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The fate of the Lifshitz tail for condensed bosons

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Abstract. We determine the extent to which Lifshitz tail states can be defined in a condensed Bose system. This provides a justification for the inert-layer picture in the study of helium on Vycor. We argue that, in three dimensions, hard-core bosons can be trapped by a sufficiently deep potential well despite a strong tendency for all particles to participate in the Bose–Einstein condensate. This is demonstrated by a variant of the conventional spin–boson problem. We find that phase fluctuations in the condensate tend to depress particle exchange between the trap and the rest of the system and hence has an enhancing effect in terms of Lifshitz-tail localization. However at *low* densities (near onset of condensation) we argue that the condensate will be relatively enhanced compared to the inert layer model, in agreement with experiment.

1. Introduction

Torsion balance studies of ^{4}He films on Vycor have shown that there is a critical coverage nc below which superfluidity is lost. Recent specific heat experiments have also found that the lambda peak moves to $T = 0$ as n approaches n_c [1]. The disorder in the Vycor substrate has been associated with this behaviour—Hertz *et al* [2] have suggested that there is an Anderson-localized 'Bose glass' phase below the critical coverage. This Bose glass is envisaged to occur when the chemical potential lies in the localized part of the Hartree–Fock single-particle spectrum. It should be noted that interparticle repulsion is necessary to prevent the physically unrealistic situation where all the particles condense into the lowest localized (Lifshitz tail) states. Bose condensation can be restored by raising the chemical potential above the mobility edge since there is no barrier to the infinite occupation of an extended state.

A phenomenological language has also evolved over the years parallel to the theoretical efforts. It has often been suggested that the adsorbed monolayer of ^{4}He atoms that exists below n_c will survive at higher coverages where superfluidity is observed. In the language of localization theory, such a picture suggests that some particles remain in localized Lifshitz tail states of the substrate potential so that others may form an extended condensate over a much smoother landscape. Although this may be a plausible picture for a classical liquid film, it ignores the indistinguishable nature of the atoms. Since the identity of particles is a key concept behind the phenomenon of Bose condensation, this 'inert layer' picture has become a point of contention in the study of superfluid films.

It is fairly difficult to make precise arguments in the Bose glass phase and most work has concentrated on the superfluid side of the transition. Fisher and coworkers

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[3] have discussed this in the context of a scaling hypothesis. This is partly supported by results from renormalization group calculations such as the work of Giamarchi and Shultz [4] on the one-dimensional case. One of their conclusions is that the observed critical exponents are inconsistent with the inert-layer model. In this paper, we would adopt a more microscopic approach to understand how such a layer might exist (even though it may not play an important part in the critical behaviour of the localization transition.) Unlike previous work, our formulation faces directly the issue of the particle identity.

Let us briefly discuss how the disorder in the substrate can be screened out in the system and when an inert-layer picture becomes necessary in such a context. At weak disorder, there is the mechanism of 'condensate screening' where the condensate wavefunction is distorted over the length scale of the healing length to screen out variations in the potential [5]. (Weak disorder can be defined as the case when the potential fluctuations are small compared with the Hartree potential experienced by an additional test particle.) It can be shown that this is most effective in the limit of high density ($n \to \infty$) and weak local interactions ($U \to 0$) such that the Hartree potential Un remains constant. In this limit, the system is totally condensed even when the chemical potential is in the Lifshitz tail of the bare potential. Away from this limit, the $1/n$ corrections show that the zero-point fluctuations (principally in the phase of the condensate wavefunction) are enhanced by the presence of disorder. It is tempting to associate these fluctuations with incipient localization occuring in the wider excursions in the components of the random potential which are not effectively screened by this condensate mechanism, e.g. deep traps over a region smaller than the healing length. In other words, an inert-layer picture becomes relevant in the case of imperfect condensate screening in the sense that some uncondensed particles may occupy the Lifshitz tail states of the single-particle theory and thus plug up the worst excesses of the random potential. This would leave a weak residual potential which allows a condensate to form. The condensate screening mechanism can then screen out this residual disorder further. This distinction between screening via localized states and the condensate parallels the non-linear and linear screening in a disordered Fermi system.

To compare between linear screening by the condensate φ and the formation of trapped states ϕ, we may start with the simplest (Hartree–Fock) wavefunction with one trapped state:

$$\Phi = \sum_{j=1}^{N} \sum_{i \neq j} \varphi_0(x_i)\phi(x_j). \tag{1}$$

Even in the absence of disorder, it is plausible that Φ has a lower energy than a uniform condensate, if the interactions are sufficiently strong—the condensate would be depressed in the vicinity of ϕ allowing one boson to 'self-trap'. It is interesting to note that weakly trapped states are possible if the trapped particle is distinguishable from the rest. However, for identical particles, strong coupling is necessary before self-trapping occurs [6]. This behaviour illustrates the extreme circumstances necessary for the coexistence of the condensate with localized particles. Disorder does not alter this conclusion. It is the purpose of this paper to investigate this strong-coupling regime in the presence of disorder. In the next section we will give a variational treatment using the trial wavefunction (1). The virtual exchange processes between a trapped particle and the condensate will be explored in section 3. This is discussed in terms of a variant of the conventional spin–boson model. Finally, we would discuss how the concept of Lifshitz tail states in a Bose condensed system can be defined more precisely.

2. Weak hopping on a lattice

To be more specific in our discussion, let us focus our attention on the Bose Hubbard model:

$$H = -t \sum_{(nn')} c_n^\dagger c_{n'} + \tfrac{1}{2} U \sum_n n_n^2. \tag{2}$$

The operators $c\dagger$ and c create and annihilate bosons at site n. In this section, we will argue that a *single-particle* trapping instability may occur in the strong-coupling limit using the trial wavefunction (1). We have discussed in previous work [6] the *weak* trapping of a distinguishable particle where the spatial extent of the wavefunction of the trapped particle is large compared to the healing length. As mentioned above, this has no analogue in the case of identical particles. This can be seen by comparing the variational theories based on symmetrized and unsymmetrized versions of (1). Bose statistics encourages the particles to occupy states with strong overlaps so that a totally condensed trial state appears quite stable when the interaction parameter $g = U/t$ is small. To pursue this further, let us consider the stability of a tightly-bound wavepacket in the weak-hopping (or strong repulsion) limit where $g \ll 1$. To avoid the mathematical difficulties in determining the spatial structure of such a wavepacket, we will simplify the trial state to a particle trapped at a *single site*. This is stable when there is no hopping ($t = 0$), allowing us to treat the hopping term in (2) perturbatively. The discussion of the zero-point fluctuations between the trap and the condensed system is postponed to the next section.

First of all, let us switch off the hopping integral t entirely. This means that there will be no kinetic energy cost for localising the particle and trapping phenomena can be easily seen, in particular revealing the role of non-orthogonality of the trapped state. Indeed the ground state of the $t = 0$ system will be a Mott insulator. The particles are evenly distributed on the lattice. The energy per particle is approximately $\frac{1}{2}U(\overline{n} - 1)$ (or zero below monolayer coverage) instead of $\frac{1}{2}U\overline{n}$ for the condensed state. There is no need to look at single-particle instabilities to understand this ground state. However, if we would like to see single-particle self-trapping or the binding of a particle due to a potential well, this zero-hopping case is not a useful starting point.

To obtain a more suitable model, let us suppose that the hopping is finite everywhere *except* around a site where it is particularly weak. Such a model will give us an extended condensate as well as the possibility of localization at the special site. The theoretical motivation to look at this situation is to investigate the competition between the (Hartree) energy advantage in localization and the more subtle effects arising from Bose statistics which encourages condensation. It will be shown that the trapping of a single particle is indeed lower in energy than the condensed state in a certain region of the parameter space.

Consider first the case when $t = 0$ near the defect site. We will use the lattice spacing as the unit of length. The lattice analogue of the trial wavefunction (1) is used. The variational equations for the amplitudes at the defect site are:

$$\begin{aligned} \left[\varphi^2 - 1 + V + \frac{2}{\overline{n}}\phi^2\right] \varphi + S[\,3\varphi^2 - 1\,]\,\phi = 0 \\ \left[(2 - \overline{n}S^2)\varphi^2 + \frac{V}{U\overline{n}}\right] \phi - 2S\varphi\phi^2 = \frac{\epsilon}{U\overline{n}}\phi \end{aligned} \tag{3}$$

where V is the potential due to a defect and $\overline{n}$ is the average number density on the lattice. The overlap of the wavefunctions is $S = \sum_n \varphi_n \phi_n$. Since we have no hopping from the defect site, there is no tendency for the wavefunction of the localized state to spread from that site. This can be checked explicitly. Therefore, we can put $\phi = 1$ at the defect and zero elsewhere. The condensate will be assumed to exist in the rest of the system so that φ is unity everywhere except on the defect. Hence, the condensate amplitude φ_0 on the defect is the only variable left.

We can investigate the self-trapping of a particle by neglecting the defect potential: $V = 0$. The totally condensed system of N particles should always be a solution. Its total energy is $\frac{1}{2}U\overline{n}N$. $\varphi_0 = 0$ is another solution corresponding to disjoint wavefunctions so that there is no overlap between the localized state and the condensate at all—there is a 'complete hole' in the condensate. Compared with the condensed state, this state has an energy of $\Delta H = \frac{1}{2}U\overline{n}(\overline{n} - 2)$ and is therefore lower in energy when $\overline{n} < 2$. A state with a 'partial hole' in the condensate can also be found for $\overline{n} > 1$. The condensate density at the special site is $\varphi_0^2 = (\overline{n} - 1)/2\overline{n}$. Its energy relative to the condensed state is $\Delta H = \frac{1}{8}U(\overline{n}^2 + 2\overline{n} - 7)$ so that it is negative for $1 < \overline{n} < 2\sqrt{2} - 1$. However, this solution is not the lowest in energy. Therefore, we find that the trapped state digs a complete hole in the condensate for $\overline{n} < 2$. As expected, this occurs when the system is sufficiently dilute, corresponding to the strong-coupling limit of the previous paper. In this simple example, we can see that the localized state is not necessarily stable even if there is no kinetic energy cost in its formation! As already mentioned, we have to attribute its disappearance above $\overline{n} = 2$ to a 'rule-of-thumb' tendency of the particles to occupy the same single-particle state.

Let us restore the defect potential V. For a repulsive potential ($V > 0$), one might expect that the complete-hole localization would occur away from the defect. However there is also the possibility that a trapped state becomes easier to form because the concomitant hole in the condensate is favoured at the repulsive defect. This effect is able to stabilize the localized state at high densities if $1 - 2/\overline{n} < V/U\overline{n} < 1$. For $V > U\overline{n}$, the condensate is completely repelled from the defect site and, seeing the bare potential, the extra particle does not localize there. For an attractive defect, the increase in the local condensate density discourages localization at the defect if it is sufficiently deep: $V/2U\overline{n} < 1 - 1/\overline{n}$. The results are summarized in figure 1. (We have ignored the possibility of partial holes.)

Having studied this zero-hopping case, we may ask whether it can be regarded as a limiting case of a weak-hopping régime for the localization instability. After all, some of the states considered are highly localized and are likely to possess a high kinetic energy when the hopping is restored. Therefore, we should investigate whether a perturbative solution in the hopping t can be obtained from the states considered above. We will restrict attention to the weak-hopping limit where the localized state ϕ does not spread beyond one lattice site from the defect. The variational equations

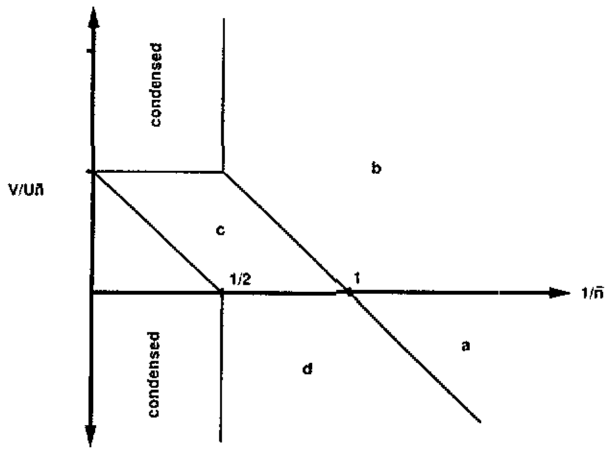

Figure 1. Trapping at weak-hopping limit. Regions (a) and (c): hole on defect. Regions (b) and (d): hole away from defect. Only regions (a) and (b) remain for non-zero hopping.

are now given by

$$-\frac{t}{U\overline{n}}\sum_{\delta}(\varphi_{n+\delta}-\varphi_n)+\left[\varphi_n^2-1+V_n+\frac{2}{\overline{n}}\phi_n^2\right]\varphi_n+S\left[3\varphi_n^2-1\right]\phi_n=0$$

$$-\frac{t}{U\overline{n}}\sum_{\delta}(\phi_{n+\delta}-\phi_n)+\left[(2-\overline{n}S^2)\varphi_n^2+V\right]\phi_n-2S\varphi_n\phi_n^2=\frac{\epsilon}{U\overline{n}}\phi_n \qquad (4)$$

where δ joins nearest neighbours. To look for solutions confined to the defect and its nearest neighbours, we can take the solution with a complete hole in the condensate and consider perturbations $O(t) \ll U\overline{n}$ on the amplitude of the condensate at the defect and on the amplitude of the localized state around it. This perturbation is small on a square lattice provided that

$$3t/2U \ll 1-\overline{n}+V/2U \qquad (5)$$

and other conditions $[(t/U\overline{n})^2 \ll 8\overline{n}, t \ll 2(V+2U\overline{n})]$ to ensure that the kinetic energy is not high enough to prevent localization over so few sites. These extra conditions are unimportant because they only serve to give us the simplest perturbative answer. On the other hand, the first condition (5) implies that some of the trapped solutions of the $t=0$ case are *unstable* to the introduction of hopping. In particular, only the states in the region

$$V/2U\overline{n} > 1-1/\overline{n} \qquad \text{and} \qquad \overline{n} < 2 \qquad (6)$$

can be regarded as the zero-hopping limit of the localized states.

The variational approach in this section suggests strongly that the particles may become localized and hence not participate in Bose–Einstein condensation. For a homogeneous system, this gives an absolute limit on the instability of the condensed phase to a Mott transition. However, it is unlikely that the actual instability can be described by single-particle processes. For instance, the collective fluctuations of the phase of the order parameter (as the number fluctuations are suppressed when the interactions are strong) may be more significant in the destruction of Bose condensation. More importantly, single-particle trapping are of interest in *inhomogeneous* systems where they may be the local precursors of the instability to a Bose glass phase.

3. Bound states in condensed systems: a spin–boson model

Consider a Bose system with a sufficiently low density such that the variational approach in the previous section allows some particles to be pulled out of the condensate to occupy bound states in deep local fluctuations of a random potential. This can be regarded as a picture of the possible 'inert layer' found in Vycor experiments. How do these particles coexist with the condensate? Heuristically, one would expect that each trapped particle will be coupled to the condensate by virtual hopping excitations out of its binding potential. In other words, the zero-point fluctuations in the ground state consists of a continuous exchange of particles between the potential well and its condensed environment. If the binding energy in the potential is decreased, then we might expect a transition or gradual crossover to the screening limit of [5] where no particles occupy localized states. We will attempt to formalize this physical picture in this section.

To simplify the problem, we will consider a lattice model where each localized particle is confined to one site only. This avoids the necessity of knowing about the structure of the localized wavefunction within the wells. Since we are interested in the exchange between the well and the condensate, we can exclude the possibility of the multiple occupancy at the defect site by considering hard-core bosons. If we further suppose that the parameters of the system can be adjusted so that these defects are dilute, then we can treat the sites as independent two-level systems (empty or occupied). From now on, we will focus on one particular defect site.

As is well known, a lattice system of hard-core bosons can be represented by a spin-half XY model. However, further approximations are necessary to circumvent the mathematical difficulties of such a model. In particular, we will observe the hard-core constraint at the defect site only. Bose–Einstein condensation will be assumed to exist in the rest of the system. If the spin-up state represents an occupied site, then the on-site term in the Hamiltonian is

$$H_{\text{spin}} = -\tfrac{1}{2}\Delta_0(\sigma^z + 1) \tag{7}$$

where σ^z is the z-component of the Pauli matrix and $\Delta_0 = \mu - V$ is the energy to remove a trapped particle and place it in the condensate. It should be positive to trap a particle. V is the site energy at the defect. μ is the chemical potential introduced to conserve the total particle number $\frac{1}{2}(\langle\sigma^z\rangle + 1) + \sum_n \langle c_n^\dagger c_n\rangle$.

The rest of the system is approximated by the finite-interaction Bose Hubbard model with random site energies. The interaction U plays the rôle of a pseudopotential. We will discuss this later. The hopping between the trap and the condensate occurs at a special site R so that the total Hamiltonian is given by:

$$H = H_{\text{Anderson}} + H_{\text{spin}} - t\,(\sigma^+ c_R + \sigma^- c_R^\dagger). \tag{8}$$

In this model, the defect site is singled out as a special site which the condensate does not penetrate so that there is no repulsion between the condensate and the trapped particle. Hence, in contrast to the models discussed previously, the condensate density is not depressed at site $\boldsymbol{R}$. Indeed, the opportunity to take part in the exchange process with the trapped site will produce a local bulge in the condensate. Thus, this model is designed to illustrate the hopping exchange between the trapped states and a Bose-condensed environment (see figure 2).

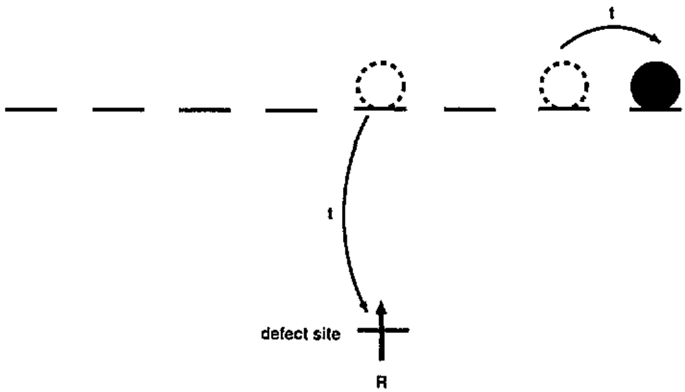

Figure 2. A defect site coupled to a uniform Bose system.

3.1. *A mean-field description*

Let us now consider the mean-field solution to this model. In other words, we will focus on the hopping of a particle between the trap and the condensate. In the language of this spin model, the existence of a condensate means that the spin experiences a field proportional to t which causes it to cant towards the xy-plane. Suppose that the canted spin makes an angle θ with the z-axis $(0 < \theta < \pi)$. The wavefunction of the system is then of the form:

$$|\Psi\rangle = \mathrm{e}^{\mathrm{i}\phi} \cos\tfrac{1}{2}\theta \mid \uparrow; N \text{ condensed}\rangle + \mathrm{e}^{-\mathrm{i}\phi} \sin\tfrac{1}{2}\theta \mid \downarrow; N+1 \text{ condensed}\rangle. \qquad (9)$$

The azimuthal direction ϕ of the spin can only be determined relative to the global phase of the condensate. (Compare with Josephson coupling.) Choosing the condensate wavefunction to be real, we can fix $\phi = 0$ so that ϕ is 'aligned' with the condensate phase. In terms of the Bose system, the trial state is a *superposition of two permanents*—one describes a trapped particle outside a condensate and the other describes a totally condensed state. On a technical level, the adoption of this two-permanent variational wavefunction (9) is the main difference between the approach in this section and those in the previous one, where only a single permanent was used. In this context, we have allowed for more freedom in our variational ground state. (Of course, we have also traded away other degrees of freedom, such as the spatial structure of the trapped state, to make the problem tractable.) Indeed, this is necessary if we wish to discuss the hopping exchange between the trap and the condensate.

Because it is advantageous to exploit the hopping term fully, we will assume that the condensate wavefunction is of the same form for both spin states; this ensures the maximum overlap of the total wavefunctions when hopping. The non-linear Schrödinger equation (NLSE) for the condensate wavefunction φ is obtained from minimizing the Hamiltonian:

$$-t\sum_{\delta}(\varphi_{n+\delta}-\varphi_n)+U\overline{n}(\varphi_n^2-1)\varphi_n=\frac{t\sin\theta}{2\overline{n}^{1/2}}\,\delta_{nR} \tag{10}$$

where we have substituted $\mu = -zt + U\overline{n}$ for the chemical potential. The source term describes the effect of the exchange with the spin which encourages a bulge in the condensate as already mentioned. The angle of the spin depends in turn on the local condensate amplitude:

$$\tan\theta=\frac{2t\overline{n}^{1/2}}{\Delta_0}\,\varphi_R. \tag{11}$$

The occupation of the defect is $\cos^2\frac{1}{2}\theta$. As expected, this quantity decreases from unity when the hopping into the condensate is introduced. As in the XY model, the xy-component of the canted spin indicates the participation of the particle in the condensate. To be more precise, it indicates the admixture of the totally-condensed state with the trapped-particle state.

The 'homogeneous' case can be obtained by setting $V = 0$ and choosing the mean-field occupation of the hard-core site to be the same as the number density asymptotically far away from the bulge in the condensate. One possible procedure is to fix $\overline{n}$ and adjust U such that the chemical potential $\mu = \Delta_0(V = 0)$ gives us the desired $\langle S_z\rangle$ for the spin state. Therefore, as already mentioned, U is treated as a *pseudopotential* for the dilute hard-core gas from which we started in this section. For instance, a filled lattice requires $\theta = 0$ and hence both $\Delta_0(V = 0)$ and U must diverge, reflecting the fact that the hard-core condition has to be enforced rigorously.

The coupled equations for the spin direction and the condensate distortion can be simplified when θ remains close to zero. This limit arises when the kinetic-energy advantage $t\overline{n}^{1/2} \sim t$ of hopping into the condensate is nullified by a much greater cost Δ_0 of leaving the well—i.e. weak hopping and a deep trap. In such a case, the source term in (10) is linearly related to the local value of the condensate wavefunction, having the same effect as a local potential well $(-t^2/\Delta_0)\,\delta_{nR}$. The depth of this well can be understood in terms of the virtual hopping process where the condensate and the trap exchange a particle. An estimate of the magnitude of the condensate at R can be obtained by balancing the energy $-(t^2/\Delta_0)\varphi^2$ for taking advantage of this well and the repulsive energy cost $\frac{1}{2}U\overline{n}^2\varphi^4$. This gives $\varphi_R^2 \simeq 1 + (t/U\overline{n})(t/\Delta_0)$ if the deviation from unity is small. Note that this bulge in the condensate is small when the trap is deep or the hopping is weak $(\Delta_0/t \gg 1)$. This is expected because the defect site is inaccessible to the condensate if a particle is tightly bound there.

Having discussed lower spin state, we will now turn to the excited state. This corresponds to a spin flip: $\theta \to \pi - \theta$ and $\phi \to \phi + \pi$ (keeping the same associated condensate wavefunction.) For $\theta \simeq 0$, this excited state is predominantly a number excitation, i.e. the trapped particle has jumped out of the defect site. In other words, the particle appears to be occupying the condensed-phase analogue of a Lifshitz tail state. The new excitation energy, which we shall denote by Δ, is not surprisingly similar to the original trapping energy Δ_0. As the depth of the trap is reduced so that $\Delta_0 \to 0$, both the lower and higher spin states cant towards the xy-plane. The difference in the occupation of the defect site between the two states is $\cos\theta$ so that it decreases as $\theta \to \frac{1}{2}\pi$. Hence, the excitation loses its number-like character, becoming 'phase-like' in the sense that its azimuthal angle ϕ is *antiparallel* to the phase of the condensate. This is reflected in the excitation energy (for $\theta \to \frac{1}{2}\pi$) which can be estimated by the effect of the phase flip on the spin–condensate coupling in the Hamiltonian: $\Delta \simeq 2t\overline{n}^{1/2}\varphi_R$. Hence, in the limit of a weak trap or strong hopping ($\Delta_0/t\overline{n}^{1/2} \to 0$), the system can be interpreted as a *Josephson weak link* between the trap and the condensate with a finite 'charging energy' Δ.

Therefore, we can see that the mean-field solution to the ground state has a gradual crossover from a bound-state picture to a Josephson-like picture of the system.

3.2. Hopping fluctuations

Let us now examine the zero-point fluctuations in the system. In a homogeneous system, these are the collective fluctuations of the condensate. In the long-wavelength limit, they are predominantly fluctuations in the phase of the condensate wavefunction. In the present model, this phase is in fact coupled to the azimuthal angle ϕ that parametrizes the spin state in (9). Variations in this angle does not alter the variational ground-state energy. Therefore, we can expect that the quantum fluctuations in our system to be similarly dominated by gapless Goldstone modes. In addition, the virtual exchange of particles between the trap and the rest of the system can be studied. We will focus on these processes because we are interested in the survival of trapped states in the presence of a condensate. Therefore, in the treatment that follows, we will not consider the effect of the trap on the condensate and we will simply assume that the number density of the condensate is $\widetilde{n}$. For the dilute system we are discussing, significant depletion of the condensate is expected so that $\widetilde{n} \ll \overline{n}$.

It is convenient to rotate the axis of quantization to coincide with the mean-field spin direction:

$$\sigma^z \to \cos\theta\ \sigma^z - \sin\theta\ \sigma^x \qquad \sigma^x \to \cos\theta\ \sigma^x + \sin\theta\ \sigma^z \qquad \sigma^y \to \sigma^y. \tag{12}$$

From the discussion of the previous sections, we know that we should be studying the dilute limit of our system for trapping. Therefore, the conventional Bogoliubov c-number procedure can be employed in a first approximation: $c_n \to \widetilde{n}^{1/2}\varphi_n + c_n$. The spin part of the Hamiltonian becomes:

$$H_{\text{spin}} \to -\tfrac{1}{2}\Delta\,\sigma^z \qquad \text{where} \qquad \Delta = \Delta_0 \sec\theta. \tag{13}$$

Δ is the new splitting as discussed in the mean-field description. Note that this is always larger than the original trapping energy Δ. The coupling between the spin and the rest of the system is described by:

$$H_1 = -\tfrac{1}{2}t\left[\,\mathrm{i}\sigma^y(c_R - c_R^\dagger) + (\cos\theta\ \sigma^x + \tfrac{1}{2}\sin\theta\,(\sigma^z - 1))(c_R + c_R^\dagger)\,\right]. \tag{14}$$

The Hamiltonian for the bosons can be truncated at the quadratic level so that a Bogoliubov transformation can be performed. The formal description of the Bogoliubov transformation with an inhomogeneous condensate has been given our previous paper [5]. However, we will only be concerned with the effect of the long-wavelength phase fluctuations on the trapped state. Since the bulge in the condensate should not extend to length scales larger than the healing length, we will ignore the inhomogeneous corrections and use the Bogoliubov excitations of a uniform system.

We can now express the Hamiltonian in terms of the Bogoliubov excitations,

$$H = -\tfrac{1}{2}\Delta\sigma^z + \sum_k \Omega_k \alpha_k^\dagger \alpha_k + H_1$$

$$H_1 = -\frac{t}{2\mathcal{N}^{1/2}} \sum_k \left[\mathrm{i}\sigma^y (u_k + v_k)(\alpha_k - \alpha_k^\dagger) + \right.$$

$$\left. (u_k - v_k)(\cos\theta\, \sigma^x + \tfrac{1}{2}\sin\theta\, (\sigma^z - 1))(\alpha_k + \alpha_k^\dagger) \right] \tag{15}$$

where u_k and v_k are the coherence factors. Ω_k is the dispersion relation for the Bogoliubov excitations. It should be linear at long wavelengths: $\Omega_k \simeq ck$. The phonon velocity c is given by $c^2 = 2tU\tilde{n}$. (R is chosen as the origin. $\mathcal{N}$ is the number of sites.)

This is an example of the 'spin-boson problem' which has been exhaustively studied. For a review, see Leggett *et al* [7]. We will now use this model to argue that the 'Lifshitz tail state' is stable in three dimensions with respect to its coupling to a condensed system provided that the trapping energy Δ_0 is much greater than the hopping matrix element t. The two-dimensional case is more subtle.

Let us focus on the first term of H_1 which represents the strongest coupling:

$$H_2 = -\sum_k \mathrm{i}\sigma^y g_k (\alpha_k - \alpha_k^\dagger) \tag{16}$$

where $g_k = t(u_k + v_k)/2\mathcal{N}^{1/2} \sim k^{-1/2}$ at long wavelengths. We may attempt to tackle this coupling perturbatively when the trap is deep. The ground state energy then lowered from $-\frac{1}{2}\Delta$ by

$$\sum_k \frac{g_k^2 |\langle 0|\, \sigma^y\, (\alpha_k - \alpha_k^\dagger)\, |\downarrow\ k\rangle|^2}{\Delta + \Omega_k} = \sum_k \frac{g_k^2}{\Delta + \Omega_k} \simeq \frac{t^2 U \tilde{n}}{2\Delta\mathcal{N}} \sum_k \frac{1}{\Omega_k} \tag{17}$$

in the limit of strong trapping $\Delta > \Delta_0 \gg \Omega_c$. $|0\rangle$ is the ground state at zero coupling, i.e. spin-up eigenstate in the Bogoliubov vacuum. Ω_c is the bandwidth of the Bogoliubov excitations. This expression converges in two and three dimensions. The fractional change in the ground-state energy is $-C(t/\Delta)(\Omega_c/\Delta)$ where C is a dimension-dependent constant of the order of unity. This perturbative result is what might be expected when the energy cost for hopping out of the well is high.

We may also adopt a variational approach to examine when the effect of the coupling overwhelms the influence of trapping energy. We follow the approach of Silbey and Harris [8] here and use the canonical transformation:

$$U = \exp\left[-\mathrm{i}\sigma^y \sum_k \frac{f_k}{\Omega_k} (\alpha_k + \alpha_k^\dagger) \right] \tag{18}$$

where f_k is the variational parameter. The variational energy of the state $U\,|0\rangle$ is

$$\langle U^{-1} H U \rangle = -\tfrac{1}{2}\Delta_{\mathrm{R}} + \sum_k \frac{1}{\Omega_k} (f_k^2 - 2 f_k g_k)$$

$$\Delta_{\mathrm{R}} = \Delta \exp\left[-2 \sum_k f_k^2 / \Omega_k^2 \right]. \tag{19}$$

We can regard Δ_R as a renormalized spin splitting. The exponential reduction in the effective spin splitting originates from the reduced overlap of the two different phonon wavefunctions associated with each spin state. However, one should be careful in interpreting this canonical transformation as introducing different c-number shifts in the Bogoliubov phonons according to the influence of the spin-up and spin-down states. (This would be the case if we replaced σ^y with σ^z in the transformation.) As we have seen in the mean-field theory, this tends to decouple the two spin states and the system will be unable to take advantage of the hopping between the trap and its environment. On the contrary, the spin-up and spin-down states have in fact become strongly admixed because of this reduction in the splitting. Therefore, the hopping term tends to decouple the eigenstates of σ^y.

The stationary points in the energy are given by $f_k = g_k/[1 + \Delta_R\Omega_k^{-1}]$. For our coupling function $g_k \sim k^{-1/2}$, it can be shown that a local minimum is obtained only if $\Delta_R = 0$ so that $f_k = g_k$. The variational energy is then given by $\Lambda = -\sum_k g_k^2/\Omega_k$. The low-$k$ contribution to this quantity diverges logarithmically in two dimensions! In other words, the spectrum for the linearized model here does not have a lower bound. The infinitely negative contribution comes from the σ^y term. The actual pathology of an unbounded energy spectrum is of course an artefact of the approximations made. The finite compressibility of the actual Bose system and hence the anharmonicity in its gas of Bogoliubov excitations should prevent this from occurring. Nevertheless, this problem indicates that the perturbative consideration of single hops between the trap and its surroundings is inadequate in two dimensions.

In three dimensions, the variational energy is $\Lambda \simeq -\frac{3}{8}(t^2U\tilde{n}/\Omega_c^2) \sim -t$. When $|\Lambda| > \frac{1}{2}\Delta$, this variational energy will be lower than the perturbative result. Anticipating that the variational state is quite different from the perturbative one, a condition for the stability of the trapped state should be $t \ll \Delta$.

How different are the variational and perturbative methods in dealing with the coupling term H_2? It has already been mentioned that the variational ansatz admixes the eigenstates of σ^z strongly and decouples the eigenstates of σ^y. To compare the two states , one might naïvely say that the perturbative state is simply the leading correction to the decoupled state $|0\rangle$ in the Taylor expansion of the variational state $U|0\rangle$ with $f_k = g_k$. More quantitatively, we can compute their overlap $S = \langle \mathrm{pert}|U|0\rangle$. The exponent in U can be normal-ordered using $\exp(A+B) = \exp A \exp B \exp -\frac{1}{2}[A, B]$, giving

$$U(f_k = g_k) = \exp\left[-\mathrm{i}\sigma^y \sum_k g_k \alpha_k^\dagger/\Omega_k\right] \exp\left[-\mathrm{i}\sigma^y \sum_k g_k \alpha_k/\Omega_k\right] \times \exp\left[-\tfrac{1}{2}\sum_k g_k^2/\Omega_k^2\right]. \tag{20}$$

The last c-number factor is the same as $(\Delta_R/\Delta)^{1/4}$ and it *vanishes* due to an infra-red divergence in the exponent. Therefore, the variational state $U|0\rangle$ does not have any overlap with wavefunctions constructed perturbatively from the decoupled system! In other words, all the matrix elements of U vanishes in the representation of the Hilbert space which uses the eigenstates of the decoupled system as a basis set. U has been called an 'improper unitary operator' and the states generated by it from the eigenstates of the decoupled system are said to form an 'improperly equivalent' Hilbert space [9]. In condensed matter physics, this is better known as the 'orthogonality catastrophe', first formulated by Anderson [10] in terms of a metallic analogue of the present problem. It is a generic feature that may arise in systems with an infinite number of degrees of freedom. In our case, it arises as an infra-red pathology, i.e. in the thermodynamic limit, when the wavefunctions of the macroscopic number of excited Bogoliubov quasiparticles associated with the eigenstates of σ^y have no overlap at all. As hinted above, this is the origin of the vanishing Δ_R which is an off-diagonal transition matrix element for the σ^y eigenstates. In the language of the problem of dissipative tunnelling between double wells, this corresponds to a particle being stuck in one of the wells [11].

Following Beck *et al* [12], we may describe a second-order transition between the two régimes we are discussing. The order parameter is identified as $p = \sum_k \mathrm{i} g_k(\alpha_k - \alpha_k^\dagger)$ which implies a c-number shift to the Bogoliubov quasiparticles. A random phase approximation gives $\langle\sigma^y\rangle = p/2\Lambda$ and a Hamiltonian of the form

$$H_{\mathrm{RPA}} = -\tfrac{1}{2}\Delta\sigma^z - p\sigma^y + \sum_k \Omega_k \beta_k^\dagger \beta_k + p^2/4\Lambda \tag{21}$$

where β_k and $\beta_k^\dagger$ are Bogoliubov operators after the subtraction of their expectation values. For this Hamiltonian, the expectation value of σ^y is given in terms of p as $p/(4p^2 + \Delta^2)^{1/2}$. To make this calculation self-consistent, we see that $p = 0$ for $\Lambda < \Delta/4$ and there is a second-order transition to finite p at $\Lambda = \Delta/4$. This transition in terms of the Bogoliubov quasiparticles has to be treated with caution because the c-number shift may well be suppressed by the anharmonic effects which we have ignored. Nevertheless, it gives an energy scale for the validity of the mean-field picture. It should be noted that the energy Λ does not feature prominently in the discussion of the conventional spin–boson literature (e.g. [7]). This is because it has been compensated explicitly by a counterterm. Such a formulation would enable one to isolate the effect of a 'classical' dissipative term on the quantum dynamics of the spin. However, this is not the purpose of the present investigation.

4. Discussion and conclusions

We now see that there is some parallel with the case of fermions in a random potential. There, if the mobility edge is below the Fermi energy, the ground state consists of both localized and extended single-particle states, if the fermions do not interact. There are excited states where holes reside in the localized states.

Both of these results have their counterparts in the bosonic case, at least at the Hartree–Fock level, as indicated in section 2. As well as the condensate wavefunction being multiply occupied, a localized state was occupied in the ground state. This presence of non-macroscopically occupied single particle states in the ground state is the prerequisite for a sensible definition of a 'hole' excited state in a Bose system. In the case of the uniform condensate, the only state that is occupied is the condensate, there is no discernible change in the occupancy if one particle is removed. However in the case of a singly occupied state occuring in the ground state, the change in occupancy is not negligible if it is removed. Thus an approximately orthogonal excited state would consist of taking the particle from the localized state and placing it in the condensate. This implies that at the Hartree–Fock level, a Lifshitz tail can be said to exist in a Bose system.

Interaction amongst the bosons presents a mechanism for the ground state to be a superposition of the fully condensed state and the state with one boson in the tail state. The condensate and localized state may be thought of as the two components in a Josephson junction, with the 'charging energy' increasing as the energy of the tail state becomes more negative. This suggests a gradual transition to a fully condensed state as the depth of the tail state is decreased, with the hole excited state becoming a phase excitation. At the Bogoliubov level we saw that this picture might breakdown—there being a genuinely 'localized' state if the well depth was large enough, at least in three dimensions. In two dimensions the results were difficult to interpret due to infrared divergences, requiring consideration of anharmonicity among the Bogoliubov excitations.

The simplest application of these results to a spatially random potential is the following. In the Vycor experiments, localization sets in at low coverages, however one peculiarity of the results is that the condensate fraction is *larger* than $n - n_c^*$ close to the transition, where n_c^* is the critical coverage *extrapolated* from high coverages (see figure 3). This implies that the 'inert layer' *dissolves* to some extent as the transition approaches. We may ask if there is some sign of this in our work. Let us consider the inequality that determines whether the trapped solution is the ground state: it is $|\Lambda| < \alpha\Delta$, where α is a constant of order unity as we saw in the last section. How does this change as the density of bosons is lowered? Λ contains one power of n in both the numerator and in the denominator (through Ω_c), so it does not vary with n. However, Δ contains one power of n through the Hartree contribution to the chemical potential, and so Δ decreases as $n \to n_c$.

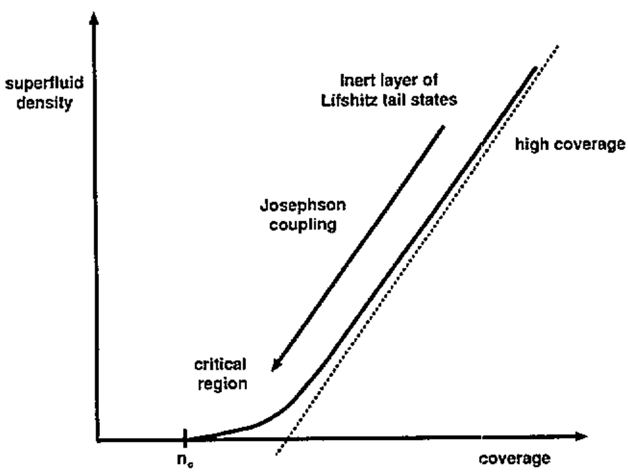

Figure 3. A schematic diagram of the condensate fraction as afunction of coverage.

The consequence of the decrease in Δ and the constancy of Λ is that the inequality for the stability of the trapped state may be violated at low density. Assuming a distribution of trap depths, as the density is lowered there will be a liberation of bosons from the traps that form the inert layer, which will place the condensate fraction above the naïve estimate (linear extrapolation from high density). These details of this process are beyond the scope of this paper.

In summary, we have argued that Lifshitz tail states can coexist with the condensate in a Bose system, justifying the inert-layer picture in the study of helium on Vycor. In three dimensions, hard-core bosons can be trapped by a sufficiently deep potential well despite a strong tendency for all particles to participate in the Bose–Einstein condensate. We found that phase fluctuations in the condensate tend to depress particle exchange between the trap and the rest of the system and hence has an enhancing effect in terms of Lifshitz-tail localization. However at *low* densities (near onset of condensation) the condensate will be relatively enhanced compared to the inert layer model, in agreement with experiment.

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