Mott insulator transition in an ultracold Bose gas

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A Bose gas in an optical lattice can be described by the following model Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i, \tag{1}$$

where the operator $\hat{a}_i$ ($\hat{a}_i^\dagger$) destroys (creates) an atom at the site i. The notation $\langle i,j \rangle$ in the first sum of Eq. (1) indicates that the sum is restricted only to i and j that are nearest neighbors in the lattice. Defining $w_i(\mathbf{r}) = w(\mathbf{r} - \mathbf{r}_i)$ to be the wavefunction of an atom at the ith site of the lattice, the field operator can be written as follows:

$$\hat{\Psi}(\mathbf{r}) = \sum_i w_i(\mathbf{r}) \hat{a}_i. \tag{2}$$

In particular we will consider the case of a three dimensional cubic lattice with periodic boundary conditions: l is the elementary step in the lattice, M the total number of sites and the total number of atoms N is equal to the total number of sites, i.e. $N = M$. Even if the coefficients U and J can be calculated from the lattice parameters and the interatomic potential, here we shall consider them to be given parameters of the problem. In what follows, we will consider only repulsive interactions $U > 0$.

In what follows the aim is to give an interpretation to the experimental results obtained in Munich in the group of T. W. Hänsch [M. Greiner *et al.*, Nature **415**, 39 (2002))].

1. **Superfluid phase**.

   Let

   $$\hat{a}_s^\dagger = \frac{1}{\sqrt{M}} \sum_i \hat{a}_i^\dagger, \tag{3}$$

   be the operator creating one particle in the mode

   $$\phi(\mathbf{r}) = \frac{1}{\sqrt{M}} \sum_i w_i(\mathbf{r})\,. \tag{4}$$

   Consider the following state:

   $$|\mathrm{SF}\rangle = \frac{1}{\sqrt{N!}} \left(\hat{a}_s^\dagger\right)^N |0\rangle \tag{5}$$

   and give a physical interpretation. In particular calculate:

(a) the one-body density matrix $\rho^{(1)}(i,j) = \langle \hat{a}_i^\dagger \hat{a}_j \rangle$ and the single-particle correlation function $g^{(1)}$.

(b) the density fluctuations $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$

(c) the expectation value $\langle \mathcal{H} \rangle$

2. **Mott insulator phase**. Consider the following state:

$$|\mathrm{MI}\rangle = \Big(\prod_i \hat{a}_i^\dagger \Big) |0\rangle, \tag{6}$$

and give a physical interpretation in terms of Fock states for each site. In particular, calculate the one-body density matrix, the density fluctuations and the average energy. Is there a Bose Einstein Condensate macroscopically populated?

3. Determine which of the states $|\mathrm{SF}\rangle$ or $|\mathrm{MI}\rangle$ has lower energy as a function of the ratio U/J. Discuss qualitatively how the transition from a superfluid state to a Mott insulator state can be driven by modifying the parameters of the optical lattice.

4. Discuss the qualitative differences that may help to distinguish the insulating state from the superfluid state in an experience in the lab:

   (a) Determine the spectrum of the excited states of the system in the two limiting cases: $U = 0$ and $J = 0$. For the $U = 0$ case consider the following operators:

$$\hat{a}_{\mathbf{q}}^\dagger = \frac{1}{\sqrt{M}} \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\, \hat{a}_i^\dagger, \tag{7}$$

   creating a particle in the mode

$$\psi_{\mathbf{q}}(\mathbf{r}) = \frac{1}{\sqrt{M}} \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\, w_i(\mathbf{r})\,. \tag{8}$$

   Here $\mathbf{q}$ is the wavevector in the lattice

$$q_\alpha = \frac{2\pi n_\alpha}{\mathcal{N} l} \qquad \alpha = x, y, z \tag{9}$$

   where $\mathcal{N}^3 = N$, n_x, n_y, n_z are integers and $-\mathcal{N}/2 \le n_\alpha < \mathcal{N}/2$. Diagonalize the Hamiltonian with the help of these operators. In the two cases $U = 0$ and $J = 0$ determine if there is an energy gap between the ground state and the first excited state, in the limit $N \to \infty$.