Hard-Sphere Bose Gas in Random External Potentials

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We consider a dilute hard-sphere Bose gas in random external potentials at low temperatures, in $D=3$, using the technique of pseudopotentials and the Bogliubov transformation. At absolute zero, the random potentials can deplete the Bose condensate, though not completely. On the other hand, they generate an amount of normal fluid equal to $\frac{4}{3}$ the condensate depletion. This is a localization effect that can destroy superfluidity at absolute zero. General features of the superfluid density in the neighborhood of this transition point agree qualitatively with experimental results on helium in porous media.

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We report on some results concerning the low-temperature properties of a dilute hard-sphere Bose gas in random external potentials in three dimensions. Such a model is a crude simulation of superfluid helium in porous media [1]. The spongelike media are here idealized as random distributions of hard-sphere potentials. To make the problem tractable, we further assume that the randomness is sufficiently dilute, and the temperature sufficiently low, that the hard spheres can be approximated by delta-function pseudopotentials [2]. We also assume that the potentials are distributed with uncorrelated randomness. Thus, the very large pores that are apparently present in the experimental media are not taken into account here. The purpose of this study is not to construct a quantitative model for the experiments, but to illuminate some qualitative features. We are able to show, for example, that at absolute zero superfluidity can be destroyed by the randomness, through an effect suggestive of boson localization.

From a theoretical point of view, the interparticle interactions are necessary to prevent a total condensation into a single localized orbital in the external potential. Thus, unlike the much-studied case of fermions, one does not have the luxury of treating the potentials as perturbations on a free-particle Hamiltonian. Here we do the next best thing, namely, start with the simplest soluble problem involving interparticle interactions—a dilute hard-sphere gas at low temperatures [2,3]. This approach differs from previous efforts on this subject [4,5], in that ours is a microscopic low-density low-temperature model, rather than a phenomenological "tight-binding" model. It may illuminate the problem from a different angle.

We consider a grand ensemble with chemical potential μ, with Hamiltonian H given by (with $\hbar=1$)

$$H-\mu N=\int d^3x\,\psi^\dagger[-(1/2m)\nabla^2-\mu+U]\psi+\tfrac{1}{2}v_0\int d^3x\,\psi^\dagger\psi^\dagger\psi\psi\,, \tag{1}$$

where $\psi(x)$ is the field operator for nonrelativistic boson of mass m, $N=\int d^3x\,\psi^\dagger\psi$ is the number operator, $U(x)$ is the external potential, and $v_0=4\pi a/m$, where a is the hard-sphere diameter. The ground-state energy is rendered finite by subtracting an appropriate divergent constant [3].

The external potential $U(x)$ may be pictured as a sum of randomly located scattering centers of random strengths, either attractive or repulsive. We assume $\langle U(x)U(y)\rangle_{\rm av}\propto\delta^3(x-y)$, and characterize the potentials by a single parameter R_0,

$$V^{-1}\langle|U_k|^2\rangle_{\rm av}=R_0\,, \tag{2}$$

where V is the total volume of the system, U_k is the Fourier transform of $U(x)$, and the subscript av denotes a quenched average over potentials. It has dimension (energy)^2(length)^3, and is (average density)×(mean-square strength) of the individual scatterers, the strength being measured by the spatial integral of the potential. Keeping R_0 fixed while varying the density of the bosons is like varying the coverage of the liquid helium in a porous medium.

Proceeding in a standard fashion [3], we introduce free-particle annihilation and creation operators a_k and $a_k^\dagger$, and assume the single level with $k=0$ is macroscopically occupied, with occupation number N_0. We refer to $n_0=N_0/V$ as the condensate density. In the expansion of H in terms of a_k and $a_k^\dagger$, we neglect all off-diagonal terms except those of the forms $v_0a_0^\dagger a_0^\dagger a_ka_k$ and $U_ka_0^\dagger a_k$, and their Hermitian conjugates. We then replace all occurrences of a_0 and $a_0^\dagger$ by the c number $N_0^{1/2}$. Thus, the only processes considered are the annihilation of a pair $\{k,-k\}$ into the condensate through the hard-sphere interaction, the scattering of a single particle k into the condensate by the random potentials, and the corresponding inverse processes. The effective Hamiltonian is

$$H_{\rm eff}-\mu N=V(-\mu n_0+\tfrac{1}{2}v_0n_0^2)+\sum_{k\neq 0}\left(\frac{k^2}{2m}-\mu+2v_0n_0\right)a_k^\dagger a_k$$
$$+\left(\frac{n_0}{V}\right)^{1/2}\sum_{k\neq 0}(U_ka_k^\dagger+U_{-k}a_k)+\tfrac{1}{2}v_0n_0\sum_{k\neq 0}(a_ka_{-k}+a_k^\dagger a_{-k}^\dagger)+\frac{v_0}{V}\left[\sum_{k\neq 0}a_k^\dagger a_k\right]^2. \quad (3)$$

The last term is important when the condensate becomes depleted. We treat it in a mean-field fashion by making the replacement

$$\frac{1}{V}\left[\sum_{k\neq 0}a_k^\dagger a_k\right]^2\to n'\sum_{k\neq 0}a_k^\dagger a_k\,, \quad (4)$$

where n' is a parameter to be determined later. The small parameters in our perturbation theory are a and R_0.

The effective Hamiltonian is diagonalized by a Bogoliubov transformation

$$a_k=\frac{c_k-\alpha_kc_{-k}^\dagger}{(1-\alpha_k^2)^{1/2}}-\frac{1}{\omega_k}\left(\frac{n_0U_k}{V}\frac{1-\alpha_k}{1+\alpha_k}\right)^{1/2}, \quad (5)$$

where

$$\alpha_k=1+x-\sqrt{x(x+2)},\quad \omega_k=v_0n_0\sqrt{x(x+2)}\,,$$
$$x=\frac{k^2}{2mn_0v_0}+\Delta,\quad \Delta=\frac{v_0(n_0+n')-\mu}{v_0n_0}. \quad (6)$$

We set $\Delta=0$, to ensure that the quasiparticle spectrum ω_k has no energy gap, in conformity with general theorems [6]. This condition determines n'. The diagonalized quench-averaged Hamiltonian has the form

$$H_{\rm eff}-\mu N=V(-\mu n_0+\epsilon_0)+\sum_{k\neq 0}\omega_kc_k^\dagger c_k\,,$$
$$\epsilon_0=\frac{2\pi an_0^2}{m}\left[1+\frac{128}{15\sqrt{\pi}}(n_0a^3)^{1/2}\right]+\frac{2-\sqrt{2}}{\sqrt{\pi}}mn_0^{3/2}a^{1/2}R_0. \quad (7)$$

The first term recovers well-known results [3].

The grand partition function $Q=\mathrm{Tr}\exp[-\beta(H-\mu N)]$ is a sum over N_0, but we keep only the largest term. Thus, μ and N_0 are determined by the two conditions [7]

$$\frac{\partial}{\partial n_0}\frac{\ln Q}{V}=0,\quad n=n_0+\frac{1}{V}\sum_{k\neq 0}\langle a_k^\dagger a_k\rangle\,, \quad (8)$$

where n is the particle density and $\langle\ \rangle$ denotes grand ensemble average. From these conditions we can obtain n' and n_0 as functions of n and the temperature.

The average number of particles with nonzero momentum represents a depletion of the condensate

$$\frac{1}{V}\sum_{k\neq 0}\langle a_k^\dagger a_k\rangle=n_1+n_R\,,$$
$$n_1=\frac{8\sqrt{\pi}}{3}(n_0a)^{3/2}+\frac{4}{\sqrt{\pi}\lambda^3}\int_0^\infty dt\frac{t^2(t+\theta/2)}{(t^2+\theta)^{1/2}\{\exp[t(t^2+\theta)^{1/2}]-1\}}\,,$$
$$n_R=\frac{m^2}{8\pi^{3/2}}\left(\frac{n_0}{a}\right)^{1/2}R_0\,,$$
$$\lambda=\sqrt{2\pi\beta/m},\quad \theta=2\beta v_0n_0\,, \quad (9)$$

where n_1 arises from the hard-sphere interactions [3,7]. It is very small at absolute zero, and rises quadratically with increasing temperature. The term n_R corresponds to condensate depletion due to scattering of condensate particles with the random potentials. The fractional depletion is of the order of $m^2R_0/\sqrt{na}$. The factor $1/\sqrt{a}$ underscores the fact that the system would collapse if there were no interparticle interactions. The depletion can be substantial within the validity of our approximations. On the other hand, there cannot be total depletion, for $n_0=0$ is not a possible solution at absolute zero, for any finite R_0. (See below.)

The superfluid density n_s is obtained by considering the response of the momentum density to an externally imposed velocity field [8,9]. The relevant response function is

$$R^{ij}(x,t)=\langle[g^i(x,t),g^j(0,0)]\rangle$$
$$=\int\frac{d^3k\,d\omega}{(2\pi)^4}e^{i(k\cdot x-\omega t)}R^{ij}(k,\omega)\,, \quad (10)$$
$$g^j(x,t)=(2i)^{-1}\psi^\dagger(x,t)\overleftrightarrow{\partial}^j\psi(x,t)\,,$$

where $\psi(x,t)$ is a Heisenberg operator. The static susceptibility is given by

$$\chi^{ij}(k)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{R^{ij}(k,\omega)}{\omega-i\epsilon}$$
$$\equiv\frac{k^ik^j}{k^2}A(k^2)+\left(\delta_{ij}-\frac{k^ik^j}{k^2}\right)B(k^2). \quad (11)$$

The transverse susceptibility $B(0)$ is the normal fluid mass density. The superfluid mass density is accordingly $\rho_s=\rho-B(0)$, where ρ is the total mass density.

Using particle conservation, one can show that $A(0)=\rho$, which is a form of the f-sum rule. Thus one sometimes writes $\rho_s = A(0) - B(0)$. However, this is not valid for the present calculation, because particle conservation was violated in replacing a_0 by a c number. We have in effect truncated the Hilbert space, leaving out the subspace spanned by single-particle states of zero momentum. Thus, computations involving the time evolution of zero-momentum particle states would be falsified. On the other hand, the nonzero momentum sector should be unaffected (as long as second-order effects of the zero-momentum states are unimportant). In the present context, this means that we can trust a calculation of $B(0)$ but not $A(0)$. Accordingly, we calculate the superfluid density through $\rho - B(0)$, and not $A(0) - B(0)$ [10].

The calculation of $B(0)$ is quite tedious. The superfluid density $n_s = \rho_s/m$ is found to be

$$\begin{aligned} n_s &= n - n_2 - \tfrac{4}{3} n_R, \\ n_2 &= -\frac{1}{3m}\int \frac{d^3p}{(2\pi)^3} p^2 \frac{\partial n_p}{\partial \omega_p} \\ &= \frac{8}{3\sqrt{\pi}\lambda^3}\int_0^\infty dt \frac{t^4 \exp[-t(t^2+\theta)^{1/2}]}{\{1-\exp[-t(t^2+\theta)^{1/2}]\}^2}, \end{aligned} \tag{12}$$

where $n_p = [\exp(\beta\omega_p) - 1]^{-1}$ is the average number of phonons. There is an elementary derivation of n_2 based on Gallilean invariance in the absence of random potentials [11], but we know of no intuitive way to obtain the term $4n_R/3$. The factor $\frac{4}{3}$ indicates that the random potentials generate more normal fluid than they took from the condensate. This makes it possible to destroy superfluidity at absolute zero. To see this, note that from $n_R = n - n_0 - n_1$ and $n_s = n - \frac{4}{3} n_R$, we have

$$n_s = \tfrac{1}{3}[4(n_0 + n_1) - n], \tag{13}$$

which vanishes when the condensate is roughly $\frac{3}{4}$ depleted by the random potentials. This result means that part of the condensate, which is made up of zero-momentum particles, belongs to the normal fluid, i.e., they are dragged along by the random potentials. This indicates localization, or formation of bound states of macroscopic extensions.

We can obtain n_0 at low temperatures ($T \to 0$) from (8) by iteration. Using this result, we then calculate n_s as a function of n and T. Neglecting a term of order $(na^3)^{1/2}$ for simplicity, we have

$$\begin{aligned} \frac{n_0}{n} &\approx e^{-2\phi} - \frac{1}{\cosh\phi}\left[\frac{T}{T_1}\right]^2 + \frac{K_1(\phi)}{(na^3)^{1/2}}\left[\frac{T}{T_1}\right]^4, \\ \frac{n_s}{n} &\approx \tfrac{1}{3}(4e^{-2\phi} - 1) + \tfrac{4}{3} e^{\phi}\tanh\phi\left[\frac{T}{T_1}\right]^2 \\ &\quad - \frac{K_2(\phi)}{(na^3)^{1/2}}\left[\frac{T}{T_1}\right]^4, \end{aligned} \tag{14}$$

where

$$\begin{aligned} \sinh\phi &= \frac{m^2 R_0}{16\pi^{3/2}\sqrt{na}}, \\ T_1 &= \sqrt{3/2}\,\pi^{-5/4} m^{-1} n^{3/4} a^{1/4}, \\ K_1(\phi) &= \frac{3}{1280}\frac{e^{4\phi}}{\sqrt{2\pi}}, \\ K_2(\phi) &= \frac{e^{5\phi}}{16\pi^{9/2}}\left[1 + \frac{\pi^4}{20\sqrt{2}}\tanh\phi\right]. \end{aligned} \tag{15}$$

At $T=0$, n_0 never vanishes. On the other hand, $n_s = 0$ at $\phi = \ln\frac{4}{2}$, which corresponds to a critical density n_c given by $n_c a^3 = (m^2 a R_0)^2/36\pi^3$. This value lies within the regions of validity of our approximation.

Figure 1 shows a 3D plot of n_s as given by (14), for certain values of a and R_0. The surface has a nose shape, which describes a kind of "reentrant" behavior. Generally, n_s rises quadratically with T, goes through a maximum, and then vanishes linearly at a critical temperature, which is roughly given by $T_c \propto an/m$, except near the tip of the "nose." The critical index is thus the same as that for the ideal Bose gas. This is in agreement with experimental results on liquid helium in porous media. But the nonmonotonic behavior of n_s has not been detected so far.

It may seem curious that n_s initially increases with T. We have to remember, however, that n_s is strongly suppressed by the random potentials at $T=0$. As T starts to increase, the suppression is lessened, because less normal fluid is generated by the random potentials, due to the fact that n_0 decreases.

Going back to (8), we can study the thermodynamic behavior near $n_0 = 0$, i.e., the Bose-Einstein transition point of the ideal gas. In this region our model is similar to a soluble one [12], in which ω_k is replaced by $k^2/2m$.

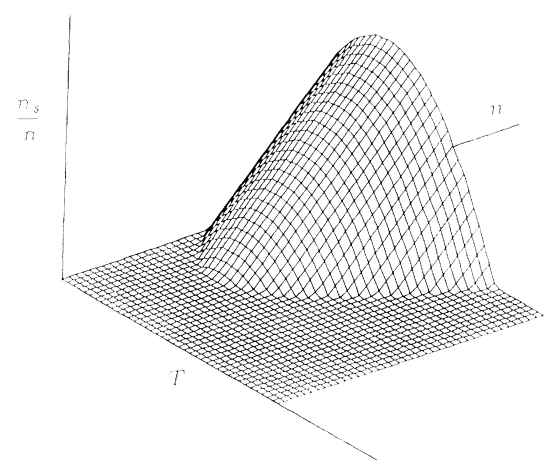

FIG. 1. Superfluid density as function of temperature and density, in the neighborhood of the superfluid transition point at absolute zero.

The isotherms are of the van der Waals type, exhibiting first-order phase transitions, with a very narrow transition region, of order $(na^3)^{1/2}$. The presence of random potentials does not change the qualitative behavior. Because scattering between quasiparticles has been neglected, however, the model cannot be taken seriously in this domain.

In regard to low-temperature phase transitions, our theory is of the mean-field type, because all fluctuations in the condensate have been ignored. In this approximation, the condensate cannot react to the destruction of superfluidity. For this reason, no specific heat singularities appear at the transition point, and the condensate remains structureless in the region $n < n_c$, the so-called "Bose glass" phase. These inadequacies can be remedied only by improving on the Bogoliubov transformation, which we are attempting to do.

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