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Phase transitions in three-dimensional bosonic systems in optical lattices

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Abstract. We formulate the collective quantum field theory for three-dimensional bosonic optical lattices and evaluate its consequences in a mean-field approximation to two collective fields, proposed by Cooper *et al* (2011 *Phys. Rev.* A **83** 053622), and in a lowest-order variational perturbation theory. It is shown that the present mean-field approximation predicts some essential features of the experimentally observed dependence of the critical temperature on the coupling strength and a second-order quantum phase transition. In contrast to a recent prediction for atomic gases given by Cooper *et al*, our finding indicates no superfluid state with zero condensate fraction.

Keywords: Hubbard model (theory), Bose–Einstein condensation (theory), phase diagrams (theory), optical lattices

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Contents

1. Introduction **2**

2. Collective quantum field theory of the 3D Bose–Hubbard model **5**
2.1. The condensed phase 7
2.2. Normal and anomalous densities 11
2.3. The symmetric phase 14

3. Variational perturbation theory in optical lattices **14**
3.1. The fractions $n_{\mathbf{u}}$ and δ in VPT 17

4. Results and discussion **18**
4.1. The quantum phase transition in the theory with two collective quantum fields and VPT 18
4.2. The critical temperature T_c^0 for ideal cases 19
4.3. The shift in T_c caused by the interaction 20

5. Conclusion **24**

Acknowledgments **25**

Appendix A **25**

Appendix B **27**

References **27**

1. Introduction

Optical lattices are gases of ultracold atoms trapped in periodic potentials created by periodically arranged intersecting standing waves of laser light. The interest in experimental and theoretical investigations of these artificial crystals is caused by the following two factors [1].

(1) Neutral atoms in these optical lattices have several attractive features that make them interesting candidates for use in the realization of a quantum computer [2].

(2) They may be used to simulate various lattice models of fundamental importance in condensed matter physics, since they permit controlled studies of solid-state physics in which one can fine-tune the interaction strength for various geometries of the lattices. In particular, it is possible to control the Hamiltonian parameters and study various regimes of system parameters.

The lattice of bosons with short-range repulsive pair interaction trapped in an optical lattice may be described by a Hamiltonian of Bose–Hubbard type:

$$H = -J \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{j}} + \frac{U}{2} \sum_{\mathbf{i}}^{N_s} \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{i}} \hat{b}_{\mathbf{i}} + \sum_{\mathbf{i}}^{N_s} (\varepsilon_{\mathbf{i}} - \mu) \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{i}}, \tag{1}$$

where: $\hat{b_{\mathbf{i}}}^{\dagger}$ and $\hat{b_{\mathbf{i}}}$ are the bosonic creation and annihilation operators on the site i; the sum over $\langle \mathbf{i}, \mathbf{j} \rangle$ includes only pairs of nearest neighbors; J is the hopping amplitude, which is responsible for the tunneling of an atom from one site to another neighboring site; U is the on site repulsion energy; and N_s is the number of sites.

At zero temperature with an *integer filling factor* $\nu \equiv N/N_s$, where N is the total number of atoms, a system of bosons described by the Hamiltonian (1) could be in a superfluid (SF) or in a Mott insulator (MI) phase. Clearly the quantum phase transition (QPT) between these two phases is ruled by the dimensionless interaction strength parameter $u = U/J$. For small u, the hopping term dominates the system, favoring it being in the SF phase. For large $u \gg 1$, on the other hand, the system exhibits a MI phase.

A critical interaction strength $u_{\mathrm{crit}} = 29.34$ was found for $d = 3$ by Monte Carlo calculations [3] at a filling factor of $\nu = 1$, and this agrees well with the experimental data [4].

To make for easier reading, we summarize some specific features of these two phases. The SF phase is characterized by a long-range correlation, a continuous (gapless) excitation spectrum and a finite compressibility. Since there exists a condensate with a finite number of particles, $n_{\mathbf{0}}$, the gauge symmetry is spontaneously broken in accordance with theorems of Bogoliubov and Ginibre. In contrast, in the MI phase, there is no long-range correlation or breaking of the gauge symmetry. The excitation spectrum has a gap and the system is incompressible, since the number of atoms per site is fixed. The mobilities of the atoms are completely different in the two phases. In the SF phase they can easily move from one site to another site by tunneling, whereas in the MI phase, they are localized.

Finite-temperature phases of optical lattices have been studied by means of quantum Monte Carlo (QMC) calculations as well as experimentally for $d = 3$. As expected, the system behaves as a normal fluid (NF) at $T > T_c$. A most interesting observation was made in [3, 4]: in contrast to the case for a system of dilute Bose gases, the critical temperature is downshifted at the transition to the MI phase.

Theoretical approaches based on the Bose–Hubbard model, which is not exactly soluble even in one dimension, have been summarized recently in textbooks [5]–[7]. Most of them use perturbative expansions in powers of J/U and give qualitatively a good description of the phase transition boundary [8, 9]. As to the nonperturbative approaches, they mainly exploit the Gutzwiller ansatz, where the wavefunction is expanded in local Fock states with variational coefficients. Although such an approach is good even in the description of the dynamics of the system [10]–[13], since it is exact for $d \to \infty$, its reliability decreases dramatically for $d = 1$.

Among the various kinds of existing mean-field theories in the literature, the bosonic dynamical mean-field theory (B-DMFT) seems to be the most powerful. Originally proposed by Byczuk and Vollhardt [14] and further developed by Anders *et al* [15], the

J. Stat. Mech. (2014) P01003

B-DMFT maps the Bose–Hubbard model onto the self-consistent solution of a bosonic impurity model with coupling to a reservoir of normal and condensed bosons. The net output of this procedure is excellent. It gives us an accurate description of the phase diagrams, the condensate order parameter and other observables of the cubic lattice Bose–Hubbard model, as obtained by QMC calculations. However, although the B-DMFT is numerically exact and flexible, it is computationally expensive, since one has to use continuous time QMC evaluations in order to solve its equations. Moreover, strictly speaking, the Hugenholtz–Pines theorem (see section 2.2 below) does not hold in B-DMFT (see figure 10 of [15]).

The application of nonperturbative renormalization group theory has revealed new scaling properties of optical lattices. Rancon and Dupuis [16] have recently shown that thermodynamic quantities of the Bose–Hubbard model can be expressed using universal scaling functions of the dilute Bose gas universality class.

As to the Bogoliubov theory, it provides an accurate description of the excitation spectrum for the SF phase, but fails to describe the SF $\rightarrow$ MI transition. In fact, the first application of a mean-field approach was made in the Hartree–Fock–Popov (HFP) approximation to optical lattices by Stoof *et al* [17]. By studying the dependence of the condensate number $n_{\mathbf{0}}$ on u, i.e. $n_{\mathbf{0}}(U/J)$, they observed that $n_{\mathbf{0}}$ never reaches zero, even in the strong-coupling limit ($u \rightarrow \infty$), implying that this approximation is unable to predict a QPT of SF $\rightarrow$ MI. In contrast to this, the two-loop approximation given by the present authors in [18] suggests the existence of such a QPT, but the critical value of u_{crit} was found to be rather small: $u_{\mathrm{crit}}(\text{two loops}) \approx 6$ for $d = 3$. So, the question of the power of an approximation, based on mean-field theory, other than B-DMFT, to adequately describe phase diagrams of optical lattices remains open. It is, therefore, desirable to develop a nonperturbative approach which would be suitable for dimensions $d = 1, 2, 3$.

An alternative approach to the treatment of dilute Bose gases has recently been proposed by Cooper *et al* [19, 20] under the name of *leading-order auxiliary field theory* (LOAF). They found a way of fixing the degeneracy in the elimination of the interaction by auxiliary collective pair and density fields by choosing a special form of a generalized Hubbard–Stratonovich transformation. Although their approach gives no QPT for a homogeneous Bose gas at zero temperature, it predicts a desirable second-order BEC transition at finite temperatures and exhibits a positive shift in the critical temperature T_{c} that is consistent with Monte Carlo and other calculations [21, 22]. One of the novel features of those calculations is that for $T > T_{\mathrm{c}}$ it predicts a novel type of superfluid phase that does not have a condensate [23]. Although such a phase has not been observed yet, it was justified by the existence of a nonzero anomalous density δ, in the region $T_{\mathrm{c}} < T \leq T^*$, where T^* is the temperature of transition to the normal phase.

In the present work we shall formulate a similar theory with two collective quantum fields for discrete systems such as optical lattices and ask the following questions.

- Does it predict a SF $\rightarrow$ MI quantum phase transition?
- Does it predict the suppression of T_{c} at large u?
- Does it predict a new phase, mentioned above, for optical lattices too?

J. Stat. Mech. (2014) P01003

Our results will be compared with those from another well-known mean-field approximation, the Hartree–Fock–Bogoliubov (HFB) approximation, which is widely used to describe BEC in homogeneous Bose gases and in triplons [24, 25] in magnetic insulators, and will also be extended here to optical lattices. Below we use $\hbar = k_{\mathrm{B}} = 1$.

The paper is organized as follows. In sections 2 and 3 we shall derive collective quantum field theory and HFB approaches for optical lattices, respectively. The results and discussions will be presented in section 4, and the conclusions will be stated in section 5.

2. Collective quantum field theory of the 3D Bose–Hubbard model

In the Wannier representation, the Euclidean action corresponding to the Bose–Hubbard Hamiltonian is given by [18]

$$\mathcal{A}(\psi^*,\psi) = \int_0^\beta \mathrm{d}\tau \Bigg\{ \sum_{\mathbf{i}} \psi^*(\mathbf{x_i},\tau)[\partial_\tau - \mu]\psi(\mathbf{x_i},\tau) - J\sum_{\langle i,j\rangle} \psi^*(\mathbf{x_i},\tau)\psi(\mathbf{x}_j,\tau) + \frac{U}{2}\sum_{\mathbf{i}} \psi^*(\mathbf{x_i},\tau)\psi^*(\mathbf{x_i},\tau)\psi(\mathbf{x_i},\tau)\psi(\mathbf{x_i},\tau)\Bigg\}, \tag{2}$$

where μ is the chemical potential and $\beta = 1/T$. The lattice points lie at the positions [26]

$$\mathbf{x_i} = \mathbf{i}\, a, \tag{3}$$

where a is the lattice spacing, and

$$\mathbf{i} \equiv (i_1, i_2, \ldots, i_d), \tag{4}$$

are integer-valued vectors.

The partition function Z, and the grand thermodynamic potential Ω, can be found from

$$Z = \int D\psi^* D\psi \mathrm{e}^{-\mathcal{A}(\psi^*,\psi)}, \tag{5}$$

$$\Omega = -T \ln Z. \tag{6}$$

The ground state expectation value of an operator $\hat{O}(\psi^*,\psi)$ can be expressed as a functional integral:

$$\langle \hat{O} \rangle = \frac{1}{Z}\int \mathcal{D}\psi^*\mathcal{D}\psi \hat{O}(\psi^*,\psi)\mathrm{e}^{-\mathcal{A}(\psi^*,\psi)}. \tag{7}$$

With the help of a Hubbard–Stratonovich transformation, the interaction term in (2) can be eliminated by adding to the action in the exponent of (5) a dummy action [27]:

$$\mathcal{A}_{\mathrm{pair}}[\psi^*,\psi,\Delta,\Delta^*] = \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \left\{ \frac{1}{2U}|\Delta(\mathbf{x_i},\tau) - U\psi(\mathbf{x_i},\tau)\psi(\mathbf{x_i},\tau)|^2 \right\} \tag{8}$$

J. Stat. Mech. (2014) P01003

containing a *pair field* Δ. After this we form the path integral $\int \mathcal{D}\Delta\mathcal{D}\Delta^* \mathrm{e}^{-\mathcal{A}_{\mathrm{pair}}[\psi^*,\psi,\Delta,\Delta^*]}$, and integrate out the pair field. This produces a multiplication of the partition function Z by a trivial constant factor.

It has been emphasized in [27] and the textbook [28] that this procedure is highly degenerate. Actually, instead of (8), one could just as well have introduced a plasmon field $\varphi(\mathbf{x},\tau)$ by adding to the action in the exponent of (5) a dummy action

$$\mathcal{A}_{\mathrm{pl}}[\psi^*,\psi,\varphi] = \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \left\{ -\frac{1}{2U} \left[\varphi(\mathbf{x_i},\tau) - U\psi^*(\mathbf{x_i},\tau)\psi(\mathbf{x_i},\tau)\right]^2 \right\}, \tag{9}$$

and forming a functional integral $\int \mathcal{D}\varphi \mathrm{e}^{-\mathcal{A}_{\mathrm{pair}}[\psi^*,\psi,\varphi]}$, which again multiplies Z by a trivial constant.

Diagrammatically, the degeneracy is caused by the fact that the sum of all collective field diagrams will always produce the same result if evaluated to *all* orders in perturbation theory. Each of these collective fields reproduces all effects of the interaction if it is integrated functionally. A difference appears if the evaluation is restricted to a mean-field approximation. Then it depends on the dominance of certain dynamical effects which field is preferable.

In principle, we can also add a combination of $\mathcal{A}_{\mathrm{pair}}$ and $\mathcal{A}_{\mathrm{pl}}$, and still leave the physical properties of the system unchanged—for instance $\mathcal{A}_{\mathrm{pl}} \cosh^2\theta - \mathcal{A}_{\mathrm{pair}} \sinh^2\theta$. Diagrammatically, however, the degeneracy cannot be easily verified since a calculation of the diagrams to all orders is really impossible. It can only be done to some finite order, for instance in a loop expansion, so the mathematical equivalence is initially of little use.

One method for avoiding the degeneracy and making the collective field approach unique was pointed out a long time ago [29]. It is based on an extension of the standard effective action $\Gamma[\Psi^*,\Psi]$, whose functional expansion terms are the one-particle irreducible vertex functions of the theory. The symbol Ψ denotes the expectations of the field $\psi(x,\tau)$. A unique version of collective fields can be introduced by going to a *higher effective action* $\mathcal{A}[\Psi^*,\Psi,\Delta,\Delta^*,\Phi]$. While the ordinary effective action $\Gamma[\Psi^*,\Psi]$ is derived from a Legendre transformation of the generating functional of the theory, $W[\eta,\eta^*]$, in which additional source terms $\eta\psi^* + \eta^*\psi$ have been added to the action, the higher effective action is obtained from the Legendre transformation of a generating functional $W[\eta,\eta^*,j,K,K^*]$ in which additional sources have been added to the action coupled to the density and the pair fields. The higher effective action will depend on the expectations of the fields $\psi,\psi^*,\rho\propto\psi^*\psi,\Delta\propto\psi\psi$ and $\Delta^*\propto\psi^*\psi^*$. At the end, it must merely be *extremized*, and no extra functional integrals can cause any double counting of Feynman diagrams. The expansion terms in the higher effective action are the two-particle irreducible vertex functions of the theory.

Another method that also abandons the fluctuations of the collective fields in favor of a collective classical field has been developed in recent years from a generalization of a variational approach to path integrals [30] to all orders in perturbation theory. It was extremely successful and has led to the most accurate theory of critical phenomena [31] so far, named variational perturbation theory (VPT) (for a review paper see [32]).

A third method which has recently been proposed and applied [19, 20] uses the combination of both fully fluctuating collective fields implied by the above dummy action

$\mathcal{A}_{\rm pl}\cosh^2\theta - \mathcal{A}_{\rm pair}\sinh^2\theta$ for the particular value $\sinh\theta = 1$. This choice is preferable if we want the mean-field approximation to exhibit excitations that have no energy gap, to comply with the Nambu–Goldstone theorem. After a trivial change of the normalization of plasmon and pair fields in the total action $\mathcal{A} + \mathcal{A}_{\rm pl}\cosh^2\theta - \mathcal{A}_{\rm pair}\sinh^2\theta$ one arrives at

$$\mathcal{A} = \mathcal{A}_\psi[\psi^*,\psi] + \mathcal{A}_\varphi[\varphi] + \mathcal{A}_\Delta[\Delta,\Delta^*], \tag{10}$$

with

$$\begin{aligned}\mathcal{A}_\psi[\psi^*,\psi] = \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \Big\{ &\psi^*(\mathbf{x_i},\tau)[\partial_\tau - \mu + \varphi(\mathbf{x_i},\tau)\cosh\theta]\psi(\mathbf{x_i},\tau) \\ &- \frac{1}{2}\sinh\theta[\Delta\psi^*(\mathbf{x_i},\tau)\psi^*(\mathbf{x_i},\tau) + \Delta^*\psi(\mathbf{x_i},\tau)\psi(\mathbf{x_i},\tau)]\Big\} \\ &- J\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i,j}} \psi^*(\mathbf{x_i},\tau)\psi(\mathbf{x_j},\tau),\end{aligned} \tag{11}$$

$$\mathcal{A}_\varphi[\varphi] = -\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \frac{\varphi^2(\mathbf{x_i},\tau)}{2U}, \qquad \mathcal{A}_\Delta[\Delta,\Delta^*] = \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \frac{\Delta(\mathbf{x_i},\tau)\Delta^*(\mathbf{x_i},\tau)}{2U}. \tag{12}$$

At the level of the fully fluctuating fields φ, Δ, Δ^*, the parameter θ is still arbitrary; this will be fixed in section 2.1.

Now we consider separately two regions, with and without a condensed phase.

2.1. The condensed phase

In this phase, the $U(1)$ gauge symmetry is spontaneously broken. It can be studied after a Bogoliubov shift of the field [33]

$$\psi(x_\mathbf{i},\tau) = \psi_\mathbf{0} + \widetilde{\psi}(x_\mathbf{i},\tau), \tag{13}$$

with

$$\psi_\mathbf{0} = \sqrt{\nu n_\mathbf{0}}, \tag{14}$$

where the $n_\mathbf{0} = N_\mathbf{0}/N$ is the condensate fraction. It is a constant in the absence of a magnetic trap. The fluctuating field $\tilde{\psi}(x,\tau)$ must satisfy the condition

$$\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \tilde{\psi}(x_\mathbf{i},\tau) = 0. \tag{15}$$

Substituting (13) into (11), and decomposing the quantum field $\tilde{\psi}(\mathbf{x_i},t)$ into its real and imaginary parts $\psi_1(\mathbf{x_i},t)$ and $\psi_2(\mathbf{x_i},t)$ as follows:

$$\begin{aligned}\tilde{\psi}(\mathbf{x_i},t) &= \frac{1}{\sqrt{2}}(\psi_1(\mathbf{x_i},t) + \mathrm{i}\psi_2(\mathbf{x_i},t)), \\ \tilde{\psi}^*(\mathbf{x_i},t) &= \frac{1}{\sqrt{2}}(\psi_1(\mathbf{x_i},t) - \mathrm{i}\psi_2(\mathbf{x_i},t)),\end{aligned} \tag{16}$$

we may separate the action as follows:

$$\mathcal{A} = \mathcal{A}_0 + \mathcal{A}_2 + \mathcal{A}_\Delta + \mathcal{A}_\varphi, \tag{17}$$

with

$$\begin{aligned}\mathcal{A}_0 = &-N_\mathrm{s}\beta\nu n_{\mathbf{0}}(\mu + Jz_0) \\ &+ \nu n_{\mathbf{0}} \sum_{\mathbf{i}} \int_0^\beta \mathrm{d}\tau \left[\cosh\theta\varphi(x_{\mathbf{i}},\tau) - \tfrac{1}{2}\sinh\theta\left(\Delta(x_{\mathbf{i}},\tau) + \Delta^*(x_{\mathbf{i}},\tau)\right)\right],\end{aligned} \tag{18}$$

$$\begin{aligned}\mathcal{A}_2 = &\tfrac{1}{2}\sum_{\mathbf{i}} \int_0^\beta \mathrm{d}\tau \sum_{a,b=1,2} \left[\mathrm{i}\varepsilon_{ab}\tilde{\psi}_a(x_{\mathbf{i}},\tau)\partial_\tau\tilde{\psi}_b(x_{\mathbf{i}},\tau) + \tilde{\psi}_a(x_{\mathbf{i}},\tau)X_a\tilde{\psi}_b(x_{\mathbf{i}},\tau)\delta_{ab}\right] \\ &- \frac{J}{2}\int_0^\beta \mathrm{d}\tau \sum_{\langle\mathbf{i},\mathbf{j}\rangle}\sum_a \tilde{\psi}_a(x_{\mathbf{i}},\tau)\tilde{\psi}_a(x_j,\tau),\end{aligned} \tag{19}$$

where $\mathcal{A}_\Delta$ and $\mathcal{A}_\varphi$ are given in equation (12), ε_{ab} is an antisymmetric tensor with $\varepsilon_{12} = -\varepsilon_{21} = 1$, $z_0 = 2d$, and

$$\begin{aligned}X_1 &= -\mu + \varphi(x_{\mathbf{i}},\tau)\cosh\theta - \tfrac{1}{2}\sinh\theta\left(\Delta^*(x_{\mathbf{i}},\tau) + \Delta(x_{\mathbf{i}},\tau)\right), \\ X_2 &= -\mu + \varphi(x_{\mathbf{i}},\tau)\cosh\theta + \tfrac{1}{2}\sinh\theta\left(\Delta^*(x_{\mathbf{i}},\tau) + \Delta(x_{\mathbf{i}},\tau)\right).\end{aligned} \tag{20}$$

For a homogeneous system the condensate is uniform and it is convenient to decompose the fluctuations into a Fourier series as follows [34, 35]:

$$\tilde{\psi}_a(\mathbf{x}_{\mathbf{i}},\tau) = \frac{1}{\beta\sqrt{N_\mathrm{s}^d}}\sum_{\mathbf{q},\omega_n}{}' \int_0^\beta \psi_a(\mathbf{q},\omega_n)\mathrm{e}^{-\mathrm{i}\omega_n\tau}\exp\left[\mathrm{i}\mathbf{x}_{\mathbf{i}}\mathbf{p}_{\mathbf{q}}\right] \tag{21}$$

where the $\omega_n = 2\pi nT$ are Matsubara frequencies, and $\mathbf{p}_{\mathbf{q}} \equiv \{q_1, q_2, \ldots, q_d\}\ 2\pi/N_\mathrm{s}a$, with $q_{\mathbf{i}}$ running from 1 to $N_\mathrm{s} - 1$, are the discrete-valued momentum vectors in the Brillouin zone. The momentum sum is explicitly

$$\frac{1}{N_\mathrm{s}}\sum_{\mathbf{q}}{}' \equiv \frac{1}{N_\mathrm{s}^d}\sum_{q_1=1}^{N_\mathrm{s}-1}\sum_{q_2=1}^{N_\mathrm{s}-1}\cdots\sum_{q_d=1}^{N_\mathrm{s}-1}. \tag{22}$$

The prime on the symbol indicates that the $\mathbf{p} = 0$-mode is omitted since it is contained in the subtracted $\psi_{\mathbf{0}}$. This will be useful for avoiding possible infrared divergencies, especially for $d < 3$.

In momentum space, the quadratic term $\mathcal{A}_2$ reads

$$\mathcal{A}_2 = \tfrac{1}{2}\sum_{\mathbf{q},\mathbf{q}',m,n} \psi_a(\mathbf{q},\omega_n)G^{-1}_{ab}(\mathbf{q},\omega_n;\mathbf{q}',\omega_m)\psi_b(\mathbf{q}',\omega_m), \tag{23}$$

with the propagator

$$G(\omega_n,\mathbf{q}) = \frac{1}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})}\begin{pmatrix}\varepsilon(\mathbf{q}) + X_2 - Jz_0 & \omega_n \\ -\omega_n & \varepsilon(\mathbf{q}) + X_1 - Jz_0\end{pmatrix}, \tag{24}$$

J. Stat. Mech. (2014) P01003

where the bare dispersion $\varepsilon(\mathbf{q})$ and phonon dispersion $\mathcal{E}(\mathbf{q})$ are given by

$$\varepsilon(\mathbf{q}) = 2J\left(d - \sum_{\alpha=1}^{d}\cos(2\pi q_\alpha/N_\mathrm{s})\right), \tag{25}$$

$$\mathcal{E}(\mathbf{q}) = \sqrt{(X_1 + \varepsilon(\mathbf{q}) - Jz_0)(X_2 + \varepsilon(\mathbf{q}) - Jz_0)}. \tag{26}$$

In the long-wavelength limit, $\varepsilon(\mathbf{q})$ behaves like

$$\varepsilon(\mathbf{q}) \approx J\frac{4\pi^2}{N_\mathrm{s}^2}\mathbf{q}^2 = Ja^2\mathbf{p}^2 + \cdots. \tag{27}$$

By comparison with the usual momentum dependence of a free single-particle energy $\mathbf{p}^2/(2M)$, we identify the particle mass $M = 1/(2Ja^2)$.

Note that in coordinate space the Green function is defined by

$$\begin{aligned} G_{ab}(\mathbf{x_i}, \tau; \mathbf{x_j}, \tau') &\equiv G_{ab}(\mathbf{x_i} - \mathbf{x_j}, \tau - \tau') \\ &= \langle \psi_a(\mathbf{x_i}, \tau)\psi_b(\mathbf{x_j}, \tau')\rangle \\ &= \frac{1}{N_\mathrm{s}\beta}\sum_n\sum_q \mathrm{e}^{\mathrm{i}\omega_n(\tau-\tau')}\mathrm{e}^{\mathrm{i}\mathbf{q}(\mathbf{x_i}-\mathbf{x_j})}G_{ab}(\omega_n, \mathbf{q}). \end{aligned} \tag{28}$$

The thermodynamics of the system can be calculated from the partition function Z, which is a functional integral over all fields ψ_1, ψ_2, φ, and the Δ and Δ^*:

$$Z = \int \mathcal{D}\psi_1\mathcal{D}\psi_2\mathcal{D}\varphi\mathcal{D}\Delta\mathcal{D}\Delta^*\mathrm{e}^{-\mathcal{A}_0-\mathcal{A}_2-\mathcal{A}_\Delta-\mathcal{A}_\varphi}. \tag{29}$$

The first integrations by ψ_1 and ψ_2 are Gaussian and may be evaluated easily by using well-known formula

$$\begin{aligned} \int \mathcal{D}\psi_1\mathcal{D}\psi_2\, \exp\Bigg[&-\tfrac{1}{2}\sum_{a,b=1,2}\int \psi_a(x)G^{-1}_{ab}(x,y)\psi_b(y)\,\mathrm{d}x\,\mathrm{d}y \\ &- \int j_1(x)\psi_1(x)\mathrm{d}x - \int j_2(x)\psi_2(x)\,\mathrm{d}x\Bigg] \\ = \sqrt{\mathrm{Det}\,G}\,\exp&\left[\sum_{a,b=1,2}\int j_a(x)G_{ab}(x,y)j_b(y)\,\mathrm{d}x\,\mathrm{d}y\right]. \end{aligned} \tag{30}$$

The integrations over the fluctuating collective fields, however, cannot be performed exactly, since they are nontrivially contained in $\sqrt{\mathrm{Det}\,G}$. As usual in these circumstances, we resort to the saddle point approximation [27][3]. In the absence of a trap, we may assume the saddle point to lie at constant values of $\varphi(x_\mathbf{i}, \tau)$ and $\Delta(x_\mathbf{i}, \tau)$:

$$\varphi(x_\mathbf{i}, \tau) = \varphi_0, \qquad \Delta(x_\mathbf{i}, \tau) = \Delta^*(x_\mathbf{i}, \tau) = \Delta_0. \tag{31}$$

[3] See section 4.3 in [36].

Then the integrals over ψ_a become trivial and we may use the formula $\mathrm{Det}\, G = \mathrm{e}^{\mathrm{Tr}\ln G}$ in equations (29) and (30) to derive the following effective potential:

$$\Omega = \frac{T}{2}\sum_q\sum_n \ln(\omega_n^2 + \mathcal{E}^2(\mathbf{q})) + N_\mathrm{s}\nu n_\mathbf{0}(\varphi' - \Delta) + \frac{N_\mathrm{s}\Delta^2}{2U\sinh^2\theta} - \frac{N_\mathrm{s}(\varphi' + \mu + Jz_0)^2}{2U\cosh^2\theta}, \tag{32}$$

with

$$\Delta \equiv \Delta_0 \sinh\theta, \qquad \varphi' = \varphi_0\cosh\theta - \mu - Jz_0. \tag{33}$$

The spectrum of density fluctuations is now, from (26),

$$\mathcal{E}^2(\mathbf{q}) = (\varepsilon(\mathbf{q}) + \varphi' - \Delta)(\varepsilon(\mathbf{q}) + \varphi' + \Delta). \tag{34}$$

The sum over $\mathbf{p}$ may be calculated for $d = 3$ by approximating (22) as follows:

$$\frac{1}{N_\mathrm{s}}\sum_\mathbf{q} f(\varepsilon(\mathbf{q})) \to \int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3\, f(\varepsilon_\mathbf{q}), \tag{35}$$

with the lattice dispersion:

$$\varepsilon_\mathbf{q} = 2J\sum_{\alpha=1}^{3}\left[1 - \cos\pi q_\alpha\right]. \tag{36}$$

Note that on lattices, the momentum integrals are always finite, so there is no need for renormalizing the coupling constant. This is in contrast to the case for atomic gases. However, if we want to express the coupling constant in terms of the scattering length a_s that is observable for low-energy atomic gases, where the quadratic coupling constant g must be renormalized to a finite value g_R by the addition of a diverging integral $1/g_\mathrm{R} = 1/g + \int \mathrm{d}^3p/(2\pi)^3\varepsilon(\mathbf{p})$, the relation $a_\mathrm{s} = Mg_\mathrm{R}/4\pi$ can be employed only after a corresponding addition of a finite sum (see the remarks after equation (93)).

Another remark concerns the frequency sum in (32), which is initially divergent. In fact, to evaluate a frequency sum such as $\sum_{n=-\infty}^{\infty}\ln(a^2 + \omega_n^2)$ with $\omega_n = 2\pi nT$, one must first differentiate it with respect to a, perform the summation over n, and integrate the result over a [36]. This procedure gives an additional divergent constant, which may be removed by an additive renormalization of the energy [37]. The subtraction can actually be justified by calculating the path integral as a product of individual integrals for each slice of a sliced time axis, as introduced originally by Feynman [36].

Therefore, in the thermodynamic potential Ω, one subtracts from Ω the one for the 'ideal' case:

$$\Omega(U = T = 0) = \tfrac{1}{2}\sum_q(\varepsilon(\mathbf{q}) - \mu - Jz_0) = \tfrac{1}{2}\sum_q(\varepsilon(\mathbf{q}) + \varphi'), \tag{37}$$

and deals only with the subtracted expression

$$\Omega_\mathrm{ren} = \Omega(U,T) - \Omega(U = 0, T = 0) = \tfrac{1}{2}\sum_q(\mathcal{E}(\mathbf{q}) - \varepsilon(\mathbf{q}) - \varphi') + N_\mathrm{s}\nu n_\mathbf{0}(\varphi' - \Delta)$$
$$+ \frac{N_\mathrm{s}\Delta^2}{2U\sinh^2\theta} - \frac{N_\mathrm{s}(\varphi' + \mu + Jz_0)^2}{2U\cosh^2\theta} + T\sum_q \ln(1 - \mathrm{e}^{-\beta\mathcal{E}(\mathbf{q})}), \tag{38}$$

J. Stat. Mech. (2014) P01003

where we have performed summation via the Matsubara frequency by using formula

$$\sum_{n=-1}^{\infty} \ln(\omega_n^2 + a^2) = a\beta + 2\ln(1 - \mathrm{e}^{-\beta a}) + \text{divergent const.} \tag{39}$$

For brevity, we shall suppress writing down the subtraction in Ω_{ren}.

In equilibrium, the thermodynamic potential reaches a minimum with respect to parameters $n_{\mathbf{0}}, \varphi'$ and Δ. Thus we minimize Ω with respect to $n_{\mathbf{0}}$:

$$\frac{\partial \Omega}{\partial n_{\mathbf{0}}} = N_{\mathrm{s}}\nu(\varphi' - \Delta) = 0, \tag{40}$$

and get

$$\varphi' = \Delta. \tag{41}$$

Inserting this into (34) leads to the well-known Bogoliubov phonon dispersion

$$\mathcal{E}(\mathbf{q}) = \sqrt{\varepsilon(\mathbf{q})}\sqrt{\varepsilon(\mathbf{q}) + 2\Delta}, \tag{42}$$

which is linear in $\mathbf{q}$ for small momentum, thus respecting the Nambu–Goldstone theorem.

Minimizing the thermodynamic potential Ω with respect to Δ gives the equation

$$\Delta = U\sinh^2\theta\left[\nu n_{\mathbf{0}} + \frac{\Delta}{N_{\mathrm{s}}}\sum_{\mathbf{q}}\frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}\right], \tag{43}$$

where $c_{\mathbf{q}}$ stands for

$$c_{\mathbf{q}} = \tfrac{1}{2} + f_\beta(\mathcal{E}(\mathbf{q})) = \tfrac{1}{2}\coth\left(\beta\mathcal{E}(\mathbf{q})/2\right), \qquad f_\beta(\omega) = 1/(\mathrm{e}^{\beta\omega} - 1). \tag{44}$$

Minimizing Ω with respect to φ', thereby taking into account the relation $\partial\mathcal{E}(\mathbf{q})/\partial\varphi' = (\varepsilon(\mathbf{q}) + \varphi')/\mathcal{E}(\mathbf{q})$, gives the following equation:

$$N_{\mathrm{s}}\nu n_{\mathbf{0}} + \sum_{q}\left[\frac{(\varepsilon(\mathbf{q}) + \varphi')c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2}\right] - \frac{N_{\mathrm{s}}(\varphi' + \mu + Jz_0)}{U\cosh^2\theta} = 0. \tag{45}$$

This will serve for determining the uncondensed fraction $n_{\mathbf{u}}$.

2.2. Normal and anomalous densities

According to the general rules of statistical mechanics, the total number of particles N is conjugate to the chemical potential:

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V}. \tag{46}$$

Applying this to (38) gives

$$N = \frac{N_{\mathrm{s}}(\varphi' + \mu + Jz_0)}{U\cosh^2\theta}. \tag{47}$$

Using (47) in (45), we obtain

$$N = N_{\rm s}\nu n_{\mathbf{0}} + \sum_q \left[\frac{(\varepsilon(\mathbf{q}) + \varphi')c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2}\right] \equiv N_{\mathbf{0}} + N_{\mathbf{u}}. \tag{48}$$

Here $N_{\mathbf{0}}$ is a total number of condensed atoms, and $n_{\mathbf{0}} = N_{\mathbf{0}}/N_{\rm s}\nu$ is the *condensate fraction*. The uncondensed atoms have a fraction

$$n_{\mathbf{u}} = \frac{N_{\mathbf{u}}}{N} = \frac{1}{\nu N_{\rm s}} \sum_q \left[\frac{(\varepsilon(\mathbf{q}) + \varphi')c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2}\right]. \tag{49}$$

It satisfies the trivial relation $n_{\mathbf{0}} + n_{\mathbf{u}} = 1$.

Note that the term $-\frac{1}{2}$ in the square bracket of (49) is due to the renormalization procedure (38), and guarantees that at $T = 0$ all particles of the ideal gas (which has $U = 0$ and $\Delta = 0$) are condensed, so $n_{\mathbf{u}}(U = 0, T = 0) = 0$.

When the $U(1)$ gauge symmetry is broken, a Bose system is characterized not only by the expectation values of the fluctuating part of the ψ-field with the normal density $n_{\mathbf{u}} = \langle\tilde{\psi}^*\tilde{\psi}\rangle$, but also with an anomalous density, defined by

$$\delta(x_{\mathbf{i}}, \tau, x_j, \tau') = \langle\tilde{\psi}(x_{\mathbf{i}}, \tau)\tilde{\psi}(x_j, \tau')\rangle. \tag{50}$$

Clearly, for a homogeneous system in equilibrium, and in particular, for periodic optical lattices without a magnetic trap, δ does not depend on the coordinates, i.e. $\delta(x_{\mathbf{i}}, \tau, x_j, \tau') = \text{const}$ as was emphasized in [38]. Omission of the anomalous averages makes all calculations not self-consistent, the dynamics non-conserving, and the thermodynamics incorrect. It ruins the order of the phase transition and renders the system unstable. It was also shown in [38] that a $\delta = 0$ type of mean-field approach referred to in the literature as Hartree–Fock–Popov (HFP) approximations [24] leads to a discontinuity in the magnetization curve for antiferromagnetic material with the triplon BEC. Thus we must always allow for $\delta \neq 0$.

Let us calculate this expectation value from the formula

$$\delta = \frac{1}{\nu}\langle\tilde{\psi}(x_{\mathbf{i}}, \tau)\tilde{\psi}(x_{\mathbf{i}}, \tau)\rangle = \frac{1}{2\nu}[\langle\tilde{\psi}_1(x_{\mathbf{i}}, \tau)\tilde{\psi}_1(x_{\mathbf{i}}, \tau)\rangle - \langle\tilde{\psi}_2(x_{\mathbf{i}}, \tau)\tilde{\psi}_2(x_{\mathbf{i}}, \tau)\rangle]$$
$$\frac{1}{2\nu}[G_{11}(0) - G_{22}(0)]. \tag{51}$$

In momentum space, the propagator can be rewritten as

$$G_{ab}(\omega_n, \mathbf{q}) = \frac{1}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})} \begin{pmatrix} \varepsilon(\mathbf{q}) + 2\Delta & \omega_n \\ -\omega_n & \varepsilon(\mathbf{q}) \end{pmatrix}, \tag{52}$$

where we used equations (20), (24), and (42). Using in (51) the equations (28) and (52), one obtains

$$\delta = \frac{1}{2\nu N_{\rm s}\beta} \sum_n \sum_{\mathbf{q}} \frac{2\Delta}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})} = \frac{\Delta}{\nu N_{\rm s}} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} = \frac{\Delta}{\nu N_{\rm s}} \sum_{\mathbf{q}} \frac{1}{\mathcal{E}(\mathbf{q})} \left(\frac{1}{2} + \frac{1}{{\rm e}^{\beta\mathcal{E}(\mathbf{q})} - 1}\right). \tag{53}$$

J. Stat. Mech. (2014) P01003

In terms of δ, the Δ-equation (43) may be rewritten in the following compact form:

$$\Delta = U\nu(n_{\mathbf{0}} + \delta)\sinh^2\theta, \tag{54}$$

with $n_{\mathbf{0}} = 1 - n_{\mathbf{u}}$, and $n_{\mathbf{u}}$ given by (49).

It is well known that the Goldstone theorem for a dilute Bose gas with a spontaneous broken symmetry is equivalent to the celebrated Hugenholtz–Pines theorem [39], according to which the self-energy $\Sigma_{\rm cl}$ and the anomalous self-energy $\Delta_{\rm cl}$ satisfy

$$\Sigma_{\rm cl} - \Delta_{\rm cl} = \mu. \tag{55}$$

In appendix A we shall show that a similar equation holds for optical lattices:

$$\Sigma_{\rm cl} - \Delta_{\rm cl} = \mu + Jz_0, \tag{56}$$

with $\Sigma_{\rm cl} = \varphi_0\cosh\theta$, $\Delta_{\rm cl} = \Delta$.

The only parameter that so far remains free in the initial action (11) is θ. It may be chosen such that the quasiparticle energy $\mathcal{E}(\mathbf{q})$ reduces, in the one-loop approximation [18], to the gapless Bogoliubov dispersion

$$\mathcal{E}(\mathbf{q})_{\rm one\,loop} = \sqrt{\varepsilon(\mathbf{q})}\sqrt{\varepsilon(\mathbf{q}) + 2U\nu}. \tag{57}$$

Indeed, in this approximation we get from (54), $\Delta \approx U\nu\sinh^2\theta$, and from (42), $\mathcal{E}(\mathbf{q}) \approx \sqrt{\varepsilon(\mathbf{q})}\sqrt{\varepsilon(\mathbf{q}) + 2U\nu\sinh^2\theta}$. This is the place where we fix the θ to satisfy

$$\sinh^2\theta = 1, \qquad \cosh^2\theta = 2, \tag{58}$$

as was announced earlier.

Summarizing this section, we present the full expression for Ω:

$$\Omega = \frac{1}{2}\sum_{\mathbf{q}}[\mathcal{E}(\mathbf{q}) - \varepsilon(\mathbf{q}) - \Delta] + \frac{N_{\rm s}\Delta^2}{2U} - \frac{N_{\rm s}(\Delta + \mu + Jz_0)^2}{4U} + T\sum_{\mathbf{q}}\ln(1 - {\rm e}^{-\beta\mathcal{E}(\mathbf{q})}), \tag{59}$$

with

$$\mu = 2\nu U - \Delta - Jz_0. \tag{60}$$

The last equation follows from (47). The self-energy Δ in (59) and (60) is defined through the following set of nonlinear algebraic equations:

$$\begin{aligned}
&\Delta = U\nu(n_0 + \delta), \qquad n_0 = 1 - n_{\mathbf{u}},\\
&n_{\mathbf{u}} = \frac{1}{\nu N_{\rm s}}\sum_{\mathbf{q}}\left[\frac{c_{\mathbf{q}}(\varepsilon(\mathbf{q}) + \Delta)}{\mathcal{E}(\mathbf{q})} - \frac{1}{2}\right],\\
&\delta = \frac{\Delta}{\nu N_{\rm s}}\sum_{\mathbf{q}}\frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})},
\end{aligned} \tag{61}$$

where $c_{\mathbf{q}}$ is given in (44) and U, J, ν, T are input parameters.

J. Stat. Mech. (2014) P01003

2.3. The symmetric phase

When $n_{\mathbf{0}} = 0$, the Hamiltonian (1) is symmetric under the transformation $\psi \to \mathrm{e}^{\mathrm{i}\alpha}\psi$ and equation (40) makes no sense. Then $\varphi' \neq \Delta$, and the energy spectrum has a gap with the dispersion

$$\mathcal{E}(\mathbf{q}) = \sqrt{(\varepsilon(\mathbf{q}) + \varphi' - \Delta)(\varepsilon(\mathbf{q}) + \varphi' + \Delta)}. \tag{62}$$

The main equations in this regime with $T > T_{\mathrm{c}}$ are

$$\Delta = U\nu\delta, \qquad \delta = \frac{\Delta}{\nu N_{\mathrm{s}}} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}, \qquad \nu = \frac{1}{N_{\mathrm{s}}} \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \varphi')c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right]. \tag{63}$$

The set of equations (63) with the energy spectrum equation (62) may have a solution $\Delta \neq 0$, $\varphi' > \Delta$, leading to an exotic state with no condensate but with a finite anomalous density: $n_{\mathbf{0}} = 0, \delta \neq 0$. It was shown in [23] that this phase has a nonzero SF fraction. The upper boundary of such a state was denoted by T^*, and was determined by solving the equations (63) with $\Delta = 0, \varphi' > 0$. Thus it was theoretically predicted that ultracold dilute atomic gases possess a superfluid state at $T_{\mathrm{c}} < T \leq T^*$ without Bose condensation in the one-body channel [23]. However, to date, such states have not been observed experimentally. In section 4 we shall investigate the possible existence of such a state for optical lattices, with a negative outcome.

3. Variational perturbation theory in optical lattices

It is interesting to compare our result with those of variational perturbation theory [31]. To lowest order, this is equivalent to the HFB approximation used in the operator formalism [40]. To do this, let us formulate the HFB approximation for optical lattices in the functional integral framework.

The starting point is again (2) in which we perform the Bogoliubov shift (13) and separate the action as follows:

$$\mathcal{A} = \mathcal{A}_{(0)} + \mathcal{A}_{(1)} + \mathcal{A}_{(2)} + \mathcal{A}_{(3)} + \mathcal{A}_{(4)}, \tag{64}$$

where

$$\begin{aligned}
\mathcal{A}_{(0)} &= \beta N_{\mathrm{s}} \nu n_{\mathbf{0}} \left[\frac{U}{2} \nu n_{\mathbf{0}} - \mu - J z_0 \right], \\
\mathcal{A}_{(1)} &= \sqrt{\nu n_{\mathbf{0}}} [-\mu - J z_0 + U \nu n_{\mathbf{0}}] \int \mathrm{d}\tau \sum_{\mathbf{i}} (\tilde{\psi}(\mathbf{x_i}, \tau) + \tilde{\psi}^*(\mathbf{x_i}, \tau)), \\
\mathcal{A}_{(2)} &= \int_0^\beta \mathrm{d}\tau \left\{ \sum_{\mathbf{i}} \tilde{\psi}^*(\mathbf{x_i}, \tau)[\partial_\tau - \mu]\tilde{\psi}(\mathbf{x_i}, \tau) + \frac{U}{2} \nu n_{\mathbf{0}} \right. \\
&\quad \times \sum_{\mathbf{i}} \left[\tilde{\psi}^2(\mathbf{x_i}, \tau) + 4\tilde{\psi}^*(\mathbf{x_i}, \tau)\tilde{\psi}(\mathbf{x_i}, \tau) + \tilde{\psi}^*(\mathbf{x_i}, \tau)\tilde{\psi}^*(\mathbf{x_i}, \tau) \right] \\
&\quad \left. - J \sum_{\langle i,j \rangle} \tilde{\psi}^*(\mathbf{x_i}, \tau)\tilde{\psi}(\mathbf{x}_j, \tau) \right\},
\end{aligned} \tag{65}$$

$$\mathcal{A}_{(3)} = U\sqrt{\nu n_{\mathbf{0}}}\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}}[\tilde{\psi}^*(\mathbf{x_i},\tau)\tilde{\psi}^2(\mathbf{x_i},\tau) + \tilde{\psi}^*(\mathbf{x_i},\tau)\tilde{\psi}^*(\mathbf{x_i},\tau)\tilde{\psi}(\mathbf{x_i},\tau)],$$

$$\mathcal{A}_{(4)} = \frac{U}{2}\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}}[\tilde{\psi}^*(\mathbf{x_i},\tau)\tilde{\psi}(\mathbf{x_i},\tau)]^2.$$

After this we add and subtract the following terms:

$$\mathcal{A}_{(\Sigma)} = \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \left\{\Sigma_{\mathrm{cl}}\tilde{\psi}^*(\mathbf{x_i},\tau)\tilde{\psi}(\mathbf{x_i},\tau) + \tfrac{1}{2}\Delta_{\mathrm{cl}}[\tilde{\psi}^*(\mathbf{x_i},\tau)\tilde{\psi}^*(\mathbf{x_i},\tau) + \tilde{\psi}(\mathbf{x_i},\tau)\tilde{\psi}(\mathbf{x_i},\tau)]\right\}, \tag{66}$$

with variational parameters Σ_{cl} and Δ_{cl}. The subscripts cl emphasize that these are variational parameters which, in contrast to the earlier fields φ and Δ, are not meant to be functionally integrated.

Using again real and imaginary parts of the complex fields $\tilde{\psi}, \tilde{\psi}^*$ as in (16), we rewrite $\mathcal{A}$ as

$$\mathcal{A} = \mathcal{A}_{(0)} + \mathcal{A}_{\mathrm{free}} + \mathcal{A}_{\mathrm{int}}, \tag{67}$$

where

$$\begin{aligned}
\mathcal{A}_{\mathrm{free}} &= \tfrac{1}{2}\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \sum_{a,b=1,2} \psi_a(\mathbf{x_i},\tau)[\mathrm{i}\varepsilon_{ab}\partial_\tau + Y_a\delta_{ab}]\psi_b(\mathbf{x_i},\tau),\\
\mathcal{A}_{\mathrm{int}} &= \mathcal{A}^{(2)}_{\mathrm{int}} + \mathcal{A}^{(3)}_{\mathrm{int}} + \mathcal{A}^{(4)}_{\mathrm{int}},\\
\mathcal{A}^{(2)}_{\mathrm{int}} &= \tfrac{1}{2}\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}}\{\psi_1^2(\mathbf{x_i},\tau)[3U\nu n_{\mathbf{0}} - \Sigma_{\mathrm{cl}} - \Delta_{\mathrm{cl}}]\\
&\quad + \psi_2^2(\mathbf{x_i},\tau)[U\nu n_{\mathbf{0}} - \Sigma_{\mathrm{cl}} + \Delta_{\mathrm{cl}}]\},\\
\mathcal{A}^{(3)}_{\mathrm{int}} &= \tfrac{1}{2}U\sqrt{2\nu n_{\mathbf{0}}}\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}}[\psi_1^3(\mathbf{x_i},\tau) + \psi_1(\mathbf{x_i},\tau)\psi_2^2(\mathbf{x_i},\tau)],\\
\mathcal{A}^{(4)}_{\mathrm{int}} &= \tfrac{1}{8}U\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}}[\psi_1^2(\mathbf{x_i},\tau) + \psi_2^2(\mathbf{x_i},\tau)]^2,
\end{aligned} \tag{68}$$

where

$$Y_1 = -\mu - Jz_0 + \Sigma_{\mathrm{cl}} + \Delta_{\mathrm{cl}}, \qquad Y_2 = -\mu - Jz_0 + \Sigma_{\mathrm{cl}} - \Delta_{\mathrm{cl}}. \tag{69}$$

The free part of the action, $\mathcal{A}_{\mathrm{free}}$ in equation (68), gives rise to the propagator to be used in the perturbation expansion. In the momentum representation of the field equation (21), the propagator is given by

$$G(\omega_n,\mathbf{q}) = \frac{1}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})}\begin{pmatrix}\varepsilon_{\mathbf{q}} + Y_2 & \omega_n\\ -\omega_n & \varepsilon_{\mathbf{q}} + Y_1\end{pmatrix}, \tag{70}$$

with $\mathcal{E}^2(\mathbf{q}) = (\varepsilon_{\mathbf{q}} + Y_1)(\varepsilon_{\mathbf{q}} + Y_2)$. One obtains, to lowest order,

$$\Omega = -T\ln Z = -T\ln Z_0 - T\ln Z_{\mathrm{free}} + T\langle\mathcal{A}_{\mathrm{int}}\rangle, \tag{71}$$

J. Stat. Mech. (2014) P01003

where $Z_0 = \mathrm{e}^{-\mathcal{A}_{(0)}}$, $Z_{\rm free} = \int \mathcal{D}\psi_1\mathcal{D}\psi_2\mathrm{e}^{-\mathcal{A}_{\rm free}} = 1/\sqrt{\mathrm{Det}\, G^{-1}}$, $\langle \mathcal{A}_{\rm int}\rangle = \{\int \mathcal{D}\psi_1\mathcal{D}\psi_2\mathcal{A}_{\rm int}\, \mathrm{e}^{-\mathcal{A}_{\rm free}}\}/Z_{\rm free}$.

Now we evaluate

$$\begin{aligned} \langle \psi_a^2(\mathbf{x_i},\tau)\rangle &= G_{aa}(0) = \frac{\sigma_a}{N_{\rm s}}, \qquad \langle \psi_a^4(\mathbf{x_i},\tau)\rangle = \frac{3\sigma_a^2}{N_s^2}, \\ \langle \psi_1^2(\mathbf{x_i},\tau)\psi_2^2(\mathbf{x_i},\tau)\rangle &= \frac{\sigma_1\sigma_2}{N_{\rm s}^2}, \qquad \langle \mathcal{A}_{\rm int}^{(3)}\rangle = 0, \end{aligned} \tag{72}$$

with

$$\sigma_1 = T\sum_{\mathbf{q},n}\frac{\varepsilon_{\mathbf{q}}+Y_2}{\omega_n^2+\mathcal{E}^2(\mathbf{q})}, \qquad \sigma_2 = T\sum_{\mathbf{q},n}\frac{\varepsilon_{\mathbf{q}}+Y_1}{\omega_n^2+\mathcal{E}^2(\mathbf{q})}, \tag{73}$$

and find the following thermodynamic potential:

$$\begin{aligned} \Omega = N_{\rm s}\nu n_{\mathbf{0}}\left(-\mu - Jz_0 + \frac{U}{2}\nu n_{\mathbf{0}}\right) + \frac{1}{2}\sum_q[\mathcal{E}(\mathbf{q}) - \varepsilon d(\mathbf{q}) + \mu + Jz_0] \\ + T\sum_{\mathbf{q}}\ln(1-\mathrm{e}^{-\beta\mathcal{E}(\mathbf{q})}) + \frac{U\nu}{8N}[3\sigma_1^2+3\sigma_2^2+2\sigma_1\sigma_2] \\ + \tfrac{1}{2}\sigma_1(3U\nu n_{\mathbf{0}} - Y_1 - Jz_0 - \mu) + \tfrac{1}{2}\sigma_2(U\nu n_{\mathbf{0}} - Y_2 - Jz_0 - \mu), \end{aligned} \tag{74}$$

where we have again subtracted $\Omega(T=0,\ U=0)$.

The parameters $\Sigma_{\rm cl}$ and $\Delta_{\rm cl}$ are now determined variationally by requiring that they minimize the thermodynamic potential, i.e., we require $\partial\Omega/\partial\Sigma_{\rm cl} = 0$ and $\partial\Omega/\partial\Delta_{\rm cl} = 0$ [41], or equivalently

$$\frac{\partial\Omega}{\partial Y_1} = 0, \qquad \frac{\partial\Omega}{\partial Y_2} = 0. \tag{75}$$

These equations yield

$$\begin{aligned} Y_1 &= 3U\nu n_{\mathbf{0}} - \mu - Jz_0 + \frac{U}{2N_{\rm s}}(3\sigma_1+\sigma_2), \\ Y_2 &= U\nu n_{\mathbf{0}} - \mu - Jz_0 + \frac{U}{2N_{\rm s}}(\sigma_1+3\sigma_2). \end{aligned} \tag{76}$$

The gaplessness of the energy spectrum is now imposed by hand. In fact, by requiring the relation (56), we get from (69) $Y_2 = 0$, which leads to the dispersion

$$\mathcal{E}(\mathbf{q}) = \sqrt{\varepsilon(\mathbf{q})}\sqrt{\varepsilon(\mathbf{q})+2\Delta}, \tag{77}$$

where $\Delta = Y_1/2$. This leads to the equations

$$\Delta = U\nu n_{\mathbf{0}} + \frac{U}{2N_{\rm s}}(\sigma_1-\sigma_2), \qquad \mu + Jz_0 = U\nu n_{\mathbf{0}} + \frac{U}{2N_{\rm s}}(\sigma_1+3\sigma_2). \tag{78}$$

Here, we draw the reader's attention to the self-consistency of the HFB approximation as far as the chemical potential is concerned. In fact, the stationary condition $\partial\Omega/\partial n_{\mathbf{0}} = 0$ with Ω given by (74) leads to the following equation for μ:

$$\mu + Jz_0 = U\nu n_{\mathbf{0}} + \frac{U}{2N_{\rm s}}(3\sigma_1+\sigma_2), \tag{79}$$

which is in contrast to equation (78).

To make the theory self-consistent, Yukalov and one of the authors [42] proposed introducing two chemical potentials: namely, μ_0, which corresponds to the equation (79), and μ_1, corresponding to equation (78). Being responsible for subsystems of condensed and uncondensed particles respectively they, naturally, coincide in the normal phase, where $Y_1 = Y_2 = 0$. In the present work, however, we follow the standard procedure of identifying μ in (78) as a chemical potential from which we determine the particle densities by differentiation of Ω.

3.1. The fractions $n_{\mathbf{u}}$ and δ in VPT

Applying the well-known relation $N = -\partial\Omega/\partial\mu$ to Ω in (74) gives

$$N = N_{\mathrm{s}}\nu n_{\mathbf{0}} + \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \Delta)c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right] \equiv N_{\mathbf{0}} + N_{\mathbf{u}}, \tag{80}$$

and hence

$$n_{\mathbf{u}} = \frac{N_{\mathbf{u}}}{N_{\mathrm{s}}} = \frac{1}{\nu N_{\mathrm{s}}} \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \Delta)c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right], \tag{81}$$

where the $\mathcal{E}(\mathbf{q})$ is Bogoliubov's dispersion given in (77).

For the anomalous density δ we obtain

$$\delta = \frac{1}{\nu}\langle\tilde{\psi}(\mathbf{x_i}, \tau)\tilde{\psi}(\mathbf{x_i}, \tau)\rangle = \frac{1}{2N_{\mathrm{s}}\beta\nu}[G_{11}(0) - G_{22}(0)] = \frac{(\sigma_1 - \sigma_2)}{2N_{\mathrm{s}}\nu} = -\frac{\Delta}{\nu N_{\mathrm{s}}} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}, \tag{82}$$

where we used equations (70) and (73).

Using now (82) in (78) gives the equation

$$\Delta = U\nu(n_{\mathbf{0}} + \delta), \tag{83}$$

which is formally the same as the one before (54) with (58). The only difference between these two approximations is in the sign of the anomalous density; we have, in general, $\delta > 0$ in the collective quantum field theory and $\delta < 0$ in the HFB case.

Summarizing, we collect here the main equations in both approximations:

$$\Delta = U\nu(n_{\mathbf{0}} + \delta), \qquad n_{\mathbf{0}} = 1 - n_{\mathbf{u}}, \tag{84}$$

$$\delta = \xi \frac{\Delta}{\nu N_{\mathrm{s}}} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}, \tag{85}$$

$$\mathcal{E}(\mathbf{q}) = \sqrt{\varepsilon(\mathbf{q})}\sqrt{\varepsilon(\mathbf{q}) + 2\Delta}, \tag{86}$$

$$c_{\mathbf{q}} = \frac{1}{2} + \frac{1}{\mathrm{e}^{\beta\mathcal{E}(\mathbf{q})} - 1}, \tag{87}$$

$$\mu = 2U\nu - \Delta - Jz_0, \tag{88}$$

$$\xi = \begin{cases} -1, & \text{HFB} \\ +1, & \text{two collective quantum fields and LOAF,} \end{cases} \tag{89}$$

where $n_{\mathbf{u}}$ is given by (81).

Table 1. Critical parameters of Bose–Hubbard model versus filling factor ν in the approach using two collective quantum fields. $u_c = (U/J)_c$ is given in the second row. The critical temperatures of ideal optical lattices for $d = 3$ are listed in units of J in the third row. The fourth row presents approximated values of t_c^0 (see equation (96)).

ν	1	2	3	4	5
$u_c = (U/J)_c$	56.08	95.4	134.3	173	211.7
$t_c^0 = T_c^0/J$	5.6	9.69	13.70	17.70	21.67
t_c^0 in small q approximation	5.06	10.07	15.2	20.25	25.32

Note that similar relations hold for atomic gases. A difference occurs for the $T > T_c$ phase. There one may use replacements listed in appendix B. In fact, in the normal phase, $n_{\mathbf{0}} = 0$, HFB theory gives

$$\Delta = U\nu\delta = -\frac{U\Delta}{\nu N_s}\sum_{\mathbf{q}}\frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}. \tag{90}$$

Since the right-hand side of this equation is negative, while the left-hand side is positive, at least for optical lattices, equation (90) has only the solution $\Delta = 0$. This means that in the normal phase $n_{\mathbf{0}} = 0$ and $\delta = 0$ (see equation (85)) simultaneously. Therefore HFB theory does not predict a superfluid phase without a condensate, thus being in contrast to the results obtained by Cooper *et al* in [23] at the mean-field level.

From the above discussions it is easy to understand that VPT gives no shift in T_c due to interaction. In fact, when $T \to T_c$, the condensed fraction $n_{\mathbf{0}} \to 0$, and hence $\Delta \to 0$. The expression for $n_{\mathbf{u}}$ will coincide with that for the ideal gas, i.e., equation (81) becomes

$$\nu = \frac{1}{N_s}\sum_{\mathbf{q}}\frac{1}{e^{\beta\varepsilon(\mathbf{q})} - 1} \equiv \frac{1}{N_s}\sum_{\mathbf{q}}\frac{1}{e^{\varepsilon(\mathbf{q})/T_c^0} - 1}, \tag{91}$$

which means that $T_c = T_c^0$ for the HFB case and, hence, $\Delta T_c = T_c - T_c^0 = 0$.

4. Results and discussion

4.1. The quantum phase transition in the theory with two collective quantum fields and VPT

First we discuss the existence of QPT in optical lattices for two collective quantum fields at the mean-field level and for the HFB approximation. It has been shown that for dilute atomic Bose gases the collective quantum field approximation does not predict a QPT [20] while the HFB case does [38]. Below we show that in the case of $d = 3$ optical lattices the situation is vice versa. This can be understood in the following way. Let us rewrite the main equation at $T = 0$ as

$$n_{\mathbf{0}}(\Delta) = \frac{\Delta}{U\nu} - \delta(\Delta). \tag{92}$$

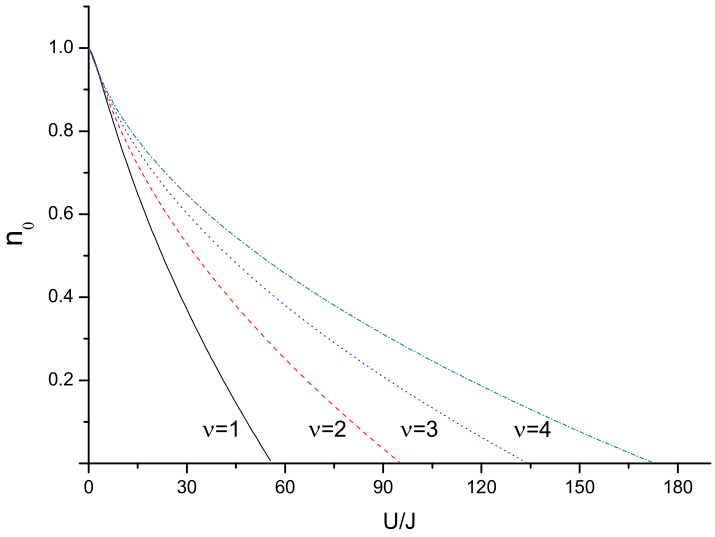

Figure 1. The condensed fraction n_0 at zero temperature as a function of $u = U/J$ for various filling factors, ν. It is seen that n_0 goes to zero smoothly and vanishes at $u_{\rm crit}$. This may be compared with the following results from Gutzwiller's approximation: $u_{\rm crit}(\nu = 1) = 34.97$, $u_{\rm crit}(\nu = 2) = 59.39$, $u_{\rm crit}(\nu = 3) = 83.56$, $u_{\rm crit}(\nu = 4) = 107.66$.

It is clear that for an interacting system, $U \neq 0$ and $\Delta \neq 0$. Since in the collective quantum field theory $\delta(\Delta) > 0$, equation (92) may have the solution $n_{\mathbf{0}}(\Delta) = 0$ with $\Delta \neq 0$ (see table 1). However, in the HFB approximation $\delta(\Delta) < 0$, and $n_{\mathbf{0}}(\Delta)$ in (92) may have as the only solution $n_{\mathbf{0}} > 0$ for $\Delta \neq 0$. Note that in the case of dilute atomic gases at $T = 0$ [43]

$$\delta(\Delta) = \begin{cases} -8\rho\sqrt{\gamma/\pi} < 0 & \text{two collective quantum fields} \\ +8\rho\sqrt{\gamma/\pi} > 0 & \text{HFB,} \end{cases} \tag{93}$$

with the dimensionless *gas parameter* $\gamma = a_{\rm s}^3\rho$ that characterizes the interaction strength of the gas after renormalization. It is formed from the s-wave scattering length $a_{\rm s}$ and the particle density ρ. This sign change is responsible for the dilute atomic gases having a QPT in the HFB approximation, but not in the theory with two collective quantum fields at the mean-field level. In figure 1, the condensed fraction n_0 as a function of $u = U/J$ is presented for $\nu = 1, 2, 3, 4$. This may be compared with $u_{\rm crit} = 6(\sqrt{\nu} + \sqrt{\nu + 1})^2$ given in Gutzwiller's approximation. It is seen that although the theory with two collective quantum fields predicts a rather large value for $u_{\rm crit}$ (see table 1), it gives a desirable second-order phase transition.

4.2. The critical temperature $T_{\rm c}^0$ for ideal cases

Before we study the shift of $T_{\rm c}$, let us estimate the critical temperature $T_{\rm c}^0$ for the free optical lattice with $U = 0$. Assuming $\Delta = 0$ in equation (63), we obtain the well-known

formula

$$\nu = \int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 \frac{1}{\mathrm{e}^{\varepsilon_q/T_\mathrm{c}^0}-1}. \tag{94}$$

Introducing dimensionless parameters $t_\mathrm{c}^0 = T_0^c/J, \hat{\varepsilon}_\mathbf{q} = \varepsilon_\mathbf{q}/2J = \sum_{\alpha=1}^3(1-\cos\pi q_\alpha)$, we may rewrite (94) as

$$\nu = \int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 \frac{1}{\mathrm{e}^{2\hat{\varepsilon}_\mathbf{q}/t_\mathrm{c}^0}-1} \tag{95}$$

which can be considered as a nonlinear equation for t_c^0 at a given filling factor ν. Our numerical estimations for t_c^0 are given in table 1. It is seen that for $\nu = 1$, $T_\mathrm{c}^0 = 5.6J$, which is in consistent with other estimates given in [3, 33].

Note that T_c^0 can be approximated as $T_\mathrm{c}^0 = 5.6J\nu^{0.825}$ in the range $\nu \in (1,5)$ including also non-integer values. In the third row of table 1, approximated values of t_c^0 are presented. The approximation, say, the spherical approximation at small momentum, is obtained by making the following replacements in (95):

$$\int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3\, f(\mathbf{q}) \to \frac{\pi}{2}\int_0^{q_d} q^2\mathrm{d}q\, f(q), \qquad \hat{\varepsilon}_\mathbf{q} \to \frac{\pi^2}{2}\mathbf{q}^2, \qquad (\mathrm{e}^{\varepsilon_q/T_\mathrm{c}^0}-1)^{-1} \to \frac{T_\mathrm{c}^0}{\varepsilon(\mathbf{q})}, \tag{96}$$

where the Debye momentum q_D defined by the equation

$$1 = \int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 = \frac{\pi}{2}\int_0^{q_d} q^2\mathrm{d}q, \tag{97}$$

equals $q_\mathrm{d} = (6/\pi)^{1/3} \approx 1.24$ for $d = 3$. This gives $T_\mathrm{c}^0/J = 2\nu\pi(\pi/6)^{1/3}$. It is seen that this approximation works with roughly 10% accuracy for $\nu \le 3$.

4.3. The shift in T_c caused by the interaction

We are now prepared for estimating the shift $\Delta T_\mathrm{c}/T_\mathrm{c}^0 = (T_\mathrm{c} - T_\mathrm{c}^0)/T_\mathrm{c}^0$ analytically. Above we have shown that the shift $\Delta T_\mathrm{c}/T_\mathrm{c}^0 = 0$ for VPT or equivalently for the HFB case. For LOAF, the integrals in the main equations are dominated by small momenta. At $T \to T_\mathrm{c}$ for $n_\mathbf{0} = 0$, $n_\mathbf{u} = 1$ they are given by

$$\Delta = U\Delta\int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 \frac{f_B(\mathcal{E}(\mathbf{q}))}{\mathcal{E}(\mathbf{q})}, \tag{98}$$

$$1 = \frac{1}{\nu}\int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 \frac{(\varepsilon_\mathbf{q}+\Delta)}{\mathcal{E}(\mathbf{q})} f_B(\mathcal{E}(\mathbf{q})), \tag{99}$$

with $\mathcal{E}(\mathbf{q}) = \sqrt{\varepsilon_\mathbf{q}}\sqrt{\varepsilon_\mathbf{q}+2\Delta}$, $f_B(\mathcal{E}(\mathbf{q})) = 1/(\mathrm{e}^{\beta_c\mathcal{E}(\mathbf{q})}-1)$, $\beta_c = 1/T_\mathrm{c}$.

Note that in (98) we may assume $\Delta \neq 0$ and divide both sides of (98) by Δ. The critical temperature of ideal gas T_c^0 is the solution of equation (99) with $\Delta = 0$, i.e.,

$$1 = \frac{1}{\nu}\int_0^1 \frac{\mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3}{\mathrm{e}^{\varepsilon_\mathbf{q}/T_\mathrm{c}^0}-1}. \tag{100}$$

Now we introduce dimensionless variables:

$$\Delta = u^2\kappa^2 T_{\rm c}^0, \qquad T_{\rm c} = T_{\rm c}^0\alpha, \qquad T_{\rm c}^0 = Jt_{\rm c}^0, \qquad \varepsilon_{\mathbf{q}} = 2J\hat{\varepsilon}_{\mathbf{q}}, \qquad \mathcal{E}(\mathbf{q}) = 2J\hat{\mathcal{E}}(\mathbf{q}), \tag{101}$$

with $\hat{\varepsilon}_{\mathbf{q}} = \sum_\alpha(1-\cos\pi\mathbf{q}_\alpha)$, $\hat{\mathcal{E}}(\mathbf{q}) = \sqrt{\hat{\varepsilon}_{\mathbf{q}}}\sqrt{\hat{\varepsilon}_{\mathbf{q}} + u^2\kappa^2 t_{\rm c}^0}$, $\Delta T_{\rm c}/T_{\rm c}^0 = \alpha - 1$ and $t_{\rm c}^0$ given in the third row of table 1.

The scaled equations can be rewritten as follows:

$$0 = 1 - \frac{u}{2}\int_0^1 \frac{f_B(\hat{\mathcal{E}}(\mathbf{q}))\mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3}{\hat{\mathcal{E}}(\mathbf{q})}, \tag{102}$$

$$0 = 1 - \frac{1}{\nu}\int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 \frac{\hat{\varepsilon}_{\mathbf{q}} + u^2\kappa^2 t_{\rm c}^0/2}{\hat{\mathcal{E}}(\mathbf{q})} f_B(\hat{\mathcal{E}}(\mathbf{q})), \tag{103}$$

with $f_B(\hat{\mathcal{E}}(\mathbf{q})) = 1/(\mathrm{e}^{2\hat{\mathcal{E}}(\mathbf{q})/\alpha t_{\rm c}^0} - 1)$.

Bearing in mind (100), we may rewrite (103) as

$$\int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 \left\{\frac{1}{\mathrm{e}^{2\hat{\mathcal{E}}(\mathbf{q})/t_{\rm c}^0} - 1} - \frac{\hat{\varepsilon}_{\mathbf{q}} + u^2\kappa^2 t_{\rm c}^0/2}{\hat{\mathcal{E}}(\mathbf{q})(\mathrm{e}^{2\hat{\mathcal{E}}(\mathbf{q})/\alpha t_{\rm c}^0} - 1)}\right\} = 0. \tag{104}$$

The nonlinear equations (102) and (104) should be solved with respect to κ and α with given numbers $u = U/J$ and $t_{\rm c}^0$. To do this we make replacements (96). Then equations (102) and (104) can be rewritten as

$$1 - \frac{u\alpha t_{\rm c}^0}{4\sqrt{2}\pi^2}\int_0^{\varepsilon_{\rm D}} \frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon}(\varepsilon + u^2\kappa^2 t_{\rm c}^0)} = 0, \tag{105}$$

$$\int_0^{\varepsilon_{\rm D}} \frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon}}\left\{1 - \frac{\alpha(\varepsilon + u^2\kappa^2 t_{\rm c}^0/2)}{\varepsilon + u^2\kappa^2 t_{\rm c}^0}\right\} = 0, \tag{106}$$

where $\varepsilon_{\rm D} = \pi^2 q_{\rm D}^2/2 = (\pi^2/2)(6/\pi)^{2/3}$.

The integrations in (105) and (106) are easily done and yield

$$0 = \sqrt{2}(6\pi^2)^{1/3}(1-\alpha) + u\alpha\kappa\sqrt{t_{\rm c}^0}\arctan\tilde{\theta} \tag{107}$$

$$0 = 4\pi^2\kappa - \sqrt{2}\alpha\sqrt{t_{\rm c}^0}\arctan\tilde{\theta}, \tag{108}$$

where $\tilde{\theta} = \sqrt{2}(6\pi^2)^{1/3}/(2\kappa u\sqrt{t_{\rm c}^0})$. Excluding α from (108) and inserting it into (107) gives

$$\alpha = \frac{2\sqrt{2}\pi^2\kappa}{\sqrt{t_{\rm c}^0}\arctan\tilde{\theta}}, \tag{109}$$

$$0 = 4\kappa\pi^{8/3}6^{1/3} - \sqrt{2t_{\rm c}^0}[(6\pi^2)^{1/3} + 2u\kappa^2\pi^2]\arctan\tilde{\theta}. \tag{110}$$

Now we consider separately two regimes:

(1) *The weakly interacting regime.* Expanding (109) and (110) in linear order of u we get

$$\alpha = \frac{4\pi^2\kappa\sqrt{2}}{\sqrt{t_{\rm c}^0}} + \frac{8\kappa^2 u}{3}\left(\frac{6}{\pi}\right)^{2/3}, \tag{111}$$

J. Stat. Mech. (2014) P01003

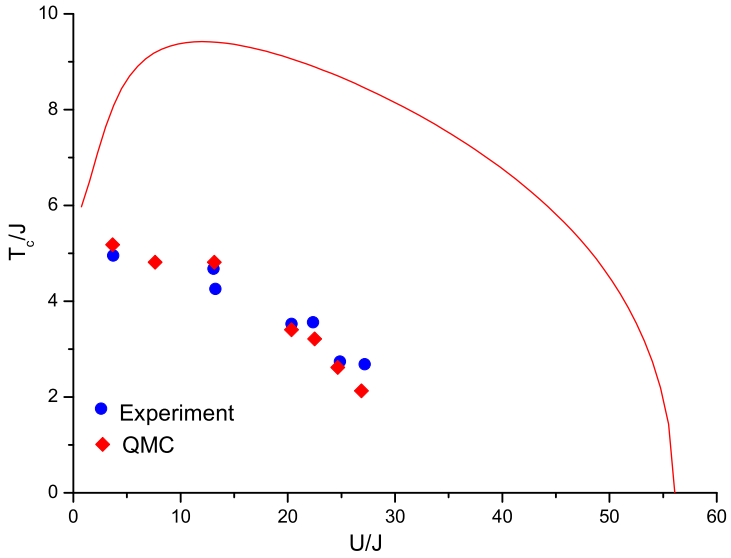

Figure 2. Behavior of T_c (in units of J) as a function of U/J in the saddle point approximation for the theory with two collective fields for $\nu = 1$. The circles show experimental values given in [4], and the solid diamonds are from the Monte Carlo calculations of [3]. Note the initial rise that was found also in atomic gases in [22].

$$\kappa = \frac{\sqrt{2t_c^0}}{8\pi}. \tag{112}$$

Now inserting κ into (111) we finally obtain

$$\alpha = 1 + \frac{ut_c^0}{12}\left(\frac{6}{\pi^4}\right)^{2/3} + O(u^2), \tag{113}$$

and hence

$$\frac{\Delta T}{T_c^0} = \alpha - 1 = \frac{ut_c^0}{12}\left(\frac{6}{\pi^4}\right)^{2/3} + O(u^2), \tag{114}$$

which means that for small coupling constant, i.e. $(U/J) < 1$, the shift is positive and increases with U/J.

(2) *The strongly interacting regime.* In this region, Δ/u^2 and, hence, κ is small, so we may use a linear approximation in κ in equations (109), (110):

$$\alpha = \frac{4\pi^2\kappa\sqrt{2}}{\sqrt{t_c^0}}, \tag{115}$$

$$0 = \frac{\sqrt{2t_c^0}(6\pi^5)^{1/3}}{2} - \kappa[2ut_c^0 + 4(6\pi^8)^{1/3}]. \tag{116}$$

This leads to the following equation:

$$\alpha = \frac{2\pi^{8/3}6^{1/3}}{ut_c^0 + 2\pi^{8/3}6^{1/3}} = \frac{T_c}{T_c^0}, \tag{117}$$

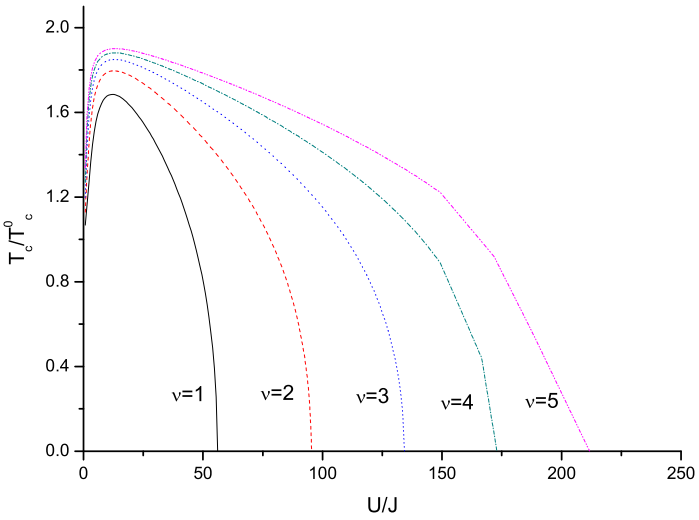

Figure 3. The same curves as in figure 1 but for $\nu = 1, 2, 3, 4, 5$.

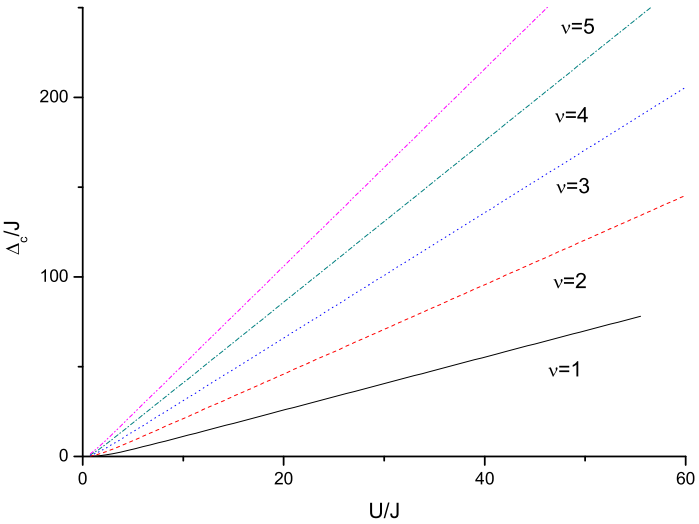

Figure 4. The critical Δ_c versus u for various filling factors ν.

from which one may conclude that T_c decreases with increasing u, i.e.

$$\frac{\Delta T_c}{T_c^0} = \alpha - 1 = -\frac{ut_c^0}{ut_c^0 + 2\pi^{8/3}6^{1/3}} < 0. \tag{118}$$

Thus, our analytical estimate shows that the critical temperature T_c as a function of the coupling constant U, i.e. the function $T(u)$, first increases and then decreases with increasing u for optical lattices. The suppression of T_c at large coupling constant is in agreement with experimental measurements [4].

In figure 2 we present T_c (in units of J) versus u for $\nu = 1$. The solid line corresponds to the exact numerical calculation, i.e., the numerical solutions of equations (98), (99). The experimental points (circles) are taken from [4], and solid diamonds are from Monte Carlo calculations taken from [3]. The suppression of T_c at large coupling constant is found for integer $\nu \geq 1$ also, as is seen in figure 3.

In figure 4 we present the critical values of the self-energy $\Delta_c = \Delta(T = T_c)$ in units of J versus (U/J). Observe that when J is fixed, Δ_c increases with increasing u and ν. On the other hand we observed that Δ_c in units of $T_c^0(\nu)$, i.e. $\Delta_c(T = T_c)/T_c^0(\nu)$ versus u, is almost independent of ν, e.g., $(\Delta_c/T_c^0)|_{\nu=1} = 7.656$ and $(\Delta_c/T_c^0)|_{\nu=4} = 7.780$ at $u = 42.0$.

Now we consider the behavior of Δ for $T > T_c$. It was suggested by Cooper *et al* [23] that in the temperature range $T \in (T_c, T^*)$ there exists a $U(1)$ symmetric phase with $n_{\mathbf{0}} = 0$ but $\delta \neq 0$. This would imply the existence of a superfluid state without a condensate. However, in solving (63) for Δ and φ', we could not find, for optical lattices, any solution with $\Delta \neq 0, \varphi' \neq 0$. Instead, the equations for $T > T_c$ have a solution with $\Delta = 0$, $\varphi' = 2U\nu - Jz_0 - \mu$. In this normal state with $\delta = 0$, the filling factor that characterizes the particle density is determined by the well-known equation

$$\nu = \frac{1}{N_s}\sum_{\mathbf{q}} \frac{1}{e^{\beta(\varepsilon_{\mathbf{q}} - 2U\nu - Jz_0 - \mu)} - 1} = \int_0^1 dq_1\, dq_2\, dq_3 \frac{1}{e^{\beta(\varepsilon_{\mathbf{q}} - 2U\nu - Jz_0 - \mu)} - 1}, \tag{119}$$

with the bare dispersion $\varepsilon_{\mathbf{q}} = 2J\sum_{\alpha=1}^{3}(1 - \cos \pi q_\alpha)$.

The chemical potential of interacting bosons in $T > T_c$ may be evaluated self-consistently from equation (119) with input parameters ν, J, U, and T, or given by an external field (pumping) as in the case of triplons [24, 25].

5. Conclusion

In this paper we have developed a collective quantum field theory and variational perturbation theories for $d = 3$ optical lattices at very low temperatures. Both approximations satisfy the Hugenholtz–Pines theorem. We have shown that a treatment with two collective quantum fields in the saddle point approximation predicts a second-order quantum phase transition that is missed in the VPT [44]. Unfortunately, the predicted critical value of $(U/J)_c$, e.g. for $\nu = 1$, is nearly twice as large as the experimental one. Note that the main equations of the previously mentioned approximation LOAF [19] (recall section 1) and VPT are formally the same. The difference is in the sign of the anomalous density δ, as is seen from equations (84)–(89). We obtained an analytical estimation for the shift of the critical temperature T_c due to the point interaction, for both weak and strong interactions. It is zero for VPT, while it has a nontrivial dependence on the coupling strength (U/J) in the collective quantum field treatment as well as in the LOAF approximation. The general behavior of the phase diagram compares qualitatively well with existing experimental and *ab initio* quantum Monte Carlo results. Similar behaviors, e.g. suppression of the critical temperature at large gas parameter for homogeneous interacting Bose gases, have also been found in path-integral Monte Carlo simulations [45]. As to the dependence of the critical temperature on the filling factor, T_c/T_c^0 increases with increasing ν at fixed U/J. From figures 1 and 2 one may conclude that in order to describe the phase transitions in optical lattices more accurately, the present theory should be extended beyond the saddle point approximation used in equation (31), or in the spirit of B-DMFT [15]. We have found no exotic superfluid state with finite anomalous density but zero condensate. Therefore, the temperatures T^* and T_c introduced by Cooper *et al* [23] coincide. The system is in a superfluid state for

J. Stat. Mech. (2014) P01003

$0 \leq T \leq T_c$, and in a normal state for $T > T_c$. It is natural that the condensation will always be present in the one-body channel (see equation (13)).

Acknowledgments

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Appendix A

Below we derive the Hugenholtz–Pines theorem

$$\Sigma_{\rm cl} - \Delta_{\rm cl} = \mu + Jz_0, \tag{A.1}$$

of section 2 for optical lattices. The normal, $\Sigma_{\rm cl}$, and anomalous, $\Delta_{\rm cl}$, self-energies in (A.1) correspond to the normal, $G_{\rm n}(r,r') = \langle T_\tau \tilde{\psi}(r)\tilde{\psi}^+(r')\rangle$, and anomalous, $G_{\rm an}(r, r') = -\langle T_\tau \tilde{\psi}(r)\tilde{\psi}(r')\rangle$, Green functions respectively. In the Cartesian parameterization of the quantum field (16) we have

$$\Sigma_{\rm cl} = \tfrac{1}{2}[\Pi_{11} + \Pi_{22}], \tag{A.2}$$
$$\Delta_{\rm cl} = \tfrac{1}{2}[\Pi_{22} - \Pi_{11}], \tag{A.3}$$

where the Π_{ab} are defined by Dyson–Beliaev equations [46]:

$$(\hat{G}^{-1})_{ab} - (\hat{G}_0^{-1})_{ab} = \Pi_{ab}, \tag{A.4}$$

and the Green function $\hat{G}_0$ corresponds to the noninteracting situation:

$$G_0^{-1}(\omega_n, \mathbf{q}) = \begin{pmatrix} \varepsilon(\mathbf{q}) - \mu - Jz_0 & -\omega_n \\ \omega_n & \varepsilon(\mathbf{q}) - \mu - Jz_0 \end{pmatrix}. \tag{A.5}$$

The interacting Green function $\hat{G}^{-1}$ is defined in equation (24). Using (20), (33), (24), (A.5) in (A.4) gives

$$\Pi_{11} = X_1 + \mu = \cosh\theta\varphi_0 - \Delta, \qquad \Pi_{22} = X_2 + \mu = \cosh\theta\varphi_0 + \Delta,$$
$$\Pi_{12} = \Pi_{21} = 0. \tag{A.6}$$

Inserting (A.6) into (A.2) and (A.3), one derives

$$\Sigma_{\rm cl} = \varphi_0 \cosh\theta, \qquad \Delta_{\rm cl} = \Delta, \tag{A.7}$$

and hence

$$\Sigma_{\rm cl} - \Delta_{\rm cl} = \varphi_0 \cosh\theta - \Delta = \varphi' + \mu + Jz_0 - \Delta, \tag{A.8}$$

where we have used equation (33). As has been shown in section 2, in the condensed phase $\varphi' = \Delta$, and equation (A.8) becomes equivalent to the Hugenholtz–Pines theorem, i.e. to equation (A.1).

The relation (A.1) in the HFB approximation can be proved in a similar way.

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Table B.1. The formal similarity between Hamiltonians (1) and (B.1).

Quantity	Homogeneous atomic gases	3D Bose–Hubbard model	Comment
Volume	V	N_s	N_s—number of sites
Density	$\rho = N/V$	$\nu = N/N_\mathrm{s}$	ν—filling factor
Bare dispersion	$\varepsilon(\mathbf{q}) = \mathbf{q}^2/2m$	$\varepsilon(\mathbf{q}) = 2J\sum_{\alpha=1}^{3}(1-\cos\pi q_\alpha)$	No additional magnetic trap
Chemical potential	μ	$\mu + Jz_0$	$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_T$
Momentum summation	$\frac{1}{V}\sum_q f(\varepsilon(\mathbf{q})) = \frac{1}{2\pi^2}\int_0^\infty q^2\,\mathrm{d}q f(\varepsilon(q))$	$\frac{1}{N_\mathrm{s}}\sum_q f(\varepsilon(\mathbf{q})) = \int_0^1 \mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 f(\varepsilon(q))$	$d = 3$
Normalization of densities	$\rho_0 + \rho_1 = \rho$	$n_0 + n_1 = 1$	In the condensed phase. No disorder.

Appendix B

Here we present the formal equivalence between the Bose–Hubbard Hamiltonian (1) in the Wannier representation and the standard Hamiltonian for homogeneous dilute atomic gases:

$$H = \int \mathrm{d}\mathbf{r}\, \Psi^\dagger(\mathbf{r}) \left[-\frac{\vec{\nabla}^2}{2m} - \mu \right] \Psi(\mathbf{r}) + \frac{g}{2} \int \mathrm{d}\mathbf{r}\, [\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})]^2, \tag{B.1}$$

where g is the constant of contact interatomic interaction. Using the replacements listed in table B.1 we obtain for Ω and the extremality equations for dilute atomic gases versus optical lattices the relevant quantities as derived in sections 2 and 3. Of course, an appropriate renormalization procedure is implied for dilute atomic gases.

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