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Speculations on Bose-Einstein Condensation and Quantum Crystals*

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It is shown, by almost rigorous arguments, that there exist many-body states of a system of interacting bosons which exhibit both crystalline order and Bose-Einstein condensation into the zero-momentum eigenstate of the single-particle density matrix. The implications of this result are discussed in relation to theories of superfluidity and the nature of quantum crystals.

I. INTRODUCTION

Little is known about the connection between Bose-Einstein condensation and superfluidity. It has, for example, been conjectured that Bose-Einstein condensation is sufficient to insure superfluidity and the converse has also been put forward as being plausible. In this paper, we shall be concerned with model states for a system of strongly interacting bosons. These states are all normalizable and symmetric and are thus possible states for such a system. We shall show – almost rigorously – that these model states can simultaneously exhibit both Bose-Einstein condensation and crystalline ordering. The presence of crystalline order would presumably prevent the appearance of any normal superfluid properties.

Given the existence of these model states the question arises whether they are, in some sense, sufficiently good approximations to the true states of a physical system that our conclusions are applicable to that system. For example, if one of our model states were a sufficiently good approximation to the ground state of solid helium four then we could conclude that the quantum crystal would possess a Bose-Einstein condensate . The physical applicability of our results is discussed in Sec. V.

Our "almost rigorous" proof is based on a theorem which is presented in Sec. II and on a conjecture which is put forward in Sec. III. In Sec. IV, we discuss the conclusions that can be drawn from the theorem and conjecture. Section V is devoted to generalizations and a discussion of the applicability of our conclusions to solid helium four.

II. THEOREM

The theorem we present has recently been proved by Reatto[1] and is a generalization of earlier work by Onsager and Penrose.[2] Consider N bosons in a volume V, then any Jastrow state

$$\psi_N = \prod_{i\neq j} f(r_{ij}) = \exp\Big[-\tfrac{1}{2}\sum_{i\neq j} u(r_{ij})\Big] , \qquad (2.1)$$

with $u(r)$ such that

$$u(r) = \infty , \quad r < a$$

$$u(r) > 0 , \quad a < r < b$$

$$\text{and} \quad |u(r)| < |Ar^{-3-\epsilon}|, r > b , \qquad (2.2)$$

with A, a, b, and ϵ positive constants, has a Bose-Einstein condensate in the zero-momentum state. These conditions on $u(r)$ imply that it has a hard core, is bounded below and has a finite range. The proof of this theorem is completely rigorous except that the thermodynamic limit of $[(N+1) \times Q_N/Q_{N+1}]$ is assumed to exist. Here Q_N is the normalization constant for Ψ_N. This limit can be formally identified as the activity of a classical system of N particles with a pair potential proportional to $u(r)$. It is almost universally accepted that this identification of the activity is indeed correct, and if this is granted, then the proof becomes completely rigorous.

The theorem can be extended to include states which have the zero-point motion of the long-wavelength density waves built into them.[3] When these correlations are included our model states have the form

$$\Psi_N = \prod_{i\neq j} f(r_{ij}) = \exp\Big[-\tfrac{1}{2}\sum_{i\neq j} u(r_{ij}) - \tfrac{1}{2}\sum_{i\neq j}\chi(r_{ij})\Big] , \qquad (2.3)$$

where $u(r)$ fulfills the same conditions as before and $\chi(r)$ is given by the equation

$$\chi(r) = (1/N)\sum_{k<k_c}{}' e^{i\vec{k}\cdot\vec{r}}\,\frac{2mc}{\hbar k} . \qquad (2.4)$$

The prime on the summation means that the $k=0$ term is omitted. Since $\chi(r)$ behaves like r^{-2} for large r we have added to $u(r)$ a long-range function. With the same proviso as we have already mentioned, it can be proved that this model state has a Bose-Einstein condensate. It is interesting to note that an alternative condition which allows both theorems to be proved is that the variational energy per particle should exist in the thermodynamic limit.[1]

III. CONJECTURE

The wave functions given by Eqs. (2.1) and (2.3) lead to probability distributions of the form

$$P_N = \Psi_N^2 = \exp[-\sum_{i\neq j} v(r_{ij})]\,, \qquad (3.1)$$

where $v(r_{ij})$ is either $u(r_{ij})$ or $u(r_{ij}) + \chi(r_{ij})$. If we introduce an effective potential $\varphi(r)$, an effective temperature T_{eff} and set $\varphi(r)/k_B T_{\text{eff}} = v(r)$ then this quantum-probability distribution is identical with the classical Gibbs distribution for N particles interacting with a two-body potential $\varphi(r)$ at a temperature T_{eff}. The conjecture we make is that, for a wide class of potentials $\varphi(r)$, or equivalently functions $v(r)$, the probability distribution P_N will exhibit crystalline ordering at sufficiently high densities and fluid ordering at low densities. We make this conjecture because it is widely accepted that the Gibbs distribution is in principle capable of describing all the phases of a single classical system. If $\varphi(r)$ were a typical intermolecular potential, for example a Lennard-Jones potential, then there is no reason to doubt that if the density of the system is increased sufficiently then a phase transition will take place to a crystalline state and this would be well described by the single Gibbs distribution. For a small number of particles ($\sim 10^3$), this has been demonstrated by machine calculations. There is also strong evidence[4] that a crystalline transition occurs with the $u(r)$ that is often used for helium work, namely, $u(r) = (b/r)^m$ with $m = 4$ or 5. We do not know exactly for which potentials $\varphi(r)$ crystallization will take place. It is, however, sufficient for the purposes of our discussion that there are some, but we see no reason not to believe that there are many. We finally comment on the presence of the long-range potential $\chi(r)$. The arguments[3] that lead to the introduction of this type of correlation are equally valid for the solid phase of helium and we would indeed expect the N-body probability distribution for the crystalline phase to have this factor. Consequently, we do not believe that it in any way affects the conjecture that this kind of probability distribution will exhibit crystalline ordering. It would be interesting to determine with computer experiments the range of potentials for which our conjecture is valid.

IV. CONCLUSIONS

If we combine the theorem we presented in Sec. II with the conjecture of Sec. III, then we conclude that Bose-Einstein condensation can occur in a state which exhibits crystalline ordering.

The theoretical implications of this result are twofold. First, it is certain that crystalline ordering would prevent the appearance of anything like normal superfluid properties and we can, therefore, conclude that the existence of a Bose-Einstein condensation is not sufficient to insure superfluidity. This is of course well known for the ideal Bose gas.[5] Our arguments extend this result to strongly interacting systems. Second, the presence of Bose-Einstein condensation with crystalline ordering tells us that the momentum distribution in such states is radically different from that in normal crystalline states.

Whether or not our arguments have any physical implications depends on how accurately our states represent real physical systems. We shall defer the discussion of this until Sec. V. For the moment we merely remark that there are good reasons to believe that these states – or simple generalizations of them – do give a reasonable description of real boson systems. If this is granted then we speculate that solid helium four may have a Bose condensate in the zero-momentum state. It is unlikely to occur in any other crystal because the phenomenon clearly requires large exchange effects and these are present only in solid helium. This kind of ordering is unlikely to set in without a phase transition and, thus, we are led to speculate that there might be an undetected phase transition in the solid phase of helium four. It is, unfortunately, impossible to say where in the solid phase the transition might take place. It cannot be along the exact continuation of the λ line in the liquid phase, as this would contradict the phase rule. It might indeed be suppressed to much lower temperatures in the solid phase.

V. GENERALIZATIONS AND DISCUSSION

The theorem and conjecture we have discussed was based on explicit two-particle correlations in our model states – although of course these explicit two-particle correlations lead to implicit many-particle correlations. The theorem can easily be generalized to states which include n-particle explicit correlations, provided suitable restrictions are placed on the effective potential function $u_n(r_1 \cdots r_n)$. These restrictions are essentially the same as one stated in Sec. II, namely, that u should have a hard core, and be bounded below and have a finite range. The introduction of n-particle effective potentials in the equivalent classical probability distribution will surely not affect our conclusion that it will exhibit crystalline order at high densities. The only circumstance in which this statement might be untrue is if the n-particle correlations completely dominated the two-particle correlations. Then we would be dealing with a very unusual equivalent classical system and would, consequently, be uncertain whether crystallization will take place. Apart from this possibility, our conclusions are valid for this much wider class of wave functions.

We now speculate that a wave function of this type will give an accurate description of the exact states of solid and liquid helium four. We make this statement because the arguments presented above allow us to include in the wave function as complicated explicit correlations as we like. It is of course true that there are other states one can envisage which do not satisfy our condition, for example, a linear combination of Jastrow states. Indeed, if no state in this wide class of model wave functions adequately describes the spatial correlations of a real-quantum crystal, then these correlations must be fundamentally different from those which occur in a classical crystal. For these reasons, we believe that our speculation about real physical systems are on much firmer grounds than would appear at first sight.

Finally, we comment on the proof by Onsager and Penrose[2] that a state with crystalline order cannot have a Bose-Einstein condensate in the zero-momentum state. This proof is based on a particular class of model states in which each particle is localized on a lattice site, each site is occupied by a particle and symmetry is ignored. If either of the latter restrictions is removed, then the original proof fails.[6] In particular, if there are vacancies in the model state and symmetry is ignored, then a condensate exists and this condensation would presumably persist if symmetry were taken into account. It is now interesting to note that we expect all the model states we have discussed to lead to crystalline order with vacancies present. This is because the equivalent classical system would be expected, on physical grounds, to lead to crystallization with a finite fraction of vacancies. We may therefore add one final speculation, namely, that a quantum crystal can only have a Bose-Einstein condensate if it has a finite fraction of vacancies. We see no reason, whatsoever, to suppose that a quantum crystal cannot have a finite fraction of vacancies at absolute zero. Liquid helium exists at absolute zero and this suggests that a crystal with a finite amount of spatial disorder could exist at absolute zero. If, on the other hand, a finite fraction of vacancies can only exist at elevated temperatures, then it might be impossible to have a Bose-Einstein condensate because of the high temperature. We pointed out in Sec. IV that it is almost impossible to predict the temperature at which such a condensation might occur.

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[1]L. Reatto, Phys. Rev. (to be published).

[2]O. Penrose and L. Onsager, Phys. Rev. 104, 576 (1956).

[3]L. Reatto and G. V. Chester, Phys. Rev. 155, 88 (1967).

[4]W. L. Macmillan, Phys. Rev. 138, A442 (1965).

[5]L. Landau, J. Phys. USSR V, 71 (1941).

[6]L. Reatto (private communication) has shown that a symmetrical state of this kind with vacancies has a Bose-Einstein condensate. This state thus provides us with an extremely simple example of a state with crystalline order and a Bose-Einstein condensate.