Bosons in optical lattices

Marc Cheneau

February 3, 2020

Caution: these notes were written for the sole use of your teacher. There are not a full-featured lecture report and may contain errors.

1 Optical lattices

Optical lattices are periodic potentials for ultracold atoms created by the interference pattern of several far-off-resonance laser beams. The origin of the potential is the AC Stark shift (also called *dipolar potential* or *light shift*) of the electronic levels induced by the interaction of the atomic electric dipole with the local laser field. In this first section we remind you of a few important properties of the dipolar potential. A more complete introduction can be found in a review article by Grimm, Weidemüller, and Ovchinnikov (2000).

1.1 Two-level atom

We denote by d_0 the reduced dipole of the electronic transition, and by ω_0 its angular frequency. The dipolar potential induced by a far-off-resonant laser field with an angular frequency ω and a local amplitude $\mathcal{E}(\mathbf{r})$ is given by the relation:

$$V(\mathbf{r}) = \frac{d_0^2 \mathcal{E}(\mathbf{r})^2}{4\hbar\bar{\Delta}} , \quad \text{with} \quad \frac{1}{\bar{\Delta}} = \frac{1}{\omega - \omega_0} + \frac{1}{\omega + \omega_0} .$$

This relation is obtained within a perturbative approach, and valid to lowest order in $d_0\mathcal{E}/\hbar\bar{\Delta}$. The off-resonance condition is to be considered with respect to the natural transition linewidth Γ: the detuning $\Delta = \omega - \omega_0$ between the laser and the electronic transition must satisfy the inequality $\Delta \gg \Gamma$.

We note two important properties:

- the dipolar potential is proportional to the square of the electric field amplitude, that is to the light intensity;
- the sign of the dipolar potential depends on the detuning Δ. The potential can either be negative and minimum where the light intensity is maximum, or positive and maximum where the light intensity is maximum.

1.2 Multi-level atom

For a real atom, the light field usually interacts with more than one electronic transition. Within the perturbative approach, the total dipolar potential is simply the sum of the dipolar potentials associated with each transition:

$$V(\mathbf{r}) = \sum_i \frac{d_i^2 \mathcal{E}(\mathbf{r})^2}{4\hbar\bar{\Delta}_i} \ .$$

1.3 Rotating wave approximation

As long as the detuning Δ remains very small compared to ω_0, one can neglect the term proportional to $1/(\omega + \omega_0)$ and keep only the term proportional to $1/(\omega - \omega_0)$. This approximation is called **rotating wave approximation**. Note that there are many orders of magnitudes between the transition linewidth and the transition frequency, which leave plenty of room for a light field to be far off-resonant, while still justifying the rotating wave approximation.

1.4 Optical lattices

The simplest instance of an optical lattice is obtained by interfering two counter-propagating laser fields of same frequency. Writing both laser fields

$$\mathcal{E}_0 \cos(kx - \omega t) \quad \text{and} \quad \mathcal{E}_0 \cos(-kx - \omega t) \ ,$$

the total field amplitude at a position $\mathbf{r}$ and time t is given by

$$\mathcal{E}(\mathbf{r}, t) = \mathcal{E}(x) \cos(\omega t) \quad \text{with} \quad 2\mathcal{E}_0 \sin(kx) \ .$$

The dipolar potential therefore reads:

$$V(\mathbf{r}) = V(x) = V_0 \ \sin^2(kx) \ , \quad \text{with} \quad V_0 = \frac{d_0^2 \mathcal{E}_0^2}{4\hbar\bar{\Delta}} \ .$$

2 Single-particle eigenstates in a periodic potential

In this section we restrict the discussion to a *one-dimensional geometry*, and assume that particles are able to move only along the x-axis.

2.1 Bloch theorem

Let us consider for a moment a generic periodic potential $V(x)$ of period a. This can be a sinusoidal potential, or a more complex potential. The **Bloch theorem** states that the energy eigenstates of the single-particle Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \ ,$$

are parameterized by two **quantum numbers**, denoted n and q, and can be put in the form:

$$\varphi_{n,q}(x) = e^{iqx} u_{n,q}(x) \ , \tag{1}$$

where the functions $u_q(x)$ are themselves periodic with period a. These eigenstates are called **Bloch states** or **Bloch waves**. The functions $u_{n,q}(x)$ are called **Bloch functions**.

The quantum number q is called the **quasimometum**. It is a real number defined modulo $2k$. One usually restricts the values of q to the so-called **first Brillouin zone** $[-k; k[$ (or $]-k; k]$). The quantum number n is a positive integer.

Although the quasimometum of a particle in a periodic potential bares resemblance with the momentum of a free particle, the two quantities should not be mixed up. A Bloch state *does not* have a well defined momentum. Instead, owing to the periodicity in space of the Bloch function $u_q(x)$, it has overlap with all plane waves with a wave-vector $q + 2jk$:

$$\varphi_{n,q}(x) = e^{iqx} \sum_{j \in \mathbb{Z}} c_{n,j}(q)\, e^{2ijkx} \ , \quad c_j(q) \in \mathbb{C} \ . \tag{2}$$

2.2 Energy bands

The eigenenergies of the periodic Hamiltonian are smooth functions of q and verify the following inequality:

$$\varepsilon_{n-1}(q) < \varepsilon_n(q) \ , \ \ \forall\, (n, q) \ .$$

This means that the spectrum consists of **bands** separated by gaps of forbidden energies. Each band forms a continuum parametrized by the quasimometum q. The quantum number n is called the **band index**.

When the depth of the periodic potential increases, the gaps between the energy bands become wider and the bands become more flat. In the so-called tight-binding limit, which we will introduce later one, and for simple sinusoidal potentials as given in **??**, the energy bands verify:

$$E_n(q) \simeq 2J_n \cos(aq) \ ,$$

where J_n is a real number having the properties $J_n = (-1)^{n+1}|J_n|$ and $|J_{n+1}| > |J_n|$.

2.3 Tight-binding limit

The single-particle eigenstates in a periodic potential are *delocalised* in space and characterised by the quasimometum, a quantity which bares some resemblance with the momentum of free particles. The amplitude of the wavefunctions, however, is modulated by the underlying potential and low-energy states have

more weight arounf the potential minima than around the potential maxima. In deep lattices, this modulation gets so strong that it may become advantageous to describe the particle's state using a basis of *localised* wavefunctions. In this section we explain how to construct such functions, called Wannier functions, present their main properties, and derive the Hamiltonian matrix elements in this basis. We will see that, in the limit of deep lattices, particles must tunnel through the energy barrier to move from one lattice site to another.

2.3.1 Wannier functions

A wavefunction localised around a minimum $x = ja, j \in \mathbb{Z}$ of the potential $V(x)$ can be constructed by summing all Bloch waves multiplied by a phase factor ensuring that the waves coherently add up at the point $x = ja$:

$$w_{n,j}(x) = \left(\frac{a}{2\pi}\right)^{1/2} \int_{-k}^{+k} \mathrm{d}q \; e^{-ijaq} \, \varphi_{n,q}(x) \; . \tag{3}$$

This procedure should be performed within a given energy band. It results in a set of functions called Wannier functions: $\{w_{n,j}(x)\}$, $n \in \mathbb{N}, j \in \mathbb{Z}$. From the above definition we can immediately deduce that:

- the Wannier states form an orthonormal basis of the Hilbert space;
- the Wannier states *are not* eigenstates of the Hamiltonian;
- the Wannier functions belonging to a given energy band but centred on different minima of the potential are all identical: $w_{n,j}(x) = w_{n,0}(x - ja)$.

The decomposition of Wannier states in the basis of Bloch states can be inverted to obtain the decomposition of Bloch states in the basis of Wannier states:

$$\varphi_{n,q}(x) = \left(\frac{a}{2\pi}\right)^{1/2} \sum_{j \in \mathbb{Z}} e^{ijaq} \, w_{n,j}(x) \; , \tag{4}$$

where we have made use of the equality $\sum_{j\in\mathbb{Z}} e^{ijaq} = (2\pi/a)\,\delta(q)$.

The exact form of Wannier functions depends on the arbitrary choice of absolute phase made when defining the Bloch states. One can show, however, that there exists a unique phase choice for which the Wannier functions have the following useful properties:

- the Wannier functions are real;
- they are either even or odd with respect to $x = 0$ or $x = a/2$;
- they tend to zero exponentially away from their centre.

For the lattice potential $V(x) = V_0 \sin^2(kx)$, this definition of the Bloch states corresponds to choosing $\varphi_{n,q}(0)$ a real positive number when n is even, and $(\mathrm{d}\varphi_{n,q}/\mathrm{d}x)(0)$ a real positive number when n is odd.

2.4 Tunnelling amplitudes

The Wannier states are no energy eigenstates. The matrix elements of the Hamiltonian in the Wannier state basis are formally defined by the relation

$$J_{n,n'}(j,j') \equiv \langle w_{n',j'}|\hat{H}|w_{n,j}\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\; w^*_{n',j'}(x)\left[\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right] w_{n,j}(x)\;.$$

A more useful expression can be obtained using the decomposition of Wannier states in the Bloch state basis:

$$\begin{aligned} J_{n,n'}(j,j') &= \frac{a}{2\pi}\int_{-k}^{+k}\mathrm{d}q' \int_{-k}^{+k}\mathrm{d}q\; e^{ij'aq'}\, e^{-ijaq}\,\langle\varphi_{n',q'}|\hat{H}|\varphi_{n,q}\rangle \\ &= \frac{a}{2\pi}\int_{-k}^{+k}\mathrm{d}q' \int_{-k}^{+k}\mathrm{d}q\; e^{ij'aq'}\, e^{-ijaq}\, E_n(q)\,\langle\varphi_{n',q'}|\varphi_{n,q}\rangle\;. \end{aligned}$$

Since the Bloch state basis is orthonormal, we can replace $\langle\varphi_{n',q'}|\varphi_{n,q}\rangle$ by the product of the Kronecker symbol $\delta_{n,n'}$ and the delta function $\delta(q-q')$. This gives:

$$\begin{aligned} J_{n,n'}(j,j') &= \frac{a}{2\pi}\int_{-k}^{+k}\mathrm{d}q' \int_{-k}^{k}\mathrm{d}q\; e^{ij'aq'}\, e^{-ijaq}\, E_n(q)\,\delta_{n,n'}\,\delta(q-q') \\ &= \frac{a}{2\pi}\int_{-k}^{+k}\mathrm{d}q\; e^{-i(j-j')aq}\, E_n(q)\,\delta_{n,n'}\;. \end{aligned}$$

The Hamiltonian thus couples only Wannier states from the same energy band. Also, the coupling between Wannier states appears to be a function of $j-j'$ only. Physically, the coupling between Wannier states means that a particle initially localised around a lattice site j will be able to *move* to neighbouring lattice sites by *tunnelling* through the potential barrier that separates the sites. For this reason, the Hamiltonian matrix elements in the Wannier state basis are often called **tunnelling amplitudes**, or **tunnel coupling**.

In deep lattices, the tunnelling amplitudes decay exponentially with $|j-j'|$ and one can neglect the tunnel couplings when $|j-j'|>0$. This is the so-called **tight-binding limit**. Within this limit, only neighbouring lattice sites are coupled via the tunnelling amplitude

$$J_n = \frac{a}{2\pi}\int_{-k}^{+k}\mathrm{d}q\; E_n(q)\;.$$

Also, the dynamics is usually restricted to a *single band* because the gap between energy bands is large.

3 Interacting bosons in a lattice

Until now, we have discussed the physics of a single particle in a periodic lattice. We now consider a far more complex system, namely a system of interacting,

identical particles. This problem is relevant in condensed-matter physics, as many properties of crystalline solids can be understood by considering the motion of electrons in the periodic ionic potential. Experiments with ultracold atoms in optical lattices are very good examples of *quantum simulation* as they offer a complementary perspective on this problem. See for instance Jaksch and Zoller (2005). The lattice geometry can be tuned almost at will by changing the configuration of interfering laser beams: wavelength, number of beams, angle and relative phase between them, etc. One can study both fermionic and bosonic particles, depending on the atomic species and isotope. The interactions between atoms can be modified using Feshbach resonances. And much more...

In the following we will restrict the discussion to the case of **indistinguishable bosonic particles in the tight-binding limit**. The interaction between particles will be modelled as a **2-body contact interaction**. We will furthermore suppose that the particles are confined in the **lowest energy band**. This model of particles in a periodic potential is called the **bosonic Hubbard model**.

3.1 The bosonic Hubbard Hamiltonian

The best suited formalism to describe a system of indistinguishable particles is in terms of Fock states. As a single-particle basis, we use the set of Wannier states. A Fock state $|\prod_j n_j\rangle$ thus represents a state where each lattice site j is occupied by n_j particles and the total particle number is $N = \sum_j n_j$.

The Hamiltonian expressed in the Fock basis of Wannier states reads:

$$\hat{H} = \sum_j \left\{ J\hat{a}_j^\dagger \hat{a}_{j+1} + J\hat{a}_{j+1}^\dagger \hat{a}_j + \frac{U}{2}\hat{n}_j(\hat{n}_j - 1) \right\} . \tag{5}$$

The operators $\hat{a}_j$ and $\hat{a}_j^\dagger$ are the annihilation and creation operators for our bosonic particles. The operator $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$ counts the number of particles in the site j.

The terms $J\hat{a}_j^\dagger \hat{a}_{j+1}$ and $J\hat{a}_{j+1}^\dagger \hat{a}_j$ correspond to the kinetic energy. They physically describe the tunnel coupling between the sites j and $j+1$, with an amplitude $J = J_{n=0} < 0$. The term $U\hat{n}_j(\hat{n}_j - 1)/2$ describes the interaction between the particles: if n_j particles occupy a site j, there are $n_j(n_j - 1)/2$ pairs of interacting particles, each with an interaction energy U. The interaction energy is proportional to the interaction strength $g = 4\pi\hbar^2 a_{\mathrm{sc}}/m$, where a_{sc} is the s-wave scattering length introduced in a previous lecture.

Whether we are interested in treating a problem with a fixed number of particles or in the grand-canonical ensemble, one will in both cases consider the free energy, rather than the Hamiltonian:

$$\hat{H} - \mu\hat{N} = \sum_j \left\{ J\hat{a}_j^\dagger \hat{a}_{j+1} + J\hat{a}_{j+1}^\dagger \hat{a}_j + \frac{U}{2}\hat{n}_j(\hat{n}_j - 1) - \mu\hat{n}_j \right\} ,$$

where μ is the chemical potential and $\hat{N} = \sum_j \hat{n}_j$ is the operator counting the total number of particles.

One can also account for the presence of an external trapping potential $V_{\text{trap}}(x)$ in addition to the lattice potential:

$$\hat{H} = \sum_j \left\{ J\hat{a}_j^\dagger \hat{a}_{j+1} + J\hat{a}_{j+1}^\dagger \hat{a}_j + \frac{U}{2}\hat{n}_j(\hat{n}_j - 1) + V_{\text{trap}}(ja)\hat{n}_j \right\} .$$

3.2 Hamiltonian in the Bloch state basis

It can be instructive to look at the Hubbard Hamiltonian also in the Bloch state basis. Introducing the annihilation and creation operators in a Bloch state with quasimomentum q, written $\hat{a}(q)$ and $\hat{a}^\dagger(q)$, on shows that

$$\hat{H} = \int_{-k}^{+k} \mathrm{d}q \, \frac{\hbar^2 q^2}{2m} \hat{n}(q) + \frac{g}{2} \iint_{-k}^{+k} \mathrm{d}q' \mathrm{d}q \, \hat{a}^\dagger(q')\hat{a}^\dagger(q)\hat{a}^\dagger(q)\hat{a}^\dagger(q') \, . \tag{6}$$

Note that, in the presence of an external trapping potential, the Bloch states are no longer eigenstates of the single-particle Hamiltonian because the discrete translation invariance of the Hamiltonian is broken.

3.3 Experimental control over the parameters of the model

In the context of optical lattices, the parameter J can be tuned by varying the lattice depth V_0, which is simply achieved by varying the intensity of the interfering laser beams. Changing the lattice depth indeed modifies the spread of the Wannier functions, and thus the value of the overlap integrals defining the tunnelling amplitudes (see **??**). The interaction parameter U, which depends on the s-wave scattering length, can be modulated by means of a Feshbach resonance.

4 The transition from a superfluid to a Mott insulator

In this section we focus on the nature of the **ground-state** in the bosonic Hubbard model. We will see how it radically changes depending on the strength of the interactions, revealing the existence of a **quantum phase transition**.

4.1 Competition between the kinetic and interaction energies

The kinetic and interaction energy terms are non-commuting. The first is diagonal in the Bloch state basis, while the second is diagonal in the Wannier state basis. The nature of the many-body ground state therefore depends on the relative magnitude of J and U.

When $J \gg U$, the ground state will tend to minimize the kinetic energy rather than the interaction energy. This is achieved by putting most particles in the Bloch state with quasimomentum $q = 0$, up to small corrections in U/J. Such state can be described as a Bose–Einstein condensate and displays a *superfluid character*.

When $J \ll U$, we have the opposite situation. The ground state will tend to minimize the interaction energy by localizing each particle in a lattice site in such a way that the density fluctuations are small. If the number of particles in the system is equal to an integer number times the number of lattice site, the interaction energy will reach an absolute minimum when the number of particles per site (called the *lattice filling*) is fixed to that integer number. When this is the case, the ground state displays an *insulating character* because setting a particle in motion costs at least a finite energy U.

The intermediate regime where $J \sim U$ turns out to be very difficult to work out analytically. In the next section we will attempt to cover the whole parameter range using a mean-field approximation, which will reveal the existence of a phase transition.

4.2 Mott insulator vs band insulator

The only way a system of bosonic particles in a periodic potential can be an insulator is when interactions between the particles are strong, as we just discussed. Such insulator is called a **Mott insulator**. For fermions, there can exist another type of insulator, called **band insulator**. It is obtained trivially at integer filling, when all single-particle states from the lowest energy bands are occupied by exactly one fermion. In such situation, setting a particle into motion costs at least an energy equal to the gap between the highest occupied energy band and the one just above. There is no need for interactions between the fermionic particles to realize a band insulator. It is only a consequence of the band structure and the Pauli exclusion principle. Most condensed matter materials with an insulating character are actually band insulators, and not Mott insulators.

4.3 Mean-field approximation

In this context, the mean-field approximation rests on the hypothesis that a significant fraction of the particles form a Bose–Einstein condensate in the Bloch state with $q = 0$. We thus focus a priori on the regime where $J \ll U$. Denoting $|0\rangle$ the many-body ground state, this hypothesis can be formerly expressed by writting:

$$\langle \hat{a}_j \rangle = \Psi_0 \; ; \quad \langle \hat{a}_j^\dagger \rangle = \Psi_0^* \; ,$$

where Ψ_0 is the condensate wavefunction and the condensed fraction is $|\Psi_0|^2 = n_0$. Here we will further assume that the condensate wavefunction is a real number: $\Psi_0 = \Psi_0^*$.

Then we neglect all two-body correlations in the bosonic Hubbard Hamiltonian by making the replacement:

$$\hat{a}_j^\dagger \hat{a}_{j'} \simeq \langle \hat{a}_j^\dagger \rangle \hat{a}_{j'} + \hat{a}_j^\dagger \langle \hat{a}_{j'} \rangle - \langle \hat{a}_j^\dagger \rangle \langle \hat{a}_{j'} \rangle = \Psi_0 (\hat{a}_j + \hat{a}_{j'}^\dagger) - \Psi_0^2 \ .$$

We are thus left with the mean-field Hamiltonian:

$$\hat{H}^{\mathrm{mf}} = \sum_j \left\{ 2J \left[\Psi_0 (\hat{a}_j + \hat{a}_j^\dagger) - \Psi_0^2 \right] + \frac{U}{2} \hat{n}_j (\hat{n}_j - 1) \right\} \ .$$

Within the mean-field approximation, we see that the Hamiltonian is the sum of *un-coupled local Hamiltonians*:

$$\hat{H}^{\mathrm{mf}} = \sum_j \hat{H}_j \quad \text{with} \quad \hat{H}_j = 2J \left[\Psi_0 (\hat{a}_j + \hat{a}_j^\dagger) - \Psi_0^2 \right] + \frac{U}{2} \hat{n}_j (\hat{n}_j - 1) \ .$$

The ground state of the mean-field Hamiltonian can therefore be written as the product of local ground states:

$$|0\rangle = \prod_j |0\rangle_j \ ,$$

where $|0\rangle_j$ minimizes the local free energy $\hat{H}_j - \mu \hat{n}_j$.

In order to determine the local ground states, we expand them in the Fock basis:

$$|0\rangle_j = \sum_n c_n |n\rangle_j \ .$$

Here, $|n\rangle_j$ is the Fock state with n particles in the Wannier state centered on the site j and the coefficients c_n are complex numbers which do not depend on j since all lattice sites are equivalent. We then write that the local ground state is an eigenstate of the free energy:

$$(\hat{H}_j - \mu \hat{n}_j) |0\rangle_j = E_j |0\rangle_j \ ,$$

and project both members of the equation onto a Fock state $|n\rangle_j$ to obtain the equation:

$$E_j c_n = 2J\Psi_0 \left(\sqrt{n+1}\, c_{n+1} + \sqrt{n}\, c_{n-1} \right) + \left[\frac{U}{2} n(n-1) - \mu - \Psi_0^2 \right] c_n \ .$$

We end up with a set of coupled equations for the coefficients c_n, whose solution depends on E_j and Ψ_0. Minimizing E_j with respect to Ψ_0 finally yields the mean-field ground state as a function of μ, U and J.

4.4 Mean-field phase diagram

5 Experimental signatures of the superfluid-to-insulator transition

Transport properties are easily accessed in condensed matter experiments (think of an electrical resistance measurement), but not so easily in ultracold atom experiments. The quantity that is most often measured with ultracold atoms is the *momentum distribution*. The *spatial distribution* of atoms inside the confinement potential can also be measured, provided the experimental setup is equipped with a high-resolution imaging system. We will see now how these two quantities are affected by the superfluid-to-Mott insulator transition.

5.1 Momentum distribution

The momentum distribution in a many-particle state $|\Phi\rangle$ is formally defined by the relation

$$\rho(p) = \langle\Phi|\hat{a}^\dagger(p)\hat{a}(p)|\Phi\rangle \ .$$

Here, the annihilation and creation operators act on the plane-wave basis and the momentum p should not be confused with the quasimomentum q. In order to calculate this expectation value, we can express the annihilation and creation operators in the basis of Wannier states. Introducing the field operator $\hat{P}si(x)$, we can procedd as follows for the annihilation operator:

$$\begin{aligned}
\hat{a}(p) &= \int_{-\infty}^{+\infty} \mathrm{d}x \; e^{-ipx/\hbar} \, \hat{\Psi}(x) \\
&= \sum_j \left[\int_{-\infty}^{+\infty} \mathrm{d}x \; e^{-ipx/\hbar} \, w_j(x) \right] \hat{a}_j \\
&= \sum_j \tilde{w}_j(p) \, \hat{a}_j \\
&= \tilde{w}_0(p) \sum_j e^{-ija} \, \hat{a}_j \ .
\end{aligned}$$

For the last step of the derivation we have introduced the Fourier transform of the Wannier wavefunction $w_j(x)$, denoted by $\tilde{w}_j(p)$, and we have made use of the property $w_j(x) = w_0(x - ja)$. For the creation operator we obtain similarly:

$$\hat{a}^\dagger(p) = \tilde{w}_0^*(p) \sum_j e^{ija} \, \hat{a}_j^\dagger \ .$$

We can now rewrite the momentum distribution in the form

$$\rho(p) = |\tilde{w}_0(p)|^2 \sum_{j,j'} e^{-ip(j-j')a/\hbar} \, \langle\Phi|\hat{a}_{j'}^\dagger \, \hat{a}_j|\Phi\rangle \ .$$

The expectation values in the right-hand side have a very clear meaning: they correspond to the **first-order correlation function**, $g^{(1)}(j, j')$, which measures the **phase coherence** of the state Φ between the lattice sites j and j'. It is thus a **signature of the presence of a Bose–Einstein condensate**.

The first experimental evidence of the superfluid-to-Mott insulator transition in ultracold atomic gases was actually obtained by measuring the atomic momentum distribution after releasing the atoms from the optical lattice potential, see Greiner et al. (2002).

5.2 Density fluctuations

Next to the momentum distribution, density fluctuations can be used to probe the transition from a superfluid to a Mott insulator. Density fluctuations are characterised by the **second-order correlation function**:

$$\begin{aligned} g^{(2)}(j, j' = j) &\equiv \langle \Phi | \hat{a}_j^\dagger \, \hat{a}_j^\dagger \, \hat{a}_j \, \hat{a}_j | \Phi \rangle \\ &= \langle \Phi | \hat{n}_j (\hat{n}_j - 1) | \Phi \rangle \ . \end{aligned}$$

The second-order correlation function is directly proportional to the interaction energy in the Hubbard Hamiltonian. It is minimized in the insulating phase and takes large values in the superfluid state. The variation of local density fluctuations across the superfluid-to-Mott insulator could be observed for the first time in 2011 by the team at Max Planck Institute for Quantum Optics using the in-situ fluorescence imaging technique Endres et al. (2011).

6 References

Endres, M., Marc Cheneau, T. Fukuhara, C. Weitenberg, P. Schauß, C. Gross, L. Mazza, et al. 2011. "Observation of Correlated Particle-Hole Pairs and String Order in Low-Dimensional Mott Insulators." *Science* 334 (6053): 200–203. https://doi.org/10.1126/science.1209284.

Greiner, M., Olaf Mandel, Tilman Esslinger, Theodor W. Hänsch, and Immanuel Bloch. 2002. "Quantum Phase Transition from a Superfluid to a Mott Insulator in a Gas of Ultracold Atoms." *Nature* 415 (6867): 39–44. https://doi.org/10.1038/415039a.

Grimm, R., Matthias Weidemüller, and Yu. B. Ovchinnikov. 2000. "Optical Dipole Traps for Neutral Atoms." In *Advances in Atomic, Molecular, and Optical Physics*, edited by B. Bederson and H. Walther, 42:95–170. Academic Press.

Jaksch, Dieter, and Peter Zoller. 2005. "The Cold Atoms Hubbard Toolbox." *Annals of Physics* 315 (1): 52–79. https://doi.org/10.1016/j.aop.2004.09.010.