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Superconductor-insulator phase transition in the boson Hubbard model

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We investigate the superconductor-insulator phase transition in the two-dimensional boson Hubbard system with short-range interactions. Fluctuations of *both* the phase and the amplitude of the superfluid order parameter are included in the determination of the phase diagram at zero and finite temperatures. The mean-field phase boundary is compared to quantum Monte Carlo results. We also calculate the frequency-dependent conductivity in the vicinity of the phase transition and find it universal at the multicritical point.

I. INTRODUCTION

Strong-coupling problems continue to be the focus of theoretical and experimental efforts in the last decade. Especially, puzzles in low dimensions and in the presence of disorder have attracted much attention recently. Parallel with the intensive thrust toward cracking the fermionic problems, there is an increasing appreciation of the relevance of the bosonic issues as well. This originates in part from the numerous experimental systems, the essence of which is adequately captured by bosonic physics, and in part from the many unresolved theoretical challenges.

The most intriguing experimental examples are helium in disordered media, such as in Vycor[1] and aerogel,[2] and disordered superconductors, of the homogeneously disordered[3] or granular[4] variety. The central phase transition in all of these systems is the (superconductor or superfluid)-to-insulator transition. This interest was further fueled by the recent discovery of a possibly universal critical resistance right *at* the phase boundary, which separates the insulating and superconducting phases in these systems.[5] Besides these, a very recently emerging field is that of the quantum spin glasses. A great part of the attention to these systems is due to the fact that a large variation in types of randomness, geometry, and symmetry classes is accessible both experimentally[6] and theoretically.[7,8]

At the same time, the ordered systems still hold many new surprises when longer-range interactions are included. These typically introduce frustration in the system and lead to unexpected new phases. Early on, it was realized that a coexistence of off-diagonal long-range order and diagonal long-range order may arise, leading to an exotic new phase, the "supersolid" regime in *XXZ*-type models.[9] Also, numerous types of frustrated Heisenberg models were introduced as they are expected to provide further insights into the nature of doped high-temperature superconductors. The many complexities of their phase diagrams have been explored just recently.[10,11] Simultaneously, data became available on genuinely new types of ordered systems as well. Complex new spin systems are argued to support some of the theoretically predicted exotic phases.[12] Also, advances in lithographic techniques enable experimentalists to create large-scale Josephson-junction arrays in the truly quantum regime and to study genuinely new, quantum phase transitions.[13]

This revival was induced in no small part by the comprehensive work of Fisher *et al.*[14] They provided arguments to determine qualitatively the phase diagram of the strongly correlated boson system, the so-called "boson Hubbard model." Motivated by earlier work,[15] they introduced several scaling arguments to determine the critical exponents in one dimension and to give bounds on them in higher dimensions. Many of their predictions have been borne out by numerical studies[16,17] and often compared favorably with experimental data as well.[1,3] However, analytic studies of the disordered models in higher dimensions have proved to be quite prohibitive to date. As mentioned above, a further intriguing experimental finding was that of a possibly universal resistance *at* the insulator-superconductor transition. This issue was recently attacked by calculating the resistivity at a special point of the phase boundary in the ordered model.[18] In that work several models related to the original one were studied which are expected to be in the same universality class. Recently, careful numerical studies on the disordered systems have provided further evidence in favor of a universal resistance at the transition, even though the actual value is quite different from the experimental numbers.[19,20]

In our work we concentrate on some questions which were left open in previous studies. Up to now, only a qualitative sketch of the phase diagram has been presented analytically. As several numerical studies of the phase diagram are available, a quantitative analytic determination of the phase boundaries and comparison with the data are clearly called for. This is what we perform in Sec. II, using the "coarse-graining" approximation.[21] We find a surprisingly good—better than 10%—quantitative agreement between quantum Monte Carlo (QMC) data and our results for the phase boundary. In Sec. III we calculate the frequency-dependent conductivity of the full boson Hubbard model in the vicinity of the transition everywhere along the phase boundary. At the multicritical point, we find a conductivity independent of the parameters of the original model. Section IV summarizes our results. The calculational details are given in the Appendixes.

II. COARSE-GRAINING PHASE DIAGRAM

We start with the boson Hubbard (BH) model on a two-dimensional square lattice with on-site Coulomb interactions only:

$$H=-\sum_i \mu\hat{n}_i+\tfrac{1}{2}V\sum_i \hat{n}_i(\hat{n}_i-1)-\tfrac{1}{2}J\sum_{\langle ij\rangle}(\hat{\Phi}_i^\dagger\hat{\Phi}_j+\text{H.c.})\ . \tag{1}$$

Here $\hat{\Phi}_i^\dagger$ ($\hat{\Phi}_i$) creates (annihilates) a charged boson on lattice site i and the chemical potential $\mu\geq 0$ controls the total number of bosons, $\sum_i\hat{n}_i=\sum_i\hat{\Phi}_i^\dagger\hat{\Phi}_i$. The hopping term is restricted to bonds between nearest-neighbor sites. In the absence of disorder, the boson system is either insulating or superconducting at $T=0$. The phase diagram can be sketched by starting with $J=0$.[14] In this limit every site is occupied by an integer number of bosons. For $n-1<\mu/V<n$, the boson occupation number is pinned at the integer value n. In this regime the system has an energy gap V against particle-hole excitations and hence a vanishing compressibility. Thus this state is a Mott-type insulator. Reintroducing $J>0$, the gain in kinetic energy by hopping the bosons around reduces and eventually overcomes the cost of the on-site repulsion. Therefore one expects that the energy gap will decrease with increasing J and correspondingly the insulating region on the μ/V-vs-J/V plane takes a lobelike shape, both of them vanishing at a critical value of J/V, where the boson states become extended.[16,22] Being at $T=0$, the system then certainly turns into a superfluid in this parameter region.

The critical phenomena related to the zero-temperature insulator-superconductor transition are driven by density fluctuations at a generic point of the phase boundary, with exponents computed in Ref. 3. At the tips of the lobes, however, the density is pinned at its commensurate value. Thus the phase fluctuations dominate and the critical behavior is that of an XY model in $d+1$ dimensions.[21]

In the following we show how the phase diagram can be mapped out quantitatively on the mean-field level. For this purpose we express the partition function of the boson Hubbard model as a coherent-state path integral[23] in imaginary times $0<\tau<\beta=1/T$ (in units where $k_B=\hbar=1$):

$$Z=\int\prod_i \mathcal{D}\Phi_i^*\mathcal{D}\Phi_i\exp[-(S_0+S_1)]\ , \tag{2a}$$

$$S_0=\int_0^\beta d\tau\sum_i[\Phi_i^*(\partial_\tau-\mu)\Phi_i+\tfrac{1}{2}V\Phi_i^*\Phi_i(\Phi_i^*\Phi_i-1)]\ , \tag{2b}$$

$$S_1=-\frac{J}{2}\int_0^\beta d\tau\sum_{\langle ij\rangle}(\Phi_i^*\Phi_j+\text{c.c.})\ . \tag{2c}$$

The complex c-number fields $\Phi_i(\tau)$ satisfy the periodic boundary condition $\Phi_i(\beta)=\Phi_i(0)$.

We choose the action S_0 to involve on-site terms only, and the hopping part will be treated as a perturbation. The standard procedure is to decouple the latter by a Hubbard-Stratonovich (HS) transformation.[21] As the order parameter for superfluidity manifests itself only in this hopping term, expanding in it is the correct way to build a Ginzburg-Landau effective action. Explicitly, we use

$$\exp(-S_1)=\int\mathcal{D}x_{\mathbf{q}}(\tau)\mathcal{D}x_{\mathbf{q}}^*(\tau)\exp\left[-\pi\int_0^\beta d\tau\sum_{\mathbf{q}}|x_{\mathbf{q}}(\tau)|^2+\int_0^\beta d\tau\sum_{\mathbf{q}}\sqrt{\pi J_{\mathbf{q}}}[x_{\mathbf{q}}^*(\tau)\Phi_{\mathbf{q}}(\tau)+\text{c.c.}]\right]\ . \tag{3}$$

Following the steps of the coarse-graining procedure[21] we perform a cumulant expansion of e^{-S_1} to leading order in the auxiliary HS fields $x_i(\tau)$. The expectation value $\langle x_i\rangle$ is linearly related to $\langle\Phi_i\rangle$, and the HS fields therefore serve as an order-parameter field for superfluidity. For the determination of the phase diagram, it is already sufficient to obtain the effective action to quadratic order in the order-parameter fields. The partition function to this order is given by

$$Z\simeq Z^{\text{CG}}=Z_0\int\mathcal{D}x_{\mathbf{q}}(\tau)\mathcal{D}x_{\mathbf{q}}^*(\tau)\exp\left[-\pi\int_0^\beta d\tau\sum_{\mathbf{q}}|x_{\mathbf{q}}(\tau)|^2+\pi\int_0^\beta d\tau\int_0^\beta d\tau'\sum_{\mathbf{q}}J_{\mathbf{q}}x_{\mathbf{q}}^*(\tau)x_{\mathbf{q}}(\tau')G(\tau-\tau')\right]\ , \tag{4}$$

where we have introduced the correlation function

$$G(\tau-\tau')=\langle\Phi_i^*(\tau)\Phi_i(\tau')\rangle_0=\frac{1}{Z_0}\int\mathcal{D}\Phi^*\mathcal{D}\Phi\ \Phi_i^*(\tau)\Phi_i(\tau')\exp(-S_0) \tag{5}$$

and Z_0 is the partition function for $J=0$. For a cubic lattice in d dimensions, the kinetic-energy dispersion is given by

$$J_{\mathbf{q}}=J\sum_{\mu=1}^{d}\cos(q_\mu)\ , \tag{6}$$

where we set the lattice constant equal to unity. For the calculation of the correlation function $G(\tau)$ with the Φ^4 action

Eq. (2b), we restrict the paths to Gaussian fluctuations in the "sombrero potential,"[24] i.e., around the saddle point Φ_0 of the action S_0, which is determined by $|\Phi_0|^2=\frac{1}{2}+\mu/V$. This approximate evaluation of $G(\tau)$ is most accurate for $\mu/V\gg 1$, that is, the steeper the minimum valley in the sombrero potential, i.e., for large boson numbers when charge fluctuations on a single site are small. We parametrize the boson fields by $\Phi(\tau)=[|\Phi_0|+A(\tau)]e^{i\varphi(\tau)}$. Then the quadratic part of the action for the phase and amplitude fluctuations around the saddle point takes the form

$$S_0^{\text{eff}}=-\frac{\beta V}{2}|\Phi_0|^4+|\Phi_0|\int_0^\beta d\tau\{2V|\Phi_0|A^2(\tau)+i[|\Phi_0|+2A(\tau)]\partial_\tau\varphi(\tau)\} \ . \tag{7}$$

In this representation the values of the phase which differ by integer multiples of 2π are equivalent; thus, the path integral for $G(\tau)$ also includes a summation over winding numbers as well,[25]

$$G(\tau-\tau')=\frac{1}{Z_0}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}d\varphi_0\int_{\varphi_0}^{\varphi_0+2\pi n}\mathcal{D}\varphi\int\mathcal{D}A\;\Phi^*(\tau)\Phi(\tau')\exp(-S_0^{\text{eff}}) \ . \tag{8}$$

Here we have dropped the site index as the different sites are decoupled by the HS transformation. As the phase and amplitude fluctuations are coupled, we have to calculate three separate contributions to the correlation function $G(\tau)$:

$$\begin{aligned}G(\tau)=&|\Phi_0|^2\langle e^{i[\varphi(\tau)-\varphi(0)]}\rangle_0\\&+|\Phi_0|\langle[A(\tau)+A(0)]e^{i[\varphi(\tau)-\varphi(0)]}\rangle_0\\&+\langle A(\tau)A(0)e^{i[\varphi(\tau)-\varphi(0)]}\rangle_0 \ .\end{aligned} \tag{9}$$

All three correlation functions can be straightforwardly computed with the quadratic action of Eq. (7). For brevity, we give here explicitly the result for the pure phase correlator only and present the complete expressions for the other correlation functions in Appendix A. We get

$$\langle e^{i[\varphi(\tau)-\varphi(0)]}\rangle_0=\frac{\vartheta_3(\pi[|\Phi_0|^2+\tau/\beta],q)}{\vartheta_3(\pi|\Phi_0|^2,q)}e^{-V\tau(1-\tau/\beta)/2} \ . \tag{10}$$

Here $q=\exp(-2\pi^2/\beta V)$ and $\vartheta_3(z,q)$ is the Jacobi theta function[26] defined by

$$\vartheta_3(z,q)=1+2\sum_{n=1}^{\infty}\cos(2nz)q^{n^2} \ , \tag{11}$$

which appears in Eq. (10) as a consequence of the winding-number summation. The analytic properties of the ϑ function guarantee the β periodicity of $G(\tau)$. Given $G(\tau)$, the partition function in the coarse-graining approximation is

$$Z^{\text{CG}}=Z_0\int d^2x_{\mathbf{q}}(\omega_\mu)\exp\left[-\frac{1}{\beta}\sum_{\mathbf{q}\mu}(1-J_{\mathbf{q}}G_\mu)|x_{\mathbf{q}}(\omega_\mu)|^2\right] \ . \tag{12}$$

The corresponding mean-field boundary to the superfluid phase is then determined from

$$0=1-J_{\mathbf{q}=0}G_{\mu=0}=1-Jd\int_0^\beta d\tau\,G(\tau) \ . \tag{13}$$

The (imaginary) time integral of the correlation function $G(\tau)$ can be analytically performed by applying Liouville's identity[26] for the ϑ functions or alternatively by the Poisson summation formula. The algebraic steps for the calculation of $G(\omega_\mu)$ are outlined in Appendix B

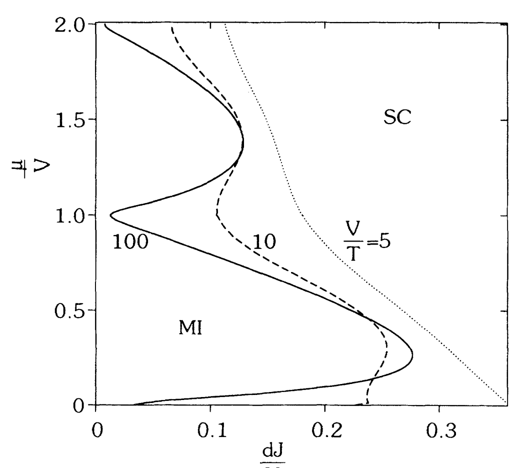

FIG. 1. Coarse-graining phase boundary for the Bose Hubbard model at the different temperatures $V/T=100$ (solid line), 10 (dashed line), and 5 (dotted line) between the Mott-insulating (MI) and superconducting (SC) phases. d is the dimension of the lattice.

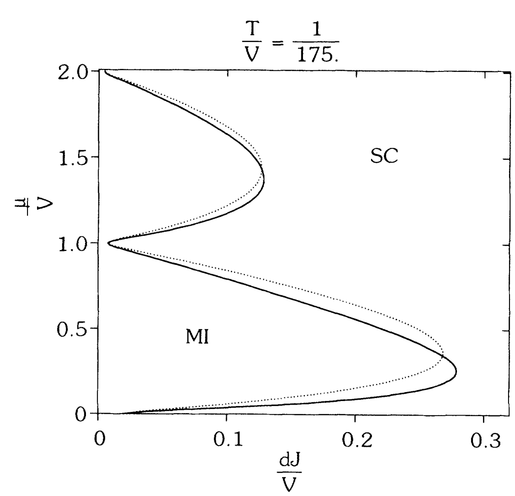

FIG. 2. Comparison between the phase boundaries with (solid line) and without (dotted line) the inclusion of amplitude fluctuations for a fixed temperature $T/V=\frac{1}{175}$.

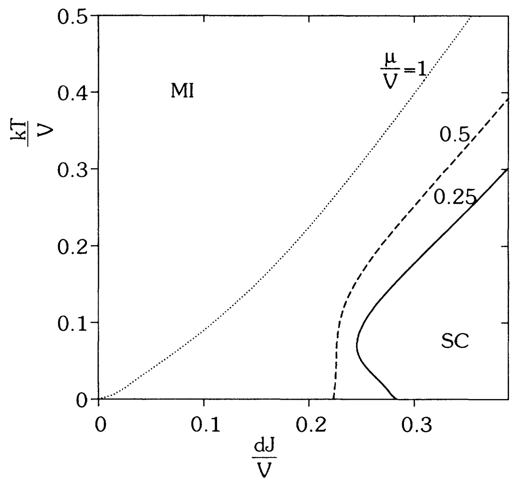

FIG. 3. Superconducting transition temperature vs dJ/V for different values of the chemical potential.

for the phase correlator.

In Fig. 1 we plot the resulting phase boundary in the μ/V-vs-J/V plane for different temperatures. For the lowest temperature, we clearly recognize the first two Mott-insulating lobes. In the zero-temperature limit, the superconducting phase extends in a cusplike shape down to a value of J, which vanishes linearly with temperature for all integer values of μ/V. The critical values of J/V at the tips of the lobes follow an envelope function which scales as $\sim 1/|\Phi_0|^2$. For $d=2$ the coarse-graining result for the critical value is given by $J_c/V=0.139$. QMC calculations on the same model[17] yield $J_c/V\approx 0.13$, a surprisingly good agreement.[27] Also, the asymmetric shape of the lobes is very similar to what was recently found in QMC calculations for the $d=1$ BH chain.[16,22] The asymmetry and in particular the downtilt of the lobes are actually enhanced by the amplitude fluctuations. This is shown in Fig. 2, where we compare the phase diagrams with and without the inclusion of amplitude fluctuations. We may contrast this result also to the analogously obtained results for pure quantum phase models. There the phase boundary appears perfectly periodic with respect to external offset charges, which play the same role as the chemical potential in the BH model.[28]

With increasing temperature the superfluid phase is expected to shrink, and indeed the lobelike structures are smoothened and the phase boundary is shifted to larger critical values of J/V. At the tips of the lobes, however, the temperature dependence is nonmonotonic. This is more clearly displayed in Fig. 3, which reveals the reentrant features at low temperatures. This behavior is the same as found in some early works on quantum phase models for Josephson-junction arrays.[29,30] Recently, it was also shown that the inclusion of Ohmic resistive processes enhances the phenomenon even further.[31] As this reentrant behavior was invoked[32] to account for the pronounced dip in the temperature dependence of the resistivity in samples close to the superfluid-insulator transition,[4] this issue should merit further investigation. Utilizing independent methods, such as QMC, is called for to decide whether or not fluctuations around the saddle point suppress this feature of the mean-field approximation.

III. CONDUCTIVITY NEAR THE INSULATOR SUPERCONDUCTOR TRANSITION

The coarse-graining approximation scheme that led us to derive the effective Ginzburg-Landau action [Eq. (4)] allows also for an explicit evaluation of the frequency-dependent conductivity. For the longitudinal component on the imaginary frequency axis $\sigma_{xx}(i\omega)$, we apply the general formula:[18,28,33]

$$\sigma_{xx}(i\omega)=-\frac{\hbar}{\omega}\sum_i\int_0^{\hbar\beta}d\tau\, e^{i\omega\tau}\frac{\partial^2 \ln Z}{\partial A_i^x(\tau)\partial A_0^x(0)}\Bigg|_{\mathbf{A}=0}. \tag{14}$$

(In this section we explicitly display $\hbar$ in all formulas in order to introduce later on the quantum unit of resistance $R_q=h/4e^2$.) The functional derivatives in Eq. (14) are with respect to a component of the vector potential in one of the space directions, say, x. The vector potential $\mathbf{A}$ is introduced by the usual Peierls description, which adds a phase factor to the hopping between nearest-neighbor sites:

$$J_{ij}\to J\exp\left[i\frac{e^*}{\hbar c}\int_i^j \mathbf{A}\cdot d\mathbf{l}\right], \tag{15}$$

where $e^*=2e$ is the charge of the lattice bosons. Using the functional-integral representation of the partition function from Eq. (2), it is straightforward to perform the derivatives, yielding the familiar result[18,34]

$$\sigma_{xx}(i\omega)=-\frac{4e^2}{\hbar\omega}\langle e^x_{\rm kin}\rangle-\frac{\hbar}{\omega}\sum_i\int_0^{\hbar\beta}d\tau\, e^{i\omega\tau}\langle j_i^x(\tau)j_0^x(0)\rangle . \tag{16}$$

The kinetic energy associated with links oriented in the x direction, $e^x_{\rm in}$, and the paramagnetic current density operator j_i^x are given in terms of the c-number Bose fields by

$$e^x_{\rm kin}=-\frac{J}{2N}\sum_i(\Phi_i^*\Phi_{i+x}+\text{c.c.}), \tag{17a}$$

$$j_i^x=i\frac{eJ}{\hbar}(\Phi_i^*\Phi_{i+x}-\text{c.c.}). \tag{17b}$$

Rewriting σ_{xx} explicitly in terms of the momentum and time-dependent Bose fields leads to

$$\sigma_{xx}(i\omega)=\frac{4e^2}{\hbar\omega}\left[\frac{1}{2N}\sum_{\mathbf{k}}J_{\mathbf{k}}\langle\Phi_{\mathbf{k}}^*(0)\Phi_{\mathbf{k}}(0)\rangle-\frac{1}{N}\sum_{\mathbf{k},\mathbf{q}}J^2\int_0^{\hbar\beta}d\tau\, e^{i\omega\tau}\sin k_x\sin q_x\langle\Phi_{\mathbf{k}}^*(\tau)\Phi_{\mathbf{k}}(\tau)\Phi_{\mathbf{q}}^*(0)\Phi_{\mathbf{q}}(0)\rangle\right]. \tag{18}$$

The frequency-dependent conductivity is then obtained by the usual analytic continuation $i\omega \rightarrow \omega + i\delta$. Clearly, if the bracket approaches a finite value as $\omega \rightarrow 0$, then the real part of $\sigma_{xx}(\omega)$ will contain a δ-function contribution implying a state with zero resistance.

The required correlation functions are most conveniently obtained if we use a generating functional by adding a fictitious time-dependent field term to the kinetic energy part of the action

$$S_1[\Phi] \rightarrow -\int_0^{\hbar\beta} d\tau \sum_{\mathbf{k}} [J_{\mathbf{k}} + v_{\mathbf{k}}(\tau)] \Phi_{\mathbf{k}}^*(\tau) \Phi_{\mathbf{k}}(\tau) \ . \tag{19}$$

Since the additional term only shifts the kinetic energy, the HS decoupling and coarse-graining procedure can still be performed with straightforward changes and the correlation functions follow from functional differentiation of the partition function of Eq. (3):

$$\langle \Phi_{\mathbf{k}}^*(0) \Phi_{\mathbf{k}}(0) \rangle = \frac{1}{Z^{\mathrm{CG}}} \frac{\delta Z^{\mathrm{CG}}}{\delta v_{\mathbf{k}}(\tau)} \bigg|_{v=0} , \tag{20a}$$

$$\langle \Phi_{\mathbf{k}}^*(\tau) \Phi_{\mathbf{k}}(\tau) \Phi_{\mathbf{q}}^*(0) \Phi_{\mathbf{q}}(0) \rangle = \frac{1}{Z^{\mathrm{CG}}} \frac{\delta^2 Z^{\mathrm{CG}}}{\delta v_{\mathbf{k}}(\tau) \delta v_{\mathbf{q}}(0)} \bigg|_{v=0} . \tag{20b}$$

While the result for the kinetic energy is immediately found to be

$$\langle e_{\mathrm{kin}}^x \rangle = -\frac{1}{2\beta N} \sum_{\mathbf{q}\mu} \frac{J_{\mathbf{q}} G_\mu}{1 - J_{\mathbf{q}} G_\mu} , \tag{21}$$

the result for the Φ^4 correlation function is considerably more complex. We find

$$\int_0^{\hbar\beta} d\tau\, e^{i\omega\tau} \langle \Phi_{\mathbf{k}}^*(\tau) \Phi_{\mathbf{k}}(\tau) \Phi_{\mathbf{q}}^*(0) \Phi_{\mathbf{q}}(0) \rangle = \frac{\delta_{\mathbf{kq}}}{4\beta} \sum_\mu \frac{G_\mu}{J_{\mathbf{k}}} \frac{1}{1 - J_{\mathbf{k}} G_\mu} \left[\frac{1 + J_{\mathbf{k}} G(\omega_\mu + \omega)}{1 - J_{\mathbf{k}} G(\omega_\mu + \omega)} + \frac{1 + J_{\mathbf{k}} G(\omega_\mu - \omega)}{1 - J_{\mathbf{k}} G(\omega_\mu - \omega)} \right] . \tag{22}$$

As a special property of the effective Ginzburg-Landau action, the momentum dependence of the correlation functions in Eqs. (21) and (22) is entirely determined through the tight-binding dispersion $J_{\mathbf{k}}$. As we show in Appendix C, it is precisely this property which allows us to verify the natural expectation that inside the Mott phase there should not be a δ-function contribution at zero frequency.

We can therefore focus on the finite-frequency behavior of the conductivity in the close vicinity of the insulator-superconductor transition. Here it is sufficient to perform a gradient expansion in the Ginzburg-Landau action. We expand G_μ to second order in frequency and introduce the coefficients $a_{\mathbf{k}}$, $b_{\mathbf{k}}$, and $c_{\mathbf{k}}$ by writing

$$1 - J_{\mathbf{k}} G_\mu \simeq a_{\mathbf{k}} - b_{\mathbf{k}} i\omega_\mu - c_{\mathbf{k}} (i\omega_\mu)^2 , \tag{23a}$$

$$a_{\mathbf{k}} = 1 - J_{\mathbf{k}} G_{\mu=0}, \quad b_{\mathbf{k}} = J_{\mathbf{k}} \frac{\partial G(z)}{\partial z} \bigg|_{z=0} , \tag{23b}$$

$$c_{\mathbf{k}} = \frac{1}{2} J_{\mathbf{k}} \frac{\partial^2 G(z)}{\partial z^2} \bigg|_{z=0} .$$

With the temporal gradient expansion, we can immediately perform the Matsubara frequency summations in Eqs. (21) and (22) by standard finite-temperature techniques. Omitting the algebraic details, we obtain, for the real part of the conductivity at $T=0$ after analytic continuation to the real-frequency axis,

$$\mathrm{Re}\sigma_{xx}(\omega) = R_q^{-1} \frac{\pi^2}{4N} \sum_{\mathbf{k}} \sin^2(k_x) \frac{J^2}{J_{\mathbf{k}}^2} \frac{1}{c_{\mathbf{k}}^2 A_{\mathbf{k}}^3} (1 + 3 b_{\mathbf{k}} A_{\mathbf{k}}) \times [\delta(\omega - 2A_{\mathbf{k}}) + \delta(\omega + 2A_{\mathbf{k}})] . \tag{24}$$

Here we introduced the short notation $A_{\mathbf{k}} = (b_{\mathbf{k}}^2/4 + a_{\mathbf{k}} c_{\mathbf{k}})^{1/2}$.

The result [Eq. (24)] reveals a charge excitation gap $\Delta = b_0/c_0$ for particle-hole excitations in the Mott insulator. On the phase boundary where $a_{\mathbf{k}=0}$ vanishes and for frequencies close above the Mott-Hubbard gap, only small momenta contribute to the sum in Eq. (24). Hence σ_{xx} can be evaluated explicitly to leading order in $\omega - \Delta > 0$. In two dimensions we find

$$\mathrm{Re}\sigma_{xx}(\omega)|_{\mathrm{PB}} = R_q^{-1} \frac{\pi}{8} \left[1 - \frac{\Delta^2}{\omega^2} \right] (1 + \tfrac{3}{2} b_0 \Delta) \theta(\omega - \Delta) , \tag{25}$$

which agrees with the leading-order results of Refs. 18 and 28. At the particle-hole symmetric points of the phase boundary where the transition occurs at fixed integer densities to the delocalized superfluid, the coefficient $b_{\mathbf{k}}$ vanishes. This is demonstrated in Appendix B as a special property of the boson-field correlation function $G(\tau)$. As a consequence, σ_{xx} is gapless at the tip and given by the universal number $\sigma^* = (\pi/8) R_q^{-1}$ in agreement with the results obtained by other groups.[18,28,35] This universal number is unique to two dimensions[36] and is a direct consequence of the vanishing "engineering" dimension of the conductivity. If we apply the same analysis to dimensions $d \neq 2$, we find σ^* to vanish for $d > 2$ and to be infinite in one dimension. The universal conductivity does not depend on the coefficients of the gradient expansion and is therefore insensitive to whether or not amplitude fluctuations of the boson fields are included in the effective Ginzburg-Landau action.

IV. CONCLUSION

In conclusion, we have provided an explicit calculation for the mean-field phase boundary between the Mott-insulating and superfluid phases of the short-range boson Hubbard model. The path-integral formulation of the coarse-graining procedure allows the treatment of phase and amplitude fluctuations on equal footing. As the critical properties of the quantum phase transition are governed by the density fluctuations at a generic point and by the phase fluctuations at the multicritical point, the simultaneous treatment of *both* of these contributions can only provide a complete picture. One expects an improvement in the quantitative agreement with other methods, e.g., quantum Monte Carlo results, and indeed we find that the two sets of data differ by less than 10%. We also computed the general expression for the frequency-dependent conductivity at zero temperature. We found a universal conductivity at the particle-hole symmetric multicritical point, in agreement with earlier work. We found that its value remained unaffected by the inclusion of the amplitude fluctuations. Qualitatively, new charge-ordered phases will appear if finite-range Coulomb interactions are included.[37] The related supersolid phenomena, however, require different mean-field techniques, and we are currently investigating those, together with the effects of truly long-range $1/r$ Coulomb interactions.

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APPENDIX A

The calculation of the $\langle \Phi^*(\tau)\Phi(0)\rangle$ correlation function involves also mixed amplitude and phase fluctuations as indicated in Eq. (9). With the action Eq. (7), they can be explicitly calculated and expressed in terms of Jacobi ϑ functions similar to the pure phase correlator. The two required mixed correlation functions are given by

$$\langle [A(\tau)+A(0)]e^{i[\varphi(\tau)-\varphi(0)]}\rangle_0 = -\langle e^{i[\varphi(\tau)-\varphi(0)]}\rangle_0 \frac{1}{V|\Phi_0|}\frac{\partial}{\partial\tau}\ln\vartheta_3\left[\pi\left[|\Phi_0|^2+\frac{\tau}{\beta}\right],q\right], \tag{A1}$$

$$\langle A(\tau)A(0)e^{i[\varphi(\tau)-\varphi(0)]}\rangle_0 = \langle e^{i[\varphi(\tau)-\varphi(0)]}\rangle_0 \frac{1}{4|\Phi_0|^2}\left\{\frac{1}{\beta V}+\left[\frac{1}{2}-\frac{\tau}{\beta}\right]^2+\frac{1}{V^2}\frac{1}{\vartheta_3(\pi|\Phi_0|^2,q)}\frac{\partial^2}{\partial\tau^2}\vartheta_3\left[\pi\left[|\Phi_0|^2+\frac{\tau}{\beta}\right],q\right]\right\}. \tag{A2}$$

Here $q = \exp(-2\pi^2/\beta V)$ is the same argument of the ϑ function as used in Eq. (10).

APPENDIX B

The Fourier transform of the Bose-field correlation function $G(\tau)$ is most conveniently calculated by applying the Poisson summation formula. It allows us to rewrite the Jacobi theta functions as

$$\begin{aligned}\vartheta_3\left[\pi|\Phi_0|^2,\exp\left[-\frac{2\pi^2}{\beta V}\right]\right] &= \sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} dx\,\exp(i2\pi x|\Phi_0|^2)\exp(i2\pi xm)\exp\left[-\frac{2\pi^2}{\beta V}x^2\right] \\ &= \sum_{m=-\infty}^{\infty}\left[\frac{\beta V}{2\pi}\right]^{1/2}\exp\left[-\frac{\beta V}{2}(|\Phi_0|^2-m)^2\right].\end{aligned} \tag{B1}$$

We consider here only the phase correlator of Eq. (10) and evaluate

$$G(\omega_\mu) = \frac{|\Phi_0|^2}{\vartheta_3(\pi|\Phi_0|^2,\exp(-2\pi^2/\beta V))}\int_0^\beta d\tau\,\vartheta_3\left[\pi\left[|\Phi_0|^2+\frac{\tau}{\beta}\right],\exp\left[-\frac{2\pi^2}{\beta V}\right]\right]\exp\left[-\frac{V\tau}{2}\left[1-\frac{\tau}{\beta}\right]\right]\exp(i\omega_\mu\tau). \tag{B2}$$

Applying Poisson's formula to both theta functions in Eq. (B2) makes the integral straightforward and the result is

$$G(\omega_\mu) = |\Phi_0|^2\sum_{m=-\infty}^{\infty}\exp\left[-\frac{\beta V}{2}\varphi_m^2\right]\frac{1-\exp[-\beta V(\varphi_m+\frac{1}{2})]}{V(\varphi_m+\frac{1}{2})-i\omega_\mu}\Bigg/\sum_{m=-\infty}^{\infty}\exp\left[-\frac{\beta V}{2}\varphi_m^2\right]. \tag{B3}$$

Here we used the short notation $\varphi_m = |\Phi_0|^2 - m = \frac{1}{2}+\mu/V-m$. This form clearly emphasizes the special role for integer values of μ/V, at which $G(\omega_\mu=0)$ diverges like $1/T$ in the low-temperature limit. This divergence is responsible for the $T=0$ cusps in the phase boundary between the different lobes. The periodicity with respect to μ/V, however, is not perfect because of the $|\Phi_0|^2$ prefactor, which is responsible for the downtilt and the shrinking of the lobes with increasing μ, i.e., increasing number of bosons. The amplitude correlators add similar structured but more involved terms to $G(\omega_\mu)$.

Equation (B3) also allows one to extract the properties of the coefficients in the temporal gradient expansion used in Sec. III for the calculation of the frequency-dependent conductivity. We find, e.g., for the linear coefficient $b_{\mathbf{k}}$ that $\partial G(z)/\partial z|_{z=0}$ diverges near integer values of $\mu/V=n$ and that it vanishes for $\mu/V=n+\frac{1}{2}$. At these points on the phase boundary, $\sigma_{xx}(\omega)$ is gapless. All these results still hold when the amplitude correlators are included in $G(\omega_\mu)$.

APPENDIX C

The general formula for the frequency-dependent conductivity in Eq. (18) shows that the weight of the δ function, which appears at $\omega=0$ after the analytic continuation to the real-frequency axis, vanishes if

$$\frac{1}{N}\sum_{\mathbf{k}} J\cos(k_x)\langle\Phi_{\mathbf{k}}^*(0)\Phi_{\mathbf{k}}(0)\rangle=\frac{1}{N}\sum_{\mathbf{k}} J^2\sin^2(k_x)\int_0^\beta d\tau\langle\Phi_{\mathbf{k}}^*(\tau)\Phi_{\mathbf{k}}(\tau)\Phi_{\mathbf{k}}^*(0)\Phi_{\mathbf{k}}(0)\rangle\ . \tag{C1}$$

In order to show that this relation holds, we perform a partial integration[18] with respect to $\cos(k_x)$. Since the correlation functions—evaluated by functional differentiation of the coarse-graining partition function—depend on the momentum only through $J_{\mathbf{k}}$, we have

$$\frac{1}{N}\sum_{\mathbf{k}} J\cos(k_x)\langle\Phi_{\mathbf{k}}^*(0)\Phi_{\mathbf{k}}(0)\rangle=\frac{1}{N}\sum_{\mathbf{k}} J^2\sin^2(k_x)\frac{\partial}{\partial J_{\mathbf{k}}}\langle\Phi_{\mathbf{k}}^*(0)\Phi_{\mathbf{k}}(0)\rangle\ . \tag{C2}$$

Applying Eq. (18), the interchange of partial and functional differentiation yields

$$\begin{aligned}\frac{\partial}{\partial J_{\mathbf{k}}}Z^{\mathrm{CG}}\langle\Phi_{\mathbf{k}}^*(0)\Phi_{\mathbf{k}}(0)\rangle&=\frac{\delta}{\delta v_{\mathbf{k}}(0)}\frac{\partial Z^{\mathrm{CG}}}{\partial J_{\mathbf{k}}}\bigg|_{v=0}=\frac{\delta}{\delta v_{\mathbf{k}}(0)}\int_0^\beta d\tau\frac{\delta Z^{\mathrm{CG}}}{\delta v_{\mathbf{k}}(\tau)}\bigg|_{v=0}\\&=\int_0^\beta d\tau\, Z^{\mathrm{CG}}\langle\Phi_{\mathbf{k}}^*(\tau)\Phi_{\mathbf{k}}(\tau)\Phi_{\mathbf{k}}^*(0)\Phi_{\mathbf{k}}(0)\rangle\ .\end{aligned} \tag{C3}$$

From this result Eq. (B1) immediately follows, proving the absence of a $\delta(\omega)$ contribution to the conductivity in the Mott phase.

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