Temperature-dependent excitation spectra of ultra-cold bosons in optical lattices

T. A. Zaleski*, T. K. Kopéć
Institute of Low Temperature and Structure Research,
Polish Academy of Sciences, POB 1410, 50-950 Wroclaw 2, Poland

Trapping ultra-cold atoms in optical lattices provides a unique environment for investigating quantum phase transitions between strongly correlated superfluid and Mott insulator phases. However, one of the major complications in the analysis of experiments are criteria for identifying the superfluid phase. Sharp features occurring while entering ordered state have been recognized as a signature of superfluidity. Here, we show that sharp peaks are not necessarily a reliable diagnostic of phase coherence in these systems. Using the combined Bogoliubov method and the quantum rotor approach for phase variables, we calculate the momentum and energy-resolved single-particle spectral function at arbitrary temperature and its shape in the presence of the superfluid phase. We find that in the two-dimensional system even at $T > 0$, where condensate fraction vanishes, the remnants of the sharp coherence peak are present. In contrast, such a feature is not observed for the bosons loaded in the three-dimensional lattice.

I. INTRODUCTION

Loading of ultra-cold atoms into an optical lattice allows to study an “artificial solid” that is undisturbed by any imperfections present in real materials [1]. It also allows to investigate a regime of strong correlations, when the energy of interactions between particles overcomes their kinetic energy [2, 3]. For example, in the realm of condensed matter physics, they manifest, e.g., in optical excitation spectra, which shows spectral weight transfers connecting different energy scales [4]. In the discussion of photoemission on solids, and in particular on the correlated electron systems, the most powerful and commonly used approach is based on the Green’s-function formalism. In this context, the propagation of a single electron in a many-body system is described by the time-ordered one-electron Green’s propagator. A common approach in describing strong electron correlations is based on consideration of the Hubbard model [5, 6]. In the context of bosonic systems, these properties can be also studied in systems of ultra-cold gases in optical lattices via methods based on a response to scattering of photons: radio-frequency spectroscopy [7], Raman spectroscopy [8] and Bragg spectroscopy [9–11]. These experiments reveal the band structure of these systems, which can be used to compare the quantum phases with their condensed-matter counterparts. One key piece of evidence for the Mott insulator phase transition is the loss of global phase coherence of the matter wave function. However, there are many possible sources of phase decoherence in these systems. Substantial decoherence can be induced by quantum or thermal depletion of the condensate, so loss of coherence is not a proof that the system resides in the Mott insulator ground state. Although the initial system can be prepared at a relatively low temperature, the ensuing system after ramp-up of the lattice has a temperature which is usually higher due to adiabatic and other heating mechanisms. Recent experiments have reported temperatures on the order of $k_B T \sim 0.9 t$ where $t$, the hopping parameter, measures the kinetic energy of bosons [12]. At such temperatures, the effects of excited states become important, motivating investigations of the the finite temperature phase diagrams, showing the interplay between quantum and thermal fluctuations.

In the present paper we study combined effects of a confining lattice potential and finite temperature on the excitation spectra of the Bose-Hubbard model in two and three dimensions. The relevant part of the low-energy excited states involve one or two particles of the many-body ground-state and they are respectively connected to the momentum $k$ and energy $\omega$-dependent one-particle spectral function $A(k\omega)$, which describes the probability of removing a particle from the system and creating an excitation. This is precisely the quantity, which we want to study in the present paper. To this end, we perform calculations of the one-particle spectral function for the Bose-Hubbard model on the square and cubic lattice using a recently developed the quantum U(1) rotor approach [13]. The collective variables for phase are isolated in the form of the space–time fluctuating phase field governed by the U(1) symmetry. As a result interacting particles appear as a composite objects consisting of bare bosons with attached U(1) gauge fields. This allows us to write the boson Green’s function in the space-time domain as the product of the U(1) phase propagator and the bare boson correlation function. The problem of calculating the spectral line shapes now becomes one of determining the convolution of phase and bare boson Green’s functions.

The plan of the paper is as follows: first, in Section II we introduce the microscopic Bose-Hubbard model that is an accepted description of strongly interacting bosons in an optical lattice. Furthermore, in Sections III and IV we briefly present the used method and arrive at the expressions for the one-particle spectral function. This allows us to present in Section V the resulting excitation

*Corresponding author. Tel.: +48 713435021; fax: +48 713441029. E-mail address: t.zaleski@int.pan.wroc.pl (T.Zaleski).
spectra of bosons in two- and three-dimensional optical lattice and discuss the influence of the temperature on the shape of spectral lines and the presence of superfluid phase. Finally, we conclude and summarize our results in the final Section VI.

II. MODEL AND WAY OF TREATMENT

A. Hamiltonian

Ultra-cold bosonic atoms in move an in optical lattice within a tight-binding scheme. They are well described by the microscopic Bose-Hubbard Hamiltonian \[ \mathcal{H} \]. The atoms are neutral, so their interactions are realized via collision. This results in an on-site repulsion, which is responsible for inter-bosonic correlations. As a result, we consider a second quantized, bosonic Hubbard Hamiltonian in the form \[ \mathcal{H} = -t \sum_{ \langle \mathbf{r}, \mathbf{r}' \rangle } \left[ a^\dagger(\mathbf{r}) a(\mathbf{r}') + a^\dagger(\mathbf{r}') a(\mathbf{r}) \right] + U \sum_{ \mathbf{r} } n(\mathbf{r}) n(\mathbf{r}') , \] (1)

The hopping of bosons between neighboring lattice sites \( \mathbf{r} \) and \( \mathbf{r}' \) is described by the first term with tunneling element \( t \) and operators \( a^\dagger(\mathbf{r}) \) and \( a(\mathbf{r}') \), which create and annihilate bosons (thus, \( n(\mathbf{r}) = a^\dagger(\mathbf{r}) a(\mathbf{r}) \) is a boson number operator). Summation \( (\mathbf{r}, \mathbf{r}') \) runs over nearest neighbors of a regular two- (2D) or three-dimensional (3D) lattice. The on-site repulsion depending on the number of atoms occupying every lattice site is given by \( U \) term. Finally, the chemical potential \( \mu \) (with \( \mathcal{P} = \mu + U/2 \)) controls the total number of bosons introduced to the lattice (with \( N \) being the total number of lattice sites). The Hamiltonian and its modifications have been widely studied within the recent years using both analytical \[ 18-20, 21, 22 \] and numerical \[ 21, 22 \] methods.

B. Path integral formulation

The statistical sum of the system can be expressed in a path integral form with use of complex fields, \( a(\mathbf{r}\tau) \) depending on the imaginary time \( 0 \leq \tau \leq \beta = 1/k_B T \) (with \( T \) being the temperature)

\[ Z = \int [ \mathcal{D}\pi \mathcal{D}a ] e^{-S[\pi, a]} , \] (2)

where the action \( S \) is given by

\[ S[\pi, a] = \int_0^\beta d\tau \left[ \mathcal{H}(\tau) + \sum_{ \mathbf{r} } \pi(\mathbf{r}\tau) \frac{\partial}{\partial \tau} a(\mathbf{r}\tau) \right] . \] (3)

The complex fields \( a(\mathbf{r}\tau) \) satisfy the periodic condition \( a(\mathbf{r}\tau) = a(\mathbf{r}\tau + \beta) \). We use a recently proposed method based on a combination of Bogoliubov and quantum rotor approaches. Our way of treatment of the model has been presented in details in Ref. \[ 23 \], so here we restrict ourselves to listing the main steps only.

III. SINGLE-PARTICLE CORRELATION FUNCTION

In order to determine spectral properties of the model, it is necessary to determine the one-particle Green’s function of the system defined as:

\[ G(\mathbf{r} - \mathbf{r}'; \tau - \tau') = \langle a(\mathbf{r}\tau) a^\dagger(\mathbf{r}'\tau') \rangle_a , \] (4)

where statistical averaging

\[ \langle \ldots \rangle_a = \frac{1}{Z} \int [ \mathcal{D}\pi \mathcal{D}a ] \ldots e^{-S[\pi, a]} . \] (5)

The Green function can be expressed using Fourier transform:

\[ G(\mathbf{r}; \tau) = \frac{1}{\beta N} \sum_{ \mathbf{k}, m } G(\mathbf{k}\omega_m) e^{i\mathbf{k}\mathbf{r} + i\omega_m \tau} , \] (6)

where \( \omega_m = 2\pi m/\beta \) is Matsubara frequency with \( m \) being an integer value. The spectral function is defined as the imaginary part of the Green’s function:

\[ A(\mathbf{k}\omega) = 2\text{Im} G(\mathbf{k}; i\omega_m + \omega + i0^+) \] (7)

and relation of \( A(\mathbf{k}\omega) \) to the function given in Eq. (6) is established through the Hilbert transform:

\[ G(\mathbf{k}\omega_m) = -\int_{-\infty}^{+\infty} dw \frac{A(\mathbf{k}\omega)}{2\pi i\omega_m - \omega} . \] (8)

Furthermore, from the Eqs. (7) and (8) a sum rule appears:

\[ \frac{1}{N} \sum_{ \mathbf{k} } \int_{-\infty}^{+\infty} d\omega A(\mathbf{k}\omega) = 1 , \] (9)

which means that the spectral function is normalized. From the spectral function, one can extract the excitation spectrum and the strength of the excitation modes.

IV. INTRODUCTION OF PHASE VARIABLES

In order to advance calculations of the Green function in Eq. (4), we resort on the quantum rotor approach (see, Ref. \[ 12 \]) combined with the Bogoliubov method \[ 24 \] that has been recently proposed and successfully applied to systems of bosons in optical lattices. This scenario provides a picture of quasiparticles and energy excitations in the strong-interaction limit, where the transition between the superfluid and the Mott state is driven by phase fluctuations. The essence of the approach is the separation
of the original Bose field into its amplitude and fluctuating phase that was absent in the original Bogoliubov treatment. As a result, one arrives at a formalism where the one-particle correlation functions are treated self-consistently and permit us to investigate a whole range of phenomena described by the Bose-Hubbard Hamiltonian. Furthermore, the phase fluctuations are described within the quantum spherical model \[22\], which goes beyond the mean-field approximation, including both quantum and spatial correlations. The method is based on a local gauge transformation to the new bosonic variables:

\[ a(\mathbf{r}\tau) = b(\mathbf{r}\tau)e^{i\phi(\mathbf{r}\tau)}, \]

which allows extraction of the phase variable \( \phi(\mathbf{r}\tau) \), whose ordering naturally describes the superfluid–Mott-insulator transition, and the amplitude \( b(\mathbf{r}\tau) \), which is related to the superfluid density. As a result, the original Green’s function defined in Eq. (4) takes a form of a product of the phase and bosonic correlators:

\[ G(\mathbf{r}\tau;\mathbf{r}'\tau') = G_\phi(\mathbf{r}\tau;\mathbf{r}'\tau')G_b(\mathbf{r}\tau;\mathbf{r}'\tau'), \]

which are defined as:

\[ G_b(\mathbf{r}\tau;\mathbf{r}'\tau') = \langle b(\mathbf{r}\tau)b(\mathbf{r}'\tau') \rangle_b, \]

\[ G_\phi(\mathbf{r}\tau;\mathbf{r}'\tau') = \langle e^{i\phi(\mathbf{r}\tau)-i\phi(\mathbf{r}'\tau')} \rangle_\phi. \]

In the Fourier space the relation in Eq. (11) becomes:

\[ G(\mathbf{k}\omega_m) = \frac{1}{\beta N} \sum_{\mathbf{k}',\omega_{m'}} G_b(\mathbf{k}'\omega_{m'}\omega_m)G_\phi(\mathbf{k}-\mathbf{k}',\omega_m-\omega_{m'}), \]

where the spectral decomposition of each constituent in Eq. (13) is given by:

\[ G_x(\mathbf{k}\omega_m) = -\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{A_x(\mathbf{k}\omega)}{i\omega_m - \omega}, \]

with \( x = b, \phi \). Furthermore, we separate the bosonic amplitude \( b(\mathbf{r}\tau) \) into the condensed \( b_0 \) and non-condensed \( b_d(\mathbf{r}\tau) \) part, following the Bogoliubov approach\[24\]:

\[ b(\mathbf{r}\tau) = b_0 + b_d(\mathbf{r}\tau). \]

The superfluid order parameter becomes:

\[ \Psi_B \equiv \langle a(\mathbf{r}\tau) \rangle = b_0\psi_B, \]

where \( \psi_B \) is the phase order parameter defined as:

\[ \psi_B = e^{i\phi(\mathbf{r}\tau)}. \]

As a result, the spectral function corresponding to the original Green’s function in Eq. (7) can be expressed as follows:

\[ A(\mathbf{k}\omega) = b_0^2A_\phi(\mathbf{k}\omega) + \psi_B^2A_b(\mathbf{k}\omega) \]

\[ -\frac{1}{N} \sum_{\mathbf{k}'} \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} A_b(\mathbf{k}'\omega')A_\phi(\mathbf{k}-\mathbf{k}';\omega-\omega') \]

\[ \times \left[ \frac{1}{e^{-\beta\omega} - 1} - \frac{1}{e^{-\beta(\omega-\omega')} - 1} \right], \]

where the first and the second terms represent macroscopic ordered states resulting from emergence of bosonic Bogoliubov amplitude \( b_0 \) and phase order parameter \( \psi_B \), respectively. They will lead to appearance of sharp coherence peaks in the excitation spectrum for non-zero values of \( b_0 \) and \( \psi_B \). The last is the remaining disordered part of the spectrum. The spectral functions \( A_b(\mathbf{k}\omega) \) and \( A_\phi(\mathbf{k}\omega) \) can be written explicitly following our earlier work (see, Ref. [13] for details):

\[ A_b(\mathbf{k}\omega) = E_{\pm}(\mathbf{k})\delta(\omega - E_k) - E_{-}(\mathbf{k})\delta(\omega + E_k) \]

\[ A_\phi(\mathbf{k}\omega) = \frac{\pi}{\Xi(\mathbf{k})} \left\{ \delta \left[ \frac{\omega}{U} + v \left( \frac{\pi}{U} \right) - \Xi(\mathbf{k}) \right] - \delta \left[ \frac{\omega}{U} + v \left( \frac{\pi}{U} \right) + \Xi(\mathbf{k}) \right] \right\}, \]

where:

\[ E_k = 2\sqrt{t(\varepsilon_0 - \varepsilon_k)(t(\varepsilon_0 - \varepsilon_k) + Ub_0^2)} \]

\[ E_{\pm}(\mathbf{k}) = 2\pi \left\{ \frac{2t(\varepsilon_0 - \varepsilon_k) + Ub_0^2}{2E_k} \pm \frac{1}{2} \right\} \]

\[ \Xi(\mathbf{k}) = \sqrt{\frac{\delta\lambda}{U} + \frac{2t}{U^2}b_0^2(\varepsilon_0 - \varepsilon_k) + v^2 \left( \frac{\pi}{U} \right)}. \]

Furthermore, \( v(x) = x - |x| - \frac{1}{2} \), with \( |x| \) being the floor function (giving the greatest integer bigger or equal to \( x \)) and the Bogoliubov amplitude \( b_0 \) can be determined \[22\]:

\[ b_0^2 = \frac{4t}{U} + \frac{\pi}{U}. \]

Next, \( \delta\lambda \) is the parameter, which arises in the quantum rotor treatment \[12, 13\] that measures “the distance from criticality” in the high-temperature phase (\( \delta\lambda = 0 \) at the critical point and in the ordered, low-temperature phase). Values of \( \delta\lambda \) (in the disordered phase) and the phase order parameter \( \psi_B \) (in the ordered phase) and are given by the equation (see, Ref. [13]):

\[ 1 - \psi_B^2 = \frac{1}{\beta N} \sum_{\mathbf{k}} \coth \left\{ \frac{\beta U}{4\Xi(\mathbf{k})} \left[ \Xi(\mathbf{k}) - v \left( \frac{\pi}{U} \right) \right] \right\} \]

\[ + \frac{1}{\beta N} \sum_{\mathbf{k}} \coth \left\{ \frac{\beta U}{2} \left[ \Xi(\mathbf{k}) + v \left( \frac{\pi}{U} \right) \right] \right\}. \]

Finally, the lattice structure factor in Eq. (20) is defined as

\[ \varepsilon_\mathbf{k} = \frac{1}{2} \sum_{\mathbf{d}} e^{i\mathbf{kd}}. \]
The spectrum is gapless, with two narrow coherence lines: the inner one results from the presence of non-zero Bogoliubov amplitude, while the outer reflects existence of the phase-ordered phase. The remainder of the spectrum is smeared and comes from incoherent (although strongly interacting) atoms. The increase of interactions between atoms $t/U$ leads to growth of phase fluctuations, which ultimately destroy the superfluid phase and drive the system into the Mott insulator. However, as temperature increases, thermal fluctuations melt away both the superfluid and Mott-insulating phases, introducing the normal phase $\rho_B = 0$.

A. Two-dimensional system

In the two-dimensional system the long-range phase order occurs only at zero temperature (see, Fig. 2). Any increase of the temperature destroys the superfluid phase ($\rho_B = 0$). This results in immediate disappearance of sharp coherence peak associated with the phase order parameter, however value of $\delta\lambda$ is small so the gap at $k = 0$ is not noticeable. Surprisingly, in higher temperatures the peak seems to be restored, although it is now a part of the incoherent particle spectrum resulting from convolution of phase and bosonic spectral functions (see, Fig. 3). Finally, further increase of the temperature leads to the peak being replaced by a dip. The temperature evolution of the peak is presented in Fig. 4 (its coordinates in the momentum space have been denoted by a red circle in Fig. 4). As a result, in two-dimensional system there is an evidence of the quasi long-range phase order in finite temperatures. Another influence of thermal fluctuations on excitation spectra visible in Fig. 3 is smearing around the inner edges of bands (for low values of $|\omega/U|$). Because the effect is subtle, additional energy cuts have been presented in Figs. 5-8 (and similar figures for the three-dimensional system in the following section).

B. Three-dimensional system

The evolution of the excitation spectra with increasing temperature in the three-dimensional system is presented in Figs. 5-8. At $T = 0$, for chosen values of $t/U = 0.045$ and $\mu/U = 0.5$, the system is in the superfluid state, which is signaled by presence of both coherence peaks: resulting from non-zero Bogoliubov amplitude $b_0$ and long-range phase order ($\psi_B \neq 0$). With the temperature being raised, the weight of the phase order peak decreases (see, Fig. 6), and at criticality it disappears completely (see, Fig. 7). Above the critical temperature, a gap opens at $k = 0$. However, it may become hidden, since thermal fluctuations also smear the inner edges of the bands, thus filling the gap with long tails of the decaying bands (see, Fig. 8).
VI. CONCLUSIONS

The present paper extends our previous work (see, Ref. [13]), which examined the excitation spectra at $T = 0$ to finite temperatures. For the bosonic system in optical lattice, as temperature increases, thermal fluctuations melt away both the superfluid and Mott-insulating phases, introducing the normal phase. We have determined the combined effects of two and three dimensional lattice potential trapping and temperature for a system of strongly interacting bosons on several lattice structures. In order to understand the properties of cold atoms in optical lattices, we examined the dependence of momentum and energy-resolved excitation spectra on the temperature. We showed that the general effect of thermal fluctuations was twofold: first, the weight of the coherence peaks resulting from the phase ordering being decreased with raising temperature. Second, there was smearing of the inner edges of one-particle bands tending to fill the excitation gap. However, in the two dimensional system,
was recreated (though this time it did not signal the superfluid phase). As a result, the existence of the sharp peaks in the excitation spectra may not necessarily be a reliable diagnostic tool of long-range order in these systems. This is similar to results of Kato, et al. who showed that sharp peaks in the time-of-flight experiments are not an unequivocal proof of superfluidity [25]. On the other hand, in the present paper, the three-dimensional system

in which the long-range ordered state exists only at zero temperature, in the finite temperatures the sharp peak

was recreated (though this time it did not signal the superfluid phase). As a result, the existence of the sharp peaks in the excitation spectra may not necessarily be a reliable diagnostic tool of long-range order in these systems. This is similar to results of Kato, et al. who showed that sharp peaks in the time-of-flight experiments are not an unequivocal proof of superfluidity [25]. On the other hand, in the present paper, the three-dimensional system

did not exhibit any remnants of the phase-order coherence peak above the critical temperature. This fact that may have important consequences for long range properties in lower dimensions. The quantitative values for the excitation spectra presented here provide benchmarks for continuing efforts to emulate the Bose-Hubbard model on optical lattices, and demonstrate consistency between strongly interacting atoms and phenomena observed in condensed-matter systems.

Acknowledgments

We would like to acknowledge support from the Polish National Science Centre (Grant No. 2011/03/B/ST3/00481).

[1] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature 415, 39 (2002).
[2] I. Bloch, Nat. Phys. 1, 23 (2005).
[3] I. Hen and M. Rigol, Phys. Rev. A 82, 043634 (2010).
[4] T. K. Kopeć, Phys. Rev. B 67, 014520 (2003).
[5] J. Hubbard, Proc. Roy. Soc. A 276, 238 (1963).
[6] N. F. Mott, Metal-insulator transition (Taylor and Francis, London, 1990).
[7] J. T. Stewart, J. P. Gaebler, D. S. Jin, Nature 454, 744 (2008).
[8] T.-L. Dao, A. Georges, J. Dalibard, C. Salomon, and I. Carusotto, Phys. Rev. Lett. 98, 240402 (2007).
[9] S.B. Papp, J. M. Pino, R. J. Wild, S. Ronen, C. E. Wie- 
man, D. S. Jin, and E. A. Cornell, Phys. Rev. Lett. 101, 135301 (2008).
[10] D. Clément, N. Fabbri, L. Fallani, C. Fort, and M. In- 
guscì, New J. Phys. 11, 103030 (2009).
[11] P. T. Ernst, S. Götze, J. S. Krauser, K. Pyka, D.-S. Lühmann, D. Pfannkuche, and K. Sengstock, Nature Phys. 6, 56 (2010).
[12] T. P. Polak and T. K. Köpec, Phys. Rev. B 76, 094503 (2007).
[13] T. A. Zaleski, Phys. Rev. A 85, 043611 (2012); J. Phys. B: At. Mol. Opt. Phys. 45, 145303 (2012).
[14] K. Jimenez-Garcia, R. L. Compton, Y.-J. Lin, W. D. Phillips, J. V. Porto, and I. B. Spielman, Phys. Rev. Lett. 105, 110401 (2010).
[15] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and 
P. Zoller, Phys. Rev. Lett. 81, 3108 (1998).
[16] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B 40, 546 (1989).
[17] S. Sachdev, Quantum Phase Transitions (Cambridge University Press, Cambridge, 1999).
[18] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B 40, 546 (1989).
[19] J. K. Freericks, H. R. Krishnamurthy, Y. Kato, N. Kawashima, and N. Trivedi, Phys. Rev. A 79, 053631 (2009).
[20] T. P. Polak and T. K. Köpec, J. Phys. B 42, 095302 (2009).
[21] C. Kollath, A. M. Läuchli, and E. Altman, Phys. Rev. 
Lett. 98, 180601 (2007).
[22] B. Capogrosso-Sansone, S. G. Söyler, N. Prokof’ev, and 
B. Svistunov, Phys. Rev. A 77, 015602 (2008).
[23] T. A. Zaleski and T. K. Köpec, Phys. Rev. A 84, 053613 (2011).
[24] N. N. Bogoliubov, J. Phys. (USSR) 11, 23 (1947) [Izv. 
Academii Nauk USSR 11, 77 (1947)].
[25] T. Vojta, Phys. Rev. B 53, 710 (1996).
[26] T. A. Zaleski and T. K. Köpec, J. Phys. A: Math. Theor. 43, 425303 (2010).
[27] K. W. Mahmud, E. N. Duchon, Y. Kato, N. Kawashima, 
R. T. Scalettar, and N. Trivedi, Phys. Rev. B 84, 054302 (2011).
[28] Y. Kato, Q. Zhou, N. Kawashima, and N. Trivedi, Nature 
Phys. 4, 614 (2008).