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Spectral Weight Of Excitations In Bose Hubbard Model

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Abstract. We obtain excitation spectra in the superfluid and the Mott Insulator phases of Bose Hubbard model near unit filling within Random Phase Approximation (RPA) and calculate its spectral weight. This gives a transparent description of contribution of each excitation towards the total Density of States (DOS) which we calculate from these spectral weights.

Keywords: Bose Hubbard Model, Phase transitions, Excitations.
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INTRODUCTION

Great control and flexibility over ultracold gases loaded in optical lattice has led itself as a important tool to study quantum phase transitions in precise way [1]. Bosonic gases in such lattice are described by Bose-Hubbard Models, which predicts many novel phases including much studied superfluid (SF) and Mott-insulating (MI) phases. These models have received great interest ever since proposal and experimental realization of Bose Hubbard model [2,3]. Varity of theoretical techniques like Quantum Monte Carlo, DMRG, mean field theory have been employed to study its phase diagram and excitations. These are in good agreement with each other.

Although great amount of work has been done on calculating excitations and density of states (DOS) of these excitations for this model, a proper description of spectral weight of each excitation and its contribution towards DOS is lacking. In this letter we obtain excitations within Random Phase Approximation (RPA) within mean felid theory of Bose Hubbard Model and calculate the spectral weight for each of them. Further we calculate Density of States corresponding to each of these excitations. In next section we give model and method of calculation. In final section we present the results obtained**.**

MODEL AND METHOD

Model describing bosons in optical lattice is given by

$$H = -t\sum_{\langle i,j\rangle}(a_i^{+}a_j + h.c) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i \qquad (1)$$

where t is the hopping amplitude and summation $<i,j>$ runs over all the nearest neighboring sites. $a^{+}_i(a_i)$ and n_i are, respectively, the boson creation (annihilation) and number operators at site i. U is the onsite repulsion strength and μ is chemical potential.

Mean Field Theory

Hamiltonian (1) can be solved by using mean field approximation which reduces the full Hamiltonian into summation over single site Hamiltonian [4]. This is done by writing creation (annihilation) operators as a average value and fluctuations, i.e. $a_i=<a_i>+\delta a_i$ ($a^{+}_i=<a^{+}_i>+\delta a^{+}_i$). Introducing superfluid order parameter $\psi=<a_i>$, Hamiltonian (1) can be re-written as $H = \sum_i H_i^{MF} - t\sum_{<ij>}(\delta a_i^{+}\delta a_j + H.C)$ where

$$H_i^{MF} = -zt(a_i^{+} + a_i)\psi + \frac{U}{2}n_i(n_i - 1) - \mu\, n_i + zt\psi^2$$

and z is the coordination number of the lattice. We scale all parameters by setting $zt=1$. Mean field Hamiltonian is solved by operating it on number basis $|0>,|1>...|n_{max}>$ and calculating ψ self-consistently. Here n_{max} is maximum number of bosons allowed per site to truncate the single site Hilbert space and it depends on onsite interaction U and μ. This gives us eigen energies E_α and eigen states $|i\alpha>$ of the single site Hamiltonian. The boson density $\rho=<n_i>$ is calculated from the ground state. Non-zero order parameter ψ shows a superfluid phase whereas vanishing order parameter with integer ρ predicts Mott insulating phase. Phase diagram is plotted in Figure (1) where we focused near density $\rho=1$.

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Excitations within Random Phase Approximations

The excitations are obtained from the single particle Green's Function defined by $g_{i,j}(t) = -i\theta(t)\langle[a_i(t), a^+{}_j(0)]\rangle$ where $\theta(t)$ is Heaviside step function. We construct standard basis operator [5] using the mean field states; we define $L^i_{\alpha\alpha'}=|i\alpha><i\alpha'|$. The single particle Green's function can be written as $g_{i,j}(t) = \sum_{\alpha\alpha'\beta\beta'} T^{ij}_{\alpha\alpha'\beta\beta'} G^{ij}_{\alpha\alpha'\beta\beta'}(t,)$ where $T^{ij}_{\alpha\alpha'\beta\beta'}=<i\alpha|a^+{}_i|i\alpha'><j\beta|a_j|\beta'>$ and $G^{ij}_{\alpha\alpha'\beta\beta'}(t) = -i\theta(t)\langle[L^i_{\alpha\alpha'}(t), L^j_{\beta\beta'}(0)]\rangle$. We solve equation of motion for $G^{ij}{}_{\alpha\alpha'\beta\beta'}$ within Random Phase Approximation and Fourier transforming it into momentum and energy space, we get

$$(\omega - E_\alpha + E_{\alpha'})G_{\alpha\alpha'\beta\beta'}(k,\omega) = \frac{1}{2\pi}P_{\alpha\alpha'}\delta_{\alpha\beta'}\delta_{\beta\alpha'} + \varepsilon_k P_{\alpha\alpha'}\sum_{\mu\nu}\breve{T}_{\alpha\alpha'\nu\mu}G_{\mu\nu\beta\beta'}(k,\omega)$$

where $P_{\alpha\alpha'}=< L_{\alpha\alpha}>-< L_{\alpha'\alpha'}>$, $\breve{T}_{\alpha\alpha'\beta\beta'}= T_{\alpha\alpha'\beta\beta'}+ T_{\beta\beta'\alpha\alpha'}$ and $\varepsilon_k = -\frac{1}{3}\sum_{j=x,y,z}\cos(\pi k_j)$

Solving the equation of motion for the Green function and writing it in the form

$$g_{\alpha\alpha'\beta\beta'}(k,\omega) = \sum_i \frac{A_i'(k)}{\omega - \omega_i(k)} \qquad (2)$$

we get excitation spectra $\omega_i(k)$ and its spectral weights $A'_i(k)$. Summation i runs for all excitations. Density of states for each excitation $\omega_i(k)$ is calculated by $N_i(\omega) = -\frac{1}{\pi}\sum_k \mathrm{Im}[g_i(k,\omega^+)]$ where $\omega^+ = \omega + i\delta$; we have added small complex part to ω. Results of these calculations have been shown in the next section.

RESULTS

The phase diagram of model (1) near unit density is shown in Figure (1). We choose few characteristic points shown in the figure by red dots to obtain the excitations. For example excitations at point (a) (density ρ=0.5) in Figure (1) are plotted in the Figure (2). Here we choose $k_y=k_z=0$ and plot excitations as function of k_x. First particle (green line) and hole (blue line) excitations are gapless consistent with the SF nature of the phase. The first gapped particle (red line) excitation has finite weight, however first gapped hole (orange line) excitation has almost zero weight. This is because for ρ=0.5 it is easy to create particle excitation than hole excitation. In all cases we see that spectral weights for excitations near to k_x=0 are dominant and it reduces as we increase k_x. We have not shown particle and hole excitations which have zero spectral weights.

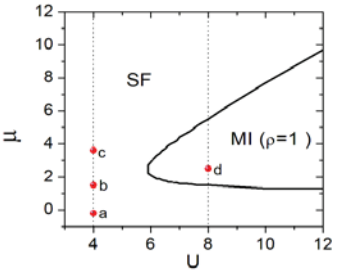

FIGURE 1. Mean field phase diagram of model (1) near unit density. Red dots are the points where excitations are calculated and presented below.

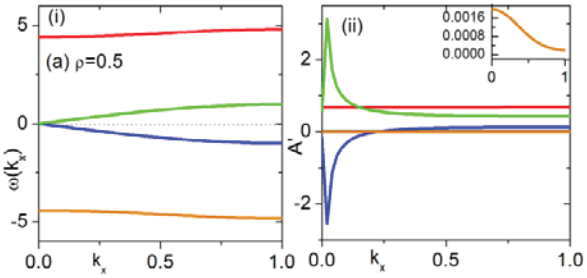

FIGURE 2. (i) Excitation spectra for point (a) in figure (1). (ii) represents corresponding spectral weights. Excitation and corresponding spectral weight are represented by same coloured line. (inset) Weight for lowest hole excitation.

Density of States (DOS) for each of these excitations, using the same colour coding, is plotted in figure (3).

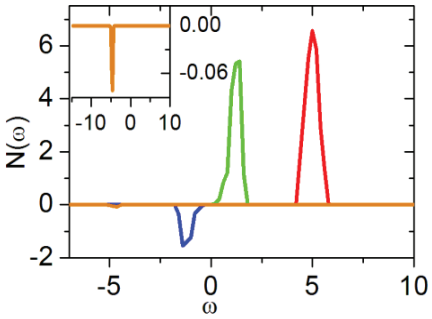

FIGURE 3. DOS of excitations of figure (2).

Similar plots for points (b) (with ρ=1.04) and (c) (ρ=1.5) are given in figure (4). As we increase the density, but continue to be in the SF phase, several higher excitations contributes to the DOS since the spectral weight of these excitations are finite. Both particle and hole excitations contributes significantly.

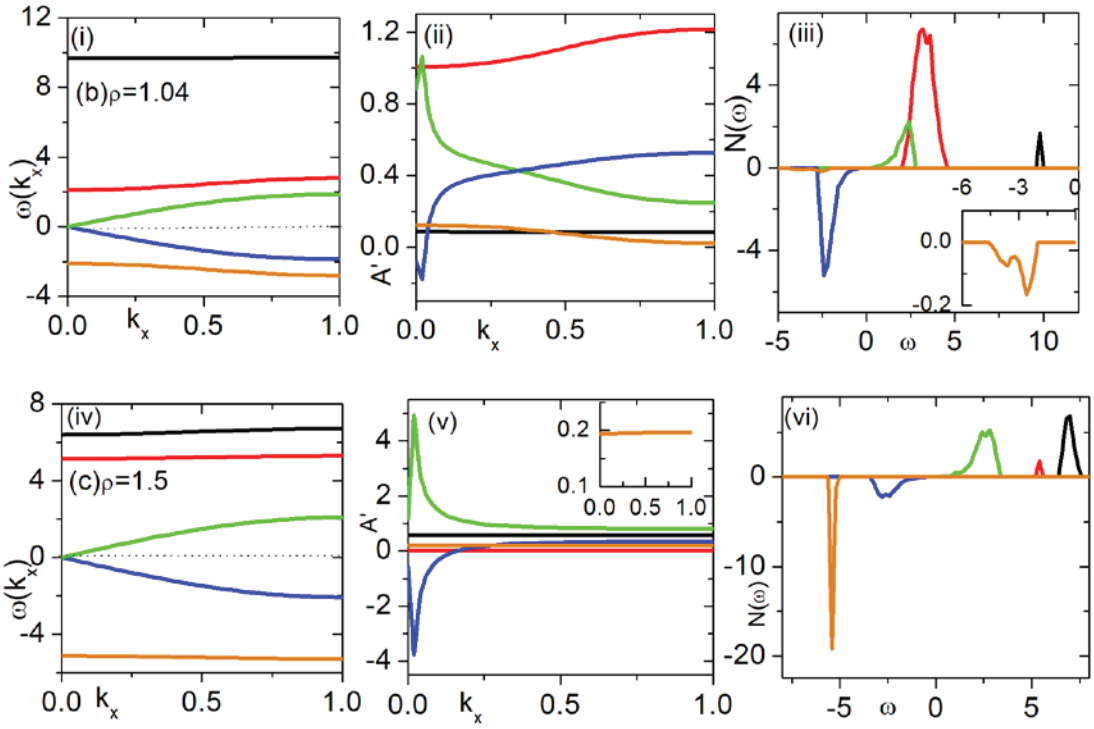

FIGURE 4. Excitations (i) and (iv), their spectral weights (ii) and (v) and DOS (iii) and (vi), respectively, for density ρ=1.04 (point (b) in figure (1)) and ρ=1.5 (points (c) in figure (1)).

For Mott insulator, near the lower edge of lobe (point (d)), the excitations and their weights are given in figure (5). Both particle and hole excitations have finite gap. Hole excitation has smaller gap compare to particle excitation. Since the point we choose is closer to the lower edge of the lobe, the hole excitation has higher spectral weight. The corresponding density of state is given in figure (6).

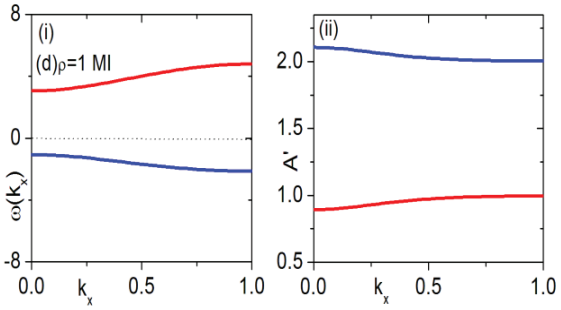

FIGURE 5. Excitations (i) and weights (ii) for point (d) in figure (1). Only excitations which have finite spectral weight have shown here.

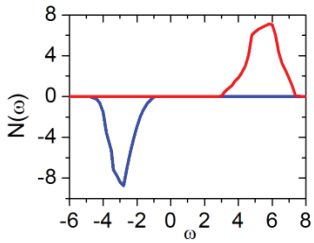

FIGURE 6. DOS of excitations of figure (5) in MI phase.

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