spectrum for an imperfect Bose gas, namely[12]

$$\epsilon(p)=\left[\left(\frac{p^2}{2m}\right)^2+\tfrac{1}{2}\Lambda\left(\frac{\hbar}{ma}\right)^2p^2\frac{\sin(pa/\hbar)}{pa/\hbar}\right]^{1/2}, \quad (11)$$

where Λ is a monotonically increasing function of the density of the system and is determined by the implicit relationship

$$\frac{4\pi^2\rho a^3}{m}=\Lambda\int_0^\infty\frac{x\sin^2x}{x^3+\Lambda\sin x}\,dx, \quad (12)$$

and expresses it in the form (1), one obtains

$$c=(\tfrac{1}{2}\Lambda)^{1/2}\hbar/ma, \quad \gamma=\tfrac{1}{12}(a/\hbar)^2(1-3/\Lambda). \quad (13)$$

At low densities, where $\Lambda\simeq 8\pi\rho a^3/m\ll 1$, one obtains the Bogoliubov expressions[17]

$$c\simeq(4\pi\rho a\hbar^2/m^3)^{1/2}, \quad \gamma\simeq -m/32\pi\rho a\hbar^2. \quad (14)$$

Equations (12)-(14) display the same qualitative trend for γ as the empirical values do. Of course, the density at which the zero of γ occurs is much smaller than the one encountered in liquid helium nevertheless, the appearance of a γ which is negative at low densities and becomes positive at higher densities is strongly suggestive of the possibility that an improved theory of elementary excitations in a Bose liquid may explain the observed behavior of γ quantitatively as well.

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Phase Diagram of a Charged Bose Gas

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The phase diagram of a charged Bose gas is drawn. We discuss the domains of existence of the solid, fluid, and superfluid phases. It is predicted that superdense helium can be superfluid at densities higher than 10^6 g/cm^3.

The purpose of this note is to draw the phase diagram of a system of charged bosons of mass m and charge e; embedded in a uniform background of opposite charge which ensures overall electrical neutrality. This model might be of astrophysical interest.[1] In a white dwarf or in the outer layers of a neutron star, the atoms are pressure ionized, and the electrons form a very inert[2] uniform Fermi sea; if the nuclei are bosons, as it is the case for instance for helium, we do have a charged Bose gas in a uniform background. The density-temperature diagram that we obtain is drawn in Fig. 1, and will now be explained.

When classical statistical mechanics applies, there are two possible phases, fluid and solid. A simple dimensional argument[3] says that the transition between these phases occurs when the thermal energy kT is some well-defined fraction Γ^{-1} of a characteristic Coulomb energy $e^2/\bar{r}$ ($\bar{r}$

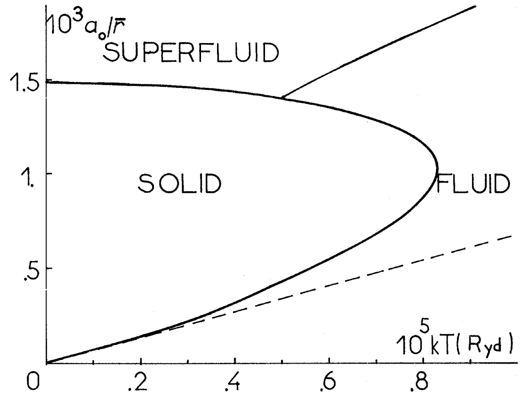

FIG. 1. Phase diagram of the charged Bose gas in the density-temperature plane. The inverse ionic sphere radius $\bar{r}^{-1} = (4\pi/3)^{1/3}\rho^{1/3}$, in units of $(10^3 a_0)^{-1}$ (a_0 is the ionic Bohr radius), is drawn versus KT, in units of 10^{-5} ionic Ry. The solid curves separate the solid, fluid, and superfluid regions. The straight dashed line represents what the melting line would be if there were no quantum effects [Eq. (1)].

is a characteristic interparticle distance related to the number density ρ by $\rho = 3/4\pi\bar{r}^3$). It is easy to check that, along the melting line

$$\rho = (3/4\pi)(\Gamma kT/e^2)^3, \tag{1}$$

if ρ and T are small enough, the de Broglie wavelength $(2\pi\hbar^2/mkT)^{1/2}$ is negligible with respect to $\bar{r}$; therefore, classical statistical mechanics does apply, and the melting line actually follows (1) in the lower left region of the phase diagram. The constant Γ has been evaluated by computer experiments[3,4] and in the following we shall adopt the value $\Gamma = 140$ of Ref. 4. Although the transition is likely to be of first order, its width has been estimated to be extremely small,[4] and will henceforth be neglected.

If we go to higher densities, quantum effects become important. The state of the system depends on ρ only through the dimensionless variable $r_s = \bar{r}/a_0$ (a_0 is the ionic Bohr radius $\hbar^2/me^2$; for helium nuclei, $a_0 = 1.80 \times 10^{-13}$ cm). It is convenient to express all energies and temperatures in ionic rydbergs $\mathcal{R} = me^4/2\hbar^2$ (for helium nuclei, $\mathcal{R}$ corresponds to a temperature of 1.85×10^{10} °K). Let us first consider the zero-temperature case. As the density increases, the zero-point vibrations of the solid become more and more important, and ultimately the solid melts[5] (the system approaches an ideal Bose gas as the density goes to infinity and r_s goes to zero[6]). The density at which this "pressure melting" occurs, at zero temperature, will now be estimated by comparing the energies of the fluid and solid phases, both obtained by variational calculations.

For describing the fluid (which is actually a superfluid as will be shown below), we use a Bijl-Jastrow trial wave function,

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \exp[-\tfrac{1}{2} \sum_{i>j=1}^{N} u(|\vec{r}_i - \vec{r}_j|)], \tag{2}$$

and choose for $u(r)$ a simple form suggested by the theory of plasma oscillations. In terms of the collective coordinates

$$\rho_{\vec{k}} = \sum_{i=1}^{N} \exp(-i\vec{k}\cdot\vec{r}_i), \tag{3}$$

an approximate Hamiltonian, which describes the plasma oscillations in a volume Ω, is

$$H = \frac{1}{2\Omega} \sum_{\vec{k}\neq 0} \frac{m}{\rho k^2} (|\dot{\rho}_{\vec{k}}|^2 + \omega^2 |\rho_{\vec{k}}|^2), \tag{4}$$

where $\omega = (4\pi e^2\rho/m)^{1/2}$ is the plasma frequency; the term $\vec{k} = 0$ is excluded since the average density is a fixed quantity. The ground state of H is

$$\Psi = \exp\left(-\frac{1}{2\Omega} \sum_{\vec{k}\neq 0} \frac{m\omega}{\hbar\rho k^2} |\rho_{\vec{k}}|^2\right), \tag{5}$$

which is of the form (2) with

$$u(r) = \frac{a}{\Omega} \sum_{\vec{k}\neq 0} \frac{4\pi}{k^2} e^{i\vec{k}\cdot\vec{r}}, \tag{6}$$

$$a = m\omega/2\pi\hbar\rho = (me^2/\pi\hbar^2\rho)^{1/2}. \tag{7}$$

In the limit of an infinite system, $u(r)$ would just be a/r; since this is a long-ranged function, some care has to be exercised, and the infinite-system limit should not be taken too early. Since (4) is only an approximate Hamiltonian, we do not fix a at the value given by (7). Rather, from now on, we shall consider (2) and (6) as a reasonable trial wave function, where a is an adjustable parameter which is to be determined by minimizing the expectation value of the *exact* Hamiltonian. Through standard manipulations, the kinetic energy expectation value is easily shown to be

$$\left\langle \Psi \left| \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m}\right) \Delta_i \right| \Psi \right\rangle = N \frac{\pi\hbar^2 a\rho}{2m}. \tag{8}$$

The evaluation of the potential-energy expectation value requires no new numerical calculations, because if (5) is used, $|\Psi|^2$ is the *classical* statistical-mechanical distribution function of a system of charged particles of charge e', at a temperature T, such that $e'^2/kT = a$ (of course e' has nothing to do with the actual charge e of the bosons). Therefore, the expectation value of the potential energy is simply related to the average potential energy U_c of this classical charged gas,

$$\left\langle \Psi \left| \sum_{i>j=1}^{N} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \right| \Psi \right\rangle = \frac{e^2}{e'^2} U_c; \qquad (9)$$

the nice feature is that U_c has already been tabulated in former computer experiments[3,4] on the classical gas.[7] Minimizing the total energy (8) plus (9) with respect to a provides the energy of the fluid as a function of r_s. In the range $30 < r_s < 400$, the best a varies from a value of the order of that given by (7) to a value about 50% higher.

To describe the solid, we use a product of one-particle Gaussian wave-functions centered on the sites of a bcc lattice. Minimizing the energy with respect to the Gaussian width parameter gives for this energy E a value practically equal to the Einstein harmonic-solid result[8]

$$E = -1.792/r_s + 3/r_s^{3/2}, \qquad (10)$$

where the energy is in rydbergs.

We find that the fluid and solid energies as functions of r_s intersect at $r_s = 360$, or equivalently $\rho_m = 5.1 \times 10^{-9} a_0^{-3}$; this value ρ_m is the melting density at zero temperature. At this point, $E = -4.5 \times 10^{-3}$ Ry and $a = 29 r_s a_0$. The uncertainty in this melting density is hard to estimate since both the fluid and solid energies are variational results and lie very close to each other over a wide range of values of r_s. Two remarks can be made concerning the error introduced by the variational method: First, in the fluid phase, a comparison can be made with a previous variational calculation,[9] which used a two-parameter trial wave function more general than (6). Our energies lie above those of Ref. 9, as they should, but the relative energy gained by introducing the second parameter decreases from 25% at $r_s = 1$ to 10% at $r_s = 20$ and is likely to become very small in the transition region ($r_s \sim 400$). The second remark concerns the solid phase: There, an alternative to the use of the Hartree variational method is the use of quasiharmonic theory[10] which yields the following ground-state energy per particle:

$$E = -1.792/r_s + 2.66/r_s^{3/2}. \qquad (11)$$

Although, in the transition region, (11) and (10) are quite close, the sensitivity of the location of the transition density to the approximation used is such that, if (11) is used instead of (10), the melting value becomes $r_s = 120$ instead of 360. Since (11) is not necessarily an upper bound to the exact ground-state energy, whereas (10) is, we feel that it is somewhat more consistent to look for the intersection of the variational energy curve of the fluid phase with the variational energy (10) of the solid phase.

We have thus far obtained estimates of the melting density in the two extreme cases: the purely classical (low ρ, low T) region and the purely quantum ($T = 0$) region. In order to interpolate the melting line in the intermediate region, we make the following two approximations: (a) We assume the validity of Lindemann's melting criterion, which states that a solid melts whenever the rms displacement of particles from their equilibrium (i.e., lattice) positions reaches a certain fraction γ, independent of density and temperature, of the nearest-neighbor distance d [$d^2 = 3(\pi/3)^{2/3} r_s^2 a_0^2$ in the case of a bcc lattice]; (b) in order to calculate γ at each density and temperature, we use quasiharmonic theory. A justification for approximation (a) is the fact that, in the two extreme regions, the values of γ at melting are reasonably close. At $T = 0$, for $r_s = 360$, the quasiharmonic theory yields $\gamma = 0.2$, whereas in the classical region, for $\Gamma = 140$, an "exact" Monte Carlo calculation[4] yields $\gamma = 0.18$. As to approximation (b), its use is justified, at least in part, by the fact that, in the classical case, at melting ($\Gamma = 140$) the quasiharmonic theory[11] yields a value $\gamma = 0.17$ very close to the "exact" value 0.18. The constant value of γ which we finally choose to determine the whole melting line is the value $\gamma = 0.17$, yielded by quasiharmonic theory at melting in the classical limit; as a consequence of this choice, the zero-temperature melting density is shifted to $r_s = 670$.

Actually, we found it more convenient to replace the exact harmonic spectrum by a much simpler, isotropic, Debye-like spectrum which yields exact first, second, and fourth moments of the frequency distribution function.[12] This spectrum, which will be discussed in more detail elsewhere, greatly simplifies the computation of γ as a function of ρ and T, while yielding thermodynamic properties in excellent agreement with those obtained using the full harmonic spectrum.

The melting line, obtained by drawing the locus of points in the (p, T) plane for which $\gamma(p, T) = 0.17$, is shown in Fig. 1. The temperature beyond which no solid can exist, because the Lindemann ratio is always larger than the melting value 0.17, is 0.83×10^{-5} Ry (ionic), which corresponds to $2400AZ^4$ °K for nuclei of atomic mass A and atomic number Z. This maximum temperature is relatively sensitive to the value chosen for the critical Lindemann ratio. If the value $\gamma = 0.2$, which was found for the $T=0$ transition, were chosen, a maximum temperature 1.96×10^{-5} Ry would result.

It should be noted that a "closed" melting line of the type described here had already been proposed by Kirzhnits,[5] whose calculation was based on a crude Einstein oscillator model and the assumption that melting occurs whenever the ratio of potential energy over kinetic energy is of order 1. However, this criterion is too crude a picture for a charged Bose gas because the previous ratio is actually much larger (of order Γ), which explains why Kirzhnits's numerical predictions differ by several orders of magnitude from the present ones.

Finally, there must be a transition line between fluid and superfluid phases, since the system must be an ordinary fluid under classical conditions (i.e., when the temperature is high enough for a given density) and a superfluid at low temperature and high density[6]; incidentally, our trial Bijl-Jastrow wave function necessarily describes a superfluid.[13] The precise location of the fluid-superfluid transition line will require further work. Here, we have used the free-Bose-gas approximation $\rho = 2.612(mkT/2\pi\hbar^2)^{3/2}$. It can be guessed that the Coulomb interactions will not drastically displace the transition line (note that the strong interactions which exist in ordinary helium do not prevent the λ transition temperature from being of the same order of magnitude as the free-Bose-gas condensation temperature). The fluid-superfluid transition line intersects the melting line at a triple point, the coordinates of which are $r_s^{-1} = 1.4\times 10^{-3}$, $kT = 0.5\times 10^{-5}$ Ry.

In the case of helium nuclei, the maximum temperature at which the solid exists is 150 000°K. The triple point lies at $\rho_t = 0.75\times 10^6$ g/cm^3 and $T_t = 90\,000$°K, and the zero-temperature melting density is $\rho_m = 0.92\times 10^6$ g/cm^3. Therefore, the domain of the superfluid phase extends to lower densities than it had previously been estimated.[14]

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