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Particle-hole character of the Higgs and Goldstone modes in strongly-interacting lattice bosons

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We study the low-energy excitations of the Bose-Hubbard model in the strongly-interacting superfluid phase using a Gutzwiller approach. We extract the single-particle and single-hole excitation amplitudes for each mode and report emergent mode-dependent particle-hole symmetry on specific arc-shaped lines in the phase diagram connecting the well-known Lorentz-invariant limits of the Bose-Hubbard model. By tracking the in-phase particle-hole symmetric oscillations of the order parameter, we provide an answer to the long-standing question about the fate of the pure amplitude Higgs mode away from the integer-density critical point. Furthermore, we point out that out-of-phase symmetric oscillations in the gapless Goldstone mode are responsible for a full suppression of the condensate density oscillations. Possible detection protocols are also discussed.

Introduction. Ultra-cold atoms in optical lattices provide an ideal platform to explore the properties of strongly-interacting lattice systems. A prominent example of their capability to reproduce prototypical lattice Hamiltonians is given by the experimental realization of the Bose-Hubbard model [1–7]. Indeed, the superfluid to Mott insulator transition has been characterized at a very high level of accuracy, exhibiting an excellent agreement between experiments and theoretical predictions at zero [5, 8–11] and finite temperature [12–16]. The ground-state properties of the Bose-Hubbard model have been thoroughly investigated through time-of-flight imaging [5], measure of noise correlations [17] and single-site microscopy [18]. Excitations have been also addressed through tilting of the lattice [5], Bragg spectroscopy [19] and lattice depth modulation [8].

A very intriguing feature of the Bose-Hubbard model is the existence of a strongly-interacting superfluid phase. With respect to a weakly-interacting superfluid, a clear distinctive property of the superfluid close to the Mott lobes is the strong particle or hole character of the phonons. A further signature of strong correlations is the existence of gapped modes [20–23], in contrast to the weakly-interacting limit, where the gapless Goldstone mode exhausts all of the spectral weight. The measurement of the first gapped mode in the short wavelength limit using Bragg spectroscopy [24] and in the large wavelength limit using lattice modulation [25] has been recently reported. When the first gapped mode consists of a pure amplitude oscillation of the superfluid order parameter [26–32], it is granted the label of *Higgs mode*, in analogy with the Higgs boson in particle physics [23].

A pure amplitude mode, decoupled from the phononic phase mode, has been predicted to exist when the Bose-Hubbard model is effectively described by a relativistic $O(2)$ field theory, since an effective particle-hole symmetry ensures Lorentz invariance and the resulting de-

coupling of phase and amplitude degrees of freedom [20, 28, 33, 34]. This $O(2)$ theory describes both the vicinity of the critical point of the superfluid to Mott transition at integer filling in dimensions $d \geq 2$ and hard-core bosons at half-integer filling [35]. An important issue regards the fate of the Higgs mode away from criticality and towards the weakly-interacting regime [23]. To the best of our knowledge, no clear answer about this question has been provided yet.

In this Letter, we find an emergent particle-hole symmetry for the first gapped mode on a curve connecting two Lorentz-invariant points of the model, starting from the tip of the insulating lobes. This result relies on higher-energy excitations and provides an answer to the long-standing debate about the conditions of existence of a pure-amplitude *Higgs* mode in the Bose-Hubbard model away from criticality. Moreover, we show that a distinct particle-hole symmetry condition for the gapless Goldstone mode produces a suppression of the condensate density oscillations in proximity of the Mott lobes and, specifically, in correspondence to the boundary between particle and hole superfluidity. We speculate that such a suppression may be responsible for an increase in the critical temperature of the normal to superfluid transition.

Model and theory. We consider bosonic particles in a d -dimensional square lattice described by the Bose-Hubbard model

$$H = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + \text{H.c.}) + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i, \quad (1)$$

where J is the hopping amplitude, U the on-site interaction, μ the chemical potential, and $\langle i,j \rangle$ represents all pairs of nearest-neighboring sites. For large enough dimensions, e.g. $d = 3$, it is appropriate to study the excitations of the system by means of a time-dependent Gutzwiller ansatz $|\psi\rangle = \prod_i \sum_n c_{i,n}(t) |n\rangle_i$.

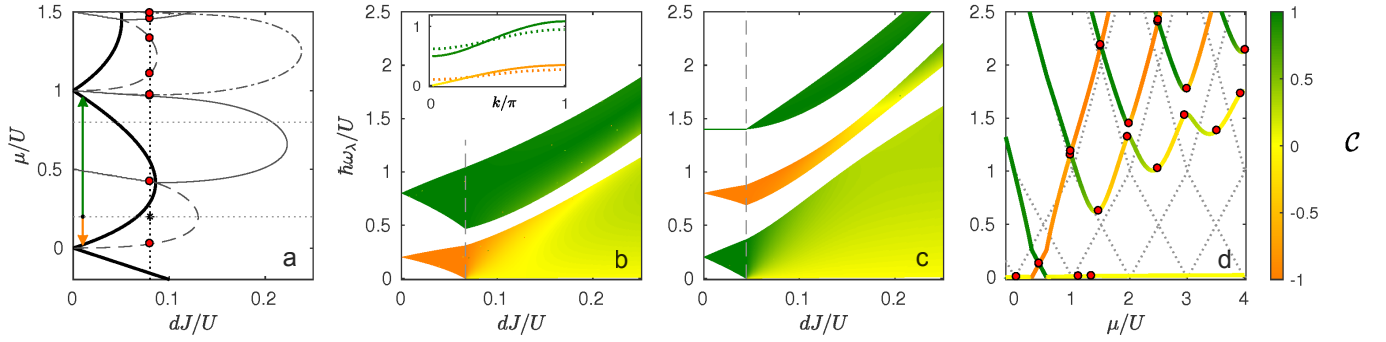


FIG. 1. (a) Mean-field phase diagram of the Bose-Hubbard model in $d = 3$ dimensions: thick lines are the Mott lobes. Single-particle (-hole) excitations in the Mott phase are indicated by the green (orange) arrows. Dashed, solid and dashed-dotted grey arcs indicate the condition of particle-hole symmetry $\mathcal{C} = 0$ at $\mathbf{k} \approx 0$ for the Goldstone, first and second gapped modes, respectively. (b,c) Lowest bands for $k = k_x = k_y = k_z$ as a function of dJ/U for $\mu/U = 0.2$ (b) and $\mu/U = 0.8$ (c) (see horizontal dotted lines in (a)). The vertical dashed line indicates the phase transition. Inset in (b): Excitation spectrum as a function of k/π in the strongly interacting superfluid at $dJ/U = 0.08$ and $\mu/U = 0.2$ (star in (a)) compared with the excitation spectrum in the Mott phase at $dJ/U = 0.04$ and $\mu/U = 0.2$ (dotted lines). In all figures, color code indicates the value of \mathcal{C} , quantifying the particle-hole character for each mode. Particle-hole symmetry is found when $\mathcal{C} = 0$. (d) Grey dotted lines $\pm m\mu/U$ are the m -holes (or m -particles) excitation energies in the Mott phase at $J = 0$. Thick lines: Excitation energies $\hbar\omega_{\mathbf{k},\lambda}/U$ for modes $\lambda = 1 \dots 4$ at $k = \pi/100$ along the vertical dotted line in (a), namely as a function of μ/U for $dJ/U = 0.08$. The points of particle-hole symmetry are highlighted by the red dots (see also (a)).

The coefficients $c_{i,n}(t)$ satisfy the equations of motion obtained from the Lagrangian $L[c, c^*] \equiv i\hbar \sum_{i,n} c_{i,n}^* \partial_t c_{i,n} - \langle H \rangle$. We define $c_{i,n}(t) = [\bar{c}_n + \delta c_{i,n}(t)] e^{-i\omega_0 t}$ [36–38], where \bar{c}_n are the ground state parameters, ω_0 describes the time dependence at equilibrium, and $\delta c_{i,n}(t)$ are the small oscillations with respect to the equilibrium configuration. Linearizing the equations of motion with respect to $\delta c_{i,n}(t)$ and introducing the Ansatz $\delta c_{i,n}(t) = u_{\mathbf{k},n} e^{i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k}} t)} + v_{\mathbf{k},n} e^{-i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k}} t)}$, one obtains Bogoliubov-like equations for the coefficient $u_{\mathbf{k},n}$ and $v_{\mathbf{k},n}$, which can be chosen to be real. To describe the excitations above the ground state, we select the solutions at positive energy $\omega_{\mathbf{k},\lambda} > 0$, where $\lambda = 1, 2, \dots$ identifies the different branches of the spectrum. The corresponding eigenvectors satisfy $\vec{u}_{\mathbf{k},\lambda} \cdot \vec{u}_{\mathbf{k},\lambda'} - \vec{v}_{\mathbf{k},\lambda} \cdot \vec{v}_{\mathbf{k},\lambda'} = \varepsilon \delta_{\lambda,\lambda'}$, with $\varepsilon > 0$. For practical convenience, we take $\varepsilon = 1$.

Given a certain observable A , an excitation λ produces a perturbation with respect to the ground state value $\delta A_\lambda = \langle A \rangle_\lambda - \bar{A}$, which we consider up to linear order in $\delta c_{i,n}$. For the order parameter $\psi_i = \langle a_i \rangle$, this reads

$$\delta \psi_{i,\lambda} = \mathcal{U}_{\mathbf{k},\lambda} e^{i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k},\lambda} t)} + \mathcal{V}_{\mathbf{k},\lambda} e^{-i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k},\lambda} t)}, \quad (2)$$

where

$$\begin{aligned} \mathcal{U}_{\mathbf{k},\lambda} &= \sum_n \sqrt{n+1} \left(\bar{c}_n u_{\mathbf{k},n+1}^{(\lambda)} + \bar{c}_{n+1} v_{\mathbf{k},n}^{(\lambda)} \right), \\ \mathcal{V}_{\mathbf{k},\lambda} &= \sum_n \sqrt{n+1} \left(\bar{c}_{n+1} u_{\mathbf{k},n}^{(\lambda)} + \bar{c}_n v_{\mathbf{k},n+1}^{(\lambda)} \right). \end{aligned} \quad (3)$$

The quantities $|\mathcal{U}_{\mathbf{k},\lambda}|^2$ and $|\mathcal{V}_{\mathbf{k},\lambda}|^2$ are the quasi-particle and quasi-hole excitation strengths, respectively [37, 38].

Particle-hole symmetry. For each mode and momentum, we define particle-hole symmetry the condition

$|\mathcal{U}_{\mathbf{k},\lambda}| = |\mathcal{V}_{\mathbf{k},\lambda}|$, identified by the zeros of the function $\mathcal{C} = (|\mathcal{U}_{\mathbf{k},\lambda}| - |\mathcal{V}_{\mathbf{k},\lambda}|) / (|\mathcal{U}_{\mathbf{k},\lambda}| + |\mathcal{V}_{\mathbf{k},\lambda}|)$ [39]. To understand the existence of lines of particle-hole symmetry, it is helpful to recall how the excitations in the Mott phase evolve into the phononic and gapped modes of the strongly-interacting superfluid [22]. In the weakly-interacting Bogoliubov regime, phonons present a strong particle and hole admixture. In contrast, close to the Mott lobes, the phononic excitations of the strongly-interacting superfluid inherit the pure particle or hole character of the Mott excitation that becomes gapless at the transition (see Fig. 1(a)). For negative (positive) doping with respect to integer filling, phononic excitations of the strongly-interacting superfluid appear with $|\mathcal{V}_{\mathbf{k},1}| \gg |\mathcal{U}_{\mathbf{k},1}|$ ($|\mathcal{U}_{\mathbf{k},1}| \gg |\mathcal{V}_{\mathbf{k},1}|$), indicating dominant hole (particle) character (see Fig. 1(b-c), respectively). At negative (positive) doping, the second lowest Mott excitation is gapped at the transition and is transformed into the first gapped mode of the superfluid phase, which conversely has particle (hole) character $|\mathcal{U}_{\mathbf{k},2}| \gg |\mathcal{V}_{\mathbf{k},2}|$ ($|\mathcal{V}_{\mathbf{k},2}| \gg |\mathcal{U}_{\mathbf{k},2}|$) (see Fig. 1(b-c), respectively).

It is instructive to realize that also higher excited modes inherit their particle-hole character from underlying pure m -particle and m -hole excitations (see Fig. 1(d)). The energy crossing between such excitations turn into anti-crossings due to the coupling introduced by a non-vanishing order parameter in the superfluid phase. The dominant particle or hole character from the underlying modes is retained, except in the vicinity of the anti-crossing points, where hybridization leads to a point of perfect particle-hole symmetry for each mode. In the weakly-interacting regime all excitations become particle-dominated. Hence, the regions of dominant hole-

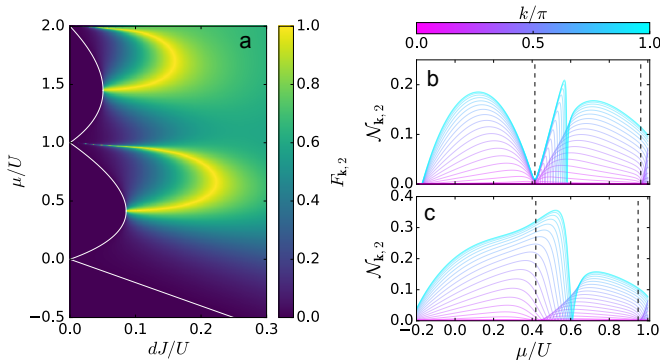


FIG. 2. (a) Flatness $F_{\mathbf{k},2}$ for the first gapped mode ($\lambda = 2$) as a function of dJ/U and μ/U for $k = k_x = k_y = k_z = \pi/100$; the bright yellow curves are the points where this mode corresponds to pure amplitude oscillation of the order parameter. As a reference, the white lines indicate the Mott to superfluid phase boundaries. (b) Density oscillation $\mathcal{N}_{\mathbf{k},2}$ as a function of μ/U for fixed $dJ/U = 0.0858$, corresponding to the tip of the lobe. (c) As in (b) for $dJ/U = 0.115$. Purple to light blue line color indicates k varying from 0 to π . Vertical dashed lines highlight the zeros of $\mathcal{N}_{\mathbf{k},2}$ at $k \approx 0$ (see (a)).

character are confined in the strongly-interacting superfluid regime and bounded by a line of perfect particle-hole symmetry ($\mathcal{C} = 0$, see grey curves in Fig. 1(a)). This picture highlights the role played by energetically-close excitations in determining the particle-hole symmetry condition for the different modes. In particular, the idea of particle-hole symmetry arising close to energy level crossings explains why particle-hole symmetry is recovered for all modes in the vicinity of the tip of the lobes (μ/U close to half-integer values) and at very small J/U and half-integer filling (μ/U close to integer values) (see Fig. 1(a,d)).

In the following, we are going to discuss how in-phase and out-of phase oscillations of the order parameter (namely the relative sign of $\mathcal{U}_{\mathbf{k},\lambda}$ and $\mathcal{V}_{\mathbf{k},\lambda}$) at the particle-hole symmetry condition determine profoundly-different physical properties of the two lowest-lying excitations [40].

Pure amplitude (Higgs) mode. A long-standing debate has taken place about the conditions for the existence of a gapped mode in the Bose-Hubbard model and its interpretation as a pure amplitude oscillation of the superfluid order parameter [23]. Due to this sought-after property, the first gapped mode is often referred to as Higgs mode. Within the linear approximation (see Eq. (2)), pure amplitude oscillations of the order parameter $\psi_{i,\lambda}$ are found when the imaginary part of $\delta\psi_{i,\lambda}$ vanishes, namely when $\mathcal{I}_{\mathbf{k},\lambda} = \mathcal{U}_{\mathbf{k},\lambda} - \mathcal{V}_{\mathbf{k},\lambda} = 0$. Conversely, vanishing real part ($\mathcal{R}_{\mathbf{k},\lambda} = \mathcal{U}_{\mathbf{k},\lambda} + \mathcal{V}_{\mathbf{k},\lambda} = 0$) corresponds to pure phase excitations of the order parameter. To quantify the amplitude and phase components of the oscillations of the order parameter in any mode λ , it is useful to define the

flatness parameter

$$F_{\mathbf{k},\lambda} = \frac{\mathcal{R}_{\mathbf{k},\lambda} - \mathcal{I}_{\mathbf{k},\lambda}}{\mathcal{R}_{\mathbf{k},\lambda} + \mathcal{I}_{\mathbf{k},\lambda}} \in [-1, 1]. \quad (4)$$

A positive flatness indicates a mode with dominant amplitude character and a negative flatness indicates a mode with dominant phase character.

In Fig. 2(a), we show the flatness of the first gapped mode ($\lambda = 2$) at small momentum $\mathbf{k} \approx 0$. This mode becomes purely amplitude-like ($F_{\mathbf{k},2} = 1$) on the clear yellow curve in the $(\mu/U, J/U)$ phase diagram. The pure amplitude Higgs mode emerges at the tip of each Mott lobe, where it is indeed expected to exist, but quickly moves towards larger fillings as J/U increases and bends back towards $J/U \rightarrow 0$ and μ/U integer. This behaviour confirms the expectations based on Fig. 1 and related discussion. We stress that the initial and final point of the curve $\mathcal{I}_{\mathbf{k},\lambda} = 0$ are Lorentz invariant points of the model.

Let us now define the density oscillations

$$\delta n_{i,\lambda} = 2\mathcal{N}_{\mathbf{k},\lambda} \cos(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k},\lambda}t), \quad (5)$$

with $\mathcal{N}_{\mathbf{k},\lambda} = \sum_n \bar{c}_n n(u_{\mathbf{k},n}^{(\lambda)} + v_{\mathbf{k},n}^{(\lambda)})$. In correspondence of the particle-hole symmetry condition $\mathcal{I}_{\mathbf{k},\lambda} = 0$, the continuity equation yields $\mathcal{N}_{\mathbf{k},\lambda} = 0$, as confirmed by our calculations (see Fig. 2(b,c)). This property identifies the pure amplitude character of a mode λ with an exchange of particles between the condensate and the normal fraction.

It is important to note that the pure amplitude character of the first gapped mode is obtained on slightly different curves depending on the momentum of the excitations. Moreover, the density response is significant only in the short wavelength limit and it is suppressed for $\mathbf{k} \rightarrow 0$ (see Fig. 2(b,c)). These facts should be taken into account when looking for the Higgs mode in possible experiments [24].

Suppression of condensate density oscillations in the Goldstone mode. Particle and hole excitations of equal amplitude but opposite sign ($\mathcal{R}_{\mathbf{k},\lambda} = \mathcal{U}_{\mathbf{k},\lambda} + \mathcal{V}_{\mathbf{k},\lambda} = 0$) [41] directly imply vanishing condensate density oscillations

$$\delta\rho_{c,i,\lambda} = \delta|\psi_{i,\lambda}|^2 = 2\mathcal{P}_{\mathbf{k},\lambda} \cos(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k},\lambda}t), \quad (6)$$

with $\mathcal{P}_{\mathbf{k},\lambda} = \bar{\psi}(\mathcal{U}_{\mathbf{k},\lambda} + \mathcal{V}_{\mathbf{k},\lambda})$. Vanishing condensate density oscillations are found on arc-shaped lines in the phase diagram in the vicinity of, and in particular below, each Mott lobe (dark blue curves in Fig. 3(a)). The suppression of $\delta\rho_c$ for mode $\lambda = 1$ occurs for distinct values \mathbf{k} on slightly different curves, which all lie above half-integer filling and end in the vicinity of the tip of the lobe (see Fig. 3(b,c)). Consistently, it will never be possible to satisfy the condition $\mathcal{R} = 0$ in the weakly-interacting limit, where the Goldstone mode alone exhausts the spectral function sum-rule $|\mathcal{U}_{\mathbf{k},1}|^2 - |\mathcal{V}_{\mathbf{k},1}|^2 = 1$.

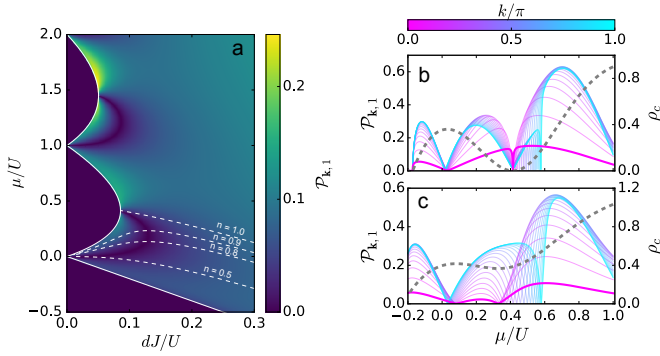


FIG. 3. (a) Amplitude of the condensate density fluctuations $P_{\mathbf{k},1}$ for the Goldstone mode ($\lambda = 1$) as a function of dJ/U and μ/U for $k = k_x = k_y = k_z = \pi/100$; Constant density $\bar{n} = 0.5, 0.8, 0.9, 1$ contours (white lines). (b) $P_{\mathbf{k},1}$ as a function of μ/U for fixed $J/U = 0.0858$, corresponding to the tip of the lobe. (c) As in (b) for $J/U = 0.115$. Purple to light blue line color indicates k varying from 0 to π . Grey dashed lines show the condensate density ρ_c in the ground state.

In the superfluid hydrodynamic regime, the condensate density oscillations of the Goldstone mode at low momenta couple only to the density oscillations $\delta\rho_c = (\partial\rho_c/\partial n)_J \delta n$. This equality has been numerically verified by independently calculating the oscillations $\delta\rho_c, \delta n$ at $\mathbf{k} \approx 0$ from Eqs. (5, 6) and the quantity $\partial\rho_c/\partial n$ in the ground state. Hence, the condensate density oscillations at $\mathbf{k} \approx 0$ vanish in correspondence of the maxima and the minima of the condensate density at constant J (see thick purple and dashed curves in Fig. 3(b,c)).

Remarkably, the suppression of condensate density oscillations at $\mathbf{k} \approx 0$ occurs at the boundary between particle and hole superfluidity, usually defined as $(\partial\mu/\partial J)_n = 0$ [38]. Indeed, the mean-field free energy per site Ω depends on the condensate density as $\Omega = -zJ\rho_c + \dots$, where $z = 2d$ is the coordination number in a hypercubic lattice. Using the thermodynamic relations $\mu = (\partial\Omega/\partial n)_J$ and $\rho_c = -(1/z)(\partial\Omega/\partial J)_n$, we obtain $(\partial\mu/\partial J)_n = -z(\partial\rho_c/\partial n)_J$.

Particularly interesting are the maximum of condensate density and the absence of condensate fluctuations found on the lower branch of each $\mathcal{R} = 0$ curve in Fig. 3(a). This suggests the presence of a condensate that is extremely robust against thermal fluctuations for temperatures smaller than the Goldstone mode bandwidth and, as a possible consequence, an increase of the normal to superfluid critical temperature. This conjecture is supported by a qualitative comparison with quantum Monte Carlo results [15] showing the critical temperature as a function of density at fixed J/U . In Ref. [15], for small J and filling smaller than unity, a maximum of critical temperature is found above half-integer filling, in apparent agreement with the particle-hole symmetry condition $\mathcal{R} = 0$ found in this work. Moreover, the fact that the maximum of the critical temperature

found in Ref. [15] is of the order of the hopping amplitude, namely, according to our calculation, smaller than the Goldstone mode bandwidth, validates an estimation of the critical temperature based on the thermal occupation of the Goldstone mode only. In this respect, the microscopic nature of the lowest-lying excitations and in particular their particle-hole symmetry seems to play a crucial role. From a broader perspective, these findings may be relevant to understand the influence of Mott physics (Mottness) on the low-temperature phase diagram of cuprates [42]. Indeed, recent experiments have shown that – among other effects [43] – at the optimal doping corresponding to the maximum of the superconducting dome, a transition from hole to particle transport [44] and a change in the charge transfer process [45, 46] occur.

Discussion. The unambiguous detection of particle-hole symmetry in the excitations of a strongly-interacting superfluid requires to independently resolve the amplitude and phase oscillations of the order parameter, or in other words, to reconstruct the single-particle Green's function in the laboratory. Pioneering experiments in this directions have been performed in the early days of Bose-Einstein condensation with two-pulse Bragg spectroscopy [47, 48]. One can also consider more sophisticated experimental techniques that are presently being developed, namely ARPES-like schemes [49, 50], or higher band Bragg spectroscopy [51]. Proposals of lattice-assisted spectroscopy to emulate a STM (Scanning Tunneling Microscopy) in ultra-cold atomic setups [52] and energy-resolved atomic scanning probes for the density of states [53] have also been recently put forward. Beyond ultracold atoms realizations, Higgs and Goldstone modes may appear in hybrid systems coupling Bose-Einstein condensates to optical cavities [54]. A more speculative possibility of quantum simulating the collective modes in the Bose-Hubbard model is offered by arrays of strongly-nonlinear optical or circuit-QED resonators [55–57], inspired by the recent realization of Mott insulator states of light [58]. In such optical systems, the full statistics of the quantum field is in fact directly accessible from a photoluminescence experiment [59].

Conclusions. In this Letter, we have discussed the emergent particle-hole symmetry of the low-energy excitations in the homogeneous Bose-Hubbard model. For the Goldstone mode, particle-hole symmetry induces a suppression of condensate density oscillations at the boundary between hole and particle superfluidity and a possible consequent increase of the normal to superfluid critical temperature. Most remarkably, particle-hole symmetry also allows us to predict a gapped pure-amplitude Higgs mode on a curve connecting the integer-density critical point (tip of the lobe) and the hard-core limit at half-integer density.

The particle-hole symmetry condition is met in the strongly-interacting superfluid when an excitation arises

ing from the Mott phase with predominant hole character acquires the predominant particle character typical of the weakly-interacting limit. In this sense, particle-hole symmetry relies on very general and fundamental properties of single-particle excitations. Future studies could be devoted to understand the impact of quantum corrections. On one hand, the development of a quantized theory for the excitations would allow one to investigate the effect of quantum and thermal fluctuations, to address the lifetime of the different excitation modes and to explore finite temperature physics. On the other hand, a whole new interesting regime is expected to arise when decreasing the dimensionality of the optical lattice. In this respect, since the single-site Gutzwiller approximation used in this work is not reliable in systems with a small coordination number, an improvement of our theory could be given by a cluster Gutzwiller approach [25, 60], which accounts for short-range quantum correlations also in two-dimensional lattices.

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