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Introduction to Ultracold Atoms Superfluid – Mott insulator transition

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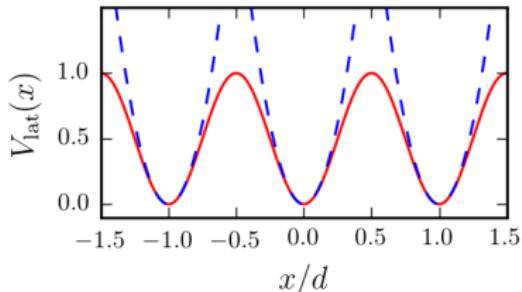
- ➊ Wannier functions and tight-binding limit
- ➋ Bose-Hubbard model
- ➌ Ground state : Superfluid -Mott insulator transition
 - Phase coherence
 - Dynamics and transport
 - Shell structure
- ➍ A glance at fermions

In a deep lattice potential, atoms are tightly trapped around the potential minima.

Harmonic approximation for each well :

$$V_{\text{lat}}(x \approx x_i) \approx \frac{1}{2} m_a \omega_{\text{lat}}^2 (x - x_i)^2,$$
$$\hbar \omega_{\text{lat}} = 2 \sqrt{V_0 E_R}.$$

The bands are centered around the energy
 $\overline{E}_n \approx (n + 1/2) \hbar \omega_{\text{lat}}$.



First correction : quantum tunneling across the potential barriers, as in tight-binding methods used in solid-state physics (Linear Combination of Atomic Orbitals)

This is best handled using a new basis, formed by so-called *Wannier functions*.

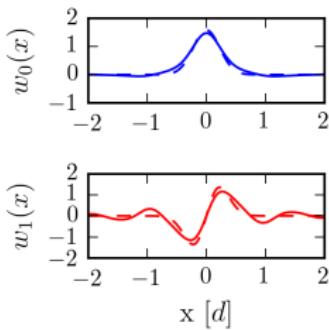
Wannier functions

Wannier functions : discrete Fourier transforms with respect to the site locations of the Bloch wave functions,

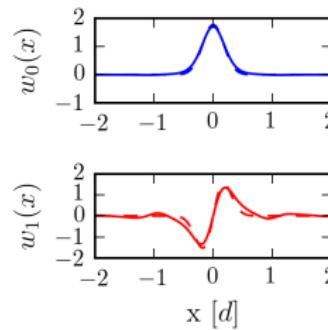
$$w_n(x - x_i) = \frac{1}{\sqrt{N_s}} \sum_{q \in BZ1} e^{-iqx_i} \phi_{n,q}(x).$$

- All Wannier functions can be deduced from $w_n(x)$ by translation of $x_i = id$.
- There are exactly N_s such functions per band (as many as Bloch functions).
- Wannier functions form a basis of Hilbert space (*not* an eigenbasis of \hat{H}).

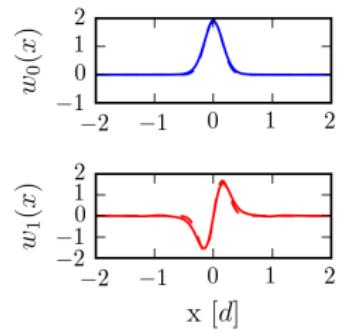
$$V_0 = 4 E_R$$



$$V_0 = 10 E_R$$



$$V_0 = 20 E_R$$



Cautionary note: Bloch functions are defined up to a q -dependent phase which needs to be fixed to obtain localized Wannier functions [W. Kohn, Phys. Rev. (1959)].

Second quantized formalism (useful for the interacting case).

Bloch basis :

$$H = \sum_{n,k \in BZ1} \varepsilon_n(k) \hat{b}_{n,k}^\dagger \hat{b}_{n,k}.$$

$\hat{b}_{n,k}$: annihilation operator for Bloch state (n, k) .

Wannier basis :

$$H = - \sum_{n,i,j} J_n(i-j) \hat{a}_{n,i}^\dagger \hat{a}_{n,j},$$

$\hat{a}_{n,i}$: annihilation operator for Wannier state $w_n(x - x_i)$.

Tunneling energies :

$$J_n(i-j) = \int dx w_n^*(x - x_j) \left(\frac{\hbar^2}{2M} \Delta - V_{\text{lat}}(x) \right) w_n(x - x_i).$$

(also called hopping parameters)

$$H = - \sum_{n,i,j} J_n(i-j) \hat{a}_{n,i}^\dagger \hat{a}_{n,j},$$

Tunneling energies :

$$\begin{aligned} J_n(i-j) &= \frac{1}{N_s} \sum_{q,q' \in BZ1} e^{-i(qx_i - q'x_j)} \underbrace{\int dx u_{n,q}^*(x) \left(\frac{\hbar^2}{2M} \Delta - V_{\text{lat}}(x) \right) u_{n,q'}(x)}_{= -\varepsilon_n(q) \delta_{n,n'} \delta_{q,q'}} \\ &= -\frac{1}{N_s} \sum_{q \in BZ1} \varepsilon_n(q) e^{-iq \cdot (x_i - x_j)}. \end{aligned}$$

$J_n(i-j)$ depend only on the relative distance $x_i - x_j$ between the two sites.

- On-site energy ($i = j$): Mean energy of band n

$$J_n(0) = -\frac{1}{N_s} \sum_{q \in BZ1} \varepsilon_n(q) = -\overline{E}_n$$

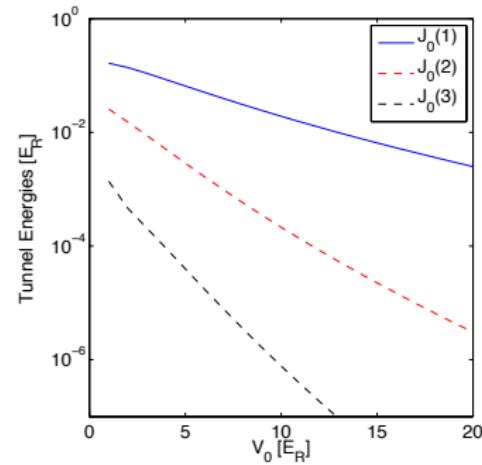
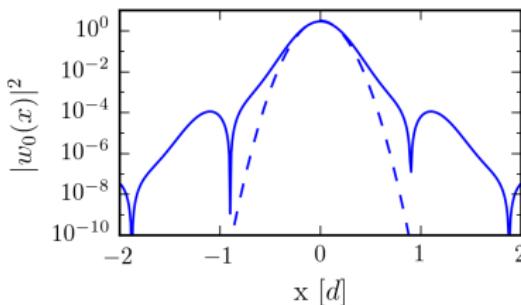
- Nearest-neighbor tunneling ($j = i \pm 1$):

$$J_n(1) = -\frac{1}{N_s} \sum_{q \in BZ1} \varepsilon_n(q) e^{iqx} = -J_n$$

Tight-binding limit

For deep lattices (roughly $V_0 \gg 5E_R$), the tunneling energies fall off very quickly with distance:

Wannier function for $V_0 = 10 E_R$:



Two useful approximations :

- **Tight-binding approximation** : keep only the lowest terms
- **Single-band approximation** : keep only the lowest band—drop band index and let $J_0(1) \equiv J$

$$\hat{H}_{TB} = \bar{E}_0 \sum_i \hat{a}_i^\dagger \hat{a}_i - J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j,$$

Cubic lattice potential :

$$V_{\text{lat}} = V_0 \sum_{\alpha} \sin(k_{\alpha}x_{\alpha})^2$$

Dispersion relation :

$$\epsilon_{\mathbf{n}}(\mathbf{q}) = \sum_{\alpha=x,y,z} \epsilon_{n_{\alpha}}(q_{\alpha}),$$

- $\epsilon_n(q)$: 1d dispersion relation,
- \mathbf{n} : a triplet of integers indexing the various bands
- \mathbf{q} : quasi momentum $\in \text{BZ1} :] -\pi/d, \pi/d]^3$.

Bloch functions :

$$\phi_{\mathbf{n},\mathbf{q}}(\mathbf{r}) = e^{i\mathbf{q} \cdot \mathbf{r}} u_{n_x, q_x}(x) u_{n_y, q_y}(y) u_{n_z, q_z}(z).$$

Wannier functions :

$$W_{\mathbf{n}}(\mathbf{r} - \mathbf{r}_{\mathbf{n}}) = w_{n_x}(x - n_x d_x) w_{n_y}(y - n_y d_y) w_{n_z}(z - n_z d_z).$$

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Basic Hamiltonian for bosons interacting *via* short-range forces :

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}},$$

$$\hat{H}_0 = \int d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2M} \Delta + V_{\text{lat}}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}),$$

$$\hat{H}_{\text{int}} = \frac{g}{2} \int d^{(3)}\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}).$$

- $\hat{\Psi}(\mathbf{r})$: field operator annihilating a boson at position \mathbf{r} ,
 - $V_{\text{lat}}(\mathbf{r})$: lattice potential,
 - $g = \frac{4\pi\hbar^2 a}{M}$: coupling constant,
 - scattering length $a > 0$: repulsive interactions.
-
- Not simpler in the Bloch basis.
 - Can be drastically simplified in the Wannier basis

Basis of Wannier functions $W_\nu(\mathbf{r} - \mathbf{r}_i)$:

$$\hat{\Psi}(\mathbf{r}) = \sum_{\nu,i} W_\nu(\mathbf{r} - \mathbf{r}_i) \hat{a}_{\nu,i}.$$

- \mathbf{r}_i : position of site i ,
- ν : band index
- $\hat{a}_{\nu,i}$: annihilation operator

Single-particle Hamiltonian :

- Tight-binding approximation : keep only the lowest terms
- Single-band approximation : keep only the lowest band–drop band index,
 $J_0(1) \equiv J$

$$\hat{H}_0 \longrightarrow \hat{H}_{TB} = - \sum_{\langle i,j \rangle} J \hat{a}_i^\dagger \hat{a}_j$$

Interacting bosons in the Wannier basis

Basis of Wannier functions $W_\nu(\mathbf{r} - \mathbf{r}_i)$:

$$\hat{\Psi}(\mathbf{r}) = \sum_{\nu,i} W_\nu(\mathbf{r} - \mathbf{r}_i) \hat{a}_{\nu,i}.$$

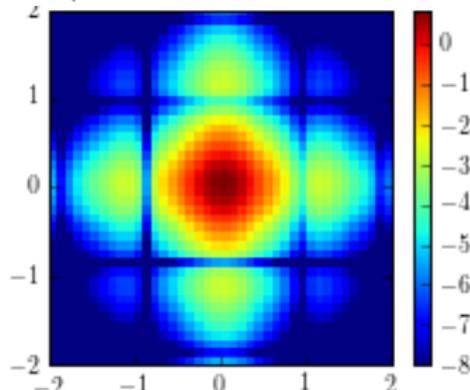
- \mathbf{r}_i : position of site i ,
- ν : band index
- $\hat{a}_{\nu,i}$: annihilation operator

Interaction Hamiltonian :

$$\hat{H}_{\text{int}} \longrightarrow \hat{H}_{\text{int}} = \frac{1}{2} \sum_{ijkl} U_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l$$

$$U_{ijkl} = g \int d\mathbf{r} W^*(\mathbf{r} - \mathbf{r}_i) W^*(\mathbf{r} - \mathbf{r}_j) W(\mathbf{r} - \mathbf{r}_k) W(\mathbf{r} - \mathbf{r}_l)$$

$\log(|W(x, y, 0)|^2)$ for $V_0 = 5E_R$:



In the tight binding regime, strong localization of Wannier function $W(\mathbf{r} - \mathbf{r}_i)$ around \mathbf{r}_i .
On-site interactions ($i = j = k = l$) are strongly dominant:

$$\hat{H}_{\text{int}} \approx \frac{1}{2} \sum_i U_{iiii} \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i + \dots$$

Bose Hubbard model

- ① Single band approximation
- ② Tight-binding approximation
- ③ On-site interactions

Bose-Hubbard model :

$$H_{\text{BH}} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1).$$

$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$: operator counting the number of particles at site i .

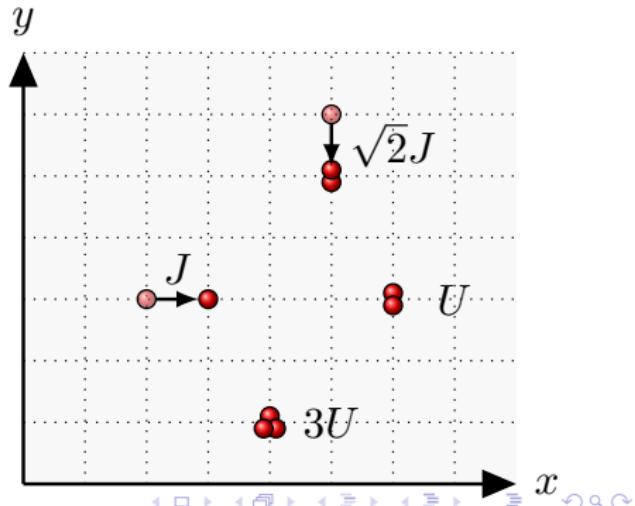
- Tunneling energy :

$$J = \frac{\max \varepsilon(\mathbf{q}) - \min \varepsilon(\mathbf{q})}{2z}$$

$z = 6$: number of nearest neighbors

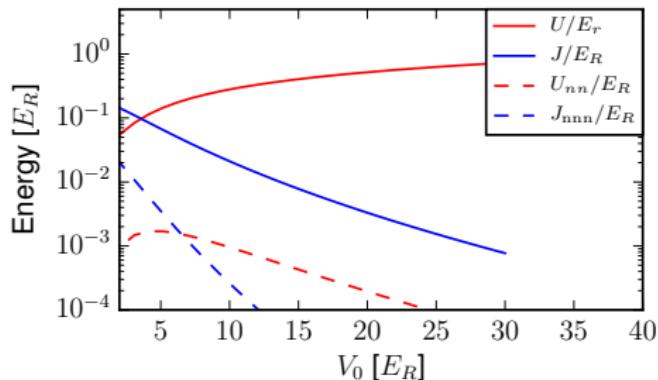
- On-site interaction energy :

$$U = g \int d\mathbf{r} w(\mathbf{r})^4.$$



Parameters of the Bose Hubbard model

Calculation for ^{87}Rb atoms [$a=5.5 \text{ nm}$] in a lattice at $\lambda_L = 820 \text{ nm}$:



Harmonic oscillator approximation :

$$\frac{\Delta_{\text{band}}}{E_R} \approx \frac{\hbar\omega_{\text{lat}}}{E_R} = \sqrt{\frac{2V_0}{E_R}}, \quad \frac{U}{E_R} \approx \sqrt{\frac{8}{\pi}} k_L a \left(\frac{V_0}{E_R} \right)^{3/4}.$$

① Single band approximation :

- $V_0 \gg E_R$
- $U \ll \Delta_{\text{band}}$: $k_L a \ll \left(\frac{E_R}{V_0} \right)^{1/4}$

② Tight-binding approximation : $V_0 \gg 5E_R$

③ On-site interactions : $V_0 \gg E_R$

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BEC in the lowest energy Bloch state $\mathbf{q} = 0$:

$$|\Psi\rangle_N = \frac{1}{\sqrt{N!}} \left(\hat{b}_{\mathbf{q}=0}^\dagger \right)^N |\emptyset\rangle = \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{N_s}} \sum_i \hat{a}_i^\dagger \right)^N |\emptyset\rangle$$

- Fixed number of particles N : canonical ensemble

Probability to find n_i atoms at one given site i :

$$p(n_i) \approx e^{-\bar{n}} \frac{\bar{n}^{n_i}}{n_i!} + \mathcal{O}\left(\frac{1}{N}, \frac{1}{N_s}\right)$$

Poisson statistics, mean \bar{n} , standard deviation $\sim \sqrt{\bar{n}}$

In the thermodynamic limit $N \rightarrow \infty, N_s \rightarrow \infty$, one finds the same result as for a coherent state with the same average number of particles N :

$$|\Psi\rangle_{\text{coh}} = \mathcal{N} e^{\sqrt{N} \hat{b}_{\mathbf{q}=0}^\dagger} |\emptyset\rangle = \prod_i \left(\mathcal{N}_i e^{\sqrt{n_i} \hat{a}_i^\dagger} |\emptyset\rangle \right)$$

- Fluctuating number of particles N : grand canonical ensemble
 $H_{\text{BH}} \rightarrow G = H_{\text{BH}} - \mu N$

Coherent state wavefunction in the grand canonical ensemble :

$$|\Psi\rangle_{\text{coh}} = \prod_i |\alpha_i\rangle, \quad |\alpha_i\rangle = \mathcal{N}_i \sum_{n_i=0}^{\infty} \frac{\alpha_i^{n_i}}{\sqrt{n_i!}} |n_i\rangle_i, \quad \hat{a}_i |\alpha_i\rangle = \alpha_i |\alpha_i\rangle$$

with $\{\alpha_i\}_{i=1,\dots,N_s}$ the variational parameters.

One can relate the presence of the condensate to a non-zero expectation value of the matter wave field $\alpha_i = \langle \hat{a}_i \rangle$, playing the role of an order parameter :

- Condensate wavefunction : $\alpha_i = \langle \hat{a}_i \rangle = \sqrt{\frac{N}{N_s}} e^{i\phi}$
- Mean density : $\bar{n} = |\alpha_i|^2 = \text{condensate density}$

Spontaneous symmetry breaking point of view.

Starting point to formulate a Gross-Pitaevskii (weakly interacting) theory :

variational ansatz with self-consistent α_i determined by the total (single-particle + interaction) Hamiltonian.

"Adiabatic continuation" from the ideal Bose gas.

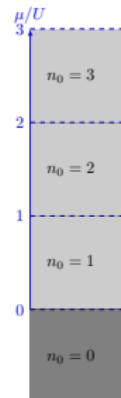
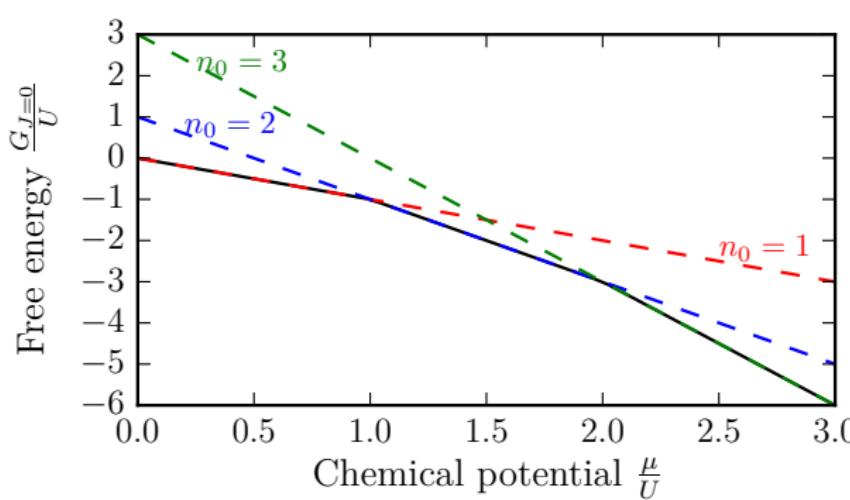
"Atomic" limit $J = 0$

Lattice \equiv many independent trapping wells

Many-body wavefunction : product state running over all lattice sites $|\Psi\rangle = \prod_i |\psi_i\rangle$

Free energy for one well: $G_{J=0} = \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i$

$\langle n_i \rangle = n_0 = \text{int}(\mu/U) + 1$: integer filling that minimizes \mathcal{H}_{int} .



- $\mu/U = p$ integer : $n_0 = p$ and $n_0 = p + 1$ degenerate
 - on-site wave function = any superposition of the two Fock states.
 - density $\langle n_i \rangle \in [p, p + 1]$.

Variational wavefunction :

$$|\Psi\rangle_{\text{Gutzwiller}} = \prod_i |\phi_i\rangle,$$
$$|\phi_i\rangle = \sum_{n_i=0}^{\infty} c(n_i) |n_i\rangle_i.$$

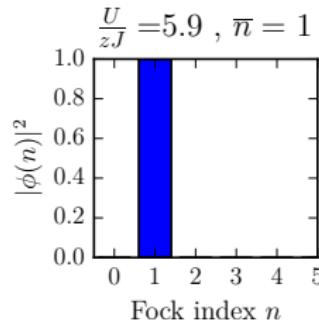
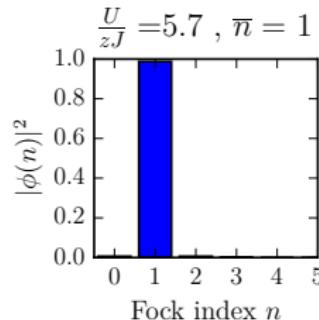
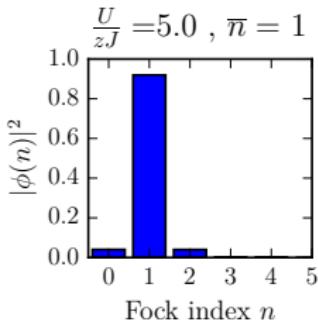
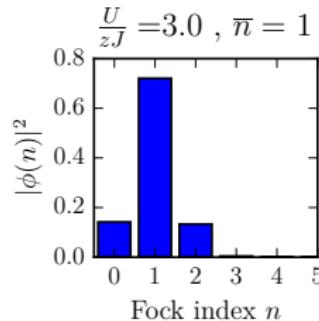
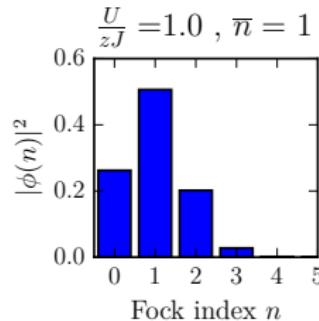
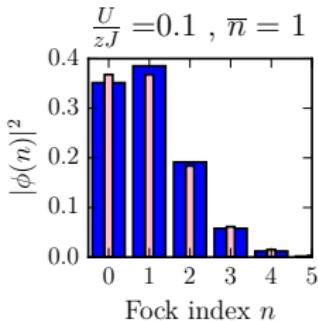
- Correct in both limits $J \rightarrow 0$ and $U \rightarrow 0$,
- Minimize $\langle \Psi | H_{\text{BH}} - \mu \hat{N} | \Psi \rangle$ with respect to $\{c(n_i)\}$ with the constraint $\sum_{n=0}^{\infty} |c(n)|^2 = 1$ for a given μ ,
- Equivalently : minimize $\langle \Psi | H_{\text{BH}} | \Psi \rangle$ with respect to $\{c(n_i)\}$ with the constraints $\sum_{n=0}^{\infty} |c(n)|^2 = 1$, $\sum_{n=0}^{\infty} n|c(n)|^2 = \bar{n}$.

Gutzwiller ansatz for the ground state

Uniform system : $|\phi\rangle_i$ identical for all sites i

Strong interactions $U \geq J$: on-site number fluctuations become costly.

The on-site statistics $p(n_i)$ evolves from a broad Poisson distribution to a peaked one around some integer n_0 closest to the average filling : **number squeezing**.



Condensate fraction (Gutzwiller ansatz)

Variational wavefunction :

$$|\Psi\rangle_{\text{Gutzwiller}} = \prod_i |\phi_i\rangle,$$
$$|\phi_i\rangle = \sum_{n_i=0}^{\infty} c(n_i) |n_i\rangle_i.$$

Condensate fraction f_c : normalized population of the quasi-momentum state $\mathbf{q} = 0$,

$$f_c = \frac{1}{N} \langle \hat{b}_{\mathbf{q}}^\dagger \hat{b}_{\mathbf{q}} \rangle_{\mathbf{q}=0} = \frac{1}{NN_s} \sum_{i,j} \langle \hat{a}_i^\dagger \hat{a}_j \rangle,$$

taken in the thermodynamic limit (TL) $N, N_s \rightarrow \infty$.

For the Gutzwiller state: $\langle \hat{a}_i^\dagger \hat{a}_i \rangle = \bar{n}$, or $\langle \hat{a}_i^\dagger \hat{a}_j \rangle = \alpha_i^* \alpha_j$ for $i \neq j$

$$f_c = \frac{1}{N_s} + \frac{|\alpha|^2}{\bar{n}} \left(1 - \frac{1}{N_s} \right) \xrightarrow{\text{TL}} \frac{|\alpha|^2}{\bar{n}}$$

- Non-interacting/Gross-Pitaevskii case ($U \rightarrow 0$): $\alpha = \sqrt{\bar{n}} \implies f_c = 1$,
- Fock states with n_0 atoms per site ($J = 0$): $\alpha = 0 \implies f_c \xrightarrow{\text{TL}} 0$.

Superfluid-Mott insulator transition

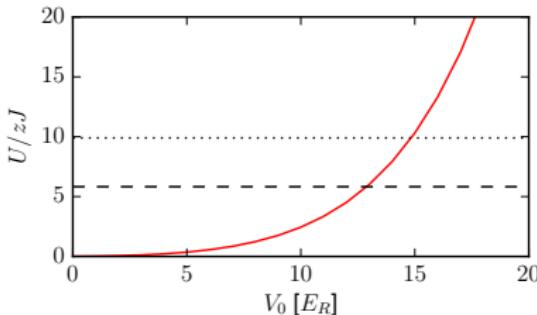
Transition from a delocalized superfluid state to a localized Mott insulator state above a critical interaction strength U_c

Superfluid:

- non-zero condensed fraction $|\alpha|^2$
- on-site number fluctuations
- Gapless spectrum
- Long wavelength superfluid flow can carry mass across the lattice

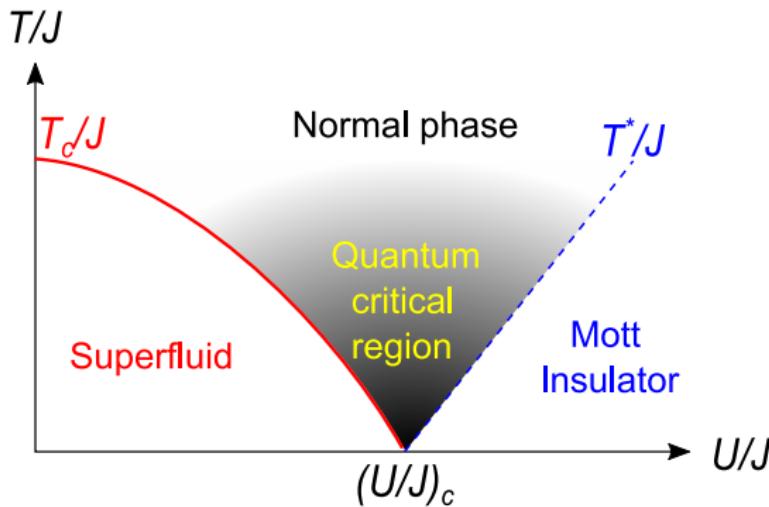
Mott insulator :

- zero condensed fraction
- on-site occupation numbers pinned to the *same* integer value
- Energy gap $\sim U$ (far from transition)
- No flow possible unless one pays an extensive energy cost $\sim U$



Quantum phase transitions

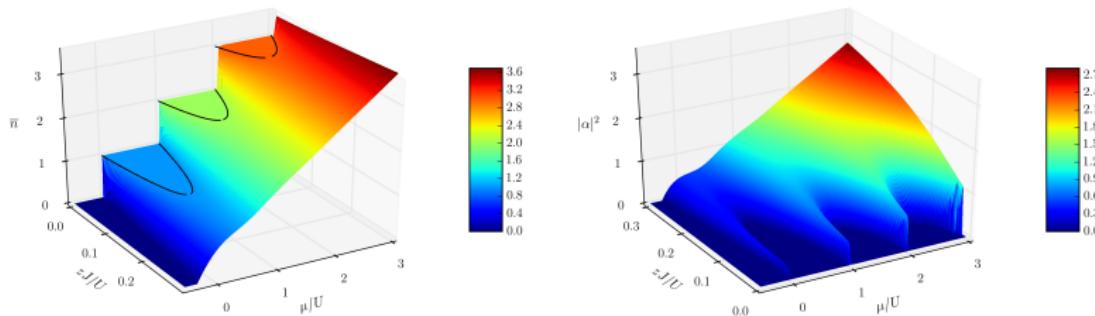
Mott transition : prototype of a quantum phase transition driven by two competing terms in the Hamiltonian



- Different from standard phase transition (competition between energy and entropy)
- Thermal crossover in the Mott insulator regime
- Strongly fluctuating quantum critical region

Mean-field phase diagram

Generalization to incommensurate fillings:



Superfluid stable when

$$\mu_{n_0}^{(+)} \leq \mu \leq \mu_{n_0+1}^{(-)}.$$

$\mu_{n_0}^{(\pm)}$: upper/lower boundaries of the Mott region with occupation number n_0

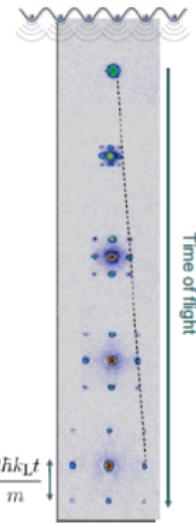
$$\mu_{n_0}^{(\pm)} = U(n_0 - \frac{1}{2}) - \frac{zJ}{2} \pm \sqrt{U^2 - 2UzJ(2n_0 + 1) + (zJ)^2}$$

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Time-of-flight interferences

Evolution of field operator after suddenly switching off the lattice :

$$\hat{\psi}(\mathbf{r}, t=0) = \sum_i W(\mathbf{r} - \mathbf{r}_i) \hat{a}_i \rightarrow \hat{\psi}(\mathbf{k}) \propto \tilde{W}(\mathbf{K}) \sum_i e^{i\mathbf{K} \cdot \mathbf{r}_i} \hat{a}_i$$



Time of flight signal, far-field regime ($\mathbf{K} = \frac{M\mathbf{r}}{\hbar t}$) :

$$n_{\text{tof}}(\mathbf{K}) = \langle \hat{\psi}^\dagger(\mathbf{K}) \hat{\psi}(\mathbf{K}) \rangle \approx \mathcal{G}(\mathbf{K}) \mathcal{S}(\mathbf{K})$$

- $\mathcal{G}(\mathbf{K}) = \left(\frac{M}{\hbar t}\right)^3 |\tilde{W}(\mathbf{K})|^2$ smooth envelope
- $\mathcal{S}(\mathbf{K}) = \sum_{i,j} e^{i\mathbf{K} \cdot (\mathbf{r}_j - \mathbf{r}_i)} \langle \hat{a}_i^\dagger a_j \rangle$ structure factor.

Key quantity : single-particle correlation function (also called $g^{(1)}(\mathbf{r}, \mathbf{r}')$)

$$\mathcal{C}(i, j) = \langle \hat{a}_i^\dagger a_j \rangle$$

Determines the structure factor and the interference pattern (or lack thereof)

Time-of-flight interferences across the Mott transition

$$\mathcal{C}(i, j) = \langle \hat{a}_i^\dagger a_j \rangle$$

$$\mathcal{S}(\mathbf{K}) = \sum_{i,j} e^{i\mathbf{K} \cdot (\mathbf{r}_j - \mathbf{r}_i)} \langle \hat{a}_i^\dagger a_j \rangle$$

Superfluid/BEC :

Mott insulator :

$$\mathcal{C}_{\text{BEC}}(i, j) = \sqrt{\bar{n}_i \bar{n}_j}$$

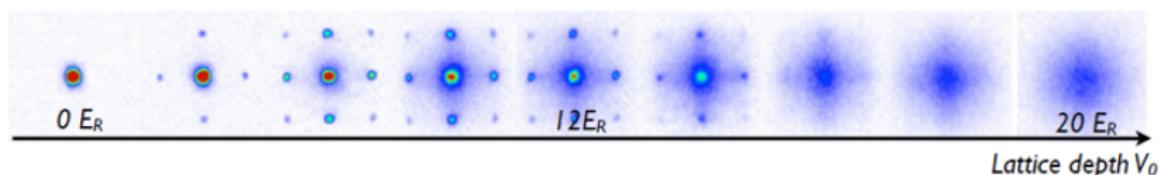
$$\mathcal{C}_{\text{Mott}}(i, j) = n_0 \delta_{i,j}$$

$$\mathcal{S}_{\text{SF}}(\mathbf{K}) \approx \left| \sum_i e^{i\mathbf{K} \cdot \mathbf{r}_i} \sqrt{\bar{n}_i} \right|^2,$$

$$\mathcal{S}_{\text{Mott}}(\mathbf{K}) \approx N_s$$

Bragg spots (height $\sim N_s^3$, width $\sim 1/N_s$)

Featureless



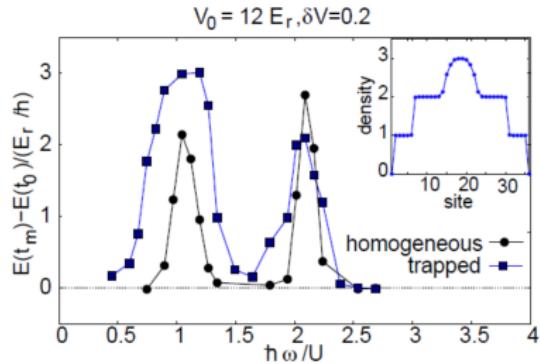
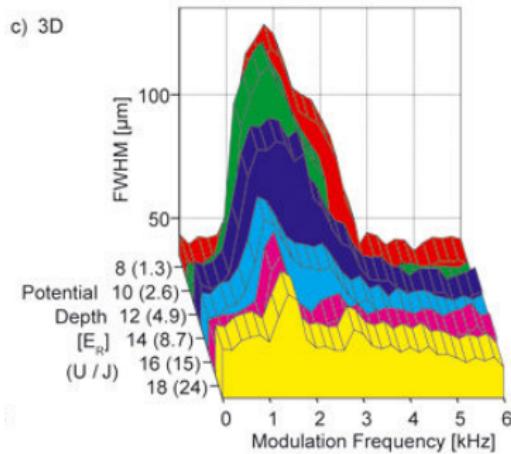
Ramping back down

M. Greiner et al., Nature 2002

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Probing the transition : lattice shaking

- Modulation of the lattice height : $V_0(t) = V_0 + \delta V_0 \cos(\omega_{\text{mod}} t)$
- Main effect for deep lattices : $\delta \hat{V} = -\delta J \cos(\omega_{\text{mod}} t) \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j$
- **Superfluid regime** : broad response at all frequencies
- **Mott insulator regime** : Coupling to particle-hole excitations \implies peaks at $\omega_{\text{mod}} \approx \frac{U}{\hbar}$



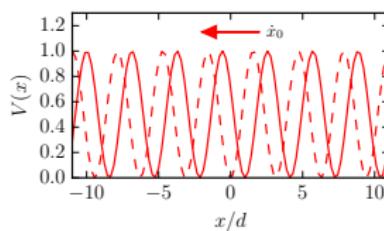
Th.: Kollath et al., PRL 2006

Exp: Schori et al., PRL 2004

Uniformly accelerated lattice : $V_{\text{lat}}[x - x_0(t)]$ with $x_0 = -\frac{Ft^2}{2m}$

Lab frame:

$$H_{\text{lab}} = \frac{p^2}{2m} + V_{\text{lat}}[x - x_0(t)]$$

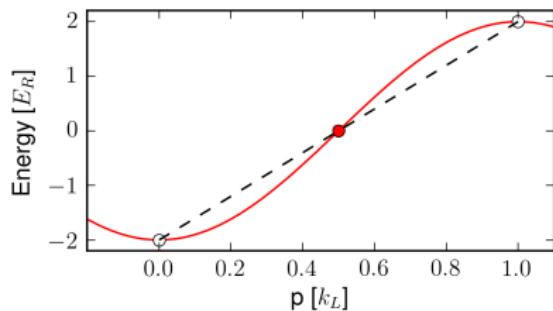
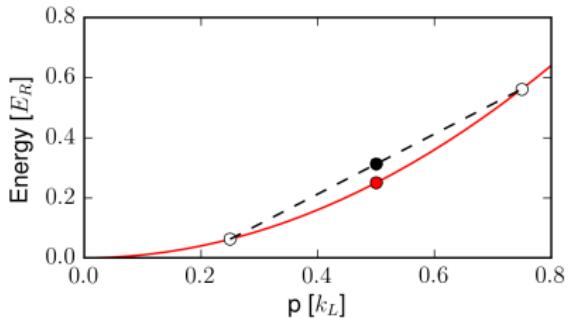


Non-interacting atoms undergo Bloch oscillations.

What happens with interactions ?

Collision of two atoms with momentum \mathbf{p}_0 :

$$2\mathbf{p}_0 = \mathbf{p}_1 + \mathbf{p}_2$$
$$2\varepsilon(\mathbf{p}_0) = \varepsilon(\mathbf{p}_1) + \varepsilon(\mathbf{p}_2)$$



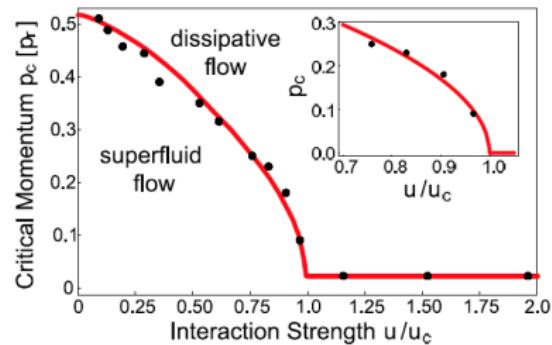
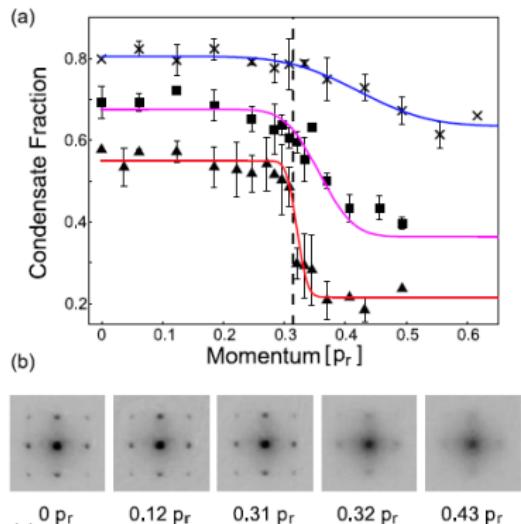
Because of the band structure, collisions redistributing quasi-momentum in the Brillouin zone are kinematically allowed in a lattice (for $|q| > \frac{\pi}{2d}$ in 1D).

This leads to a *dynamical instability* of wavepackets exceeding a certain critical velocity ($v_c = \frac{\hbar k_L}{M}$ in 1D).

Probing the transition : moving lattice and critical momentum

MIT experiment [Mun et al., PRL 2007]:

- moving lattice dragging the cloud along
- $p_r = \hbar k_L$: momentum unit
- cycle the lattice back and forth through the cloud (period 10 ms)



Critical point near $U/J \approx 34.2(2)$

Mean field theory predicts 34.8 , quantum Monte-Carlo 29.3 : ?

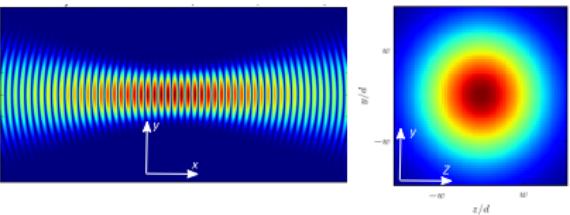
- ➊ Wannier functions and tight-binding limit
- ➋ Bose-Hubbard model
- ➌ Ground state : Superfluid -Mott insulator transition
 - Phase coherence
 - Dynamics and transport
 - Shell structure
- ➍ A glance at fermions

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Non-uniform lattices : Harmonic trapping

Actual laser beams have Gaussian profile :
Lattice potential of the form

$$V_{1D} = -V_0 \cos^2(k_L x) e^{-2\frac{y^2+z^2}{w^2}}.$$



In the Wannier basis, additional potential energy term :

$$\delta V_x \approx \sum_i \frac{1}{2} M \Omega^2 (y_i^2 + z_i^2) \hat{a}_i^\dagger \hat{a}_i,$$

with $\Omega^2 \approx \frac{8V_0}{M w_x^2} \left(1 - \frac{k_L \sigma_w}{2}\right)$.

For a 3D lattice :

$$\delta V \approx \sum_i \underbrace{\frac{1}{2} M \Omega^2 (x_i^2 + y_i^2 + z_i^2)}_{V_h(\mathbf{r}_i)} \hat{a}_i^\dagger \hat{a}_i,$$

with V_h a harmonic potential.

An insulator is incompressible :

Within a Mott lobe, changing the chemical potential does not change the density.

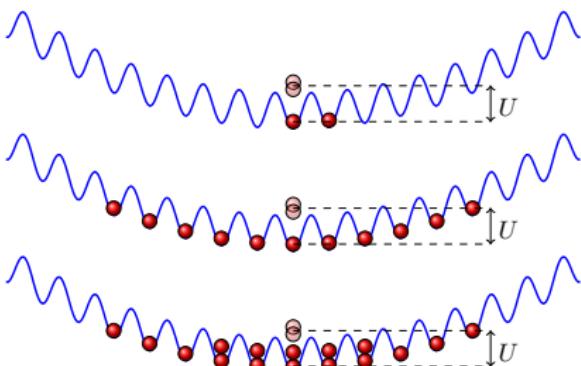
Consequence of the gap for producing particle/hole excitations, which vanishes at the phase boundaries.

Consequence : non-uniform density profile in a trap

Simple picture in 1D :

Filling the lattice atom by atom in the atomic limit ($J = 0$)

Formation of shells due to competition between interaction and potential energy



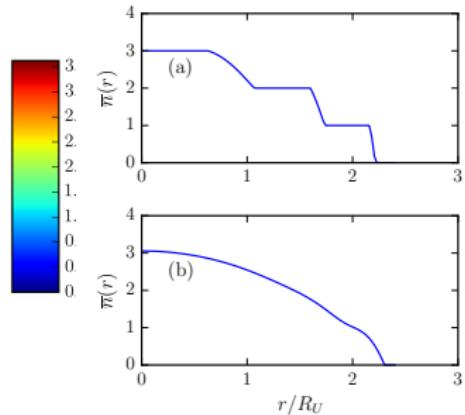
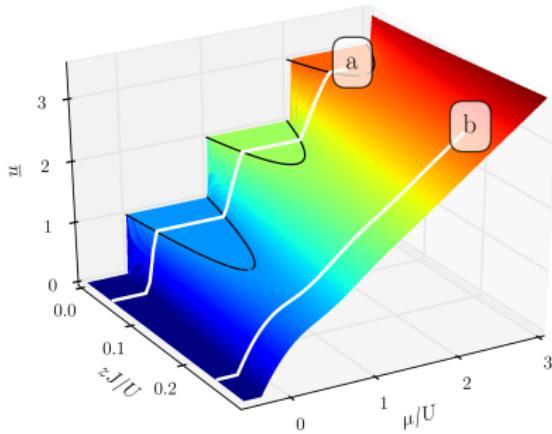
Local density approximation

Local density approximation for a smooth potential :

$$\mu_{\text{loc}}(\mathbf{r}) = \mu - V_h(\mathbf{r}),$$

μ : global chemical potential fixed by constraining the total atom number to N

Density profile given by the equation of state $n[\mu]$ for the uniform system, evaluated at $\mu = \mu_{\text{loc}}(\mathbf{r})$.



- **Mott insulator (a):** density changes abruptly; plateaux with uniform density
- **Superfluid (b):** density changes smoothly from the center of the cloud to its edge

Single-site imaging of Mott shells

Munich experimental setup (Sherson *et al.* 2010) :

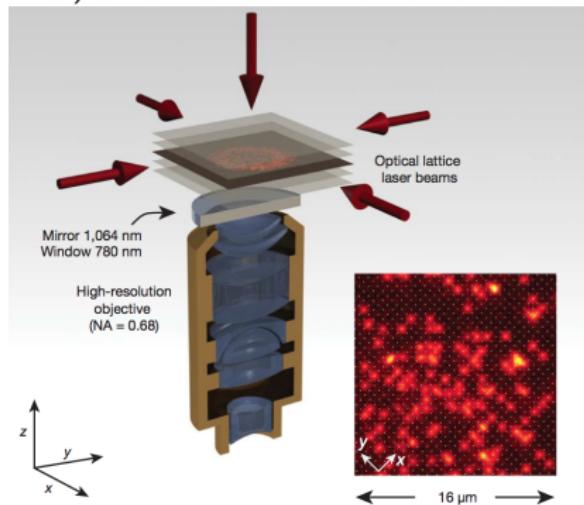
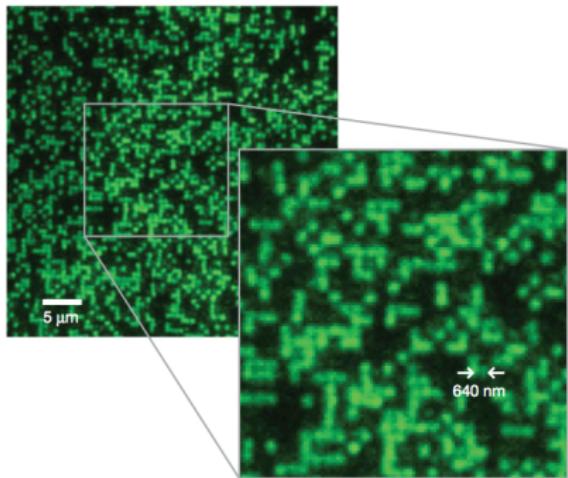


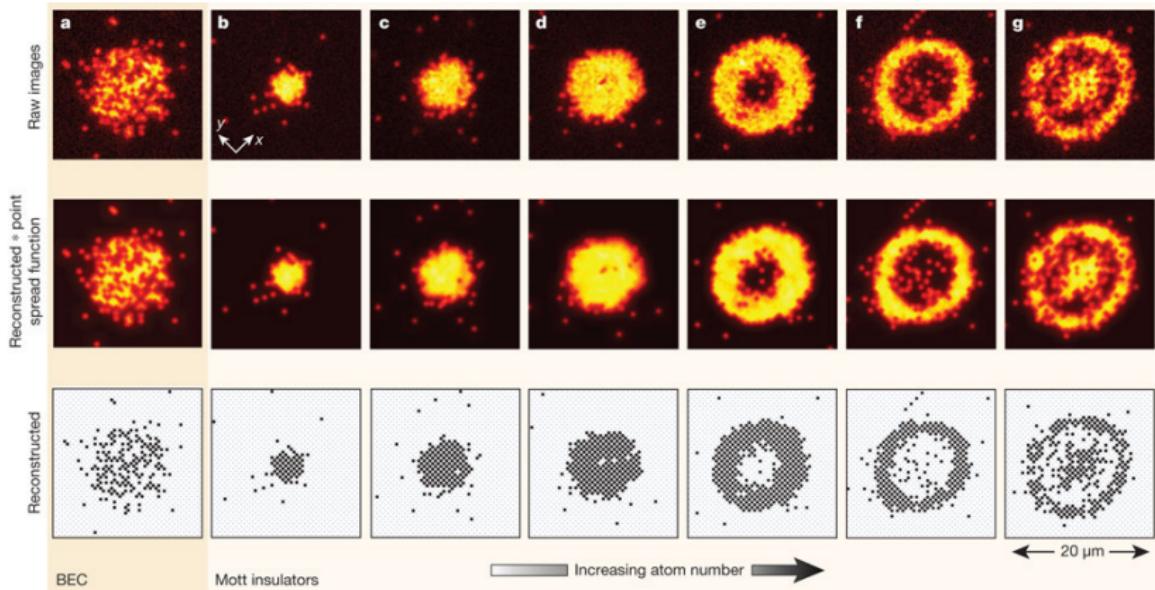
image of a dilute gas

image of a Bose-Einstein condensate in a 2D lattice [Bakr *et al.*, 2010]:



Single-site imaging of Mott shells

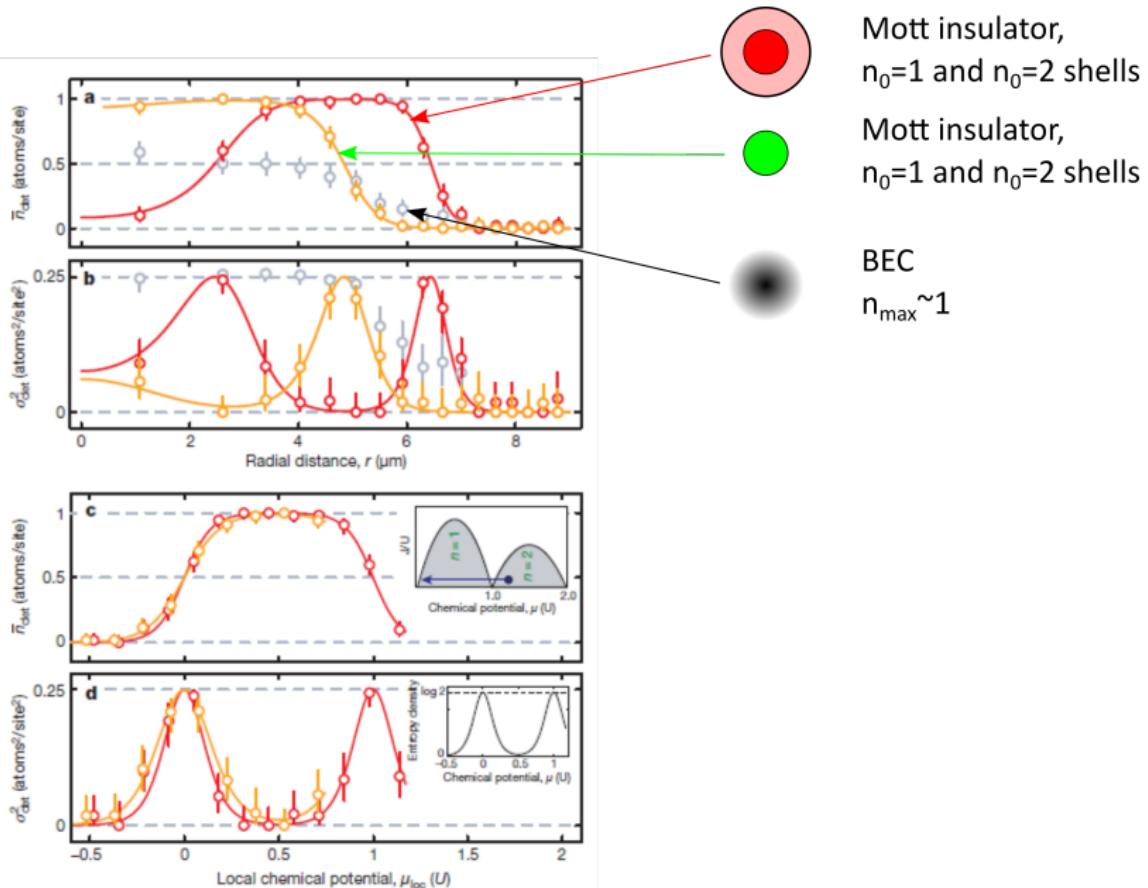
In-situ images of a BEC and of Mott insulators [Sherson et al., Nature 2010]:



Total atom number (or chemical potential) increases from left to right.

Lowest row : reconstructed map of the atom positions, obtained by deconvolution of the raw images to remove the effect of finite imaging resolution.

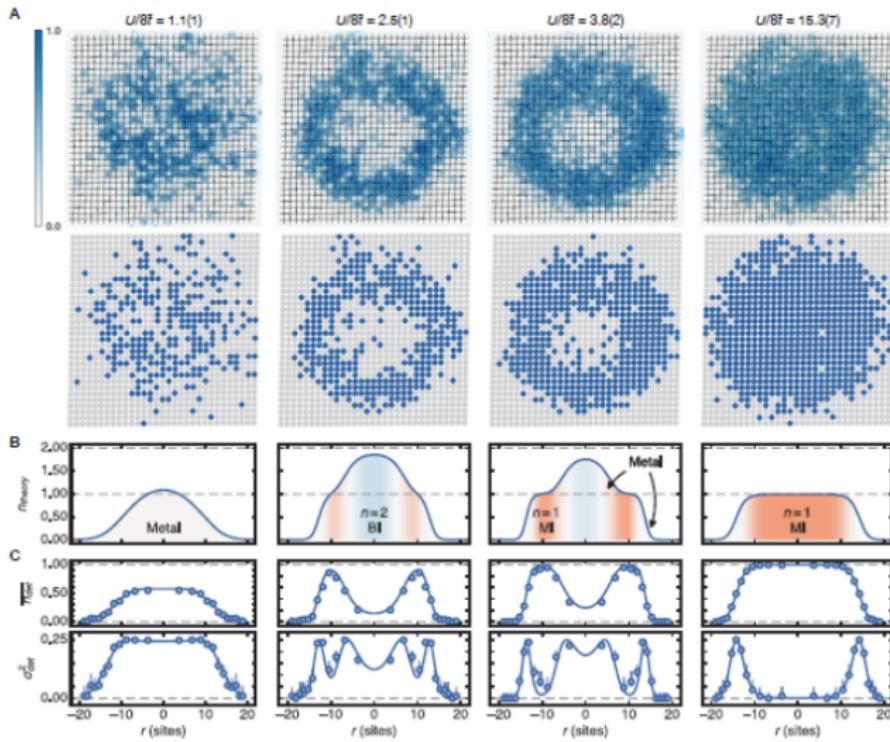
Mott shells and LDA



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A glance at fermions

Two-component fermions with repulsive interactions: Fermionic Mott insulator



[Greif et al., arxiv1511.06366 (2015)]

Fermionic quantum gas microscopes also demonstrated in : Haller et al., arxiv1503.02005 (2015); Cheuk et al., arxiv1503.02648 (2015); Omran et al., arxiv1510.04599 (2015).

Two-component repulsive Hubbard model :

- antiferromagnetic Néel phase below $S_c/Nk_B \lesssim 0.5$
- d -wave superconductors ? unknown but certainly much lower entropy.

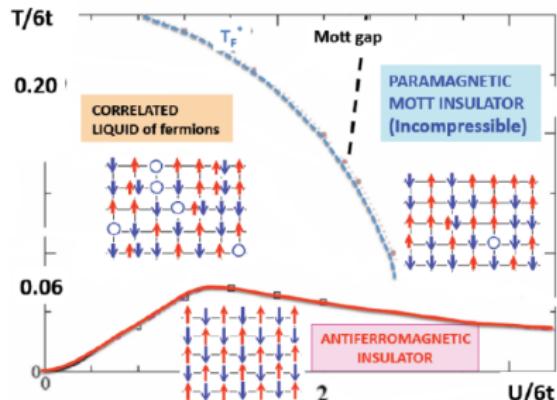


figure from [Georges & Giamarchi, arxiv1308.2684 (2014)]

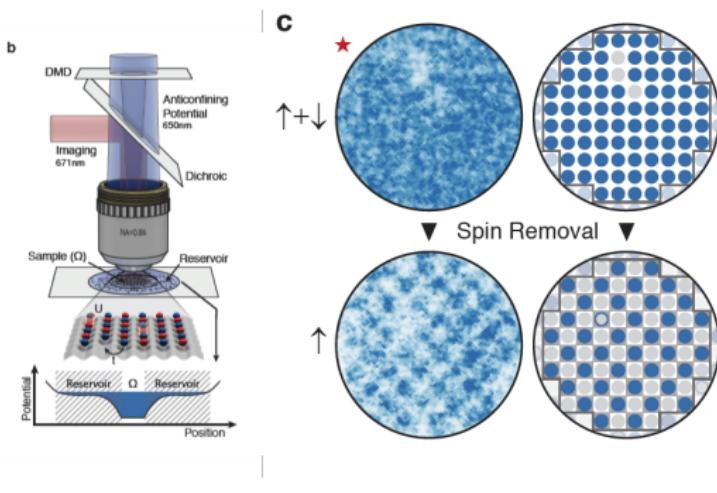
- Experiments are actually not performed at temperatures low enough that one can safely take the limit $T = 0$. achieve $S/Nk_B \sim 1$,
- many interesting phases are awaiting below that scale
- limits of the current “cooling then adiabatic transfer” technique,

New methods to cool atoms directly in the lattice needed.

See reviews for a more detailed discussion :
 [McKay & DeMarco, , Rep. Prog. Phys. 74, 0544401 (2011)],
 [Georges & Giamarchi, arxiv1308.2684 (2014)]

Observation of antiferromagnetic ordering

Recent realization of magnetic ordering in M. Greiner's group (Harvard University)



[Marurenko et al., Nature 2017]

- Spin-resolved quantum gas microscopy (right picture)
- Density of spin \uparrow atoms displays a checkerboard pattern characteristic of Néel ordering.
- key experimental advance : using carefully shaped trap potential to create high- and low-entropy regions; Néel ordering occurs only in the latter.

The End