

Instability in a Two-Dimensional Dilute Interacting Bose System

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The formalism of Ursell operators provides a self-consistent integral equation for the one-particle reduced operator. In three dimensions this technique yields values of the shift in the Bose-Einstein condensation (BEC) transition temperature, as a function of the scattering length, that are in good agreement with those of Green's function and quantum Monte Carlo methods. We have applied the same equations to a uniform two-dimensional system and find that, as we alter the chemical potential, an instability develops so that the self-consistent equations no longer have a solution. This instability, which seems to indicate that interactions restore a transition, occurs at a non-zero value of an effective chemical potential. The non-linear equations are limited to temperatures greater than or equal to T_c , so that they do not indicate the nature of the new stable state, but we speculate concerning whether it is a Kosterlitz-Thouless state or a "smeared" BEC, which might avoid any violation of the Hohenberg theorem, as described in an accompanying paper.

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1. INTRODUCTION

Interest in Bose systems and Bose-Einstein condensation (BEC) has been expanding in recent years, stimulated in part by the experimental work on alkali atoms in magnetic traps.¹ Much of the theoretical work has involved mean-field theories, such as those based on the Gross-Pitaevskii equation.² However, some theoretical analyses have recently reconsidered the properties of three-dimensional (3D) homogeneous systems with the inclusion of dynamic correlations that go beyond mean-field theory. Here we extend the

methods to dilute systems in two-dimensions (2D).

In 3D, these techniques have provided computations of the change in the BEC transition temperature as a function of the repulsive interactions in a dilute Bose gas.^{3,4,5} Ref. ³ reports results from an Ursell operator approach,⁶ which are confirmed by non-perturbative Green's function methods.^{4,5} The two techniques give equivalent non-linear self-consistent equations for the self-energies and the distribution functions. Each method finds that a dilute Bose system with repulsive interactions reduces its self-energy by spatial rearrangements of particles with low velocities, and that the low- k quasi-particle energies behave as $k^{2-\eta}$ near the transition. (The constant η is equal to 1/2 in lowest order approximation, and smaller in higher order.) Both methods predict that there is an increase of the critical temperature as the repulsive interactions are turned on, a result confirmed by quantum Monte Carlo calculations.⁷

There may soon be a number of experiments involving 2D systems for, say, alkali atoms or for spin-polarized hydrogen in traps or in homogeneous settings. The usefulness of the Ursell approach in 3D suggests studying 2D systems by the same approach. Here we solve the self-consistent equation for the self-energy as a function of the chemical potential. In 3D, as the chemical potential is increased from large negative values, one reaches a critical value where the phase transition takes place; an effective chemical potential that includes the effects of mean-field and dynamic correlations vanishes signaling the transition. We carry out a similar program here and find that at a finite value of the effective chemical potential the equations no longer have a self-consistent solution, again signaling some sort of transition.

The Hohenberg theorem⁹ states that a 2D system cannot undergo a BEC into a single state, but recent work shows that a "smeared" condensation is not forbidden by this theorem.¹⁰ In this mode of BEC, no single state is extensively occupied, but each of the states in a band has a large, although non-extensive, occupation, with enough states in the band that its total occupation is extensive. Furthermore, one knows that superfluidity occurs in 2D via a Kosterlitz-Thouless transition.⁸ It is even possible that the KT transition and a smeared BEC are equivalent.¹¹ Since our theory has not yet been extended to regimes in which there is macroscopic occupation of a single state or of a band of states, we are unable to tell what transition is signaled by our instability.

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2. URSELL OPERATOR APPROACH

We use the method of Ursell operators,⁶ an approach that allows the generalization of the usual cluster expansion to all orders in statistical effects, while still allowing the possibility of including interactions in lower order. A basic quantity is the second Ursell operator given by

$$U_2(1, 2) = e^{-\beta H_2(1,2)} - e^{-\beta(H_1(1)+H_1(2))} \quad (1)$$

where H_1 is a single-particle Hamiltonian and H_2 a two-particle Hamiltonian. A particular problem in 2D is that the matrix elements of this operator do not approach a constant at small k ; indeed, for hard-core scattering, the leading term is proportional to $1/\ln(ka)$, where a is the hard-core radius. However, we will see that we can, to good approximation, avoid that complication and use a k -independent U_2 matrix element, as in 3D.

The Ursell operator method gives an integral equation for the one-particle reduced density ρ_1 with Fourier transform ρ_k . When the occupation of all states is small (no BEC), one finds,³ to lowest order in the interaction, that ρ_k is given by a free-particle distribution function with a self-consistent, k -dependent effective chemical potential: $\rho_k = [e^{\beta(\varepsilon_k - \tilde{\mu}_k)} - 1]^{-1}$, where $\varepsilon_k = \hbar^2 k^2 / 2m$ and $\tilde{\mu}_k = \mu - \Delta\mu_k$ is the effective chemical potential. The leading correction to the chemical potential is given by $\beta\Delta\mu_k = -\ln[1 - \Delta\xi_k]$, where

$$\Delta\xi_k = -\frac{2\lambda^2}{(2\pi)^2} \int d\mathbf{k}' \frac{\rho_k e^{\beta\Delta\mu_{k'}}}{\ln(|\mathbf{k} - \mathbf{k}'| \bar{a})} \quad (2)$$

with \bar{a} equal to a times a constant of order unity. (In 3D the log factor does not occur and so $\Delta\xi$ is independent of k .) We have solved these equations by iteration and find that $\Delta\xi_k$ is a very weak function of k , so that one might as well set the logarithm to a constant. A constant correction to the chemical potential or, equivalently, the single-particle energy is simply a mean-field, which can cause no fundamental change, and certainly no phase transition, in the Bose gas. Ignoring the logarithm is equivalent to using a momentum-independent matrix element of U_2 , which is what we use in the next order approximation.

If we add corrections second order in the interaction we necessarily develop velocity-dependent terms in the distribution function. We find that the effective chemical potential change is

$$\beta\Delta\mu_k = -\ln[1 - \Delta\xi_0 - \delta\xi_k] \quad (3)$$

where, with our assumption of constant interaction, we now have

$$\Delta\xi_0 = \frac{\alpha}{(2\pi)^2} \int d\mathbf{k} \rho_{\mathbf{k}} e^{\beta\Delta\mu_k} \quad (4)$$

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with α a parameter measuring the strength of the interaction. The second-order correction in Eq.(3) is

$$\delta\xi_{\mathbf{k}} = -\frac{\alpha^2}{2(2\pi)^4} \int d\mathbf{k}' \rho_{\mathbf{k}'} e^{\beta\Delta\mu_{\mathbf{k}'}} \int d\mathbf{q} \rho_{\mathbf{k}'-\mathbf{q}} \rho_{\mathbf{k}+\mathbf{q}} e^{\beta(\Delta\mu_{\mathbf{k}'-\mathbf{q}}+\Delta\mu_{\mathbf{k}+\mathbf{q}})} \quad (5)$$

The quantities $\Delta\xi_0$ and $\delta\xi_{\mathbf{k}}$ are equivalent to self-energies in the Green's function approach.⁴

There are a variety of calculational procedures that can be followed to compute $\delta\xi_{\mathbf{k}}$. If one assumes that $\rho_{\mathbf{k}}$ is dependent only on the magnitude of \mathbf{k} , then this quantity can be reduced to a four-fold numerical integral. By changes of variables this integral can be done in several ways. Alternatively, one can introduce the Fourier transform of $\rho_{\mathbf{k}} e^{\beta\Delta\mu_{\mathbf{k}}}$; since Eq.(5) is a convolution, the computation reduces to doing the Fourier transform and a one-dimensional integral. The procedure used is to pick a value of the real chemical potential, compute the interaction corrections, and iterate. As in the 3D case, $\delta\xi_{\mathbf{k}}$ has a minimum at $k = 0$ and rises monotonically. As one increases μ from very negative values, as would happen in 3D in a system approaching criticality, the minimum in $\delta\xi_{\mathbf{k}}$ deepens and the curvature at $k = 0$ sharpens. The value of $|\tilde{\mu}_k|$ decreases during this process. This feature is caused by dynamic correlations that lead to rearrangements of particles with small k .

Unexpectedly, at a particular value of μ , with $|\tilde{\mu}_k|$ still *nonvanishing*, the iteration becomes unstable and the self-consistent solution disappears as shown in Fig. 1. This result is quite robust and occurs independently of the numerical method used. At the instability $|\delta\xi_0|$, instead of converging to a self-consistent value as one iterates, increases rapidly until the process predicts a positive value of $\tilde{\mu}_0$, at which point the iterations must halt. Passing through $\tilde{\mu}_0 = 0$ would seem to indicate the onset of BEC. Since the theory has not been extended into any condensed regime we are unable to say what the new stable phase might be.

Since one knows that there is a KT phase in 2D, one might expect that our theory is showing an instability towards that phase. A second possibility arises from the proof in an accompanying paper,¹⁰ which shows that the Hohenberg theorem does not rule out what we term as a ‘‘smeared’’ BEC, as defined in the Introduction. It will be interesting to extend the theory to cover such a possibility.

One can go to higher orders in the approximation scheme and sum all ‘‘bubble’’ diagrams, in which case one finds

$$\delta\xi_{\mathbf{k}} = \frac{\alpha^2}{2(2\pi)^4} \int d\mathbf{k}' \rho_{\mathbf{k}'} e^{\beta\Delta\mu_{\mathbf{k}'}} \left\{ \frac{\int d\mathbf{q} \rho_{\mathbf{q}} \rho_{\mathbf{k}+\mathbf{q}+\mathbf{k}'} e^{\beta(\Delta\mu_{\mathbf{q}}+\Delta\mu_{\mathbf{k}+\mathbf{q}+\mathbf{k}'})}}{1 - \frac{\alpha^2}{2} \int d\mathbf{q} \rho_{\mathbf{q}} \rho_{\mathbf{k}+\mathbf{q}+\mathbf{k}'} e^{\beta(\Delta\mu_{\mathbf{q}}+\Delta\mu_{\mathbf{k}+\mathbf{q}+\mathbf{k}'})}} \right\} \quad (6)$$

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We find that the instability persists, although the iterations now have a somewhat different behavior. As one iterates, values of $\Delta\xi_0$ and $\delta\xi_{\mathbf{k}}$ conspire to make the subsequent values of these quantities oscillate about an average value. Either this oscillation dies out eventually to a self-consistent value or grows until it becomes completely unstable.

3. DISCUSSION

Because of the success of the Ursell approach in 3D, namely, its good agreement with the results of other powerful approaches, we have confidence that it should yield reliable results in 2D. Our results show an instability in this case, but we are unable, at this time, to determine if this is the signal of a true phase transition, what is the order of such a transition, or what might be the stable state to which the system proceeds. It is known that perturbation theory breaks down near the BEC phase transition⁴⁻⁶, and that applies here as well. Nevertheless, the unknown sum of the diagrams associated with interparticle correlations must give some negative result, because the mean-field theory can be seen as a variational evaluation with the same wave function as an ideal gas, and the inclusion of correlations can only reduce the free energy and bring the system closer to instability. As μ and the density increase, it seems then that an instability must ultimately take place. Possibilities are that we are seeing a KT transition or, perhaps more interestingly, a transition to a “smeared” Bose-Einstein condensation, which our accompanying article shows is possible.¹⁰ Thus the present paper is really a progress report and we will need further research to resolve the questions it raises.

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5. FIGURE CAPTION

FIG. 1 Change in the effective chemical potential for $k = 0$ as a function of the real chemical potential. For the interaction strength used the instability occurs at $\beta\mu > 0.13$, beyond which the plot shows successive final

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iteration values just before failure rather than self-consistent values. BEC criticality occurs when $\mu + \Delta\mu = 0$, i.e., when the $\Delta\mu_0$ touches the diagonal μ line.

REFERENCES

1. M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Science* **269**, 198 (1995); K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995); C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995).
2. F. Dalfovo, S. Giorgini, L. Pitaevskii, and S. Stringari, *Rev. Mod. Phys.* **71**, 463 (1999).
3. M. Holzmann, P. Grüter, and F. Laloë, *Europhys. Journ. B* **10**, 739 (1999).
4. G. Baym, J.-P. Blaizot, M. Holzmann, F. Laloë, and D. Vautherin, *Phys. Rev. Lett.* **83**, 1703 (1999).
5. G. Baym, J.-P. Blaizot, and J. Zinn-Justin, *Europhys. Lett.* **49**, 150 (2000).
6. P. Grüter and F. Laloë, *J. Phys. I France* **5**, 181 (1995); **5**, 1255 (1995); P. Grüter, F. Laloë, A. E. Meyerovich, and W. Mullin, *J. Phys. I France* **7**, 485 (1997); F. Laloë, in *Bose-Einstein Condensation*, edited by A. Griffin, D. W. Snoke, and S. Stringari, Cambridge Univ. Press (1995).
7. M. Holzmann and W. Krauth, *Phys. Rev. Lett.* **83**, 2687 (1999).
8. J. M. Kosterlitz and D. J. Thouless, *J. Phys. C* **6**, 1181 (1973); V. L. Berezinskii, *Sov. Phys. JETP* **32**, 493 (1971).
9. P.C. Hohenberg, *Phys. Rev.* **158**, 383 (1967).
10. W. J. Mullin, M. Holzmann, and F. Laloë, (This conference).
11. V. N. Popov, *Functional Integrals in Quantum Field Theory and Statistical Physics*, (Reidel Publishing Company, Dordrecht, 1983).