

# Effect of fluctuations on the superfluid-supersolid phase transition on the lattice

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(Received 12 February 2008; revised manuscript received 4 March 2008; published 8 September 2008)

We derive a controlled expansion into mean field plus fluctuations for the extended Bose-Hubbard model, involving interactions with many neighbors on an arbitrary periodic lattice, and study the superfluid-supersolid phase transition. Near the critical point, the impact of (thermal and quantum) fluctuations on top of the mean field grows, which entails striking effects, such as negative superfluid densities and thermodynamical instability of the superfluid phase—earlier as expected from mean-field dynamics. We also predict the existence of long-lived “supercooled” states with anomalously large quantum fluctuations.

DOI: 10.1103/PhysRevA.78.033604

PACS number(s): 03.75.Kk, 67.80.kb, 03.75.Lm

## I. INTRODUCTION

The question of whether macroscopic quantum coherence can prevail in the presence of periodic order, ultimately leading to the existence of a supersolid, has been intensely debated for five decades [1–3]. Of late, this topic has seen a renewed surge of interest, partly due to the observations in [4] indicating potential signatures of a supersolid phase of <sup>4</sup>He. Because of the inherent complexity of <sup>4</sup>He, it is useful to gain further understanding by studying supersolid phases in other systems such as the Bose-Hubbard model, which can be realized experimentally via cold bosonic atoms in optical lattices [5]. For on-site interactions only, the phase diagram at  $T=0$  contains the superfluid and the Mott insulator state [6,7]. Adding interactions across sites (next nearest or higher) in a so-called extended Bose-Hubbard model, a superfluid-supersolid phase transition may occur [8–12] in addition to further Mott-type phases. Here the term supersolid is associated to an order parameter (with a well-defined phase) which is, in contrast to the homogeneous superfluid ground state, not the same for all lattice sites, but periodically modulated. At the heart of supersolid formation is the generic phenomenon that an instability towards density modulations occurs if the excitation spectrum dips below zero for a finite wave vector.

Within mean-field theory, i.e., neglecting all fluctuations, properties of the supersolid phase were studied in [13]. However, the evanescent excitation energies at the transition suggest that (thermal and quantum) fluctuations should play an important role near the critical point. The impact of these fluctuations can be taken into account with quantum Monte Carlo simulations (see, e.g., [8,12]). Despite the strength of this method, these simulations are always restricted to a specific (low-dimensional) lattice of finite size and a small sample of the full Hilbert space. In the following, we consider an arbitrary periodic lattice and develop an analytic expansion into mean-field plus fluctuations where the size of the fluctuations and the validity of the expansion is *controlled* by a small parameter. Therefore, our derivation is complementary to other numerical and analytical approaches using, for example, duality to vortex field theory [14]. To the

end of devising a controlled mean-field expansion, we begin by introducing the concept of weighted operator sums in the next section.

## II. WEIGHTED OPERATOR SUMS

We consider the extended Bose-Hubbard model on an arbitrary lattice as described by the Hamiltonian

$$\hat{H} = \sum_{\alpha\beta} \left( T_{\alpha\beta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta} + \frac{1}{2} V_{\alpha\beta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\alpha} \hat{a}_{\beta} \right), \quad (1)$$

where  $\alpha, \beta$  label the lattice sites and  $\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\beta}$  are the associated bosonic creation or annihilation operators. The kinetic term is determined by the hopping matrix  $T_{\alpha\beta}$  and the interaction part by  $V_{\alpha\beta}$ . (Both matrices are real and symmetric.) Since the above Hamiltonian cannot be diagonalized analytically, we have to employ some approximations. To this end, we introduce the concept of weighted operator sums defined via

$$\hat{X}_S[f] = \frac{1}{|S|} \sum_{\alpha \in S} f_{\alpha}(\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\alpha}), \quad (2)$$

with a set  $S \subset \mathbb{N}$  of  $|S|$  elements  $\alpha \in S$  and a function  $f_{\alpha}$  of order one, i.e., which does not scale with  $|S|$ . Hence the limit  $\lim_{|S| \rightarrow \infty} \hat{X}_S[f]$  exists (in an appropriate sense, e.g., as a weak limit) while all single addends are suppressed by  $1/|S|$  for large  $|S|$ . Examples for the form (2) include all (local) one-site operators such as  $\hat{X}_{\{\alpha\}}[\mathbf{1}] = \hat{a}_{\alpha}$  for  $|S|=1$  as well as the (global) Fourier components  $\sum_{\alpha} \hat{a}_{\alpha} \exp\{ik\alpha\}/L = \hat{a}_k/\sqrt{L}$  with  $|S|=L$  being the total number of sites for a one-dimensional chain  $S=[1, L]$ . Now, considering the commutator between two such weighted operator sums

$$[\hat{X}_S[f], \hat{X}_{S'}[f']] = \frac{|S \cap S'|}{|S| \times |S'|} \hat{X}_{S \cap S'}[f''], \quad (3)$$

with  $f''_{\alpha}(\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\alpha}) = [f_{\alpha}(\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\alpha}), f'_{\alpha}(\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\alpha})]$ , we find that they are suppressed for large  $|S|$  due to  $|S \cap S'| \leq \min\{|S|, |S'|\}$ . Hence the limit  $\lim_{|S| \rightarrow \infty} \hat{X}_S[f]$  commutes with all other weighted operator sums (including all local operators) and can thus be

approximated by a  $c$  number within the relevant Hilbert space generated by weighted operator sums acting on the ground (or thermal) state. This motivates the following asymptotic expansion for large  $|S| \gg 1$ ,

$$\hat{X}_S[f] = \hat{C}_0[f] + \frac{\hat{C}_{1/2}[f]}{\sqrt{|S|}} + \frac{\hat{C}_1[f]}{|S|} + \dots, \quad (4)$$

where the leading term  $\hat{C}_0[f]$  can be approximated by a  $c$  number and the subleading operators  $\hat{C}_{1/2}[f]$  and  $\hat{C}_1[f]$  generate the commutator (3), of order  $1/|S|$ .

Applying the concept of weighted operator sums to operators like  $\hat{X}_\Sigma[\mathbf{1}] = \sum_\beta \hat{a}_\beta / L$  or other Fourier components, we arrive at the mean-field expansion

$$\hat{a}_\alpha = \psi_\alpha + \hat{\chi}_\alpha + O(1/\sqrt{L}), \quad (5)$$

where  $\psi_\alpha$  denotes the mean field and corresponds to the leading parts  $\hat{C}_0[f]$  in Eq. (4) while the fluctuations  $\hat{\chi}_\alpha$  with  $\langle \hat{\chi}_\alpha \rangle = 0$  incorporate the noncommuting remainders. Note that (in contrast to [15]) the filling  $n_\alpha = \langle \hat{a}_\alpha^\dagger \hat{a}_\alpha \rangle = |\psi_\alpha|^2 + \langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle$  is here not assumed to be large;  $|\psi_\alpha|^2$  is the condensate part and  $\langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle$  is the remaining thermal or quantum depletion. Hence the fluctuations  $\hat{\chi}_\alpha$  are not necessarily small compared to the mean field  $\psi_\alpha$ : e.g., for half-filling  $n_\alpha = 1/2$ , the variance is obviously of order one. In order to simplify the full equation of motion derived from Eq. (1) [ $\hbar = 1$ ],

$$i\partial_t \hat{a}_\alpha = \sum_\beta (T_{\alpha\beta} \hat{a}_\beta + V_{\alpha\beta} \hat{n}_\beta \hat{a}_\alpha), \quad (6)$$

we assume that the interaction  $V_{\alpha\beta}$  involves a large number  $D \gg 1$  of sites  $\beta$  on a roughly equal footing. This could be the case, for example, for long-range interactions or for a large number of spatial dimensions. For normalized potentials  $\sum_\beta V_{\alpha\beta} \equiv V_\Sigma = O(1)$ , we may then apply the concept of weighted operator sums (2) to the term  $\sum_\beta V_{\alpha\beta} \hat{n}_\beta$  and obtain

$$\sum_\beta V_{\alpha\beta} \hat{n}_\beta = \sum_\beta V_{\alpha\beta} \langle \hat{n}_\beta \rangle + O(1/\sqrt{D}) \quad (7)$$

from Eq. (4). However, one must be careful: simply replacing  $\hat{n}_\beta$  by  $n_\beta$  in Eq. (6), we would lose the phonon modes. The subleading term  $O(1/\sqrt{D})$  can only be neglected if there is no *other* small (or large) term involved. This is precisely the case for modes with long wavelengths over many lattice sites, where the sum over  $T_{\alpha\beta} \hat{a}_\beta$ , for example, is also very small and hence the  $O(1/\sqrt{D})$  contributions become relevant. In order to describe long-wavelength modes correctly, we insert Eq. (5) into Eq. (6) to obtain the Gross-Pitaevskii equation

$$i\partial_t \psi_\alpha = \sum_\beta (T_{\alpha\beta} \psi_\beta + V_{\alpha\beta} [|\psi_\beta|^2 + \langle \hat{\chi}_\beta^\dagger \hat{\chi}_\beta \rangle] \psi_\alpha), \quad (8)$$

where we have replaced  $\sum_\beta V_{\alpha\beta} \hat{\chi}_\beta^\dagger \hat{\chi}_\beta$  by its expectation value according to the above arguments, plus the remaining fluctuation part

$$i\partial_t \hat{\chi}_\alpha = \sum_\beta \{ T_{\alpha\beta} \hat{\chi}_\beta + V_{\alpha\beta} [|\psi_\beta|^2 + \langle \hat{\chi}_\beta^\dagger \hat{\chi}_\beta \rangle] \hat{\chi}_\alpha + V_{\alpha\beta} [\psi_\beta^* \hat{\chi}_\beta + \psi_\beta \hat{\chi}_\beta^\dagger] (\psi_\alpha + \hat{\chi}_\alpha) \}. \quad (9)$$

Again, the second line is suppressed by  $O(1/\sqrt{D})$  and will only be relevant for long-wavelength modes, which involve a sum over many sites  $\alpha$ . In this case, however, the  $c$ -number term  $\sum_\alpha \psi_\alpha$  will dominate the fluctuation term  $\sum_\alpha \hat{\chi}_\alpha$  in view of Eq. (4) and hence we may approximate the bracket  $(\psi_\alpha + \hat{\chi}_\alpha)$  in the second line by  $\psi_\alpha$ , arriving at a linear operator equation

$$i\partial_t \hat{\chi}_\alpha = \sum_\beta (T_{\alpha\beta} \hat{\chi}_\beta + V_{\alpha\beta} [|\psi_\beta|^2 + \langle \hat{\chi}_\beta^\dagger \hat{\chi}_\beta \rangle] \hat{\chi}_\alpha + V_{\alpha\beta} [\psi_\beta^* \hat{\chi}_\beta + \psi_\beta \hat{\chi}_\beta^\dagger] \psi_\alpha) + O(1/\sqrt{D}), \quad (10)$$

which corresponds to the Bogoliubov-de Gennes equations for the fluctuations. Note that the approximation from Eq. (9) to Eq. (10) neglects the exchange of particles between the condensate  $|\psi_\alpha|^2$  and the thermal or quantum depletion  $\langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle$ . This exchange is governed by the subleading term  $\sum_\beta V_{\alpha\beta} \psi_\beta^* \langle \hat{\chi}_\beta \hat{\chi}_\alpha \rangle$ , which could be added to Eq. (8).

### III. QUASIPARTICLE MODES

In order to introduce quasiparticle modes, we assume translational invariance, i.e., that  $T_{\alpha\beta}$  and  $V_{\alpha\beta}$  only depend on the distance  $\alpha - \beta$  and that the condensate density is homogeneous  $|\psi_\alpha| = |\psi|$ . Nevertheless, we may still have a constant phase gradient  $\eta$  in our sample, i.e., we set  $\psi_\alpha = |\psi| \exp\{-i\mu t + i\eta\alpha\}$ . In this case, we may diagonalize Eq. (10) via a Fourier transformation

$$i\partial_t \hat{\chi}_k = (T_{k+\eta} + V_\Sigma n + V_k |\psi|^2) \hat{\chi}_k + V_k \psi^2 \hat{\chi}_{-k}^\dagger. \quad (11)$$

Note that in more than one spatial dimension,  $\alpha$  and  $\beta$  as well as  $k$  and  $\eta$  will be multi-indices (labeling the real and the inverse lattice, respectively) and  $\eta\alpha$  is a scalar product. Assuming reflection invariance  $T_k = T_k^* = T_{-k}$  and  $V_k = V_k^* = V_{-k}$  for the lattice, we see that this symmetry  $k \rightarrow -k$  is broken for the modes  $\hat{\chi}_k$  by the phase gradient  $\eta$ . The quasiparticle Hamiltonian

$$\begin{aligned} \hat{H}_\chi &= \sum_k \left\{ \hat{\chi}_k^\dagger (T_{k+\eta} + V_\Sigma n + |\psi|^2 V_k) \hat{\chi}_k + \frac{V_k}{2} (\psi^2 \hat{\chi}_k^\dagger \hat{\chi}_{-k}^\dagger + \text{H.c.}) \right\} \\ &= \sum_k \omega_k^\dagger \hat{b}_k^\dagger \hat{b}_k, \end{aligned} \quad (12)$$

can be diagonalized via the Bogoliubov transformation  $\hat{\chi}_k = u_k \hat{b}_k + v_k \hat{b}_{-k}^\dagger$  with  $|u_k|^2 - |v_k|^2 = 1$ . This yields the Bogoliubov coefficients

$$u_k = \frac{1}{1 - l_k^2}, \quad v_k = \frac{l_k}{1 - l_k^2},$$

$$l_k = \sqrt{w_k^2 + 2w_k - 1 - w_k}, \quad w_k = \frac{\bar{T}_k}{V_k |\psi|^2}. \quad (13)$$

For  $w_k = -2$ , the coefficients diverge due to  $l_k = 1$  (leading to the instability for  $\eta = 0$ , to be discussed below). The quasiparticle frequencies obey the dispersion relation ( $T_{k=0} = 0$ )

$$\omega_k^\pm = \frac{1}{2}(T_{k+\eta} - T_{k-\eta}) \pm \sqrt{\bar{T}_k^2 + 2|\psi|^2 V_k \bar{T}_k}, \quad (14)$$

where  $\bar{T}_k = (T_{k+\eta} + T_{k-\eta})/2$  and thus the branches are connected by  $\omega_k^+ = -\omega_{-k}^-$ .

In the continuum limit, i.e., for small  $k \ll 1$ , we may approximate  $T_k \approx k^2/(2m)$  due to  $T_k = T_k^* = T_{-k}$  and  $T_{k=0} = 0$  with the mass  $m$  being determined by the hopping rates. For small phase gradients  $\eta \ll k \ll 1$ , we then reproduce the usual Galilei shift

$$(\omega_k^\pm + vk)^2 = |\psi|^2 V_k \frac{k^2}{m} + \frac{k^4}{(2m)^2}, \quad (15)$$

where  $v = \eta/m$  is superfluid velocity. Now, even for purely positive  $V_{\alpha\beta}$ , the Fourier transform  $V_k$  may become negative for some  $k$  and hence the dispersion relation may develop dips (similar to the roton dip in superfluid  $^4\text{He}$ ). If  $V_k$  is sufficiently negative (compared to  $T_k$ ), the dispersion curve  $\omega_k$  may even dive below zero. Ignoring the fluctuations discussed below, the onset of instability,  $\omega_k = 0$ , marks the end of the (homogeneous) superfluid phase and the beginning of the supersolid phase where  $|\psi_\alpha|$  is periodic, i.e., inhomogeneous. The phase gradient  $\eta$  favors the supersolid phase, i.e., the transition superfluid  $\rightarrow$  supersolid occurs earlier for nonvanishing  $\eta$ . For  $\eta = T = 0$ , the frequencies  $\omega_{k=\pm k_*}$  at the roton wave number become imaginary beyond the critical point and hence these modes start to grow exponentially. For  $\eta > 0$  and  $T = 0$ , the transition occurs earlier and is slower since the frequency  $\omega_{k=\pm k_*}$  becomes negative, but not imaginary.

Hence only the coupling to some environment (fixed by the lattice) induces an instability of these quasiparticle modes. On the other hand, the depletion  $\langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle$  due to thermal or quantum fluctuations favors the superfluid phase since it reduces (for a fixed filling  $n$ ) the condensate fraction  $|\psi|^2$  and thus weakens the term  $|\psi|^2 V_k$  in Eq. (14) responsible for the roton dip. Ergo, heating up the supersolid state may yield the superfluid phase (as long as the condensate does not disappear altogether  $\psi = 0$ ), which will become important for the discussion of ‘‘supercooled’’ states which we turn to in Sec. V.

#### IV. SUPERFLUID DENSITY

Now let us study the response of the system to a small phase gradient  $\hat{a}_\alpha \rightarrow \hat{a}_\alpha \exp\{i\eta\alpha\}$ , which determines the superfluid fraction. The interaction part  $\frac{1}{2}V_{\alpha\beta}\hat{a}_\alpha^\dagger\hat{a}_\beta^\dagger\hat{a}_\alpha\hat{a}_\beta$  of the Hamiltonian (1) does not change, but the kinetic term yields

$$\frac{\partial \hat{H}}{\partial \eta} = -i \sum_{\alpha\beta} T_{\alpha\beta} (\alpha - \beta) \hat{a}_\alpha^\dagger \hat{a}_\beta, \quad (16)$$

which is a measure for the total current  $\partial \hat{H} / \partial \eta \propto \hat{J}$ , cf. the Fourier expansion in Eq. (12). For example for  $T_{\alpha\beta} \propto \delta_{\alpha,\beta+1} + \delta_{\alpha,\beta-1} - 2\delta_{\alpha,\beta}$  [15], we get the usual expression  $\hat{J} \propto i(\hat{a}_{\alpha+1}^\dagger \hat{a}_\alpha - \text{H.c.})$ . In the continuum limit of  $T_k \approx k^2/(2m)$ , we obtain

$$\hat{J} \propto \frac{\partial \hat{H}}{\partial \eta} = \frac{1}{m} \sum_k (\eta |\psi|^2 + k \hat{\chi}_k^\dagger \hat{\chi}_k) \rightarrow J_\psi + \hat{J}_\chi, \quad (17)$$

where the first term  $\eta |\psi|^2$  in the parentheses is the condensate (i.e., mean-field) contribution  $J_\psi$  and the second one,  $\hat{J}_\chi$ , stems from the fluctuations. Inserting the Bogoliubov transformation  $\hat{\chi}_k = u_k \hat{b}_k + v_k \hat{b}_{-k}^\dagger$ , we find

$$\langle \hat{\chi}_k^\dagger \hat{\chi}_k \rangle_0 = \frac{\bar{T}_k + |\psi|^2 V_k}{2\sqrt{\bar{T}_k^2 + 2\bar{T}_k |\psi|^2 V_k}} - \frac{1}{2} = \langle \hat{\chi}_{-k}^\dagger \hat{\chi}_{-k} \rangle_0, \quad (18)$$

i.e., the expectation value of the fluctuation part in the ground state vanishes  $\langle \hat{J}_\chi \rangle_0 = 0$ . Even though the quasiparticle frequencies are different in opposite directions for a nonvanishing phase gradient  $\eta$ ,  $\omega_k \neq \omega_{-k}$ , the Bogoliubov coefficients are still symmetric  $|u_k| = |u_{-k}|$  and  $|v_k| = |v_{-k}|$ . Because of the symmetry  $l_k = l_{-k}$ , from Eq. (13), quantum depletion does not contribute to the current [17].

In a thermal ensemble, as described by the density matrix  $\hat{\mathcal{Q}} = \exp\{-\hat{H}_\chi/T\}/Z$ , however, quasiparticle modes with  $\omega_k \neq \omega_{-k}$  will have different occupation numbers and hence we do get a contribution to the total flux from the fluctuations  $\langle \hat{J} \rangle \propto \sum_k (\eta |\psi|^2 + k \langle \hat{b}_k^\dagger \hat{b}_k \rangle)$ . Clearly, near the superfluid-supersolid phase transition, the major contributions occur around the roton minima at  $\pm k_*$ . Here, we consider for simplicity one spatial dimension only, but the main results apply to higher dimensions as well. Let us first study the case  $\eta = 0$ . In the continuum limit  $k \ll 1$ , we may use a Taylor expansion

$$\omega_k^2 = 2T_k |\psi|^2 V_k + T_k^2 \approx \omega_*^2 + \gamma^2 (k - k_*)^2, \quad (19)$$

around the roton minimum at the critical wave number  $k_* \ll 1$ , where  $\gamma$  is the curvature of the roton dip. Approaching the phase transition corresponds to the limit  $\omega_*^2 \rightarrow 0$  and for small  $\omega_*$  with  $\omega_* \ll T$ , the leading term scales as

$$\frac{1}{L} \sum_k \langle \hat{b}_k^\dagger \hat{b}_k \rangle = O\left(\frac{T \ln \omega_*}{\gamma}\right). \quad (20)$$

At the critical point  $\omega_* = 0$ , the  $k$  integral over the thermal distribution  $\langle \hat{b}_k^\dagger \hat{b}_k \rangle \approx T/\omega_k$  becomes weakly divergent near the roton dip at  $k_*$  where  $\omega_k \approx \gamma|k - k_*|$ , leading to the logarithmic singularity  $\ln \omega_*$ .

Now, adding a small phase gradient, one roton minimum is lifted and the other one approaches the  $\omega = 0$  axis even closer. Hence the thermal quasiparticle occupation numbers

$\langle \hat{b}_k^\dagger \hat{b}_k \rangle$  react in opposite ways and induce a net current, which is opposite to the condensate flux  $\eta |\psi|^2$ . The change due to  $\omega_* \rightarrow \omega_* \pm v k_*$  scales as

$$\langle \hat{J}_\chi \rangle \propto \frac{1}{L} \sum_k k \langle \hat{b}_k^\dagger \hat{b}_k \rangle = O\left(\frac{T v k_*^2}{\omega_* \gamma}\right). \quad (21)$$

For small enough  $\omega_*$  or, alternatively, for large enough temperatures  $T > T_{\text{cr}} = O(\omega_* m \gamma |\psi|^2 / k_*^2)$ , the current induced by the thermal fluctuations can easily compensate the condensate (mean-field) contribution  $\eta |\psi|^2$ . Thus, the superfluid fraction can be significantly reduced and may even become negative (which is also occurring in  $\pi$ -Josephson junctions [16]), i.e., the phase gradient  $\eta$  entails a net current  $\langle \hat{J} \rangle$  in the *opposite* direction.

Such a negative superfluid density induces a thermodynamical instability [18]: As discussed before, the current  $\langle \hat{J} \rangle$  is a measure for the response of the system to a phase gradient  $\langle \partial \hat{H} / \partial \eta \rangle$ . Inserting the canonical ensemble  $\hat{\rho} = \exp\{-\hat{H}/T\}/Z$ , we see that the expectation value  $\langle \partial \hat{H} / \partial \eta \rangle = \partial F / \partial \eta$  equals the change of the free energy  $F = E - TS = \langle \hat{H} \rangle + T \langle \ln \hat{\rho} \rangle$ . Since a stable equilibrium state in an isothermal environment corresponds to a minimum of the free energy, a negative superfluid density  $\partial \langle \hat{J} \rangle / \partial \eta < 0$  shows that the system is unstable against the spontaneous generation of local phase gradients (since  $\eta=0$  is a maximum of the free energy).

Note that a negative superfluid density does not require a large thermal depletion: as we may infer from Eq. (20), the thermal occupation number  $\sum_k \langle \hat{b}_k^\dagger \hat{b}_k \rangle$  scales merely logarithmically with  $\omega_*$  and hence it can be much smaller than the condensate fraction  $|\psi|^2$  (e.g., for  $T \leq \gamma$  and  $k_* \ll 1 \rightsquigarrow k_* \ln \omega_* < 1$ ). Of course, in addition to thermal occupation, the condensate is also depleted by quantum effects. This quantum depletion survives at zero temperatures and is given by Eq. (18) via  $\langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle = \sum_k \langle \hat{\chi}_k^\dagger \hat{\chi}_k \rangle / L$ . With the same approximations as in Eq. (20), we get again merely a logarithmic dependence

$$\langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle_0 = O\left(\frac{k_*^2 \ln \omega_*}{m \gamma}\right). \quad (22)$$

Consequently, a vanishing superfluid density  $\partial \langle \hat{J} \rangle / \partial \eta = O(\eta)$ , which marks the end of the (homogeneous) superfluid phase may occur even when the total (thermal plus quantum) depletion is very small,  $|\psi|^2 \gg \langle \hat{\chi}_\beta^\dagger \hat{\chi}_\beta \rangle$ , and hence the condensate fraction is still near one. Note that this behavior is opposite to (bulk) superfluid  $^4\text{He}$ , where the superfluid fraction (near 100% for low temperatures) strongly exceeds the condensate part (of order 10%).

## V. “SUPERCOOLED” STATES

Although the depletion was small,  $|\psi|^2 \gg \langle \hat{\chi}_\beta^\dagger \hat{\chi}_\beta \rangle$ , in the cases under consideration, we would like to stress that the presented controlled mean-field expansion (5) can also be

applied to the case of large depletions  $\langle \hat{\chi}_\beta^\dagger \hat{\chi}_\beta \rangle = O(|\psi|^2)$ . This generalization can be achieved by demanding that  $V_k$  is strongly peaked at the origin  $V_{k=0} = V_\Sigma = O(1)$  and much smaller otherwise  $V_{|k|>k_0} \ll 1$  such that the width  $k_0$  of the peak at the origin is much smaller than the typical  $k$  values (position  $k_*$  and breadth  $1/\sqrt{\gamma}$ ) associated with the roton dips (where  $\langle \hat{\chi}_k^\dagger \hat{\chi}_k \rangle$  yields the major contribution). To see how this works, let us compare  $\sum_\beta V_{\alpha\beta} \hat{\chi}_\beta$ , which must be small within our approach, with the depletion  $\langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle = \sum_k \langle \hat{\chi}_k^\dagger \hat{\chi}_k \rangle / L$ . Calculating the squared norm  $\langle |\sum_\beta V_{\alpha\beta} \hat{\chi}_\beta|^2 \rangle$ , we get  $\sum_k |V_k|^2 \langle \hat{\chi}_k^\dagger \hat{\chi}_k \rangle / L$ . Similarly, higher orders yield a sum over several wave numbers containing Fourier components at linear combinations of roton wave numbers  $V_{k \pm k'}$ . Consequently, all these terms are suppressed even though the quantum depletion may be large.

Given these requirements, one may obtain “supercooled” states, which are long-lived superfluid phases in a parameter region where the true ground state is supersolid. In order to demonstrate the main idea, let us consider the following *gedanken* experiment: We start in the superfluid phase at  $T=0$ , where 90% of the particles are in the condensate  $|\psi|^2$  and 10% in the quantum depletion  $\langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle$ . Now we remove 80% of the particles (e.g., by a Raman transition with no momentum transfer incurred) by decreasing the condensate part  $|\psi|^2$  only, i.e., we leave the modes with  $k \neq 0$  forming the quantum depletion untouched. Simultaneously, we increase the interaction strength  $V_k$  (e.g., via a Feshbach resonance) such that the product  $|\psi|^2 V_k$  remains constant, leaving the quasiparticle spectrum intact. After that procedure, half of the remaining particles are in the condensate  $|\psi|^2$  and the other half are in the quantum depletion  $\langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle = |\psi|^2$ . These anomalously large quantum fluctuations are caused by the increased interaction  $V_k$ , which is so strong that the true ground state (with this filling  $n = |\psi|^2 + \langle \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha \rangle$ ), having significantly smaller depletion, is supersolid. However, the immediate transition to the supersolid state is prevented by the fact that only half the particles are in the condensate. Because the quasiparticle modes have the same positive energies as before, the system is linearly stable. Similar to the thermodynamical instability caused by a negative superfluid density, the decay to the true supersolid ground state is mediated by the subdominant term  $\sum_\beta V_{\alpha\beta} \psi_\beta^* \langle \hat{\chi}_\beta \hat{\chi}_\alpha \rangle$ . Ergo, the predicted supercooled state is long lived and thus might be accessible to an experimental verification.

## VI. CONCLUSION

In summary, by means of a controlled expansion into powers of the small parameter  $1/\sqrt{D}$ , yielding the mean field  $\psi$  plus (thermal and quantum) fluctuations  $\hat{\chi}_\alpha$ , we are able to study the impact of these fluctuations onto the superfluid-supersolid phase transition analytically. In addition to the instabilities indicating the end of the (homogeneous) superfluid phase known from mean-field dynamics, which occur when the roton dip touches the  $\omega=0$  axis, the fluctuations induce a thermodynamic instability even *before* reaching the classical critical point  $\omega_*=0$ . This breakdown of the homogeneous superfluid is associated with a negative superfluid



density and occurs rather slowly, since changes of the mean field  $\psi$  induced by fluctuations  $\hat{\chi}_\alpha$  are governed by the subdominant term  $\sum_\beta V_{\alpha\beta} \psi_\beta^* \langle \hat{\chi}_\beta \hat{\chi}_\alpha \rangle$  in Eq. (10), which is effectively a  $O(1/\sqrt{D})$  correction to the Gross-Pitaevskii equation (8). Finally, even though the thermodynamical instability effect is governed by thermal fluctuations, quantum fluctuations do also generate intriguing phenomena near the critical point like supercooled states.

## ACKNOWLEDGMENTS

We thank G. E. Volovik for helpful discussions. This work was supported by the Australian Research Council, the Emmy Noether Programme of the German Research Foundation (DFG, Grant No. SCHU 1557/1-2,3), as well as the DFG Grant No. FI 690/3-1.

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- [1] O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956).  
 [2] A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP **29**, 1107 (1969).  
 [3] A. J. Leggett, Phys. Rev. Lett. **25**, 1543 (1970).  
 [4] E. Kim and M. H. W. Chan, Nature (London) **427**, 225 (2004); A. J. Leggett, Science **305**, 1921 (2004).  
 [5] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).  
 [6] K. Xu, Y. Liu, D. E. Miller, J. K. Chin, W. Setiawan, and W. Ketterle, Phys. Rev. Lett. **96**, 180405 (2006).  
 [7] M. Greiner *et al.*, Nature (London) **415**, 39 (2002).  
 [8] G. G. Batrouni, R. T. Scalettar, G. T. Zimányi, and A. P. Kampf, Phys. Rev. Lett. **74**, 2527 (1995).  
 [9] V. W. Scarola and S. Das Sarma, Phys. Rev. Lett. **95**, 033003 (2005).  
 [10] D. L. Kovrizhin, G. Venketeswara Pai, and S. Sinha, Europhys. Lett. **72**, 162 (2005).  
 [11] K. Góral, L. Santos, and M. Lewenstein, Phys. Rev. Lett. **88**, 170406 (2002); S. Yi, T. Li, and C. P. Sun, *ibid.* **98**, 260405 (2007).  
 [12] S. Wessel and M. Troyer, Phys. Rev. Lett. **95**, 127205 (2005); D. Heidarian and K. Damle, *ibid.* **95**, 127206 (2005); R. G. Melko *et al.*, *ibid.* **95**, 127207 (2005).  
 [13] C. Josserand, Y. Pomeau, and S. Rica, Phys. Rev. Lett. **98**, 195301 (2007).  
 [14] A. A. Burkov and L. Balents, Phys. Rev. B **72**, 134502 (2005).  
 [15] R. Schützhold, M. Uhlmann, Y. Xu, and U. R. Fischer, Phys. Rev. Lett. **97**, 200601 (2006).  
 [16] L. N. Bulaevskii, V. V. Kuzii, and A. A. Sobyenin, JETP Lett. **25**, 290 (1977).  
 [17] Note, however, that an opposite current could also be generated by pure quantum effects due to nonequilibrium phenomena: approaching the transition too fast, we get nonadiabatic excitations,  $\langle \hat{b}_k^\dagger \hat{b}_k \rangle > 0$ , which are stronger for small  $\omega_k$ .  
 [18] Thermodynamical stability within the supersolid phase has been discussed, e.g., in G. G. Batrouni and R. T. Scalettar, Phys. Rev. Lett. **84**, 1599 (2000); P. Sengupta, L. P. Pryadko, F. Alet, M. Troyer, and G. Schmid, Phys. Rev. Lett. **94**, 207202 (2005).