Quantum phase transitions in optical lattices beyond the Bogoliubov approximation

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We study the quantum phase transition from a superfluid to a Mott insulator in optical lattices using a Bose-Hubbard Hamiltonian. For this purpose we develop 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 the 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 the following two factors [1].

(1) Neutral atoms in these optical lattices have a number of effective 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 the Bose-Hubbard Hamiltonian:

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

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

Clearly the SF 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 for easier reading here, we clarify 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 number of particles $N_0 \neq 0$, the gauge symmetry is spontaneously broken in accordance with the Bogoliubov and Ginibre theorems. In contrast, in the MI phase, there is no long-range correlation or 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 the above quantum phase transition, depending on the starting point. In the experiments by Greiner *et al.* [4] one first creates a Bose-Einstein condensate 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 the ground state of the harmonic plus the periodic potential. It seems to be that the first method is good for observing SF $\to$ MI transitions, while the second one is good for MI $\to$ SF transitions.

Similarly, most theoretical approaches can be divided into two classes: SF $\to$ MI and MI $\to$ SF. The latter are based on the Ginzburg-Landau theory as described, for instance, in Ref. [8]. They are well suited for analysis of the time-of-flight pictures and the resulting visibility at zero and finite temperatures. In the former class (SF $\to$ MI) one uses a

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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 the last lines in Sec. IV).

(1) The mean-field Hamiltonian, which features single boson terms, does not conserve the total number of bosons [14].

(2) Tunneling of uncondensed atoms is neglected.

(3) The critical value $\kappa_{\rm crit}$ does not depend on the lattice dimension.

Nevertheless, prediction of the 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 spin excitations in magnetic insulators, 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 0 for finite values of κ, implying that this approximation is unable to predict a possible phase transition to an MI 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 when we go beyond these approximations.

In the present work we investigate BEC in optical lattices by applying a two-loop approximation and treating the result by variational perturbation theory (VPT) [18]. It is 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 0 at $\kappa \sim 6$–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 the functional formalism for the 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 the condensate fraction vs input parameters U, J, and ν. The quantum corrections to the energy of the system are discussed in Sec. V. In Sec. VI we present numerical results and discussion. Section VII summarizes our results.

II. ACTION AND PROPAGATORS IN THE BOSE-HUBBARD MODEL

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

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

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

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

with λ the wavelength of the laser light. The lattice points lie at 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 action (2) is equivalent to the well-known Bose-Hubbard model, (1).

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

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

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

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

where $\omega_n(\mathbf{x})$ are Wannier functions. In the tight-binding limit and pseudopotential approximation, $V(\mathbf{x}-\mathbf{x}') = 4\pi a\delta(\mathbf{x}-\mathbf{x}')/m$, Eqs. (7) and (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, action (2) can be rewritten as follows:

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

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 is 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 go into a BEC state. The necessary and sufficient condition for BEC is 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 $\nu = N/N_s$ is the filling factor, and the condensate fraction, $n_0 = N_0/N$, is constant for a regular lattice without a 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:

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

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

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

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

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

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

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

$$X_1 = -\mu + 3U\nu n_0, \quad X_2 = -\mu + U\nu n_0. \tag{23}$$

For a homogeneous 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 $\mathbf{q} = \{q_1,q_2,\ldots,q_d\}$, 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 the noncondensed modes. In momentum space the quadratic term $S^{(2)}$ is as follows:

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

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

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

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

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

where

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

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

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

Note that, in deriving (26)–(30), the following relations were used:

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

III. EFFECTIVE POTENTIAL IN THE TWO-LOOP APPROXIMATION

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

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

$$S_{\rm cl} = S^0 = N_s \int dt \left\{ \mu \nu n_0 + J z_0 \nu n_0 - \frac{U}{2} \nu^2 n_0^2 \right\}, \quad (34)$$

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

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

$$\mathcal{L}_{\rm int}(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t)) = v_3\left[\varphi_1(\mathbf{x_i},t)\varphi_2^2(\mathbf{x_i},t) + \varphi_1^3(\mathbf{x_i},t)\right] + v_4\left[\varphi_1^4(\mathbf{x_i},t) + \varphi_2^4(\mathbf{x_i},t) + 2\varphi_1^2(\mathbf{x_i},t)\varphi_2^2(\mathbf{x_i},t)\right] \equiv \mathcal{L}_3 + \mathcal{L}_4, \quad (37)$$

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

The perturbative framework is based on the propagator $G_{ab}(k,\omega)$ given in (29). The effective potential $\mathcal{V}$ can be evaluated by Eq. (13), where the only connected, irreducible diagrams in the partition function $Z = \int \mathcal{D}\varphi_1 \mathcal{D}\varphi_2 \exp(iS(\varphi_1,\varphi_2))$ should be taken into account. The grand thermodynamic potential, i.e., the 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:

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

where we have introduced the notation

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

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 the factor $\exp(iS_0)$ in Eq. (38):

$$\mathcal{V}_0 = \frac{i}{T} \ln e^{iS_0} = \frac{N_s \nu n_0}{2} [U \nu n_0 - 2(\mu + J z_0)]. \quad (40)$$

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

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

where $M(\omega,\mathbf{q})$ is given by Eq. (28). One notes that the frequency sum, and, with it, the ω integration, is divergent. In fact, to evaluate a frequency sum such as $\sum_{n=-\infty}^{n=\infty} \ln(a^2 + \omega_n^2)$, with $\omega_n = 2\pi n T$, one differentiates it with respect to a and, after performing 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 subtracting from $\mathcal{V}$ the thermodynamic potential for the ideal gas [27]:

$$\mathcal{V}_{1L}^{\rm ren} = \mathcal{V}_{1L}(U) - \mathcal{V}_{1L}(U=0) = \frac{1}{2} \sum_{\mathbf{q}} \mathcal{E}(\mathbf{q}) - \frac{1}{2} \sum_{\mathbf{q}} \mathcal{E}(\mathbf{q}) \Big|_{U=0} = \frac{1}{2} \sum_{\mathbf{q}} [\mathcal{E}(\mathbf{q}) - \varepsilon(\mathbf{q}) + \mu + J z_0], \quad (42)$$

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

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

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

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

$$\langle \mathcal{L}_{\rm int} \rangle_0 = \langle \mathcal{L}_4 \rangle_0 = v_4 \left\{ \langle \varphi_1^4 \rangle_0 + \langle \varphi_2^4 \rangle_0 + 2 \langle \varphi_1^2 \varphi_2^2 \rangle_0 \right\}. \quad (44)$$

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 in (38). As for the term $\mathcal{L}_4(\varphi_a(\mathbf{x_i},t)) \mathcal{L}_4(\varphi_a(\mathbf{x_i},t))$, it should also be omitted since its contribution is beyond two-loop corrections. Therefore

$$\mathcal{V}_{2L} = \frac{i}{T} \ln \left\{ 1 + i \sum_{\mathbf{i}} \langle \mathcal{L}_4(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t)) \rangle_0 + \frac{i^2}{2} \sum_{\mathbf{i},\mathbf{j}} \times \int dt dt' \langle \mathcal{L}_3(\varphi_1(\mathbf{x_i},t),\varphi_2(\mathbf{x_i},t)) \mathcal{L}_3(\varphi_1(\mathbf{x_j},t),\varphi_2(\mathbf{x_j},t)) \rangle_0 \right\}. \quad (45)$$

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

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

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

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

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)

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

The third term,

$$\begin{aligned}\langle \mathcal{L}_3\mathcal{L}_3\rangle_0 = v_3^2\big[&\left\langle\varphi_1(x)\varphi_2^2(x)\varphi_1(y)\varphi_2^2(y)\right\rangle_0\\ &+2\left\langle\varphi_1(x)\varphi_2^2(x)\varphi_1^3(y)\right\rangle_0+\left\langle\varphi_1^3(x)\varphi_1^3(y)\right\rangle_0\big],\end{aligned} \tag{50}$$

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

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

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

Now, using (46), (50), and (51) in Eq. (45), we finally obtain

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

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

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

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

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

where the following integrals are introduced,

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

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

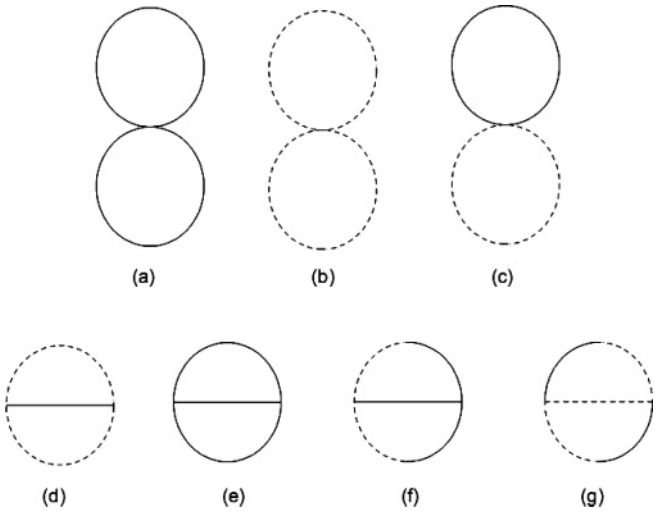

FIG. 1. Vacuum diagrams in a two-loop approximation. Solid and dashed lines correspond to G_{11} and G_{22}, respectively, while a mixed line corresponds to G_{12} (or G_{21}).

IV. THE CONDENSATE FRACTION IN VPT

To evaluate the condensate fraction n_0 as an explicit function of U/J and v, we use the following strategy, referred to as a VPT [18].

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

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

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

(2) Impose the extremalization condition,

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

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

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

with

$$n_{01}(\mu) = -\frac{\mathcal{V}'_{1L}(\mu,n_{00})}{\mathcal{V}''_0(\mu,n_{00})},$$

$$n_{02}(\mu) = -\frac{n^2_{01}(\mu)\mathcal{V}'''_0(\mu,n_{00}) + 2\mathcal{V}'_{2L}(\mu,n_{00}) + 2n_{01}(\mu)\mathcal{V}''_{1L}(\mu,n_{00})}{2\mathcal{V}''_0(\mu,n_{00})}, \quad (60)$$

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

(4) Introduce a variational parameter M as

$$\mu = M + r\eta, \quad (61)$$

with the abbreviation

$$r = \frac{\mu - M}{\eta}, \quad (62)$$

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

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

$$M_{\rm opt} = Uv - Jz_0. \quad (63)$$

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

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

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

$$\frac{\partial\mathcal{V}_0(n_0,\mu)}{\partial n_0} = -N_s[v\tilde{\mu} - Uv^2n_0], \quad (65)$$

$$\frac{\partial\mathcal{V}_{1L}(n_0,\mu)}{\partial n_0} = -\frac{Uv}{2}\sum_{\mathbf{q}}\frac{(2\tilde{\mu} - 3Uvn_0 - 2\varepsilon(\mathbf{q}))}{\mathcal{E}(\mathbf{q})}, \quad (66)$$

$$\frac{\partial\mathcal{V}^{(1)}_{2L}(n_0,\mu)}{\partial n_0} = \frac{U^2v}{4}\sum_{\mathbf{q}}\frac{(\tilde{\mu} - \varepsilon(\mathbf{q}))\,[(\tilde{\mu} - 4Uvn_0 - \varepsilon(\mathbf{q}))I_{10}(n_0,\mu) - (\tilde{\mu} - \varepsilon(\mathbf{q}))I_{20}(n_0,\mu)]}{\mathcal{E}^3(\mathbf{q})}, \quad (67)$$

where the following relations are used:

$$\frac{\partial\mathcal{E}(\mathbf{q})}{\partial n_0} = -\frac{Uv}{\mathcal{E}(\mathbf{q})}(2\mu - 3Uvn_0 - 2\varepsilon(\mathbf{q}) + 2Jz_0), \quad (68)$$

$$\frac{\partial I_{10}}{\partial n_0} = \frac{Uv}{2N_s}\sum_{\mathbf{q}}\frac{(\mu - \varepsilon(\mathbf{q}) + Jz_0)(\mu - 3Uvn_0 - \varepsilon(\mathbf{q}) + Jz_0)}{\mathcal{E}^3(\mathbf{q})}, \quad (69)$$

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

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

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

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) and (71) into Eq. (56), one gets $\Omega(\mu)$ as a function of μ as

$$\begin{aligned}
\Omega(\mu) &= \mathcal{V}(\mu,\bar{n}_0) = \Omega_0(\mu)+\eta\Omega_1(\mu)+\eta^2\Omega_2(\mu),\\
\Omega_0(\mu) &= -\frac{N_s(\mu+Jz_0)^2}{2U},\\
\Omega_1(\mu) &= \frac{1}{2}\sum_{\mathbf{q}}[\mathcal{E}_\mu(\mathbf{q})+\mu-\varepsilon(\mathbf{q})+Jz_0],\\
\Omega_2(\mu) &= \mathcal{V}^{(2)}_{2L}[\mu,n_{00}(\mu)]+\frac{UN_s}{8}\left[2I^2_{10}(\mu)-4I_{10}(\mu)I_{20}(\mu)-6I^2_{20}(\mu)-1\right].
\end{aligned} \tag{74}$$

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

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

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

$$\begin{aligned}
n_1 &= n^{1L}_1+n^{2L}_1,\\
n^{1L}_1 &= \frac{1}{2\nu N_s}\sum_{\mathbf{q}}\left[\frac{\varepsilon(\mathbf{q})+U\nu}{\mathcal{E}_0(\mathbf{q})}-1\right],
\end{aligned} \tag{76}$$

$$\begin{aligned}
n^{2L}_1 &= \frac{1}{N_sU\nu^2}\frac{\partial\mathcal{V}^{(2)}_{2L}}{\partial n_0}\bigg|_{n_0=n_{00}}-\frac{1}{\nu N_s}\frac{\partial\mathcal{V}^{(2)}_{2L}}{\partial\mu}\bigg|_{\mu=\mu_0}-\frac{(I_{10B}-I_{20B})^2}{4\nu^2}\\
&\quad-\frac{U}{4N_s\nu}\sum_{\mathbf{q}}\frac{[(I_{10B}-I_{20B})(2U^2\nu^2-\varepsilon^2(\mathbf{q}))+U\nu\varepsilon(\mathbf{q})(2I_{20B}-1)]}{\mathcal{E}^3_0(\mathbf{q})}.
\end{aligned} \tag{77}$$

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

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

Now we compare the present approximation with Gutzwiller's.

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

(2) As seen from Eqs. (76) and (77), in Bogoliubov-type approximations the uncondensed particles have momentum distribution $n_q = \langle a_q^\dagger a_q \rangle$ varying as q^{-4} for large momentum [29], while in the 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. (79) can be rewritten as

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

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

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

with $\mathcal{E}_0(\mathbf{q})$ given in Eq. (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, the expression

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

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

VI. RESULTS AND DISCUSSION

First, we discuss the condensate fraction, n_0 vs U/J. In Fig. 2(a) 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 cannot reach 0 within moderate values of U/J. More precisely $n_0[\text{oneloop}] = 0$ 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 Sec. I. It is shown in Fig. 2(b) that in the Gutzwiller approach n_0 reaches 0 at $U/J \simeq 34.8$ [30]. Note that a similar behavior of n_0 vs U/J with exactly the same κ_{crit} was found by Stoof *et al.* in a decoupling approximation in the second-order perturbation theory [16].

The SF fraction for two values of ν, $\nu = 1$ (dotted line) and $\nu = 2$ (solid line) is shown in Figs. 3(a) and 3(b) for $D = 3$ and $D = 1$, respectively. It is shown that the critical values of U/J as well as a whole $n_0(U/J,\nu)$ are not as sensitive to the filling factor. The fact that the SF fraction does not crucially depend on ν has been observed also in Bogoliubov [9] as well as HFB [17] approximations. This is in contradiction to the prediction by the Gutzwiller single-site approximation [10], where the dependence is rather strong:

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

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

On the other hand as shown in Fig. 3(b), 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 $D = 1$ were obtained by Danshita and Naidon in their time-evolving block decimation (TEBD) method [23]. However, note that the TEBD method takes several days of computer calculations, while the present

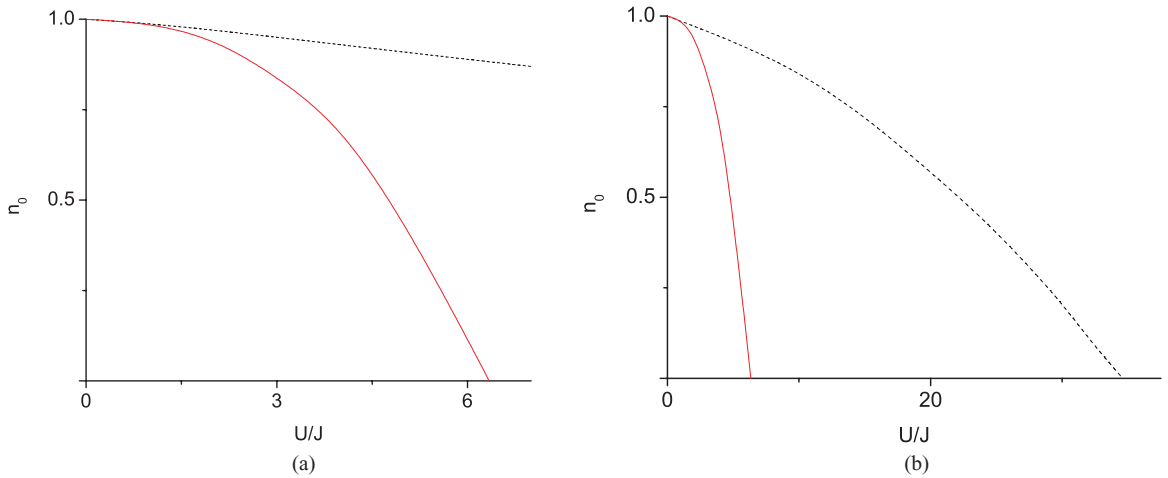

FIG. 2. (Color online) Superfluid fraction n_0 as a function of U/J for $\nu = 1$, $D = 3$. (a) In one-loop (dashed line) and two-loop (solid line) approximations. (b) Here the dashed line was obtained with the Gutzwiller approach, and the solid line with the present one.

approach takes 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. 3(a) and 3(b).

The ground-state energy per particle E/N vs U/J in units of 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 0. It is shown that quantum corrections due to diagrams in Fig. 1 are not significant for small $U/J < 1$. The dependence of E/N on the filling factor ν is illustrated in Figs. 5(a) and 5(b). It is shown 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 the path integral formalism to calculate second-order quantum corrections to the energy density as well as to the SF fraction in cubic optical lattices. Instead of using the standard formalism with complex field operators from the 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 SF fraction, n_0, goes to 0 at $U/J \sim 6$ for $\nu = 1,2,3$, and this is interpreted as a quantum phase transition from the SF to the MI 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: $\kappa_{\rm crit}^{\rm exp}(D = 2) = 16.8$ and $\kappa_{\rm crit}^{\rm exp}(D = 3) = 29.34$, for $\nu = 1$. It appears that a more reliable 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, a 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

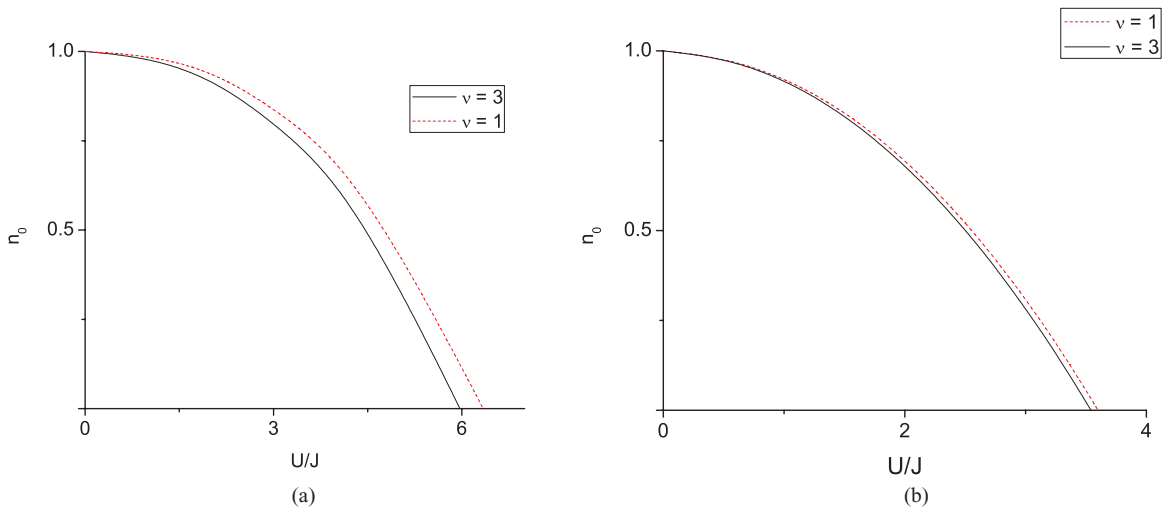

FIG. 3. (Color online) Superfluid fraction as a function of U/J for $\nu = 1$ (dashed line) and $\nu = 3$ (solid line) for (a) $D = 3$ and (b) $D = 1$ in a two-loop approximation.

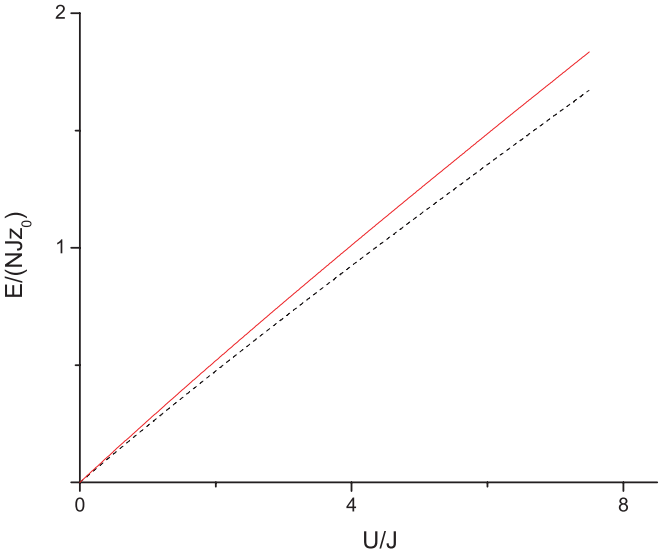

FIG. 4. (Color online) Energy per atom in units of Jz_0 in one-loop (solid line) and two-loop (dashed line) approximations for $\nu = 1$ for $D = 3$.

a quantum phase transition from an SF to a MI state. Within a two-loop approximation we have derived an explicit expression for the ground-state energy of the optical lattice.

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APPENDIX

In the 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, $-\pi/a \leqslant k_\alpha \leqslant \pi/a$. 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:

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{(\omega^2 - \mathcal{E}^2 + i\epsilon)} = -\frac{i}{2\mathcal{E}}, \tag{A1}$$

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{(\omega^2 - \mathcal{E}^2 + i\epsilon)^2} = \frac{i}{4\mathcal{E}^3}, \tag{A2}$$

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\omega^2}{(\omega^2 - \mathcal{E}^2 + i\epsilon)^2} = -\frac{i}{4\mathcal{E}}, \tag{A3}$$

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \frac{d\omega_1 d\omega_2}{4\pi^2} \frac{1}{[\omega_1^2 - \mathcal{E}_1^2 + i\epsilon][\omega_2^2 - \mathcal{E}_2^2 + i\epsilon][(\omega_1+\omega_2)^2 - \mathcal{E}_3^2 + i\epsilon]} = \frac{1}{4\mathcal{E}_1\mathcal{E}_2\mathcal{E}_3(\mathcal{E}_1+\mathcal{E}_2+\mathcal{E}_3)}, \tag{A4}$$

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \frac{d\omega_1 d\omega_2}{4\pi^2} \frac{\omega_1\omega_2}{[\omega_1^2 - \mathcal{E}_1^2 + i\epsilon][\omega_2^2 - \mathcal{E}_2^2 + i\epsilon][(\omega_1+\omega_2)^2 - \mathcal{E}_3^2 + i\epsilon]} = \frac{1}{4\mathcal{E}_3(\mathcal{E}_1+\mathcal{E}_2+\mathcal{E}_3)}. \tag{A5}$$

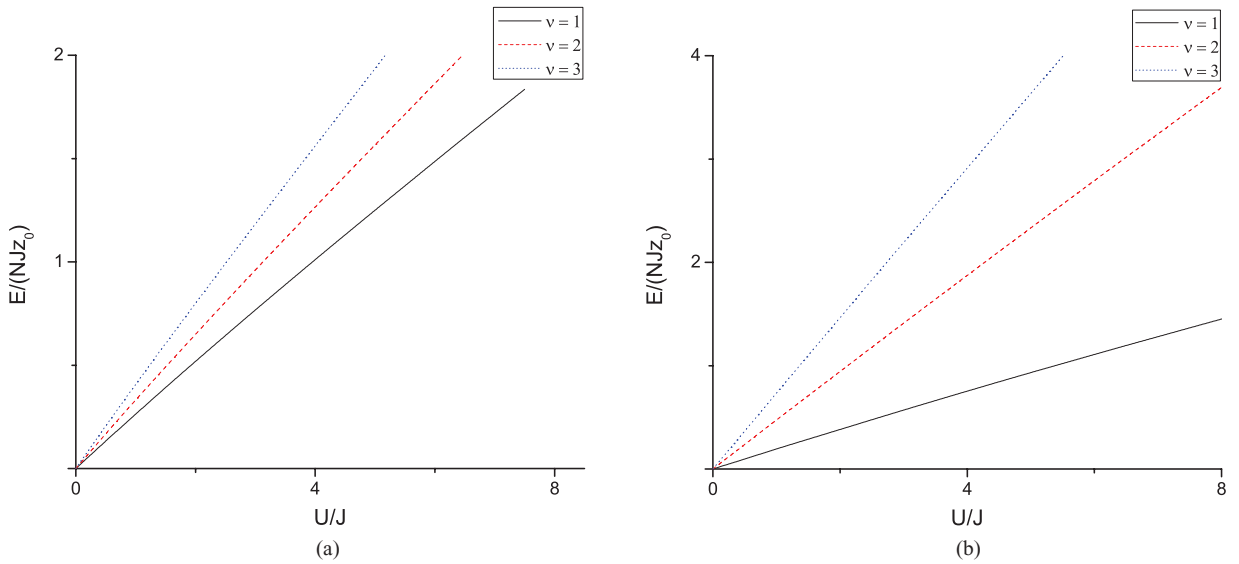

FIG. 5. (Color online) Energy per atom in units of Jz_0 for various values of the filling parameter ν for (a) $D = 3$ and (b) $D = 1$.

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

$$I_{12}(\mathbf{q}) = \int \frac{d\omega}{2\pi} \frac{i\omega}{(\omega^2 - \mathcal{E}^2(\mathbf{q}) + i\epsilon)}, \tag{A6}$$

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 a formula given in the literature [26],

$$\frac{1}{\beta}\sum_{n=-\infty}^{\infty} \frac{e^{i\eta\omega_n}(b + i\omega_n)}{\omega_n^2 + a^2}\bigg|_{\eta\to 0} = \frac{1}{2}\left(\frac{b}{a} - 1\right) + \frac{b}{a(e^{\beta a} - 1)}, \tag{A7}$$

where $\omega_n = 2\pi nT$, $\beta = 1/T$. The zero-temperature limit, $T \to 0$, of (A7) leads to

$$I_{12}(\mathbf{q}) = -\tfrac{1}{2}, \tag{A8}$$

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 the term -1 in the square brackets in 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 the trace log term in Eq. (41), it must be taken into account properly. How to do that has been shown in a textbook [32]. Strictly speaking, the integral

$$L(\mathcal{E}) = \int \frac{d\omega}{2\pi} \ln(\omega^2 - \mathcal{E}^2) \tag{A9}$$

appearing in the trace log is divergent. To evaluate it, one may differentiate (A9) with respect to $\mathcal{E}^2$,

$$\frac{\partial L(\mathcal{E})}{\partial \mathcal{E}^2} = -\int \frac{d\omega}{2\pi} \frac{1}{(\omega^2 - \mathcal{E}^2)}, \tag{A10}$$

and use (A1) to obtain

$$\frac{\partial L(\mathcal{E})}{\partial \mathcal{E}^2} = \frac{i}{2\mathcal{E}}. \tag{A11}$$

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

$$L(\mathcal{E}) = \int \frac{d\omega}{2\pi} \ln(\omega^2 - \mathcal{E}^2) = i\mathcal{E} + \text{constant}. \tag{A12}$$

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

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