

Excitation spectra of bosons in optical lattices from the Schwinger-Keldysh calculation

T. D. Graß,¹ F. E. A. dos Santos,² and A. Pelster^{3,*}

¹*ICFO-Institut de Ciències Fotòniques, Mediterranean Technology Park, E-08860 Castelldefels, Barcelona, Spain*

²*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany*

³*Fachbereich Physik, Universität Duisburg-Essen, Lotharstraße 1, D-47048 Duisburg, Germany*

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Within the Schwinger-Keldysh formalism we derive a Ginzburg-Landau theory for the Bose-Hubbard model which describes the real-time dynamics of the complex order parameter field. Analyzing the excitations in the vicinity of the quantum phase transition, it turns out that particle-hole dispersions in the Mott phase map continuously onto corresponding amplitude-phase excitations in the superfluid phase, which have been detected recently by Bragg spectroscopy measurements.

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I. INTRODUCTION

Within the last decade ultracold atoms in optical lattices [1,2] have become a standard tool for studying quantum-statistical many-body effects. Due to their high tunability, these systems represent an almost-perfect test ground for a large variety of solid-state models. In particular, the experimental observation of the seminal quantum phase transition from the Mott insulating (MI) to the superfluid (SF) phase, exhibited by a single-band Bose-Hubbard (BH) system of spinless or spin-polarized bosons, has recently attracted a lot of attention [3,4]. Although the occurrence of this quantum phase transition is evident from the momentum distributions of time-of-flight measurements, its precise location cannot be determined from them. Recently, however, more detailed information about the collective excitations of this system could also be achieved by exciting the system via lattice modulation [5] or by Bragg spectroscopy [6–8]. Deep in the SF phase, the observed gapless excitation spectrum can be well understood within a Bogoliubov theory [9]. Approaching the phase boundary, a time-dependent dynamic Gutzwiller calculation [7], a slave-boson method [10], and a random-phase approximation [11,12] have predicted an additional SF gapped mode, which recently could be confirmed experimentally in the strongly interacting regime [7]. When the MI phase is reached, both SF modes turn continuously into particle and hole excitations which are also found by mean-field theory [9]. Due to their finite energy gaps, they characterize the insulating phase in a unique way.

A field-theoretic ansatz describing the system in both the insulating and the SF regime was first considered in Ref. [13], where an effective action was obtained via two successive Hubbard-Stratonovich transformations. The same action can also be obtained by the Ginzburg-Landau approach developed in Refs. [14] and [15], which is technically based on resumming a perturbative hopping expansion. As explicitly shown in Refs. [14–18], the practical advantage of this nonperturbative approach is that it provides a generalization of mean-field theory by taking into account higher hopping orders in a straightforward systematic way. However, the Landau theory in Ref. [14] is restricted to a static description of the

SF-MI transition at zero temperature. A finite-temperature Ginzburg-Landau theory developed in Ref. [15] also yields dynamic results via an analytic continuation but is restricted to near-equilibrium situations. Since time-resolved measurements [19] have become possible within the last years, a real-time description of quantum systems is desirable. Therefore, we follow Ref. [20] and modify the imaginary-time approach from Ref. [15] by converting it to real time, thus requiring techniques which were first introduced by L.V. Keldysh [21] and J. Schwinger [22].

This so-called Schwinger-Keldysh formalism, which we briefly introduce in Sec. II, is believed to be suited to describe any kind of nonequilibrium problems of Hamiltonian systems. However, in the present paper we restrict ourselves to studying with this formalism the equilibrium problems of the time-independent BH model. To this end we derive a Ginzburg-Landau functional by combining a perturbative hopping expansion of the free energy in Sec. III, with a subsequent resummation due to a Legendre transformation in Sec. IV. Extremizing this functional leads to equations of motion for the order parameter fields, which are solved in Sec. V. This yields a plethora of equilibrium results like the phase boundary and the excitation spectra in Sec. VI, which are compared with the corresponding imaginary-time approach of Ref. [15]. While both descriptions agree qualitatively and, at zero temperature, also quantitatively, a subtle difference in the four-point Green function reveals an unexpected mismatch at finite temperature. Thereby we are able to show that both formalisms do not describe the same physical situation, as we discuss in detail in Sec. VII. Finally, a summary of the present work and an outlook, how to generalize it to nonequilibrium situations, are given in Sec. VIII.

II. SCHWINGER-KELDYSH FORMALISM

To introduce the Schwinger-Keldysh formalism, we consider the Green functions of a many-body system. In general, these are averages over a product of creation operators $\hat{a}_i^\dagger$ and annihilation operators $\hat{a}_i$, where the index i collects the degrees of freedom of the system. In our case, it just denotes the respective lattice site. At zero temperature, the averaging process is purely quantum mechanical, whereas for finite temperature the thermal fluctuations are also taken

*axel.pelster@uni-duisburg-essen.de

into account. In equilibrium systems, that is, those with a Hamiltonian constant in time, introducing imaginary-time variables puts the thermal averaging formally on an equal footing with the dynamic evolution of a time-dependent system at zero temperature.

For both cases, perturbative treatments are well known, which are based on reducing the nontrivial real or imaginary dynamics of the operators in the Heisenberg picture to the trivial dynamics of operators in the Dirac picture, which is determined by some solvable part $\hat{H}_0$ of the full Hamiltonian $\hat{H}$. The remaining part $\hat{H}_1$ then enters the time-evolution operator $\hat{U}(t, t_0)$ which acts on the states. In the case of a real-time evolution, for instance, it reads $\hat{U}(t, t_0) = \hat{T} \exp[-i \int_{t_0}^t dt \hat{H}_{1D}(t)]$, where $\hat{T}$ is the time-ordering operator, and $\hbar$ has been set to 1.

In the zero-temperature formalism (ZTF), the Green functions are defined as ground-state expectation values of time-ordered operator products in the Heisenberg picture, that is, $\langle \hat{T}[\hat{a}_{i_1H}^\dagger(t_1) \cdots \hat{a}_{i_nH}(t_n)] \rangle_{\hat{H}}$, where $\langle \bullet \rangle_{\hat{H}}$ denotes the expectation value with respect to the ground state of the Hamiltonian $\hat{H}$. Applying the translation formula from the Heisenberg to the Dirac picture to this expression, that is, $\hat{a}_H(t) = \hat{U}(t_0, t) \hat{a}_D(t) \hat{U}(t, t_0)$, where t_0 is the initial time, we find for each operator a forward and a backward time evolution. But due to the time ordering, these various pieces can be straightened to one single forward evolution from t_0 to the largest time within the operator product and a subsequent backward evolution. The latter, however, cancels due to a connection between the ground state of the full and that of the unperturbed system, which is provided by the Gell-Mann-Low theorem [23]. In this way, we not only get rid of the backward evolution, but also reduce the expectation value to the one of the known, unperturbed ground state. Finally, we get $\langle \hat{T}[\hat{U}(\infty, -\infty) \hat{a}_{i_1D}^\dagger(t_1) \cdots \hat{a}_{i_nD}(t_n)] \rangle_{\hat{H}_0}$, where the nontrivial part of the averaging process enters only via a forward evolution along a straight time path, which has been extended to infinity. In this way, the perturbation theory is reduced to a Taylor expansion of the time-evolution operator $\hat{U}(\infty, -\infty)$.

In the following, however, we also consider finite temperatures, so in the Green functions the average $\langle \bullet \rangle_{\hat{H}}$ now denotes a thermal average with respect to the equilibrium of $\hat{H}$, that is, $\text{Tr}(\bullet e^{-\beta \hat{H}}) / \text{Tr}(e^{-\beta \hat{H}})$, where $\beta = 1/k_B T$ is, as usual, the inverse temperature. If there is no evolution along the real-time axis, then the scheme of the ZTF described above can be taken over to an artificially introduced imaginary-time axis. Evolution along this axis somehow imitates the thermal averaging process, so the backward evolution in imaginary dynamics of the operator product can be directly canceled against the perturbative part of the thermal density matrix $e^{-\beta \hat{H}}$. In this way, the imaginary-time formalism (ITF) also puts all nontrivial $\hat{H}_1$ contributions of the Green functions into a straight time evolution.

The situation becomes more complicated for a time-dependent many-body system at finite temperature, where the backward evolution along the real-time axis cannot be canceled by the Gell-Mann-Low theorem as in the ZTF. To realize the consequences of this, let us consider for simplicity the product $\hat{O}_{2H}(t_2) \hat{O}_{1H}(t_1)$ of two arbitrary operators in the Heisenberg picture. If $t_1 > t_2$, the translation from the Heisenberg into the Dirac picture yields $\hat{U}(t_0, t_2) \hat{O}_{2D}(t_2) \hat{U}(t_2, t_1) \hat{O}_{1D}(t_1) \hat{U}(t_1, t_0)$,

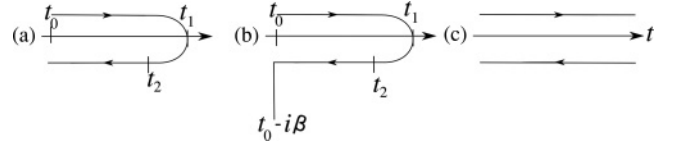


FIG. 1. Contours of time evolution: (a) Schwinger contour; (b) interaction contour; (c) Keldysh contour.

which represents a time evolution along a closed contour as depicted in Fig. 1(a), with $\hat{O}_{2D}(t_2)$ being located on the backward path of the contour. For the opposite case $t_2 > t_1$, the closed contour extends from t_0 to t_2 , and the condition to maintain the order of the operators now is that $\hat{O}_{1D}(t_1)$ appears on the forward path. In both cases it obviously plays no role which part of the contour is assigned to the last operator.

By providing each operator with a corresponding path index $P = \pm$, where $+$ stands for the forward and $-$ for the backward path, the positions of the operators on the contour can be fixed. With this we are able to define a contour-ordering operator $\hat{T}_c$, which brings the $+$ operators in time order, while acting as an anti-time-ordering operator $\hat{A}$ on the $-$ operators. Such contour-ordered operator products are the most natural generalization of the time-ordered products considered in the ZTF. Thus the relevant Green functions are given by quantities like $\langle \hat{T}_c[\hat{a}_{i_1H}^{P_1}(t_1) \cdots \hat{a}_{i_nH}^{P_n}(t_n)] \rangle_{\hat{H}}$. But even after transforming into the Dirac picture, that is, $\langle \hat{T}_c[\hat{U}(t_0, t_>) \hat{U}(t_>, t_0) \hat{a}_{i_1D}^{P_1}(t_1) \cdots \hat{a}_{i_nD}^{P_n}(t_n)] \rangle_{\hat{H}_0}$, where $t_>$ is the biggest time appearing in the operator product, the perturbative part of the Hamiltonian is not completely isolated within the time-evolution operator, since it still appears in the thermal average. We might manage this by extending the time-evolution contour to the complex plane as shown in Fig. 1(b), yielding a third path.

However, it is widely believed in the literature that, if we perform the initial time limit $t_0 \rightarrow -\infty$, the imaginary part of that contour can be neglected for initially uncorrelated systems [24,25]. We follow this tradition and discuss its limitations at the end of this paper. With this simplification and by extending the contour to the infinite future, we get the time-evolution contour from Fig. 1(c), encircling completely the real-time axis. It is a closed path, and we, therefore, refer to this formalism as the closed time path formalism (CTPF).

Then the contour-ordered Green functions can be defined as

$$G_{(i)}^{(P)}(\{t\}) \equiv i^{n+m-1} \langle \hat{T}_c[\hat{S}^\dagger \hat{S} \hat{a}_{i_1}^{P_1}(t_1) \cdots \hat{a}_{i_n}^{P_n}(t_n) \times \hat{a}_{i_{n+1}}^{P_{n+1}}(t_{n+1}) \cdots \hat{a}_{i_{n+m}}^{P_{n+m}}(t_{n+m})] \rangle_{\hat{H}_0}, \quad (1)$$

where, for simplicity, we have waived the index for the Dirac picture, as we do so for the rest of this paper. With the curly brackets $\{X\}$, we abbreviated the union of variables $X_1, \dots, X_{n+m}$. In this expression, the perturbation enters only in the time evolution $\hat{S}^\dagger \hat{S} = \hat{T}_c \exp[-i \int_{-\infty}^{\infty} dt \hat{H}_1^\dagger(t) - \hat{H}_1(t)]$.

The Green functions from Eq. (1) can systematically be derived from a generating functional. To this end, we have to introduce artificial currents $j_i^P(t)$ and their complex conjugate $\bar{j}_i^P(t)$, which linearly couple to the corresponding creation and annihilation operators $\hat{a}_i^{P\dagger}(t)$ and $\hat{a}_i^P(t)$. With

such a source term, the new Hamiltonian reads $\hat{H}^P[j, \bar{j}](t) = \hat{H}_0^P(t) + \hat{H}_1^P(t) + \sum_i [j_i^P(t) \hat{a}_i^{P\dagger}(t) + \bar{j}_i^P(t) \hat{a}_i^P(t)]$. Assigning the source term to the perturbative part, we have to substitute $\hat{S}$ by $\hat{S}[j^+, \bar{j}^+] = \hat{T} \exp(-i \int_{-\infty}^{\infty} dt [\hat{H}_1^+(t) + \sum_i [j_i^+(t) \hat{a}_i^{+\dagger}(t) + \text{c.c.}]])$, and similarly for the backward evolution operator $\hat{S}^\dagger$. The generating functional is then defined as

$$\mathcal{Z}[j^+, j^-, \bar{j}^+, \bar{j}^-] = \langle \hat{T}_c \{ \hat{S}^\dagger[j^-, \bar{j}^-] \hat{S}[j^+, \bar{j}^+] \} \rangle_{\hat{H}_0}, \quad (2)$$

yielding the Green functions as its functional derivatives,

$$G_{i_1 \dots i_n, i_{n+1} \dots i_{n+m}} = \frac{\delta^{n+m} \mathcal{Z}[j, \bar{j}]}{\delta \bar{j}_{i_1} \dots \delta \bar{j}_{i_n} \delta j_{i_{n+1}} \dots \delta j_{i_{n+m}}} \Big|_{j=0}, \quad (3)$$

where both path indices and temporal variables have been waived for simplicity.

Path-ordered quantities, though naturally arising within the Keldysh formalism, lack a clear physical interpretation, so it is convenient to define the linear combinations

$$X^\Sigma(t) = [X^+(t) + X^-(t)]/\sqrt{2}, \quad (4)$$

$$X^\Delta(t) = [X^+(t) - X^-(t)]/\sqrt{2}. \quad (5)$$

A good discussion of different choices for a suitable basis can be found in Ref. [26]. To see how the path-ordered Green functions given in Eq. (1) transform under this so-called Keldysh rotation, it is most instructive to consider the two-point functions. Writing them in the form of a 2×2 matrix, the transformation is given by

$$\begin{pmatrix} G_{ij}^{++}(t; t') & G_{ij}^{+-}(t; t') \\ G_{ij}^{-+}(t; t') & G_{ij}^{--}(t; t') \end{pmatrix} \rightarrow \begin{pmatrix} A_{ij}(t; t') & G_{ij}^R(t; t') \\ G_{ij}^A(t; t') & 0 \end{pmatrix}, \quad (6)$$

where $G^{R,A}$ are the well-known retarded (advanced) Green function and A is the anticommulator function. In the case of bosons, they are defined as [27]

$$G_{ij}^R(t; t') \equiv i\theta(t - t') \langle [\hat{a}_{iH}(t), \hat{a}_{jH}^\dagger(t')] \rangle_{\hat{H}}, \quad (7)$$

$$G_{ij}^A(t; t') \equiv -i\theta(t - t') \langle [\hat{a}_{iH}(t), \hat{a}_{jH}^\dagger(t')] \rangle_{\hat{H}}, \quad (8)$$

$$A_{ij}(t; t') \equiv i \langle [\hat{a}_{iH}(t), \hat{a}_{jH}^\dagger(t')]_+ \rangle_{\hat{H}}. \quad (9)$$

Here, $[\bullet, \bullet]_+$ denotes the anticommutator, while the commutator is given by $[\bullet, \bullet]$, and θ stands for the Heaviside function. To see how these quantities arise from the Keldysh rotation in Eq. (6), we must note that the definitions in Eqs. (7)–(9) can be rewritten in terms of contour-ordered products, $\hat{T}_c[\hat{a}_{iH}^P(t) \hat{a}_{jH}^{P\dagger}(t')]$. It then turns out that these can be summarized to one single product of $\hat{a}^\Sigma$ and $\hat{a}^\Delta$ operators or their Hermitian conjugates, respectively. We find

$$G_{ij}^R(t; t') = i \langle \hat{T}_c [\hat{a}_{iH}^\Sigma(t) \hat{a}_{jH}^\Delta(t')] \rangle_{\hat{H}}, \quad (10)$$

$$G_{ij}^A(t; t') = i \langle \hat{T}_c [\hat{a}_{iH}^\Delta(t) \hat{a}_{jH}^\Sigma(t')] \rangle_{\hat{H}}, \quad (11)$$

$$A_{ij}(t; t') = i \langle \hat{T}_c [\hat{a}_{iH}^\Sigma(t) \hat{a}_{jH}^\Sigma(t')] \rangle_{\hat{H}}. \quad (12)$$

Since in the next section we calculate the path-ordered Green functions perturbatively, we stress that these relations hold not only for the exact Green functions, but also in any order of perturbation theory [28]. Furthermore, it can be shown for arbitrary n -point functions that the Keldysh rotation always yields, among other functions, the retarded and advanced

Green functions. For practical calculations it is also relevant to note that operator products of the kind $\hat{T}_c \hat{O}_1^\Delta \dots \hat{O}_n^\Delta$ are identically 0 [24], so among the Keldysh-rotated n -point functions, we always find a vanishing one.

III. PERTURBATION THEORY

In the previous section we have introduced the general formalism of separating the nontrivial real-time dynamics and thermodynamics from the rest of a Green function by performing a translation from the Heisenberg to the Dirac picture. In view of concrete applications, we must now define the respective unperturbed and perturbed parts of the considered Hamiltonian.

Bosons in an optical lattice are described by the BH Hamiltonian [1,2] given as $\hat{H}_{BH} = \hat{H}_0 + \hat{H}_1$, where we have introduced a decomposition into the local part,

$$\hat{H}_0 = \sum_i \left[\frac{U}{2} \hat{a}_i^\dagger \hat{a}_i (\hat{a}_i^\dagger \hat{a}_i - 1) - \mu \hat{a}_i^\dagger \hat{a}_i \right], \quad (13)$$

and the nonlocal hopping term,

$$\hat{H}_1 = - \sum_{i,j} J_{ij} \hat{a}_i^\dagger \hat{a}_j. \quad (14)$$

Here $\hat{a}_i(\hat{a}_i^\dagger)$ denotes the bosonic annihilation(creation) operator at lattice site i , μ the chemical potential, U the on-site interaction parameter, and J_{ij} the hopping matrix element, being equal to $J > 0$ for nearest neighbors only.

The main feature of this Hamiltonian is a quantum phase transition from an MI phase to an SF phase due to the competition between kinetic energy, that is, hopping between sites, and local on-site interactions. Therefore, it is natural to consider the hopping as a perturbation, if we are interested in the MI phase, whereas in the SF phase the interaction represents the perturbation. However, a perturbative description of the critical behavior between the two regimes would then be doomed to fail. But we are in the lucky situation that in the SF phase a *resummed* hopping expansion can also be considered as a $1/D$ expansion of an D -dimensional system and, thus, might allow for a proper description of the quantum phase transition. To show this, we note that, in the presence of a condensate, the hopping parameter J must be rescaled according to the dimensional scaling law $J \rightarrow J/D$ to have a finite energy in infinite dimensions [29]. This means that within a hopping expansion all n th-order hopping loops are suppressed by a factor $1/D^{n-1}$. By resumming the one-particle irreducible contributions up to the n th hopping order, we therefore get an effective $(1/D)$ expansion up to the $(n-1)$ th order. Although we restrict ourselves in this paper to the lowest order $n=1$, we get a theory which, given a nonzero condensed fraction, is exact for infinite dimensions or infinite-range hopping [30]. In this way we find for $D \geq 2$ that the quantum phase transition can be well described in a quantitative way.

Finally, we must add a source term to the Hamiltonian, yielding $\hat{H}[j, \bar{j}](t) = \hat{H}_{BH} + \hat{H}_S(t)$, with

$$\hat{H}_S[j, \bar{j}](t) = \sum_i [\hat{a}_i^\dagger(t) j_i(t) + \text{c.c.}]. \quad (15)$$

A similar source term has already been introduced for defining a generating functional in Eq. (2), but there it was only a technical tool. Although we set the currents to 0 in the end, here this term acquires a physical meaning, since it explicitly breaks the underlying U(1) symmetry of the original BH Hamiltonian. Only this symmetry breaking makes it possible to have a non-vanishing condensate amplitude $\langle \hat{a}_i(t) \rangle$, which characterizes the SF phase and can be taken as an order parameter field $\Psi_i(t)$ for describing the MI-SF transition within a Ginzburg-Landau theory. From definition (15) it is clear that the currents $j_i(t)$ and $\bar{j}_i(t)$ are the conjugate variables of the order parameter fields $\bar{\Psi}_i(t) = \langle \hat{a}_i^\dagger(t) \rangle$ and $\Psi_i(t) = \langle \hat{a}_i(t) \rangle$, now appearing explicitly within the Hamiltonian $\hat{H}[j, \bar{j}](t)$.

Ginzburg-Landau theories are in general based on a fourth-order expansion of the thermodynamic potential in the order parameter field [31]. To derive it for the underlying BH model, we start from the free energy. For small order parameter fields we can assume that also the influence of the symmetry-breaking currents is small, so we can write down the free energy as a power series with respect to these currents $j_i(t)$ and $\bar{j}_i(t)$. It is then possible to replace the currents via a Legendre transformation by the order parameter fields $\bar{\Psi}_i(t) = \langle \hat{a}_i^\dagger(t) \rangle$ and $\Psi_i(t) = \langle \hat{a}_i(t) \rangle$, so that we finally end up with the so-called effective action that serves as a Ginzburg-Landau functional.

Noting that the generating functional $\mathcal{Z}[j^+, j^-, \bar{j}^+, \bar{j}^-]$ defined in Eq. (2) has a structure similar to that of the partition function in statistical mechanics, we get an analog of the free energy by taking the logarithm:

$$\mathcal{F}[j^+, j^-, \bar{j}^+, \bar{j}^-] = -i \ln \mathcal{Z}[j^+, j^-, \bar{j}^+, \bar{j}^-]. \quad (16)$$

As described in Sec. II, the functional $\mathcal{Z}$ is given by a forward and a backward evolution in time, where the operators and currents appearing on both time paths have to be distinguished from each other. Before starting a perturbative expansion of this functional, however, it turns out to be feasible to perform a Keldysh rotation, which mixes the quantities on the forward and backward path as defined by Eqs. (4) and (5). Under this rotation, the source term transforms as $j_i^+ \hat{a}_i^{++} - j_i^- \hat{a}_i^{-+} = j_i^\Sigma \hat{a}_i^{\Delta+} + j_i^\Delta \hat{a}_i^{\Sigma+}$, and for the hopping term we have $\hat{a}_i^{++} \hat{a}_j^+ - \hat{a}_i^{-+} \hat{a}_j^- = \hat{a}_i^{\Delta+} \hat{a}_j^\Sigma + \hat{a}_i^{\Sigma+} \hat{a}_j^\Delta$. It turns out to be helpful to introduce the vector quantities $\mathbf{j}_i = (j_i^\Delta, j_i^\Sigma)^T$ and $\hat{\mathbf{a}}_i^\dagger = (\hat{a}_i^{\Sigma\dagger}, \hat{a}_i^{\Delta\dagger})$. Then the generating functional reads

$$\begin{aligned} \mathcal{F}[\mathbf{j}, \bar{\mathbf{j}}] = & -i \ln \left(\hat{T}_c \exp \left(-i \int_{-\infty}^{\infty} dt \left\{ \sum_{ij} J_{ij} \hat{\mathbf{a}}_j^\dagger \sigma^1 \hat{\mathbf{a}}_i \right. \right. \right. \\ & \left. \left. \left. + \sum_i [\bar{\mathbf{j}}_i(t) \cdot \hat{\mathbf{a}}_i(t) + \text{c.c.}] \right\} \right) \right)_{\hat{H}_0}, \end{aligned} \quad (17)$$

where σ^1 is the Pauli matrix [32].

Instead of straightforwardly expanding this functional in the hopping parameter J and in the vector currents $\mathbf{j}$ and $\bar{\mathbf{j}}$, we first note that the logarithm has the nice property of making $\mathcal{F}[\mathbf{j}, \bar{\mathbf{j}}]$ an extensive quantity. Thus the linked-cluster theorem [33,34] applies: It states that, whereas the expansion of $\mathcal{Z}$ is built up by the Green functions, which have been defined in the

path-ordered basis in Eq. (1), the functional $\mathcal{F}$ can be expanded in a series of *connected* Green functions or cumulants C :

$$C_{i_1 \dots i_n; i_{n+1} \dots i_{n+m}} = \frac{\delta^{n+m} \mathcal{F}[j, \bar{j}]}{\delta \bar{j}_{i_n} \dots \delta \bar{j}_{i_1} \delta j_{i_{n+1}} \dots \delta j_{i_{n+m}}} \Big|_{j=0}^{\bar{j}=0}. \quad (18)$$

For simplicity, we have suppressed here, again, both the time variables and the Keldysh indices.

These cumulants are much simpler objects than the Green functions: Whereas, roughly speaking, the Green functions may describe any particle creation and annihilation processes, the cumulants decompose them into their independent contributions. What is meant by this can be illustrated by considering only the unperturbed system $\hat{H}_0$ in (13). Here, each lattice site i can be considered as an independent system and we could define generating functionals $\mathcal{Z}_i^{(0)}[\mathbf{j}_i, \bar{\mathbf{j}}_i]$ in each subsystem. We would find that the Green functions of the whole system could be derived from $\mathcal{Z}^{(0)}[\mathbf{j}, \bar{\mathbf{j}}] = \prod_i \mathcal{Z}_i^{(0)}[\mathbf{j}_i, \bar{\mathbf{j}}_i]$. Whereas an expansion of each $\mathcal{Z}_i^{(0)}[\mathbf{j}_i, \bar{\mathbf{j}}_i]$ in the currents would be completely local, the expansion of $\mathcal{Z}^{(0)}[\mathbf{j}, \bar{\mathbf{j}}]$ would contain highly nonlocal objects as well. Nevertheless, it is clear, that these nonlocal Green functions arise as products of local Green functions, and it must therefore be possible to find a decomposition. This mixing is circumvented from the beginning, if we consider instead $\mathcal{F}^{(0)}[\mathbf{j}, \bar{\mathbf{j}}] = -i \sum_i \ln \mathcal{Z}_i^{(0)}[\mathbf{j}_i, \bar{\mathbf{j}}_i]$, where the logarithm has turned the product of subsystems into a sum of them.

In a system with hopping, of course, the situation is not that simple, but if we expand $\mathcal{F}[\mathbf{j}, \bar{\mathbf{j}}]$ not only in the currents, but also in the hopping parameter J , the expansion still contains only the local cumulants of the unperturbed system, and the hopping simply appears as a link between two cumulants. For an expansion up to fourth order in the currents, we need the unperturbed cumulants $C_i^{K_1 K_2(0)}(t_1; t_2)$ and $C_i^{K_1 K_2 K_3 K_4(0)}(t_1, t_2; t_3, t_4)$, where $K = \Sigma, \Delta$ denotes the respective Keldysh index. All the cumulants have only one site index due to their locality. Note that cumulants describing an unequal number of annihilation and creation processes vanish in the unperturbed system, since $\hat{H}_0$ commutes with the local number operator $\hat{n}_i \equiv \hat{a}_i^\dagger \hat{a}_i$. Their relations to the unperturbed Green functions can be derived from Eqs. (3) and (18) and read explicitly

$$C_i^{K_1 K_2(0)}(t_1; t_2) = G_{ii}^{K_1 K_2(0)}(t_1; t_2) \quad (19)$$

and

$$\begin{aligned} C_i^{K_1 K_2 K_3 K_4(0)}(t_1, t_2; t_3, t_4) &= G_{iiii}^{K_1 K_2 K_3 K_4(0)}(t_1, t_2; t_3, t_4) - i C_i^{K_1 K_3(0)}(t_1; t_3) C_i^{K_2 K_4(0)}(t_2; t_4) \\ &\quad - i C_i^{K_1 K_4(0)}(t_1; t_4) C_i^{K_2 K_3(0)}(t_2; t_3). \end{aligned} \quad (20)$$

The unperturbed Green functions are obtained by setting $J = 0$ in Eq. (1). Explicitly, they read

$$G_{ij}^{K_1 K_2(0)}(t_1; t_2) = \frac{\text{Tr}\{e^{-\beta \hat{H}_0} \hat{T}_c [\hat{a}_i^{K_1}(t_1) \hat{a}_j^{K_2\dagger}(t_2)]\}}{\text{Tr}\{e^{-\beta \hat{H}_0}\}} \quad (21)$$

and

$$\begin{aligned} G_{ijkl}^{K_1 K_2 K_3 K_4(0)}(t_1, t_2; t_3, t_4) &= \frac{\text{Tr}\{e^{-\beta \hat{H}_0} \hat{T}_c [\hat{a}_i^{K_1}(t_1) \hat{a}_j^{K_2\dagger}(t_2) \hat{a}_k^{K_3\dagger}(t_3) \hat{a}_l^{K_4\dagger}(t_4)]\}}{\text{Tr}\{e^{-\beta \hat{H}_0}\}}. \end{aligned} \quad (22)$$

To obtain an expansion of Γ as a power series in J , Ψ , and $\bar{\Psi}$, we first insert the expansion of $\mathcal{F}[\mathbf{j}, \bar{\mathbf{j}}]$ from Eq. (27) into the definition of Ψ in Eq. (28), yielding an expression of the order parameter fields as a power series in J , $\mathbf{j}$, and $\bar{\mathbf{j}}$. In the diagrammatic notation, the derivative in Eq. (28) is obtained by taking away a black square with an ingoing leg from the graphs in $\mathcal{F}$ and, if there is more than one such square within one graph, by applying the usual product rule of differentiation. With this we obtain for the order parameter fields, which we denote by white squares, the following expression:

$$\begin{aligned} \Psi_i(t) \equiv \square \xrightarrow{it} &= \blacksquare \xrightarrow{i} \circ \xrightarrow{t} + \blacksquare \xrightarrow{i} \bullet \xrightarrow{t} + \frac{1}{2} \blacksquare \xrightarrow{i} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \\ &+ \frac{1}{2} \left[2 \blacksquare \xrightarrow{i} \bullet \xrightarrow{t} \bullet \xrightarrow{t} + \blacksquare \xrightarrow{i} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \right. \\ &\left. + \blacksquare \xrightarrow{i} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \right]. \end{aligned} \quad (31)$$

Variables fixed by the derivative appear explicitly in the diagrams; for all other variables the previous summation convention continues to hold.

Inverting expression (31) iteratively in J and $\mathbf{j}$, we find a power series of $\mathbf{j}[\Psi, \bar{\Psi}](J)$. In zeroth hopping order and first order in the currents, only the first diagram in Eq. (31) must be taken into account. Thus, the inversion reads

$$\blacksquare \xrightarrow{it} = \square \xrightarrow{i} \circ \xrightarrow{t}, \quad (32)$$

where the white circle stands for the inverse cumulant $[\mathbf{C}_i(t_1; t_2)]^{-1}$. Note that the triangular structure of $\mathbf{C}_i(t_1; t_2)$ is conserved under inversion:

$$[\mathbf{C}_i(t_1; t_2)]^{-1} = \begin{pmatrix} 0 & [\mathbf{C}_i^{\Delta\Sigma(0)}(t_1; t_2)]^{-1} \\ [\tilde{\mathbf{C}}_i^{\Sigma\Delta(0)}(t_1; t_2)]^{-1} & [\tilde{\mathbf{C}}_i^{\Sigma\Sigma(0)}(t_1; t_2)]^{-1} \end{pmatrix}, \quad (33)$$

where we have introduced the abbreviation

$$\begin{aligned} [\tilde{\mathbf{C}}_i^{\Sigma\Sigma(0)}(t_1; t_2)]^{-1} &\equiv -\mathbf{C}_i^{\Sigma\Sigma(0)}(t_1; t_2) [\mathbf{C}_i^{\Delta\Sigma(0)}(t_1; t_2)]^{-1} \\ &\times [\mathbf{C}_i^{\Delta\Sigma(0)}(t_1; t_2)]^{-1}. \end{aligned} \quad (34)$$

Reinserting this in the second diagram in Eq. (31), we get the inversion up to the first hopping order,

$$\blacksquare \xrightarrow{it} = \square \xrightarrow{i} \circ \xrightarrow{t} - \sum_j J_{ij} \square \xrightarrow{j} \sigma^1 \quad (35)$$

and, finally, taking into account the currents up to third order, we get

$$\begin{aligned} \blacksquare \xrightarrow{it} &= \square \xrightarrow{i} \circ \xrightarrow{t} - \frac{1}{2} \blacksquare \xrightarrow{i} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \\ &- \sum_j J_{ij} \left[\square \xrightarrow{j} + \frac{1}{2} \blacksquare \xrightarrow{j} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \right] \sigma^1. \end{aligned} \quad (36)$$

Note that the lines between a cumulant and its inverse are not internal lines; that is, they do not represent a hopping. Inserting the result from Eq. (36) into Eq. (30) together with (27) and discarding any diagram which is higher than first order in the

hopping or higher than fourth order in the order parameter fields, we finally find the effective action in the shape of a Ginzburg-Landau functional in first hopping order:

$$\begin{aligned} \Gamma^{(4,1)}[\Psi, \bar{\Psi}] &= -\square \xrightarrow{i} \circ \xrightarrow{t} \square + \int_{-\infty}^{\infty} dt \sum_{ij} \square \xrightarrow{it} [J_{ij} \sigma^1] \xrightarrow{j} \square \\ &+ \frac{1}{4} \blacksquare \xrightarrow{i} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \bullet \xrightarrow{t} \square. \end{aligned} \quad (37)$$

Comparing the graphical content of the effective action in Eq. (37) with the corresponding one of the free energy in Eq. (27), we find that it has a much simpler structure: In the last two diagrams of the free energy the hopping connects two cumulants, yielding a so-called one-particle reducible diagram, that is, a diagram which might be divided into two diagrams by cutting one single line. In the effective action, however, these diagrams do not appear, and only the one-particle irreducible diagrams remain [35,36].

At this point, it is helpful to express result (37) in analytic terms. However, while in the diagrammatic approach, apart from a straightforward redefinition of the diagrams, it makes no difference if we work in real space or in Fourier space, the analytic expression is simplified considerably by a Fourier transformation. Therefore, we define the transformation into frequency space,

$$f(\omega) = \int_{-\infty}^{\infty} dt f(t) e^{i\omega t}, \quad (38)$$

and into wave vector space,

$$f_{\vec{k}} = \sum_i f_i e^{-i\vec{k} \cdot \vec{r}_i}. \quad (39)$$

For conjugate variables, for example, $\bar{\Psi}$, the corresponding conjugate transformations hold.

Since the unperturbed Hamiltonian $\hat{H}_0$ in (13) is not explicitly time dependent, the unperturbed cumulants may depend only on the differences in their time variables. As we explicitly see in the Appendix, where all the relevant cumulants are calculated in frequency space, this independence from an absolute time yields a Dirac δ function in frequency space. Thus we are able to define

$$\mathbf{C}_i(\omega_1; \omega_2) \equiv \delta(\omega_1 - \omega_2) \mathbf{c}_i(\omega_1), \quad (40)$$

and we have

$$\mathbf{C}(\omega_1, \omega_2; \omega_3, \omega_4) \sim \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4). \quad (41)$$

Regarding the spatial variables, the homogeneity of J_{ij} assures that the hopping term becomes local by a transformation into wave-vector space. In a cubic lattice with lattice spacing a , for instance, we get

$$J_{ij} \rightarrow 2J \sum_{v=1}^3 \cos(k_v a) \equiv J_{\vec{k}}. \quad (42)$$

As all cumulants are local, the transformation into wave vector space always yields a $\vec{k}$ dependence in the form of $\delta_{\vec{k}, \vec{0}}$. Since a summation over $\vec{k}$ must also be performed, we can completely suppress the wave-vector indices of the cumulants.

The effective action then reads in terms of Fourier transformed quantities:

$$\Gamma^{(4,1)} = - \sum_{\vec{k}} \int d\omega \bar{\Psi}_{\vec{k}}(\omega) [\mathbf{c}(\omega)]^{-1} - \sigma_1 J_{\vec{k}} \Psi_{\vec{k}}(\omega) + \frac{1}{4} \sum_{\{\vec{k}\}} \int d\{\omega\} \delta_{\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4} \bar{\Psi}_{\vec{k}_1}(\omega_1) [\mathbf{c}(\omega_1)]^{-1} \\ \times \bar{\Psi}_{\vec{k}_2}(\omega_2) [\mathbf{c}(\omega_2)]^{-1} \mathbf{C}(\omega_1, \omega_2; \omega_3, \omega_4) [\mathbf{c}(\omega_3)]^{-1} \Psi_{\vec{k}_3}(\omega_3) [\mathbf{c}(\omega_4)]^{-1} \Psi_{\vec{k}_4}(\omega_4). \quad (43)$$

Now we can show that this expression of the effective action contains resummed hopping processes. To this end, we consider the first term in Eq. (43), which is of second order in the fields: $[\mathbf{c}(\omega)]^{-1} [1 - J_{\vec{k}} \sigma^1 \mathbf{c}(\omega)]$. Expanding this expression into a geometric sum yields $\{\mathbf{c}(\omega) \sum_n [J_{\vec{k}} \sigma^1 \mathbf{c}(\omega)]^n\}^{-1}$. Diagrammatically, this represents the inverse of a sum of arbitrarily long hopping “chains.” Thus, by means of a resummation, any of these terms is automatically taken into account within the effective action. This is the clue which transforms the initial perturbative hopping expansion for the free energy into an effective $1/D$ expansion for the effective action, from which we may expect reliable results not only in the MI but also in the SF phase.

We conclude this section by showing how to extract physical information from the effective action given by Eq. (43). The easiest and most direct way to do so is by noting that the physical situation corresponds to vanishing currents. Due to Legendre identities this means that

$$\bar{\mathbf{J}}_{\vec{k}}(\omega) = \frac{\delta \Gamma}{\delta \Psi_{\vec{k}}(\omega)} \stackrel{!}{=} 0, \quad (44)$$

and the complex conjugate of this equation. We refer to these equations as the *equations of motion*, as they determine the order parameter field. In the next section we deal with their solutions. This will yield both the phase boundary, if we consider the static case, and the excitation spectra, in the dynamical case.

V. EQUATIONS OF MOTION

Analyzing the structure of the effective action Γ in (43), we find that the second-order term $\bar{\Psi}^\Sigma \Psi^\Sigma$ is related to the vanishing cumulant $C^{\Delta\Delta}$ and the fourth-order term $\bar{\Psi}^\Sigma \bar{\Psi}^\Sigma \Psi^\Sigma \Psi^\Sigma$ is related to the vanishing cumulant $C^{\Delta\Delta\Delta\Delta}$. This means that all nonvanishing terms in Eq. (43) contain Ψ^Δ at least to first order. Since the first component in Eq. (44) is given by $\delta\Gamma/\delta\Psi^\Sigma = 0$, all the terms in this equation will contain Ψ^Δ or $\bar{\Psi}^\Delta$ as a factor. As we aim at solving the equations of motion with the ansatz $\Psi^+(t) = \Psi^-(t)$, that is, with an order parameter field which is independent of the time path, we are looking for solutions $\Psi^\Delta = 0$. Thus, we find that the first component in Eq. (44) is always trivially fulfilled. The second component reads

$$\frac{\delta \Gamma}{\delta \Psi_{\vec{k}}^\Delta(\omega)} = -\bar{\Psi}_{\vec{k}}^\Sigma(\omega) \left(\frac{1}{G^{A(0)}(\omega)} - J_{\vec{k}} \right) + \frac{1}{4} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \int_{-\infty}^{\infty} d\omega_3 \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3} \delta_{\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}} [C^{\Delta\Delta\Delta\Sigma(0)}(\omega_1, \omega_2; \omega_3, \omega) \\ + C^{\Delta\Delta\Sigma\Delta(0)}(\omega_1, \omega_2; \omega, \omega_3)] \frac{\bar{\Psi}_{\vec{k}_1}^\Sigma(\omega_1) \bar{\Psi}_{\vec{k}_2}^\Sigma(\omega_2) \Psi_{\vec{k}_3}^\Sigma(\omega_3)}{G^{A(0)}(\omega_1) G^{A(0)}(\omega_2) G^{R(0)}(\omega_3) G^{A(0)}(\omega)} \stackrel{!}{=} 0. \quad (45)$$

The four-point cumulants $C^{K_1 K_2 K_3 K_4(0)}(\omega_1, \omega_2; \omega_3, \omega_4)$ are symmetric in $\{\omega_1, K_1\} \leftrightarrow \{\omega_2, K_2\}$ and $\{\omega_3, K_3\} \leftrightarrow \{\omega_4, K_4\}$, such that $C^{\Delta\Delta\Delta\Sigma(0)}(\omega_1, \omega_2; \omega_3, \omega_4) = C^{\Delta\Delta\Sigma\Delta(0)}(\omega_1, \omega_2; \omega_4, \omega_3)$. Thus, from the initial 16 four-point cumulants, only 1 has to be calculated. This is done in the Appendix, where explicit expressions for the retarded and advanced Green functions $G^{R(0)}$ and $G^{A(0)}$ are also derived. There we see, furthermore, that $2C^{\Delta\Delta\Delta\Sigma(0)}(\omega_1, \omega_2, \omega_3, \omega_4)$ coincides with the advanced four-point function $C^{A(0)}(\omega_1, \omega_2; \omega_3, \omega_4)$, which is defined as the thermal average of multiple commutators times Heaviside step functions (cf. [24]). As the complex conjugates of advanced Green functions are retarded Green functions, the complex conjugate of Eq. (44) amounts to interchanging the respective retarded and advanced functions.

Due to the triple frequency integrals and the triple wave-vector sums, Eq. (45) is not straightforwardly solved. To continue analytically, we now assume the equilibrium ansatz $\Psi_{\vec{k}}^\Sigma(\omega) = \delta(\omega) \delta_{\vec{k},0} \bar{\Psi}_{\text{eq}}^\Sigma$ of a spatially homogeneous and temporally constant order parameter field. With that ansatz, all integrals and sums become trivial, and we get the algebraic equation:

$$\frac{1}{G^{A(0)}(0)} - J_0 = \frac{C^{A(0)}(0,0;0,0) \bar{\Psi}_{\text{eq}}^\Sigma \Psi_{\text{eq}}^\Sigma}{4G^{A(0)}(0)G^{A(0)}(0)G^{R(0)}(0)G^{A(0)}(0)}. \quad (46)$$

Later we read off from this equation physically important results like the phase boundary. At the moment we only need the information that this equation defines an equilibrium value Ψ_{eq}^Σ around which we perform a harmonic approximation for the effective action, Eq. (45), with the ansatz $\Psi_{\vec{k}}^K(\omega) = \Psi_{\text{eq}}^K + \Psi_{\vec{k}}^K(\omega)$. This yields

$$\Gamma[\Psi^\Delta, \bar{\Psi}^\Delta, \Psi^\Sigma, \bar{\Psi}^\Sigma] \approx \frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \left\{ \frac{\delta^2 \Gamma}{\delta \Psi_{\vec{k}_1}^\Sigma(\omega_1) \delta \bar{\Psi}_{\vec{k}_2}^\Delta(\omega_2)} \bigg|_{\text{eq}} \bar{\Psi}_{\vec{k}_2}^\Delta(\omega_2) \Psi_{\vec{k}_1}^\Sigma(\omega_1) + \frac{\delta^2 \Gamma}{\delta \bar{\Psi}_{\vec{k}_1}^\Sigma(\omega_1) \delta \Psi_{\vec{k}_2}^\Delta(\omega_2)} \bigg|_{\text{eq}} \right. \\ \left. \times \Psi_{\vec{k}_2}^\Delta(\omega_2) \bar{\Psi}_{\vec{k}_1}^\Sigma(\omega_1) + \frac{\delta^2 \Gamma}{\delta \Psi_{\vec{k}_1}^\Sigma(\omega_1) \delta \Psi_{\vec{k}_2}^\Delta(\omega_2)} \bigg|_{\text{eq}} \Psi_{\vec{k}_2}^\Delta(\omega_2) \Psi_{\vec{k}_1}^\Sigma(\omega_1) + \frac{\delta^2 \Gamma}{\delta \bar{\Psi}_{\vec{k}_1}^\Sigma(\omega_1) \delta \bar{\Psi}_{\vec{k}_2}^\Delta(\omega_2)} \bigg|_{\text{eq}} \bar{\Psi}_{\vec{k}_2}^\Delta(\omega_2) \bar{\Psi}_{\vec{k}_1}^\Sigma(\omega_1) \right\}. \quad (47)$$

Other derivatives either vanish or lead to terms which are of second order in Ψ^Δ . They would vanish when the resulting equations of motion are solved by $\Psi^\Delta = 0$. Evaluating explicitly the respective derivatives in Eq. (47) yields the linearized expression:

$$\begin{aligned} & \left[\frac{1}{G^{R(0)}(\omega)} - J_{\bar{k}} - \frac{|\Psi_{\text{eq}}|^2 C^{R(0)}(\omega, 0; 0, \omega)}{2G^{A(0)}(0)G^{R(0)}(0)G^{R(0)}(\omega)G^{R(0)}(\omega)} \right] \\ & \times \Psi_{\bar{k}}^\Sigma(\omega) - \frac{|\Psi_{\text{eq}}|^2 C^{R(0)}(\omega, -\omega; 0, 0)}{4G^{A(0)}(-\omega)G^{R(0)}(0)G^{R(0)}(\omega)G^{R(0)}(0)} \\ & \times \bar{\Psi}_{-\bar{k}}^\Sigma(-\omega) \stackrel{!}{=} 0. \end{aligned} \quad (48)$$

This equation and its complex conjugate form a set of linear equations determining four degrees of freedom: the phase and amplitude of the order field at both positive and negative frequencies ω . To obtain the dispersion relations, it is sufficient to restrict ourselves to the real part of the equation of motion. To see this we relate the linearized equation of motion to the

Green functions. We start with the statement

$$\left. \frac{\delta^2 \mathcal{F}}{\delta \bar{j}_i^\Delta \delta j_j^\Sigma} \right|_{j=\bar{j}=0} = G_{ij}^A. \quad (49)$$

Making use of the product rule for functional derivatives, we find the identity

$$\begin{aligned} \delta_{ij} = \frac{\delta j_i^\Delta}{\delta j_j^\Delta} = \sum_k \left(\frac{\delta j_i^\Delta}{\delta \Psi_k^\Delta} \frac{\delta \Psi_k^\Delta}{\delta j_j^\Delta} + \frac{\delta j_i^\Delta}{\delta \bar{\Psi}_k^\Delta} \frac{\delta \bar{\Psi}_k^\Delta}{\delta j_j^\Delta} \right. \\ \left. + \frac{\delta j_i^\Delta}{\delta \Psi_k^\Sigma} \frac{\delta \Psi_k^\Sigma}{\delta j_j^\Delta} + \frac{\delta j_i^\Delta}{\delta \bar{\Psi}_k^\Sigma} \frac{\delta \bar{\Psi}_k^\Sigma}{\delta j_j^\Delta} \right), \end{aligned} \quad (50)$$

and a similar one from $0 = \delta \bar{j}_i^\Delta / \delta j_j^\Delta$. With the Legendre identity

$$\Psi_i^\Sigma = \frac{\delta \mathcal{F}}{\delta \bar{j}_i^\Delta}, \quad (51)$$

which is dual to (44), we are finally able to relate the second derivatives of the effective action Γ to the advanced two-point functions,

$$G_k^A(\omega) = \frac{\left. \frac{\delta^2 \Gamma}{\delta \bar{\Psi}_{-\bar{k}}^\Delta(-\omega) \delta \Psi_{-\bar{k}}^\Sigma(-\omega)} \right|_{\text{eq}}}{\left. \frac{\delta^2 \Gamma}{\delta \bar{\Psi}_{-\bar{k}}^\Delta(-\omega) \delta \Psi_{-\bar{k}}^\Sigma(-\omega)} \right|_{\text{eq}} \left. \frac{\delta^2 \Gamma}{\delta \Psi_{\bar{k}}^\Delta(\omega) \delta \bar{\Psi}_{\bar{k}}^\Sigma(\omega)} \right|_{\text{eq}} - \left. \frac{\delta^2 \Gamma}{\delta \Psi_{-\bar{k}}^\Delta(-\omega) \delta \Psi_{\bar{k}}^\Sigma(\omega)} \right|_{\text{eq}} \left. \frac{\delta^2 \Gamma}{\delta \bar{\Psi}_{\bar{k}}^\Delta(\omega) \delta \bar{\Psi}_{-\bar{k}}^\Sigma(-\omega)} \right|_{\text{eq}}}, \quad (52)$$

and the complex conjugate expression for the retarded Green function. We now see that the equation of motion, (48), is solved, when the SF Green function, (52), diverges. As this divergence must take place in both the real and the imaginary part of the Green function, it is sufficient to consider just one of them to find the excitations. As shown in the Appendix, it is much simpler to find an expression for the real part. However, the imaginary part contains information about the spectral weights, as we show in Sec. VIB.

VI. RESULTS

The nontrivial solutions of Eq. (45) can be divided into two classes which we work out at $T = 0$. How to perform the $T = 0$ limit for the respective Green functions and cumulants is shown in the Appendix.

A. Phase boundary

Static solutions are obtained from Eq. (46). The right-hand side of Eq. (46) does not explicitly depend on the hopping parameter, but it is multiplied by $|\Psi_{\text{eq}}|^2 \geq 0$. Thus, its sign is independent of J . The left-hand side of Eq. (46) depends explicitly on J and changes its sign at some critical value $J_{\text{PB}}(\mu, U)$, which is obtained by setting the left-hand side of Eq. (46) equal to 0. From (A3) and (A9) we get explicitly

$$J_{\text{PB}}(\mu, U) = -\frac{(Un - \mu - U)(Un - \mu)}{6(\mu/U + 1)}. \quad (53)$$

For $J < J_{\text{PB}}$ at a given μ and U , only $\Psi_{\text{eq}} = 0$ solves Eq. (46), and thus we are in the disordered, that is, MI phase. For $J > J_{\text{PB}}$, the system is SF. A plot of the phase boundary, (53), for $T = 0$ and $0 \leq \mu/U \leq 1$ is shown on the left side of Fig. 3 for $n = 1$. In the considered first hopping order, this quantum phase diagram is identical to the mean-field result [9], with a deviation from recent high-precision Monte Carlo data [37] of about 25%. Within a Landau expansion the second-order hopping contribution was recently calculated analytically in Ref. [14], decreasing the error to less than 2%. A numerical evaluation of higher hopping orders has even been shown to converge to a quantum phase diagram which is indistinguishable from the Monte Carlo result [16–18].

For obtaining dynamic solutions we have to consider the linearized equation of motion Eq. (48). Numerically, we obtain the dispersion relations shown in Fig. 3, where the MI-SF transition can clearly be observed by a qualitative change in the excitations of the system.

B. MI spectra

In the MI phase, we find the gapped particle-hole excitations from mean-field theory [9]. At the phase boundary, we have to distinguish the tip from the rest of the lobe in accordance with the critical theory of the BH model [30,31]. While at the tip of the m th lobe, that is, at $\mu_m/U = \sqrt{m(m+1)} - 1$, both excitations become gapless and linear for small $|k|$, off the tip, at $\mu > \mu_m$ ($\mu < \mu_m$), only the particle (hole) mode becomes gapless and remains with a finite effective mass.

Since in the MI phase and at the phase boundary we have $|\Psi_{\text{eq}}| = 0$, we are able to determine analytic solutions of the

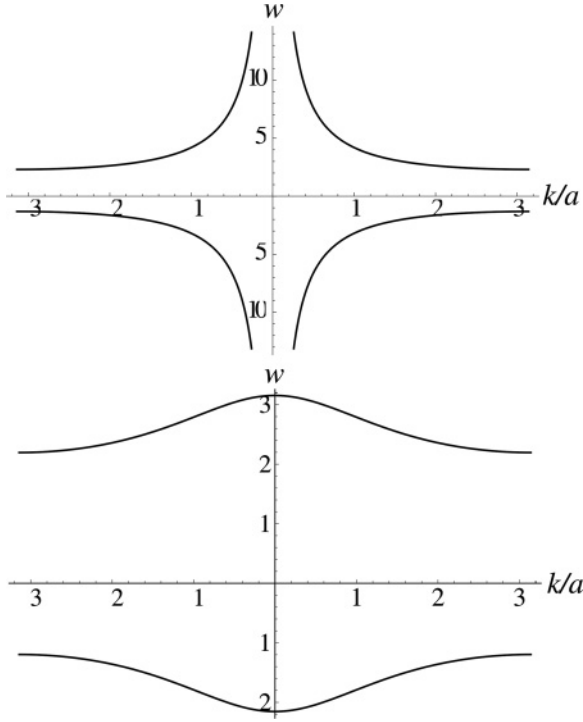


FIG. 2. Spectral weights at the lobe tip (top) and for $J/U = 0.02$ (bottom) as a function of $k = \vec{k} \cdot \vec{e}_x$.

equations of motion, Eq. (48):

$$\omega_{\pm}(\vec{k}) = \frac{1}{2\hbar} \left[U(2n-1) - 2\mu - J_{\vec{k}} \pm \sqrt{U^2 - 2J_{\vec{k}}U(2n+1) + J_{\vec{k}}^2} \right]. \quad (54)$$

The Green function in Eq. (52) reduces in the MI phase to

$$G_{\vec{k}}^{\text{R(MI)}}(\omega) = \left[\frac{1}{G_{\vec{k}}^{\text{R(0)}}(\omega)} - J_{\vec{k}} \right]^{-1}. \quad (55)$$

Comparing this with the general spectral representation of the retarded (advanced) Green functions [38],

$$G_{\vec{k}}^{\text{R/A}}(\omega) = \int_{-\infty}^{\infty} d\omega' \rho(\omega', \vec{k}) \left(\frac{\text{P}}{\omega - \omega'} \pm i\pi \delta(\omega - \omega') \right), \quad (56)$$

where P denotes the principal value of the integration across the singularity and $\rho(\omega, \vec{k})$ denotes the spectral function, we can also obtain information about the spectral weights of the excitations, that is, how much of the total excitation energy is stored in each excitation. To this end we have to divide Eq. (55) into its real and imaginary part, where the latter is due to an infinitesimal $i\epsilon$ shift of the poles from the real axis into the complex plane (see the Appendix). By performing the limit $\epsilon \rightarrow 0$, we find

$$\rho(\omega, \vec{k}) = \delta(\omega - \omega_+(\vec{k}))w_+(\vec{k}) + \delta(\omega - \omega_-(\vec{k}))w_-(\vec{k}), \quad (57)$$

with the respective weights

$$w_{\pm}(\vec{k}) = \frac{1}{2} \left(1 \pm \frac{U(1+2n) - J_{\vec{k}}}{\sqrt{U^2 - 2J_{\vec{k}}U(2n+1) + J_{\vec{k}}^2}} \right). \quad (58)$$

Note that they do not depend on the chemical potential. At the tip of the lobe, both weights diverge at $\vec{k} = \vec{0}$. We can check the spectral function, (57) and (58), by noting that it obeys the sum rule [38]:

$$\int_{-\infty}^{\infty} d\omega \rho(\omega, \vec{k}) = 1. \quad (59)$$

The spectral weights are plotted for two different ratios J/U in Fig. 2.

C. SF spectra

By increasing the hopping we reach the SF phase, where long-range correlations arise. Due to the resummation, our effective action, Eq. (43), contains infinite chain diagrams and is, thus, able to describe such a long-range order. Being restricted to first-order diagrams, however, it does not account for large number fluctuations, which play a role as one moves deeper into the SF phase. In this section, we thus restrict ourselves to a SF regime in the vicinity of the Mott lobes. The validity of our theory in the opposite limit of very small interactions is discussed in Sec. VI E.

As the correlations break the phase-rotational symmetry of the system, resulting in a finite equilibrium value of the order field Ψ_{eq} , the structure of Eq. (48) becomes much more complicated than in the MI phase, and we therefore restrict ourselves to determining the dispersion relations. As argued above, they already follow from the real part of Eq. (48); that is, we can neglect the imaginary parts of the Green functions.

Interestingly, we find all solutions to be symmetric under changing of the sign of the frequency ω in accordance with the RPA approximation in Ref. [12]. As there are no excitations with negative energy, the important quantity can only be the absolute value of ω . Thus, the number of solutions reduces to two, which allows for mapping them onto the MI spectra.

We find that the gapless mode rapidly loses its mass and has to be identified with the Goldstone mode which arises due to the broken U(1) symmetry. Indeed, within the Ginzburg-Landau theory it turns out, in the limit $\vec{k} \rightarrow \vec{0}$ and $\omega \rightarrow 0$, that the excitation $\Psi_{\vec{k}}(\omega)$ stems from variations of the phase. Within a slave-boson approach it has even been shown in Ref. [10] that, also for general wave vectors $\vec{k}$, phase variations dominate this excitation. Thus density variations arise which make this mode sensitive to Bragg spectroscopy. Recently, the whole sound mode has been measured via Bragg spectroscopy far away from the phase boundary and could be well described via a Bogoliubov fit [6]. Analytical results for this mode can be obtained by expanding Eq. (48) for small ω and small $\vec{k}$ up to second order. The resulting algebraic equation is solved by the ansatz $\omega = c|\vec{k}|$. Defining the dimensionless quantities $\tilde{\mu} = \mu/U$ and $\tilde{J} = J/U$, we find that the sound velocity c of the Goldstone mode at $T = 0$, which is given by the dimensionless

quantity,

$$\tilde{c}(n, \tilde{\mu}, \tilde{J}) = \frac{c(n, \mu, J, U)}{aU/\hbar} \quad (60)$$

$$\begin{aligned} \tilde{c}(1, \tilde{\mu}, \tilde{J}) = & \{[\tilde{J}\tilde{\mu}^2(1 + \tilde{\mu})^3(3 - 2\tilde{\mu})(-3 + 8\tilde{\mu} - 10\tilde{\mu}^2 + 4\tilde{\mu}^3 + \tilde{\mu}^4)^2((\tilde{\mu} - 1)\tilde{\mu} + 6\tilde{J}(1 + \tilde{\mu}))]/ \\ & \times [36\tilde{J}(1 - \tilde{\mu})^3\tilde{\mu}^3(-27 + 108\tilde{\mu} + 9\tilde{\mu}^2 - 92\tilde{\mu}^3 + 3\tilde{\mu}^4 - 24\tilde{\mu}^5 + 7\tilde{\mu}^6) - (-1 + \tilde{\mu})^3\tilde{\mu}^3 \\ & \times (27 - 135\tilde{\mu} + 36\tilde{\mu}^2 + 172\tilde{\mu}^3 - 210\tilde{\mu}^4 + 294\tilde{\mu}^5 - 196\tilde{\mu}^6 + 60\tilde{\mu}^7 + 15\tilde{\mu}^8 + \tilde{\mu}^9) + 18\tilde{J}^2(1 + \tilde{\mu})^2 \\ & \times (27 - 270\tilde{\mu} + 1359\tilde{\mu}^2 - 3860\tilde{\mu}^3 + 5950\tilde{\mu}^4 - 4512\tilde{\mu}^5 + 1198\tilde{\mu}^6 + 100\tilde{\mu}^7 + 135\tilde{\mu}^8 - 66\tilde{\mu}^9 + 3\tilde{\mu}^{10})]\}^{1/2}. \end{aligned} \quad (61)$$

In addition to that sound mode, however, a gapped mode also survives the quantum phase transition or arises again if we depart from the lobe tip. It can be smoothly mapped onto one of the respective MI modes, which is shown in the plot of both the effective masses and the gaps on the right side in Fig. 3. The existence of such a SF gapped mode is in accordance with theoretical results obtained in Refs. [10–13]. Comparing the gap with the one obtained in the RPA approximation, we find a perfect quantitative agreement at the phase boundary, but for an increasing hopping J , our approach predicts a slower increase in the gap than found in Ref. [12]. This gapped mode is interpreted in Refs. [7] and [10] as an amplitude excitation which corresponds to an exchange between condensed and noncondensed particles at a constant overall density. Although Eq. (48) does not allow *pure* amplitude excitations, we can back this interpretation of predominant amplitude excitations by observing that the zero-momentum energy transfer at the phase boundary corresponds to the creation of a particle-hole pair. Recently, progress has been made by experimentally confirming the existence of this SF gapped mode, even in weakly interacting SFs, where the sound mode is in good agreement with the prediction of the Bogoliubov theory [7].

D. Critical exponents

From our excitation spectra we can directly read off the dynamical critical exponent z , which is $z = 1$ at the tip, where a relativistic dispersion relation is found, and $z = 2$ off the tip, where the system behaves like a normal Bose gas. This is in agreement with the critical theory of the BH model [30,31]. Physically, the difference between the “generic” transition off the lobe tip and the “XY-like” one at the tip is caused by the density variations that are only absent at the lobe tip. Writing the gap Δ as a function of $J - J_{\text{PB}}(\mu)$, that is, of the distance to the phase boundary, we find that $\Delta \sim [J - J_{\text{PB}}(\mu)]^{z\nu}$ with the mean-field exponent $\nu = 1/2$ for any *vertical* phase transition (see Fig. 4). Since vertical transitions really cross the phase boundary, their exponents can be obtained analytically by considering only the behavior within the Mott phase. At the tip, there is also the possibility of touching the phase boundary horizontally, that is, without entering the MI phase. We find that this is a special case of the generic transitions with $z\nu = 1$, where $z = 1$ and $\nu = 1$ are obtained numerically.

along any lattice direction. Here n gives the occupation number of the MI lobe, above which the SF theory is constructed. For $n = 1$, for instance, we find the explicit result

E. Gross-Pitaevskii limit

Although conceptually designed for a description of the system in the Mott phase and at the onset of superfluidity, it turns out that the resummed hopping expansion also provides access to the weak-coupling regime, if we expand the Green functions in U . To see this, one must note that our strong-coupling expansion contains all local quantum fluctuations, while nonlocal quantum fluctuations are only included to first order through the hopping expansion. The correct physics in the small U limit is known to be reproduced by the Gross-Pitaevskii (GP) theory, which is the first-order U expansion. For this reason, our theory, which contains the first-order hopping contribution as well as contributions of all orders in U , is supposed to reduce to the GP theory if one expands it to first order in U . Indeed, we find that, in the lowest nontrivial order, the Green functions do not depend on temperature and reduce to

$$G^{\text{R/A}(0)}(\omega_1; \omega_2) = -2\pi \frac{1}{\mu + \omega} \delta(\omega_1 - \omega_2) + O(U) \quad (62)$$

$$\begin{aligned} C^{\text{R/A}(0)}(\omega_1, \omega_2; \omega_3, \omega_4) &= -2\pi \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) \\ &\times \frac{2U}{(\mu + \omega_1)(\mu + \omega_2)(\mu + \omega_3)(\mu + \omega_4)} \\ &+ O(U^2). \end{aligned} \quad (63)$$

Inserting this into Eq. (45) leads, after a Fourier transformation into real time and space, to the equation of motion,

$$i \frac{\partial \Psi_i^\Sigma}{\partial t} = - \sum_j J_{ij} \Psi_j^\Sigma - \mu \Psi_i^\Sigma + \frac{U}{2} \Psi_i^\Sigma |\Psi_i^\Sigma|^2, \quad (64)$$

which is the lattice version of the GP equation [39]. From this follows the Bogoliubov sound mode of a fully condensed system [9], which is given by

$$\omega_{\vec{k}} = \sqrt{\epsilon_{\vec{k}}^2 + 2Un\epsilon_{\vec{k}}}, \quad (65)$$

where $\epsilon_{\vec{k}} = 6J - J_{\vec{k}}$ denotes the free dispersion. For small $|\vec{k}|$, this dispersion is linear with the sound velocity,

$$\frac{c}{a/\hbar} = \sqrt{2J(\mu + 6J)}, \quad (66)$$

which coincides with the limit $\tilde{c}U$ from Eq. (61) for $U \rightarrow 0$.

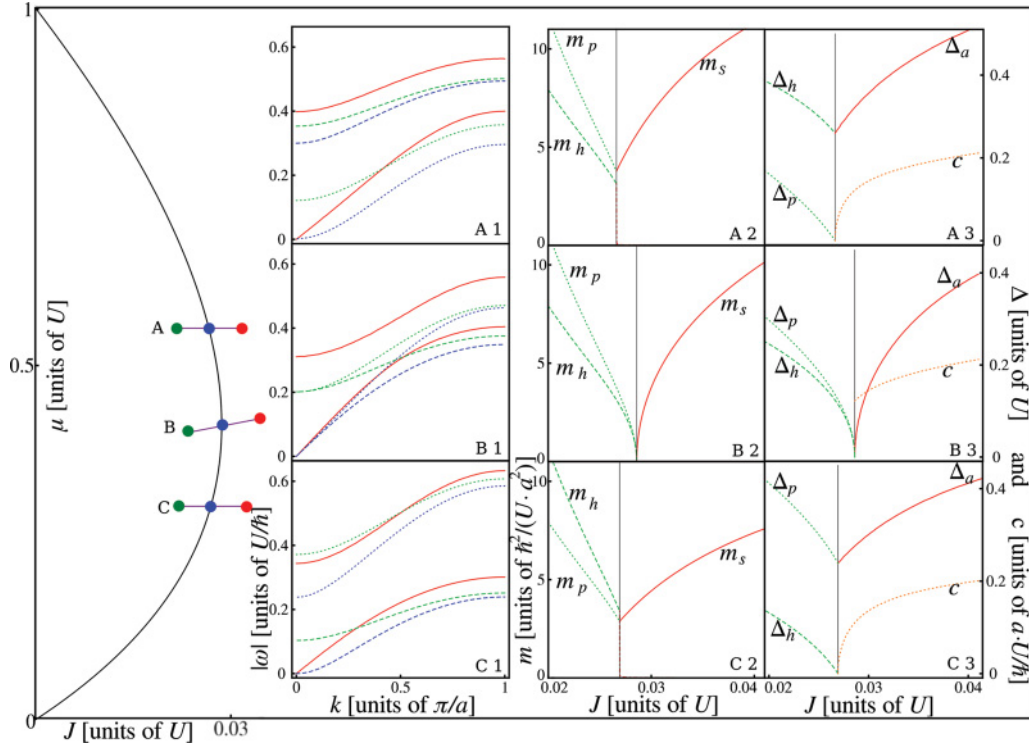


FIG. 3. (Color online) Excitations in the $\mathbf{k} = (1,0,0)$ direction are plotted in A1–C1 for different values of μ/U and J/U , which are marked in the phase diagram (left). In the MI phase (green lines) and on the phase boundary (blue lines), the two $T = 0$ modes can be interpreted as particle (dotted lines) and hole (dashed lines) excitations. At the tip of the Mott lobe (B), both modes become gapless, whereas for larger(smaller) chemical potentials μ , only the gap of the particle (hole) mode vanishes. In the SF phase (red), the gapless mode turns into a sound mode, but a gapped mode is also present everywhere in the SF phase. The smooth transition from the MI excitation to the SF excitation is further analyzed in A2–C2 and A3–C3, where the effective mass m and the gap Δ of each mode are plotted as a function of J/U . The sound velocity c of the massless SF excitation, plotted in A3–C3, vanishes at the phase boundary except at the tip, indicating the existence of a different universality class in this configuration.

We thus have shown that, by throwing away higher orders of U , our theory agrees exactly with the GP approximation predicting only a gapless mode. It is thus interesting to ask what happens if we instead take into account *all* interaction contributions and choose U to be small, that is, solve the *full* equations of motion numerically for small values of U . We find that the gapped mode converges to the constant dispersion $\omega(\vec{k}) = 2\mu$, if U becomes negligibly small. As the chemical potential μ corresponds to the energy needed to add or take away one noninteracting particle from a lattice site, this gapped excitation may be interpreted as the creation of a particle-hole pair. This result agrees qualitatively with recent experimental findings [7] based on Bragg spectroscopy.

VII. COMPARISON WITH EQUILIBRIUM THEORY

Finally, we compare our results with those obtained within a similar Ginzburg-Landau theory in imaginary time [15]. Whereas at $T = 0$ both formalisms yield identical results, a mismatch occurs for finite temperature. This is surprising, since both formalisms are considered to be equivalent in equilibrium [24,25], but there also exists a number of papers in which possible disagreements of the CTPF and the ITF are discussed [40–43].

To localize this mismatch, we note that the equations of motions in the ITF have the same structure as ours in Eq. (48), but the retarded and advanced cumulants have to be replaced by the analytical continuation of the thermal Green functions to real frequencies. For the two-point function we find that the analytical continuation yields exactly the retarded and advanced functions. However, in the case of the four-point functions, the thermal Green function has a decomposition into lower cumulants, while the retarded and advanced Green functions do not have a similar decomposition (see the Appendix and Ref. [44]). Apart from this missing cumulant decomposition terms, both formalisms agree completely, but these terms, which vanish for $T = 0$, might become large if the temperature increases.

We note that the decomposition vanishes for retarded and advanced Green functions due to the choice of our time-evolution contour in Sec. II. On the Keldysh contour the path of the largest-time operator plays no role, which results in the vanishing of contour-ordered products of Δ -indexed operators and, therefore, of any possible decompositions of the retarded and advanced Green functions. Obviously, the path of the largest-time operator would play a role, if both the forward and the backward path were not chosen to be along the real-time axis, for example, if we shifted the backward axis by $-i\beta$ as proposed in Ref. [45]. Thus we can conclude that the Keldysh

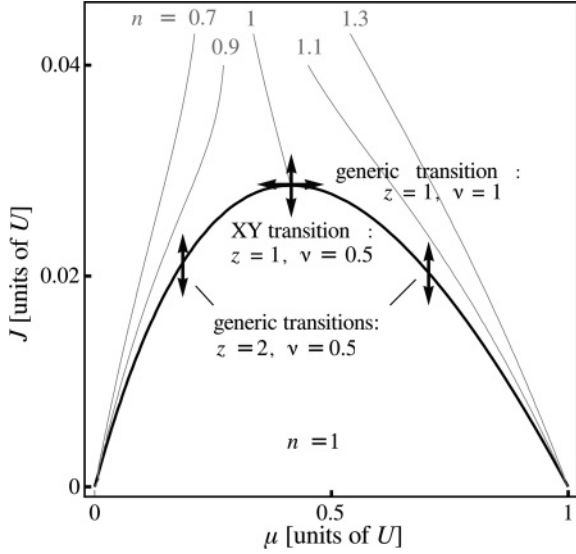


FIG. 4. The critical exponents depend on the position and direction of the phase transition. The gray lines of constant densities in the SF phase are obtained via a thermodynamic effective action based on an analog expansion in imaginary time [15].

formalism working with a purely real time-evolution contour is not able to produce the correct equilibrium configuration of the full system for a finite temperature. This result is supported by Ref. [46], where it is argued that throwing away the imaginary part of the time-evolution contour reduces the generating functional $\mathcal{Z}$ to 1, whereas along the full contour it really represents the partition function.

This formal argumentation can be backed by a more physical picture: The Keldysh theory describes the time evolution of a many-body system starting in a thermal equilibrium at a given temperature, which is destroyed by some perturbation. In our case, where a time-independent hopping is taken as the perturbation, the scenario described can be considered a quench which has occurred in the infinite past, so at any finite time the system is assumed to have equilibrated into a new equilibrium state. Apart from the question whether this assumption really holds for the BH model [47], we cannot expect the new equilibrium to be found at the same temperature, as after the Hamiltonian is changed, the conserved energy has to be distributed among new degrees of freedom. It is, therefore, important to note that the temperature in the Keldysh formalism is the temperature *before* perturbing the system, which is the only possible choice in a nonequilibrium system, but for describing an equilibrated, time-independent system, one might rather be interested in the temperature *after* equilibration, which is also the temperature considered in the ITF.

This explains why the results from our Keldysh method do not agree quantitatively with the ITF results. To achieve this, we would have to take into account the imaginary axis, as then the initial thermal equilibrium is defined with respect to the perturbed Hamiltonian, but obviously a third path on the contour would complicate the calculation considerably. This is certainly a handicap if one wishes to study relaxation into equilibrium within the Keldysh formalism, but the fact that the temperature is defined differently in the ITF than

in the Keldysh formalism, might, in contrast, also allow for calculating the heating of the system due to a quench by applying both formalisms and comparing the results.

The agreement of both formalisms at $T = 0$ can be understood as a consequence of the Gell-Mann-Low theorem [23], stating that the systems remains in the ground state if a perturbation is adiabatically switched on. Since the Keldysh ansatz has pushed this switching into the infinite past, no additional assumptions about its adiabatic properties had to be made [25].

VIII. SUMMARY AND OUTLOOK

We have developed a real-time and finite-temperature Ginzburg-Landau theory for the BH model by applying the Schwinger-Keldysh formalism of a closed time-path reviewed in Sec. II. The perturbative hopping contributions for the free energy have been resummed via a Legendre transformation, yielding a large D expansion for the effective action. Therefore, we have been able not only to extract the phase boundary from the equations of motion (44), but also to calculate the excitation spectra in the SF phase: There, the particle-hole excitations from the MI phase turn smoothly into a gapped amplitude and a gapless phase mode. Surprisingly, we obtain reliable results even in the limit of small U , where our theory turns into the GP theory.

A comparison with a similar theory making use of imaginary times [15] has shown an unexpected mismatch due to the negligence of the imaginary part of the time-evolution contour. In the future this should be overcome by a new calculation which explicitly includes this imaginary path. Thereby, one should also be able to test our assumption that the Schwinger-Keldysh formalism, which neglects the imaginary part of the contour, describes a system at constant temperature. Neglecting temperature changes due to hopping, which is exact at $T = 0$ and a good approximation at low temperatures as encountered in the experiments, our theory already works in full agreement with the ITF. Therefore, it could, thus, be directly applied to BH Hamiltonians with time-dependent hopping parameters J , which are relevant in collapse and revival experiments [19]. Including a possible time dependence of U might be more problematic, but since the relevant quantity is J/U , we are able to keep U constant and put effectively all time dependencies into the hopping parameter [48]. As the Schwinger-Keldysh formalism is especially suited for treatment of such time-dependent perturbations, this generalization causes no further difficulties, but obviously a linearization of the equation of motion around an equilibrium is no longer possible. Applying suitable numerical methods, one should be able to solve the equations of motion and obtain nonequilibrium results with the formalism developed here.

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APPENDIX: CALCULATION OF THE CUMULANTS

As worked out in Sec. V, the equations of motion depend on the retarded and advanced two- and four-point cumulants. Written in the Keldysh basis, the retarded and advanced Green functions are given as averages of contour-ordered operator products, with one operator $\hat{O}^\Sigma$ and the rest of the operators $\hat{O}^\Delta$. If the Σ -indexed operator is an annihilation operator, we have the retarded function; otherwise, it is the advanced one. From this, it can be directly seen that advanced and retarded functions are linked via complex conjugation. We thus need to calculate explicitly only one of the two. Any cumulant decomposition of these functions necessarily involves $\langle \hat{T}_c \hat{O}^\Delta \hat{O}^\Delta \rangle$ or $\langle \hat{O}^\Delta \rangle$, both being 0, since they contain exclusively Δ -indexed operators. Therefore, the decomposition of the retarded (advanced) Green functions contains Green functions of lower order, and we do not have to distinguish between retarded (advanced) cumulants and the corresponding Green functions. However, we should note that the unperturbed cumulants are always local, whereas the unperturbed Green functions may also describe independent processes on distinct sites. In this Appendix, however, we completely suppress spatial variables and assume locality for all objects.

Starting with the two-point function, we first rewrite it by making use of the Heaviside step function,

$$\begin{aligned} G^{R(0)}(t_1; t_2) &= i \langle \hat{T}_c \hat{a}^\Sigma(t_1) \hat{a}^{\Delta\dagger}(t_2) \rangle_{\hat{H}_0} \\ &= i \theta(t_1 - t_2) \text{Tr}[e^{-\beta \hat{H}_0} \hat{a}(t_1) \hat{a}^\dagger(t_2) \\ &\quad - \hat{a}^\dagger(t_2) \hat{a}(t_1)] / \mathcal{Z}^{(0)}, \end{aligned} \quad (\text{A1})$$

where $\mathcal{Z}^{(0)} = \text{Tr} e^{-\beta \hat{H}_0}$. The traces are best calculated in the occupation number basis solving the eigenvalue problem,

$$\hat{H}_0 |n\rangle \equiv E_n |n\rangle, \quad (\text{A2})$$

where the energy eigenvalues are given by

$$E_n = \frac{U}{2} n(n-1) - \mu n. \quad (\text{A3})$$

The retarded Green functions can thus be written as

$$\begin{aligned} G^{R(0)}(t_1; t_2) &= i \theta(t_1 - t_2) \sum_{n=0}^{\infty} e^{-\beta E_n} [(n+1) e^{-i(E_{n+1}-E_n)(t_1-t_2)} \\ &\quad - n e^{-i(E_n-E_{n-1})(t_1-t_2)}] / \mathcal{Z}^{(0)}, \end{aligned} \quad (\text{A4})$$

with the partition function

$$\mathcal{Z}^{(0)} = \sum_{n=0}^{\infty} e^{-\beta E_n}. \quad (\text{A5})$$

To determine the Fourier transform of (A4) according to Eq. (38), we use the integral representation of the step function:

$$\theta(t_1 - t_2) = \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{i/2\pi}{x + i\epsilon} e^{-i(t_1-t_2)x} dx. \quad (\text{A6})$$

In the following we suppress the limit symbol for brevity. Furthermore, we make use of the Fourier representation of the Dirac δ function:

$$\delta(\omega_1 - \omega_2) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega_1 - \omega_2)t} dt. \quad (\text{A7})$$

Performing the substitution $t \equiv t_1 - t_2$, we get at first

$$\begin{aligned} G^{R(0)}(\omega_1; \omega_2) &= \delta(\omega_2 - \omega_1) \frac{-1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} e^{-\beta E_n} \int_{-\infty}^{\infty} \frac{dx}{x + i\epsilon} \\ &\quad \times \int_{-\infty}^{\infty} dt [(n+1) e^{-i(E_{n+1}-E_n-\omega_2+x)t} \\ &\quad - n e^{-i(E_n-E_{n-1}-\omega_2+x)t}]. \end{aligned} \quad (\text{A8})$$

Evaluating both integrals then yields the result

$$\begin{aligned} G^{R(0)}(\omega_1; \omega_2) &= 2\pi \delta(\omega_1 - \omega_2) \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} e^{-\beta E_n} \\ &\quad \times \left(\frac{n+1}{E_{n+1} - E_n - \omega_2 - i\epsilon} - \frac{n}{E_n - E_{n-1} - \omega_2 - i\epsilon} \right). \end{aligned} \quad (\text{A9})$$

To get the advanced two-point function, we must only replace the minus sign in front of the ϵ with a plus sign.

The procedure for calculating the retarded four-point function is much the same. At first we express it in terms of Heaviside functions:

$$\begin{aligned} C^{\Sigma\Delta\Delta\Delta}(t_1, t_2; t_3, t_4) &= \frac{-i}{2} \{ \theta(t_1 - t_2) \theta(t_2 - t_3) \theta(t_3 - t_4) \\ &\quad \times \langle [[[\hat{a}(t_1), \hat{a}(t_2)], \hat{a}^\dagger(t_3)], \hat{a}^\dagger(t_4)] \rangle_{\hat{H}_0} \\ &\quad + \theta(t_1 - t_3) \theta(t_3 - t_2) \theta(t_2 - t_4) \\ &\quad \times \langle [[[\hat{a}(t_1), \hat{a}^\dagger(t_3)], \hat{a}(t_2)], \hat{a}^\dagger(t_4)] \rangle_{\hat{H}_0} \\ &\quad + \theta(t_1 - t_3) \theta(t_3 - t_4) \theta(t_4 - t_2) \\ &\quad \times \langle [[[\hat{a}(t_1), \hat{a}^\dagger(t_3)], \hat{a}^\dagger(t_4)], \hat{a}(t_2)] \rangle_{\hat{H}_0} \}_{t_3 \leftrightarrow t_4}. \end{aligned} \quad (\text{A10})$$

Here, the symbol $t_3 \leftrightarrow t_4$ means that we still have to symmetrize the expression in these variables. Apart from a factor 2, it is identical to the usual definition of retarded n -point functions [40]. We define

$$2C^{\Sigma\Delta\Delta\Delta}(t_1, t_2; t_3, t_4) \equiv C^R(t_1, t_2; t_3, t_4). \quad (\text{A11})$$

Again, the thermal averages can be evaluated by tracing the operator products in the occupation number basis. Then the resulting expression is Fourier transformed in the same way as before when dealing with the two-point function. Since the number of different terms is much bigger now [44], we do not write them down explicitly. The whole function depends only

on time differences; thus one Fourier transformation leads to the Dirac function, $\delta(\omega_1 + \omega_2 - \omega_3 - \omega_4)$. From the Fourier representation of the three Heaviside functions, we now get three different infinitesimal frequency shifts $\pm i\epsilon_i$. The real part of the four-point function is found by setting all $\epsilon_i = 0$,

whereas the imaginary part is obtained by carefully taking the limits $\epsilon_i \rightarrow 0$. Since the knowledge of the latter is needed only for the spectral weights, and not for the spectrum itself, we only give here the real part of the four-point function, which has a relatively compact form:

$$\begin{aligned} \text{Re } C^R(\omega_1, \omega_2; \omega_3, \omega_4) = & -2\pi \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) \sum_{n=0}^{\infty} \frac{e^{-\beta E_n}}{\mathcal{Z}(0)} \\ & \times \left\{ \frac{n(n+1)}{(E_n - E_{n-1} - \omega_1)(E_{n+1} - E_n - \omega_4)} \left(\frac{1}{E_n - E_{n-1} - \omega_3} - \frac{1}{E_{n+1} - E_n - \omega_2} \right) \right. \\ & + \frac{n(n+1)}{(E_n - E_{n-1} - \omega_3)(E_{n+1} - E_n - \omega_1)} \left(\frac{1}{E_n - E_{n-1} - \omega_2} - \frac{1}{E_{n+1} - E_n - \omega_4} \right) \\ & + \frac{-(n+2)(n+1)}{(E_{n+1} - E_n - \omega_4)(E_{n+2} - E_n - \omega_1 - \omega_2)} \left(\frac{1}{E_{n+1} - E_n - \omega_1} + \frac{1}{E_{n+1} - E_n - \omega_2} \right) \\ & + \frac{n(n-1)}{(E_n - E_{n-1} - \omega_4)(E_n - E_{n-2} - \omega_1 - \omega_2)} \left(\frac{1}{E_n - E_{n-1} - \omega_1} + \frac{1}{E_n - E_{n-1} - \omega_2} \right) \\ & + \frac{2(n+1)^2}{(E_{n+1} - E_n - \omega_1)(E_{n+1} - E_n - \omega_2)(E_{n+1} - E_n - \omega_4)} \\ & \left. + \frac{-2n^2}{(E_n - E_{n-1} - \omega_1)(E_n - E_{n-1} - \omega_2)(E_n - E_{n-1} - \omega_4)} \right\}_{\omega_3 \leftrightarrow \omega_4, \omega_2 \leftrightarrow \omega_1}. \end{aligned} \quad (\text{A12})$$

If we wish to take the zero-temperature limit $\beta \rightarrow \infty$ in Eq. (A9) or (A12), we must note that there is one occupation number, n_0 , which represents the commensurate ground state of the unperturbed system, and thus $E_{n_0} < E_n$ for any integer $n \neq n_0$. By factoring out $e^{-\beta E_{n_0}}$ in the

Boltzmann sums in both the denominator and the numerator, all terms in the sum with $n \neq n_0$ remain with a factor $e^{-\beta(E_n - E_{n_0})} \rightarrow 0$ for $\beta \rightarrow \infty$. Thus only the term with $n = n_0$ is not suppressed and survives the zero-temperature limit.

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