PROBLEMS OF STATISTICAL PHYSICS IN STRONGLY ELONGATED BODIES

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Abstract

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PROBLEMS OF STATISTICAL PHYSICS IN STRONGLY ELONGATED BODIES

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In a number of works (see, for example, ([1,2])) the following fact was noted: in an ideal Bose gas enclosed in a strongly elongated box (for example, if the sides of the box are related by $L_2 = L_3 = e^{\gamma L_1}$, $\gamma > 0$, and $L_1 \to \infty$), Bose condensation occurs at a temperature lower than the usual critical temperature T_c (in other words, at a temperature $T < T_c$ it may happen that the ratio of the number n_0 of particles in the ground level to the volume V tends to zero as $V \to \infty$). From this fact the conclusion is drawn that in strongly elongated samples (films and threads) superfluidity and superconductivity set in at lower temperatures than in cubic ones ([1,2]). Such reasoning is at least doubtful.

First of all, one can prove that for an ideal Bose gas enclosed in a box with sides $L_1 \leq L_2 \leq L_3$, the limit of all thermodynamic functions as $L_1 \to \infty$ will be the same as for a cubic box. In particular, the phase-transition temperature, determined from thermodynamic functions (for example, from the jump $\partial C_v/\partial T$), does not depend on the manner in which the volume of the box tends to infinity. The same can be said of correlation functions; in particular, the momentum density, for any manner in which the sides of the box tend to infinity, is, as usual, equal in the limit to $\rho_0\delta(\mathbf{k}) + \rho_1$, with the only difference that ρ_0 is no longer equal to $\lim n_0/V$. Visually one may say that when $L_1 \ll L_3$, other levels lie very close to the ground level, and condensation occurs not at the ground level but around it. More precisely, for $T < T_c$ a macroscopic number of particles have momenta lying in a sphere of radius ε, where $\varepsilon \to 0$ as $L_1 \to \infty$. Namely, if by $N(\varepsilon)$ we denote the number of particles with momenta $\leq \varepsilon$ and define ε_0 by the equality $N(\varepsilon_0) = \nu V$, then for $\nu < \rho_0$

$$\varepsilon_0 = \sqrt{\alpha}\,\rho^{1/3} \exp\left[-c\alpha^{-1}(1-\alpha^{3/2})\rho^{1/3}L_1\right] \quad \text{for } L_1 \ll L_2 = L_3 \text{ (film)}; \qquad (1)$$

$$\varepsilon_0 = c\alpha/(1-\alpha^{3/2})\rho^{1/3}L_1^2 \quad \text{for } L_1 = L_2 \ll L_3 \text{ (thread)};$$

here $\alpha = T/T_c$, and c is contained between positive constants depending only on ν.

The inverse quantity ε_0^{-1} has the meaning of a correlation length in the direction of the side L_3. We see that, although the correlation length tends to infinity as $L_1 \to \infty$, it may be $\ll L_3$ (which is equivalent to the absence of condensation at the ground level).

Let us outline proofs of some of the facts listed above.

Let $T < T_c$ and

$$\rho_0 = \rho - \int d^3k\, n(\mathbf{k}^2, 0),$$

where

$$n(\mathbf{k}^2, \mu) = \left[\exp\{h^2\mathbf{k}^2/2mT - \mu/T\} - 1\right]^{-1}.$$

Since μV tends to zero no faster than $1/V$ as $L_1 \to \infty$, in the case $L_2 = L_3 \geq \exp(\gamma L_1)$, $\gamma > 0$, representing $N(\varepsilon)/V$ in the form

$$\frac{N(\varepsilon)}{V} = \frac{1}{V} n(0, \mu_V) + \frac{1}{V} \sum_{\substack{k_1=0,\ \mathbf{k}^2\neq 0 \\ |\mathbf{k}|<\varepsilon}} n(\mathbf{k}^2, \mu_V) + \frac{1}{V} \sum_{\substack{k_1\neq 0 \\ |\mathbf{k}|<\varepsilon}} n(\mathbf{k}^2, \mu_V),$$

one can show that in the limit $L_1 \to \infty$

$$\frac{N(\varepsilon)}{V} = \frac{1}{V} n(0, \mu_V) + \frac{1}{L_1} \int_{|\mathbf{k}|<\varepsilon} d^2k\, n(k^2, \mu_V) + \int_{|\mathbf{k}|<\varepsilon} d^3k\, n(k^2, \mu_V) + O\left(\frac{1}{L_1}\right).$$

To estimate the error in replacing sums by integrals, multiple sums are represented as repeated sums, and for single sums one uses the estimate

$$\left| \sum_{m+1}^{p} f(x) - \int_m^p f(x)\, dx \right| < f(m) - f(p),$$

valid for a monotonically decreasing function $f(x)$.

Taking the double integral and noting that

$$\frac{n(0, \mu_V)}{V} + \frac{2\pi mT}{L_1 h^2} \left| \ln\left(1 - \exp\left(\frac{\mu_V}{T}\right)\right) \right| = \rho_0 + O\left(\frac{1}{L_1}\right),$$

we obtain

$$\frac{N(\varepsilon)}{V} = \rho_0 + \int_{|\mathbf{k}|<\varepsilon} d^3k\, n(k^2, 0) - \frac{2\pi mT}{L_1 h^2} \left| \ln \left(1 - \exp\left[-\frac{h^2\varepsilon^2}{2mT} + \frac{\mu_V}{T} \right] \right) \right| + O\left(\frac{1}{L_1}\right). \tag{2}$$

From (2) it is clear that

$$\lim_{L_1\to\infty} \frac{N(\varepsilon)}{V} = \rho_0 + \int_{|\mathbf{k}|<\varepsilon} d^3k\, n(k^2, 0),$$

which coincides with the case of a cubic box. Formula (2) also yields expression (1) for ε_0. The case $L_1 = L_2 \ll L_3$ is analogous.

As an example of proving the assertion about thermodynamic functions, let us carry it out for the heat capacity

$$C_V = \frac{1}{VT^2} \sum_{\mathbf{k}} f(\mathbf{k}^2, -\mu_V) \exp\left(-\frac{\mu_V}{T}\right),$$

where

$$f(\mathbf{k}^2, \varepsilon) = \left[\frac{(hk)^4}{4m^2} + \frac{(hk)^2}{2m}\varepsilon \right] \frac{\exp(h^2k^2/2mT)}{\left[\exp\{h^2k^2/2mT + \varepsilon/T\} - 1\right]^2}.$$

For $T < T_c$, for any $\varepsilon > 0$ there exists V_0 such that for $V > V_0$

$$\frac{1}{VT^2} \sum_{\mathbf{k}} f(\mathbf{k}^2, \varepsilon) < C_V < \frac{1}{VT^2} \sum_{\mathbf{k}} f(\mathbf{k}^2, 0) + M \left[\exp\left(-\frac{\mu_V}{T}\right) - 1 \right], \tag{3}$$

where

$$M = \frac{1}{VT^2} \sum_{\mathbf{k}} f(\mathbf{k}^2, 0) < \infty.$$

Taking the limiting transitions in (3), first $L_1 \to \infty$ and then $\varepsilon \to 0$, it is easy to see that $\lim_{L_1\to\infty} C_V$ will always be the same as for a cubic box.

For a nonideal Bose or Fermi gas with finite radius of interaction, one can show that the limit F of the free-energy density

$$F_V = \frac{1}{V} T \ln \mathrm{Sp} \exp\left(-\frac{H}{T}\right)$$

in a box of volume V, as the dimensions of the box tend to infinity, does not depend on the manner of approach.

An analogous assertion can also be proved for correlation functions, if they are defined with the aid of Bogolyubov "quasiaverages." Thus, for macroscopic samples of elongated shape, the density of free energy may be regarded as the same as for cubic samples. However, since the chief interest is in thin films and filaments, in which a lowering of the critical temperature may occur because of the violation of the macroscopicity condition, it is of interest to estimate

rate of convergence of F_V to F. It can be shown that $F_V - F \to 0$ as $V \to \infty$ as $1/L_1$.

For lattice models of statistical physics one can give the following estimate. If the Hamiltonian has the form

$$H = \sum_{m,n} \sum_{\mathbf{x},\mathbf{y}} H_{m,n}(\mathbf{x} \mid \mathbf{y}) a^+(x_1) \dots a^+(x_m) a(y_1) \dots a(y_n),$$

where $H_{m,n}(x_1, \dots, x_m \mid y_1, \dots, y_n)$ are translationally invariant functions of lattice points x_k, y_l, then

$$-\frac{12c}{L_1}|F| \le F_V - F \le \frac{3c}{L_1} \sum_{m,n} \sum_{\mathbf{x},\mathbf{y}} |H_{m,n}(\mathbf{x} \mid \mathbf{y})| \, |L_{m,n}(\mathbf{x} \mid \mathbf{y})|.$$

Here L_1 is the smallest side of the box, $L_1 \ge c$; $L_{m,n}(x_1, \dots, x_m \mid y_1, \dots, y_n)$ are correlation functions (i.e., statistical averages $\langle a^+(x_1) \dots a(y_n) \rangle$ in the limit of infinite volume); the summation is over $x_2, \dots, x_m, y_2, \dots, y_n$ running over the lattice (x_1 is fixed); c is the radius of interaction.

In proving this estimate it is convenient to use the formalism of L-functionals proposed by one of the authors (see ([5,6]); below we use the terminology and notation of those notes). Let Λ be a translationally invariant L-functional for which

$$\min(\bar{H}(L) - T\bar{S}(L))$$

is attained, where $\bar{H}(L)$ is the energy density of the functional L; $\bar{S}(L)$ is the density of its entropy; the minimum is taken over all translationally invariant L-functionals (as indicated in ([6]), $\min(\bar{H}(L) - T\bar{S}(L)) = F$; the functional Λ describes the equilibrium state in infinite volume). For the restriction Λ_V of the functional Λ to the parallelepiped V, one can prove that

$$\frac{1}{V} S(\Lambda_V) \ge \bar{S}(\Lambda),$$

and $\left|\bar{H}(\Lambda) - \frac{1}{V} H_V(\Lambda_V)\right|$ is easily estimated. Since

$$F_V \le \frac{1}{V}(H_V(\Lambda_V) - TS(\Lambda_V)),$$

we obtain an upper estimate for F_V. If the equilibrium state in the parallelepiped V, specified by the inequalities $0 \le x_i < L_i$, corresponds to the L-functional

M, then in the parallelepiped V_1, defined by the relations $-c \leq x_i < L_i + c$, we construct an L-functional M_1 as the product of the functional M on V and the unit functional on $V_1 \setminus V$. Next we divide the lattice into parallelepipeds W_α obtained by parallel translation of V_1; in each of the W_α we define an L-functional by translating the functional M_1 in parallel, and consider the product N of all these L-functionals. Using the fact that

$$F \leq \bar{H}(N) - T\bar{S}(N) \leq \frac{L_1 \ldots L_\nu}{(L_1 + 2c) \ldots (L_\nu + 2c)} (H_V(M) - TS(M)),$$

we obtain an upper estimate for F.

The statements formulated above do not completely prove the independence of the temperature of the onset of superfluidity and superconductivity from the shape of the box, since these phenomena are determined by the spectrum of elementary excitations. The question of the independence of the spectrum of elementary excitations from the degree of elongation of the box remains open in the general case; however, for the model Hamiltonian considered by Luban ([4]), it can be verified that the spectrum of elementary excitations calculated with the help of the ideology of "quasiaverages" (i.e., by introducing into the Hamiltonian an infinitely small perturbation $(\nu a_0 + \nu^* a_0^+)\sqrt{V}$) does not depend on the way in which the dimensions of the box tend to infinity.

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Note: Figure translations are in progress. See original paper for figures.