Polarons and Bose decondensation: A self-trapping approach

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(Received 24 June 1991)

An additional, quantum, particle interacting with a Bose condensate forms self-trapped "polaron" if the interaction is sufficiently strong. This is contrasted with the case where the additional particle is *identical* with those in the condensate, where the "self-trapping" would be interpreted as a consequence of a Mott transition. There the transition to the self-trapped state, if it exists, is abrupt, unlike the impurity case. An external potential enhances self-trapping in the nonidentical case.

I. INTRODUCTION

Low-temperature investigations probing the behavior of foreign particles in superfluid ^{4}He have made use of two broad categories of impurities: ^{3}He (e.g., Ref. 1) and ions[2,3] (e.g., He anions or metal cations). The Fermi-liquid nature of the former seems unaffected while the latter particles seem to form heavy, classical entities. As a simple generic model of these systems, we may consider a quantum particle interacting with a Bose condensate of ^{4}He atoms. It is possible to imagine that a foregin particle might be "self-trapped" in the distortion that has been created around it by its interaction with ^{4}He atoms. Such a scenario is plausible if the interaction is sufficiently strong compared to the kinetic-energy costs of creating this new, correlated, ground state. (Whether the ground state is actually *inhomogeneous*, due to the localization of the self-trapped particle, will be considered in the concluding section.) It is tempting to associate the cases of the ^{3}He and ionic impurities with the untrapped and trapped regimes of this model, respectively. This issue will be clarified in this paper for a model system. In particular, the dimensional dependence will be discussed.

A subject apparently unrelated to the impurity problem is Bose "decondensation" and its associated precursor effects. Zero-temperature destruction of a Bose condensate occurs in at least two instances—the solidification of ^{4}He under pressure and the (assumed) localization of ^{4}He in thin films at low coverages (e.g., Ref. 4). Additionally, this may occur in superconducting thin films in a magnetic field (e.g., Refs. 5 and 6). The possibility of a relationship between self-trapping and decondensation lies in replacing the foreign particle by one of the bosons. Could the self-trapping of this *boson* signify an instability to decondensation? Finally, with ^{4}He on rough surfaces in mind, we consider how disorder may encourage self-trapping to occur in local regions. Such "Lifshitz tail states" in the condensed phase may be regarded as the precursor to bulk decondensation.

We will discuss the above issues in the context of the Bose Hubbard model with on-site repulsion U and nearest-neighbor hopping t. The system is Bose condensed in the noninteracting case. Although the condensate is depleted when a weak interaction is introduced, the system is believed to remain a gapless fluid. At strong coupling, however, a commensuration effect becomes important when the average site occupancy, $\bar{n}$, becomes close to an integer. The system is locked into a uniform state with integral site occupation if the hopping integral t is small compared with U. There is an energy gap ($E_{\rm gap} \lesssim U$) for excitations because such excitations involve particles hopping out of a site creating a potential well of depth U in the local Hartree energy. At a site connected by m hops to the center of the localized state, the wave function should be of the form $(t/E_{\rm gap})^m$ (using perturbation theory) so that the particle has a localization length $\lambda_{\rm loc} \sim 1/\ln(E_{\rm gap}/t)$. Similarly, there is a gap for the addition or removal particles so that the system is incompressible. This Mott insulating state becomes unstable ($E_{\rm gap} \to 0$) when t becomes comparable to U so that the cost in kinetic energy is too great to localize the particles. The converse process of the particles becoming localized as the interaction is increased may be thought of as being a self-consistent form of self-trapping.

Indeed, a variant of the Hubbard model with infinite-range hopping can be solved in a mean-field approach and the transition between the Mott insulator and the liquid phases is demonstrated in that case.[7] The hard-core limit ($U \to \infty$) has recently been solved exactly by Tóth[8] and Penrose,[9] who find that the ground state is always condensed away from integral filling. For general U and t, the Hubbard model has been solved in one dimension,[10] showing a transition from the gapless to the gapped state occurs when $U/t > 4\sqrt{3}$ at an average occupancy of unity. [This should be contrasted with the one-dimensional (1D) model with δ-function repulsion where no such transition occurs.[11–13]] In higher dimensions where the gapless state is believed to be superfluid, there are unfortunately no exact solutions. Nevertheless, Fisher *et al.*[7] have used scaling arguments to make predictions about the critical exponents for such quantities as the superfluid density. Chui[14] has also studied the solidification problem in a continuum using a density-functional theory.

Another solvable limit of the Hubbard model has been investigated by Lee and Gunn.[15] The limit consists in taking $U \to 0$ and $\bar{n} \to \infty$ simultaneously, so that the product (the Hartree potential) remains constant. In this limit the ground state is always condensed and can be described by a nonlinear Schrödinger equation. Corrections away from this limit may be calculated using a Bogoliubov theory. An additional advantage of this limit is that an inhomogeneous potential can be treated in the same framework. The inclusion of disorder raises the possibility of an Anderson-localized insulating phase—the compressible "Bose glass."[16,7] As already mentioned, the conclusions of this paper would have implications for the nature of the insulating phase.

Let us now consider the dimensional dependence of the self-trapping. We will only examine the instability of one particle leaving the condensate to form a localized state by itself. This process is a highly excited process in the limit of weak coupling, $U \to 0$. (Consideration of the case with an identical particle being self-trapped is complicated by the issue of orthogonality of the states[17] and will be discussed later in this paper.) A crude estimate of the cost in kinetic energy is $t\bar{n}^{2/d}$, approximating the size of the localized state with the interparticle spacing. Another energy cost comes from the local distortion of the condensate necessary to accommodate the localized particle. An estimate using the compressibility of the condensate is $\hbar c \bar{n}^{1/d}$. Since the reduction in repulsive energy is $\sim U\bar{n}$, the instability is expected at low density in one dimension and high density in three dimensions and above. (In contrast, the different dimensional dependence of a Coulombic interaction means that the Wigner crystallization of electrons is expected to occur at low density for $d=1,2,3$.) It is interesting to note that any attractive shallow potential, such as the depression created by the particle in the condensate, has at least one bound state in one and two dimensions.[18,19] We will discuss the relevance of this general result to our problem later.

By restricting the discussion to only one localized particle, one cannot approach the superfluid-solid transition. For the homogeneous system, the particles may localize together at the same time so that there is no intermediate phase where only a fraction of the particles are self-trapped. Alternatively, there may be an instability to a cluster of self-trapped particles whose size diverges as the transition is approached. Nevertheless, single-particle instabilities should give an absolute limit on the stability of the condensed phase. Moreover, it is conceivable in an *inhomogeneous* system that the instability would occur preferentially in certain places while the rest of the system remains condensed. Therefore, it is reasonable to examine this restricted problem as a starting point. This coexistence of localized and condensed particles is related to the "inert layer" model for ^{4}He films on Vycor. Alternatively, in the context of localization theory, the one-particle instability considered here can be regarded as the remnant of the Lifshitz tail states of the Bose-glass phase.

II. AN IMPURITY PROBLEM: NONLINEAR SCHRÖDINGER EQUATION

For the sake of generality, this "impurity" atom can be given a mass m' and repulsive interaction u' different from the condensate particles. In this section, a variational wave function will be used to investigate the instability. We will find that a weakly trapped state exists for a strong interaction or heavy impurity. In fact, as we will see in the next section, this situation does not arise if the localized particle is identical with the rest because Bose statistics tends to favor strong overlap between occupied states, leading to Bose-Einstein condensation.

As in our previous paper,[15] we will adopt a variational approach in the continuum limit. The Hamiltonian is

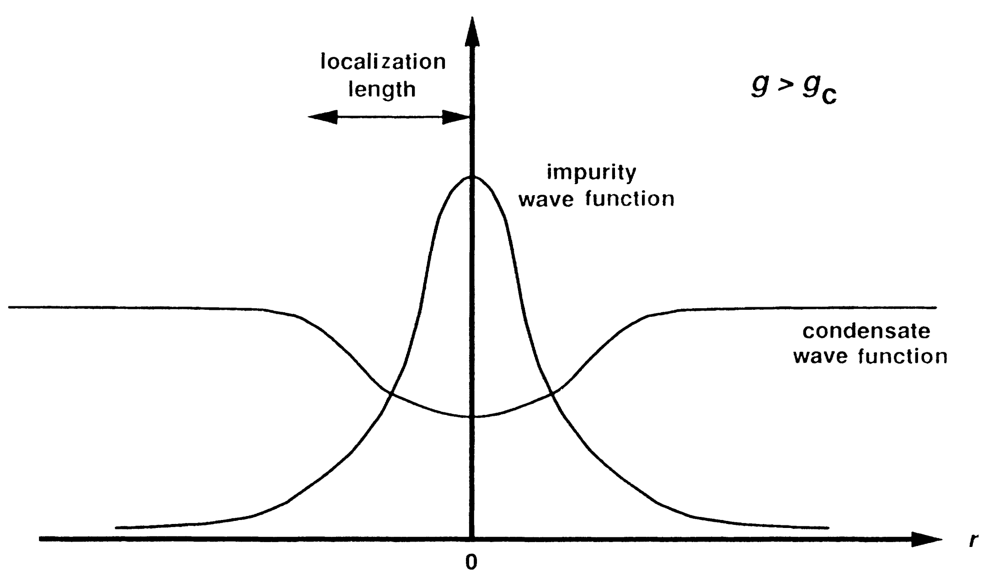

FIG. 1. Schematic wave functions for the trapping regime.

$$H=-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2-\frac{\hbar^2}{2m'}\nabla_{\mathbf{R}}^2+\frac{1}{2}u\sum_{\substack{i,j=1\\(i\neq j)}}^{N}\delta(\mathbf{r}_i-\mathbf{r}_j)+u'\sum_{i=1}^{N}\delta(\mathbf{r}_i-\mathbf{R}) \ . \tag{1}$$

Let us consider the variational wave function

$$\Psi=\frac{1}{V^{N/2}}\phi(\mathbf{R})\prod_{i=1}^{N}\varphi(\mathbf{r}_i) \ , \tag{2}$$

where $\phi(\mathbf{R})$ is the impurity wave function normalized by $\int\phi^2 d\mathbf{r}=1$ (unlike the condensate wave function φ which is normalized to unity per unit volume, see Fig. 1). (Note that, although we will be considering a spatially localized wave function, the true ground state may be a superposition of such states; this point will be discussed further in the concluding section.) Let us use $u\rho$ as the unit of energy and the healing length λ of the condensate as the unit of length ($\lambda=1$). In order to maintain the same normalization condition, let us use a dimensionless wave function $\phi\rightarrow\lambda^{d/2}\phi$. The coupled Euler-Lagrange equations for the two wave functions are

$$\left[-\frac{1}{2}\nabla^2+\varphi^2+\frac{\beta}{\rho\lambda^d}\phi^2\right]\varphi=E\varphi \ ,$$
$$(-\tfrac{1}{2}\alpha\nabla^2+\beta\varphi^2)\phi=\varepsilon\phi \ , \tag{3}$$

where $\alpha=m/m'$ and $\beta=u'/u$. The mass ratio α is small when the impurity is massive. The interaction ratio β is large when the impurity is strongly repelled from the other particles. These equations always have the trivial solution of a delocalization impurity (i.e., constant ϕ and $\varepsilon=\beta$). This is, in fact, the only solution in our previous dense, but weakly interacting, limit where the number of particles in a healing volume diverges: $\rho\lambda^d\rightarrow\infty$. However, away from this limit, the last term on the left-hand side of the first equation represents the "feedback" process where the impurity atom causes a local depression in the condensate. From the second equation, this distortion in the local Hartree potential acts as a well to trap the impurity in a bound state ($\varepsilon<\beta$). Therefore, it is reasonable to expect a self-trapped ground state to exist when the feedback is strong enough (e.g., a strongly repulsive impurity with $\beta\gg1$).

Is there a perturbative solution to the pair of nonlinear equations (3) which marks the onset of the self-trapping instability? This corresponds to the case of *weak trapping* where the distortion of the condensate is small and the size of localized state λ_{loc} is consequently large. More quantitatively, the effect of the impurity feedback can be treated perturbatively if it is much smaller than the Hartree term. Since the magnitude of ϕ should scale as $\lambda_{\text{loc}}^{-d/2}$, the dimensionless quantity $\eta=\beta/\rho\lambda_{\text{loc}}^d$ has to be much less than unity. Let us use η as an expansion parameter for the distortion in the condensate so that the equation for φ can be linearized. Write

$$\varphi=\varphi_0+\eta\varphi_1+O(\eta^2)$$

and

$$E=E_0+\eta E_1+O(\eta^2) \ .$$

Since the condensed limit should be recovered as $\eta\rightarrow0$, $\varphi_0=1+O(1/V)$, $E_0=1$, and $E_1\sim O(1/V)$. The linearized equations are

$$(-\tfrac{1}{2}\nabla^2+2)\varphi_1=-\lambda_{\text{loc}}^{-d}\phi^2 \ ,$$
$$(-\tfrac{1}{2}\alpha\nabla^2+2\beta\eta\varphi_1)\phi=(\varepsilon-\beta)\phi \ . \tag{4}$$

Eliminating the condensate distortion from the equations, one obtains a nonlocal nonlinear Schrödinger equation (NLSE) for the localized wave function:

$$\left[-\tfrac{1}{2}\nabla^2-2g\int G(\mathbf{r}-\mathbf{r}')\phi^2(\mathbf{r}')d\mathbf{r}'\right]\phi=\tilde{\varepsilon}\phi \ , \tag{5}$$

where $g=\beta^2/\alpha\rho\lambda^d$ is the coupling constant for self-trapping. It should be noted that g is not necessarily small in this perturbation theory. In a $d=2$ tight-binding model, it translates into $g=U/t$. We can see that the feedback is strong when the kinetic-energy cost is low (massive impurity) or when the repulsion is strong. We can also see from the form of the coupling constant of the feedback that the mean-field theory of our previous paper[15] (which has no feedback) breaks down when the number of particles in a healing volume is small. $\tilde{\varepsilon}=(\varepsilon-\beta)/\alpha$ should be negative for a self-trapped solution. The nonlocal kernel $G(\mathbf{r})$ is the Green's function satisfying

$$(-\tfrac{1}{2}\nabla^2+2)G(\mathbf{r})=\delta(\mathbf{r}) \ . \tag{6}$$

This is a short-ranged kernel because it decays exponentially for separations much greater than $\lambda/2$. In one dimension, its asymptotic form is $\frac{1}{2}e^{-2|x|}$. In two dimensions,

$$G(\mathbf{r})=\frac{1}{\pi}K_0(2|\mathbf{r}|) \ , \tag{7}$$

where K_0 is the zero-order modified Bessel function of the first kind.

Equation (5) minimizes the energy functional:

$$F[\phi]=\tfrac{1}{2}\int|\nabla\phi|^2d\mathbf{r}-g\int\int\phi^2(\mathbf{r})G(\mathbf{r}-\mathbf{r}')\phi^2(\mathbf{r}')d\mathbf{r}\,d\mathbf{r}' \ . \tag{8}$$

The tendency for self-trapping is clearly seen as the *attractive* potential term in this effective energy. Let us start by discussing the *local* case, i.e., $2G(\mathbf{r})=\delta(\mathbf{r})$. This corresponds to a condensate of vanishingly small healing length. The kinetic term scales as $1/\lambda_{\text{loc}}^2$ while the attractive potential term scales as $-1/\lambda_{\text{loc}}^d$. Therefore, F should vary like $a/\lambda_{\text{loc}}^2-b/\lambda_{\text{loc}}^d$ when one performs a scale transformation on any trial wave function. Hence, one expects that a stable trapped state exists for $d=1$. For $d\geq3$, although a delocalized state may be stable, there should be a state of lower energy which collapses to a point ($\lambda_{\text{loc}}\rightarrow0$, $\tilde{\varepsilon}\rightarrow-\infty$). (This is known as Derrick's theorem.) The marginal dimension is two where a critical coupling constant g_c is necessary for collapse.

It is well known that the 1D *local* equation can be solved exactly and the answer verifies the argument given above. The solution is $\phi=\mathrm{sech}(x/\lambda_{\mathrm{loc}})/(2\lambda_{\mathrm{loc}})^{1/2}$ with $\bar{\varepsilon}=-1/2\lambda_{\mathrm{loc}}^2$. The localization length is $\lambda_{\mathrm{loc}}=2/g$. The distortion in the condensate is $-(\alpha g^2/8\beta)\,\mathrm{sech}^2(x/\lambda_{\mathrm{loc}})$. Therefore, the disturbance in the condensate is perturbative for $g^2 \ll 8\beta/\alpha$. Since the localization length becomes much greater than the healing length, this weak-trapping regime is expected to survive when the nonlocality of the kernel is restored.

In the 2D problem, a variational criterion can be established for the critical coupling g_c above which the NLSE encourages collapse. This is of interest because it will be argued that the nonlocal case has self-trapped solutions above the same critical value. For the local equation, the functional in (8) becomes

$$F_{\mathrm{loc}}[\phi]=\tfrac{1}{2}\int k^2|\phi_{\mathbf{k}}|^2\frac{d\mathbf{k}}{(2\pi)^2}-\frac{g}{2}\int|\rho_{\mathbf{k}}|^2\frac{d\mathbf{k}}{(2\pi)^2}\ , \tag{9}$$

where $\phi_{\mathbf{k}}$ and $\rho_{\mathbf{k}}$ are the Fourier transforms of the wave function and density, respectively. The scale transformation discussed above is

$$\phi(\mathbf{r})\to\phi'(\mathbf{r})=\kappa\phi(\kappa\mathbf{r})\ , \tag{10}$$

so that $\kappa<1$ corresponds to stretching the wave function and $\kappa>1$ corresponds to a contraction. As a result, $\rho_{\mathbf{k}}\to\rho'_{\mathbf{k}}=\rho_{\mathbf{k}/\kappa}$ and $F_{\mathrm{loc}}[\phi']=\frac{1}{2}\kappa^2(T-gR_0)$, where

$$T=\tfrac{1}{2}\int|\nabla\phi|^2 d\mathbf{r}\ ,\qquad R_0=\int\phi^4 d\mathbf{r}\ . \tag{11}$$

It is obvious from this argument that the collapse occurs if a starting wave function ϕ can be found such that $g>T/R_0$. In other words, the *critical* g_c should be the value of $(T/R_0)_{\min}$. At first sight, one might conclude that the minimum is zero corresponding to the nontrapping solution of $\phi=1/V^{1/2}$. This is *incorrect* because the scale transformation (10) on a constant ϕ does not produce collapse. Moveover, one cannot treat the constant wave function as the $\kappa\to0$ limit of a spatially varying wave function because the ratio T/R_0 is *invariant* under the scale transformation. Therefore, we have to be careful about the Hilbert space of wave functions in which the variational argument is employed. Since any trapping solution to Eqs. (3) should have exponential decay asymptotically, an appropriate choice is the space of smooth square-integrable functions defined on the infinite plane. For instance, a Gaussian ϕ gives $T/R_0=2\pi$ and $\phi\sim(1+r)e^{-r}$ gives a value of $(144/77)\pi$. In other words, each square-integrable wave function is in the Hilbert space but its infinite-size limit is not so that there is no paradox in the various limits having different values of T/R_0. A lower estimate of $g_c/2\pi\sim0.93$ can be obtained computationally. This can also be checked by attempting to solve the NLSE iteratively.

In order to progress further, the nonlocality of the kernel $G(\mathbf{r})$ has to be restored. The scaling argument above breaks down when λ_{loc} becomes comparable to the range of the kernel $\lambda/2$. The attractive potential term no longer decreases indefinitely so that the collapse of the wave function is halted for $d\geq2$, we expect that a bound state of size λ may exist for the nonlocal NLSE at large g. However, the NLSE is invalid for tightly bound solutions. These will be discussed in the next section. Nevertheless, the effect of the nonlocality is more pronounced in the marginal dimension of two—it manages to stabilize weak-trapping solutions with λ_{loc} much greater than the range of the kernel.

To see how this assertion can be proved, consider the nonlocal contribution to the variational functional F (8). In Fourier space,

$$F[\phi]=\tfrac{1}{2}\int k^2|\phi_{\mathbf{k}}|^2\frac{d\mathbf{k}}{(2\pi)^2}-2g\int\frac{|\rho_{\mathbf{k}}|^2}{k^2+4}\frac{d\mathbf{k}}{(2\pi)^2}\ . \tag{12}$$

The nonlocal corrections $F-F_{\mathrm{loc}}$ will be positive and hence *repulsive* at every $\mathbf{k}$ vector so that even long-wavelength components may be stabilized against collapse (at marginal dimension). Since we are concerned with weakly trapped solutions, we can focus on these small-k contributions. Performing a Taylor expansion in k for the kernel, we can write F as

$$F=F_{\mathrm{loc}}+\frac{g}{8}\int|\rho_{\mathbf{k}}|^2(k^2+\cdots)\frac{d\mathbf{k}}{(2\pi)^2}\ . \tag{13}$$

Performing the scale transformation (10) for a given shape, the functional varies as

$$F(\kappa)=\tfrac{1}{2}\kappa^2(T-gR_0)+\tfrac{1}{8}g\kappa^4R'_0+O(\kappa^4)\ ,\qquad R'_0=\int|\nabla\rho|^2 d\mathbf{r}\ . \tag{14}$$

Now, suppose that the stable weak trapping exists for a given coupling g and use it as the starting wave function ϕ. This minimizes F so that $\partial F/\partial\kappa=0$ at $\kappa=1$. This implies that $F_{\min}=-gR'_0/8$ and

$$g=\frac{T/R_0}{1-R'_0/2R_0}\ . \tag{15}$$

Note that the ratio R'_0/R_0 varies as $1/\lambda_{\mathrm{loc}}^2$ while T/R_0 does not. This means that the above equation can always be satisfied for any $g>(T/R_0)_{\min}$ with a wave function of any shape by an appropriate choice of size for the wave function. The optimum wave function (which minimizes $F_{\min}$) should also maximize R'_0 and R'_0/R_0 for a given g. Such a wave function should therefore minimize the numerator in (15). Hence, we come to the conclusion that the critical coupling g_c for the existence of a self-trapped solution in the nonlocal problem is the *same* as the one at which collapse occurs for the local problem. Moreover, the scaling behavior of R'_0/R_0 in (15) suggests that the size of the trapped state diverges as

$$\lambda_{\mathrm{loc}}\sim(g-g_c)^{-1/2} \tag{16}$$

as the threshold is approached from above ($g-g_c \ll g$).

How is this weak trapping related to the bound states of a shallow potential well $V\leq0$? Comparing with our NLSE, we should make the correspondence:

$$V(\mathbf{r})\leftrightarrow-2g\int G(\mathbf{r}-\mathbf{r}')\phi^2(\mathbf{r}')d\mathbf{r}'$$

so that, using (6), the strength of the well is $\int|V|d\mathbf{r}=g$.

In one dimension, the size of the bound state is $\lambda_{\rm loc} \sim 1/g$ with energy $\bar{\varepsilon} \sim -g^2$. This is therefore very close to the solution of the NLSE. In two dimensions, the bound state of a shallow well is exponentially larger than the size of the well l:

$$\lambda_{\rm loc}/l \sim e^{1/2g} \text{ with } \bar{\varepsilon} \sim \frac{1}{l^2} e^{-1/g} . \qquad (17)$$

If this result could be applied to the NLSE, it would imply that the bound state is much larger than the distortion in the condensate. However, the first equation in (4) shows that such a bound state would enlarge the distortion. An iterative procedure starting with this wave function will lead to a delocalized solution. Indeed, the weakly trapped solution of the NLSE is supported by a distortion of the condensate of a *similar* size. Hence, the shallow-well bound state ($g \to 0$) cannot be a self-consistent solution of the NLSE, giving further support to the above conclusion that a finite coupling $g \sim O(1)$ is necessary for self-trapping.

What is the effect of *inhomogeneity* on the trapping of the impurity? To be specific, let us consider a local defect in a two-dimensional system, described by a potential well $\sigma V(\mathbf{r})$ for the bosons and $\sigma' V(\mathbf{r})$ for the impurity. An interesting competition arises when the two coupling strengths σ and σ' have the same sign. Both the impurity and the condensate are attracted to this well. On the other hand, the interaction term u' would prefer to find the impurity at a region of low condensate density. If the potential is weak ($\sigma, \sigma' \ll 1$), we can discuss this problem in the weak-trapping framework as above. Potential terms have to be added to (5) so that the nonlinear Schrödinger equation becomes

$$\left[-\frac{1}{2}\nabla^2 + \frac{1}{\alpha}[\beta W + (\sigma' - \beta\sigma)V] - 2g \int G(\mathbf{r}-\mathbf{r}')\phi^2 d\mathbf{r}' \right] \phi = \bar{\varepsilon}\phi , \qquad (18)$$

where $W = \sigma V - E_0 + \varphi_0^2$ is the residual potential defined in our previous paper.[15] Recall that the eigenstates of this potential have non-negative energies and that the low-lying states are not expected to be strongly localized.

To investigate the possibility of bound states in this two-dimensional problem, we will use again the result for the single-particle Schrödinger equation that the integrated strength of a potential with bound states should be negative.[18,19] In fact, the strength of the residual potential $\int W d\mathbf{r}$ should be zero—it cannot be negative because there are no Lifshitz tail states, nor can it be positive since the spectrum has the lowest eigenstate at zero energy. This means that the system described by (18) will always have a bound state if

$$(\sigma' - \beta\sigma) \int V(\mathbf{r}) d\mathbf{r} < 0 . \qquad (19)$$

Since we are discussing a potential well, the bound state exists if $\sigma'/\sigma > \beta$. As expected, the impurity atom will be trapped by the potential well if it is sufficiently attracted to the well compared to the other particles. Therefore, we can see that the critical g_c becomes zero when the above condition is satisfied. It seems that the self-trapping effect becomes irrelevant to the onset of bound impurity states. If condition (19) is reversed in sign, then the impurity atom will not be trapped at the defect site. Instead, the onset of a bound state will probably occur elsewhere by the self-trapping mechanism when $g > g_c$. The sensitivity in two dimensions to inhomogeneities discussed here seems to be quite a generic property. It should be related to the diversity of experimental results on superfluid thin films on various substrates.

In summary, the impurity problem has weakly trapped states for $d = 1, 2$. In three dimensions and above, a similar argument suggests there are trapped states are tightly bound on the scale of the healing length when the coupling is sufficiently strong. Indeed this result is found in the problem of an electron coupled to the acoustic phonons of a lattice.[20] Toyozawa investigated the case of strong electron-lattice interactions. When the zero-point fluctuations of the phonons are included, the delocalized ground state may have an abrupt transition from a state localized to a lattice site. (There is no healing length in the lattice problem so that the lattice spacing acts as the short-distance cutoff.) This occurs when the Debye frequency of the phonons is less than the electron bandwidth. There is also a jump of several orders of magnitude in the effective mass of the electron. The hopping matrix element becomes heavily renormalized: $\omega_{\mathbf{k}} \to \omega_{\mathbf{k}} S_{\mathbf{k}}$, where $S_{\mathbf{k}} = \langle \Phi_{\mathbf{k}}(\mathbf{R}) | \Phi_{\mathbf{k}}(\mathbf{R}+\boldsymbol{\delta}) \rangle$ is the overlap integral for the wave functions of displaced lattice distortions when the impurity with momentum $\mathbf{k}$ hops from site $\mathbf{R}$ to its neighbor. A self-consistent calculation shows that there are only solutions for S close to unity or zero. The calculation is facilitated by the collapse of the electron wave function onto a site so that it does not have to be variationally determined as well.

III. A QUESTION OF IDENTITY

In the previous section, a nonlinear Schrödinger equation has been set up to describe a weak-trapping regime for an impurity atom in two dimensions. We will now discuss its analogue for identical particles. (We will continue to use the healing length λ as the unit of length and $u\rho$ as the unit of energy.) A hint that the system of identical particles is radically different is the sensitivity of the impurity system to inhomogeneities which should be contrasted with the result of our previous paper[15] that the totally condensed state is stable to the introduction of a random potential in the limit $g \to 0$. In fact, we will see that weak trapping is absent when Bose statistics are reinstated for all particles.

The variational wave function (2) describing the system with one particle outside the condensate forming a localized wavepacket has to be symmetrized now:

$$\Psi = \frac{1}{(N+1)^{1/2} V^{N/2} C_N^{1/2}} \sum_{\rm sym} \phi(\mathbf{r}_{N+1}) \prod_{i=1}^{N} \varphi(\mathbf{r}_i) , \qquad (20)$$

where C_N is the normalized integral:

$$C_N = 1 + \frac{N}{V}\int \varphi\phi \, d\mathbf{r} = 1 + \rho |S|^2 \,, \tag{21}$$

ρ is the average number of particles in a healing volume in our units. S is therefore defined as the overlap between the condensate wave function and the localized state.

The Hamiltonian has a rather complicated expectation value:

$$\langle \Psi | H | \Psi \rangle = [NC_{N-1}T_{00} + \tfrac{1}{2}(N-1)C_{N-2}R_4 + 2\rho S T_{01} + T_{11} + 2R_2 + 2\rho(1-1/N)R_3 S]/C_N \,, \tag{22}$$

where T's are the matrix elements for the kinetic energy

$$T_{00} = -\tfrac{1}{2}\int \varphi \nabla^2 \frac{d\mathbf{r}}{V} \,, \quad T_{01} = -\tfrac{1}{2}\int \varphi \nabla^2 \phi \, d\mathbf{r} \,, \quad T_{11} = -\tfrac{1}{2}\int \phi \nabla^2 \phi \, d\mathbf{r} \,, \tag{23}$$

and R's are the interaction matrix elements

$$R_4 = \int \varphi^4 \frac{d\mathbf{r}}{V}, \quad R_3 = \int \varphi^3 \phi \, d\mathbf{r}, \quad R_2 = \int \varphi^2 \phi^2 d\mathbf{r} \,. \tag{24}$$

It should be noted that integrals such as S, T_{01}, and R_3 would be absent for fermionic problems where the particles occupy mutually orthogonal states. We will see that these overlap integrals are also responsible for the difference between the system of identical particles and the impurity system discussed previously.

To find the variational ground state, we have to minimize $\mathcal{H} = \langle H \rangle$. Lagrange multipliers E and ε will be used to constrain the normalization of the condensate wave function and the localized wave function as in the previous section. The general Euler-Lagrange equations involving $\mathcal{H}$, E, and ε are quite complicated. It can be checked that they contain the totally condensed state as a solution. However, we are interested in a state with a localized ϕ. By imposing the conditions that $\varphi(\mathbf{r}) \to \varphi(\infty) \simeq 1$ and $\phi(\mathbf{r}) \to 0$ asymptotically, $\mathcal{H}$ and E can be determined in terms of the remaining Lagrange multiplier ε. The equations can then be simplified to

$$\begin{aligned} -\tfrac{1}{2}\nabla^2\varphi + \left[\varphi^2 + \frac{2}{\rho}\phi^2\right]\varphi + S(3\varphi^2 - 1)\phi = \varphi \,, \\ -\tfrac{1}{2}\nabla^2\phi + (2 - \rho S^2)\varphi^2\phi - 2S\phi^2\varphi = \varepsilon'\phi \,, \end{aligned} \tag{25}$$

where ε' is a linear combination of the Lagrange multipliers. We can see that these coupled equations reduce to the impurity case (3) with $\alpha = 1$ and $\beta = 2$ if the terms involving overlaps are dropped. In other words, the corresponding coupling constant is $g = 4/\rho$.

This comparison leads us to ask whether there is a weak-trapping solution in this identical case when the number of particles in a healing volume drops below $2/\pi$. Recall that the feedback mechanism for self-trapping requires the special state ϕ to localize at a local depression of the condensate. This means that the sign of the second term in the ϕ equation in (25) should be positive. Therefore, the condition

$$\rho S^2 < 2 \tag{26}$$

has to be satisfied for a trapped state to exist. However, for a weakly localized state of size $\lambda_{\rm loc} \gg \lambda = 1$, its overlap with the condensate is large: $S \sim \lambda_{\rm loc}^{1/2}$. Hence, we do not expect a perturbative solution to exist for the self-trapping of identical particles.

IV. DISCUSSION AND CONCLUSIONS

The results of Sec. II predict that there will be a self-trapping transition for foreign particles coupled to a condensate. Taking the condensate to be that in ^{4}He, then it seem empirically that ^{3}He and the ionic systems are on opposite sides of g_c—with the ions self-trapped. In fact, most of our effort was in investigating the marginal case of two dimensions, as naively there was the possibility of a considerable disparity between the extent of the wave function of the self-trapped particle and the distortion in the condensate. Of course, this is not relevant in the case of two-dimensional ions, as they will stick to the substrate, in preference to ^{4}He; however, it *is* relevant to the consideration of ^{3}He in ^{4}He films.

First, we return to the issue of localization of the self-trapped particle. In the limit of Ref. 15, i.e., $\bar{n} \to \infty$ and $U \to 0$, where there are no quantum fluctuations (with β scaled appropriately to yield a finite g), the problem reduces to a nonlinear Schrödinger equation, as in our approach leading to localization. However, in the *presence* of quantum fluctuations it is an open problem whether the ground state is inhomogeneous or not, in the sense of being a superposition of wave functions of the form of Eq. (2) centered at each point in space. Even in the homogeneous case, the true ground-state wave function is likely to contain correlations between the extra particle and the condensate of the form derived, for $g \gtrsim g_c$.

For the remainder of this section we will continue the discussion of the role of the identity of the self-trapped particle. We concluded that there would be no weak-trapping solution for the case of an identical particle. However, would the system support a *strongly* localized state at lower densities? We will confine the discussion in this paper to the implications of the continuum equations (25). (This question will be addressed in a lattice model in future publications.)

Suppose that the coupling constant g is much larger than unity so that a tightly bound state is formed in the corresponding impurity problem. We can now estimate how the overlap terms in (25) may alter such a solution. The most dangerous term to the self-trapping mechanism seems to be $-S\phi$ in the first equation which acts as a source for the condensate wave function wherever the special state is localized.

A crude estimate of the quantities involved can be obtained from the length scales, L_φ and L_ϕ, which are the sizes of the condensate distortion and the localized state, respectively. L_φ is expected to be of the order of the healing length. Let $\bar{\varphi}$ be the average of the condensate wave function φ over this region. For a tightly bound state, the distortion in the condensate should be large so we should expect $\bar{\varphi} \ll 1$. The wave-function overlap can be estimated as $S \sim \bar{\varphi} L_\phi$ since $\phi \sim 1/L_\phi$ in $d = 2$. Looking at the coupled equations (25) in the region of the distortions, one can see that these two scales should be roughly balanced according to the equations

$$1/2L_\varphi^2 - 2\bar{\varphi}/\rho L_\phi^2 + (\bar{\varphi}L_\phi)/L_\phi = 0 \ ,$$

$$1/2L_\phi^3 + 2\bar{\varphi}^2/L_\varphi - 2(\bar{\varphi}L_\phi)\bar{\varphi}/L_\varphi^2 = \varepsilon'/L_\phi \ .$$

The last terms on the left-hand side originate from the overlap terms. The dangerous term mentioned above turns out to be small when the coupling constant is large. Therefore, it is not unreasonable to expect a strongly localized state to exist when the repulsion among the particles becomes sufficiently strong.

It is difficult to extract further information on the strong-coupling limit where the spatial variation of the wave functions occur on the scale of the healing length. This limit corresponds to the case where there are few particles in a healing area. Since our variational approach is essentially a mean-field theory that does not consider zero-point fluctuations, it is only expected to be reliable when the distortions in the wave functions occur over length scales much larger than the healing length (i.e. weak-trapping case). Therefore, it is not supposed to be reliable in the strong-coupling limit. We will simply conclude this discussion by speculating the existence of a single-particle instability in the Bose system. This instability should give an absolute limit on the stability of the condensed phase to a Mott transition.

Finally, we should note that the result with the identical particle has an implication in the presence of a random potential. It implies that there will be no "large" localized states coexisting with a condensed Bose system, there will be only rather strongly localized Lifshitz tail states.

To conclude, the main results of this paper concern the self-trapping of particles coupled to a Bose condensate and the influence of statistics on those results. In particular, the relation of decondensation of the pure Bose system to the self-trapping.

We showed that, for a *foreign* particle, the wave function obeyed a nonlinear Schrödinger equation which was nonlocal on the scale of the healing length of the condensate. We found that this nonlocality prevented the collapse of the self-trapped state that occurs above a critical coupling constant in the local case. ^{3}He in ^{4}He and ions in ^{4}He are on the non-self-trapped and self-trapped sides of this transition. It may be possible to tune films of ^{3}He in ^{4}He through the transition by varying the ^{4}He coverage.

We found that if the foreign particle was replaced by a boson *identical* with those in the condensate, there were no weakly self-trapped solutions and we were led outside the validity of our approximations. The overlap between the putatively self-trapped boson and the condensate, S, played a crucial role showing the influence of Bose statistics as commented upon by Anderson.[17] Finally, we noted that this work predicts the lack of large Anderson localized states coexisting with a condensate.

ACKNOWLEDGMENTS

D.K.K.L. would like to thank Trinity College, Cambridge, for financial support and the Rutherford Appleton Laboratory for hospitality while part of this work was performed.

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