# Bose Hubbard Model

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## Introduction

The Bose Hubbard model is a simple theoretical model to describe the physics of interacting bosons, confined on a (mostly optical) lattice. It was introduced in 1963 by John Hubbard. It can be used in solid state physics to understand the phenomena of superconductivity qualitatively.

Within this seminar talk we first describe the optical lattices which are essential for the further understanding and experimental realization. Then the Bose Hubbard model will be introduced and the phase transition from a superfluid phase into a Mott insulating phase is derived. Some experimental results are summarized within the last section.

## Motivation

For a given problem, the first aim of theoretical physicists is to simplify a complex system into one, describable very easily, but representing the physics in a correct manner. Therefore, bosons inside the solid state (e.g. cooper pairs) will be represented by particles inside an optical lattice. The big advantage of this system rebuilding is the larger scale of the new system. It is at least three orders of magnitude bigger, because the new lattice constant is given by the laser wavelength $\lambda$:

1) optical: $d_{lat} \approx \frac{\lambda_{Laser}}{2} \approx 10^{-6}\,\mathrm{m}$
2) solid state: $d_{lat} \approx 10^{-10}\,\mathrm{m}\ \left(\text{Å}\right)$

Now have a look on figure 1. The confinement potential of the original solid state is represented by the laser potential, created by a standing wave with the depth $V_0$. Thus, a three dimensional lattice can be described by

$$V(x,y,z) = \sum_i V_0 \sin^2(ki) \ .$$

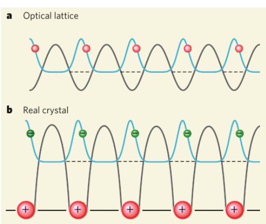


Figure 1. The solid state of matter is rebuilt using an optical lattice. The dimensions are at least three orders of magnitude larger.

The behavior of the particles, confined inside the optical lattice is described by the Boson Hubbard model.

## Optical lattice

First we have a look on the confinement potential of an optical lattice. This can be calculated by

$$\Delta E = U_{dip} = -\frac{1}{2}\langle \boldsymbol{pE}\rangle = -\frac{1}{2}\Re(\alpha(\omega))\left\langle E^2(t)\right\rangle$$

where $\boldsymbol{p}$ denotes the electric dipole moment and $\boldsymbol{E}$ the electric field. The pre-factor $1/2$ is used, because the dipole moment is an induced one. This can be rewritten as

$$U_{dip} = -\frac{1}{2\epsilon_0 c}\Re(\alpha(\omega))\cdot I \ ,$$

and connected to the laser parameters with

$$U_{dip} = \frac{3\pi c^2}{2\omega_0^3}\cdot\frac{\Gamma}{\Delta}\cdot I(x) \propto \frac{\Gamma}{\Delta}\cdot I(x) \ ,$$

where $\Gamma$ denotes the resonance damping (spontaneously photon decay rate of excited state), $\Delta \equiv \omega - \omega_0$ the laser detuning, $\omega_0$ the 2-niveau resonance and $I$ the laser intensity. Figure 2 is an graphical illustration of these parameters.

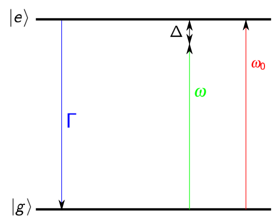


Figure 2. 2-niveau system with a ground state $|g\rangle$ and an excited state $|e\rangle$. Resonant frequency (red), laser frequency (green) and resonance damping (blue) are shown.

The scattering rate (spontaneous reemission) can be calculated to

$$\Gamma_{sc} = \frac{3\pi c^2}{2\hbar\omega_0^3}\cdot\left(\frac{\Gamma}{\Delta}\right)^2\cdot I(x) \propto \left(\frac{\Gamma}{\Delta}\right)^2\cdot I(x) \ .$$

A comparison of the dependencies in $\Gamma$ and $\Delta$ we can summarize:

- Below atomic resonance ("red" shifted) ($\omega < \omega_0$) we get
  - $\Delta < 0 \rightarrow U_{dip} < 0$
  - attractive potential

For experiments it is important to know:

Use for optical traps (at a certain potential depth)
- large detunings
- high intensities

## Bose Hubbard model

Once the particles are trapped, they can be described by the Hubbard Hamiltonian

$$H_B = -J \sum_{\langle ij \rangle} \left( \hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i \right) - \mu \sum_i \hat{n}_{bi} + \frac{U}{2} \sum_i \hat{n}_{bi} \left( \hat{n}_{bi} - 1 \right)$$

$$\left[ \hat{b}_i, \hat{b}_j^\dagger \right] = \delta_{ij}$$

- $J$: Allows hopping of bosons / Josephson tunneling
- $\mu$: Chemical potential
- $U > 0$: Repulsive interaction

Figure 3 represents these parameters graphically. We have to keep in mind, if the laser induced confinement potential is deepened $J$ will decrease.

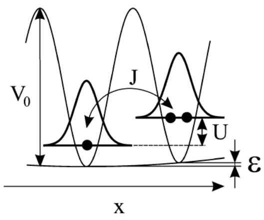


Figure 3. Explanation of the parameters in the Hubbard Hamiltonian.

Using the mean field approximation we can rewrite this Hamiltonian to

$$H_{MF} = \sum_i \left( -\mu \hat{n}_{bi} + \frac{U}{2} \hat{n}_{bi} \left( \hat{n}_{bi} - 1 \right) - \Psi_B^* \hat{b}_i - \Psi_B \hat{b}_i^\dagger \right)$$

- $\Psi_B$: variational parameter (complex)
- $\mu$: Chemical potential
- $U > 0$: Repulsive interaction

Now we use the Landau symmetry of a phase transition second order, which leads to the ground state energy $E_0$

$$E_0 = E_{00} + r \left| \Psi_B \right|^2 + \mathcal{O}\left( \left| \Psi_B \right|^4 \right) .$$

Use perturbation theory till second order we can identify $r$ to be

$$r = x_0 \cdot \left( 1 - ZJx_0 \right) ,$$

where $x_0$ is given by

$$\begin{aligned} x_0 \left( {}^{\mu}/_{U} \right) &= \frac{n \left( {}^{\mu}/_{U} \right) + 1}{Un \left( {}^{\mu}/_{U} \right) - \mu} + \frac{n \left( {}^{\mu}/_{U} \right)}{\mu - u \left( n \left( {}^{\mu}/_{U} \right) - 1 \right)} \\ &= - \frac{\mu + U}{\left( Un - \mu \right) \left( U \left( n - 1 \right) - \mu \right)} . \end{aligned}$$

For a phase transition $r$ must equal zero, which can be achieved when the term inside the bracket vanishes. This leads to

$$\frac{ZJ}{U} = \frac{\left( n - \frac{\mu}{U} \right) \left( 1 - n + \frac{\mu}{U} \right)}{1 + \frac{\mu}{U}} .$$

Figure 4 is a plot of the function above. At this point we have to point out that there is the critical point (with $n = 1$)

$$\left( {}^{ZU}/_{J} \right)_c \approx 0.172 \Leftrightarrow \left( {}^{J}/_{U} \right)_c \approx 5.8 \cdot Z . \qquad (1)$$

Here $n$ denotes the filled energy level of the system.

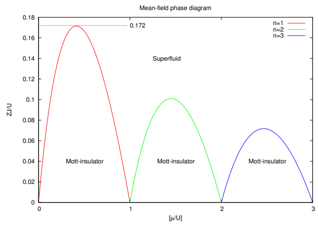


Figure 4. Phase diagram which represents the superfluid - Mott insulating transition. The critical level at $n = 1$ is derived to be $\left( {}^{J}/_{U} \right)_c \approx 5.8 \cdot Z$.

The wave-functions in both cases can be described as:

1) U=0: Superfluid phase

$$\left| \Psi_{SF} \right\rangle_{(U=0)} = \frac{1}{\sqrt{N!}} \left( \frac{1}{\sqrt{N_L}} \sum_{i=1}^{N_L} \hat{b}_i^\dagger \right)^N \left| 0 \right\rangle$$

2) J=0: Mott insulating phase

$$\left| \Psi_{MI} \right\rangle_{(J=0)} \propto \prod_{i=1}^{N_L} \left( \hat{b}_i^\dagger \right)^n \left| 0 \right\rangle$$

## Experimental evidence

In an experiment using an optical lattice ($d = 426\,\mathrm{nm}$) the SF-MI phase transition was observed with the time of flight method, using an expansion time of 15 ms. Figure 5 shows the resulting data. It can be understood as the Fourier transformation of a periodical potential, which results in $\delta$-peaks at certain values, if the matter waves can interfer - the system is in the superfluid phase (b-e). After the phase transition the wave functions are decoherent and no interference pattern is visible (g-h).

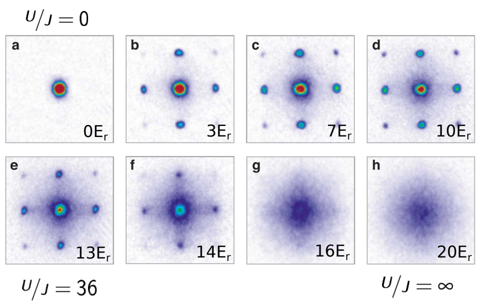


Figure 5. Interference experiment which demonstrates the SF-MI phase transition at a certain potential depth (e).

We can summarize that the experimental results are in good agreement with the former derived theory:

- SF-MI transition (experiment): ${}^{U}/_{J} = 36|_{Z=6} \rightarrow {}^{U}/_{J} = 6$
- SF-MI transition (theory): ${}^{U}/_{J} = 5.8$