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Conductivity of Strongly Correlated Bosons in the Simple Cubic Lattice — Magnetic Field and Hopping Anisotropy Effects

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We investigate optical conductivity in three dimensional system of bosons under strong magnetic field. In particular, we consider Bose Hubbard model in the strongly correlated limit, where Mott insulator phase emerges. For chosen rational number of magnetic flux per cell we show that response of the system gains complex peaks behavior on the order of frequency corresponding to on-site boson repulsive interaction. Moreover, when anisotropy in hopping energy for the direction parallel to magnetic field is tuned up, the non-monotonous behavior of the optical conductivity could appear. The obtained results can be experimentally probed in the system of ultracold atoms loaded on an optical lattice.

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1. Introduction

Response of the system to the external perturbation is one of the fundamental problems in condensed matter physics. One of such an example is an optical conductivity for strongly correlated bosonic systems [1–5]. Importance of bosonic description lays in its wide application to the currently investigated materials like high T_c superconductors [6, 7] or ultracold atoms loaded on an optical lattice [8]. Moreover the response became highly non-trivial when we additionally subject to the system strong magnetic field, what was in the past years widely investigated experimentally, e.g. Josephson Junction arrays [9, 10] or ultracold atoms [11, 12].

In this paper, we focus on the linear response theory for the Bose Hubbard model (BHM) in three dimensions where strong magnetic field plays an important role. For Mott insulator phase we show, that presence of the Hofstadter spectrum [13] split by boson interaction energy, causes the pronounced consequences in the optical conductivity spectra, where only the intra Hofstadter band transitions are allowed [5]. In particular, complex peak behavior appears dependening on the strength of external magnetic field. We compare our results with the case in which magnetic field is absent.

Moreover, we investigate anisotropy effects introduced in hopping energy. We show, that anisotropy effects have the largest influence on the system where magnetic field is non zero. In addition, the optical conductivity could depend on anisotropy in non-monotonous way. This kind of consideration, where tuning of kinetic energy of bosons is needed, could be successfully tested in ultracold atoms on an optical lattice [2, 14].

2. Theoretical description

The Bose Hubbard model is defined by the Hamiltonian

$$H = -\sum_{\langle ij\rangle} \left(J_{ij} e^{j\frac{e^*}{\hbar c} \int_j^i \mathbf{A}_0 \cdot dl} \hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right) - \mu \sum_i \hat{n}_i$$
(1)

where J_{ij} is hopping energy (non-zero only between adjacent sites), U — onsite repulsion energy, μ — chemical potential, exp $\left(i\frac{e^*}{\hbar c}\int_j^i A_0 \cdot dl\right)$ — Peierls factor with vector potential A_0 . The presence of bosons on the lattice is described by annihilation (creation) of boson on site iby using operator \hat{b}_i (\hat{b}_i^{\dagger}). Further in formulas below, we only display electric charge of boson e^* (speed of light c, lattice spacing a and reduced Planck constant \hbar we set to 1).

In the following, we consider uniform magnetic field B, resulting from Landau qauge $A_0 = B(0, x, 0)$, which is perpendicular to the *xy*-plane. To simplify notation, we introduce $f = Ba^2e^*/hc = p/q$, i.e. f counts number of magnetic fluxes per unit cell [13].

In order to investigate optical conductivity (OC) in the zero temperature limit for the Mott insulator phase, as a starting point we use formula for the real part of OC derived in Ref. [5], namely

$$\operatorname{Re}\sigma_{xx}^{\boldsymbol{A}_{0}}(\omega) = 2\pi^{2}\sigma_{Q}\sum_{\alpha}\sum_{s=\{+,-\}}\Xi_{q}^{\alpha}\left[u^{s}(\omega);p\right],\qquad(2)$$

$$\Xi_{q}^{\alpha}\left[v;p\right] = \frac{J}{U} \frac{n_{0}(1+n_{0})}{\left(\omega/U\right)^{2}\sqrt{4n_{0}(1+n_{0})+\left(\omega/U\right)^{2}}}\rho_{q,2D}^{\alpha}(v;p), \quad (3)$$

$$u^{\pm}(\omega) = \frac{U}{J} \left(2n_0 + 1\right) \left(1 \mp \sqrt{1 - \frac{1 - \left(\omega/U\right)^2}{\left(2n_0 + 1\right)^2}}\right), \quad (4)$$

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Fig. 1. Frequency dependent conductivity for different value of magnetic strength f and anisotropy η . f = 0 case is plotted with J/U = 0.02 and f = 1/2, 1/3, 1/4 is plotted with J/U = 0.03.

where in comparison to Ref. [5] we rewrite expression for OC to another form. This expression has been obtained in the approximation, where only the intra Hofstadter band transitions are taken into account [5]. Moreover, n_0 is an integer number which is equal to the average boson density per site in Mott insulator state, $\sigma_Q = (e^*)^2/h$ is a quantum conductance and $\rho_{q,2D}^{\alpha}(v;p)$ is weighted density of states for conductivity in two dimension with definition

$$\rho_{q,2D}^{\alpha}(v;p) = \frac{1}{N} \sum_{\boldsymbol{k}} \left[\partial_{k_x} \epsilon_q^{\alpha}(\boldsymbol{k};p) \right]^2 \delta\left(v - \epsilon_q^{\alpha}(\boldsymbol{k};p)/J \right), \tag{5}$$

where $\epsilon_q^{\alpha}(\mathbf{k}; p)$ is a tight binding dispersion energy, enumerated by $\alpha = 0, 1, ..., q - 1$. This dispersion depends on magnetic wave vector $\mathbf{k} = (k_x, k_y)$ and magnetic field strength f and could be explicitly derived from Harper's equations [13]. Next, to study OC in three dimensional cubic lattice, two dimension dispersion $\epsilon_q^{\alpha}(\mathbf{k}; p)$ in Eq. (5) should be replaced by $\epsilon_q^{\alpha}(\mathbf{k}; p) - 2J_z \cos k_z$, what consequently changes weighted density of states for conductivity (DOSc)

$$\rho_{q,3D}^{\alpha}(v;p) = \frac{1}{NL} \sum_{\boldsymbol{k}k_z} \left[\partial_{k_x} \left(\epsilon_q^{\alpha}(\boldsymbol{k};p) - 2J_z \cos k_z \right) \right]^2 \\ \times \delta \left(v - \epsilon_q^{\alpha}(\boldsymbol{k};p) / J + 2\eta \cos k_z \right) =$$

$$\int \mathrm{d}E\rho_{1D}(E)\rho_{q,2D}^{\alpha}(v+E;p),\tag{6}$$

where

$$\rho_{1D}(E) = \frac{1}{N_z} \sum_{k_z} \delta\left(E - 2\eta \cos k_z\right) \tag{7}$$

is a density of states for one dimension $(k_z \text{ is a wave vector})$. As we see in Eq. (7), we introduce anisotropy constance in z-direction which is denoted by $\eta = J_z/J$.



Fig. 2. Anisotropy dependence of conductivity at $\omega = U$ for different values of external magnetic field f. We set J/U = 0.02.

3. Results and discussion

Particle-hole excitations in Mott insulator phase appear, when energy subjected to the system is comparable to on-site interaction energy U. This implies that linear response of the system like OC, shows energy gap (Fig. 1a). The physical situation is similar when the strong external magnetic field is applied to the system but the shape of the response becomes non-trivial.

In particular, orbital magnetic field, introduced by Peierls factor, causes that kinetic energy of bosons acquires complex behavior. This is explicitly seen in the tight binding energy dispersion, which from well-known form $-2J(\cos k_x + \cos k_y) - 2J_z \cos k_z$ of the three dimensional cubic lattice in the absence of magnetic field f = 0, change to $\epsilon_q^{\alpha}(\mathbf{k}; p) - 2J_z \cos k_z$ where magnetic fields is present $f \neq 0$. Then, the $\epsilon_q^{\alpha}(\mathbf{k}; p)$ part of this single particle energy emerges in OC as a rich peaks structure in terms of frequency. This effect is clearly visible in Fig. 1a, e, i, m (which behavior is very similar to the quasi-three dimensional system containing for example 60 xy-layers, Ref. [15]).

It is also interesting to notice from Fig. 1a, e, i, m, that Hofstadter spectra with tiny peaks at the edges of the band [13] (see, e.g. 1/4 case), generate small OC response above Mott insulator gap, what in real experiment could give confirmation of reacher structure of tight binding dispersions.

Going further we see, that the orbital magnetic field effects are more pronounced when we study hopping anisotropy in the z-direction, i.e. when we go from $\eta = 1$ to $\eta < 1$. We plot this results for f = 1/2, 1/3, 1/4 in Fig. 1 with different non-isotropic value of anisotropy parameter, $\eta = 0.6, 0.3, 0.03$. Consequently, it is seen, that sub-band structure presented in two dimensional system is gradually approached [5].

For comparison, we plot optical conductivity for three dimensional system when magnetic field is absent (Fig. 1a, b, c, d), which shows that its qualitative behavior is almost intact when we change anisotropy factor η .

Moreover, analyzes of magnetic field and hopping anisotropy effects reveals also unusual behavior in OC spectra. Namely, we observe that for chosen value of magnetic field the OC could depend on anisotropy in nonmonotonous way. This is clearly seen in Fig. 2 where we set $\omega = U$ and f = 1/4. Here, we choose point $\omega = U$ because it should be easily accessible in ultra cold atoms experiments where parameters J and U are tunable with high precision [8]. Furthermore it is valuable to stress that the strength of the response at $\omega = U$ is lower for non-zero amplitude of magnetic field. One of the possible explanation of this effect could be assigned to the spectral weight transfer beyond the center of the band in comparison to the f = 0 case, what is seen in single particle density of states [13]. All the above results should be available experimentally in ultracold gases loaded on an optical lattice. Firstly, Mott phase was realized in such systems more than ten years ago [8]; Secondly, possible measurements of OC are under current theoretical interest, i.e. using phase modulation of the lattice [2] or by center of mass oscillation [4].

4. Summary

We have analyzed optical conductivity in Bose Hubbard model using linear response theory. In particular, strongly correlated bosons in three dimensional cubic lattice were investigated. We have shown that the response of the system above Mott insulator gap gains complex peaks behavior in comparison to the case when magnetic field is absent. Moreover, we have analyzed anisotropy in the kinetic energy of bosons, where we show that optical conductivity, for given frequency and strength of magnetic field, could have non-monotonous dependence.

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