

Extended self-energy functional approach for strongly correlated lattice bosons in the superfluid phase

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Among the various numerical techniques to study the physics of strongly correlated quantum many-body systems, the self-energy functional approach (SFA) has become increasingly important. In its previous form, however, SFA is not applicable to Bose-Einstein condensation or superfluidity. In this paper, we show how to overcome this shortcoming. To this end, we identify an appropriate quantity, which we term D , that represents the correlation correction of the condensate order parameter, as it does the self-energy for Green's function. An appropriate functional is derived, which is stationary at the exact physical realization of D and of the self-energy. Its derivation is based on a functional-integral representation of the grand potential followed by an appropriate sequence of Legendre transformations. The approach is not perturbative and, therefore, applicable to a wide range of models with local interactions. We show that the variational cluster approach based on the extended self-energy functional is equivalent to the "pseudoparticle" approach proposed in [Phys. Rev. B **83**, 134507 \(2011\)](#). We present results for the superfluid density in the two-dimensional Bose-Hubbard model, which shows a remarkable agreement with those of quantum-Monte-Carlo calculations.

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I. INTRODUCTION

Seminal experiments with ultracold gases of atoms trapped in optical lattices shed new light on strongly correlated many-body systems.¹⁻³ In these experiments, specific lattice Hamiltonians can be engineered and investigated with a remarkably high level of control, making quantum mechanical interference effects observable on a macroscopic scale. Most important as well as fundamental is the quantum phase transition of strongly correlated lattice bosons from the localized Mott phase to the delocalized superfluid phase. In the superfluid phase, a macroscopic fraction of the particles condenses into one quantum mechanical state, thus, forming a Bose-Einstein condensate, where the number of particles in the condensate is not necessarily equal to the number of superfluid particles. In experiments with ultracold gases of atoms trapped in optical lattices, the condensate density can be extracted from time-of-flight images,² which are related to the momentum distribution of the confined particles. Importantly, the finite expansion time of the particle cloud has to be taken into account when drawing the connection between these time-of-flight images and the true momentum distribution.⁴⁻⁷ However, it is probably even more challenging to measure the superfluid density itself, as it is not a ground-state property but rather related to the response of the system to a phase twisting field.⁸ Interestingly, only very recently for Bose gases without the periodic lattice potential, an optical method has been proposed to extract the superfluid density. This experiment creates a vector potential, that imposes angular momentum on normal fluid particles, while superfluid particles stay at rest.⁹

In a previous work, we extended the variational cluster approach (VCA), which is capable of dealing with strongly correlated many-body systems, to the symmetry broken superfluid phase of lattice bosons.¹⁰ Originally, the VCA had been formulated for the normal Mott phase of lattice bosons in Ref. 11 within the so-called self-energy functional approach (SFA), which was previously introduced for interacting fermionic systems.^{12,13} Our extension to the superfluid

phase in Ref. 10 follows a different path and is based on the so-called "pseudoparticle" formalism. Within this approach, we obtained the expressions for the superfluid order parameter, the anomalous Green's function, and the grand potential, which is the starting point for the variational principle [see Eqs. (1), (33), and (2) in this reference].

It should be pointed out that, while the pseudoparticle formalism is equivalent to VCA in the normal phase of both bosonic¹⁰ and fermionic¹⁴ systems, it lacks the rigorous theoretical framework provided by SFA. In particular, there is no genuine variational principle explaining why one should look for a saddle point in the grand potential. The goal of the present paper is to put the results obtained within the pseudoparticle approach into a rigorous framework by developing an extended self-energy functional approach, which is capable of dealing with the bosonic superfluid phase.

From the present work, it will become clear that this extension is not straightforward, as it involves a precise sequence of Legendre transformations with suitably chosen variables. In the search for the appropriate set of transformations, the knowledge of the final results provided by the pseudoparticle formalism proves to be useful. This fact emphasizes the advantage of the heuristic, yet straightforward, pseudoparticle approach to formulate extensions of VCA.¹⁰

The extended SFA formulated in the present paper yields the same expressions for the superfluid order parameter, for the Nambu Green's function, and for the grand potential as obtained from the pseudoparticle approach. While this might not seem to be surprising, since we were guided by the very results of the pseudoparticle approach, we argue below that our SFA extension presented here is unambiguous. The most important step in this SFA extension is to find a quantity, which we call D , which is the companion of the self-energy in the superfluid phase. Correspondingly, one has to find an appropriate universal functional of this quantity and of the self-energy, which generates the superfluid order parameter and Green's function.

As an application, we present an evaluation of the superfluid density within this extended VCA by the usual method of introducing a phase twisting field, which is equivalent to the helicity modulus¹⁵ and to winding numbers in quantum-Monte-Carlo (QMC) algorithms.^{16,17} We evaluate the superfluid density for the two-dimensional Bose-Hubbard (BH) model¹⁸ and find a remarkably excellent agreement with QMC results.

This article is organized as follows. In Sec. II, we extend the SFA to the superfluid phase and obtain the corresponding extended self-energy functional, along with the appropriate variable describing superfluidity. The evaluation of the superfluid density within this extended VCA is presented in Sec. III and applied to the BH model in two dimensions. The VCA results are compared with unbiased QMC results showing excellent agreement. Finally, we conclude and summarize our findings in Sec. IV.

II. SELF-ENERGY FUNCTIONAL APPROACH

Let us recall the key idea of the SFA due to M. Potthoff.¹² The starting point is an appropriate functional

$$\hat{\Omega}[\Sigma, G_0^{-1}, H_U] \equiv \hat{\mathcal{F}}[\Sigma, H_U] + \hat{\mathcal{E}}[\Sigma, G_0^{-1}], \quad (1)$$

which consists of a functional $\hat{\mathcal{F}}$ of the self-energy, the Legendre transform of the Luttinger-Ward functional, which is universal in the sense that it depends on the interaction part (H_U) of the Hamiltonian but not on the single-particle part. The latter enters via the free Green's function G_0^{-1} in the second functional, which is explicitly known as

$$\hat{\mathcal{E}}[\Sigma, G_0^{-1}] \equiv -\beta \text{tr} \ln (\Sigma - G_0^{-1}).$$

The functional $\hat{\Omega}[\Sigma, G_0^{-1}, H_U]$ has three key features, which are crucial for the VCA. (a) The nonuniversal part $\hat{\mathcal{E}}$ enters additively in the form of a known functional, and the many-body aspects are described by a universal functional independent of the single-particle Hamiltonian, or, equivalently, independent of G_0^{-1} . (b) The self-energy of the physical system, characterized by H_U and G_0^{-1} , is a stationary point of the functional $\hat{\Omega}$ with respect to Σ . (c) The value of $\hat{\Omega}$ at the stationary point is equal to the thermodynamic grand potential. Given these properties, one can construct a parametric family of Hamilton operators based on the same interaction part (reference systems), for which the thermodynamic grand potential, Green's function, and the self-energy can be determined exactly. This allows one to determine the exact self-energy functional for self-energies accessible by the reference systems. In this very subspace, the self-energy functional in Eq. (1) for the physical system is replaced by that of the reference system. The stationarity condition in turn allows one to determine Green's function and the self-energy of the physical system.

Our goal is to generalize this approach to the superfluid phase as well. Besides the self-energy, which is the interaction correction of the inverse Green's function, we need the corresponding companion that describes the interaction correction to the order parameter, which we call D .

Once the appropriate form of D has been determined, we need a functional

$$\hat{\Omega}_s[\Sigma, D, F, G_0^{-1}, H_U] \equiv \hat{\mathcal{F}}[\Sigma, D, H_U] + \hat{\mathcal{E}}[\Sigma, D, G_0^{-1}, F]$$

in the self-energy Σ and D with the following features. (a) $\hat{\mathcal{F}}$ is again a universal functional, now in Σ and D . The nonuniversal part $\hat{\mathcal{E}}$ is explicitly known and carries the dependence on G_0^{-1} and the symmetry breaking source field F . (b) The functional is again stationary at the exact self-energy Σ and the exact D of the physical system, characterized by H_U , G_0^{-1} , and F . (c) The value of $\hat{\Omega}_s$ at the stationary point is equal to the thermodynamic grand potential. The sought-for functional $\hat{\Omega}_s$, to be derived in this section, will turn out to be (see below for a definition of the quantities)

$$\begin{aligned} 2\beta\hat{\Omega}_s[\Sigma, D, G_0^{-1}, F] &= \hat{\mathcal{F}}[\Sigma, D] + \hat{\mathcal{E}}[\Sigma, D, G_0^{-1}, F] \quad (2) \\ \hat{\mathcal{E}}[\Sigma, D, G_0^{-1}, F] &\equiv \beta \text{Tr} \ln [(G_0^{-1} - \Sigma) G_\infty] \\ &\quad + (\bar{D} - \bar{F})(G_0^{-1} - \Sigma)^{-1}(D - F). \quad (3) \end{aligned}$$

In the normal phase, it is identical to the functional introduced by Potthoff (Ref. 12). The additional factor 2 is due to the use of Nambu Green's functions. Notice that, the expression for the grand potential obtained with the help of a so-called reference system [see Eq. (30)] below is identical to the one obtained within the pseudoparticle approach.¹⁰

A. Derivation of the grand-potential functional

We start out from the partition function Z of a bosonic many-body system, which in a functional integral representation reads

$$Z = \int \mathcal{D}A e^{-S}, \quad (4)$$

where S is the action, which in general can be written as¹⁹

$$\begin{aligned} S &= -\frac{1}{2} \int d\tau \int d\tau' \bar{A}(\tau') G_0^{-1}(\tau', \tau) A(\tau) \\ &\quad - \int d\tau [\bar{F}(\tau) A(\tau) - H_U(A(\tau))]. \quad (5) \end{aligned}$$

In view of treating the superfluid phase, we have adopted a Nambu notation in which the boson fields are expressed in a vector representation

$$A(\tau) \equiv \begin{pmatrix} a_1(\tau) \\ \vdots \\ a_N(\tau) \\ \bar{a}_1(\tau) \\ \vdots \\ \bar{a}_N(\tau) \end{pmatrix}. \quad (6)$$

The indices 1 through N denote the corresponding single-particle orbitals (for example, lattice sites) where the boson operators act, and $a_i(\tau)$ [$\bar{a}_i(\tau)$] are the fields associated with

the annihilation (creation) of a boson in the orbital i . The adjoint field is defined as

$$\bar{A}(\tau) \equiv (\bar{a}_1(\tau), \dots, \bar{a}_N(\tau), a_1(\tau), \dots, a_N(\tau)). \quad (7)$$

It can be expressed in terms of $A(\tau)$ with the help of the matrix \mathcal{T} , which exchanges the first N entries of a vector with the last N ones:

$$\bar{A}(\tau) = A(\tau)^T \mathcal{T}. \quad (8)$$

The operator \mathcal{T} has the properties $\mathcal{T}^2 = \mathbb{1}$ and $\mathcal{T} = \mathcal{T}^T$. The action in Eq. (5) also contains the source fields

$$\bar{F} \equiv (f_1, \dots, f_N, \bar{f}_1, \dots, \bar{f}_N) \quad \text{and} \quad F = \mathcal{T} \bar{F}^T,$$

which are zero for the physical system of interest, the boson interaction described by H_U , as well as the $2N \times 2N$ noninteracting Green's function matrix $G_0(\tau', \tau)$. Equation (4) with Eq. (5) defines the corresponding grand potential as a functional of G_0^{-1} and F ,

$$\hat{\Omega}_s[G_0^{-1}, F] \equiv -\frac{1}{\beta} \ln \hat{Z}, \quad (9)$$

where β is the inverse temperature. Here and in the following, we mark functionals with a hat “ $\hat{}$ ” and omit their arguments whenever they are obvious. The noninteracting Green's function has the matrix structure (see Subsec. C of the Appendix)

$$G_0^{-1}(\tau', \tau) = -\delta(\tau - \tau') \begin{pmatrix} \partial_\tau + \mathbf{t} & 0 \\ 0 & -\partial_\tau + \mathbf{t} \end{pmatrix}, \quad (10)$$

where \mathbf{t} is the single-particle Hamiltonian matrix.

In the following, we carry out a sequence of Legendre transformations starting from $\hat{\Omega}_s$, ultimately leading to a universal functional $\hat{\mathcal{F}}[\Sigma, D]$ of the self-energy Σ and of a suitable quantity D defined in Eq. (21a). The functional $\hat{\mathcal{F}}$ is the generalization of the self-energy functional¹¹⁻¹³ to the superfluid phase, where a nonvanishing expectation value $\mathcal{A}(\tau) \equiv \langle A(\tau) \rangle$ of the boson operators A exists. The functional $\hat{\mathcal{F}}$ has the properties [see Eq. (23)] that its functional derivatives with respect to Σ and D yield the disconnected Green's function and the expectation value \mathcal{A} , respectively. This procedure is inspired by Ref. 20 and extends that approach to the treatment of the superfluid phase.

We first determine the conjugate variables to G_0^{-1} and to the source fields F . The functional derivative of $\hat{\Omega}_s$ with respect to the noninteracting Green's function yields¹⁹ (see Subsec. A of the Appendix)

$$\begin{aligned} & 2\beta \frac{\delta \hat{\Omega}_s}{\delta G_{0ji}^{-1}(\tau', \tau)} \\ &= -\frac{2}{\hat{Z}} \frac{\delta}{\delta G_{0ji}^{-1}(\tau', \tau)} \\ & \quad \times \int \mathcal{D}A \exp \left\{ \frac{1}{2} \int d\tilde{\tau} \int d\tilde{\tau}' \bar{A}_l(\tilde{\tau}) G_{0ll'}^{-1}(\tilde{\tau}, \tilde{\tau}') A_{l'}(\tilde{\tau}') \right. \\ & \quad \left. + \int d\tilde{\tau} [\bar{F}_l(\tilde{\tau}) A_l(\tilde{\tau}) - H_U(\bar{a}, a)] \right\} \\ &= -\frac{1}{\hat{Z}} \int \mathcal{D}A \bar{A}_j(\tau') A_i(\tau) \exp[-S] \equiv \hat{G}_{\text{disc},ij}(\tau, \tau'). \end{aligned}$$

Here, $\hat{G}_{\text{disc},ij}(\tau, \tau')$ is the disconnected interacting time-ordered Green's function. Along with the definition of the connected Green's function $\hat{G}[G_0^{-1}, F]$, we obtain

$$2\beta \frac{\delta \hat{\Omega}_s[G_0^{-1}, F]}{\delta G_0^{-1}} = \hat{G}_{\text{disc}} \equiv \hat{G} - \hat{\mathcal{A}} \hat{\mathcal{A}}. \quad (11a)$$

For the functional derivative with respect to F , we obtain similarly

$$2\beta \frac{\delta \hat{\Omega}_s[G_0^{-1}, F]}{\delta \bar{F}} = -2\hat{\mathcal{A}}[G_0^{-1}, F]. \quad (11b)$$

The two functionals $\hat{G}[G_0^{-1}, F]$ and $\hat{\mathcal{A}}[G_0^{-1}, F]$ defined in Eq. (11) provide the exact Green's function G and order parameter A for a given noninteracting Green's function G_0^{-1} and source field F of the system. The first step toward the universal functional consists in a Legendre transformation replacing the variables F with \mathcal{A} . To this end, we invert²¹ the relation Eq. (11) making F a functional $\hat{F}[G_0^{-1}, \mathcal{A}]$ and introduce

$$\hat{\Xi}[G_0^{-1}, \mathcal{A}] = 2\beta \hat{\Omega}_s + 2\hat{F}\mathcal{A}, \quad (12)$$

where, as usual in Legendre transformations, the functional dependence on F has been eliminated in favor of \mathcal{A} by using the inverse function. It is straightforward to show that the corresponding functional derivatives give

$$\frac{\delta \hat{\Xi}}{\delta 2\mathcal{A}} = \hat{F}[G_0^{-1}, \mathcal{A}], \quad \frac{\delta \hat{\Xi}}{\delta G_0^{-1}} = \hat{G}_{\text{disc}}[G_0^{-1}, \mathcal{A}].$$

Next, we modify the functional in the following way:

$$\hat{\Xi}[G_0^{-1}, \mathcal{A}] = \hat{\Xi} + \bar{\mathcal{A}} G_0^{-1} \mathcal{A}, \quad (13)$$

such that we obtain the connected Green's function from the functional derivative with respect to G_0^{-1} . In total, we have

$$\frac{\delta \hat{\Xi}}{\delta 2\mathcal{A}} = \hat{F}[G_0^{-1}, \mathcal{A}] + \bar{\mathcal{A}} G_0^{-1}, \quad (14)$$

$$\frac{\delta \hat{\Xi}}{\delta G_0^{-1}} = \hat{G}_{\text{disc}} + \mathcal{A} \bar{\mathcal{A}} = \hat{G}[G_0^{-1}, \mathcal{A}]. \quad (15)$$

The second step is a Legendre transformation replacing the variable G_0^{-1} with G :

$$\hat{\Pi}[G, \mathcal{A}] = \hat{\Xi} - \beta \text{Tr}(G \hat{G}_0^{-1} - \mathbb{1}), \quad (16)$$

where we have expressed \hat{G}_0^{-1} as a functional of G and \mathcal{A} by inverting Eq. (15).^{19,21} We subtract an “infinite” constant $\beta \text{Tr} \mathbb{1}$ in order to keep $\hat{\Pi}[G, \mathcal{A}]$ finite. The functional derivatives of the new functional are

$$\frac{\delta \hat{\Pi}}{\delta 2\mathcal{A}} = \hat{F} + \bar{\mathcal{A}} \hat{G}_0^{-1}, \quad \frac{\delta \hat{\Pi}}{\delta G} = -\hat{G}_0^{-1}.$$

Now, we modify the functional such that we get the self-energy from the functional derivative (see Subsec. A3 of the Appendix)

$$\hat{\Pi}[G, \mathcal{A}] = \hat{\Pi} + \beta \text{Tr} \ln(G/G_\infty). \quad (17)$$

This gives

$$\frac{\delta \hat{\Pi}}{\delta 2\mathcal{A}} = \hat{F} + \bar{\mathcal{A}} \hat{G}_0^{-1}, \quad \frac{\delta \hat{\Pi}}{\delta G} = \hat{\Sigma}, \quad (18a)$$

$$\hat{\Sigma} \equiv G^{-1} - \hat{G}_0^{-1}. \quad (18b)$$

Here, we have used the Dyson equation as the defining equation for the self-energy. Furthermore, we carry out a third Legendre transformation replacing G with Σ in the usual way. Thus, we introduce

$$\hat{P}[\Sigma, \mathcal{A}] = \hat{\Pi} + \beta \text{Tr} \Sigma \hat{G} \quad (19)$$

with the properties

$$\frac{\delta \hat{P}}{\delta 2\mathcal{A}} = \hat{F} + \bar{\mathcal{A}}\hat{G}_0^{-1}, \quad \frac{\delta \hat{P}}{\delta \Sigma} = \hat{G}.$$

We modify this functional once more so that its derivative yields a new function D , which will be the companion of the self-energy in our extended self-energy approach:

$$\hat{P}[\Sigma, \mathcal{A}] = \hat{P} - \bar{\mathcal{A}}\Sigma\mathcal{A}. \quad (20)$$

The functional derivatives yield

$$\frac{\delta \hat{P}}{\delta 2\mathcal{A}} = \hat{F} + \bar{\mathcal{A}}\hat{G}_0^{-1} - \bar{\mathcal{A}}\Sigma = \hat{F} + \bar{\mathcal{A}}\hat{G}^{-1} \equiv \hat{D}, \quad (21a)$$

$$\frac{\delta \hat{P}}{\delta \Sigma} = \hat{G} - \mathcal{A}\bar{\mathcal{A}} = \hat{G}_{\text{disc}}. \quad (21b)$$

Before proceeding, let us discuss the meaning of the function D introduced in Eq. (21a). When extending SFA to the superfluid phase, one is looking for a quantity which is related to the condensed order parameter and which plays a similar role as the self-energy, in that it describes the deviation between the interacting and noninteracting case. Thus, this quantity should vanish in the noninteracting case ($H_U = 0$). The reason is that the SFA will eventually amount to an approximation for Σ and D , and we require this approximation to become exact for $H_U = 0$. Finally, D must obviously vanish in the normal phase. The expression in Eq. (21a) has precisely these features, since $\bar{\mathcal{A}}_0 = -\bar{F}G_0$, which is straightforwardly determined from the Gaussian integral for $H_U = 0$ in Eq. (5). Interestingly, the pseudoparticle approach, presented in Ref. 10, and which is based on an intuitive, yet heuristic approximation, provides the same form of D as given in Eq. (21a).

The final Legendre transformation replacing \mathcal{A} with D yields the desired functional of the self-energy and D . It represents the generalization of the self-energy functional ($F[\Sigma]$ of Refs. 11 and 12) to the superfluid phase

$$\hat{\mathcal{F}}[\Sigma, D] = \hat{P} - 2\bar{D}\hat{\mathcal{A}} \quad (22)$$

and has the properties

$$\frac{\delta \hat{\mathcal{F}}}{\delta \bar{D}} = -2\hat{\mathcal{A}}[\Sigma, D], \quad \frac{\delta \hat{\mathcal{F}}}{\delta \Sigma} = \hat{G}_{\text{disc}}[\Sigma, D]. \quad (23)$$

Similarly to $F[\Sigma]$ from Refs. 11 and 12, $\hat{\mathcal{F}}$ is (for fixed H_U) a *universal* functional of Σ and D only, from which the disconnected Green's function and the order parameter are obtained by a functional derivative [see Eq. (23)]. Given Σ and D , we can compute by Eq. (23) the corresponding values for \mathcal{A} and G_{disc} . On the other hand, for a specific physical system, uniquely defined by G_0^{-1} , F , and H_U , the definitions of the self-energy Σ [Eq. (18b)] and the modified order parameter D

[Eq. (21a)] provide another set of equations which uniquely fix Σ and D via the equations

$$\begin{aligned} \hat{G}_{\text{disc}}[\Sigma, D] &\stackrel{!}{=} (G_0^{-1} - \Sigma)^{-1} \\ &+ (G_0^{-1} - \Sigma)^{-1}(D - F)(\bar{D} - \bar{F})(G_0^{-1} - \Sigma)^{-1} \end{aligned} \quad (24a)$$

and

$$-2\bar{\mathcal{A}}[\Sigma, D] \stackrel{!}{=} -2(\bar{D} - \bar{F})(G_0^{-1} - \Sigma)^{-1}. \quad (24b)$$

As for the (original) self-energy functional approach, we seek now a functional which becomes stationary at the exact Σ and D for specific G_0^{-1} and F , and which consists of the universal functional $\hat{\mathcal{F}}$ plus a nonuniversal explicit functional of the form

$$2\beta\hat{\Omega}_s[\Sigma, D, G_0^{-1}, F, H_U] = \hat{\mathcal{F}}[\Sigma, D, H_U] + \hat{\mathcal{E}}[\Sigma, D, G_0^{-1}, F].$$

In order to yield the correct stationary point, the functional $\hat{\mathcal{E}}$ has to fulfill according to Eq. (24) the equations

$$\begin{aligned} \frac{\delta \hat{\mathcal{E}}}{\delta \Sigma} &= -(G_0^{-1} - \Sigma)^{-1} \\ &- (G_0^{-1} - \Sigma)^{-1}(D - F)(\bar{D} - \bar{F})(G_0^{-1} - \Sigma)^{-1}, \end{aligned} \quad (25a)$$

$$\frac{\delta \hat{\mathcal{E}}}{\delta D} = 2(\bar{D} - \bar{F})(G_0^{-1} - \Sigma)^{-1}. \quad (25b)$$

With these ingredients, we can now express the sought-for functional $\hat{\Omega}_s$ as

$$\begin{aligned} 2\beta\hat{\Omega}_s[\Sigma, D, G_0^{-1}, F] &= \hat{\mathcal{F}}[\Sigma, D] + \beta \text{Tr} \ln [(G_0^{-1} - \Sigma) G_\infty] \\ &+ (\bar{D} - \bar{F})(G_0^{-1} - \Sigma)^{-1}(D - F), \end{aligned} \quad (26)$$

which obviously fulfills Eq. (25). It remains to be shown that, whenever evaluated at the exact Σ and D , the functional $\hat{\Omega}_s$ corresponds, possibly apart from a constant, to the thermodynamic grand potential $\tilde{\Omega}_s$ of the system. To this end, we add up all the terms used to construct the functional. At the exact values of Σ and D , we have

$$\begin{aligned} 2\beta\hat{\Omega}_s|_{\text{exact}} &= 2\beta\tilde{\Omega}_s + 2\bar{F}\mathcal{A} + \bar{\mathcal{A}}G_0^{-1}\mathcal{A} - \beta \text{Tr} (GG_0^{-1} - \mathbb{1}) \\ &+ \beta \text{Tr} \ln (G/G_\infty) + \beta \text{Tr} \Sigma G - \bar{\mathcal{A}}\Sigma\mathcal{A} - 2\bar{D}\mathcal{A} \\ &- \beta \text{Tr} \ln (G/G_\infty) + \bar{\mathcal{A}}G^{-1}\mathcal{A} \\ &= 2\beta\tilde{\Omega}_s - 2\underbrace{(\bar{D} - \bar{F})\mathcal{A}}_{\bar{\mathcal{A}}G^{-1}} + 2\bar{\mathcal{A}}G^{-1}\mathcal{A} \\ &= 2\beta\tilde{\Omega}_s. \end{aligned}$$

We can now proceed as in Refs. 12 and 22 and construct a reference system, which can be solved (almost) exactly.²³ The reference system is described by a Hamiltonian H' which shares the same interaction H_U as the physical system, but consists of a different noninteracting Green's function G'_0 and source fields F' . The point is the following: Due to the fact that \mathcal{F} is a universal functional, it cancels out from the difference

between $\hat{\Omega}_s$ for the physical and the reference system, *with the same values of Σ and D* . In particular, this gives

$$\begin{aligned} & 2\beta\hat{\Omega}_s[\Sigma, D, G_0^{-1}, F] - 2\beta\hat{\Omega}_s[\Sigma, D, G_0'^{-1}, F'] \\ &= \beta \text{Tr} \ln \left((G_0^{-1} - \Sigma) G_\infty \right) - \beta \text{Tr} \ln \left((G_0'^{-1} - \Sigma) G_\infty \right) \\ & \quad + (\bar{D} - \bar{F})(G_0^{-1} - \Sigma)^{-1} (D - F) \\ & \quad - (\bar{D} - \bar{F}')(G_0'^{-1} - \Sigma)^{-1} (D - F'), \end{aligned} \quad (27)$$

which allows one to evaluate the functional $\hat{\Omega}_s$ exactly for the physical system as well, however, in a restricted subspace of Σ and D , representable by the parametric family of reference systems. By construction, the optimal values for Σ and D for the physical system are those of the reference system for the set of optimal variational parameters.

The variational procedure then follows and generalizes Ref. 12: First, a class of exactly solvable reference systems \hat{H}' with the same interaction as the physical system characterized by a continuum of single-particle parameters \mathbf{t}' and source fields F' is identified. In VCA, this class is obtained by dividing the original lattice into disconnected clusters with varying single-particle energies and hopping strengths. A larger subspace can be reached by adding bath sites.¹³ Then, the (connected) Green's function G' , the order parameter \mathcal{A}' , and the grand potential Ω'_s of the reference system is evaluated. With the help of Dyson's equation [Eq. (18b)], the self-energy Σ' , and Eq. (21a), D' is determined. By varying \mathbf{t}' and F' , the subspace of self-energies and D 's is spanned, which is accessible to the reference system and to which these objects for the physical system are restricted. Within this subspace, the functional $\hat{\Omega}_s$ can be evaluated exactly for arbitrary G_0 and F of the physical system. For the relevant case $F = 0$, we obtain²⁴ from Eq. (27)

$$\begin{aligned} 2\beta\Omega_s &= 2\beta\Omega'_s + \beta \text{Tr} \ln \left(-(G_0^{-1} - \Sigma') \right) \\ & \quad - \beta \text{Tr} \ln \left(-(G_0'^{-1} - \Sigma') \right) + \bar{D}(G_0^{-1} - \Sigma')^{-1} D \\ & \quad - \bar{A}' G'^{-1} \mathcal{A}, \end{aligned} \quad (28)$$

which is now a *function* of \mathbf{t}' and F' . The infinite physical system can break the symmetry spontaneously, while in the reference systems of disconnected finite clusters, a nonvanishing order parameter can only be achieved by an additional source field F' . This explains why a finite F' is required although $F = 0$ in the physical system. The SFA approximation consists in finding a stationary point of $\hat{\Omega}_s$ within this subspace of self-energies and D 's. This corresponds, quite generally, to finding a stationary point with respect to \mathbf{t}' and F' of Eq. (28), i. e., to the equations

$$\frac{\partial \Omega}{\partial \mathbf{t}'} = 0, \quad \frac{\partial \Omega}{\partial F'} = 0. \quad (29)$$

Here, we have replaced Ω_s with $\Omega \equiv \Omega_s - \frac{1}{2} \text{tr} \mathbf{t}$ which differs just by \mathbf{t}' - and F' -independent constants and, thus, does not change the saddle-point equations. The quantity Ω is the grand potential obtained from the normal-ordered Hamiltonian (see Subsec. C of the Appendix). We also introduce the grand potential of the normal-ordered reference system $\Omega'_s \equiv \Omega'_s - \frac{1}{2} \text{tr} \mathbf{t}'$. This term is also present in the pseudoparticle approach,¹⁰ where its origin is easily seen. Moreover, for

τ -independent fields and the Hamiltonian, the expectation values $\mathcal{A}(\tau)$ are τ independent as well, and Green's functions depend on the time difference only. In this way, we can rewrite Eq. (28) as

$$\begin{aligned} \Omega &= \Omega' - \frac{1}{2} \text{tr}(\mathbf{t} - \mathbf{t}') - \frac{1}{2} \text{Tr} \ln(-G) + \frac{1}{2} \text{Tr} \ln(-G') \\ & \quad + \frac{1}{2} \bar{\mathcal{A}} G^{-1}(\omega_n = 0) \mathcal{A} - \frac{1}{2} \bar{\mathcal{A}}' G'^{-1}(\omega_n = 0) \mathcal{A}', \end{aligned} \quad (30)$$

where $G(\omega_n) \equiv \int d\tau G(\tau, 0) e^{i\tau\omega_n}$ is Green's function in Matsubara space. The expression for Ω given in Eq. (30) is our main result. As can be seen, this expression is the same as Eq. (1) in Ref. 10, except for a different normalization factor, which is the number of clusters N_c . Notice that $N_c h$ in Ref. 10 is equal to $\mathbf{t} - \mathbf{t}'$ in the present paper. We thus proved that the result obtained within the pseudoparticle approach in Ref. 10 can be equivalently obtained within a more rigorous "generalized" self-energy functional approach. While the pseudoparticle approach is quite intuitive, the present self-energy approach provides a rigorous variational principle, explaining why the grand potential Ω has to be optimized with respect to the cluster parameters \mathbf{t}' and F' . In addition, as in SFA for the normal phase, it suggests more general approximations in which bath sites are used to enlarge the space of possible self-energies.^{13,25,26}

III. SUPERFLUID DENSITY

In this section, we discuss the evaluation of the superfluid density ρ_s within our extended SFA/VCA theory and present results for the two-dimensional BH model.

The superfluid density is related to the response of the system to a phase-twisting field,^{15,27} leading to twisted boundary conditions (BCs) in one spatial direction, which we choose to be the \mathbf{e}_x direction, and periodic BCs in the others. The many-body wave function $|\Psi\rangle$ has to obey these BCs and thus

$$\hat{T}(N_x \mathbf{e}_x) |\Psi\rangle = e^{i\Theta} |\Psi\rangle,$$

where the operator $\hat{T}(\mathbf{r})$ translates the particles by the vector \mathbf{r} , N_x is the lattice extension in \mathbf{e}_x direction, and Θ is the phase twist applied to the system. The twisted BCs can be mapped by a unitary transformation onto the lattice Hamiltonian, leading to complex-valued hopping integrals.^{8,28,29} The resulting Hamiltonian can be interpreted as a cylinder rolled up along the x direction, which is threaded by an effective magnetic field with total flux Θ . When a particle is translated by N_x in the \mathbf{e}_x direction, a phase $\exp[-i\Theta]$ is picked up.³⁰ Due to gauge invariance, one is free to choose where the phase is collected when the particle propagates across the lattice. The usual choice is that each hopping process in the \mathbf{e}_x direction, i. e., from site $\mathbf{r}' = (r_x - 1, r_y)$ to $\mathbf{r} = (r_x, r_y)$, is multiplied by a phase factor $\exp[-iA]$, where the associated vector potential is

$$A = \Theta / N_x. \quad (31)$$

When choosing the phase in that way, the reference system \hat{H}' also depends on the vector potential A , and the intracluster hopping terms become complex valued along the \mathbf{e}_x direction. For a Hamiltonian with nearest-neighbor hopping t , the

superfluid density is determined from³⁰

$$\rho_s = \frac{1}{t} \frac{1}{N_x N_y} \frac{\partial^2 \Omega_\Theta}{\partial A^2}, \quad (32)$$

where $N_x N_y$ is the total number of lattice sites of the physical system, and Ω_Θ is the grand potential of the physical system, subject to a phase twist Θ , as discussed above. Plugging in the vector potential of Eq. (31) yields

$$\rho_s = \frac{1}{t} \frac{N_x}{N_y} \frac{\partial^2 \Omega_\Theta}{\partial \Theta^2}. \quad (33)$$

In practice, the grand potential Ω_Θ is evaluated at the stationary point of Eq. (30) and is determined self-consistently for several values of Θ . From this data, the curvature of Ω_Θ with respect to Θ is extracted from a fit. Using the curvature, the superfluid density is evaluated according to Eq. (33). Note that a finite cluster is embedded in an essentially infinitely large system, and, thus, the limits are taken in the correct order to obtain the superfluid density.³⁰

In the following, we apply this procedure to the two-dimensional BH model¹⁸

$$\hat{H} = \sum_{(i,j)} t_{ij} a_i^\dagger a_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i,$$

where a_i^\dagger (a_i) creates (destroys) a boson particle on site i , and $\hat{n}_i = a_i^\dagger a_i$ is the occupation number operator. The hopping integrals t_{ij} are nonzero for nearest neighbors only, as indicated by the angle brackets. Specifically, $t_{ij} = -t$ for hopping processes along the \mathbf{e}_y direction and $t_{ij} = -t \exp[i A (\mathbf{r}_i - \mathbf{r}_j) \cdot \mathbf{e}_x]$ for hopping processes along the \mathbf{e}_x direction. The chemical potential, termed μ , controls the particle number, and U is the repulsive on-site interaction, which subsequently will be used as unit of energy. The reference system \hat{H}' consists of

a cluster decomposition of the physical system \hat{H} plus a $U(1)$ symmetry breaking source term

$$\hat{H}' = \sum_{\mathbf{R}} \left[\sum_{(\alpha,\beta)} t'_{\alpha\beta} a_{\alpha,\mathbf{R}}^\dagger a_{\beta,\mathbf{R}} + \frac{U}{2} \sum_{\alpha} \hat{n}_{\alpha,\mathbf{R}} (\hat{n}_{\alpha,\mathbf{R}} - 1) - \mu' \sum_{\alpha} \hat{n}_{\alpha,\mathbf{R}} - \sum_{\alpha} (a_{\alpha,\mathbf{R}}^\dagger f_{\alpha}^\dagger + f_{\alpha}^* a_{\alpha,\mathbf{R}}^\dagger) \right],$$

where the lattice site indices i have been decomposed into an index \mathbf{R} that specifies the cluster and into an index α that specifies the lattice sites within a cluster.^{10,31} Analogously to the physical system, the hopping integrals are $t'_{\alpha\beta} = -t'$ and $t'_{\alpha\beta} = -t' \exp[i A (\mathbf{r}_{\mathbf{R}\alpha} - \mathbf{r}_{\mathbf{R}\beta}) \cdot \mathbf{e}_x]$ for nearest-neighbor hopping processes along the \mathbf{e}_y and the \mathbf{e}_x direction, respectively, and zero otherwise. In our calculation, we use the chemical potential μ' and the source coupling strength f_{α} of the reference system as variational parameters in the optimization prescription. Since the reference system is complex valued, the source coupling strength f_{α} is complex valued too, i. e., $f_{\alpha} = |f_{\alpha}| \exp[i\phi_{\alpha}]$. Thus, in general, $2L$ variational parameters have to be considered, where L is the number of cluster sites. However, for different cluster sites α , the source coupling strengths f_{α} are interrelated, as can be seen from mean-field arguments, leading effectively to two variational parameters $|f|$ and ϕ , which we use—in addition to the chemical potential μ' —to treat complex-valued reference systems.

In Fig. 1, we present the superfluid density ρ_s for different sizes of the reference system ranging from $L = 1 \times 1$, over $L = 2 \times 1$, to $L = 2 \times 2$ and essentially infinitely large physical systems. For the largest cluster, we restrict the variational search space to real valued order parameters, i. e., we set $\phi_{\alpha} = 0$. Figure 1 (a) demonstrates that this choice leads to comparable results as obtained with the full variational space. Yet, for the restricted variational space, the computational effort as well as the numerical complexity is reduced, since the reference system remains real valued.

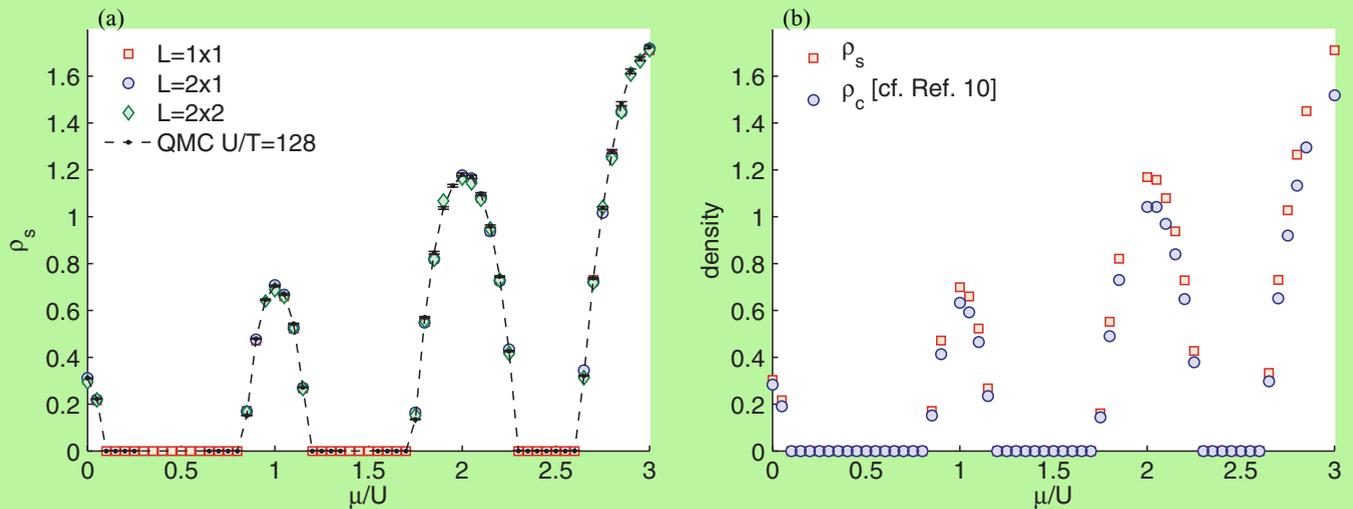


FIG. 1. (Color online) (a) Superfluid density ρ_s evaluated for constant hopping strength $t/U = 0.02$ as a function of the chemical potential μ/U . VCA results for reference systems of size $L = 1 \times 1$, $L = 2 \times 1$, and $L = 2 \times 2$ and for essentially infinitely large physical systems are compared to QMC results for physical systems of size 32×32 and inverse temperature $U/T = 128$. (b) Comparison of the superfluid density ρ_s and condensed density ρ_c for reference systems of size $L = 1 \times 1$ and essentially infinitely large physical systems (cf. Ref. 10).

Figure 1 (a) shows the superfluid density ρ_s as a function of the chemical potential μ/U evaluated for fixed hopping strength $t/U = 0.02$. The chemical potential ranges from $\mu/U = 0$ to $\mu/U = 3$. As the hopping strength is small, three regions with $\rho_s = 0$ are present, corresponding to the Mott insulating phase. In between these regions, we observe a finite superfluid density ρ_s indicating the occurrence of the superfluid phase. In addition to the VCA results, we show QMC results with error bars (barely visible) for physical systems of size 32×32 and inverse temperature $U/T = 128$. The QMC calculations were performed with the ALPS library³² and the ALPS applications.³³ Particularly, we use the stochastic series expansion representation of the partition function with directed loop updates,³⁴⁻³⁶ where the superfluid density is evaluated via the winding number.^{16,17} The superfluid density ρ_s obtained from VCA agrees remarkably well with the QMC results. Furthermore, VCA results are almost independent of the size L of the reference system, signaling convergence to the correct results even for $L = 1 \times 1$ site clusters. The superfluid density ρ_s is compared to the condensate density $\rho_c = \langle a_i \rangle$ in Fig. 1 (b) (cf. Ref. 10). It can be observed that the superfluid density is always larger than the density of the Bose-Einstein condensate. However, the difference between the two densities is rather small, since a very dilute Bose gas is investigated.

In Fig. 2, we evaluate (a) the superfluid density ρ_s and (b) the superfluid fraction ρ_s/n (n is the particle density) for a fixed chemical potential $\mu/U = 0.4$ as a function of the hopping strength t/U . The hopping strength ranges from $t/U = 0$ to $t/U = 1$, which is already very deep in the superfluid phase. For $\mu/U = 0.4$, the phase boundary between the Mott and the superfluid phase is located at $t/U \approx 0.06$. In the superfluid phase close to the phase boundary, the superfluid density rises quickly from zero, developing an almost linear behavior for $t/U \gtrsim 0.2$. In the latter parameter regime, the superfluid fraction is larger than 90%, signaling that already a very large amount of the lattice bosons is superfluid. As emphasized in Ref. 37, a relatively sharp crossover from a strongly correlated superfluid, characterized by a superfluid fraction which is well below 1, to a weakly correlated superfluid, where the superfluid fraction is almost 1, can be observed [see Fig. 2(b)]. In addition to the VCA results evaluated for reference systems of size $L = 1 \times 1$ and essentially infinitely large physical systems, we show QMC results for physical systems of size 32×32 and inverse temperature $U/T = 128$, which again exhibit perfect agreement.

In Fig. 3, we focus on the quantum critical region close to the tip of the first Mott lobe, which is the most challenging one. In particular, we evaluate the particle density n , the condensate density ρ_c , and superfluid density ρ_s . In the first row, we show results for a fixed chemical potential $\mu/U = 0.4$ as a function of the hopping strength t/U , whereas in the second row we keep the hopping strength fixed at $t/U = 0.05$ and vary the chemical potential μ/U . We compare VCA results with QMC and mean field (MF). The most important observation is that MF is far off from QMC and VCA. For $\mu/U = 0.4$, MF predicts the phase transition to be at a much smaller value of t/U than QMC and VCA. This leads to significant deviations in both the density and condensate density as compared to QMC and VCA. For fixed $t/U = 0.05$, MF does not enter the Mott region and, thus, does not predict a plateau in the density.

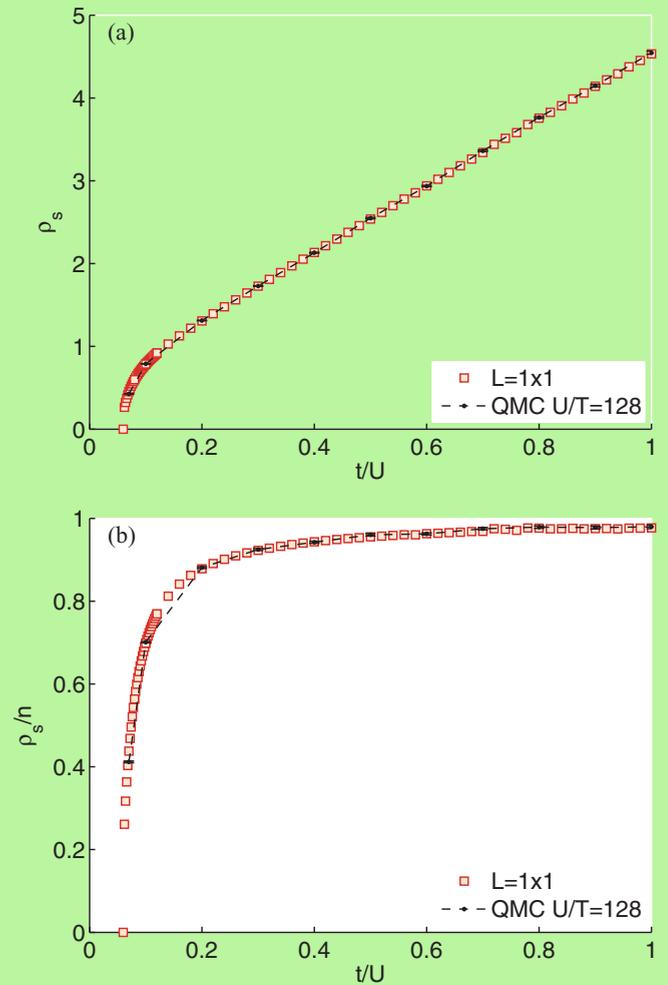


FIG. 2. (Color online) (a) Superfluid density ρ_s and (b) superfluid fraction ρ_s/n ranging deep in the superfluid phase evaluated for constant chemical potential $\mu/U = 0.4$ as a function of the hopping strength t/U . Results obtained by means of VCA for reference systems of size $L = 1 \times 1$ and essentially infinitely large physical systems are compared to QMC results for physical systems of size 32×32 and inverse temperature $U/T = 128$.

For both investigated situations (fixed μ/U and fixed t/U), the results obtained by means of VCA and QMC agree quite well. For the QMC simulations, we used lattices of size 32×32 and inverse temperatures of $U/T = 128$. The VCA results are obtained at zero temperature for clusters of size 1×1 and 2×1 , respectively, and essentially infinitely large physical systems. In this challenging regime, small differences between VCA and QMC are observable for the condensate density. For the reference system sizes considered here, results are almost identical. Larger reference systems might still reduce the difference between VCA and QMC. However, close to the phase transition, finite size and finite temperature effects might still be important for the QMC results, and, thus, a proper finite size scaling of these data might also reduce the discrepancy between the two approaches. Note that for fixed hopping $t/U = 0.05$, there is a very small region at $\mu/U \approx 0.85$, where it is difficult to numerically determine the stationary point of the grand potential. Such a region is also present between the first and the second and between the

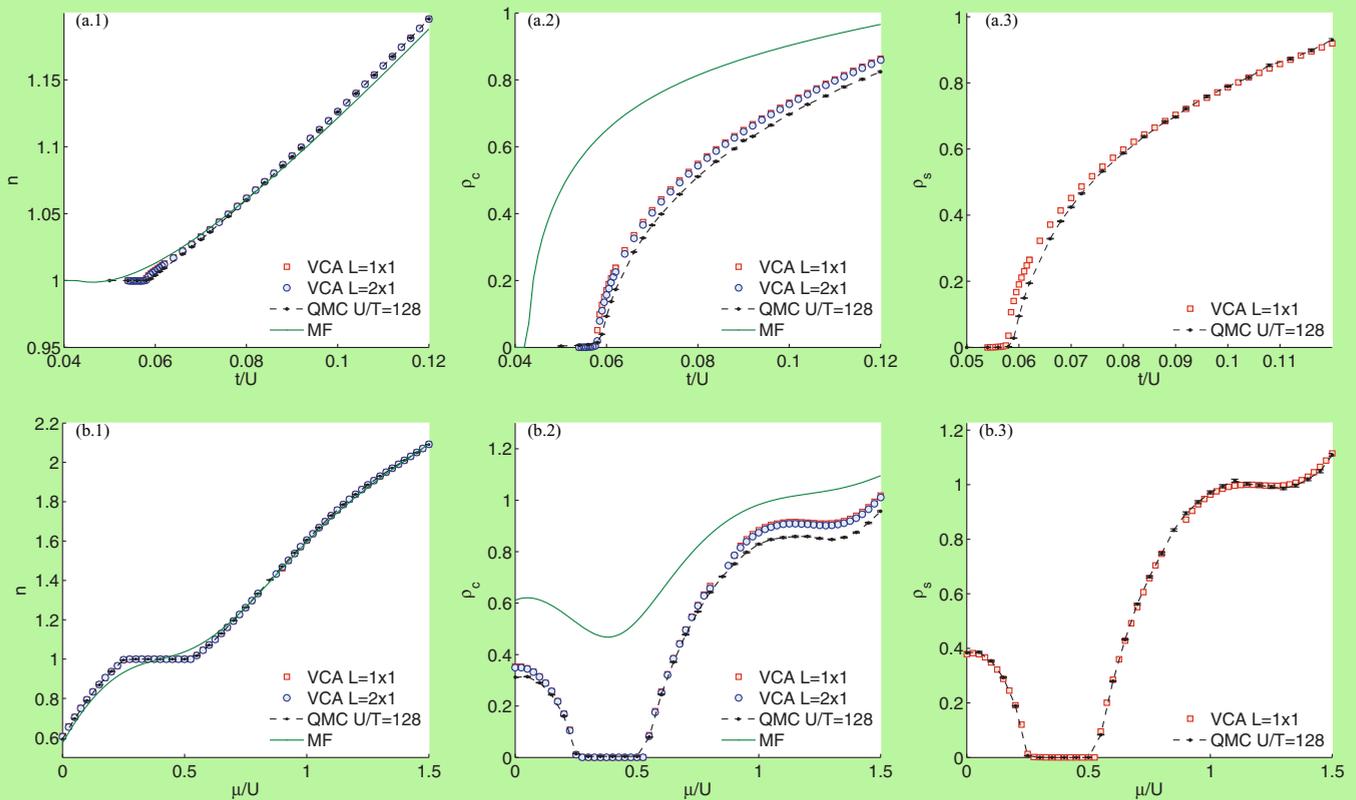


FIG. 3. (Color online) Particle density n (left), condensate density ρ_c (middle), and superfluid density ρ_s (right) evaluated around the quantum critical region close to the tip of the first Mott lobe. Comparison of the data obtained by means of VCA (for essentially infinitely large physical systems and reference systems as stated in the legends), QMC (for physical systems of size 32×32 and inverse temperatures $U/T = 128$), and mean field. (a.1)–(a.3) The first row shows results for a fixed chemical potential $\mu/U = 0.4$ as a function of the hopping strength t/U , whereas (b.1)–(b.3) the second row shows results for the fixed hopping strength $t/U = 0.05$ as a function of the chemical potential μ/U .

second and the third Mott lobes in Fig. 1. However, there it is barely visible since the spacing between two consecutive μ data points is larger than this gap. This failure appears to be related to the fact that two solutions adiabatically connected to two sectors with different particle numbers, i.e., the two neighboring Mott regions, meet and try to avoid each other. However, we want to emphasize that this problem affects only a tiny region of the phase diagram. When keeping the chemical potential fixed at $\mu/U = 0.4$, solutions can be easily found for all values of the hopping strength.

Finally, we want to emphasize that the VCA results are obtained with very modest computational effort and that excellent agreement with QMC can be observed, even for very small reference systems.

IV. CONCLUSIONS

In the present work, we extend the self-energy functional approach to the $U(1)$ symmetry broken, superfluid phase of correlated lattice bosons. A crucial point of this extension is the identification of a quantity, termed D , which is the companion of the self-energy Σ in the superfluid phase. We also identify the appropriate (nonuniversal) functional $\hat{\Omega}_s$ which is stationary at the physical values of the self-energy Σ and of D . In analogy to the self-energy, which describes the difference between the interacting and noninteracting

Green's function, the quantity D is related to the difference of the order parameter of the interacting and noninteracting systems. Thus, D is zero in the normal phase and for $U = 0$. From these relations also follows that both Σ as well as D vanish in the noninteracting case. Importantly, when the functional $\hat{\Omega}_s$ is evaluated at the exact values of Σ and D , it corresponds to the grand potential of the physical Hamiltonian. To evaluate the functional, we proceed as in the original self-energy functional approach¹² and introduce a reference system, which here corresponds to a cluster decomposition of the physical system. Importantly, the reference system shares its two-particle interaction with the physical system and can be exactly solved by numerical methods. By comparison with the functionals, the universal part of $\hat{\Omega}_s$, denoted as $\hat{\mathcal{F}}$, can be eliminated, which allows one to evaluate $\hat{\Omega}_s$ exactly on the subspace of Σ and D , spanned by the possible sets of reference systems. The results presented are shown to be equivalent to the ones obtained by a more heuristic method, the pseudoparticle approach introduced in Ref. 10, and, thus, provide rigorous variational grounds for that approach. In addition, the extended self-energy functional approach introduced here allows one to envision more general reference systems, in which bath sites are incorporated to enlarge the space of possible self-energies Σ , and possibly bridge over to the (cluster) dynamical mean-field theory (DMFT).^{12,38} For future research, it would be interesting to verify whether in

the limit of an infinite number of bath sites and for a single correlated site as a reference system, our superfluid SFA becomes equivalent to the DMFT for superfluid bosons,^{39,40} as it is the case in the normal phase.¹² For a finite number of bath sites, this is certainly not the case, since the order parameter in the reference system differs from the physical one.

We also presented how the superfluid density can be evaluated by means of this extended variational cluster approach. To this end, we applied a phase-twisting field to the system. We evaluated the superfluid density for the two-dimensional Bose-Hubbard model and compared the extended variational cluster approach results with unbiased quantum-Monte-Carlo results, yielding remarkable agreement. We want to emphasize that the extended self-energy functional approach is not only applicable to the Bose-Hubbard model but to a large class of lattice models, which exhibit a condensed phase. This includes experimentally interesting systems, such as disordered bosons, multicomponent systems (Bose-Bose mixtures or Bose-Fermi mixtures), and light matter systems.^{41,42} Strictly speaking, the method cannot treat long-range interactions, such as dipolar ones, exactly.^{43,44} However, the long-range part can be incorporated on a mean-field level.⁴⁵ In principle, the present approach can be applied to systems with broken translational invariance as well, and, for example, can consider the effect of a confining magnetic trap. However, in this case, one has to abandon the Fourier transform in the cluster vectors and work in real space and, thus, deal with larger matrices and a larger number of variational parameters. A convenient, numerically less expensive alternative, is to adopt the so-called local density approximation.⁴⁶

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APPENDIX : NOTATION AND CONVENTIONS

A. Matrix notation

1. General

In order to simplify our notation, we omit time arguments whenever this does not cause ambiguities. Therefore, two-point functions, such as Green’s functions, self-energies, etc., are interpreted as matrices in Nambu, orbital, and τ space. One-point objects such as \mathcal{A} ($\vec{\mathcal{A}}$) are interpreted as column (row) vectors in the same space. Matrix-matrix and vector-matrix products are understood throughout, whereby internal τ variables are considered to be integrated over. In addition, the transposing operator “ T ” also acts on time variables. Traces Tr contain an integral over τ and a trace tr over orbital indices, i. e., $\text{Tr } M \equiv \text{tr} \int_0^\beta d\tau M(\tau, \tau + 0^+)$, where the 0^+ leads to the well known convergence factor $e^{i\omega_n 0^+}$ in Matsubara space.

(Functional) derivatives with respect to matrices are defined “transposed”:

$$\left(\frac{\delta \hat{X}}{\delta M} \right)_{ij}(\tau, \tau') \equiv \frac{\delta \hat{X}}{\delta M_{ji}(\tau', \tau)}.$$

Finally, there are two types of products between row (in the form \bar{v}) and column (u) vectors, depending on the order: On the one hand, the product $\bar{v}u$ produces a scalar (all indices are summed/integrated over). On the other hand, inverting the order, as in $u\bar{v}$ gives a matrix, as indices are “external” and, thus, not summed over.

2. Trace in τ and in Matsubara space

In τ space, we have

$$\text{Tr } M = \beta^{-1} \text{tr} \int_0^\beta d\tau M(\tau, \tau + 0^+).$$

The transformation of $M(\tau, \tau')$ to Matsubara space is defined as

$$M(\tau, \tau') \equiv \beta^{-1} \sum_{n, n'} M(\omega_n, \omega'_n) e^{-i\omega_n \tau + i\omega'_n \tau'}.$$

The inverse transformation reads

$$M(\omega_n, \omega'_n) = \beta^{-1} \int d\tau d\tau' M(\tau, \tau') e^{i\omega_n \tau - i\omega'_n \tau'}.$$

Combining the equations above, the trace becomes

$$\begin{aligned} \text{Tr } M &= \text{tr} \int_0^\beta d\tau \beta^{-2} \sum_{n, n'} M(\omega_n, \omega'_n) e^{-i(\omega_n - \omega'_n)\tau + i\omega'_n 0^+} \\ &= \beta^{-1} \sum_n \text{tr} M(\omega_n, \omega_n) e^{i\omega_n 0^+}. \end{aligned}$$

3. Logarithm

There are some subtle points concerning logarithms of two-point functions. Although these issues are immaterial for the final result, we prefer to specify them in detail.

The logarithm of G considered as a matrix in the continuum variable τ is defined up to an infinite constant which depends on the discretization step δ (see below). In addition, the trace of the logarithm carried out in Matsubara space diverges as well (despite the convergence factor $e^{i\omega_n 0^+}$). The usual result presented in the literature (see, for instance Ref. 47) implicitly assumes that an infinite constant has been subtracted. In order to avoid these undetermined infinite terms, we subtract them explicitly at the outset with the help of the “infinite energy” Green’s function

$$\begin{aligned} G_\infty(\tau, \tau') &= \beta^{-1} \sum_n G_\infty(\omega_n) e^{-i\omega_n(\tau - \tau')} \\ G_\infty(\omega_n) &= \mathbb{1} \frac{1}{i\omega_n - E}, \end{aligned}$$

where it is understood that the $E \rightarrow +\infty$ limit is taken at the end of the calculation. This choice guarantees, for example, that $\text{Tr} \ln G/G_\infty$, where G is Green’s function in normal (i.e., not Nambu) notation, vanishes in the limit $\mu \rightarrow -\infty$, where μ is the chemical potential.

The Fourier transform defined in Subsec. A2 of the Appendix allows one to define the logarithm of G in τ space, apart from an infinite multiplicative constant, which originates from the fact that the Fourier transformation is not and cannot be normalized in the continuum limit. In particular,

$$\begin{aligned} [\ln(-G)](\tau, \tau') &= \beta^{-1} \sum_{n, n'} [\ln(-G)](\omega_n, \omega'_n) e^{-i\omega_n \tau + i\omega'_n \tau'} \\ &= \beta^{-1} \sum_n \ln[-G(\omega_n)] e^{-i\omega_n(\tau - \tau')}. \end{aligned}$$

B. Symmetry of Green's functions and other two-point functions

The action in Eq. (5) is invariant under the transformation $G_0 \rightarrow (\mathcal{T}G_0^T \mathcal{T})$, where the transposing operator “ T ” also acts on time variables and \mathcal{T} is defined in Eq. (8). This is due to the fact that

$$\begin{aligned} \bar{A}(\tau') G_0^{-1}(\tau', \tau) A(\tau) &= A(\tau')^T \mathcal{T} G_0^{-1}(\tau', \tau) \mathcal{T} \bar{A}(\tau)^T \\ &= \bar{A}(\tau) (\mathcal{T} G_0^{-1}(\tau', \tau)^T \mathcal{T}) A(\tau'). \end{aligned}$$

Therefore, we choose G_0 to obey the symmetry

$$G_0 = (\mathcal{T} G_0^T \mathcal{T}). \quad (\text{A1})$$

The same symmetry is obeyed by other two-point functions, such as the interacting Green's function G , the self-energy Σ , and their inverses.

In principle, this redundancy renders relations such as Eq. (15) noninvertible. In order to avoid this, we adopt the convention that functional inversions are carried out within the subspace of two-point functions obeying the relation Eq. (A1). In addition, we adopt the following convention for functional derivatives of an arbitrary functional $\hat{\mathcal{E}}$ with respect to a two-point function X :

$$\frac{\delta \hat{\mathcal{E}}}{\delta X} \rightarrow \frac{1}{2} \left(\frac{\delta \hat{\mathcal{E}}}{\delta X} + \frac{\delta \hat{\mathcal{E}}}{\delta \mathcal{T} X^T \mathcal{T}} \right).$$

C. Continuum limit of the functional integral

In principle, the expression Eq. (10) should be understood such that adjoint fields \bar{a} are evaluated at a later imaginary time $\tau + \delta$, whereby δ is the width of the discretization mesh of the interval $(0, \beta)$. The continuum limit $\delta \rightarrow 0$ should be taken after having carried out the functional integration (see, e.g., Ref. 48). Taking this limit at the outset amounts to neglecting the so-called “contribution from infinity.”^{49,50} This can be achieved by effectively replacing the normal-ordered Hamiltonian with a “symmetrically ordered” one, which is suitably symmetrized among possible permutation of creation and annihilation operators.⁵¹ In particular, for the noninteracting part, this amounts to replacing the operator expression $a^\dagger a$ by $\frac{1}{2}(a^\dagger a + a a^\dagger) = a^\dagger a + \frac{1}{2}$. Therefore, we should keep in mind that the grand potential $\tilde{\Omega}_s$ corresponds to such a symmetrized Hamiltonian.

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¹D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).

²M. Greiner, O. Mandel, T. Esslinger, T. W. Hansch, and I. Bloch, *Nature (London)* **415**, 39 (2002).

³I. Bloch, J. Dalibard, and W. Zwerger, *Rev. Mod. Phys.* **80**, 885 (2008).

⁴F. Gerbier *et al.*, *Phys. Rev. Lett.* **101**, 155303 (2008).

⁵S. Trotzky, L. Pollet, F. Gerbier, U. Schnorrberger, I. Bloch, N. V. Prokof'ev, B. Svistunov, and M. Troyer, *Nat. Phys.* **6**, 998 (2010).

⁶Y. Kato, Q. Zhou, N. Kawashima, and N. Trivedi, *Nat. Phys.* **4**, 617 (2008).

⁷R. B. Diener, Q. Zhou, H. Zhai, and T. L. Ho, *Phys. Rev. Lett.* **98**, 180404 (2007).

⁸R. Roth and K. Burnett, *Phys. Rev. A* **67**, 031602 (2003).

⁹N. R. Cooper and Z. Hadzibabic, *Phys. Rev. Lett.* **104**, 030401 (2010).

¹⁰M. Knap, E. Arrigoni, and W. von der Linden, *Phys. Rev. B* **83**, 134507 (2011).

¹¹W. Koller and N. Dupuis, *J. Phys. Condens. Matter* **18**, 9525 (2006).

¹²M. Potthoff, *Eur. Phys. J. B* **32**, 429 (2003).

¹³M. Potthoff, *Eur. Phys. J. B* **36**, 335 (2003).

¹⁴M. G. Zacher, R. Eder, E. Arrigoni, and W. Hanke, *Phys. Rev. B* **65**, 045109 (2002).

¹⁵M. E. Fisher, M. N. Barber, and D. Jasnow, *Phys. Rev. A* **8**, 1111 (1973).

¹⁶E. L. Pollock and D. M. Ceperley, *Phys. Rev. B* **36**, 8343 (1987).

¹⁷N. V. Prokof'ev and B. V. Svistunov, *Phys. Rev. B* **61**, 11282 (2000).

¹⁸M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, *Phys. Rev. B* **40**, 546 (1989).

¹⁹See Subsec. B of the Appendix.

²⁰M. Potthoff, *Condensed Matter Physics* **9**, 557 (2006).

²¹Here and below, we assume that the relations between conjugate variables are invertible, at least locally (see also Subsec. B of the Appendix).

²²M. Potthoff, M. Aichhorn, and C. Dahnken, *Phys. Rev. Lett.* **91**, 206402 (2003).

²³In VCA (Refs. 12,52), the reference system is typically a cluster partition of the original lattice, which can be improved by including bath sites (Refs. 25,26). However, for boson systems with $F \neq 0$ and $U < \infty$, the Hilbert space is infinite and the particle number is not conserved. Thus, neither a cluster nor a single site can be solved by exact diagonalization. However, a cutoff in the maximum number of bosons can be introduced, which still allows one to reach arbitrary accuracy.

²⁴The term with G_∞ (see Subsec. C of the Appendix) cancels out.

²⁵M. Balzer, W. Hanke, and M. Potthoff, *Phys. Rev. B* **77**, 045133 (2008).

²⁶M. Balzer, W. Hanke, and M. Potthoff, *Phys. Rev. B* **81**, 144516 (2010).

²⁷E. H. Lieb, R. Seiringer, and J. Yngvason, *Phys. Rev. B* **66**, 134529 (2002).

²⁸A. M. Rey, K. Burnett, R. Roth, M. Edwards, C. J. Williams, and C. W. Clark, *J. Phys. B* **36**, 825 (2003).

²⁹D. Poilblanc, *Phys. Rev. B* **44**, 9562 (1991).

- ³⁰D. J. Scalapino, S. R. White, and S. Zhang, *Phys. Rev. B* **47**, 7995 (1993).
- ³¹M. Knap, E. Arrigoni, and W. von der Linden, *Phys. Rev. B* **81**, 024301 (2010).
- ³²A. Albuquerque *et al.*, *J. Magn. Magn. Mater.* **310**, 1187 (2007).
- ³³F. Alet, S. Wessel, and M. Troyer, *Phys. Rev. E* **71**, 036706 (2005).
- ³⁴A. W. Sandvik and J. Kurkijärvi, *Phys. Rev. B* **43**, 5950 (1991).
- ³⁵H. G. Evertz, G. Lana, and M. Marcu, *Phys. Rev. Lett.* **70**, 875 (1993).
- ³⁶O. F. Syljuåsen and A. W. Sandvik, *Phys. Rev. E* **66**, 046701 (2002).
- ³⁷A. Rancon and N. Dupuis, *Phys. Rev. B* **83**, 172501 (2011).
- ³⁸A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).
- ³⁹K. Byczuk and D. Vollhardt, *Phys. Rev. B* **77**, 235106 (2008).
- ⁴⁰P. Anders, E. Gull, L. Pollet, M. Troyer, and P. Werner, *Phys. Rev. Lett.* **105**, 096402 (2010).
- ⁴¹M. Hartmann, F. G. Brandão, and M. B. Plenio, *Laser Photonics Rev.* **2**, 527 (2008).
- ⁴²A. Tomadin and R. Fazio, *J. Opt. Soc. Am. B* **27**, A130 (2010).
- ⁴³R. Barnett, D. Petrov, M. Lukin, and E. Demler, *Phys. Rev. Lett.* **96**, 190401 (2006).
- ⁴⁴A. Micheli, G. K. Brennen, and P. Zoller, *Nat. Phys.* **2**, 341 (2006).
- ⁴⁵M. Aichhorn, H. G. Evertz, W. von der Linden, and M. Potthoff, *Phys. Rev. B* **70**, 235107 (2004).
- ⁴⁶C. Kollath, U. Schollwöck, J. von Delft, and W. Zwerger, *Phys. Rev. A* **69**, 031601 (2004).
- ⁴⁷J. M. Luttinger and J. C. Ward, *Phys. Rev.* **118**, 1417 (1960).
- ⁴⁸L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).
- ⁴⁹E. Arrigoni, C. Castellani, M. Grilli, R. Raimondi, and G. C. Strinati, *Phys. Rep.* **241**, 291 (1994).
- ⁵⁰E. Arrigoni and G. C. Strinati, *Phys. Rev. Lett.* **71**, 3178 (1993).
- ⁵¹E. Arrigoni and G. C. Strinati, *Phys. Rev. B* **52**, 2428 (1995).
- ⁵²C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff, *Phys. Rev. B* **70**, 245110 (2004).