\right] \tag{111}$$

where [see (49)]

$$N_\varepsilon = \sum_{j: 0 \leqslant E_j^L \leqslant \varepsilon} 1 = L\frac{(2\varepsilon)^{1/2}}{\pi} \tag{112}$$

so that (110) follows immediately. ▮

The estimate (108) suffices to rule out Bose–Einstein condensation in the ordinary sense [see (2)] but in fact $\langle N_0^L \rangle$ can be computed explicitely. The calculation turns out to be simpler than that leading to (93) and we omit it.

Proposition 4. For σ, $a > 0$, we have

$$\langle N_0^L \rangle = \frac{2}{(N+2)}\frac{1}{(1-e^{-2\sigma a})} + O(e^{-aN}) \tag{113}$$

The last possibility that we have to examine is the following one: could it be that there is macroscopic occupation of some unexpected one-particle level, completely unrelated to the kinetic energy? We use the results of Section 4.1 to show that no such phenomenon occurs in this model [in other words, the Onsager–Penrose criterion (7) is not satisfied either].

Theorem 3. Let f be an arbitrary normalized wave function in $L^2[0, L]$. Then, for N and L large enough

$$\langle N_f^L \rangle \leqslant 3(N+1)^{3/4} \log(2N+1) \tag{114}$$

Proof. With the notation (4), (32), we have

$$\langle N_f^L \rangle^2 = (f, R_\Psi^L f)^2 \leqslant \|R_\Psi^L\|^2 \tag{115}$$

$$\leqslant \int_0^L dx \int_0^L dy \rho_L^2(x, y) \tag{116}$$

$$\leqslant \int_0^L dx \int_0^L dy \rho_L(x, y)\, \rho_L^{1/2}(x, x)\, \rho_L^{1/2}(y, y) \tag{117}$$

$$= L\rho(g, R_\Psi^L g) = L\rho \langle N_g^L \rangle \tag{118}$$

where we have put

$$g(x) = \left[\frac{1}{\rho L} \rho_L(x, x)\right]^{1/2} \tag{119}$$

$$\rho = \frac{N+1}{L} \tag{120}$$

Note that g is a normalized function in $L^2[0, L]$, because

$$\int_0^L dx g^2(x) = \frac{1}{\rho L} \int_0^L dx \rho_L(x, x) = \frac{1}{\rho L} \operatorname{Tr} R_\Psi^L = 1 \tag{121}$$

In deducing (117) from (116), we used the fact [obvious from (6)] that R_Ψ^L is a positive operator; this together with the continuity of $\rho_L(x, y)$ [see Proposition 3 and remark (ii) in Section 4.1] implies that the kernel of the operator satisfies the inequality

$$\rho_L(x, y) \leqslant \rho_L^{1/2}(x, x)\, \rho_L^{1/2}(y, y) \tag{122}$$

Now, by virtue of Proposition 1

$$g(x) \leqslant \{4\sigma(N+1)^{1/2}[1 + \log(N-1)] + 8\sigma\}^{1/2} \tag{123}$$

so that Corollary 1 gives, for N, L large enough

$$\langle N_g^L \rangle \leqslant 9(N+1)^{1/2}[\log(2N+1)]^2 \tag{124}$$

We have thus proved [see (118)] that for any f in $L^2[0, L]$ one has, for N and L large enough

$$\langle N_f^L \rangle^2 \leqslant 9(N+1)^{3/2}[\log(2N+1)]^2 \quad \blacksquare \tag{125}$$

Remarks. (i) In view of the current wisdom, it comes as a surprise that the singularity in the thermodynamic functions of the model [see (71)] is not accompanied by any form of Bose–Einstein condensation. However, from a mathematical view point, there is no reason why the two phenomena should be connected; indeed the thermodynamics is entirely controlled by the spectrum of the Hamiltonian, whereas condensation properties involve (through the reduced density matrix) the eigenfunctions as well (in fact only the ground state wave function if we work at zero temperature). The situation is radically different in the free gas, where occupation numbers are expressible in terms of the spectrum only (we refer here to the finite temperature case, since at $T=0$ the free gas shows always complete condensation, even if there is no finite-temperature transition).

Let us be more explicit. Consider a noninteracting Bose gas with one-particle Hamiltonian h_L (possibly including an external potential); let $\{\varepsilon_j^L\}$ be the eigenvalues of h_L. All the information relevant to the thermodynamics and the condensation properties of the system at *finite volume* is contained in $\{\varepsilon_j^L\}$, or equivalently in the distribution of the eigenvalues of h_L:

$$F_L(x) = L^{-1} \sum_{j:\varepsilon_j^L \leqslant x} 1 \tag{126}$$

But the mere knowledge of the *asymptotic* distribution of the eigenvalues

$$F(x) = \lim_{L \to \infty} F_L(x) \tag{127}$$

does *not* give access to the condensation properties of the infinitely extended model in the usual sense [see (2)]. However, both the thermodynamics of the infinite system and its generalized condensation properties [see (1)] follow from $F(x)$.[14] In that sense, a singularity in the thermodynamic functions of a free Bose gas implies existence of generalized condensation. No such connection exists in the model of the interacting gas studied in this paper (see Corollary 2). In fact, as we mentioned earlier, there is no reason why a property of this type should be expected to hold, because already at finite volume the condensation properties of an interacting gas are not determined solely by the spectrum of the multiparticle Hamiltonian.

(ii) Penrose[19] has developed an argument of general nature which provides a lower bound on the occupation of any given one-particle level in a hard core gas at zero temperature. This estimate is particularly simple in our model if we apply it to the level $\varphi_0^L(x) = C_L e^{\sigma x}$; we find

$$\langle N_0^L \rangle \geqslant \int_{|x-y|>a}^{L} dx \int_0^L dy \rho_L(x, y)\, \varphi_0^L(x)\, \varphi_0^L(y) \tag{128}$$

$$= O((N+1)\, e^{-2\sigma a(N+1)}) \tag{129}$$

A comparison between (129) and (113) shows that the general bound of Ref. 19 is rather poor in this model. But, what is more interesting, we deduce from (113), (128), (129) that the main contribution to $\langle N_0^L \rangle$ comes from the integration on the region $|x-y| \leqslant a$ in (91). This casts a serious doubt on the common belief that condensation properties are governed by the asymptotic behavior of $\rho_L(x, y)$ for $|x-y|$ large; see [15] and [20].

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