

## van der Waals limit of an interacting Bose gas in a weak external field

Philip de Smedt

*Instituut voor Theoretische Fysica, B3030 Heverlee, Belgium  
and Department of Mathematics, Rutgers University, New Brunswick, New Jersey 08903*

V. A. Zagrebnov

*Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141 980, U.S.S.R.  
(Received 18 December 1986)*

We study how the introduction of a two-body interaction changes the thermodynamic properties of the free Bose gas in a weak (scaled) external field. We show that, in the van der Waals limit, the thermodynamic pressure always is a  $C^\infty$  function of the density in one and two dimensions, while this is not so in higher dimensions. The phase transition to the superfluid phase in the latter case is discussed in more detail by looking at the local densities. We also show that the van der Waals limit for this system does not correspond to the usual mean-field approximation.

### I. INTRODUCTION

The properties of the ideal Bose gas can change drastically when an external field is switched on. This was, for instance, discussed rigorously by van den Berg and Lewis.<sup>1</sup> They show that condensation in the one- and two-dimensional free Bose gas can be induced by switching on a *scaled* external field. [They also show an example where this condensation takes the form of a macroscopic occupation of infinitely many low-lying levels (the so-called generalized Bose-Einstein condensation<sup>2</sup>).] The condensate or superfluid phase, however, only occupies a microscopic fraction of the volume (i.e., the ratio of the volume of the condensate to the volume of the box tends to zero when the box grows to infinity). Nevertheless, the condensation manifests itself in the nonanalyticity of the thermodynamic pressure and free energy as a function of density and temperature.

A hard, and up to now essentially unsolved, problem is what happens to the condensate when the particles start to interact. It is well known that, in the absence of an external field, condensation does not occur in one and two dimensions.<sup>3,4</sup> It can also be shown that, in this case, the condensation persists in the van der Waals limit in dimensions higher than three (the van der Waals limit is a limit of very long-range forces between the particles, but the range remains small compared to the overall size of the box).<sup>5</sup>

In Ref. 6 the case was considered of an ordinary external field which is strong enough to produce at least one bound state. In this case Bose-Einstein condensation persists when a mean-field type of interaction is switched on. On the other hand, a simple superstability argument shows that, when a scaled external field is present and any superstable interaction is switched on, the condensate can no longer sit on the microscopic scale (see, e.g., Ref. 7). The superfluid phase might, however, spread out over a macroscopic region. As a first step towards a better understanding of what goes on with the condensate in this case, we study in this paper the van der Waals limit of the interacting Bose gas in a scaled external field. The situation turns out to be very interesting. In contrast to the

free case, we find that the limiting thermodynamic pressure becomes a  $C^\infty$  function of both the chemical potential  $\mu$  (or density  $\rho$ ) and the temperature in dimensions  $\nu=1$  and 2, whatever the scaled external field is. Moreover, it allows an analytic extension to some complex region near the real axis. This clearly suggests that the limiting system does not have a phase transition. In dimensions  $\nu \geq 3$ , we find that there are many points where the limiting thermodynamic pressure as a function of  $\mu$  is not infinitely differentiable. In particular, there is a whole interval of  $\mu$  (densities) where the set of local densities are not  $C^\infty$ . The expressions for the pressure and local densities point out that, at some lower critical density, a superfluid phase forms which gradually occupies a greater and greater macroscopic fraction of the box when the density is increased until, at some density, it is sitting over all the box. The introduction of the interaction, therefore, completely changes the thermodynamics of the system compared to the free case. For example, the reader can think of a box filled with bosons placed in the very weak gravitation field of the earth. Were there no interactions between the particles, the superfluid phase would concentrate on the bottom of the vessel and form a microscopic film. However, when some weak but long-range force is switched on between the bosons (corresponding to the van der Waals limit), the superfluid phase will spread out over the whole box and its density will be roughly everywhere the same (as the change in the gravitation potential will be very small over the box).

The structure of the paper is as follows. In Sec. II we discuss the model and introduce some formalism. In Sec. III we derive an explicit expression for the thermodynamic pressure in the van der Waals limit. Finally, in Sec. IV we discuss its properties as well as the behavior of the local densities. We also compare these results to the results of the usual mean-field approximation. As will be shown, the properties of this system are very different.

### II. DESCRIPTION OF THE MODEL

We consider the set of  $\nu$ -dimensional cubes  $\Lambda_L = [0, L]^\nu$  with volume  $L^\nu$  and denote by  $\mathcal{H}_L^n$  the space of sym-

metric, complex, square-integrable functions on the bounded region  $\Lambda_L^n = \times_{i=1}^n \Lambda_L$ . We define as usual the Fock space  $F_L$  by

$$F_L = \bigoplus_{n=0}^{\infty} \mathcal{H}_L^n. \tag{1}$$

We assume that the particles feel a weak (scaled) external field  $V(x/L)$  and the interact via a two-body potential  $\lambda^{\nu}U(\lambda r)$ , ( $\lambda > 0$ ). We make the following two assumptions concerning  $V$  and  $U$ : First,

$$V \in C^{\infty}(\Lambda_1), \tag{2}$$

and second,

$$\hat{U}(k) \equiv \int d^{\nu}x U(x)e^{ikx} \geq 0, \quad \forall k \in R^{\nu} \tag{3a}$$

$$U(0) < \infty, \tag{3b}$$

$$|U(x)| \leq \frac{D}{|x|} \nu + \epsilon, \quad \forall x \in R^{\nu} \quad (D, \epsilon > 0) \tag{3c}$$

$$U(x) \geq 0, \quad \forall x \in R^{\nu}. \tag{3d}$$

We believe, however, that the last condition [i.e., (3d)] is not essential to derive the van der Waals limit,<sup>8,9</sup> although the derivation seems to become much more difficult if (3d) is not assumed. We note that the class of potentials satisfying conditions 3(a)–3(d) is not empty [for instance, it contains the potentials  $U(r) = a \exp(-br^2)$ ,  $a, b > 0$ ]. For convenience, we put  $X^n = (x_1, \dots, x_n)$  and  $dX^n = d^{\nu}x_1 \cdots d^{\nu}x_n$ .

Now we introduce the following quadratic forms on  $F_L$ , defined by their reductions to  $\mathcal{H}_L^n$ .

*Kinetic energy.*

$$t_L^{\infty}(\psi) = \frac{1}{2} \sum_{k=1}^n \int dX^n |\nabla_k \psi(X^n)|^2 \tag{4}$$

with domain  $S(C_0^1(\Lambda_L^n))$  ( $S$  being the usual symmetrization operator).  $t_L^0(\psi)$  is defined similarly, but with domain  $S(C^1(\Lambda_L^n))$ .<sup>10</sup> (Basically,  $\infty$  denotes Dirichlet boundary conditions, while 0 denotes Neumann boundary conditions.)

*External potential.*

$$v_L(\psi) = \sum_{k=1}^n \int dX^n V \left[ \frac{x_k}{L} \right] |\psi(X^n)|^2. \tag{5}$$

*Interaction.*

$$u_{L,\lambda}(\psi) = \sum_{\substack{i,j \\ (1 \leq i < j \leq n)}} \int dX^n \lambda^{\nu} U(\lambda(x_i - x_j)) |\psi(X^n)|^2. \tag{6}$$

We denote by  $h_{L,\lambda}^0(\psi)$  [ $h_{L,\lambda}^{\infty}(\psi)$ ] the closure of the quadratic form  $t_L^0(\psi) + v_L(\psi) + u_{L,\lambda}(\psi)$  [ $t_L^{\infty}(\psi) + v_L(\psi) + u_{L,\lambda}(\psi)$ ] and denote by  $H_{L,\lambda}^0$  ( $H_{L,\lambda}^{\infty}$ ) the associated self-adjoint operator, being the Hamiltonian for our system. In the same way we construct the mean-field Hamiltonians  $\tilde{H}_{L,a}^{0(\infty)}$  corresponding to the closure of the quadratic forms  $t_L^{0(\infty)}(\psi) + (a/2)(\psi, N_L^2 \psi)$ . Here  $N_L$  is the usual number operator, defined by

$$N_L \psi(X^n) = n \psi(X^n) \quad \forall \psi \in \mathcal{H}_L^n.$$

The thermodynamic pressure  $p_{L,\lambda}^{0(\infty)}(\mu)$  is defined by

$$p_{L,\lambda}^{0(\infty)}(\mu) = \frac{1}{\beta L^{\nu}} \ln \{ \text{Tr} \exp[-\beta(H_{L,\lambda}^{0(\infty)} - \mu N_L)] \}. \tag{7}$$

The pressure of the mean-field system  $\tilde{p}_{L,a}^{0(\infty)}(\mu)$  is defined similarly. We also define in the usual way the finite-volume Gibbs states  $\omega_{L,\lambda,\mu}^{0(\infty)}(\cdots)$ . In Sec. III we will derive an explicit expression for the thermodynamic pressure  $p_{L,\lambda}^{0(\infty)}(\mu)$  in the van der Waals limit  $\lim_{\lambda \downarrow 0} \lim_{L \rightarrow \infty}$ .

### III. DERIVATION OF THE van der WAALS LIMIT

Before stating the main theorem, we first recall some properties of the mean-field system  $\tilde{H}_{L,a}^{0(\infty)}$ .<sup>11</sup> One has

$$\tilde{p}_a(\mu) = \lim_{L \rightarrow \infty} \tilde{p}_{L,a}^0(\mu) = \lim_{L \rightarrow \infty} \tilde{p}_{L,a}^{\infty}(\mu) = \frac{(\mu - \alpha)^2}{2a} + p_0(\alpha), \tag{8a}$$

where  $\alpha$  satisfies

$$\alpha = \mu - a\rho_0(\alpha) \quad \text{if } \mu < a\rho_c,$$

$$\alpha = 0 \quad \text{if } \mu \geq a\rho_c,$$

and where

$$p_0(\alpha) = -\frac{1}{\beta} \int \frac{d^{\nu}k}{(2\pi)^{\nu}} \ln \left\{ 1 - \exp \left[ -\beta \left( \frac{k^2}{2} - \alpha \right) \right] \right\}, \tag{8b}$$

$$\alpha \leq 0$$

$$\rho_0(\alpha) = \int \frac{d^{\nu}k}{(2\pi)^{\nu}} \frac{1}{\exp \left[ \beta \left( \frac{k^2}{2} - \alpha \right) \right] - 1}, \quad \alpha \leq 0 \tag{8c}$$

$$\rho_c = \rho_0(0) \quad (\rho_c < \infty \quad \text{if } \nu \geq 3). \tag{8d}$$

We note that the mean-field system has a third-order (second-order) phase transition in dimensions  $\nu = 3, 4$  ( $\nu \geq 5$ ), when  $\mu = a\rho_c$ . At this point the density of the system is  $\rho_c$ . The rest of this section will be devoted to proving the following theorem.

#### Theorem 1

With the preceding conventions and assumptions,

$$\lim_{\lambda \downarrow 0} \lim_{L \rightarrow \infty} p_{L,\lambda}^{0(\infty)}(\mu) = \int_{\Lambda_1} d^{\nu}x \tilde{p}_a(\mu - V(x))$$

where  $a \equiv \int_{R^{\nu}} d^{\nu}x U(x)$ .

The proof consists in finding upper and lower bounds for  $p_{L,\lambda}^{0(\infty)}(\mu)$  which coincide in the van der Waals limit. One has

$$p_{L,\lambda}^{\infty}(\mu) \leq p_{L,\lambda}^0(\mu) \tag{9}$$

(see, e.g., Ref. 10). Therefore, it suffices to find an upper bound for  $p_{L,\lambda}^0(\mu)$  and a lower bound for  $p_{L,\lambda}^{\infty}(\mu)$ .

#### Upper bound for $p_{L,\lambda}^0(\mu)$

To find an upper bound, we partition the cube  $\Lambda_L$  into the cubes

$$\Lambda_{\mathbf{k}}^{(m)} = \times_{i=1}^v \left[ (k_i - 1) \frac{L}{m}, k_i \frac{L}{m} \right], \quad 1 \leq k_i \leq m \quad (m \in N).$$

Clearly,

$$\bigcup_{\mathbf{k}} (\Lambda_{\mathbf{k}}^{(m)}) = \Lambda_L \quad \text{and} \quad F_L = \otimes_{\mathbf{k}} F_{\mathbf{k}}, \quad (10)$$

where  $F_{\mathbf{k}}$  stands for the Fock space over the volume  $\Lambda_{\mathbf{k}}^{(m)}$ .

Let us now define the following quadratic forms, corresponding to the partitioning described above ( $\psi \in \mathcal{H}_L^n$ ):

$$i_{\mathbf{k}}^0(\psi) = \sum_{j=1}^n \int dX^n \chi_{\mathbf{k}}(x_j) |\nabla_j \psi(X^n)|^2 \quad (11a)$$

with domain  $S(C^1(\Lambda^n))$ , where  $\chi_{\mathbf{k}}(x)$  is the usual characteristic function of the volume  $\Lambda_{\mathbf{k}}^{(m)}$ ;

$$n_{\mathbf{k}}(\psi) = \int dX^n \left[ \sum_{j=1}^n \chi_{\mathbf{k}}(x_j) \right] |\psi(X^n)|^2, \quad (11b)$$

$$n_{\mathbf{k}}^2(\psi) = \int dX^n \left[ \sum_{j=1}^n \chi_{\mathbf{k}}(x_j) \right]^2 |\psi(X^n)|^2, \quad (11c)$$

$$\underline{v}_{\mathbf{k}}(\psi) = \underline{V}_{\mathbf{k}} n_{\mathbf{k}}(\psi), \quad (11d)$$

where

$$\underline{V}_{\mathbf{k}} = \min_{x \in \Lambda_{\mathbf{k}}^{(m)}} V \left[ \frac{x}{L} \right].$$

We then have the following.

$$\begin{aligned} u_{L,\lambda}(\psi) &= \int dX^n U_{\lambda}(X^n) |\psi(X^n)|^2 \\ &= \sum_{i_1, \dots, i_n} \int_{\Lambda_{i_1}} d^v x_1, \dots, \int_{\Lambda_{i_n}} d^v x_n U_{\lambda}(X^n) |\psi(X^n)|^2 \end{aligned} \quad (14)$$

$$= \sum'_{\{N_{\mathbf{k}}\}} P_{\{N_{\mathbf{k}}\}} \left[ \prod_{\mathbf{k}} \int_{\Lambda_{\mathbf{k}}} dX^{N_{\mathbf{k}}} \right] U_{\lambda}(X^n) |\psi(X^n)|^2, \quad (15)$$

where  $\sum'_{\{N_{\mathbf{k}}\}}$  stands for the sum over all possible choices of  $\{N_{\mathbf{k}}: N_{\mathbf{k}} \geq 0\}$  such that  $\sum_{\mathbf{k}} N_{\mathbf{k}} = n$  and

$$\int_{\mathbf{k}} dX^{N_{\mathbf{k}}} = \prod_{j=1}^{N_{\mathbf{k}}} \left[ \int_{\Lambda_{\mathbf{k}}^{(m)}} d^v x_{k_j} \right].$$

In going from (14) to (15), we have ordered the particles in such a way that the first  $N_{\mathbf{k}_1}$  particles sit in  $\Lambda_{\mathbf{k}_1}^{(m)}$ , the second  $N_{\mathbf{k}_2}$  particles in  $\Lambda_{\mathbf{k}_2}^{(m)}$  and so on. The factor  $P_{\{N_{\mathbf{k}}\}}$  is a permutation factor which counts the number of terms in (14) which yield the same contribution in (15). Now, using  $U(x) \geq 0$  [see (3d)], we find

$$\begin{aligned} u_{L,\lambda}(\psi) &\geq \sum'_{\{N_{\mathbf{k}}\}} P_{\{N_{\mathbf{k}}\}} \left[ \prod_{\mathbf{k}} \int_{\Lambda_{\mathbf{k}}} dX^{N_{\mathbf{k}}} \right] \\ &\quad \times \left[ \sum_{\mathbf{k}} U_{\lambda}(X^{N_{\mathbf{k}}}) \right] |\psi(X^n)|^2. \end{aligned}$$

Finally, we use (13), taking  $L/m > L_1$ . Then

*Proposition 1.*

$$i_L^0(\psi) = \sum_{\mathbf{k}} i_{\mathbf{k}}^0(\psi), \quad (12a)$$

$$v_L(\psi) \geq \sum_{\mathbf{k}} \underline{v}_{\mathbf{k}}(\psi), \quad (12b)$$

$\forall \lambda > 0, \forall \epsilon > 0, \exists L_0$  such that  $\forall L > L_0$ :

$$u_{L,\lambda}(\psi) \geq \frac{a(1-\epsilon)}{2} \frac{m^v}{L^v} \sum_{\mathbf{k}} n_{\mathbf{k}}^2(\psi) - \lambda^v U(0) \sum_{\mathbf{k}} n_{\mathbf{k}}(\psi), \quad (12c)$$

where  $a \equiv \int_{R^v} d^v x U(x)$ .

*Proof.* The proof of (12a) and (12b) is trivial. It remains to prove (12c). We use the following result which can be found in Ref. 12:

$\forall \lambda > 0, \forall \epsilon > 0, \exists L_1$ ,

such that  $\forall L > L_1, \forall N, \forall x_i \in \Lambda_L$ :

$$\sum_{\substack{i,j \\ (1 \leq i < j \leq N)}} \lambda^v U(\lambda(x_i - x_j)) \geq \frac{a(1-\epsilon)}{2L^v} N^2 - \lambda^v U(0)N. \quad (13)$$

Now take any  $\psi \in \mathcal{H}_L^n$  and put

$$U_{\lambda}(X^n) = \sum_{\substack{i,j \\ (1 \leq i < j \leq n)}} \lambda^v U(\lambda(x_i - x_j)).$$

Then

$$\begin{aligned} u_{L,\lambda}(\psi) &\geq \sum'_{\{N_{\mathbf{k}}\}} P_{\{N_{\mathbf{k}}\}} \left[ \prod_{\mathbf{k}} \int_{\Lambda_{\mathbf{k}}} dX^{N_{\mathbf{k}}} \right] \\ &\quad \times \left[ \frac{a(1-\epsilon)}{2} \frac{m^v}{L^v} \sum_{\mathbf{k}} N_{\mathbf{k}}^2 - \lambda^v U(0) \sum_{\mathbf{k}} N_{\mathbf{k}} \right] \\ &\quad \times |\psi(X^n)|^2. \end{aligned} \quad (16)$$

It is straightforward to check that (16) is equivalent to (12c).

Using (10) and proposition 1, an analysis similar to the one in Ref. 10 yields

$$p_{L,\lambda}^0(\mu) \leq \frac{1}{m^v} \sum_{\mathbf{k}} \tilde{p}_{L/m, a(1-\epsilon)}^0(\mu - \underline{V}_{\mathbf{k}} + \lambda^v U(0)).$$

Taking the following series of limits,

$$\lim_{m \rightarrow \infty} \lim_{\epsilon \downarrow 0} \lim_{\lambda \downarrow 0} \lim_{L \rightarrow \infty},$$

we then obtain

$$\limsup_{\lambda \downarrow 0} \lim_{L \rightarrow \infty} p_{L,\lambda}^0(\mu) \leq \int_{\Lambda_1} d^{\nu}x \tilde{p}_a(\mu - V(x)). \quad (17)$$

[The existence of  $\lim_{L \rightarrow \infty} p_{L,\lambda}^0(\mu)$ , and its equality to  $\lim_{L \rightarrow \infty} p_{L,\lambda}^{\infty}(\mu)$ , can be shown using similar arguments to the ones presented in Ref. 10.]

#### Lower bound for $p_{L,\lambda}^{\infty}(\mu)$

To obtain a lower bound for  $p_{L,\lambda}^{\infty}(\mu)$ , we divide  $\Lambda_L$  into the cubes  $\Lambda_{\mathbf{k}}^{(q,r)}$ :

$$\Lambda_{\mathbf{k}}^{(q,r)} = \prod_{i=1}^{\nu} \left[ k_i \left[ \frac{L}{q} + \frac{L}{r} \right], k_i \left[ \frac{L}{q} + \frac{L}{r} \right] + \frac{L}{q} \right],$$

$$0 \leq k_i \leq \text{Int} \left[ \frac{qr}{q+r} \right] - 1. \quad (18)$$

$\text{Int}(x)$  denotes the integral part of  $x$  and  $q, r \in \mathbb{N}$ . The volume of the cubes  $\Lambda_{\mathbf{k}}^{(q,r)}$  is  $(L/q)^{\nu}$  and the minimal distance between two such cubes is bigger than  $L/r$ . Clearly,

$$p_{L,\lambda}^{\infty}(\mu) \geq \overline{\text{Tr}}_M \exp[-\beta(H_{L,\lambda}^{\infty} - \mu N_L)], \quad (19)$$

where  $\overline{\text{Tr}}_M$  stands for the trace over the space  $G_M$  of states containing no particles outside the cubes  $\Lambda_{\mathbf{k}}^{(q,r)}$  and at most  $ML^{\nu}$  particles in each of them.  $M$  is some fixed but sufficiently large number, to be determined later on.

Let us define the quadratic forms:

$$\bar{v}_{\mathbf{k}}(\psi) = \bar{V}_{\mathbf{k}} n_{\mathbf{k}}(\psi), \quad (20)$$

where

$$\bar{V}_{\mathbf{k}} = \max_{x \in \Lambda_{\mathbf{k}}^{(q,r)}} V \left[ \frac{x}{L} \right].$$

$n_{\mathbf{k}}$  is defined as in (11b) (but with  $\Lambda_{\mathbf{k}}^{(m)}$  replaced by  $\Lambda_{\mathbf{k}}^{(q,r)}$ ). Similarly, we also define the quadratic forms  $t_{\mathbf{k}}^{\infty}$  and  $u_{\mathbf{k},\lambda}$ . The following proposition then holds.

*Proposition 2.*  $\forall \psi \in G_M$ :

$$t_L^{\infty}(\psi) = \sum_{\mathbf{k}} t_{\mathbf{k}}^{\infty}(\psi), \quad (21a)$$

$$v_L(\psi) \leq \sum_{\mathbf{k}} \bar{v}_{\mathbf{k}}(\psi), \quad (21b)$$

$$u_{L,\lambda}(\psi) \leq \sum_{\mathbf{k}} u_{\mathbf{k},\lambda}(\psi) + A(\lambda, q, r, M) L^{\nu-\epsilon} \|\psi\|^2, \quad (21c)$$

where  $A(\lambda, q, r, M)$  is some finite number depending on the choice of  $\lambda, q, r$  and  $M$ ;  $\|\psi\|$  denotes the usual  $L^2$  norm; and  $\epsilon$  is as in (3c).

*Proof:* The proof of (21a) and (21b) is again trivial. It remains to prove (21c). Clearly,  $u_{L,\lambda}(\psi)$  is equal to  $\sum_{\mathbf{k}} u_{\mathbf{k},\lambda}(\psi)$  plus the contribution  $u_{\text{int}}(\psi)$  coming from the interaction between particles sitting in different cubes  $\Lambda_{\mathbf{k}}^{(q,r)}$ . We now work out an upper bound for  $|u_{\text{int}}(\psi)|$ . The interaction between two cells  $\Lambda_{\mathbf{k}}^{(q,r)}$  and  $\Lambda_{\mathbf{l}}^{(q,r)}$  is clearly bounded by

$$(ML^{\nu})^2 K(\mathbf{k}, \mathbf{l}),$$

where  $K(\mathbf{k}, \mathbf{l})$  is the maximum of  $\lambda^{\nu} U(\lambda(x-y))$  with  $x$  in  $\Lambda_{\mathbf{k}}^{(q,r)}$  and  $y$  in  $\Lambda_{\mathbf{l}}^{(q,r)}$ .

Using the bound (3c) and summing over all cells, we

then find

$$|u_{\text{int}}(\psi)| \leq \|\psi\|^2 \left[ \frac{qr}{q+r} \right]^{\nu} \sum_{\substack{\mathbf{k} \in \mathbb{Z}^{\nu} \\ \mathbf{k} \neq 0}} \frac{\lambda^{\nu} D(ML^{\nu})^2}{\lambda^{\nu+\epsilon} L^{\nu+\epsilon} (d(\mathbf{k}))^{\nu+\epsilon}}, \quad (22)$$

where  $d(\mathbf{k})$  denotes the minimal distance between the cubes  $\Lambda_0^{(q,r)}$  and  $\Lambda_{\mathbf{k}}^{(q,r)}$  divided by  $L$ . [Here we have extended the definition (18) of the cubes  $\Lambda_{\mathbf{k}}^{(q,r)}$  to any  $\mathbf{k} \in \mathbb{Z}^{\nu}$ .] Formula (22) gives an explicit formula for  $A(\lambda, q, r, M)$  which finishes the proof of the proposition.

We now define the approximate pressure  $f_{L,\lambda}^M(\mu)$  by

$$f_{L,\lambda}^M(\mu) = \frac{1}{\beta L^{\nu}} \ln \{ \text{Tr}_M \exp[-\beta(\bar{H}_{L,\lambda}^{\infty} - \mu N^L)] \},$$

where  $\bar{H}_{L,\lambda}^{\infty}$  is the Hamiltonian of the interacting system without the external field term and  $\text{Tr}_M$  stands for the trace over the states with less than  $ML^{\nu}$  particles in the box  $\Lambda_L$ . Using (19) and Proposition 2, we obtain

$$p_{L,\lambda}^{\infty}(\mu) \geq \frac{1}{q^{\nu}} \sum_{\mathbf{k}} f_{L,\lambda}^{Mq^{\nu}}(\mu - \bar{V}_{\mathbf{k}}) - \frac{A(\lambda, q, r, M)}{L^{\epsilon}}. \quad (23)$$

It is shown in the Appendix that  $\forall \mu_0, \forall \lambda_0 > 0, \exists M$  such that  $\forall \mu < \mu_0, \forall \lambda: 0 < \lambda < \lambda_0$ :

$$\lim_{L \rightarrow \infty} f_{L,\lambda}^M(\mu) = \bar{p}_{\lambda}(\mu), \quad (24)$$

where

$$\bar{p}_{\lambda}(\mu) = \lim_{L \rightarrow \infty} \frac{1}{\beta L^{\nu}} \ln \{ \text{Tr} \exp[-\beta(\bar{H}_{L,\lambda}^{\infty} - \mu N_L)] \}.$$

Therefore, taking the limit  $L \rightarrow \infty$  of (23), we get

$$\lim_{L \rightarrow \infty} p_{L,\lambda}^{\infty}(\mu) \geq \frac{1}{q^{\nu}} \sum_{\mathbf{k}} \bar{p}_{\lambda}(\mu - \bar{V}_{\mathbf{k}}). \quad (25)$$

But it is well known (see, e.g., Ref. 5) that

$$\lim_{\lambda \downarrow 0} \bar{p}_{\lambda}(\mu) = \bar{p}_a(\mu).$$

Applying  $\lim_{q \rightarrow \infty} \lim_{r \rightarrow \infty} \lim_{\lambda \downarrow 0}$  to (25) then yields

$$\liminf_{\lambda \downarrow 0} \lim_{L \rightarrow \infty} p_{L,\lambda}^{\infty}(\mu) \geq \int_{\Lambda_1} d^{\nu}x \tilde{p}_a(\mu - V(x)). \quad (26)$$

Theorem 1 now follows by combining (9), (17), and (26).

#### IV. THERMODYNAMIC PROPERTIES OF THE LIMITING van der WAALS SYSTEM

In Sec. III we proved that

$$\begin{aligned} p(\mu) &\equiv \lim_{\lambda \downarrow 0} \lim_{L \rightarrow \infty} p_{L,\lambda}^{0(\infty)}(\mu) \\ &= \int_{\Lambda_1} d^{\nu}x \tilde{p}_a(\mu - V(x)) \\ &= \int_{\Lambda_1} d^{\nu}x \left[ \frac{(\mu - V(x) - \alpha(x))^2}{2a} + p_0(\alpha(x)) \right], \end{aligned}$$

where  $\alpha(x)$  satisfies

$$\begin{aligned} \alpha(x) &= \mu - V(x) - a\rho_0(\alpha(x)) \quad \text{if } \mu - V(x) \leq a\rho_c \\ \alpha(x) &= 0 \quad \text{if } \mu - V(x) \geq a\rho_c. \end{aligned} \quad (27)$$

[see Eqs. (8)]. We now study the behavior of  $p(\mu)$  as a function of  $\mu$  or, equivalently, as a function of the mean density  $\rho(\mu) = dp(\mu)/d\mu$ .

In one or two dimensions  $\rho_c = \infty$  and it is then easy to see that  $p(\mu)$  is a  $C^\infty$  function of  $\mu$  (and therefore also of  $\rho$ ), which allows, moreover, an analytic extension to some complex domain near the real axis.

The situation is quite different in higher dimensions where  $\rho_c < \infty$ . To sketch what goes on, let us consider the case  $\nu=3$ . (A similar analysis can be carried through in higher dimensions.) Moreover, let us assume that  $\Lambda_1$ , instead of being a cube, is a ball of radius  $R=1$ , centered around the origin, and that  $V(x)$  is a rotation invariant function, i.e.,  $V(x) = V_0(|x|)$  where  $V_0 \in C^\infty([0,1])$ . (A typical case is shown in Fig. 1.) As before, we can show that

$$p(\mu) = 4\pi \int_0^1 dr r^2 \tilde{p}_a(\mu - V_0(r)).$$

Using the fact that

$$\rho_0(\alpha) = \rho_c + \Gamma(-\frac{1}{2})(-\beta\alpha)^{1/2} + O(\alpha),$$

with  $|\alpha|$  small (Ref. 13) and formulas (8), one can verify that all derivatives of  $\tilde{p}_a(\mu)$  with respect to  $\mu$  up to fourth order exist and are bounded, except at  $\mu = a\rho_c$  where  $\tilde{p}_a''(\mu)$  and  $\tilde{p}_a^{IV}(\mu)$  are discontinuous. Now denote by  $r_i$  ( $i=1, N$ ) the set of points such that

$$V_0(r_i) = \mu - a\rho_c$$

(see Fig. 1). Using the above remarks, one checks that

$$p^{IV}(\mu) = 4\pi \int_0^1 dr r^2 \tilde{p}_a^{IV}(\mu - V_0(r)) + 4\pi C \sum_{i=1}^N \frac{dr_i}{d\mu} r_i^2,$$

where

$$C = \lim_{\mu \rightarrow a\rho_c} \tilde{p}_a'''(\mu) - \lim_{\mu \rightarrow a\rho_c} \tilde{p}_a'''(\mu).$$

A straightforward analysis then yields that  $p^{IV}(\mu)$  is discontinuous at any point  $\mu$  satisfying

$$\mu = a\rho_c + V_0(R_j) \quad (j=1, M)$$

or

$$\mu = a\rho_c + V_0(1)$$

where  $R_j$  are the extremal points of  $V_0(r)$  (see Fig. 1). The point  $\mu = a\rho_c + V_0(0)$  needs a special analysis, but also turns out to be a point of nonanalyticity of  $p(\mu)$ . How often  $p(\mu)$  is differentiable at this point depends, however, on the behavior of  $V_0(r)$  near  $r=0$ . The behavior of the local densities  $\rho(\mu; x)$  turns out to be more instructive in this respect. They are defined as follows:

$$\rho(\mu; x) = \lim_{A \rightarrow 0} \lim_{\lambda \rightarrow 0} \lim_{L \rightarrow \infty} \omega_{L, \lambda, \mu}^{(0, \infty)} \left[ \frac{N_L^{x, A}}{A^\nu L^\nu} \right],$$

where  $N_L^{x, A}$  is the operator counting the number of particles in the box

$$\Lambda_L^{x, A} = \prod_{i=1}^{\nu} [L(x_i - A), L(x_i + A)],$$

i.e.,

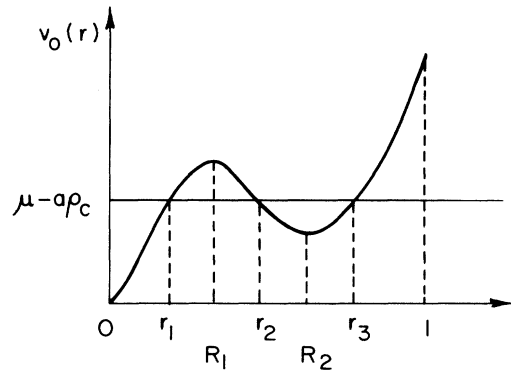


FIG. 1. A typical potential  $V_0(r)$ .

$$N_L^{x, A} \psi(X^n) = \sum_{i=1}^n \chi_A(x_i) \psi(X^n), \quad \forall \psi \in \mathcal{H}_L^n,$$

$\chi_A(x)$  being the characteristic function of  $\Lambda_L^{x, A}$ . Now consider the functions  $g_{L, \lambda}^{(0, \infty)}(\delta)$ :

$$g_{L, \lambda}^{(0, \infty)}(\delta) = \frac{1}{\beta L^\nu} \ln \{ \text{Tr} \exp[ -\beta(H_{L, \lambda}^{(0, \infty)} - \mu N_L - \delta N_L^{x, A}) ] \}.$$

As in Sec. II, we can prove that

$$\begin{aligned} g(\delta) &\equiv \lim_{\lambda \rightarrow 0} \lim_{L \rightarrow \infty} g_{L, \lambda}^{(0, \infty)}(\delta) \\ &= \int_{\Lambda_1 \cap \Lambda_1^{x, A}} d^\nu x \tilde{p}_a(\mu - V(x) + \delta) \\ &\quad + \int_{\Lambda_1 \setminus \Lambda_1^{x, A}} d^\nu x \tilde{p}_a(\mu - V(x)). \end{aligned}$$

Moreover, as  $g_{L, \lambda}^{(0, \infty)}(\delta)$  is a convex function of  $\delta$ , one has

$$\begin{aligned} \lim_{\lambda \rightarrow 0} \lim_{L \rightarrow \infty} \frac{\omega_{L, \lambda}^{(0, \infty)}(N_L^{x, A})}{L^\nu} &= \lim_{\lambda \rightarrow 0} \lim_{L \rightarrow \infty} \frac{d}{d\delta} g_{L, \lambda}^{(0, \infty)}(\delta) \Big|_0 \\ &= \frac{d}{d\delta} g(\delta) \Big|_0 \\ &= \int_{\Lambda_a \cap \Lambda_1^{x, A}} d^\nu x \left[ \frac{d}{d\mu} \tilde{p}_a(\mu) \Big|_{\mu - V(x)} \right]. \end{aligned}$$

Consequently,

$$\rho(\mu; x) = \frac{d}{d\mu} \tilde{p}_a(\mu) \Big|_{\mu - V(x)}.$$

We note that  $\rho(\mu; x)$  is a  $C^\infty$  function of  $\mu$  except at the point  $\mu = V(x) + a\rho_c$ . Clearly what goes on is the following: When the mean density of the system is increased, the local density  $\rho(\mu; x)$  increases also and all particles in the neighborhood of  $x$  sit in the normal phase. However, as soon as the local density exceeds  $\rho_c$ , any newly added particle at that point will enter the superfluid phase. We conclude that for any  $\mu$  with

$$a\rho_c + \min_{y \in \Lambda_1} V(y) \leq \mu \leq a\rho_c + \max_{y \in \Lambda_1} V(y),$$

there exists some point  $x \in \Lambda_1$ , where the local density  $\rho(\mu; x)$  is nonanalytic. A similar statement can be made

about the local densities as a function of the mean density  $\rho$ .

To end this section, we stress the difference between the system we obtain in the van der Waals limit and the system one obtains performing the usual mean-field approximation. This latter system is described by the Hamiltonian derived from the quadratic form

$$t_L^{(0\infty)}(\psi) + v_L(\psi) + \frac{a}{2} n_L^2(\psi).$$

Denoting the limiting pressure of this system by  $p_{mf}(\mu)$ , one finds

$$p_{mf}(\mu) = \int_{\Lambda_1} dx \left[ \frac{(\mu - \alpha)^2}{2a} + \rho_0(\alpha - V(x)) \right],$$

where  $\alpha$  satisfies

$$(i) \quad \alpha = \mu - a \int_{\Lambda_1} dx \rho_0(\alpha - V(x)) \quad \text{if } \mu \leq a\rho_{c,ext} + \underline{V},$$

$$(ii) \quad \alpha = \underline{V} \quad \text{if } \mu \geq a\rho_{c,ext} + \underline{V},$$

where  $\underline{V} = \min_{x \in \Lambda_1} V(x)$  and where

$$\rho_{c,ext} = \lim_{\alpha \uparrow \underline{V}} \int_{\Lambda_1} dx \rho_0(\alpha - V(x)).$$

This expression has to be compared to expression (27). Note that the mean-field pressure  $p_{mf}(\mu)$  shows a singularity only at  $\mu = a\rho_{c,ext}$  and that  $\rho_{c,ext}$  can be finite even in one or two dimensions (see, e.g., Ref. 1). It is also possible to consider the local densities  $\rho_{mf}(\mu; x)$  for this system. These have the following property [ $\forall x$  with  $V(x) > \underline{V}$ ];

$$\rho_{mf}(\mu; x) = \rho_0[\underline{V} - V(x)] \quad \text{if } \mu > a\rho_{c,ext} + \underline{V}.$$

Therefore, as soon as the mean density  $\rho$  exceeds the value  $\rho_{c,ext}$ , the local densities at points  $x$  with  $V(x) > \underline{V}$  saturate, and any newly added particles tend to sit in the minimum of the potential. This is in shrill contrast to the van der Waals limiting case where the local densities are *strictly monotonically increasing* functions of the mean density  $\rho$ . The difference between the mean-field approximation and the van der Waals limit can, however, easily be understood when one realizes that, in the first case, the interaction energy in some small box inside  $\Lambda_L$  is proportional to the total density of the system squared while, in the second case, it is proportional to the local density squared.

## ACKNOWLEDGMENTS

One of us (Ph. de S.) would like to thank the Joint Institute for Nuclear Research, Dubna, for its hospitality, as well as the Belgian National Fonds voor Wetenschappelijk Onderzoek for its financial support.

## APPENDIX

In this Appendix we present the proof of statement (24). The idea of this proof is basically already present in, e.g., Refs. 13 and 14. Choose some  $\mu_0$  and  $\lambda_0$  and assume that  $\mu < \mu_0$ ,  $0 < \lambda < \lambda_0$ . Denote by  $K^L(x)$  the distribution function

$$K^L(x) = \frac{\sum_{\{n \mid n/L^v \leq x\}} (\exp \beta \mu n) [\text{Tr}_{\mathcal{H}_n^L} \exp(-\beta \bar{H}_{L,\lambda}^\infty)]}{\exp[\beta L^v \bar{p}_{L,\lambda}^\infty(\mu)]}.$$

Then

$$\exp[\beta L^v f_{L,\lambda}^M(\mu)] = \exp[\beta L^v \bar{p}_{L,\lambda}^\infty(\mu)] \left[ 1 - \int_{(M,\infty)} K^L(dx) \right]. \quad (\text{A1})$$

Now choose any  $c > 0$ . Clearly,

$$\begin{aligned} & \int_{(M,\infty)} K^L(dx) \\ & \leq \exp(-\beta c M L^v) \int_{(0,\infty)} \exp(\beta c L^v x) K^L(dx) \\ & = \exp \left[ c \beta L^v \left[ -M + \frac{\bar{p}_{L,\lambda}^\infty(\mu + c) - \bar{p}_{L,\lambda}^\infty(\mu)}{c} \right] \right]. \end{aligned}$$

But

$$0 \leq \bar{p}_{L,\lambda}^\infty(\mu + c) \leq \bar{p}_{L,a(1-\epsilon)}^\infty(\mu_0 + c + \lambda_0^v U(0)),$$

where we have used (13) (take  $L$  large enough) and the fact that the pressure is an increasing function of  $\mu$ .

Now choose

$$M > \min_c \frac{\bar{p}_{a(1-\epsilon)}^\infty(\mu_0 + c + \lambda_0^v U(0))}{c}.$$

It is then easy to prove that for all  $0 < \lambda < \lambda_0$ ,  $\mu < \mu_0$ ,

$$\lim_{L \rightarrow \infty} \frac{1}{\beta L^v} \ln \left[ 1 - \int_{(M,\infty)} K^L(dx) \right] = 0,$$

which together with (28) proves the statement (24).

<sup>1</sup>M. van den Berg and J. T. Lewis, *Commun. Math. Phys.* **81**, 475 (1981).

<sup>2</sup>M. van den Berg, J. T. Lewis, and J. V. Pulè, *Helv. Phys. Acta* **59**, 1271 (1986).

<sup>3</sup>P. C. Hohenberg, *Phys. Rev.* **158**, 383 (1967).

<sup>4</sup>M. Bouziane and Ph. A. Martin, *J. Math. Phys.* **17**, 1848 (1976).

<sup>5</sup>J. T. Lewis, J. V. Pulè, and Ph. de Smedt (unpublished); J. T. Lewis, *Statistical Mechanics and Field Theory: Mathematical Aspects Proceedings, Groningen, 1985*, Vol. 257 of *Lecture*

*Notes in Physics*, edited by T. C. Dorlas, N. M. Hugenholtz, and M. Winnink (Springer, New York, 1986).

<sup>6</sup>V. V. Papoyan and V. A. Zagrebnoy, *Phys. Lett.* **113A**, 8 (1985).

<sup>7</sup>Ph. de Smedt, *J. Stat. Phys.* **45**, 201 (1986).

<sup>8</sup>J. Lebowitz and O. Penrose, *J. Math. Phys.* **7**, 98 (1966).

<sup>9</sup>E. Lieb, *J. Math. Phys.* **7**, 1016 (1966).

<sup>10</sup>D. W. Robinson, *The Thermodynamic Pressure in Quantum Statistical Mechanics*, Vol. 9 of *Lecture Notes in Physics* (Springer-Verlag, New York, 1971).

- <sup>11</sup>M. van den Berg, J. T. Lewis, and Ph. de Smedt, *J. Stat. Phys.* **37**, 697 (1984).
- <sup>12</sup>J. T. Lewis, J. V. Pulè, and Ph. de Smedt, *J. Stat. Phys.* **35**, 381 (1984).
- <sup>13</sup>R. M. Ziff, G. E. Uhlenbeck, and M. Kac, *Phys. Rep.* **32**, 169 (1977).
- <sup>14</sup>J. T. Lewis and J. V. Pulè, *Stochastic Analysis and Applications: Proceedings, Swonsea (1983)*, Vol. 1095 of *Lecture Notes in Mathematics*, edited by A. Trumann and D. Williams (Springer-Verlag, New York, 1984), p. 25.