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# Modulation Spectroscopy and Dynamics of Double Occupancies in a Fermionic Mott Insulator

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We calculate the rate of creation of double occupancies in a 3D Fermionic Mott insulator near half-filling by modulation of optical lattice potential. At high temperatures, incoherent holes lead to a broad response peaked at the Hubbard repulsion  $U$ . At low temperatures, antiferromagnetic order leads to a coherent peak for the hole along with broad features representing spin wave shake-off processes. This is manifested in the doublon creation rate as a sharp absorption edge and oscillations as a function of modulating frequency. Thus, modulation spectroscopy can be used as a probe of antiferromagnetic order and nature of quasiparticle excitations in the system.

Advances in experiments with cold atoms on optical lattices have made them promising candidates for simulators of lattice models which play an important part in our understanding of strongly interacting quantum systems. Recently Mott insulating states[1] have been obtained in the large  $U$  limit of the repulsive Fermionic Hubbard model[2, 3] with these systems.

Motivated by recent experiments[2], we give a theoretical formulation of the response of a Mott insulator near half-filling to modulation of optical lattice potential by relating the rate of production of double occupancies to the convolution of spectral function of holes and double occupancies (doublons) in the Mott insulator. We will show that this technique can be used to detect the presence of antiferromagnetic (AF) order and probe the nature of quasiparticle excitations (coherent vs. incoherent) in the system. We also discuss the connection of this response to optical conductivity in corresponding charged systems.

We focus on two temperature regimes: (i) the high temperature limit ( $J \ll T \sim t_h \ll U$ ), where  $T$  is the temperature,  $t_h$  the tunneling matrix, and  $J = 4t_h^2/U$  the super-exchange scale, which controls the quantum dynamics of the background spins; and (ii) The low temperature limit ( $T \ll J$ ), with an AF ordered spin background.

In the paramagnetic phase (current experiments[2]), we get a response peaked at  $\omega = U$  with a width equal to twice the bandwidth of the holes, reflecting the completely incoherent hole and doublon in this limit. We also derive a sum rule for the energy integrated rate of doublon production in this limit.

At low temperatures, the AF ordering leads to coherent propagation of quasiparticles and manifests itself in a sharp absorption edge in the production rate. Additional structures at higher energies appear as a result of shake-off processes of spin waves. Thus, lattice modulation spectroscopy can be used to observe the nature of quasiparticle excitations and detect the presence of antiferromagnetic ordering in the Mott insulating state.

**Modulation of Optical Lattice:** Repulsive fermions in optical lattices are well described by a one band Hubbard model

$$H = -t_h \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where the tunneling matrix  $t_h$  and the onsite repulsion  $U$  depend on the depth of the optical lattice  $V$  through [4]

$$t_h \sim E_r \left( \frac{V}{E_r} \right)^{\frac{3}{4}} e^{-2\sqrt{\frac{V}{E_r}}}, \quad U \sim \frac{a_s}{\lambda} E_r \left( \frac{V}{E_r} \right)^{\frac{3}{4}} \quad (2)$$

where  $E_R$  is the recoil energy of the photon,  $\lambda$  is its wavelength and  $a_s$  is the s-wave scattering length of the atoms.

The modulation of the optical potential  $V(t) = V_0 + \delta V \sin(\omega t)$  effects both  $t_h$  and  $U$ . The modulation of  $U$  can be neglected in the large  $U/t_h$  limit. The modulation of  $t_h(t) = t_h + \delta t_h \sin(\omega t)$  is related to  $V(t)$  by

$$\delta t_h = t_h \delta V \left[ \frac{3}{4V_0} - \frac{1}{\sqrt{V_0 E_r}} \right] \quad (3)$$

The single particle spectrum of the Mott insulator is formed of two bands: (a) the lower Hubbard band, which does not contain double occupancies and is exactly filled at half-filling and (b) the upper Hubbard band, which contains a single double occupancy and is completely empty at half-filling. These are separated by the Mott gap  $\sim U$ . So, the modulation of the optical barrier will produce double occupancies once the frequency of modulation exceeds the Mott gap.

**Schwinger Bosons and Slave Fermions:** In the Schwinger Boson Slave Fermion representation, we represent the singly occupied sites (spins) by two Schwinger bosons  $a_{i\sigma}^\dagger$ , the doubly occupied sites by a doublon  $d^\dagger$  and the empty sites by a holon  $h^\dagger$ . The doublon and holon are Fermions. The original Fermion creation operator can be written as  $c_{i\sigma}^\dagger = a_{i\sigma}^\dagger h_i + \sigma a_{i-\sigma} d_i^\dagger$  with the local constraint equation  $a_{i\sigma}^\dagger a_{i\sigma} + d_i^\dagger d_i + h_i^\dagger h_i = 1$ . We define the following operators:  $F_{ij}^\dagger = \sum_\sigma a_{i\sigma}^\dagger a_{j\sigma}$  and  $A_{ij}^\dagger = \sum_\sigma \sigma a_{i\sigma}^\dagger a_{j-\sigma}^\dagger$  which represent the hopping of the bosons and the creation of singlet configurations. We further make the following transformation: On B sublattice  $d^\dagger \rightarrow -d^\dagger$ . Then the unperturbed Hamiltonian is

$$H_0 = t_h \sum_{\langle ij \rangle} (d_i^\dagger d_j + h_i^\dagger h_j) F_{ij} + (d_i^\dagger h_j^\dagger A_{ij} + h.c.) + U \sum_i d_i^\dagger d_i \quad (4)$$

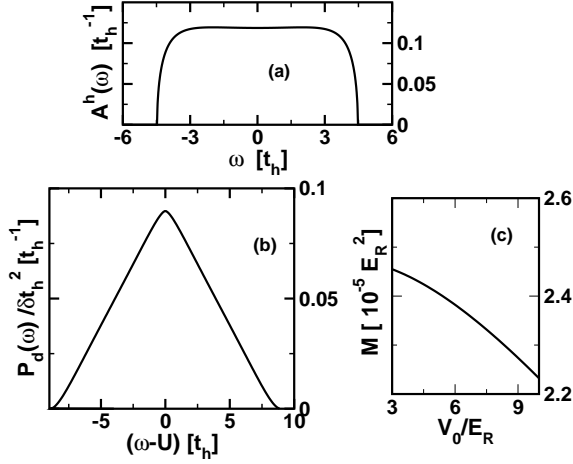


FIG. 1: (a) The density of states of a single hole in a half-filled background in the atomic limit. (b) The rate of production of double occupancies as a function of frequencies and (c) The energy integrated response in high temperature limit.

while the perturbation due to the lattice modulation is

$$H_1(t) = \delta t_h \sin[\omega t] \sum_{\langle ij \rangle} d_i^\dagger h_j^\dagger A_{ij} + h_i d_j A_{ij}^\dagger \quad (5)$$

where we have neglected terms that do not create or destroy doublons. We work with a system at half-filling, at temperatures  $T \ll U$ , where we can neglect the presence of doublons and holes in the unperturbed system. The number of doublons created in time  $t$  is given by

$$N_d(t) = \sum_n e^{-E_n/T} \langle n | U^\dagger(t) \sum_i d_i^\dagger d_i U(t) | n \rangle \quad (6)$$

where  $|n\rangle$  denotes the unperturbed states (in our case spin configurations) with energy  $E_n$  and the time evolution operator has a perturbation expansion  $U(t) = 1 - i \int_0^t dt' H_1^I(t') - \int_0^t dt' \int_0^{t'} dt'' H_1^I(t') H_1^I(t'')$ , where the standard interaction representation of an operator is given by  $\mathcal{O}^I(t) = e^{iH_0 t} \mathcal{O}(t) e^{-iH_0 t}$ . We also assume that the doublons are created by the action of the perturbation Hamiltonian only, i.e. the time evolution of the system by the unperturbed Hamiltonian conserves the number of doublons. This neglects the decay of doublons into a pair of bosons during the time evolution. This approximation is justified as long as  $T \ll U$ , since, due to energy conservation requirements, the decay of a doublon in the system is a very slow process [5]. Under these assumptions, the first order response of the system vanishes and upto second order in perturbation theory, the rate of creation of doublons is given by

$$P_d(\omega) = \frac{\pi}{2} (\delta t_h)^2 \int d\omega_1 \int d\omega_2 \sum_{\langle ij \rangle \langle lm \rangle} A_{ijlm}^s(\omega_2) A_{il}^d(\omega_1) A_{jm}^h(\omega - \omega_1 - \omega_2) \quad (7)$$

where  $\omega$  is the frequency of the perturbation,  $\mathcal{A}^{d(h)}$  is the spectral function for the doublon (hole) and  $\mathcal{A}^s$  is the Fourier transform of  $\langle A_{lm}(t) A_{ij}^\dagger(t') \rangle$ . It is to be noted that we have already used a mean field decoupling of the doublon, hole and Schwinger boson operators to arrive at the above equation. This approximation is justified at large  $U/t_h$  due to the separation of energy scales governing the hole (doublon) dynamics ( $t_h$ ) and the spin dynamics ( $J$ ).

We emphasize that the response we are calculating is not equivalent to optical conductivity in the condensed matter systems. (i) The current vertex in optical conductivity is replaced by the kinetic energy vertex. (ii) The optical conductivity involves convolution of hole spectral function with itself, whereas the calculated response involves convolution of hole and doublon spectral functions. Since the doublon spectral function is shifted by  $U$ , as we move away from half-filling, there is no response at low frequencies, whereas there would be optical response at low frequencies in a compressible state.

**High Temperature:** We now focus on the regime  $U \gg T \sim t_h \gg J$ , which is the regime of interest for the current experiments. In this limit, the quantum dynamics of the spins are irrelevant and one can replace the  $A$  operators by the probability of finding a  $\uparrow\downarrow$  or  $\downarrow\uparrow$  configuration in an ensemble where all spin configurations occur with equal weight. Thus,

$$P_d(\omega) = \frac{\pi}{2} P_s (\delta t_h)^2 \sum_{\langle ij \rangle \langle lm \rangle} \int d\omega' A_{il}^d(\omega') A_{jm}^h(\omega - \omega') \quad (8)$$

where  $P_s$  is the probability of finding relevant configurations at  $(i, j)$  and  $(l, m)$  given by  $P_s = 1/2$  if  $(i, j) = (l, m)$ ,  $P_s = 1/8$  if  $(i, j)$  and  $(l, m)$  have no overlap and  $P_s = 1/4$  if  $(i, j)$  and  $(l, m)$  share one site in common. Due to particle-hole symmetry of the problem at half-filling, we have  $\mathcal{A}^d(\omega + U) = \mathcal{A}^h(\omega)$ , so that it is enough to compute the spectral function for the holes only.

We now try to evaluate the spectral function of a single hole in a half-filled background where the spins are completely disordered. The hole is completely incoherent, i.e. it moves diffusively in the system. The spectral function of the hole in this limit has been worked out by Brinkman and Rice [6] and Kane *et al* [7] using the so called retraceable path approximation.

The Green's function has contributions from processes where the hole hops from one point to another. However, as the hole hops, it scrambles the spin configuration and a string of ferromagnetic bonds is required along the path for the process to contribute. The probability of finding such a string is given by  $(1/2)^L$ , where  $L$  is the length of the path. However, the trajectories where the hole retraces its path do not scramble the background spins and have a weight of 1 as opposed to  $(1/2)^L$ . They provide the dominant contribution to the density of states at low energies.

The easiest way to derive the spectral function is to write the Green's function as a function of the frequency  $\omega$  in the following way:  $G^{-1}(\omega) = \omega[1 - \Sigma(\omega)]$  and derive a self-consistent equation for the self energy. The first contribution to the self-energy comes from the hops to nearest neighbours

and gives  $\Sigma^{(1)}(\omega) = zt_h^2/\omega^2$ , where  $z$  is the co-ordination number of the lattice. To include the longer hops, the denominator of  $\Sigma^{(1)}$  can be modified with a higher order self-energy  $\Sigma^{(2)}(\omega) = zt_h^2/\omega^2(1 - (z-1)t_h^2/\omega^2)$ , where the factor  $z-1$  comes from excluding the initial site while considering the initial hop. This method is similar to the one used by Anderson in his original paper on localization physics [8] and gives a self energy  $\Sigma(\omega) = (z/z-1)[1/2 - \sqrt{\omega^2 - 4(z-1)t_h^2/\omega}]$ . This leads to the spectral function

$$\mathcal{A}(\omega) = \frac{1}{\pi z t_h} \left[ \frac{(5 - 9\omega^2/z^2 t_h^2)^{1/2}}{1 - \omega^2/z^2 t_h^2} \right] \quad (9)$$

The spectral function is plotted as a function of frequency in Fig 1(a). The spectrum is incoherent and has a band-width of  $2\sqrt{z-1}t_h$ . The spectral weight decreases monotonically as one goes towards the band edge. The rate of production of doublons, calculated using this spectral function is plotted in Fig 1(b). There is a peak around  $\omega = U$  with weight upto twice the bandwidth (for the holes) around it.

We note here some recent work in the paramagnetic phase using different techniques[9, 10].

**Sum Rule:** Sum-rules have played an important role in various strongly correlated systems, since they often involve less approximations and serve as useful check on both theory and experiments. In this case we consider the energy integrated rate of production of doublons  $\int d\omega P_d(\omega)$ . Using the identity  $\int_{-\infty}^{\infty} d\omega \mathcal{A}_{ij}^{d(h)}(\omega) = \delta_{ij}$  we obtain the sum rule in the high temperature limit

$$M = \int_{-\infty}^{\infty} d\omega P_d(\omega) = \frac{\pi}{4}(\delta t_h)^2 \quad (10)$$

The sum-rule is proportional to  $(\delta t_h)^2$ , which is proportional to  $t_h^2$  for a constant fractional change in the amplitude of the lattice potential. Assuming  $U/t$  is tuned by tuning the lattice potential and a constant fractional change in the amplitude of the potential ( $\delta V_0/V_0$  is held fixed), one finds that in the Mott regime, the energy integrated weight monotonically decreases with increase in  $V_0/E_R$ , as shown in Fig 1 (c).

**Low Temperature (Antiferromagnetic phase) :** We now consider the response of the system at  $T = 0$  in an AF ordered phase. As we will see, in this regime, the spectral function of holes has a sharp peak and a series of broad features. The sharp peak is reflected in the doublon creation rate as a sharp absorption edge and the broad features result in oscillations in the rate as a function of modulating frequency.

This phase is characterized by Bose condensation of  $\uparrow$  and  $\downarrow$  Schwinger Bosons on opposite (A and B) sublattices. In a  $1/S$  expansion, the fluctuations are governed by the Holstein Primakoff Hamiltonian

$$H = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \quad (11)$$

where  $\omega_{\mathbf{k}} = zJ(1 - \gamma_{\mathbf{k}}^2)^{1/2}$  is the dispersion of the spin wave

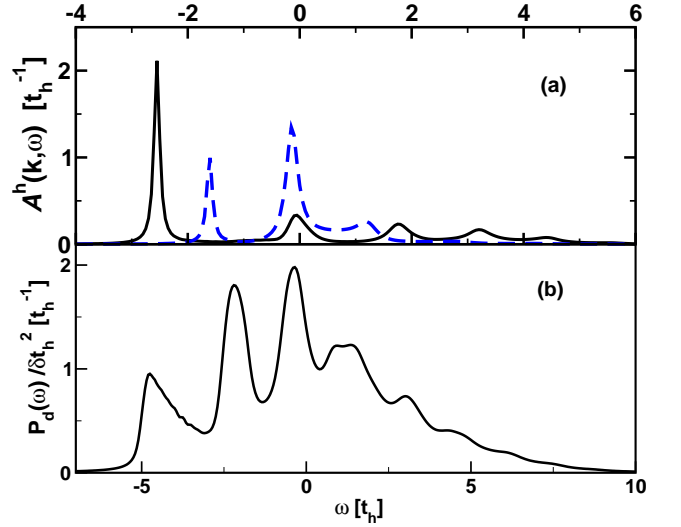


FIG. 2: (a) The spectral function of the hole at  $(\pi/2, \pi/2, \pi/2)$  (solid line) and at  $(0, 0, 0)$  (dashed line) for a system with  $U/t = 20$ . The spectral functions are broadened by an artificial broadening of  $0.06t$  (b) The rate of doublon production  $P_d(\omega)$  as a function of perturbing frequency.

with  $\gamma_{\mathbf{k}} = (1/3)[\cos k_x + \cos k_y + \cos k_z]$ , and the quasiparticle operators are given by  $\alpha_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} a_{-\mathbf{k}}^{\dagger}$  with

$$a_{\mathbf{k}} = \sum_{i \in A} a_{i\downarrow} e^{i\mathbf{k}\cdot\mathbf{r}_i} + \sum_{j \in B} a_{j\uparrow} e^{i\mathbf{k}\cdot\mathbf{r}_j} \quad (12)$$

The coherence factors  $u_{\mathbf{k}}$  and  $v_{\mathbf{k}}$  are given by  $u_{\mathbf{k}} = (1/\sqrt{2})(\omega_{\mathbf{k}}^{-1} + 1)^{1/2}$  and  $v_{\mathbf{k}} = -\text{sgn}(\gamma_{\mathbf{k}})(1/\sqrt{2})(\omega_{\mathbf{k}}^{-1} - 1)^{1/2}$ . The hole hopping Hamiltonian can be written as

$$H^h = t_h \sum_{\langle ij \rangle} h_i^{\dagger} h_j a_{i\sigma} a_{j\sigma}^{\dagger} \quad (13)$$

Replacing the  $\uparrow$  and  $\downarrow$  spins on A and B sublattice by the condensate amplitude  $\sqrt{\rho_0} = 1$ , this term can be written as

$$H^h = z t_h \sqrt{\rho_0} \sum_{\mathbf{k}\mathbf{q}} h_{\mathbf{k}}^{\dagger} h_{\mathbf{k}-\mathbf{q}} (u_{\mathbf{q}} \gamma_{\mathbf{k}-\mathbf{q}} \alpha_{\mathbf{q}} + v_{\mathbf{q}} \gamma_{\mathbf{k}} \alpha_{-\mathbf{q}}^{\dagger}) + h.c. \quad (14)$$

The motion of a hole is thus accompanied by creation of a spin wave. We calculate the self-energy of the hole in a self-consistent Born Approximation [11, 12] which is equivalent to calculating the non-crossing Feynman diagram for the self energy. At  $T = 0$ , the self-energy is given by

$$\Sigma(\mathbf{k}, \omega) = \sum_{\mathbf{q}} |\Gamma(\mathbf{k}, \mathbf{q})|^2 G(\mathbf{k} - \mathbf{q}, \omega - \omega_{\mathbf{q}}) \quad (15)$$

where the vertex function  $\Gamma(\mathbf{k}, \mathbf{q}) = z t_h \sqrt{\rho_0} (u_{\mathbf{q}} \gamma_{\mathbf{k}-\mathbf{q}} + v_{\mathbf{q}} \gamma_{\mathbf{k}})$  and the self-consistency is ensured through

$$G^{-1}(\mathbf{k}, \omega) = \omega - \Sigma(\mathbf{k}, \omega). \quad (16)$$

The spectral weight obtained from the self-consistent solution for  $J = 0.2t_h$  is plotted for two different  $\mathbf{k}$  values,  $([0, 0, 0]$  and  $[\pi/2, \pi/2, \pi/2])$  in Fig 2(a). At the lowest energy of propagation of the hole, which occurs at  $(\pi/2, \pi/2, \pi/2)$ , spin waves cannot be created (at  $T = 0$ ) and there is a coherent peak. The coherent weight is largest at this point and gradually decreases as one moves to the center of the Brillouin zone. The location of the coherent peak disperses as  $\sim J\gamma_{\mathbf{k}}^2$ , corresponding to second order hopping processes which do not scramble the AF alignment.

Beyond the coherent peak, there are additional broad features at higher energies, whose peak to peak distance scales with  $J$ . These are generated by spin wave shake-off processes[13]. The peaks correspond to 2, 4, 6, ... spin waves and are dominated by spin waves near the Brillouin zone boundary where the flat spin-wave spectrum results in a diverging density of states. This is similar to peaks in the 2-magnon Raman response in antiferromagnetic insulators[14].

In terms of the calculated spectral function, one can calculate the rate of doublon production as

$$P_d(\omega - U) = \frac{\pi}{2}(\delta t_h)^2 \kappa \sum_{\mathbf{k}} \gamma_{\mathbf{k}}^2 \int d\omega_1 A(\mathbf{k}, \omega_1) A(\mathbf{k}, \omega - \omega_1) \quad (17)$$

where  $\kappa = 1 - (1/2z) \sum_{\mathbf{k}} \gamma_{\mathbf{k}}^2 / \omega_{\mathbf{k}}$  is a vertex correction which takes care of the singlet spectral function. There is no convolution with spin spectral functions as the spin dynamics is governed by the transverse (phase) modes ( $\uparrow$  on B and  $\downarrow$  on A sublattices) and the longitudinal (amplitude) modes ( $\uparrow$  on A and  $\downarrow$  on B) of the condensate are neglected[7].

The rate of doublon production is plotted in Fig 2(b). It shows an abrupt edge at the lower end of the spectrum corresponding to the coherent spectral weight of the holes. The other oscillations in the response reflect the convolution of the coherent part with the broad incoherent peaks due to shake-off processes and that of the peaks themselves. We thus see that the presence of the AF order leaves its signature in the frequency dependence of the response.

We sketch what happens as we move away from half-filling (still remaining within the AF phase). The order parameter  $\rho_0$  decreases, weakening the scattering of the hole by the spin waves. Thus the coherent part should grow leading to a sharper edge. This is in contrast to disordering the AF phase by raising temperature, where the scattering from occupied spin wave modes reduce the coherent part.

Although our calculation is done for  $T = 0$ , we expect these qualitative features to be valid as long as the temperature is much below the Neel transition temperature.

**Comparison with Experiments:** In the experiments of Ref. [2], the modulation is kept on for a fixed number of cycles. The time of drive is proportional to  $\omega^{-1}$  and the quantity measured is proportional to  $P_d(\omega)/\omega$ . So the frequency integrated response should decrease even faster with  $U/t_h$  as compared to Fig. 1c. However, the experimental data shows a monotonic increase with  $U/t_h$ [15].

We believe this could be due to several reasons: (a) The

response might be dominated by terms beyond second order perturbation theory. This can be checked by putting on the drive for different amount of time and looking at the linearity (or lack thereof) of the number of doublons produced with time. (b) The unperturbed system is not in thermal equilibrium due to slow relaxation of the doublons created during tuning  $U/t$  [5] or (c) Relaxation of doublons while driving the system leads to a steady state behaviour. We hope the discrepancies between the theory and experiments can be settled with further experiments on this system.

**Conclusion:** We have related the rate of production of double occupancies by modulation of optical lattice in a 3D Mott insulator near half-filling to the convolution of hole and doublon spectral functions. This technique can be used to study the nature of quasiparticle excitations and detect presence of AF order in the system. In the paramagnetic phase there is a broad response peaked around  $\omega = U$ . In the ordered phase, the coherent hole is reflected as a sharp absorption edge, while shake off processes lead to oscillations.

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