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Quantum phase transitions in optical lattices beyond Bogoliubov approximation

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Abstract

We study quantum phase transition from the superfluid to a Mott insulator in optical lattices using a Bose-Hubbard Hamiltonian. For this purpose we have developed a field theoretical approach in terms of path integral formalism to calculate the second-order quantum corrections to the energy density as well as to the superfluid fraction in cubic optical lattices. Using present approach the condensate fraction and ground state energy are calculated as functions of the s-wave scattering length. In contrast to the Bogoliubov model, which is technically speaking a one-loop approximation, we carry the calculation up to two loops, and improve the result further by variational perturbation theory. The result suggests that the quantum phase transition exists.

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I. INTRODUCTION

Optical lattices are known as the gases of ultracold atoms trapped in periodic potentials created by standing waves of laser light. The actuality of experimental and theoretical investigations of these artificial crystals bound by light can be justified by following two factors [1]:

1) Neutral atoms in these optical lattices have a number of affective futures that make them interesting candidates for the realization of a quantum computer [2].

2) They may be used to stimulate various lattice models of fundamental importance to condensed matter physics to study in a controlled way in solid-state physics, since one is able to finely tune the properties and geometry of the lattices. In particular, it is possible to control the Hamiltonian parameters and study various regimes of interest. Similarly to the ordinary Bose - Einstein Condensation (BEC) of gases, the quantum phase transitions in optical lattices were first predicted theoretically [3] and have recently been observed experimentally [4].

Most of the theoretical investigations are based on Bose-Hubbard Hamiltonian:

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

where $\hat{c}_{\mathbf{i}}^{\dagger}$ and $\hat{c}_{\mathbf{i}}$ are the bosonic creation and annihilation operators on the site i; the sum over $< \mathbf{i}, \mathbf{j} >$ 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; N_s - number of sites. Presently it is well established that at very low temperature ($T \to 0$) a system of bosons described by the Hamiltonian (1) could be on superfluid (SF) or in Mott insulator (MI) phase. Clearly there would be a quantum phase transition between these two phase depending on parameters U and J. Particularly, when the hopping term is dominated, $U/J \ll 1$, the system prefers to be in the SF phase. On the other hand when the repulsion prevails the kinetic term, $U/J \gg 1$, the system would be in MI phase where each atoms is absolutely localized near a site.

Clearly the superfluid phase may consist not only of condensed particles with a number N_0, but also of N_1 uncondensed ones, whose sum $N_0 + N_1 = N$ is the total number of particles. The critical interaction strength $\kappa_{\text{crit}} \equiv (U/J)_{\text{crit}} = 29.34$ and $\kappa_{\text{crit}} = 3.6$, for $D = 3$ and $D = 1$ respectively, of the quantum phase $SF \to MI$ transition estimated

by Monte Carlo calculations [5, 6] at filling factor $\nu = 1$ is in good agreement with the experimental data.

To make easier further reading we clarify some specific features of these two phases: SF phases is characterized by long-range correlation, a continuous (gapless) excitation spectrum and a finite compressibility. Since there exists a condensate with a number of particles $N_0 \neq 0$, the gauge symmetry is spontaneously broken in accordance with Bogoliubov and Ginibre theorems. In contrast, in the Mott insulator phase, there is no long-range correlation neither breaking of gauge symmetry. The excitation spectrum has a gap and the system is incompressible, since there is a fixed number of atoms per-site. This new state of matter can survive only at zero temperature and integer filling factor ν.

It is interesting to note that there are two kinds of experiments observing above quantum phase transition, depending on the starting point. In the experiments by Greiner et al [4] one first creates a BEC in a conventional harmonic trap and then adiabatically adds the periodic optical potential. In the second method, pioneered by the Florence group [7] one uses a conventional protocol for evaporative cooling in a magnetic trap down to temperatures just above the threshold for BEC. At this point the optical lattice potential is switched on and evaporative cooling continues. In this way, the system condenses directly into a ground state of the harmonic plus periodic potential. It seems to be that the first method is good to observe SF→MI while the second one is good for MI→SF transitions.

Similarly, most of theoretical approaches can be divided into two classes: SF→MI and MI→SF ones. The latter are based on the Ginzburg - Landau theory as describes for instance in Ref. [8]. They are well suited to analyze the time-of light pictures and the resulting visibility at zero and finite temperatures. In the former class (SF→MI) one uses a perturbative scheme [9] within a decoupling (or single site) approximation due to Gutzwiller. This variational appoach which was first proposed for a fermion system [10], and further developed for bosons in Refs. [11, 12], has the following drawbacks [13] (see also last lines of Sec. IV):

- The mean field Hamiltonian which features single boson terms does not conserve the total number of bosons [14];
- Tunneling of uncondensed atoms is neglected;
- The critical value $\kappa_{\rm crit}$ does not depend on the lattice dimension.

Nevertheless, the prediction of decoupling approximation for $\kappa_{\rm crit} = 34.98$ at filling factor $\nu = 1$ is in agreement with the well established value given above. Some years ago an application of the Hartree-Fock-Popov approximation (which is widely used to study BEC of atomic gases and even triplons [15]) to optical lattices was presented by Stoof et al. [16]. Studying the dependence of the condensate number N_0 on $\kappa = U/J$, i.e. $N_0(U/J)$ they observed that N_0 never reaches zero for finite values of κ, implying that this approximation is unable to predict a possible phase transition to a Mott-insulator phase. Moreover, a Hartree-Fock-Bogoliubov (HFB) approximation applied to the Bose-Hubbard Hamiltonian gives no quantum phase transition for optical lattices [17]. Hence we find it interesting to study the possibility of such a transition if we go beyond these approximations.

In the present work we shall investigate BEC in optical lattices by applying a two-loop approximation and treating the result by variational perturbation theory (VPT) [18]. It will be shown that, while the ground state energy is rather sensitive to the filling factor in commensurate situations, this is not so for arbitrary condensate fractions $n_0 = N_0/N$. We find that n_0 goes to zero at $\kappa \sim 6 \div 6.5$ for $\nu = 1, 2, 3$ in $D = 3$ dimensions. In $D = 1$ dimension, this happens at $\kappa \sim 4$.

The plan of this paper is as follows. In Sec. II the basic equations in functional formalism for Bose-Hubbard Hamiltonian are formulated. In Sec. III we derive explicit expressions for the effective potential in two-loop order. In Sec. IV we obtain condensate fraction vs input parameters U, J, ν . The quantum corrections to the energy of the system is discussed in Sec. V. In Sec. VI we present numerical results and discussions. The last Sec. VII summaries our results.

II. THE ACTION AND PROPAGATORS IN BOSE-HUBBARD MODEL

The action at zero temperature, $(T = 0)$ that describes a gas of atoms in a periodic potential is given by

$$\begin{aligned} S(\varphi^\dagger, \varphi) \;=\; & \int dt d\mathbf{x} \left[\varphi^\dagger i\partial_t \varphi + \varphi^\dagger \frac{\vec{\nabla}^2}{2m} \varphi + \mu \varphi^\dagger \varphi - V_{\rm ext}(\mathbf{x}) \varphi^\dagger \varphi \right] \\ & - \frac{1}{2} \int \varphi^\dagger(\mathbf{x}) \varphi^\dagger(\mathbf{x}') V(\mathbf{x} - \mathbf{x}') \varphi(\mathbf{x}) \varphi(\mathbf{x}') dt d\mathbf{x} d\mathbf{x}' \end{aligned} \tag{2}$$

where the isotropic optical lattice potential is described by [4]

$$V_{\text{ext}}(\mathbf{x}) = V_0 \sum_{\alpha=1}^{D} \sin^2\left(\frac{2\pi x_\alpha}{\lambda}\right) \tag{3}$$

with λ the wave length of the laser light. The lattice points lie at the positions [19]

$$\mathbf{x_i} = \mathbf{i}\, a, \tag{4}$$

where a is the lattice spacing, and

$$\mathbf{i} \equiv (i_1, i_2, \ldots, i_d) \tag{5}$$

are integer-valued vectors. It can be shown [9, 13] that the Wannier representation of the Hamiltonian corresponding to the action (2) is equivalent to well known Bose-Hubbard model (1).

The on-site energy, $\varepsilon_{\mathbf{i}}$, the amplitude of hopping – J and on-site interaction strength U are related to $V_{\text{ext}}(\mathbf{x})$ and $V(\mathbf{x}-\mathbf{x}')$ as follows:

$$\varepsilon_{\mathbf{i}} = \int d\mathbf{x}\omega_0^\dagger(\mathbf{x}-\mathbf{x_i})\left\{-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\mathbf{x})\right\}\omega_0(\mathbf{x}-\mathbf{x_i}) \tag{6}$$

$$J_{\mathbf{i,j}} = -\int d\mathbf{x}\omega_0^\dagger(\mathbf{x}-\mathbf{x_i})\left\{-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\mathbf{x})\right\}\omega_0(\mathbf{x}-\mathbf{x_j}) \tag{7}$$

$$U = \int d\mathbf{x}\int d\mathbf{x}'\omega_0^\dagger(\mathbf{x}-\mathbf{x_i})\omega_0^\dagger(\mathbf{x}-\mathbf{x_i})V(\mathbf{x}-\mathbf{x}')\omega_0(\mathbf{x}'-\mathbf{x_i})\omega_0(\mathbf{x}'-\mathbf{x_i}) \tag{8}$$

where $\omega_n(\mathbf{x})$ are Wannier functions. In the tight-binding limit and pseudopotential approximation, $V(\mathbf{x}-\mathbf{x}') = 4\pi a\delta(\mathbf{x}-\mathbf{x}')/m$ the equations (7), (8) are simplified as:

$$J = \frac{4}{\sqrt{\pi}}E_r\left(\frac{V_0}{E_r}\right)^{3/4}\exp\left\{-2\left(\frac{V_0}{E_r}\right)^{1/2}\right\} \tag{9}$$

$$U = \frac{2\pi\omega a}{l\sqrt{2\pi}} \tag{10}$$

where $E_r = 2\pi^2/m\lambda^2$, a is the s-wave scattering length, and $l = \sqrt{1/m\omega} = (E_r/V_0)^{1/4}\lambda/4\pi$ is the harmonic oscillator length.

In terms of parameters J and U the action (2) can be rewritten as follows:

$$S(\varphi^\dagger,\varphi) = \int dt\Bigg\{\sum_{\mathbf{i}}\varphi^\dagger(\mathbf{x_i},t)[i\partial_t+\mu]\varphi(\mathbf{x_i},t) + J\sum_{<\mathbf{i,j}>}\varphi^\dagger(\mathbf{x_i},t)\varphi(\mathbf{x_j},t) - \frac{U}{2}\sum_{\mathbf{i}}\varphi^\dagger(\mathbf{x_i},t)\varphi^\dagger(\mathbf{x_i},t)\varphi(\mathbf{x_i},t)\varphi(\mathbf{x_i},t)\Bigg\} \tag{11}$$

The grand-canonical partition function Z, and the effective potential at zero temperature, $\mathcal{V}$, can be found as [20]:

$$Z = \int \mathcal{D}\varphi^\dagger \mathcal{D}\varphi e^{iS(\varphi^\dagger,\varphi)} \tag{12}$$

$$\mathcal{V} = \frac{i}{T}\ln Z \tag{13}$$

where $\int dt = T$ is the total time interval. Note that, in accordance with the background field method [21], which will be used below, in evaluation of the effective potential only connected single - particle irreducible Feynman diagrams should be included. The ground state expectation value of an operator $\hat{A}(\varphi^\dagger,\varphi)$ can be expressed as a functional integral:

$$\langle \hat{A} \rangle = \frac{1}{Z}\int \mathcal{D}\varphi^\dagger \mathcal{D}\varphi \hat{A}(\varphi^\dagger,\varphi) e^{iS(\varphi^\dagger,\varphi)} \tag{14}$$

At zero temperature the system could undergo into BEC state. The necessary and sufficient condition for Bose-Einstein condensation is the spontaneous gauge-symmetry breaking which is established by Bogoliubov shift [13]:

$$\varphi(\mathbf{x_i},t) = \sqrt{\nu n_0} + \tilde{\varphi}(\mathbf{x_i},t) \tag{15}$$

where $\nu = N/N_s$– filling factor,and the condensate fraction, $n_0 = N_0/N$, is constant for regular lattice without magnetic trap.

Substituting (15) into (11) and parameterizing quantum field $\tilde{\varphi}(\mathbf{x_i},t)$ in terms of two real-valued quantum fields $\varphi_1(\mathbf{x_i},t)$ and $\varphi_2(\mathbf{x_i},t)$ as

$$\begin{aligned} \tilde{\varphi}(\mathbf{x_i},t) &= \frac{1}{\sqrt{2}}(\varphi_1(\mathbf{x_i},t) + i\varphi_2(\mathbf{x_i},t)) \\ \tilde{\varphi}^\dagger(\mathbf{x_i},t) &= \frac{1}{\sqrt{2}}(\varphi_1(\mathbf{x_i},t) - i\varphi_2(\mathbf{x_i},t)) \end{aligned} \tag{16}$$

one may separate the action as follows

$$S = S^0 + S^{(1)} + S^{(2)} + S^{(3)} + S^{(4)} \tag{17}$$

$$S^0 = N_s \int dt \left[\mu\nu n_0 + Jz_0\nu n_0 - \frac{U}{2}\nu^2 n_0^2\right] \tag{18}$$

$$S^{(1)} = \sqrt{2\nu n_0}\Big[Jz_0 + \mu - U\nu n_0\Big]\int dt \sum_{\mathbf{i}} \varphi_1(\mathbf{x_i},t) \tag{19}$$

$$\begin{aligned} S^{(2)} = {} & \frac{1}{2}\int dt \sum_{\mathbf{i}} \sum_{a,b=1,2} \Big[-\varepsilon_{ab}\varphi_a(\mathbf{x_i},t)\partial_t\varphi_b(\mathbf{x_i},t) - \varphi_a(\mathbf{x_i},t)X_a\varphi_b(\mathbf{x_i},t)\delta_{ab}\Big] \\ & + \frac{J}{2}\int dt \sum_{<\mathbf{i},\mathbf{j}>} \sum_{a=1,2} \varphi_a(\mathbf{x_i},t)\varphi_a(\mathbf{x_j},t) \end{aligned} \tag{20}$$

$$S^{(3)} = -\frac{U\sqrt{2\nu n_0}}{2}\int dt \sum_{\mathbf{i}} \Big[\varphi_1(\mathbf{x_i},t)\varphi_2^2(\mathbf{x_i},t) + \varphi_1^3(\mathbf{x_i},t)\Big] \tag{21}$$

$$S^{(4)} = -\frac{U}{8}\int dt \sum_{\mathbf{i}} \Big[\varphi_1^4(\mathbf{x_i},t) + \varphi_2^4(\mathbf{x_i},t) + 2\varphi_1^2(\mathbf{x_i},t)\varphi_2^2(\mathbf{x_i},t)\Big]. \tag{22}$$

In (20) ε_{ab} is the antisymmetric tensor with $\varepsilon_{12} = 1, \quad \varepsilon_{21} = -1$, and

$$\begin{aligned} X_1 &= -\mu + 3U\nu n_0 \\ X_2 &= -\mu + U\nu n_0 \end{aligned} \tag{23}$$

For a homogenous system the condensate is uniform and it is convenient to decompose the fluctuations into a Fourier series [22, 23]

$$\varphi_a(\mathbf{x_j},t) = \frac{1}{\sqrt{N_s^d}}\sum_{\mathbf{q}}\int \frac{d\omega}{(2\pi)}\varphi_a(\vec{q},\omega)e^{-i\omega t}\exp\left[\frac{2i\pi\mathbf{j}}{N_s}\mathbf{q}\right] \tag{24}$$

where $\mathbf{q} = \{q_1, q_2 \dots q_d\}$ with q_i running from 1 to $N_s - 1$ is an integer-valued vector field associated with all wave vectors in the Brioullin zone: $\vec{q} = 2\pi\,\mathbf{q}/a$, and

$$\frac{1}{N_s}\sum_{\mathbf{q}} \equiv \frac{1}{N_s^d}\sum_{q_1=1}^{N_s-1}\sum_{q_2=1}^{N_s-1}\cdots\sum_{q_d=1}^{N_s-1}. \tag{25}$$

The $\vec{q} = 0$ mode, i.e. the Goldstone mode, is omitted from the sum, to achieve orthogonality between the condensate and noncondensed modes. In momentum space the quadratic term $S^{(2)}$ as follows:

$$S^{(2)} = \frac{1}{2}\int \sum_{\mathbf{q},\mathbf{q}'} \varphi_a(\mathbf{q},\omega)M_{ab}(\mathbf{q},\omega,\mathbf{q}',\omega')\varphi_b(\mathbf{q}',\omega')\frac{d\omega d\omega'}{(2\pi)^2} \tag{26}$$

$$M_{11}(\mathbf{q},\omega,\mathbf{q}',\omega') = -[X_1 + \varepsilon(\mathbf{q}) - Jz_0]\delta(\omega+\omega')\delta_{\mathbf{q},-\mathbf{q}'}, \quad M_{12}(\mathbf{q},\omega,\mathbf{q}',\omega') = i\omega, \tag{27}$$

$$M_{22}(\mathbf{q},\omega,\mathbf{q}',\omega') = -[X_2 + \varepsilon(\mathbf{q}) - Jz_0]\delta(\omega+\omega')\delta_{\mathbf{q},-\mathbf{q}'}, \quad M_{21}(\mathbf{q},\omega,\mathbf{q}',\omega') = -i\omega, \tag{28}$$

with z_0 being the number of nearest neighbors. From this we extract the Fourier transformation of the propagator of the fields φ_1, and φ_2 as the 2×2 matrix:

$$G(\omega,\mathbf{q}) = \frac{i}{\omega^2 - \mathcal{E}^2(\mathbf{q}) + i\epsilon}\begin{pmatrix} X_2 + \varepsilon(\mathbf{q}) - Jz_0 & -i\omega \\ i\omega & X_1 + \varepsilon(\mathbf{q}) - Jz_0 \end{pmatrix} \tag{29}$$

where

$$\begin{aligned} \mathcal{E}(\mathbf{q}) &= \sqrt{(X_1 + \varepsilon(\mathbf{q}) - Jz_0)(X_2 + \varepsilon(\mathbf{q}) - Jz_0)} \\ \varepsilon(\mathbf{q}) &= 2J\Big(d - \sum_{\alpha=1}^{d}\cos(2\pi q_\alpha/N_s)\Big) \end{aligned} \tag{30}$$

In coordinate space for a regular lattice the propagator is translational invariant

$$G_{ab}(\mathbf{x_i},t;\mathbf{x_j},t') \equiv G_{ab}(\mathbf{x_i}-\mathbf{x_j},t-t') = \langle \varphi_a(\mathbf{x_i},t)\varphi_b(\mathbf{x_j},t')\rangle \tag{31}$$

Note that, in deriving (26)-(30), the following relations have been used:

$$\begin{aligned}
&\sum_{<\mathbf{m},\mathbf{j}>} \exp\left[\frac{i2\pi}{N_s}(\mathbf{j}\cdot\mathbf{q}-\mathbf{m}\cdot\mathbf{p})\right] = 2N_s\delta_{\mathbf{q},\mathbf{p}}\sum_{\alpha=1}^{d}\cos(2\pi q_\alpha/N_s),\\
&\sum_{\mathbf{j}} \exp\left[\frac{i2\pi\mathbf{j}}{N_s}(\mathbf{q}-\mathbf{p})\right] = N_s\delta_{\mathbf{q},\mathbf{p}}\\
&\textstyle\sum_{<\mathbf{i},\mathbf{j}>}[1] = z_0 = 2d, \qquad \sum_{\mathbf{q}}[1] = N_s, \qquad \sum_{\mathbf{i}}[1] = N_s.
\end{aligned} \tag{32}$$

III. THE EFFECTIVE POTENTIAL IN TWO-LOOP APPROXIMATION

To organize the quantum corrections in a two-loop expansion, we separate the terms in the action (17) into a free part and interaction parts following Jackiws pioneering work [20]

$$S = S_{\rm cl} + S_{\rm free} + S_{\rm int} \tag{33}$$

$$S_{\rm cl} = S^0 = N_s\int dt\left\{\mu\nu n_0 + Jz_0\nu n_0 - \frac{U}{2}\nu^2 n_0^2\right\} \tag{34}$$

$$S_{\rm free} = \frac{1}{2}\sum_{\mathbf{i},\mathbf{j}}\int dt\varphi_a(\mathbf{x_i},t)M_{ab}(\mathbf{x_i},t;\mathbf{x_j},t)\varphi_b(\mathbf{x_j},t) \tag{35}$$

$$S_{\rm int} = \int dt\sum_{\mathbf{i}}\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t)) \tag{36}$$

$$\begin{aligned}
&\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t)) = v_3[\varphi_1(\mathbf{x_i},t)\varphi_2^2(\mathbf{x_i},t)+\varphi_1^3(\mathbf{x_i},t)]\\
&+v_4[\varphi_1^4(\mathbf{x_i},t)+\varphi_2^4(\mathbf{x_i},t)+2\varphi_1^2(\mathbf{x_i},t)\varphi_2^2(\mathbf{x_i},t)] \equiv \mathcal{L}_3+\mathcal{L}_4
\end{aligned} \tag{37}$$

where 2×2 matrix M_{ab} is given by Eqs. (27), (28) , $v_3 = -U\sqrt{\nu n_0/2}, \quad v_4 = -U/8$.

The perturbative framework is based on the propagator $G_{ab}(k,\omega)$ given in (29). The effective potential $\mathcal{V}$ can be evaluated by the Eq. (13), where the only connected, irreducible diagrams in the partition function $Z = \int\mathcal{D}\varphi_1\mathcal{D}\varphi_2\exp\left(iS(\varphi_1,\varphi_2)\right)$ should be taken into account. The grand thermodynamic potential i.e. free energy, $\Omega(n_0,\mu)$, corresponds to the minimum of $\mathcal{V}(n_0,\mu)$, such that n_0 is a solution of the equation $\partial\mathcal{V}(n_0,\mu)/\partial n_0 = 0$ [24].

Now using (34)-(36) and making expansion by $\mathcal{L}_{\rm int}$ one can represent Z as follows:

$$\begin{aligned}
&Z = e^{iS_0}\int \mathcal{D}\varphi_1\mathcal{D}\varphi_2 e^{iS_{\rm free}+iS_{\rm int}} \\
&= e^{iS_0}\int \mathcal{D}\varphi_1\mathcal{D}\varphi_2 e^{\frac{i}{2}\varphi_a M_{ab}\varphi_b}\Bigg\{1 + i\sum_{\mathbf{i}}\int dt\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t)) \\
&+\frac{i^2}{2}\sum_{\mathbf{i,j}}\int dtdt'\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t))\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_j},t),\varphi_2(\mathbf{x_j},t))\Bigg\} \\
&= \frac{e^{iS_0}}{\sqrt{\mathrm{Det}G}}\Bigg\{1 + i\sum_{\mathbf{i}}\langle\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t))\rangle_0 dt \\
&+\frac{i^2}{2}\sum_{\mathbf{i,j}}\int dtdt'\langle\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t))\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_j},t),\varphi_2(\mathbf{x_j},t))\rangle_0\Bigg\}
\end{aligned} \tag{38}$$

where we introduced the following notation

$$\langle\hat{A}(\varphi_a(\mathbf{x_i},t),\varphi_b(\mathbf{x_i},t))\rangle_0 = \hat{A}\left(\frac{\delta}{i\delta j_a(\mathbf{x_i},t)},\frac{\delta}{i\delta j_b(\mathbf{x_i},t)}\right)e^{-\frac{i}{2}j_\alpha G_{\alpha\beta}j_\beta}\Bigg|_{j=0}, \tag{39}$$

suppressing the summation and integration signs over lattice sites and times t and t' in quandratic forms, for brevity.

The classical contribution to $\mathcal{V}$ is given by factor $\exp(iS_0)$ in (38)

$$\mathcal{V}_0 \;=\; \frac{i}{T}\ln e^{iS_0} = \frac{N_s\nu n_0}{2}[U\nu n_0 - 2(\mu + Jz_0)] \tag{40}$$

The one-loop contribution to the thermodynamic potential - $\mathcal{V}_{1L}$, can be obtained by using the free part of the action (35) in (38), neglecting interaction terms:

$$\mathcal{V}_{1L} = \frac{i}{2T}\mathrm{Tr}\ln\mathrm{Det}\hat{M} = \frac{i}{2}\sum_{\mathbf{q}}\int\frac{d\omega}{(2\pi)}\ln\mathrm{Det}M(\omega,\mathbf{q}) \tag{41}$$

where $M(\omega,\mathbf{q})$ is given by (28). One notices that the frequency sum, and with it the ω integration, is divergent. In fact, to evaluate the frequency sum such as $\sum\limits_{n=-\infty}^{n=\infty}\ln(a^2+\omega_n^2)$, with $\omega_n = 2\pi nT$ one differentiates it with respect to a and, after performing the summation over n, integrates it over a. This procedure gives an additional divergent constant which may be removed by an additive renormalization of the energy [25]. Therefore, in the case of optical lattices, where the momentum integration is performed within a finite volume there is no additional ultraviolet divergency coming from q integration, but there is an infinite constant coming from the frequency summation [26]. This divergent constant can be removed by subtraction from $\mathcal{V}$ the thermodynamic potential for the ideal gas [27]:

$$\begin{aligned}
\mathcal{V}_{1L}^{\rm ren} \;&=\; \mathcal{V}_{1L}(U) - \mathcal{V}_{1L}(U=0) = \frac{1}{2}\sum_{\mathbf{q}}\mathcal{E}(\mathbf{q}) - \frac{1}{2}\sum_{\mathbf{q}}\mathcal{E}(\mathbf{q})\Bigg|_{U=0} \\
&=\; \frac{1}{2}\sum_{\mathbf{q}}[\mathcal{E}(\mathbf{q}) - \varepsilon(\mathbf{q}) + \mu + Jz_0],
\end{aligned} \tag{42}$$

where we have used Eqs.(23), (30) and performed integration by ω using formulas given in the Appendix. Further, for simplicity, we shall suppress the superscript in $\mathcal{V}_{1L}^{\rm ren}$.

The two-loop contributions to $\mathcal{V}$ are involved in second and third terms of (38) as

$$\mathcal{V}_{2L} = \frac{i}{T}\ln\left\{1 + i\sum_{\mathbf{i}}\int\langle\mathcal{L}_{\rm int}\rangle_0 dt + \frac{i^2}{2}\sum_{\mathbf{i,j}}\int dtdt'\langle\mathcal{L}_{\rm int}\mathcal{L}_{\rm int}\rangle_0\right\} \tag{43}$$

The former includes $\mathcal{L}_3(\varphi_1,\varphi_2)$ which does not contribute to Z, since it is in odd power of φ_a, and hence:

$$\langle\mathcal{L}_{\rm int}\rangle_0 = \langle\mathcal{L}_4\rangle_0 = v_4\{\langle\varphi_1^4\rangle_0 + \langle\varphi_2^4\rangle_0 + 2\langle\varphi_1^2\varphi_2^2\rangle_0\} \tag{44}$$

The same is true for $\langle\mathcal{L}_3(\varphi_a(\mathbf{x_i},t))\mathcal{L}_4(\varphi_b(\mathbf{x_i},t))\rangle_0$ coming from the third term of (38). As to the term $\mathcal{L}_4(\varphi_a(\mathbf{x_i},t))\mathcal{L}_4(\varphi_a(\mathbf{x_i},t))$ it also should be omitted since its contribution is beyond two-loop corrections. Therefore

$$\begin{aligned}\mathcal{V}_{2L} \;=\; & \frac{i}{T}\ln\left\{1 + i\sum_{\mathbf{i}}\langle\mathcal{L}_4(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t))\rangle_0\right.\\ & \left.+\frac{i^2}{2}\sum_{\mathbf{i,j}}\int dtdt'\langle\mathcal{L}_3(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t))\mathcal{L}_3(\varphi_1(\mathbf{x_j},t),\varphi_2(\mathbf{x_j},t))\rangle_0\right\}\end{aligned} \tag{45}$$

.

The second term in the logarithm in Eq.(45) can be expressed in terms of propagator as

$$\langle\mathcal{L}_4\rangle_0 = v_4\Big[3(G_{11}^2(0) + G_{22}^2(0)) + 2G_{11}(0)G_{22}(0) + 4G_{12}^2(0)\Big] \tag{46}$$

where we used the following abbreviation $x = (\mathbf{x},t)$ and the formulas

$$\begin{aligned}\langle\varphi_a(x)\varphi_b(x')\rangle_0 &= G_{ab}(x-x'),\\ \langle\varphi_a^4\rangle_0 &= 3G_{aa}^2(0),\\ \langle\varphi_1^2\varphi_2^2\rangle_0 &= G_{11}(0)G_{22}(0) + 2G_{12}^2(0),\end{aligned} \tag{47}$$

and introduced the notation

$$G_{ab}(0) = G_{ab}(x,x) = \frac{1}{N_s}\sum_{\mathbf{q}}\int\frac{d\omega}{(2\pi)}G_{ab}(\omega,\mathbf{q})e^{i\omega(t-t')}\Big|_{t\to t'} \tag{48}$$

Note that $G_{12}(0)$ is the constant (see the Appendix)

$$G_{12}(0) = \frac{1}{N_s}\sum_{\mathbf{q}}\int\frac{d\omega}{2\pi}\frac{\omega}{\omega^2 - \mathcal{E}^2(\mathbf{q}) + i\epsilon} = \frac{i}{2N_s}\sum_{\mathbf{q}}[1] = -G_{21}(0) = \frac{i}{2}. \tag{49}$$

The third term,

$$\langle \mathcal{L}_3 \mathcal{L}_3 \rangle_0 \;=\; v_3^2 \Big[\langle \varphi_1(x)\varphi_2^2(x)\varphi_1(y)\varphi_2^2(y)\rangle_0 + 2\langle \varphi_1(x)\varphi_2^2(x)\varphi_1^3(y)\rangle_0 + \langle \varphi_1^3(x)\varphi_1^3(y)\rangle_0 \Big] \quad (50)$$

includes averages with six φ_a. These may be evaluated via Wick theorem to yield

$$\begin{aligned}
&\langle \varphi_1^3(x)\varphi_1^3(y)\rangle_0 = 6G_{11}^3(x,y) \\
&\langle \varphi_1^3(x)\varphi_1(y)\varphi_2^2(y)\rangle_0 = 6G_{11}(x,y)G_{12}^2(x,y) \\
&\langle \varphi_1(x)\varphi_2^2(x)\varphi_1(y)\varphi_2^2(y)\rangle_0 = 4G_{22}(x,y)G_{12}(x,y)G_{21}(x,y) + 2G_{22}^2(x,y)G_{11}(x,y).
\end{aligned} \quad (51)$$

We have omitted one-particle reducible diagrams such as $G_{22}(0)G_{11}(x,y)G_{11}(0)$.

Now, using (46), (50)-(51) in (45), we finally obtain:

$$\begin{aligned}
\mathcal{V}_{2L} \;=\; & \frac{UN_s}{8}\Big[3G_{11}^2(0) + 3G_{22}^2(0) + 2G_{11}(0)G_{22}(0) + 4G_{12}^2(0)\Big] \\
& - \frac{iU^2\nu n_0}{2T}\sum_{\mathbf{i},\mathbf{j}} \int dtdt' \Big[G_{22}^2(\mathbf{x_i},t;\mathbf{x_j},t')G_{11}(\mathbf{x_i},t';\mathbf{x_j},t') \\
& + 3G_{11}^3(\mathbf{x_i},t;\mathbf{x_j},t') + 6G_{11}(\mathbf{x_i},t;\mathbf{x_j},t')G_{12}^2(\mathbf{x_i},t;\mathbf{x_j},t') \\
& + 2G_{12}(\mathbf{x_i},t;\mathbf{x_j},t')G_{21}(\mathbf{x_i},t;\mathbf{x_j},t')G_{22}(\mathbf{x_i},t;,\mathbf{x_j},t')\Big] \equiv \mathcal{V}_{2L}^{(1)} + \mathcal{V}_{2L}^{(2)}.
\end{aligned} \quad (52)$$

The two-loop diagrams that contribute the thermodynamic potential are shown in Fig. 1.

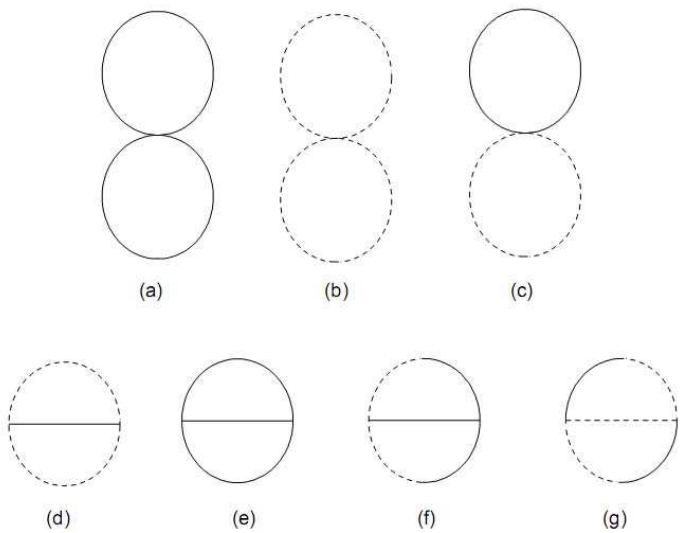


FIG. 1: Vacuum diagrams in a two-loop approximation. The solid and dashed lines correspond to G_{11} and G_{22} respectively, while the mixed line corresponds to G_{12} (or G_{21}).

We now pass to momentum space, and perform integrations over energy variables ω to obtain following analytic expression (see Appendix):

$$\mathcal{V}_{2L}^{(1)}(n_0,\mu) \;=\; \frac{U}{8}N_s\Big(3I_{10}^2+3I_{20}^2+2I_{10}I_{20}-1\Big), \tag{53}$$

$$\mathcal{V}_{2L}^{(2)}(n_0,\mu) \;=\; -\frac{U^2\nu n_0}{8N_s}\Big(I_1+3I_2-6I_3+2I_4\Big). \tag{54}$$

where following integrals are introduced

$$\begin{aligned}
I_{10}(n_0,\mu) &= \frac{1}{N_s}\sum_{\mathbf{q}}\frac{(-\tilde{\mu}+3U\nu n_0+\varepsilon(\mathbf{q}))}{2\mathcal{E}(\mathbf{q})} = G_{22}(0),\\
I_{20}(n_0,\mu) &= \frac{1}{N_s}\sum_{\mathbf{q}}\frac{(-\tilde{\mu}+U\nu n_0+\varepsilon(\mathbf{q}))}{2\mathcal{E}(\mathbf{q})} = G_{11}(0),\\
I_1(n_0,\mu) &= \textstyle\sum_{\mathbf{q}_1\neq\mathbf{q}_2}\dfrac{(-\tilde{\mu}+3U\nu n_0+\varepsilon(\mathbf{q}_1))(-\tilde{\mu}+3U\nu n_0+\varepsilon(\mathbf{q}_2))(-\tilde{\mu}+U\nu n_0+\varepsilon(\mathbf{q}_3))}{\mathcal{E}(\mathbf{q}_1)\mathcal{E}(\mathbf{q}_2)\mathcal{E}(\mathbf{q}_3)(\mathcal{E}(\mathbf{q}_1)+\mathcal{E}(\mathbf{q}_2)+\mathcal{E}(\mathbf{q}_3))},\\
I_2(n_0,\mu) &= \textstyle\sum_{\mathbf{q}_1\neq\mathbf{q}_2}\dfrac{(-\tilde{\mu}+U\nu n_0+\varepsilon(\mathbf{q}_1))(-\tilde{\mu}+U\nu n_0+\varepsilon(\mathbf{q}_2))(-\tilde{\mu}+U\nu n_0+\varepsilon(\mathbf{q}_3))}{\mathcal{E}(\mathbf{q}_1)\mathcal{E}(\mathbf{q}_2)\mathcal{E}(\mathbf{q}_3)(\mathcal{E}(\mathbf{q}_1)+\mathcal{E}(\mathbf{q}_2)+\mathcal{E}(\mathbf{q}_3))},\\
I_3(n_0,\mu) &= \textstyle\sum_{\mathbf{q}_1\neq\mathbf{q}_2}\dfrac{(-\tilde{\mu}+U\nu n_0+\varepsilon(\mathbf{q}_3))}{\mathcal{E}(\mathbf{q}_3)(\mathcal{E}(\mathbf{q}_1)+\mathcal{E}(\mathbf{q}_2)+\mathcal{E}(\mathbf{q}_3))},\\
I_4(n_0,\mu) &= \textstyle\sum_{\mathbf{q}_1\neq\mathbf{q}_2}\dfrac{(-\tilde{\mu}+3U\nu n_0+\varepsilon(\mathbf{q}_3))}{\mathcal{E}(\mathbf{q}_3)(\mathcal{E}(\mathbf{q}_1)+\mathcal{E}(\mathbf{q}_2)+\mathcal{E}(\mathbf{q}_3))}
\end{aligned} \tag{55}$$

and $\mathcal{E}(\mathbf{q}) = \sqrt{(-\tilde{\mu}+3U\nu n_0+\varepsilon(\mathbf{q}))}\sqrt{(-\tilde{\mu}+U\nu n_0+\varepsilon(\mathbf{q}))}$, $\tilde{\mu}=\mu-Jz_0$, $\mathbf{q}_3=\mathbf{q}_1-\mathbf{q}_2$.

Therefore the full effective potential in a two-loop approximation is given by

$$\mathcal{V}(\mu,n_0) = \mathcal{V}_0(\mu,n_0)+\mathcal{V}_{1L}(\mu,n_0)+\mathcal{V}_{2L}^{(1)}(\mu,n_0)+\mathcal{V}_{2L}^{(2)}(\mu,n_0) \tag{56}$$

where $\mathcal{V}_0$, $\mathcal{V}_{1L}$, $\mathcal{V}_{2L}^{(1)}$, $\mathcal{V}_{2L}^{(2)}$ are given by equations (40), (42), (53), (54) respectively. Note that for the homogenous Bose gas. Eqs. (53)-(56) were calculated before by Braaten and Nieto [28].

IV. THE CONDENSATE FRACTION IN VPT

To evaluate the condensate fraction n_0 as an explicite function of U/J and ν we shall use following strategy referred as a variational perturbation theory[18]:

1. With fixed values of input parameters introduce an auxiliary parameter, loop counter, η (η=1 at the end of calculations) to represent $\mathcal{V}$ in Eq. (56) as:

$$\mathcal{V}(\mu,n_0) = \mathcal{V}_0(\mu,n_0)+\eta\mathcal{V}_{1L}(\mu,n_0)+\eta^2\mathcal{V}_{2L}(\mu,n_0) \tag{57}$$

with $\mathcal{V}_{2L}(\mu, n_0) = \mathcal{V}_{2L}^{(1)}(\mu, n_0) + \mathcal{V}_{2L}^{(2)}(\mu, n_0)$

2. Impose the extremalization condition:

$$\frac{\partial \mathcal{V}(\mu, n_0)}{\partial n_0} = O(\eta^3) \tag{58}$$

and solve this equation with respect to n_0. Let the solution of the equation is $\bar{n}_0(\mu)$. Clearly the latter can be also represented in powers of η:

$$\bar{n}_0(\mu) = n_{00}(\mu) + \eta n_{01}(\mu) + \eta^2 n_{02}(\mu) \tag{59}$$

with

$$\begin{aligned} n_{01}(\mu) &= -\frac{\mathcal{V}'_{1L}(\mu, n_{00})}{\mathcal{V}''_0(\mu, n_{00})} \\ n_{02}(\mu) &= -\frac{n_{01}^2(\mu)\mathcal{V}'''_0(\mu, n_{00}) + 2\mathcal{V}'_{2L}(\mu, n_{00}) + 2n_{01}(\mu)\mathcal{V}''_{1L}(\mu, n_{00})}{2\mathcal{V}''_0(\mu, n_{00})} \end{aligned} \tag{60}$$

where the prime denotes the derivative with respect to n_0, e.g. $\mathcal{V}'_{1L}(\mu, n_{00}) = [\partial \mathcal{V}_{1L}(\mu, n_0)/\partial n_0]|_{n_0=n_{00}}$ and n_{00} is the solution to the equation $\mathcal{V}'_0(\mu, n_0) = 0$.

3. Inserting $\bar{n}_0(\mu)$ back to the effective potential (57) determines the free energy of the system $\Omega(\mu) = \mathcal{V}(\bar{n}_0, \mu)$

4. Introducing a variational parameter M as

$$\mu = M + r\eta \tag{61}$$

with the abbreviation

$$r = \frac{\mu - M}{\eta} \tag{62}$$

and inserting (61) into $\Omega(\mu)$ reexpand this $\Omega(M, \mu, r)$ in powers of η at fixed r.

5. Reinserting back r from (62) optimize $\Omega(M, \mu)$ with respect to the variational parameter M. This will fix μ as a function of the optimal $M = M_{opt}$, with

$$M_{opt} = U\nu - Jz_0 \tag{63}$$

6. Finally, inserting this μ into (59) one finds an explicit expression for n_0 as $n_0 = n_0(U/J, \nu)$.

Below we consider each step in detail. First, taking partial derivative with respect to n_0 from Eq. (57) one presents (58) as

$$\frac{\partial \mathcal{V}(n_0,\mu)}{\partial n_0} = \frac{\partial \mathcal{V}_0(n_0,\mu)}{\partial n_0} + \eta \frac{\partial \mathcal{V}_{1L}(n_0,\mu)}{\partial n_0} + \eta^2 \frac{\partial \mathcal{V}_{2L}^{(1)}(n_0,\mu)}{\partial n_0} + \eta^2 \frac{\partial \mathcal{V}_{2L}^{(2)}(n_0,\mu)}{\partial n_0} = 0 \tag{64}$$

$$\frac{\partial \mathcal{V}_0(n_0,\mu)}{\partial n_0} = -N_s \left[\nu\tilde{\mu} - U\nu^2 n_0\right] \tag{65}$$

$$\frac{\partial \mathcal{V}_{1L}(n_0,\mu)}{\partial n_0} = -\frac{U\nu}{2}\sum_{\mathbf{q}} \frac{(2\tilde{\mu} - 3U\nu n_0 - 2\varepsilon(\mathbf{q})}{\mathcal{E}(\mathbf{q})} \tag{66}$$

$$\frac{\partial \mathcal{V}_{2L}^{(1)}(n_0,\mu)}{\partial n_0} = \frac{U^2\nu}{4}\sum_{\mathbf{q}} \frac{(\tilde{\mu} - \varepsilon(\mathbf{q}))\left[(\tilde{\mu} - 4U\nu n_0 - \varepsilon(\mathbf{q}))I_{10}(n_0,\mu) - (\tilde{\mu} - \varepsilon(\mathbf{q}))I_{20}(n_0,\mu)\right]}{\mathcal{E}^3(\mathbf{q})} \tag{67}$$

where following relations are used

$$\frac{\partial \mathcal{E}(\mathbf{q})}{\partial n_0} = -\frac{U\nu}{\mathcal{E}(\mathbf{q})}(2\mu - 3U\nu n_0 - 2\varepsilon(\mathbf{q}) + 2Jz_0) \tag{68}$$

$$\frac{\partial I_{10}}{\partial n_0} = \frac{U\nu}{2N_s}\sum_{\mathbf{q}} \frac{(\mu - \varepsilon(\mathbf{q}) + Jz_0)(\mu - 3U\nu n_0 - \varepsilon(\mathbf{q}) + Jz_0)}{\mathcal{E}^3(\mathbf{q})} \tag{69}$$

$$\frac{\partial I_{20}}{\partial n_0} = -\frac{U\nu}{2N_s}\sum_{\mathbf{q}} \frac{(\mu - \varepsilon(\mathbf{q}) + Jz_0)(\mu - U\nu n_0 - \varepsilon(\mathbf{q}) + Jz_0)}{\mathcal{E}^3(\mathbf{q})} \tag{70}$$

In Eqs. (67) $\partial \mathcal{V}_{2L}^{(2)}/\partial n_0$ has a long expression and will be given later. Solving Eq. (64) iteratively gives Eq. (59) with

$$\begin{aligned}
n_{00}(\mu) &= \frac{\mu + Jz_0}{\nu U}, \\
n_{01}(\mu) &= -\frac{1}{2\nu}(3I_{20}(\mu) + I_{10}(\mu)) = -\frac{1}{2N_s\nu}\sum_{\mathbf{q}} \frac{(\mu + Jz_0 + 2\varepsilon(\mathbf{q}))}{2\mathcal{E}_\mu(\mathbf{q})}, \\
n_{02}(\mu) &= -\frac{1}{N_s U\nu^2}\frac{\partial \Omega_{2l}^{(2)}(n_0,\mu)}{\partial n_0}\bigg|_{n_0 = n_{00}} + \frac{1}{2N_s\nu}\sum_{\mathbf{q}}\left[-\frac{U\varepsilon^2(\mathbf{q})(I_{10}(\mu) + I_{20}(\mu))}{\mathcal{E}_\mu^3(\mathbf{q})}\right. \\
&\quad \left. + \frac{2UI_{20}(\mu)\varepsilon(\mathbf{q})(\mu + Jz_0)}{\mathcal{E}_\mu^3(\mathbf{q})} + \frac{U(\mu + Jz_0)^2(I_{10}(\mu) - I_{20}(\mu))}{\mathcal{E}_\mu^3(\mathbf{q})}\right],
\end{aligned} \tag{71}$$

where

$$\begin{aligned}
I_{10}(\mu) &= I_{10}(n_0,\mu)|_{n_0=n_{00}} = \frac{1}{2N_s}\sum_{\mathbf{q}} \frac{2\mu + 2Jz_0 + \varepsilon(\mathbf{q})}{\mathcal{E}_\mu(\mathbf{q})}, \\
I_{20}(\mu) &= I_{20}(n_0,\mu)|_{n_0=n_{00}} = \frac{1}{2N_s}\sum_{\mathbf{q}} \frac{\varepsilon(\mathbf{q})}{\mathcal{E}_\mu(\mathbf{q})}.
\end{aligned} \tag{72}$$

In this step the Goldstone boson dispersion is correctly achieved:

$$\mathcal{E}_\mu(\mathbf{q}) = \sqrt{\varepsilon(\mathbf{q})}\sqrt{\varepsilon(\mathbf{q}) + 2\mu + 2Jz_0} \tag{73}$$

Now inserting (59), (71) into (56) one gets $\Omega(\mu)$ as a function of μ as

$$\Omega(\mu) = \mathcal{V}(\mu, \bar{n}_0) = \Omega_0(\mu) + \eta\Omega_1(\mu) + \eta^2\Omega_2(\mu)$$

$$\begin{aligned}
\Omega_0(\mu) &= -\frac{N_s(\mu + Jz_0)^2}{2U}, \\
\Omega_1(\mu) &= \frac{1}{2}\sum_{\mathbf{q}}[\mathcal{E}_\mu(\mathbf{q}) + \mu - \varepsilon(\mathbf{q}) + Jz_0], \\
\Omega_2(\mu) &= \mathcal{V}^{(2)}_{2L}(\mu, n_{00}(\mu)) + \frac{UN_s}{8}[2I_{10}^2(\mu) - 4I_{10}(\mu)I_{20}(\mu) - 6I_{20}^2(\mu) - 1].
\end{aligned} \tag{74}$$

Performed one more step of VPT we finally obtain μ as an explicit function of the parameters U, J, ν:

$$\begin{aligned}
\mu &= \mu_0 + \eta\mu_1 + \eta^2\mu_2, \\
\mu_0 &= U\nu - Jz_0, \\
\mu_1 &= \frac{U}{2N_s}\sum_{\mathbf{q}}\frac{\varepsilon(\mathbf{q}) + \mathcal{E}_0(\mathbf{q})}{\mathcal{E}_0(\mathbf{q})} = U\left(I_{20B} + \frac{1}{2}\right), \\
\mu_2 &= \frac{U}{N_s}\frac{\partial\mathcal{V}^{(2)}_{2L}(\mu)}{\partial\mu}\bigg|_{\mu=\mu_0} + \frac{U(I_{10B} - I_{20B})^2}{4\nu} \\
&\quad + \frac{U^2(I_{10B} + I_{20B} - 1)}{4N_s}\sum_{\mathbf{q}}\frac{\varepsilon^2(\mathbf{q})}{\mathcal{E}_0^3(\mathbf{q})}.
\end{aligned} \tag{75}$$

and also the normal fraction, $n_1 = 1 - \bar{n}_0$ as

$$\begin{aligned}
n_1 &= n_1^{1L} + n_1^{2L}, \\
n_1^{1L} &= \frac{1}{2\nu N_s}\sum_{\mathbf{q}}\left[\frac{\varepsilon(\mathbf{q}) + U\nu}{\mathcal{E}_0(\mathbf{q})} - 1\right],
\end{aligned} \tag{76}$$

$$\begin{aligned}
n_1^{2L} &= \frac{1}{N_sU\nu^2}\frac{\partial\mathcal{V}^{(2)}_{2L}}{\partial n_0}\bigg|_{n_0=n_{00}} - \frac{1}{\nu N_s}\frac{\partial\mathcal{V}^{(2)}_{2L}}{\partial\mu}\bigg|_{\mu=\mu_0} - \frac{(I_{10B} - I_{20B})^2}{4\nu^2} \\
&\quad - \frac{U}{4N_s\nu}\sum_{\mathbf{q}}\frac{\left[(I_{10B} - I_{20B})(2U^2\nu^2 - \varepsilon^2(\mathbf{q})) + U\nu\varepsilon(\mathbf{q})(2I_{20B} - 1)\right]}{\mathcal{E}_0^3(\mathbf{q})}
\end{aligned} \tag{77}$$

In Eqs. (75), (77) $\mathcal{E}_0(\mathbf{q})$, I_{10B} and I_{20B} are given by

$$\begin{aligned}
\mathcal{E}_0(\mathbf{q}) &= \sqrt{\varepsilon(\mathbf{q})}\sqrt{\varepsilon(\mathbf{q}) + 2U\nu}, \\
I_{10B} &= \frac{1}{2N_s}\sum_{\mathbf{q}}\frac{2U\nu + \varepsilon(\mathbf{q})}{\mathcal{E}_0(\mathbf{q})}, \\
I_{20B} &= \frac{1}{2N_s}\sum_{\mathbf{q}}\frac{\varepsilon(\mathbf{q})}{\mathcal{E}_0(\mathbf{q})}.
\end{aligned} \tag{78}$$

Now we compare present approximation with Gutzwiller's.

- In Gutzwiller approach the phonon dispersion for small $\vec{q}$ is quadraric in wave number [12] rather than linear given in present approximation by Eq. (73).

- As it is seen from Eq.s (76) and (77) in Bogoliubov type approximations the uncondensed particles have momentum distribution $n_q =< a_q^\dagger a_q >$ varying as q^{-4} for large momentum [29], while in Gutzwiller approach this distribution is independent of $\vec{q}$ [12].

V. GROUND STATE ENERGY

The ground state energy of the system at zero temperature can be determined as

$$E = \Omega(\mu) + \mu N, \tag{79}$$

where $\Omega(\mu)$ in Eq. (80) can be rewritten as follows

$$\begin{aligned}
&\Omega(U,J,\nu) = \Omega_0(U,J,\nu) + \Omega_1(U,J,\nu) + \Omega_2(U,J,\nu),\\
&\Omega_0(U,J,\nu) = -\frac{UN_s\nu^2}{2}, \quad \Omega_1(U,J,\nu) = \frac{1}{2}\sum_{\mathbf{q}}[\mathcal{E}_0(\mathbf{q}) - \varepsilon(\mathbf{q})] + N_s\nu\left(\frac{U}{2} - \mu_1\right),\\
&\Omega_2(U,J,\nu) = \Omega_{2L}^{(2)}(U,J,\nu) + \frac{UN_s\left(2I_{10B}^2 - 4I_{10B}I_{20B} - 6I_{20B}^2 - 1\right)}{8} + \frac{N_s(\mu_1^2 - 2U\nu\mu_2)}{2U}
\end{aligned} \tag{80}$$

where $\Omega_{2L}^{(2)}$ is given by

$$\begin{aligned}
\Omega_{2L}^{(2)}(U,J,\nu) &= \mathcal{V}_{2L}^{(2)}(n_0 = 1, \mu = \mu_0)\\
&= -\frac{NU^2}{4N_s^2}\sum_{\mathbf{q}_1,\mathbf{q}_2}\left[\frac{U\varepsilon_3\nu(\varepsilon_1 + \varepsilon_2 + 2U\nu)}{\mathcal{E}_0(1)\mathcal{E}_0(2)\mathcal{E}_0(3)\mathcal{E}_{0T}} + \frac{2\varepsilon_1\varepsilon_2\varepsilon_3 - 2\mathcal{E}_0(1)\mathcal{E}_0(2)(\varepsilon_3 + U\nu)}{\mathcal{E}_0(1)\mathcal{E}_0(2)\mathcal{E}_0(3)\mathcal{E}_{0T}}\right],
\end{aligned} \tag{81}$$

with $\mathcal{E}_0(\mathbf{q})$ given in (78), and $\varepsilon_1 \equiv \varepsilon_{\mathbf{q}_1}$, $\mathcal{E}_0(1) \equiv \mathcal{E}_0(\mathbf{q}_1)$, $\mathcal{E}_{0T} \equiv \mathcal{E}_0(1) + \mathcal{E}_0(2) + \mathcal{E}_0(3)$.

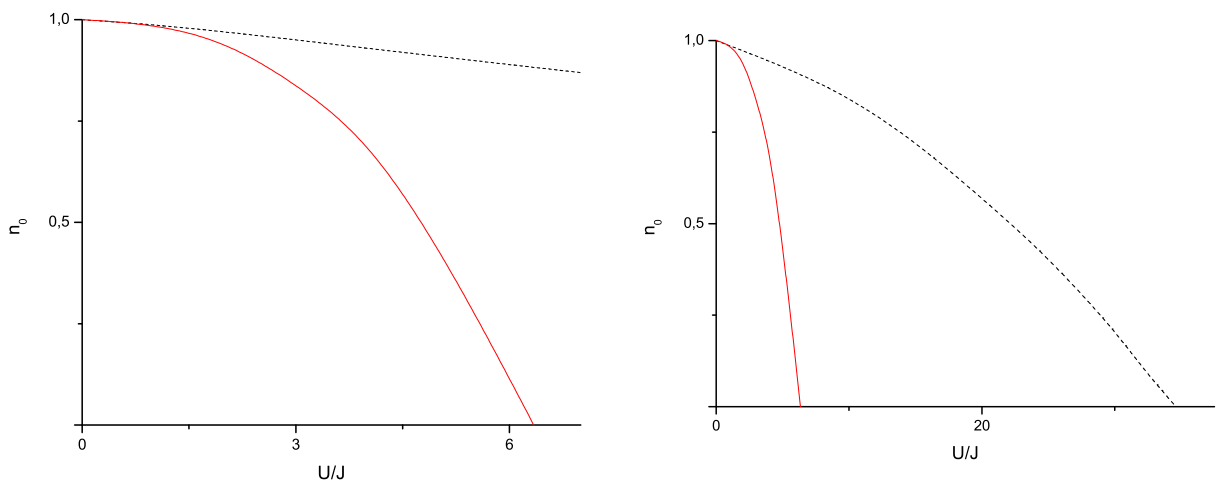
After some algebraic manipulations one obtains for the energy per particle E/N following expression

$$\begin{aligned}
\frac{E}{N} &= \frac{U(4\nu^2 + 4\nu - 1)}{8\nu} + \frac{\mu_1^2}{2U\nu} + \frac{U(I_{10B} + I_{20B})(I_{10B} - 3I_{20B})}{4\nu} + \frac{\Omega_{2L}^{(2)}(U,J,\nu)}{N}\\
&+ \frac{1}{2N_s\nu}\sum_{\mathbf{q}}[\mathcal{E}_0(\mathbf{q}) - \varepsilon(\mathbf{q})].
\end{aligned} \tag{82}$$

Here the energy of an "ideal gas " (when $U = 0$ in Bose-Hubbard Hamiltonian) has been subtracted .

VI. RESULTS AND DISCUSSIONS

Firstly we discuss the condensate fraction, n_0 vs U/J. In Fig.2a it is presented in one- and two-loop approximations, (dashed and solid curves respectively) for the filling factor $\nu = 1$ and $D = 3$. It is seen that in the one loop approximation n_0 can not reach zero within moderate values of U/J. More precisely $n_0[\text{one loop}] = 0$ at $U/J = 81.2$. On the other hand, two-loop contributions coming from the diagrams in Fig. 1 are too large: quantum phase transition occurs at $U/J \simeq 6$. Unfortunately this is rather far from the experimental value: $n_0 = 0$ at $U/J \simeq 29.34$ as pointed out in the Introduction. It is seen from Fig.2b that in Gutzwiller approach n_0 reaches zero at $U/J \simeq 34.8$ [30]. Note that the similar behavior of n_0 vs U/J with exactly the same κ_{crit} has been found by Stoof et al. in decoupling approximation in the second order perturbation theory [16].



a) b)

FIG. 2: The superfluid fraction n_0 as a function of U/J for $\nu = 1$, $D = 3$. a)In one (dashed line) and two loop approximations (solid line); b) Here the dashed line was obtained in Gutzwiller approache while the solid line in the present one.

The superfluid fraction for two values of ν , $\nu = 1$ (dotted line) and $\nu = 2$ (solid line) is shown in Fig. 3a and Fig. 3b for $D = 3$ and $D = 1$ respectively. It is seen that the critical value of U/J as well as a whole $n_0(U/J, \nu)$ are not so sensitive to the filling factor. The fact that the superfluid fraction does not crucially depend on ν has been observed also in Bogoliubov [9] as well as HFB [17] approximations. This is in contradiction with

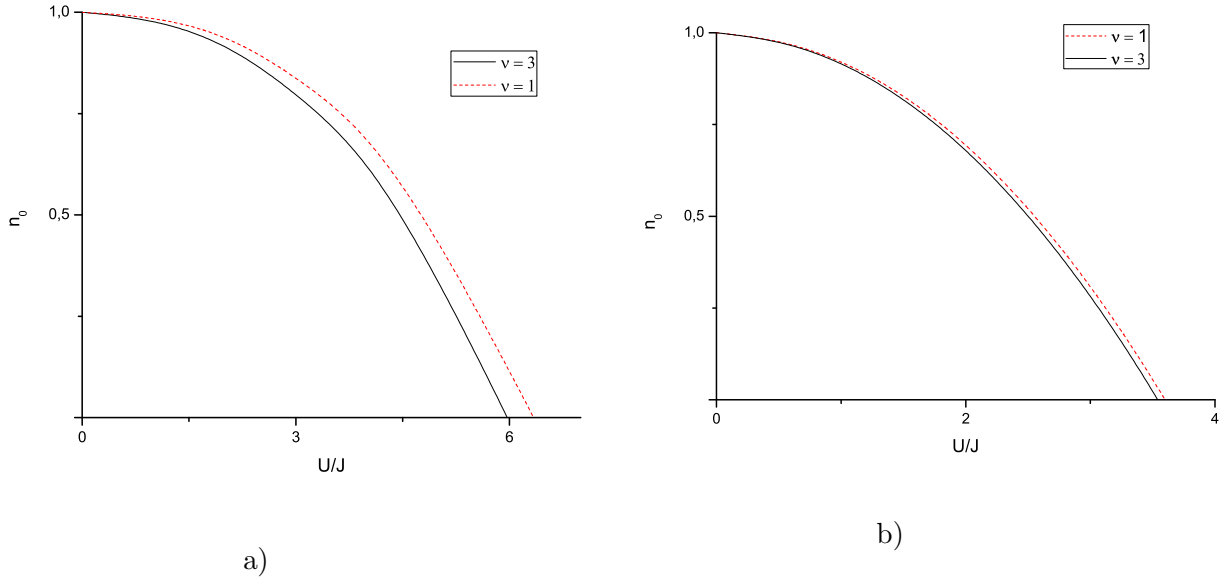


FIG. 3: The superfluid fraction as a function of U/J for $\nu = 1$ (dashed line) and $\nu = 3$ (solid line) for a) $D = 3$ and b) $D = 1$ in a two-loop approximation.

the prediction by Gutzwiller single site approximation [10] where the dependence is rather strong:

$$\kappa_{\rm crit} = z_0[\sqrt{\nu} + \sqrt{1+\nu}]^2 = 2D[\sqrt{\nu} + \sqrt{1+\nu}]^2 \tag{83}$$

Note that, although Eq. (83) gives a nice value for $\nu = 1$, $\kappa_{\rm crit} = 34.8$, it can not be considered as an absolute truth since , besides it's drawbacks, outlined above, it takes into account the lattice dimensionality in a rather simple way.

On the other hand as it is seen from Fig. 3b, for $D = 1$ the quantum phase transition, which , more strictly speaking, is a Berezinskii- Kosterlitz- Thouless transition, occurs around $U/J = 4$. This is in good agreement with Monte- Carlo predictions [6]. Similar results for $D = 1$ have been obtained by Danshita and Naidon in their time - evolving block decimation (TEBD) method [23]. However, note that TEBD method takes several days of computer calculations , while present approach does several minutes. In our calculations we used $N_s = 60$, $N = \nu N_s$, that is we considered finite size systems. This explains the smoothness of $n_0(U/J)$ in Figs. 3a and 3b.

The ground state energy per particle E/N vs U/J in units Jz_0 in one (solid line) and two (dashed line) loops is presented in Fig. 4. It is normalized such that the appropriate energy for the ideal case ($U = 0$ in the Bose-Hubbard Hamiltonian) is set to zero. It is seen

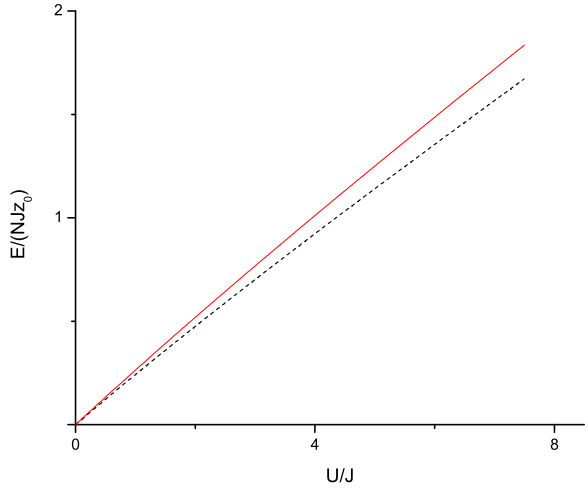


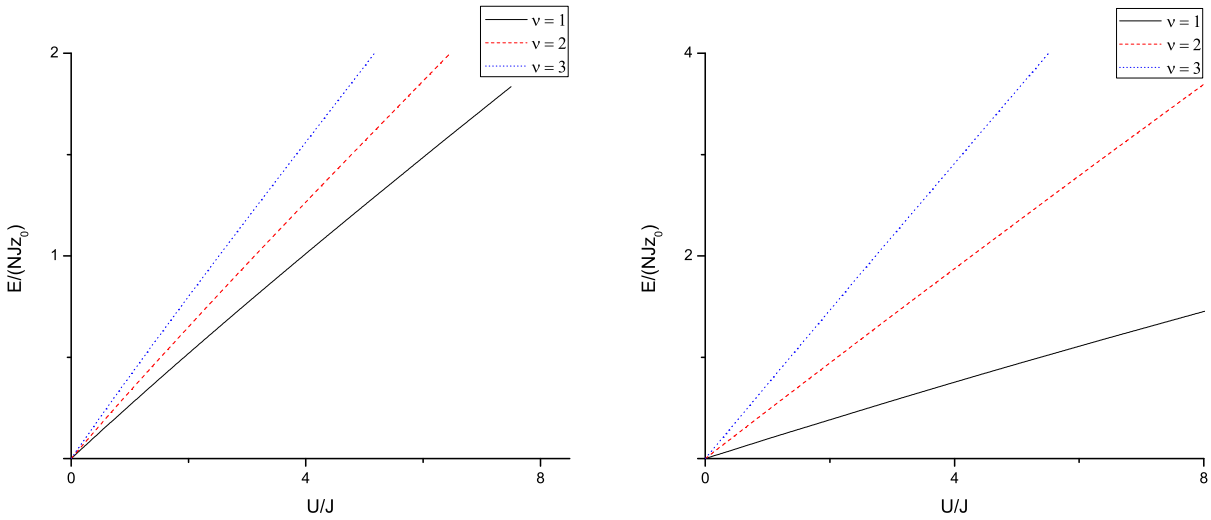
FIG. 4: The energy per atom in units Jz_0 in one (solid line) and two-loop (dashed line) approximations for $\nu = 1$ for $D = 3$.

that quantum corrections due to diagrams in Fig.1 are not significant for small $U/J < 1$. The dependence of E/N on filling factor ν is illustrated in Figs. 5a, 5b. It is seen that E is more sensitive to ν than n_0 due to the leading term (the first term in Eq. (82)) depending on ν explicitly.

VII. SUMMARY AND CONCLUSIONS

We have developed a field theoretical approach in terms of path integral formalism to calculate the second-order quantum corrections to the energy density as well as to the superfluid fraction in cubic optical lattices. Instead of using the standard formalism with complex field operatorsof condensed-matter literature, we find it more convenient to use two real fields. The thermodynamics of the system is deduced from the effective potential $\mathcal{V}$, whose minimum gives free energy Ω.

The superfluid fraction, n_0 , goes to zero at $U/J \sim 6$ for $\nu = 1, 2, 3$, and this is interpreted as a quantum phase transition from the superfluid to the Mott insulator phase. For $D = 1$, we have found a good description of the transition. Unfortunately, for $D = 2$ and $D = 3$ the critical values for the parameters are rather far from the experiment: $\kappa_{\rm crit}^{\rm exp}(D = 2) = 16.8$



a) b)

FIG. 5: The energy per atom in units Jz_0 for various values of the filling parameter ν for a) $D = 3$ and b) $D = 1$.

and $\kappa_{\rm crit}^{\rm exp}(D = 3) = 29.34$, for $\nu = 1$. It appears that a more relaible value for $\kappa_{\rm crit}$ for $D = 2, 3$ can only be reached by going beyond the present two-loop approximation. We expect that higher-order quantum corrections, for example post-Gaussian approximation [21, 31], will improve the situation, but they are hard to calculate.

Thus we have shown that going beyond the Bogoliubov approximation employed by Stoof et al. [16], one finds a quantum phase transition from a superfluid to a Mott insulator state. Within a two-loop approximation we have derived explicit expression for the ground state energy of the optical lattice.

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Appendix

In present work all the calculations are carried out in real time. Loop integrals are taken over real energies ω and over three dimensional quasimomentum $\vec{k}$ which pertains to the Brillouin zone $-\pi/a \leq k_\alpha \leq \pi/a$. So, three or six dimensional integrals, presenting in one or two-loop calculations are finite and may be evaluated numerically by using Monte - Carlo methods.

The integrals over ω are evaluated using contour integration. Some energy integrals needed for one- and two-loop calculations can be easily evaluated directly by using residue formulas:

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{(\omega^2 - \mathcal{E}^2 + i\epsilon)} = -\frac{i}{2\mathcal{E}} \tag{84}$$

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{(\omega^2 - \mathcal{E}^2 + i\epsilon)^2} = \frac{i}{4\mathcal{E}^3} \tag{85}$$

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\omega^2}{(\omega^2 - \mathcal{E}^2 + i\epsilon)^2} = -\frac{i}{4\mathcal{E}} \tag{86}$$

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{d\omega_1 d\omega_2}{4\pi^2} \frac{1}{[\omega_1^2 - \mathcal{E}_1^2 + i\epsilon][\omega_2^2 - \mathcal{E}_2^2 + i\epsilon][(\omega_1 + \omega_2)^2 - \mathcal{E}_3^2 + i\epsilon]} = \frac{1}{4\mathcal{E}_1\mathcal{E}_2\mathcal{E}_3(\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3)} \tag{87}$$

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{d\omega_1 d\omega_2}{4\pi^2} \frac{\omega_1\omega_2}{[\omega_1^2 - \mathcal{E}_1^2 + i\epsilon][\omega_2^2 - \mathcal{E}_2^2 + i\epsilon][(\omega_1 + \omega_2)^2 - \mathcal{E}_3^2 + i\epsilon]} = \frac{1}{4\mathcal{E}_3(\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3)} \tag{88}$$

In the last two integrals $\mathcal{E}_1 \equiv \mathcal{E}(\mathbf{q}_1)$, $\mathcal{E}_2 \equiv \mathcal{E}(\mathbf{q}_2)$, and $\mathcal{E}_3 \equiv \mathcal{E}(\mathbf{q}_1 + \mathbf{q}_2)$.

The integral

$$I_{12}(\mathbf{q}) = \int \frac{d\omega}{2\pi} \frac{i\omega}{(\omega^2 - \mathcal{E}^2(\mathbf{q}) + i\epsilon)} \tag{89}$$

needed for $G_{12}(0) = -(i/N_s)\sum_{\mathbf{q}} I_{12}(\mathbf{q})$ should be considered more carefully.To evaluate it we use following formula given in the literature [26]

$$\frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{e^{i\eta\omega_n}(b + i\omega_n)}{\omega_n^2 + a^2}\Bigg|_{\eta\to 0} = \frac{1}{2}\left(\frac{b}{a} - 1\right) + \frac{b}{a(e^{\beta a} - 1)} \tag{90}$$

where $\omega_n = 2\pi n T$, $\beta = 1/T$. The zero temperature limit, $T \to 0$, of (90) leads to

$$I_{12}(\mathbf{q}) = -\frac{1}{2} \tag{91}$$

so that $G_{12}(0) = (i/2N_s)\sum_{\mathbf{q}}[1]$. This constant enters into the evaluation of the constant $n_1 \sim \langle\tilde{\varphi}^\dagger\tilde{\varphi}\rangle$, and produces a term -1 in the square brackets of Eq. (76). In a homogeneous Bose gas, such a constant term can be ignored. But here, on an optical lattice, it becomes

significant, so that in the evaluation of trace log term in Eq (41), it must be taken into account properly. How to do that has been shown in the textbook [32]. Strictly speaking, the integral

$$L(\mathcal{E}) = \int \frac{d\omega}{2\pi} \ln(\omega^2 - \mathcal{E}^2) \tag{92}$$

appearing in the trace log is divergent. To evaluate it, one may differentiate (92) with respect to $\mathcal{E}^2$:

$$\frac{\partial L(\mathcal{E})}{\partial \mathcal{E}^2} = -\int \frac{d\omega}{2\pi} \frac{1}{(\omega^2 - \mathcal{E}^2)} \tag{93}$$

and use (84) to obtain

$$\frac{\partial L(\mathcal{E})}{\partial \mathcal{E}^2} = \frac{i}{2\mathcal{E}} \tag{94}$$

Integrating this once $\mathcal{E}^2$ gives

$$L(\mathcal{E}) = \int \frac{d\omega}{2\pi} \ln(\omega^2 - \mathcal{E}^2) = i\mathcal{E} + \text{constant}. \tag{95}$$

Using the method of Ref. [32] we obtain the result of Section III where the constant leads to a term term -1 in n_1 (see Eq. 76).

[1] O. Morsch and M. Oberthaler Rev. Mod. Phys. **78**, 179 (2006).

[2] R. Raussendorf, D.E. Browne and H. J. Briegel, Phys. Rev. A **68**, 022312 (2003).

[3] M. Fisher, P. B. Weichman, G. Grinstein and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).

[4] M. Greiner, O. Mandel, T. Esslinger, T. W. Hansch and I. Bloch, Nature **415**, 39 (2002).

[5] B. Capogrosso-Sansone, N. V. Prokofiev, and B. V. Svistunov, Phys. Rev. **B** 75, 134302 (2007); S. Trotzky, L. Pollet, F. Gerbier, U. Schnorrberger, I. Bloch, N. V. Prokofev, B. Svistunov and M. Troyer, Nature Phys. **6**, 998-1004 (2010).

[6] G. G. Batrouni, V. Rousseau, R. T. Scalettar, M. Rigol, A. Muramatsu, P. J. H. Denteneer, M. Troyer, Phys. Rev. Lett. **89**, 117203 (2002).

[7] S. Burger, F. S. Cataliotti, C. Fort, F. Minardi, M. Inguscio, M. L. Chiofalo and M. P. Tosi, Phys. Rev. Lett. **86**, 4447 (2001).

[8] F. E. A. dos Santos and A. Pelster, Phys. Rev. A **79**, 013614 (2009).

[9] H. T. C. Stoof, K. B. Gubbels and D.B.M. Dickerscheid *Ultracold Quantum Fields* (Springer, 2009).

[10] M. G. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963)

[11] D. S. Rokhsar and B. G. Kotliar Phys. Rev. B **44**, 10328 (1991) ; D. Jaksch, C. Bruder, et al. Phys. Rev. Lett. **81**, 3108 (1998).

[12] W. Krauth , M. Caffarel,and J. Bouchaud Phys. Rev. B **45**, 3137 (1992)

[13] V. I. Yukalov, Laser Physics **19**, 1 (2009).

[14] P. Buonsante and A. Vezzani, Phys. Rev. A **70**, 033608 (2004).

[15] Abdulla Rakhimov, Shuhrat Mardonov and E.Ya. Sherman, Ann. Phys. **326**, 2499 (2011); Abdulla Rakhimov, E. Ya. Sherman and Chul Koo Kim, Phys. Rev. B **81**, 020407(R) (2010).

[16] D. van Osten, O. van der Straten and H.T.C. Stoof Phys. Rev. A **63**, 053601 (2001).

[17] V.I. Yukalov, A. Rakhimov, S. Mardonov, Laser Phys. **21**, 264 (2011).

[18] H. Kleinert, S. Schmidt, and A. Pelster, Annalen der Physik (Leipzig) **14**, 214-230 (2005)

[19] For field theories on a lattice see H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I Superflow and Vortex Lines, World Scientific, Singapore 1989, pp. 1–756.

[20] R. Jackiw, Phys. Rev. D **9**, 1686 (1974).

[21] A. M. Rakhimov, Jae Hyung Yee, Intern. Journ. Mod. Phys. A **19**, 1589 (2004).

[22] H. Kleinert, *Converting Divergent Weak-Coupling into Exponentially Fast Convergent Strong-Coupling Expansions*, EJTP **8**, 25 (2011) `http://www.ejtp.com/articles/ejtpv8i25p15.pdf`.

[23] I. Danshita and P. Naidon , Phys. Rev. A **79**, 043601 (2009).

[24] J. O. Andersen, Rev. Mod. Phys. **76**, 599 (2004).

[25] H. Kleinert and V. Schulte-Frohlinde, *Critical Phenomena in ϕ^4-Theory*, World Scientific, Singapore, 2001.

[26] J. I. Kapusta *Finite Temperature Field Theory*, (Cambridge University Press, 1989); Michel Le Bellac *Thermal Field Theory*, (Cambridge University Press, 1996).

[27] T. Haugset, H. Haugerud and F. Ravndal, Ann. Phys. **27**, 266 (1998).

[28] E. Braaten and A. Nieto, Euro. Phys. J. B **11**, 143 (1999).

[29] V. I. Yukalov Ann. Phys. **323**, 461 (2008)

[30] K. Sheshadri, H. R. Krishnamurthy, R. Pandit and T. V. Ramakrishnan, Europhys. Lett. **22**, 257, (1993).

[31] P. M. Stevenson Phys. Rev. D **32**, 1389 (1985); Chul Koo Kim, A. Rakhimov and Jae Hyung Yee Eur. Phys. Journ. B **39**, 301 (2004); A. Rakhimov, Chul Koo Kim, Sang-Hoon Kim and Jae Hyung Yee, Phys. Rev. A **77**, 033626 (2008).

[32] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 5th ed., World Scientific (2009).