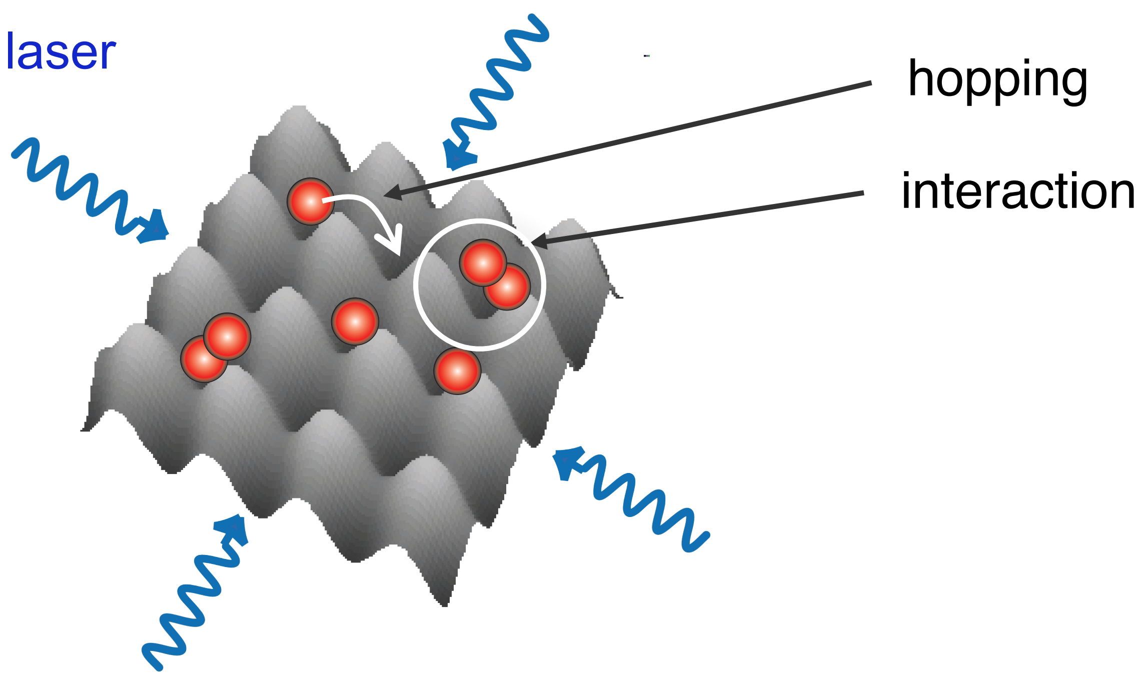
Application of 2nd Quantization:

Hubbard Models
&
Cold Atoms in Optical Lattices

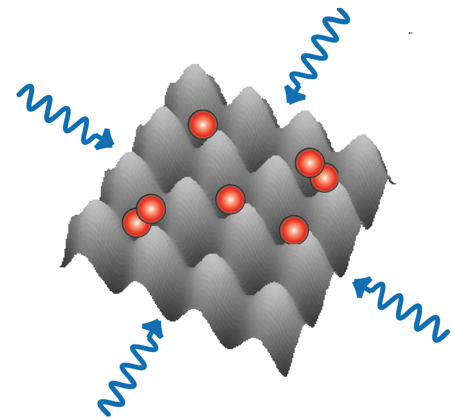
Bose Hubbard Model

System: We consider N bosonic particles moving on a lattice ("lattice gas") consisting of M lattice sites. The essential ingredients of the dynamics are

- hopping of the bosonic particles between lattice sites (kinetic energy)
- repulsive / attractive interaction between the particles (interaction energy)
- Bose statistics



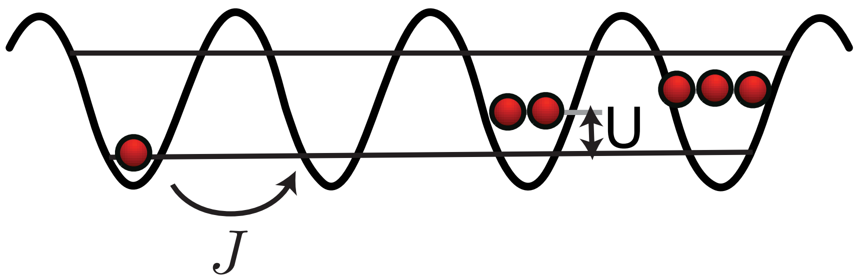
cold atoms in an optical lattice (see below)

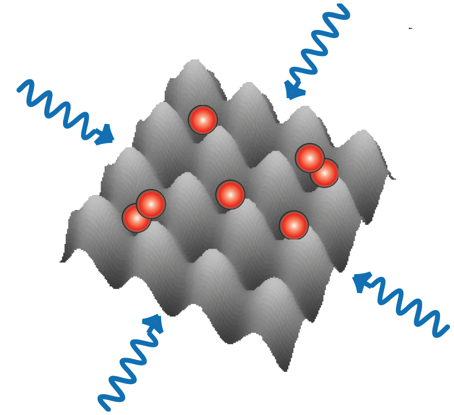


Bose Hubbard (BH) Hamiltonian:

$$\hat{H} = -J \sum_{<ij>} b_i^\dagger b_j + \frac{1}{2} U \sum_i b_i^{\dagger 2} b_i^2$$
$$= \hat{T} + \hat{V}$$

- **Second quantized notation:** b_i and $b_i^\dagger$ denote destruction and creation operators for bosons at lattice site i obeying commutation relations $\left[b_i, b_j^\dagger\right] = \delta_{ij}$. The occupation number operator for site i is $\hat{n}_i \equiv b_i^\dagger b_i$.
- **Kinetic energy:** the first term is the kinetic energy $\hat{T} = -J \sum_{<ij>} b_i^\dagger b_j$. It describes the hopping of electrons between adjacent lattice sites (notation $< i, j >$) with *tunneling amplitudes* $J > 0$.
- **Interaction energy:** the second term $\hat{V} = \frac{1}{2} U \sum_i b_i^{\dagger 2} b_i^2 \equiv \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)$ describes an *on-site interaction* U*,* when two bosons occupy the same site. (Typically we assume $U > 0$, i.e repulsive interactions to guarantee stability.)

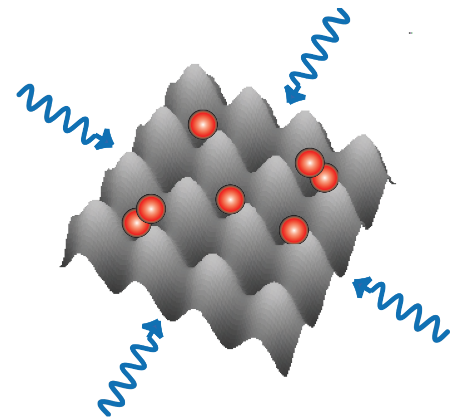




cold atoms in an optical lattice

Physical realization: (we will return to the details later)

- Atomic physics: loading cold bosonic atoms (from a Bose Einstein condensate) into an optical lattice
- Josephson junction array in mesoscopic solid state physics: in a superconductor electrons bind to form Cooper pairs, which behave as composite bosons. As JJ array is an array (lattice) of superconducing island connected by tunneling junctions.

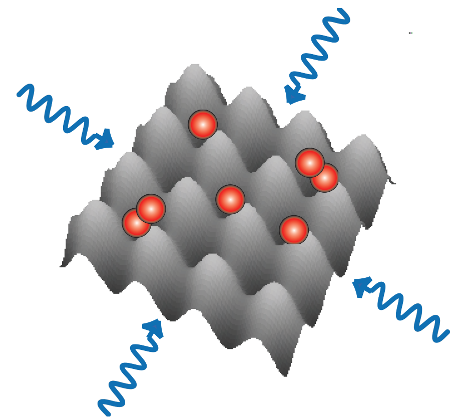


Fock space:

- On a single lattice site we have configurations with no boson, one, two etc. bosons: $|n_i\rangle_i = \frac{1}{\sqrt{n!}} b_i^{\dagger n_i} |\text{vac}\rangle$ with $n_i = 0, 1, 2, \ldots$ occupation numbers
- The total wave function of the system will be a superposition state

$$|\Psi\rangle = \sum_{\{n_i\}, \sum_i n_i = N} c_{\{n_i\}} |\{n_i\}\rangle$$

The Hamiltonian preserves the particle number $\hat{N} = \sum_i \hat{n}_i$, $\left[\hat{H}, \hat{N}\right] = 0$, which leads to the constraint $\sum_i n_i = N$.

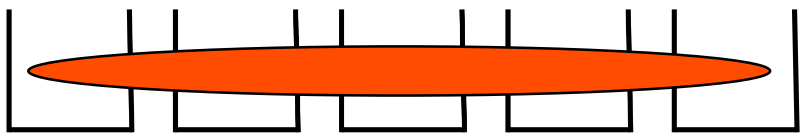


What we are interested in ...

- We will be mainly interested in the properties of the *ground state* of this system, and low energy excitations. The central question will be the *role of interactions, in particular the competition between the kinetic energy and interaction energy and the associated quantum phases and quantum phase transitions.*
- (Of course, finite temperature, and the complete phase diagram in the quantum degenerate regime are also of interest.)

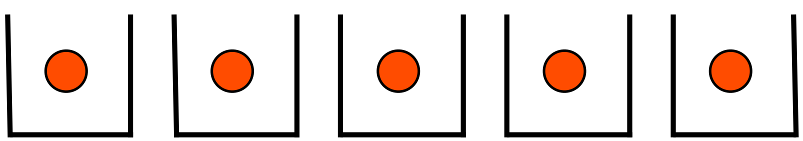
For the Bose Hubbard Model we expect ...

- for a weakly interacting gas $J \gg U$ the ground state will correspond to a *Bose Einstein condensate* (BEC). Interactions will result in a depletion of the condensate.



atoms delocalize (condense)
to minimize their energy

- with increasing interactions $J \ll U$, and depending on the filling of the lattice, other phases like a *Mott insulator* are possible.



atoms want to sit on different lattice sites to avoid seeing each other and thus to minimize their energy

- by tuning the parameter U/J the system can undergo a *quantum phase transition* from a BEC to a Mott phase at a critical U_c.

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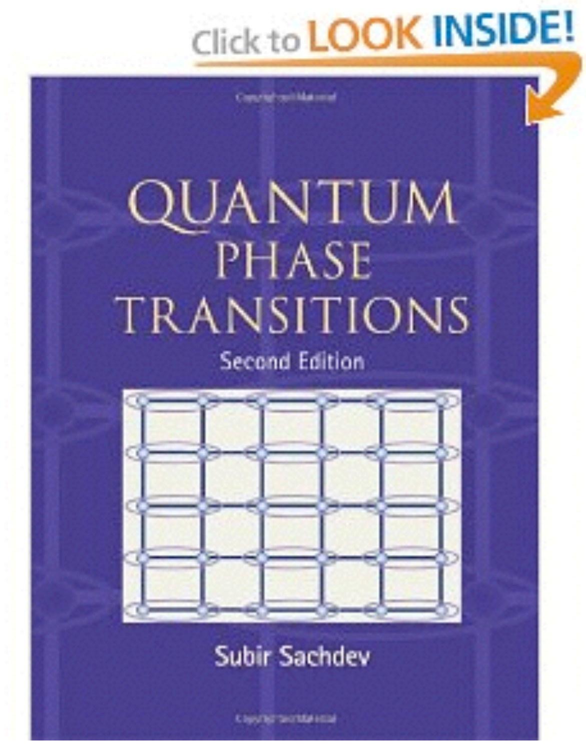


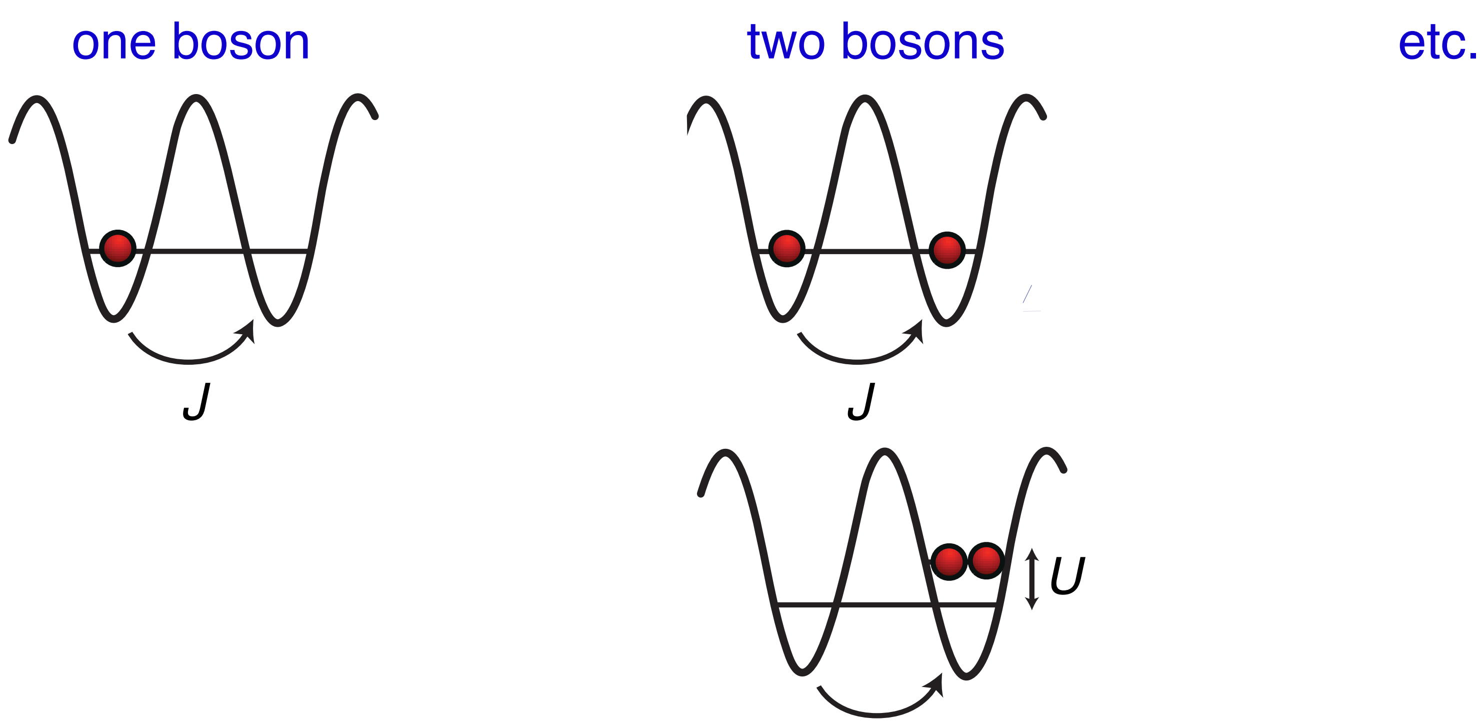
Quantum Phase Transitions
Subir Sachdev

A Toy Model: Bosons on Two Coupled Lattice Sites

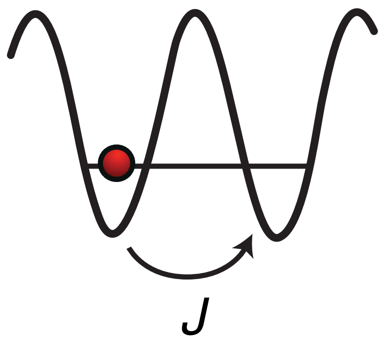
Model system: a good part of the physics of competition between hopping and interactions can be understood by considering bosons on two lattice sites.

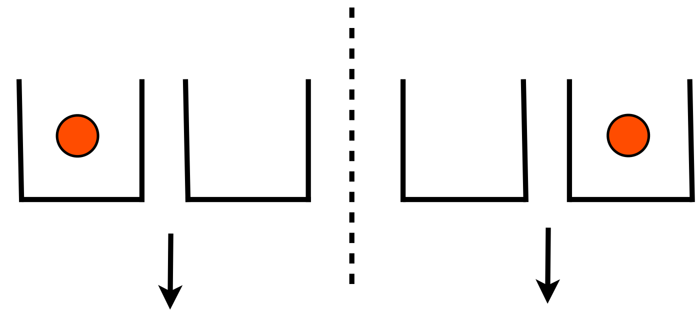
Hamiltonian

$$\hat{H} = -J(b_1^\dagger b_2 + b_2^\dagger b_1) + \frac{1}{2}U \sum_{i=1,2} b_i^{\dagger 2} b_i^2$$



One boson $N = 1$



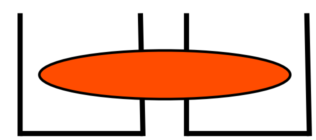


For a single particle, $N = 1$, the state space is $\left\{ |1,0\rangle \equiv b_1^\dagger |\mathrm{vac}\rangle, |0,1\rangle \equiv b_2^\dagger |\mathrm{vac}\rangle \right\}$. The Hamiltonian becomes a 2x2 matrix

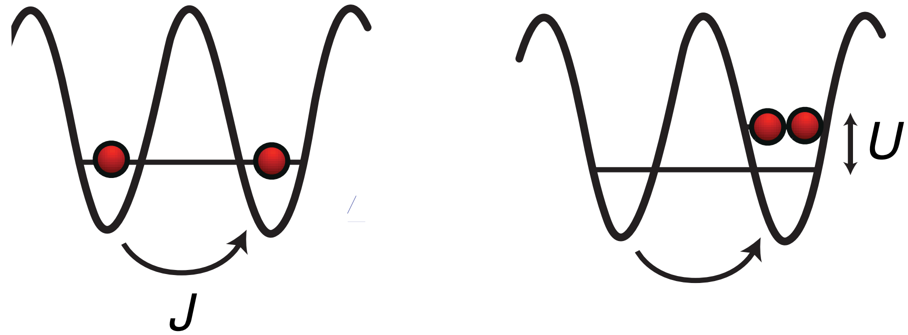
$$H = \begin{pmatrix} 0 & -J \\ -J & 0 \end{pmatrix}.$$

The ground (excited) state are the symmetric (antisymmetric) superposition

$$\frac{1}{\sqrt{2}}\left(b_1^\dagger + b_2^\dagger\right)|\mathrm{vac}\rangle \equiv \frac{1}{\sqrt{2}}\left(|1,0\rangle + |0,1\rangle\right) \quad E_0 = -J$$
$$\frac{1}{\sqrt{2}}\left(b_1^\dagger - b_2^\dagger\right)|\mathrm{vac}\rangle \equiv \frac{1}{\sqrt{2}}\left(|1,0\rangle - |0,1\rangle\right)E_1 = +J$$



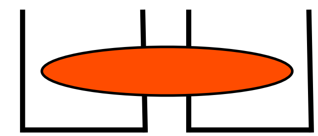
In the ground state the particle will lower its energy by delocalizing over the two lattice sites. (For one particle there is no interaction).



For two bosons, $N = 2$, we have a state space spanned by the configurations $\{|1,1\rangle, |2,0\rangle, |0,2\rangle\}$.

- In the weakly interacting limit $J \gg U \to 0$ the ground state is a "mini-condensate"

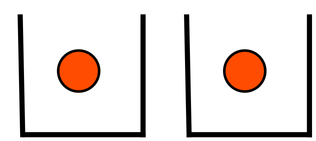
$$|\mathrm{BEC}\rangle \sim \left(b_1^\dagger + b_2^\dagger\right)^2 |\mathrm{vac}\rangle \sim \left(|2,0\rangle + \sqrt{2}\,|1,1\rangle + |0,2\rangle\right) \quad E_0 = -2J$$



i.e. the two particles occupy the same delocalized lowest-energy orbital.

- In the limit of strong interactions $J \ll U$ $(U > 0)$ the ground state is a "Mott insulator"

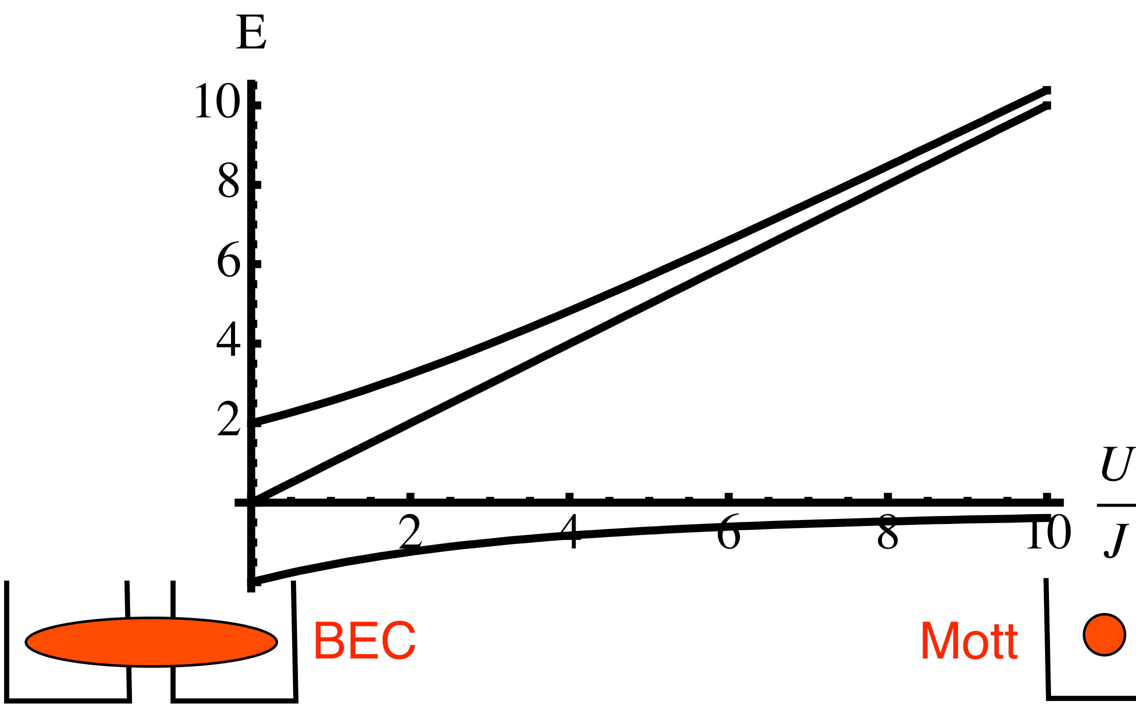
$$|\mathrm{Mott}\rangle = b_1^\dagger b_2^\dagger |\mathrm{vac}\rangle = |1,1\rangle \quad E_0 = 0$$

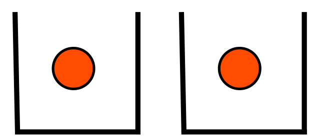


i.e. the particles occupy different lattice sites, thus avoiding the energy penalty from the strong repulsive interactions.

- In general the 3x3 Hamiltonian matrix is (with $\sqrt{2}$ in the kinetic energy term bosonic stimulation factors)[2]

$$H = \begin{pmatrix} 0 & -\sqrt{2}J & -\sqrt{2}J \\ -\sqrt{2}J & U & 0 \\ -\sqrt{2}J & 0 & U \end{pmatrix}$$



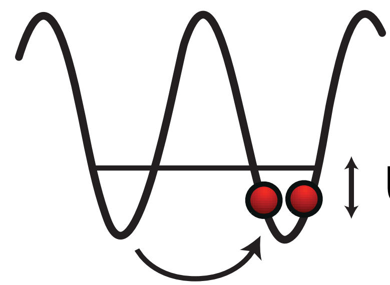


with eigenvalues and eigenvectors

$$\begin{array}{cc} U & (0,-1,1) \\ \frac{1}{2}\left(U-\sqrt{U^2+16J^2}\right) & \left(\frac{U/J+\sqrt{(U/J)^2+16}}{2\sqrt{2}},1,1\right) \\ \frac{1}{2}\left(U+\sqrt{U^2+16J^2}\right) & \left(\frac{U/J-\sqrt{(U/J)^2+16}}{2\sqrt{2}},1,1\right) \end{array}$$

Plot: We see a *crossover* between the *BEC* and the *Mott* state.

In the limit of a system with infinite number of lattice sites and infinite number of particles this crossover becomes sharper and sharper, and develops into a quantum phase transition [see Subir Sachdev, Quantum Phase Transitions (Cambridge, 1999)]. We will discuss this quantum phase transition below in a mean field theory.



Exercise:

- What happens for *attractive interactions* $U < 0$?
  - Show: For $|U| \gg J \to 0$ there are two degenerate states $|2,0\rangle$, $|0,2\rangle$
  - Show: With energy $E_0 = -|U|$, i.e. the bosons prefer to sit on the same site forming a “molecule” with binding energy $U < 0$. Including the kinetic energy results in a ground state $|2,0\rangle + |0,2\rangle$ with the molecule delocalized over two lattice sites.

    Remark: For a large number of bosons *all* particles want to sit on the same site. Typially, this situation will be unstable and the BH model might be physically unrealistic: for atoms due to the high density there will be strong collisional losses.

Remark: For a large number of bosons *all* particles want to sit on the same site. Typially, this situation will be unstable and the BH model might be physically unrealistic: for atoms due to the high density there will be strong collisional losses.

Overview of Limiting Cases: ideal BEC and Mott Phase

Non-interacting bosons (ideal BEC)

Independent bosons: Before considering the effect of interactions we must understand the (trivial) case of non-interacting bosons ($U = 0$).

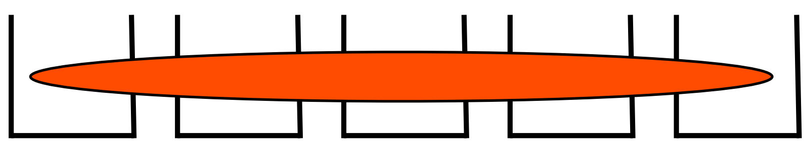
The Hubbard Hamiltonian $\hat{H} = -J \sum_{<ij>} b_i^\dagger b_j$ is quadratic in the creation and annihilation operators, and can thus be (trivially) diagonalized in quasimomentum states of the Bloch band,

$$\hat{H} = -J \sum_{<ij>} b_i^\dagger b_j = \sum_{\vec{q}} \epsilon_{\vec{q}} b_{\vec{q}}^\dagger b_{\vec{q}}.$$

(kinetic energy)

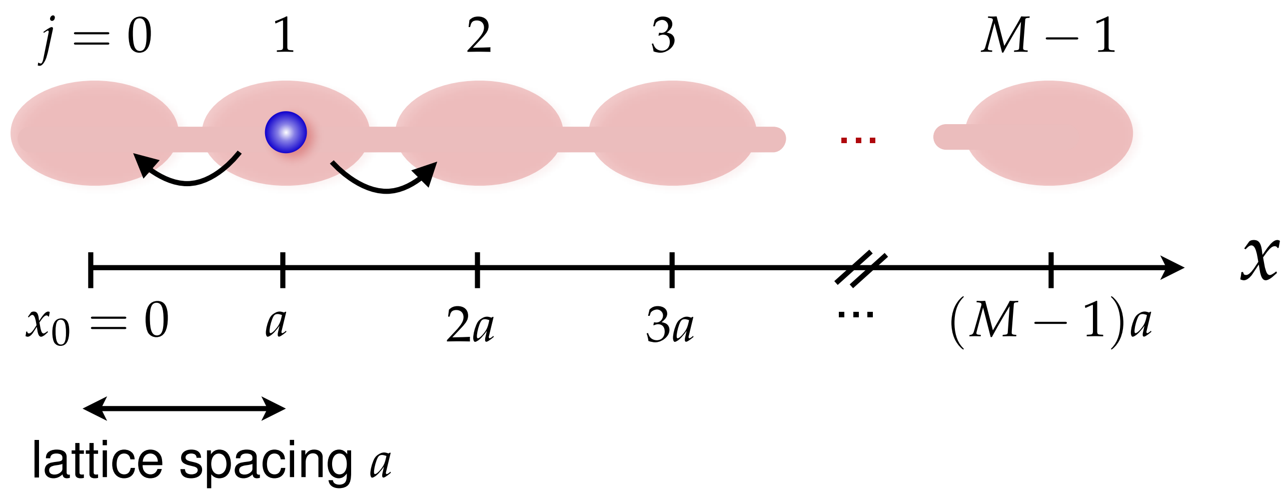
position

quasi-momentum
in Bloch band



N non-interacting particles on M lattice sites:
ground state

lattice sites:



Example: 1D

- **Bloch bands in tight binding:** For a 1D lattice with spacing a we define destruction operators for a quasimomentum $-\pi/a < q \leq \pi/a$ (Discrete Fourier Transform)

$$b_q = \frac{1}{\sqrt{M}} \sum_j e^{iqx_j} b_j \quad (x_j = ja; j = 0, \ldots, M-1)$$

for details see the following appendix

where $[b_q, b_{q'}^\dagger] = \delta_{qq'}$.

This diagonalizes the Hamiltonian

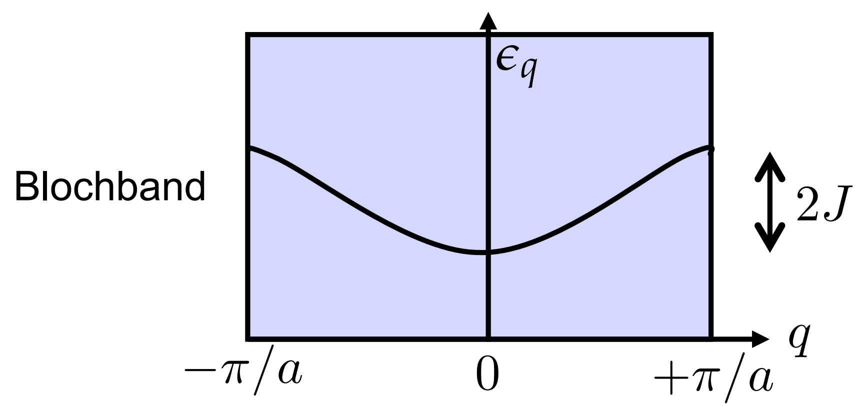
$$\hat{H} = -J \sum_j \left(b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j \right) = \sum_q \epsilon_q b_q^\dagger b_q$$

This diagonalizes the Hamiltonian

$$\hat{H} = -J \sum_j \left(b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j \right) = \sum_q \epsilon_q b_q^\dagger b_q$$

with the tight-binding dispersion relation

$$\epsilon_q = -2J \cos qa \quad (-\pi/a < q \leq \pi/a).$$

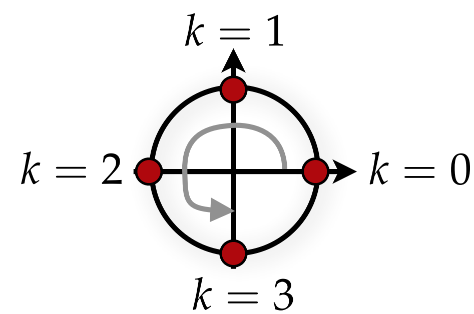


For long wavelengths $|qa| \ll 1$ we have the expansion $\epsilon_q \approx -2J + J(qa)^2 \equiv -2J + q^2/2m^*$ with effective mass m^*.

Appendix:

- The **Discrete Fourier Transform** of a vector of complex numbers $y_0, \ldots, y_{M-1}$ is defined as

$$\tilde{y}_k = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} e^{i2\pi kj/M} y_j \quad (k = 0, \ldots, M-1),$$



and its inverse is

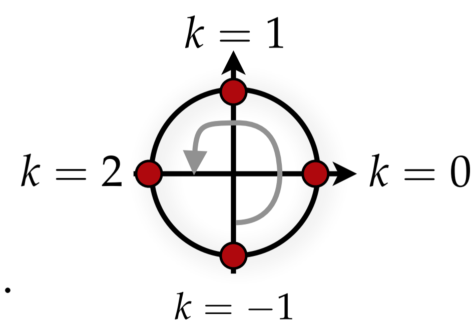
$$y_j = \frac{1}{\sqrt{M}} \sum_{k=0}^{M-1} e^{-i2\pi kj/M} \tilde{y}_k \quad (j = 0, \ldots, M-1).$$

example: M=4

Assuming for the moment M even we find it convenient for our purpose to shift the k index

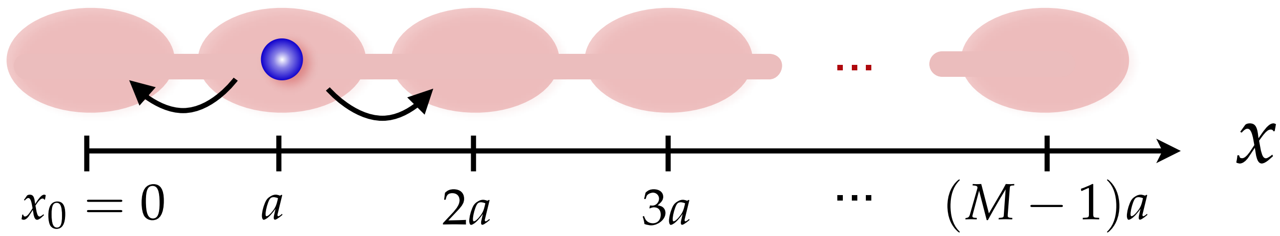
$$\tilde{y}_k = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} e^{i2\pi kj/M} y_j \quad (k = -\frac{M}{2} + 1, \ldots, \frac{M}{2}),$$

$$y_j = \frac{1}{\sqrt{M}} \sum_{k=-\frac{M}{2}+1}^{\frac{M}{2}} e^{-i2\pi kj/M} \tilde{y}_k \quad (j = 0, \ldots, M-1).$$



Exercise: consider the case M odd.

Appendix on Discrete Fourier Transforms etc.



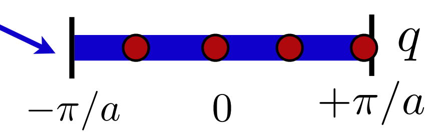
- **Destruction operators for lattice sites b_j and quasimomentum b_q.** We consider the set of bosonic destruction operators b_j on lattice sites $x_j = aj$ with lattice spacing a and $j = 0, \ldots, M-1$ with bosonic commutation relations $[b_j, b_{j'}^\dagger] = \delta_{jj'}$. We define quasimomentum destruction operators

$$\boxed{b_q = \frac{1}{\sqrt{M}} \sum_j e^{iqx_j} b_j} \quad \left(q = \frac{2\pi}{a}\frac{k}{M} \text{ with } k = -\frac{M}{2} + 1, \ldots, \frac{M}{2}\right).$$

Here q is a quasimomentum in the first Brillouin zone $-\pi/a < q \leq \pi/a$ in discretized form

$$\boxed{q = -\frac{\pi}{a} + \frac{2\pi}{a}\frac{1}{M}, -\frac{\pi}{a} + \frac{2\pi}{a}\frac{2}{M}, \ldots, 0, \ldots, +\frac{\pi}{a}.}$$

Brillouin zone



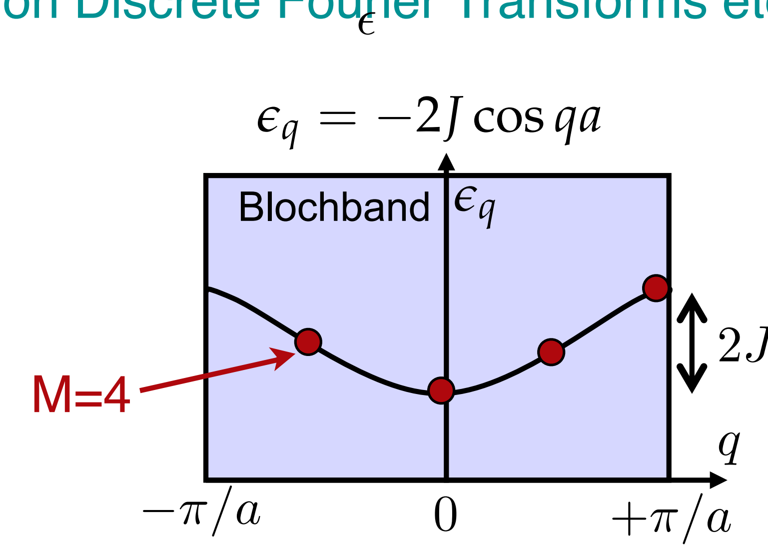
example: M=4

The inverse of the above relation is

$$\boxed{b_j = \frac{1}{\sqrt{M}} \sum_q e^{-iqx_j} b_q}$$

Note that $b_j \leftrightarrow b_q$ is just a unitary transform, and we have the bosonic commutation relations

$$[b_j, b_{j'}^\dagger] = \delta_{jj'} \leftrightarrow [b_q, b_{q'}^\dagger] = \delta_{q,q'}.$$

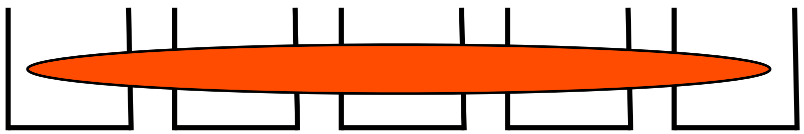


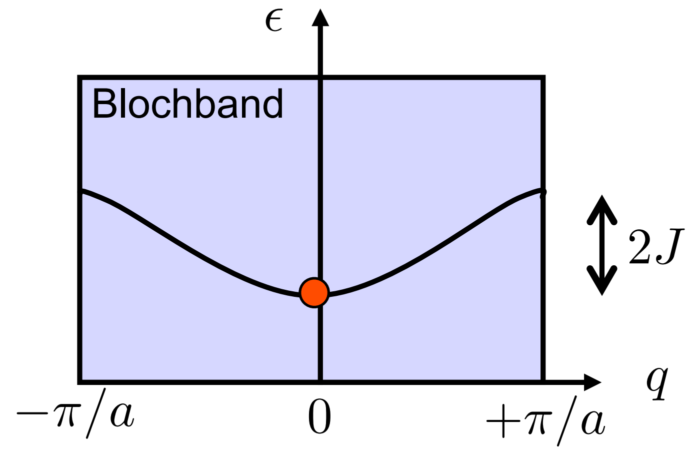
- **Exercise:** We rewrite the kinetic energy term in a momentum representation

$$
\begin{aligned}
\hat{H} &= -J\sum_j b_j^\dagger b_{j+1} + \text{h.c.} \\
&= -J\sum_j b_j^\dagger \left(\frac{1}{\sqrt{M}}\sum_q e^{-iqx_j - iqa} b_q\right) + \text{h.c.} \\
&= -J\sum_q e^{-iqa}\left(\frac{1}{\sqrt{M}}\sum_j b_j^\dagger e^{-iqx_j}\right) b_q + \text{h.c.} \\
&= \sum_q \epsilon_q b_q^\dagger b_q \quad (\epsilon_q = -2J\cos qa)
\end{aligned}
$$

where ϵ_q with $q \in (-\frac{\pi}{a}, \frac{\pi}{a}]$ is the dispersion relation of the (first) Bloch band.
Rem.: See below bandstructure in an optical lattice

N particles on M lattice sites: BEC on a lattice





- **BEC:** For N particles the ground state corresponds to a situation where all bosons occupy the lowest quasi-momentum state

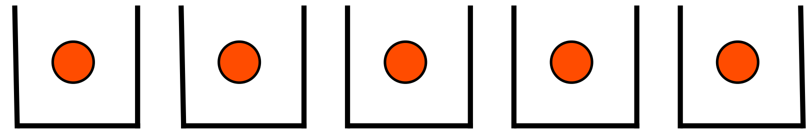
$$|\mathrm{BEC}\rangle = \frac{1}{\sqrt{N!}}\left(b^\dagger_{q=0}\right)^N |\mathrm{vac}\rangle$$
$$\equiv \frac{1}{\sqrt{N!}}\left(\frac{1}{\sqrt{M}}\sum_j b^\dagger_i\right)^N |\mathrm{vac}\rangle$$

- **Long range order:** the first order correlation function $\langle b^\dagger_i b_j\rangle \equiv \langle\Psi|\, b^\dagger_i b_j\,|\Psi\rangle$ as a function of site indices i and j is a measure of the coherence. For a BEC we have

$$\langle b^\dagger_i b_j\rangle = \mathrm{const}$$

which is the signature of long range order.

Mott phase



Limit of strong interactions: $U \gg J \to 0$

- **Commensurate filling:** For commensurate filling $N = M$ the ground state will be a Mott insulator (Fock state)

$$|\mathrm{Mott}\rangle = b_1^\dagger b_2^\dagger \dots b_{N=M}^\dagger |\mathrm{vac}\rangle = |1, 1, \dots, 1\rangle$$

with exactly $n_0 = 1$ particle per lattice site, and similarly for fillings $n_0 = 2$ etc. This state has no long-range oder

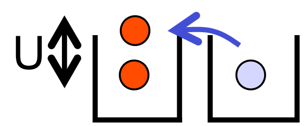
$$\langle b_i^\dagger b_j \rangle = n_0 \delta_{ij}$$

Excitations correspond to states of the type

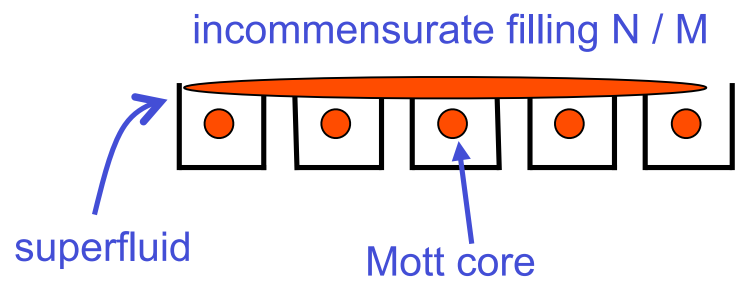
$$|1, 0, 2, 1, 1 \dots, 1\rangle$$

with excitation energy U. The excitation spectrum is gapped.

excitations: gapped ~U



robust!



- **Incommensurate filling:** there will be a Mott core, and superfluid particles on top.
  In the commensurate case the excitation spectrum will be gapped: to excite a boson we require an energy U.

Advanced Topic:
SF - MI Quantum Phase Transition in Mean Field Theory

Gutzwiller Mean Field Theory & Superfluid - Mott Insulator Quantum Phase Transition

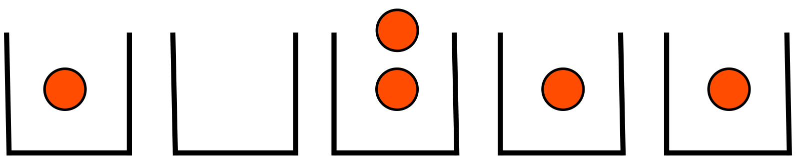
Introductory remarks:

For N particles we have we have calculated the ground state of the Bose Hubbard (BH) Hamiltonian in the two limiting cases $J \gg U \to 0$ (BEC) and $U \gg J \to 0$ (Mott insulator). For values J/U in between we cannot solve the BH Hamiltonian exactly, and thus must rely on approximations.

One approximation scheme is the **Gutzwiller mean field ansatz**. It allows us to understand the **phase diagram** as a function of J/U and particle density (or chemical potential), and the **quantum phase transition** from the superfluid to the Mott insulator phase. (For simplicity we will be only interested in the case temperature $T = 0$, i.e. understanding the ground state of the BH Hamiltonian, and not in the complete thermodynamics.)

For the top students: This is an advanced topic, and thus much more difficult than what we did before. It will not be part of the final exam. However, if you work yourself in detail through the following slides and document this by writing a short computer program to calculate the phase diagram (see below), you can elect this to be one of the exam questions, and you will get extra points if you bring your write-up with you to the final exam :-)

Gutzwiller Mean Field Theory & Superfluid - Mott Insulator Quantum Phase Transition



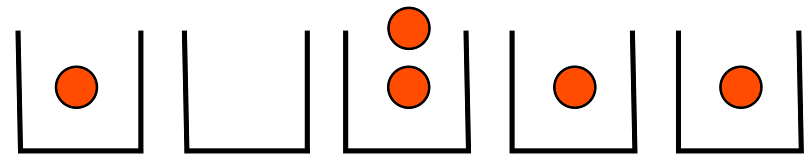
N particles on M lattice sites

http://en.wikipedia.org/wiki/Martin_Gutzwiller

Lit.:

- Subir Sachdev , Quantum Phase Transitions (Cambridge, 1999)
- K Sheshadri, HR Krishnamurthy, R Pandit, TV Ramakrishnan, Europhys. Lett. 22, 257 (1993)

Problem: We seek an approximate variational solution for the ground state of the Bose Hubbard model which produces both the BEC and the Mott phase, and describes the regime and quantum phase transition between these phases.



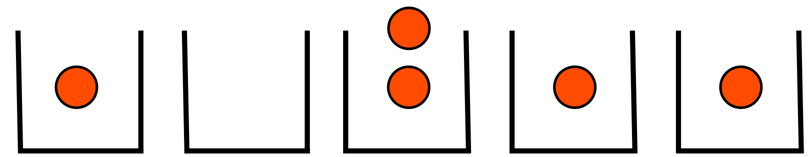
N particles on M lattice sites

Gutzwiller mean field ansatz:

$$|\Psi\rangle = \prod_{i}^{M} |\phi_i\rangle \quad \text{with } |\phi_i\rangle = \sum_{n=0}^{\infty} f_n^{(i)} |n\rangle_i$$

with $\{f_n^{(i)}\}$ variational parameters (normalization: $\sum_n \left| f_n^{(i)} \right|^2 = 1$).

- This is a *product state* over lattice sites.
  - thus all expectation values etc. can be easlily calculated :-)



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- This wave function does *not* conserve particle number (while according to $[\hat{H}, \hat{N}] = 0$ an exact wave function should!?)
  - However, it is precisely this feature will allow us to describe within a s*imple single ansatz* both the superfluid and Mott phase. Thus a bug becomes a feature when doing mean field theory. (Note that the mean field BCS wave function describing superconductivity also is non-particle number conserving!)[3]
  - Instead of a fixed N we will include $\langle\hat{N}\rangle = N$ as a constraint in our variational principle, i.e. we require only particle number conservation *in the mean*.

[3]Rem.: Actually, we could implement particle conservation in our ansatz by projecting on a fixed particle number $P_N |\mathrm{Gutzi}\rangle$, but ... we will not do so.

Variational Principle for Gutzwiller wave function

The ground state and energy is determined by $E = \langle\Psi|\, \hat{H}\, |\Psi\rangle \,/ \langle\Psi|\Psi\rangle \to \min$ over the set of variational parameters $\{f_n^{(i)}\}$.

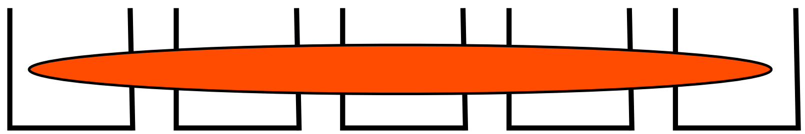
We include the constraints $\langle\hat{N}\rangle = N$ (particle number conservation) and $\forall i$ $\sum_n |f_n^{(i)}|^2 = 1$ (normalization of the wave function) via *Lagrange multipliers* μ and $\{\epsilon_i\}$, respectively,

$$\langle\hat{H}\rangle - \mu\langle\hat{N}\rangle - \sum_i \epsilon_i \sum_n |f_n^{(i)}|^2 \to \text{min}$$

with $\langle\ldots\rangle \equiv \langle\Psi|\ldots|\Psi\rangle$. The Lagrange parameter μ will have the meaning of a *chemical potential* (as familiar from statistical mechanics with the grand canonical ensemble).

[Rem.: grand canonical potential $\rho_G \sim e^{-(\hat{H}-\mu\hat{N})/kT}$ which for $T \to 0$ reduces to the above expression.]

Discussion: Before solving the varational problem by determining the $\{f_n^{(i)}\}$, we ask: *what are the manifestations of a superfluid and Mott phase in the Gutzwiller wave function?*



superfluid

$\langle b_i^\dagger b_j \rangle = const$

long range order!

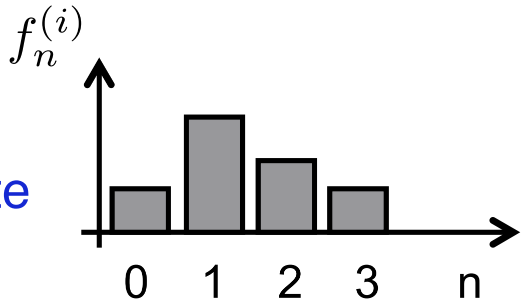
- **a superfluid phase** will manifest itsself as a non-trivial superposition $|\phi_i\rangle = \sum_{n=0}^{\infty} f_n^{(i)} |n\rangle_i$, so that the order superfluid parameter

$$\langle b_i \rangle = \langle \Psi | b_i | \Psi \rangle \equiv \langle \phi_i | b_i | \phi_i \rangle$$

$$= \sum_{m,n} f_m^{(i)*} {}_i\langle m | b_i | n \rangle_i f_n^{(i)} = \sum_{n=0}^{\infty} \sqrt{n} f_{n+1}^{(i)*} f_n^{(i)} \neq 0$$

The mean occupation per lattice site is $\langle n_i \rangle = \sum_n n |f_n^{(i)}|^2$, and we identify $|f_n^{(i)}|^2$ with the particle number distribution on a given lattice site.

superfluid:
coherent state



Example: let us assume $f_n^{(i)} = \psi^n \exp(-\frac{1}{2}|\psi|)^2/\sqrt{n!}$ (homogeneous) which corresponds to a coherent state

$$|\phi_i\rangle = \sum_{n=0}^{\infty} f_n^{(i)} |n\rangle_i = \sum_{n=0}^{\infty} \frac{\psi^n}{\sqrt{n!}} e^{-\frac{1}{2}|\psi|^2} |n\rangle_i = |\psi\rangle_{\text{coh}},$$

Then the superfluid order parameter is

$$\langle b_i \rangle = \psi \neq 0.$$

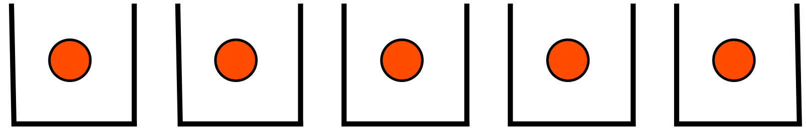
The number distribution on one lattice site is Poissonian $p_n = |f_n^{(i)}|^2 = |\psi|^{2n} \exp(-|\psi|^2)/n!$ with mean particle number $\langle \hat{n}_i \rangle = |\psi|^2$, and variance $\Delta \hat{n}_i = \langle n_i \rangle$

Rem.: The corresponding Gutzwiller wave function is a multimode coherent state

$$|\Psi\rangle = \prod_i^M |\phi_i\rangle = e^{\sum_i \psi b_i^\dagger} |\text{vac}\rangle \, .$$

A number projection would result in (compare above)

$$P_N |\Psi\rangle \sim \left(\sum_i b_i^\dagger \right)^N |\text{vac}\rangle \sim |\text{BEC}\rangle \, .$$



- **a (homogenous) Mott phase** with commensurate filling $N = n_0 M$ is represented by

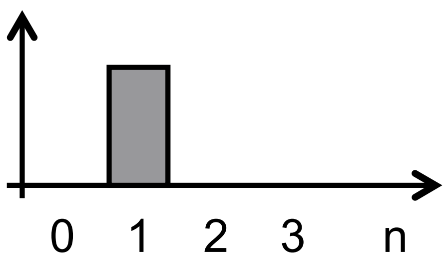
$$f_n^{(i)} = \delta_{n,n_0}$$

so that the superfluid order parameter is

$$\langle b_i \rangle = 0.$$

The mean occupation is $\langle \hat{n}_i \rangle = n_0$ and the variance is $\Delta \hat{n}_i = 0$, i.e. there is no particle fluctuations. There is no off-diagonal long range order $\langle b_i^\dagger b_j \rangle = n_0 \delta_{ij}$.

Mott:
Fock state



☺ Thus the Gutzwiller ansatz is able to describe both the superfluid and Mott limit. The hope is that it is also a reasonable approximation in between.

Exercise: Mott plateaus for $J = 0$.

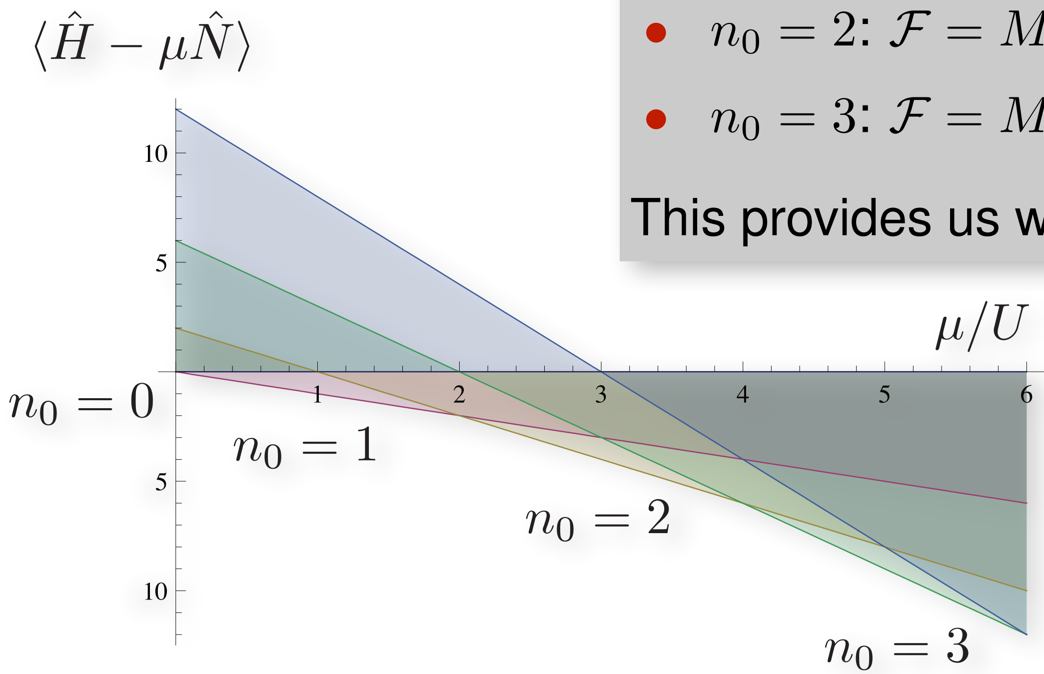
The Hamiltonian is $H = U \sum_i \hat{n}_i(\hat{n}_i - 1)$. The Fockstates $|n_0, n_0, \ldots, n_0\rangle$ are exact eigenstates with energy $E = MUn_0(n_0 - 1)$ where we assume spatial homogeneity. The $n_0 = 0, 1, 2, \ldots$ play the role of variational parameters. We seek

$$\mathcal{F} = \langle \hat{H} - \mu\hat{N} \rangle = M\tfrac{1}{2}U \left(n_0(n_0 - 1) - 2\frac{\mu}{U} n_0 \right) \rightarrow \min$$

For a given μ/U we must find $n_0 = 0, 1, .2, \ldots$ which minimizes this expression

- $n_0 = 0$: $\mathcal{F} = 0$, for $\frac{\mu}{U} < 0$
- $n_0 = 1$: $\mathcal{F} = M\frac{1}{2}U\left(-2\frac{\mu}{U}\right)$ for $0 < \frac{\mu}{U} < 1$
- $n_0 = 2$: $\mathcal{F} = M\frac{1}{2}U\left(2 - 4\frac{\mu}{U}\right)$ for $1 < \frac{\mu}{U} < 2$
- $n_0 = 3$: $\mathcal{F} = M\frac{1}{2}U\left(6 - 3\frac{\mu}{U}\right)$ for $2 < \frac{\mu}{U} < 3$ etc.

This provides us with $n = n(\frac{\mu}{U})$ which is a stair function.



Appendix: technical details ...

Variational calculation: We have ...

- The product form of the Gutzwiller wave function gives

$$\langle \hat{H} \rangle = \langle \Psi | \hat{H} | \Psi \rangle = -J \sum_{<ij>} \langle b_i^\dagger \rangle \langle b_j \rangle + \frac{1}{2} U \sum_i \langle b_i^{\dagger 2} b_i^2 \rangle$$

  We note that the kinetic energy factorizes with $\langle b_i \rangle = \sum_{n=0}^{\infty} \sqrt{n} f_{n+1}^{(i)*} f_n^{(i)} =: \psi_i$ (*superfluid order parameter*), and $\frac{1}{2} U \langle b_i^{\dagger 2} b_i^2 \rangle = \frac{1}{2} U \sum_{n=0}^{\infty} n(n-1) |f_n^{(i)}|^2$.

- $\langle \hat{n}_i \rangle = \sum_n n |f_n^{(i)}|^2$
- $\langle \phi_i | \phi_i \rangle = \sum_n |f_n^{(i)}|^2$

We vary $\{f_n^{(i)*}, f_n^{(i)}\}$ in

$$-J \sum_{<ij>} (\sum_{n=0}^{\infty} \sqrt{n} f_{n+1}^{(i)} f_n^{(i)*}) \sum_{n=0}^{\infty} \sqrt{n} f_{n+1}^{(j)*} f_n^{(j)} + \tfrac{1}{2} U \sum_i \sum_n n(n-1) |f_n^{(i)}|^2$$
$$-\mu \sum_i \sum_n n |f_n^{(i)}|^2 - \sum_i \epsilon_i \sum_n |f_n^{(i)}|^2 \quad \rightarrow \quad \min$$

to obtain the self-consistency equations

$$\left(\hat{h}_i(\{\psi, \psi^*\}) - \mu \hat{n}_i\right) |\phi_i\rangle \quad = \quad \epsilon_i \, |\phi_i\rangle \qquad (*)$$

$$\psi_i = \langle \phi_i | \, b_i \, | \phi_i \rangle \qquad (**)$$

with *local* mean field Hamiltonian in Eq. (*) defined by

$$\hat{h}_i(\{\psi, \psi^*\}) := -J \sum_{\langle j|i \rangle} \left(b_i^\dagger \psi_j + \psi_j^* b_i \right) + \tfrac{1}{2} U \sum_i b_i^{\dagger 2} b_i^2$$

where $\sum_{\langle j|i \rangle}$ denotes a sum j over neighbors of a given site i.

Let us from now on consider the *homogeneous* situation $\psi_i = \psi$ and $f_n^{(i)} = f_n$)

Exercise: write out the SE with mean field Hamiltonian for the homogeneous case. We have

$$\langle n|\, \hat{h} - \mu \hat{n}\, |m\rangle = -zJ(\sqrt{m+1}\delta_{n,m+1}\psi + \psi^* \sqrt{m}\delta_{n,m-1}) + \tfrac{1}{2}Un(n-1)\delta_{nm}$$

or

$$\begin{pmatrix} 0 & -zJ\psi^* & & & \\ -zJ\psi & -\mu & -\sqrt{2}zJ\psi^* & & \\ & -\sqrt{2}zJ\psi & U-2\mu & -\sqrt{3}zJ\psi^* & \\ & & -\sqrt{3}zJ\psi & 3U-3\mu & \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix} = \epsilon \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix}$$

with z the number of nearest neighbors.

self-consistency equations

$$\left(\hat{h}_i(\{\psi,\psi^*\}) - \mu\hat{n}_i\right)|\phi_i\rangle = \epsilon_i\,|\phi_i\rangle \quad (*)$$

$$\psi_i = \langle\phi_i|\, b_i\, |\phi_i\rangle \quad (**)$$

Computer Program: For given J, U and chemical potential μ perform the following calcuations.

1. Asume $\psi \neq 0$.
2. Solve the Schrödinger equation (*) for the lowest eigenvalue ϵ and normalized eigenvector $|\phi_i\rangle = \sum_{n=0}^{\infty} f_n\,|n\rangle_i$
3. Calculate the new ψ from the $\{f_n\}$.

Repeat until $\{f_n\}$ and thus ψ converge.

Cases: For a given $\{J, U, \mu\}$ two cases are possible:

- if $\psi \neq 0$ we have a superfluid phase, and
- if $\psi = 0$ we have a Mott phase. The transition between these phases will occur for a certain critical U_c/J. It is a second order transition.

End Appendix

This gives the phase diagram as a function of μ/U and J/U.