Light scattering detection of quantum phases of ultracold atoms in optical lattices

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Ultracold atoms loaded on optical lattices can provide unprecedented experimental systems for the quantum simulations and manipulations of many quantum phases. However, so far, how to detect these quantum phases effectively remains an outstanding challenge. Here, we show that the optical Bragg scattering of cold atoms loaded on optical lattices can be used to detect many quantum phases which include not only the conventional superfluid and Mott insulating phases, but also other important phases such as various kinds of density waves (CDW), valence bond solids (VBS), CDW supersolids and VBS supersolids.

In this paper, we will develop a systematic theory of using the optical Bragg scattering (Fig.1) to detect the nature of quantum phases of interacting bosons loaded in optical lattices. We show that the optical Bragg scattering not only couples to the density order parameter, but also the valence bond order parameter due to the hopping of the bosons on the lattice. At integer fillings, when $\vec{q}$ matches a reciprocal lattice vector $\vec{K}$ of the underlying OL, there is an increase in the optical Bragg scattering cross section as the system evolves from the Mott to the SF state due to the increase of hopping in the SF state. At 1/2 filling, in the CDW state, when $\vec{q}$ matches the CDW ordering wavevector $\vec{Q}_n$ and $\vec{K}$, there is a diffraction peak proportional to the CDW order parameter squared and the density squared respectively (Fig.3a), the ratio of the two peaks is a good measure of the CDW order parameter. In the VBS state, when $\vec{q}$ matches the VBS ordering wavevector $\vec{Q}_K$, there is a much smaller, but detectable diffraction peak proportional to the VBS order parameter squared, when it matches $\vec{K}$, there is also a diffraction peak proportional to the uniform density in the VBS state (Fig.3b). All the diffraction peaks scale as the square of the numbers of atoms inside the trap. All these characteristics can determine uniquely CDW and VBS state at 1/2 filling and the corresponding CDW supersolid and VBS supersolid slightly away from the 1/2 filling. In the following, we just take 2d optical lattices as examples. The 1d and 3d cases can be similarly discussed.

The Extended Boson Hubbard Model (EBHM) has various kinds of interactions, on all kinds of lattices and at different filling factors is described by the following Hamiltonian:

$$H_{BH} = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + h.c.) - \mu \sum_i n_i + \frac{U}{2} \sum_i n_i (n_i - 1) + V_1 \sum_i n_i n_j + V_2 \sum_{\langle ij \rangle} n_i n_k + \cdots$$

where $n_i = b_i^\dagger b_i$ is the boson density, $t$ is the nearest
neighbor hopping which can be tuned by the depth of the optical lattice potential, the $U, V_1, V_2$ are onsite, nearest neighbor (nn) and next nearest neighbor (nnn) interactions, respectively. The on-site interaction $U$ can be tuned by the Feshbach resonance [2]. Various kinds of optical lattices such as honeycomb, triangular [18], body-centered-cubic [18], Kagome lattices [19] can be realized by suitably choosing the geometry of the laser beams forming the optical lattices. There are many possible ways to generate longer range interaction $V_1, V_2, ...$ of ultra-cold atoms loaded in optical lattices. Being magnetically or electrically polarized, the $^{52}Cr$ atoms [20] or polar molecules [21] $^{40}K + ^{87}Rb$ (or $^{39}K + ^{87}Rb$) interact with each other via long-range anisotropic dipole-dipole interactions. Loading the $^{52}Cr$ or the polar molecules on a 2d optical lattice with the dipole moments perpendicular to the trapping plane can be mapped to Eqn.3 with long-range repulsive interactions $\sim p^2/r^3$ where $p$ is the dipole moment. The CDW supersolid phases studied by QMC [11] and described in [13] by the dual vortex method was numerically found to be stable in large parameter regimes in this system [22]. The generation of the ring exchange interaction has been discussed in [24]. Some of the important phases with long range interactions are listed in Fig.2. Recently, the quantum entanglement properties of the VB state was addressed in [25].

The interaction between the two laser beams in Fig.1 with the two level bosonic atoms is:

$$H_{int} = \int d^2r \left[ \frac{\hbar^2 p^2}{2m_a} + V_{OL}(\vec{r}) + \frac{\hbar \omega_a}{2} \sigma_z \right]$$

$$\left( \sigma_+ u_l(\vec{r}) + h.c. \right) \Psi(\vec{r})$$

where $\Psi(\vec{r}) = (\psi_1, \psi_2)$ is the two component boson annihilation operator, the incident and scattered lights in Fig.1a and the two incident lights in Fig.1b have frequencies $\omega_l$ and mode functions $u_l(\vec{r}) = e^{i\vec{k}_l \cdot \vec{r} + i\phi_l}$. The Rabi frequencies $\Omega$ are much weaker than the laser beams (not shown in Fig.1) which form the optical lattices. When it is far off the resonance, the laser light-atom detunings $\Delta_l = \omega_l - \omega_a$ where $\omega_a$ is the two level energy difference are much larger than the Rabi frequency $\Omega$ and the energy transfer $\omega = \omega_1 - \omega_2$ (See Fig.1a and 1b), so $\Delta_1 \sim \Delta_2 = \Delta$.

After adiabatically eliminating the upper level $e$ of the two level atoms, expanding the ground state atoms field operator $\psi_e(\vec{r}) = \sum_i b_i u_e(\vec{r} - \vec{r}_i)$ in Eqn.2 where $u(\vec{r} - \vec{r}_i)$ is the localized Wannier functions of the lowest Bloch band corresponding to $V_{OL}(\vec{r})$ and $b_i$ is the annihilation operator of an atom at the site $i$ in the Eqn.1 then we get the effective interaction between the off-resonant laser beams and the ground level $g$:

$$H_{int} = \hbar \Omega^2 \sum_{i} J_{i,i} n_i + \sum_{<ij>} N J_{i,j} b_i^\dagger b_j$$

where the interacting matrix element is $J_{i,i} = \int d\vec{r} w(\vec{r} - \vec{r}_i) u^*_i(\vec{r}) u_j(\vec{r}) w(\vec{r} - \vec{r}_j) = J_{i,j}$. The first term in Eqn.3 is the on-site term $D = n_i J_{i,i} n_i$ (See Fig.1a). The second term is the off-site term (See Fig.1b). Because the Wannier wavefunction $w(\vec{r})$ can be taken as real in the lowest Bloch band, the off-site term can be written as $K = \sum_{<ij>} J_{i,j} b_i^\dagger b_j = \sum_{<ij>} J_{i,j} (b_i^\dagger b_j + h.c.)$ which is nothing but the off-site coupling to the nearest neighbor kinetic energy of the bosons $K_{ij} = b_i^\dagger b_j + h.c.$.

It is easy to show that:

$$\dot{\hat{D}}(\vec{q}) = \frac{f_0(\vec{q})}{\hbar} \sum_{i=1}^N e^{-i\vec{q} \cdot \vec{r}_i} n_i = N f_0(\vec{q}) n(\vec{q})$$

where $\vec{q} = \vec{k}_1 - \vec{k}_2, f_0(\vec{q}) = \int d\vec{r} e^{-i\vec{q} \cdot \vec{r}} w^2(\vec{r})$ and $n(\vec{q}) = \frac{1}{\hbar} \sum_{i=1}^N e^{-i\vec{q} \cdot \vec{r}_i} n_i = \sum_{\vec{k}} b_{\vec{k}}^\dagger b_{\vec{k}+\vec{q}}$ is the Fourier transform of the density operator at the momentum $\vec{q}$. Note that $n(\vec{q}) = n(\vec{q} + \vec{K})$. The wavevector is confined to $L^{-1} < q < a^{-1}$ where the trap size $L \sim 100 \mu m$ and the lattice constant $a \sim 0.5 \mu m$ in Fig.1. In fact, more information is encoded in the off-site kinetic coupling in Eqn.3. In a
square lattice, the bonds are either oriented along the \( \hat{x} \) axis \( \vec{r}_j - \vec{r}_i = \hat{x} \) or along the \( \hat{y} \) axis \( \vec{r}_j - \vec{r}_i = \hat{y} \), we have:

\[
\tilde{K}_\square = N|f_x(\vec{q})K_{x}(\vec{q}) + f_y(\vec{q})K_{y}(\vec{q})|
\]

(5)

where \( K_\alpha(\vec{q}) = \frac{1}{\lambda} \sum_{i=1}^{N} \sum_{\beta} \cos k_\alpha b_\beta b_\beta^{\dagger} \) are the Fourier transform of the kinetic energy operator \( K_{ij} = b_\beta^{\dagger} b_\beta + h.c. \) along \( \alpha = x, y \) bonds at the momentum \( \vec{q} \) and the "form" factors \( f_\alpha(\vec{q}) = f(\vec{q}, \vec{r}_j - \vec{r}_i = \alpha) = \int d^3 \vec{r} e^{-i\vec{q}\cdot\vec{r}} w(\vec{r}) w(\vec{r} + \vec{r}_j - \vec{r}_i) \). Note that \( K_x(\vec{q}) = K_y(\vec{q} + \vec{K}) \). Following the harmonic approximation used in [2], we can estimate that \( f(\vec{q}, \vec{r}_i) \sim |e^{-\frac{1}{2}(V_0/E_r)^{-1/2}}| \), so \( |f_x(\pi,0)| \sim e^{-\frac{1}{2}(V_0/E_r)^{-1/2}} \), and the integrated scattering cross section inside the CDW region parameter [15]. The \( f_y(\vec{q},0) \) is close to 1 when \( V_0/E_r > 4 \). It is instructive to relate this ratio to that of the hopping t over the onsite interaction \( U \) in the Eqn.6 \( |f_x(\pi,0)|/|f_y(\pi,0)| \sim \frac{\lambda\sqrt{t}}{\hbar k_\alpha} \) as \( \lambda \) is the zero field scattering length and \( \alpha = \lambda / 2 = \pi/k \) is the lattice constant, using the typical values \( t/U \sim 10^{-2} \), \( a_{\alpha}/a \sim 10^{-2} \), one can estimate \(|f_y/0| \sim 10^{-3} \). Note that the harmonic approximation works well only in a very deep optical lattice \( V_0 \gg E_r \), so the above value underestimates the ratio, so we expect \(|f_y/0| \geq 10^{-3} \).

The differential scattering cross section of the light from the cold atom systems in the Fig.1 can be calculated by using the standard linear response theory:

\[
\frac{d\sigma}{d\Omega dE} = S(\vec{q},\omega) \sim \left( \frac{\Omega}{\Delta} \right)^2 N^2 |f_\alpha(\vec{q})|^2 S_N(\vec{q},\omega) + \sum_{\alpha=\pm\hat{y}} |f_\alpha(\vec{q})|^2 S_{K_\alpha}(\vec{q},\omega)
\]

(6)

where \( \vec{q} = \vec{k}_1 - \vec{k}_0, \omega = \omega_1 - \omega_2 \), the \( S_N(\vec{q},\omega) = \langle n(-\vec{q},\omega) n(\vec{q},\omega) \rangle \) is the dynamic density-density response function whose Lehmann representation was listed in [4]. The \( S_{K_\alpha}(\vec{q},\omega) = \langle K_\alpha(-\vec{q},\omega) K_\alpha(\vec{q},\omega) \rangle \) is the bond-bond response function whose Lehmann representation can be got that from of the \( S_N(\vec{q},\omega) \) simply by replacing the density operator \( n(\vec{q}) \) by the bond operator \( K_\alpha(\vec{q}) \). The integrated scattering cross section over the final energy \( \frac{d\sigma}{d\Omega} \) is proportional to the equal-time response function \( \frac{d\sigma}{d\Omega} = S(\vec{q}) \sim \left( \frac{\Omega}{\Delta} \right)^2 N^2 |f_\alpha(\vec{q})|^2 S_N(\vec{q},\omega) + \sum_{\alpha=\pm\hat{y}} |f_\alpha(\vec{q})|^2 S_{K_\alpha}(\vec{q},\omega) \).

We first look at the superfluid to Mott transition at integer filling factor \( n \). When \( \vec{q} \) is equal to the shortest reciprocal lattice vector \( \vec{K} = (2\pi,0) \), in the Mott state, \( \frac{d\sigma}{d\Omega} \sim |f_\alpha(2\pi,0)|^2 N^2 n^2 \), in the superfluid state, \( \frac{d\sigma}{d\Omega} \sim |f_\alpha(2\pi,0)|^2 N^2 n^2 + \frac{1}{2} |f_\alpha(2\pi,0)|^2 N^2 B^2 \) where \( B \) is the average kinetic energy on a bond in the superfluid side. Because \( |f_\alpha(2\pi,0)|^2 \sim |f_\alpha(2\pi,0)|^2 \sim 1 \) and \( B \) is appreciable in the superfluid side, we expect a dramatic increase of the scattering cross section

\[
\frac{d\sigma}{d\Omega} \sim 2|f_\alpha(2\pi,0)|^2 N^2 B^2
\]

across the Mott to the SF transition due to the prefactor \( N^2 \). This prediction could be tested immediately.

Surprisingly, there is no such optical Bragg scattering experiment in the superfluid yet.

In the CDW with \( \vec{Q}_n = (\pi,\pi) \) in Fig.2a, due to the lack of VBS order on both sides, the second term in Eqn.6 can be neglected, so that

\[
\frac{d\sigma}{d\Omega dE}|_{CDW} \sim \left( \frac{\Omega}{\Delta} \right)^2 N^2 |f_\alpha(\vec{q})|^2 S_N(\vec{q},\omega)
\]

(8)

which should show a peak at \( \vec{q} = \vec{Q}_n \) (Fig.3a) whose amplitude scales as the square of the number of atoms inside the trap \( |f_\alpha(\pi,\pi)|^2 N^2 m^2 \) where \( m = n_A + n_B \) is the CDW order parameter [15]. Then \( \vec{q} = \vec{K} \), then \( \mathcal{S}_{CDW}(\vec{K}) \sim |f_\alpha(2\pi,0)|^2 N^2 m^2 \) where \( f_\alpha(2\pi,0) \sim f_\alpha(\pi,\pi) \) (Fig.3a). So the ratio of the two peaks in Fig.3a is \( m^2/n^2 \) if one neglects the very small difference of the two form factors. Slightly away from 1/2 filling, the CDW in Fig.2a may turn into the CDW supersolid (CDW-SS) phase through a second order phase transition [15]. Then we have \( \langle n(\vec{q}) \rangle = m\delta_{\vec{q},\vec{Q}_n} + n\delta_{\vec{q},0} \) where \( n = n_A + n_B = 1/2 + \delta n \). The superfluid density \( \rho_s \sim \delta n \sim n - 1/2 \). The scattering cross section inside the CDW-SS: \( \mathcal{S}_{CDW-SS}(\vec{Q}_n) \sim |f_\alpha(2\pi,0)|^2 N^2 m^2 \) stays more or less the same as that inside the CDW, but \( \mathcal{S}_{CDW-SS}(\vec{K}) \sim |f_\alpha(2\pi,0)|^2 N^2 m^2 \) will increase. The B is the average bond strength due to very small superfluid component \( \rho_s \sim \delta n = n - 1/2 \) flowing through the whole lattice. So the right peak in Fig.3a will increase due to the increase of the total density and the superfluid component inside the CDW-SS phase.

Now we discuss the VBS state with \( \vec{Q}_K = (\pi,0) \) in Fig.2b. Due to the uniform distribution of the density in the VBS, when \( \vec{q} = \vec{K} \), the second term in Eqn.6 can be neglected, so there is a diffraction peak (Fig.3b) whose amplitude scales as the square of the number of atoms inside the trap \( |f_\alpha(2\pi,0)|^2 N^2 n^2 \) where \( f_\alpha(2\pi,0) \sim f_\alpha(\pi,\pi) \) and \( n = 1/2 \) is the uniform density in the VBS state. However, when one tunes \( \vec{q} \) near \( \vec{Q}_K \), the first term in Eqn.6 can be neglected, then

\[
\frac{d\sigma}{d\Omega dE}|_{VBS} \sim \left( \frac{\Omega}{\Delta} \right)^2 N^2 \sum_{\alpha=\pm\hat{y}} |f_\alpha(\vec{q})|^2 S_{K_\alpha}(\vec{q},\omega)
\]

(9)

which should show a peak at \( \vec{q} = \vec{Q}_K \) signifying the VBS ordering at \( \vec{Q}_K \) whose amplitude scales also as the square of the number of atoms inside the trap \( |f_\alpha(\pi,\pi)|^2 N^2 K^2 \) where \( K = K_\alpha - K_\beta \) is the VBS order parameter [15]. So the ratio of the VBS peak at \( \vec{q} = \vec{Q}_K \) over the uniform density peak at \( \vec{q} = \vec{K} \) is
The superfluid density $\rho = \frac{1}{n} \delta n$ is very much visible in the current optical Bragg scattering experiments. However, the smallness of $|f_\pi|^2$ is compensated by the large number of atoms $N \sim 10^6$, $|f_\pi|^2 N^2 = (|f_\pi|^2 N) \times N \sim N \times 10^6$. Therefore, the Bragg scattering cross section from the VBS order is $\geq 10^{-5}$ smaller than that at $\vec{q} = \vec{K}$ at the same incident energy $I_n$ (Fig.3b), but still $\sim 10^6$ above the background, so very much visible in the current optical Bragg scattering experiments. Slightly away from 1/2 filling, the VBS may turn into VB Supersolid (VB-SS) through a second order transition. We have $\langle K_\pi(q) \rangle = B \delta_{\vec{q},\vec{Q}} + K \delta_{\vec{q},\vec{Q}_K}$ and $\langle n(q) \rangle = (\delta n + 1/2) \delta_{\vec{q},\vec{0}}$. The superfluid density $\rho_s \sim \delta n = n - 1/2$. The scattering cross section inside VB-SS: $\tilde{\Sigma}_{VB-SS}(\vec{Q}_K) \sim |f_\pi(\pi,0)|^2 N^2 K^2$ stays more or less the same as that inside the VBS, but $\tilde{\Sigma}_{VB-SS}(\vec{K}) \sim |f_0(2\pi,0)|^2 N^2 n^2 + |f_y(2\pi,0)|^2 N^2 (\delta n)^2 B_x^2 + |f_y(2\pi,0)|^2 N^2 (\delta n)^2 B_y^2$ where $n = 1/2 + \delta n$ and the $B_x$, $B_y$ are the average bond strengths along $x$ and $y$ due to very small superfluid component $\rho_s \sim \delta n = n - 1/2$ flowing through the whole lattice. So the right peak in Fig.3b will increase due to the increase of the total density and the superfluid component inside the VB-SS phase. Very similarly, one can discuss the VBS order at $\vec{q} = \vec{Q}_K = (0,0)$. For the plaquette VBS order in Fig.2d, then one should be able to see the $S_K(\vec{q})$ peaks at both $(\pi,0)$ and $(0,\pi)$. So the dimer VBS and the plaquette VBS can also be distinguished by the optical Bragg scattering.

In this paper, we only focused on the optical Bragg scattering detections of the various ground states in a square lattice. The detections of the excitation spectra, the generalization to frustrated lattices, the effects of finite temperature and a harmonic trap will be discussed in a future publication.

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