The Mott transition in a gas of ultracold bosons

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

$$\mathcal{H} = -J \sum_{i,j} \delta_{ij}^{(1)} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i. \tag{1}$$

The $\hat{a}_i$ and $\hat{a}_i^\dagger$ respectively destroy and create an atom on the i-th site. The $\delta_{ij}^{(1)}$ function is non-vanishing and equal to 1 if and only if i and j are next-neighbor sites. Indicating with $w_i(\mathbf{r}) = w(\mathbf{r} - \mathbf{r}_i)$ the wavefunction for an atom localized on the i-th site of the lattice, the atomic field operator can be written as:

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

We focus our attention on the case of a 3D cubic lattice with periodic boundary conditions, containing a number N of atoms exactly equal to the number M of available sites. The parameters U and J can be calculated from the optical lattice parameters and the atom-atom interaction potential. Here, we shall consider them as input parameters of the problem. We shall limit our attention to the case of repulsive interactions $U > 0$.

1. Characterization of the **superfluid phase**. Consider a state of the form:

$$|\mathrm{SF}\rangle = \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{M}} \sum_i \hat{a}_i^\dagger \right)^N |0\rangle \tag{3}$$

   and try to provide a physical interpretation. In particular, evaluate:

   (a) the corresponding one-body density matrix $\rho^{(1)}(i,j) = \langle \hat{a}_i^\dagger \hat{a}_j \rangle$

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

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

   (d) the relative occupation of the different one-particle orbitals

2. Characterization of the **Mott insulator phase**. Consider a state of the form:

$$|\mathrm{MI}\rangle = \left(\prod_i \hat{a}_i^\dagger \right) |0\rangle \tag{4}$$

   and try to provide a physical interpretation in terms of Fock states for each site. In particular, evaluate the one-body density matrix, the density fluctuations, the expectation value of the energy. Does this state contain a macroscopically occupied Bose-Einstein condensate?

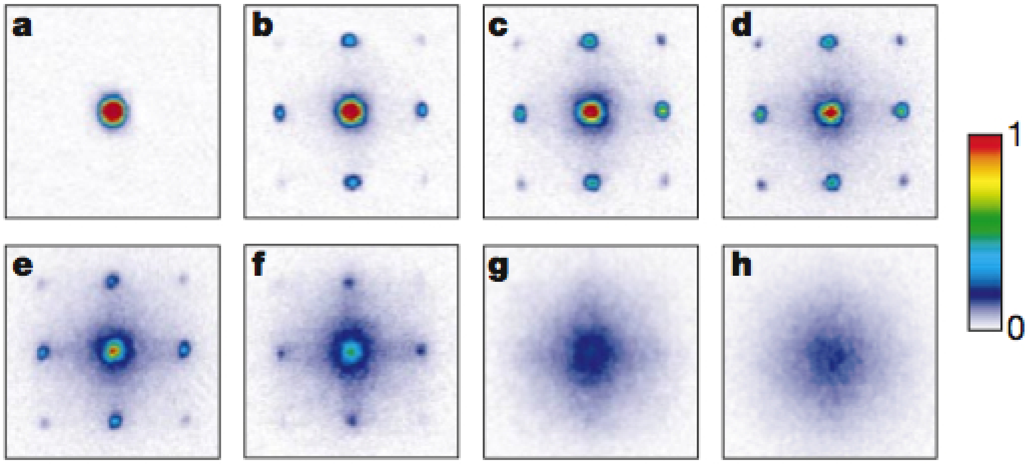

Figure 1: Momentum distribution for growing values of the lattice intensity (figure taken from M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, I. Bloch, Nature **415**, 39 (2002).

3. As a function of the ratio U/J, determine which one of the two states $|\mathrm{SF}\rangle$ or $|\mathrm{MI}\rangle$ has a lower energy. Discuss qualitatively how the transition from a superfluid to an insulator state can be induced by modifying the lattice parameters.

4. Discuss the qualitative differences that can help to distinguish an insulator state from a superfluid one in an actual experiment:

   (a) Study the spectrum of the excited states of the system in the two limiting cases $U = 0$ and $J = 0$; in particular, determine whether this spectrum shows an energy gap between the ground and the lowest excited state.

   (b) Determine the momentum distribution of the atoms in the two cases and comment the experimental figure.