• Atoms in Optical Lattices

* Due to the so-called dipole force, atoms loaded in a standing-wave formed by two counterpropagating lasers, may experience a sinusoidal external potential of the form:

$$V_{ext}(x) = V_0 \sin^2 qx$$

(q is the wavenumber of the lasers forming the standing wave and V_0 is the potential depth which is proportional to the laser intensity.)

with periodicity $d = \pi/q$

* This is a so-called <u>optical lattice</u>. One may create a 3D optical lattice by employing 3 pairs of counter-propagating lasers. (<u>Note</u>: We will discuss about other "exotic" optical lattices later in these lectures.)
* Due to its periodicity, atoms in optical lattices behave in a similar fashion as electrons in a crystal (but here with neither phonons nor defects)
* In absence of interaction the atoms in the optical lattice obey the Schrödinger equation:

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V_0 \sin^2 qx\, \psi(x)$$

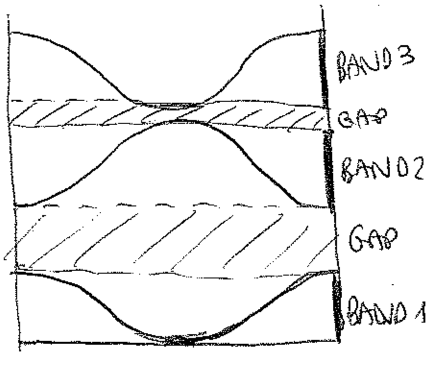
(we keep the discussion 1D for simplicity)

The stationary solutions are of the form (Bloch theorem):

$$\psi_p(x) = e^{ipx/\hbar}\, u_p(x) \quad \text{(Bloch functions)}$$

where $\begin{cases} p \text{ is the quasimomentum} \rightarrow -q \le p/\hbar \le q \quad (1^{st} \text{ Brillouin zone}) \\ u_p(x) = u_p(x+d) \end{cases}$

For a given value of p there are different eigen-energies E_{pn} which form the typical band structure of periodic potentials:



* Each band is characterized by a dispersion law $E_n(p) = E_{pn}$
* The spectrum presents forbidden gaps.
* Associated with E_{pn} we have a function $u_{pn}(x)$.

* We can introduce an alternative description, which is particularly useful for our discussion of the tight-binding regime later in this lecture. For the n-th band we define the Wannier-function at the site j

$$W_j^{(n)}(x) = \frac{1}{\sqrt{N}} \sum_q e^{-iqjd/\hbar} \psi_{qn}(x)$$

$\equiv w^{(n)}(x-jd)$ ↳ number of sites; $\psi_{qn}(x)$ ⟶ Bloch function $\Rightarrow u_{qn}(x)\, e^{iqx/\hbar}$

These functions form a complete set of orthogonal functions:

$$\int_{-d/2}^{d/2} w^{(n)}(x-jd)\, w^{(n')}(x-j'd)\, dx = \delta_{nn'}\, \delta_{j,j'}$$

Due to the factor $e^{iq(x-jd)/\hbar}$ the Wannier function is strongly localized at $x=jd$, i.e. the j-th site, and this is why this basis is so good in the tight-binding regime.

* BEC IN AN OPTICAL LATTICE: DISCRETE NONLINEAR SCHRÖDINGER EQUATION

* Let's analyze now the particular case of a BEC in an optical lattice. We will first assume that there's actually condensation, and that we may employ the GP formalism. We will soon see when this is not correct.

- We hence consider the 1D time-independent GPE:

$$\mu \psi_0(x) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_0(x) + V_{ext}(x)\, \psi_0(x) + g |\psi_0(x)|^2 \psi_0(x)$$

where now $V_{ext}(x+d) = V_{ext}(x)$ is the periodic lattice potential.

- The ground-state solution is the Bloch function with $p=0$ (in the lowest band). This is obviously clear without interactions, but the interactions do not change this fact.

* We may express any Bloch function in terms of the Wannier functions

$$\psi_{pn}(x) = \frac{1}{\sqrt{N}} \sum_j e^{ipjd/\hbar}\, w^{(n)}(x-jd)$$

In particular:

$$\Psi_0(x) = \frac{1}{\sqrt{N}} \sum_j w(x-jd)$$

(from now on I consider only the lowest band, and hence remove the band index.)

• It's quite interesting to have a look to the Fourier-Transform:

$$\tilde\Psi_0(p) = \int dx\, \Psi_0(x)\, e^{-ipx/\hbar} = \frac{1}{\sqrt{N}} \sum_j \int dx\, w(x-jd)\, e^{-ipx/\hbar}$$

$$= \frac{1}{\sqrt{N}} \sum_j \underbrace{\left[\int w(x)\, e^{-ipx/d} dx\right]}_{\tilde w(p)} e^{-ipjd/\hbar} = \tilde w(p) \underbrace{\frac{1}{\sqrt{N}} \sum_j e^{-ipjd/\hbar}}_{\sum_n \delta\left[p - \frac{2\pi\hbar}{d} n\right]}$$

Hence

$$\tilde\Psi_0(p) = \tilde w(p) \underbrace{\sum_n \delta\left[p - 2\pi \frac{\hbar}{d} n\right]}$$

→ δ-comb with peaks at $0, \pm 2\hbar q, \pm 4\hbar q, \dots$

↙ Fourier-Transform of the on-site (Wannier) wavefunction

• We may evaluate $w(x)$, and hence $\tilde w(p)$, exactly, but we may get a quite good approximation (if the lattice is deep-enough) by approximating at a lattice minimum

$$V_0 \sin^2 qx \simeq V_0 q^2 x^2 \equiv \frac{1}{2} m \omega_{eff}^2 x^2$$

We have then an effective harmonic oscillator of frequency $\omega_{eff} = \sqrt{\frac{2V_0 q^2}{m}}$

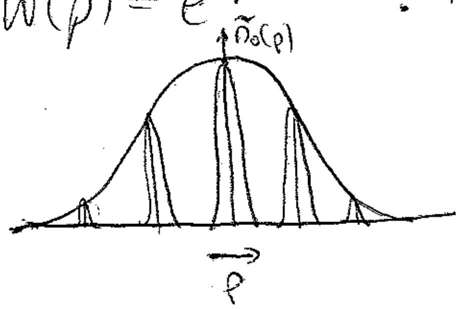
which has a ground state

$$w(x) \simeq \frac{1}{\sqrt{\sqrt{\pi}\, l_{HO}}}\, e^{-x^2/2 l_{HO}^2} \quad \text{with } l_{HO} = \sqrt{\frac{\hbar}{m\omega_{eff}}}$$

We approximate the Wannier function by this ground state. Hence:

$\tilde w(p) = e^{-p^2 l_{HO}^2/2\hbar^2}$. The momentum distribution is hence:

$$\tilde n_0(p) = |\tilde\Psi_0(p)|^2 \propto \sum_n e^{-4\pi^2 n^2 l_{HO}^2/d^2}\, \delta\left[p - \frac{2\pi\hbar n}{d}\right]$$



• We have a series of peaks with a Gaussian envelope. Since the BEC has a finite size L, the peaks aren't truly δ's, but have a finite with ~ $1/L$.

* The momentum distribution is experimentally very important, because a sudden release of the atoms, leads after expansion to a map of the initial momentum distribution into the final density distribution.

(Note: the expanded density distribution reproduces the original momentum distribution for expansion times much longer than the inverse of the original trapping frequencies and if the non-linear terms can be neglected during the expansion. The latter demand a fast-enough density decrease after releasing.)

· Hence a time-of-flight picture after releasing the BEC in the lattice will show the peaked structure showed above.

* The appearance of these interference pattern in experiments shows that the system is coherent. Indeed what it means is that the coherence length is larger than the intersite spacing.

In the previous discussion we have assumed a pure BEC.

For the case of a pure BEC the coherence length is ($l_{coherence}$) of the order of the sample size. This is why the peaks of the interference pattern have a width $\propto 1/L$. For a less coherent source, the peaks have a width $\Delta K \propto 1/l_{coherence}$.

Note that if $l_{coherence} \lesssim d$, then $\Delta K \sim 2q$, and the peaks merge.

(Note: in other words when the quasimomentum distribution gets basically flat. $\Delta K \approx q$, the quasimomentum distribution gets basically flat (the Brillouin zone saturates), and obviously the fringes disappear)

· This discussion is particularly important in our future discussion of beyond-GPE scenarios.

* The dynamics of a BEC in an optical lattice (confined to the lowest band) is better described in the frame of the so-called discrete non-linear Schrödinger equation (DNLSE). In the following we introduce the idea of DNLSE, and employ it to discuss an important problem related to the coherence of BECs in lattices, namely the problem of Josephson junction arrays of BEC.

* I reduce, again, the discussion to 1D. The NLSE (ie. the GPE) is of the form:

$$i\hbar \dot{\psi}(x,t) = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{ext}(x) + g|\psi(x)|^2\right]\psi(x)$$

where $V_{ext}(x) = V_{lattice}(x) + V_{HO}(x)$

($V_{lattice}$: lattice; V_{HO}: overall harmonic confinement (if any))

* We shall consider the situation in which only the lowest band is relevant (all relevant energies are much lower than the gap). Then we may expand $\psi(x,t)$ in the basis of Wannier functions:

$$\psi(x,t) = \sum_n w_n(x)\psi_n(t)$$

Then:

$$i\hbar \sum_n w_n(x)\dot{\psi}_n(t) = \sum_{n'}\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{ext}(x)\right) w_{n'}(x)\psi_{n'}(t)$$
$$+ g\sum_{n_1 n_2 n_3} w^*_{n_1}(x) w_{n_2}(x) w_{n_3}(x)\; \psi^*_{n_1}(t)\psi_{n_2}(t)\psi_{n_3}(t)$$

We multiply by $w_n^*(x)$ and integrate over x. Using orthogonality of the Wannier functions we get

$$i\hbar\dot{\psi}_n(t) = \sum_{n'}\left[\int dx\, w_n^*(x)\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{ext}(x)\right) w_{n'}(x)\right]\psi_{n'}(t)$$
$$+ \sum_{n_1 n_2 n_3}\left[g\int dx\, w_n^*(x) w^*_{n_1}(x) w_{n_2}(x) w_{n_3}(x)\right]\psi^*_{n_1}(t)\psi_{n_2}(t)\psi_{n_3}(t)$$

* Since the Wannier functions are very localized (for sufficiently deep lattices) then:

$$\int dx\, w_n^*(x)\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V_{ext}(x)\right]w_{n'}(x) \cong -J\left[\delta_{n',n+1}+\delta_{n',n-1}\right] + \epsilon_n\,\delta_{n',n}$$

$$g\int dx\, w_n^*(x)\,w_{n_1}^*(x)\,w_{n_2}(x)\,w_{n_3}(x) \simeq \underbrace{\int dx\,|w_n(x)|^4}_{U}\,\delta_{n_1 n}\,\delta_{n_2 n}\,\delta_{n_3 n}$$

Hence:

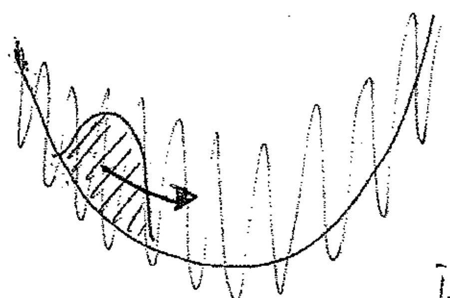
$$\boxed{i\hbar\dot{\psi}_n = -J\left(\psi_{n+1}+\psi_{n-1}\right) + \epsilon_n\psi_n + U|\psi_n|^2\psi_n}$$

This is the <u>discrete NLSE</u>

* This equation is very helpful to describe the physics of BEC in optical lattices
(<u>Note</u>: This type of discrete nonlinear equation is also well-known in nonlinear optics, in particular in the context of the so-called <u>discrete solitons</u>.)

* Although we can approximate the condensates in each lattice site as having their own wave functions, <u>tunneling between adjacent wells locks all the different condensates in phase</u> (This is what leads to the interference pattern discussed above).

. An interesting experiment on BEC coherence in optical lattices was performed in Florence in 2001. A BEC was created in an optical lattice with an overall (magnetic) trap. The trap was suddenly displaced, and then the BEC started an oscillatory motion.



. This collective motion can only be established if there's an overall coherence, in other words only if the relative phase among all adjacent sites remains locked.

· The latter is easy to understand.
A collective motion of a wavepacket demands
$\psi(x)\, e^{ikx}$ (motion with momentum $p = \hbar k$)
In a lattice, the phase at the site j would then be
$\phi_j = \phi(jd) = kjd$
at site j+1 $\longrightarrow$ $\phi_{j+1} = \phi[(j+1)d] = k(j+1)d$
$\Big\}$ $\Delta\phi = \phi_{j+1} - \phi_j = kd$

* Hence $\Delta\phi = kd$ for all neighbouring sites. Otherwise one can't mimic an overall collective motion!

· For displacement that are not very large, they observed in Florence indeed a collective motion. In absence of lattice the BEC would oscillate with a frequency equal to the harmonic one

* In the presence of the lattice they observed a substantially lower oscillation frequency.
The reason for this is because, as we already know (p. (7)), the current flowing through each Josephson junction (i.e. between each 2 wells of the lattice) has a maximum value given by the Josephson amplitude I_J, which is directly proportional to the tunneling rate. This limits the velocity the condensate can flow through the barriers and hence lowers the oscillation frequency.

* This may be easily see from the DNLSE formalism.
Let $\psi_j = \sqrt{n_j}\, e^{i\phi_j}$, then we can easily transform the DNLSE of p. (18) in the form (recall the hydrodynamic eqs. of p. (5))

$$\hbar \dot{n}_j = 2J\sqrt{n_j n_{j-1}}\,\sin[\phi_j - \phi_{j-1}] - 2J\sqrt{n_j n_{j+1}}\,\sin(\phi_{j+1} - \phi_j)$$

$$\hbar \dot{\phi}_j = -U n_j - \Omega j^2 + J\sqrt{\frac{n_{j-1}}{n_j}}\cos(\phi_j - \phi_{j-1}) + J\sqrt{\frac{n_{j+1}}{n_j}}\cos(\phi_{j+1} - \phi_j)$$

(where $\Omega = \frac{1}{2} m\omega^2 d^2$, with ω the oscillator frequency.
Note that $j = 0$ is the trap center)

• We introduce the center of mass coordinate

$$\xi(t) = \sum_j j\, n_j$$

Then one may obtain

$$\hbar \dot{\xi} = 2J \sum_j \sqrt{n_j n_{j+1}}\,\sin(\phi_{j+1} - \phi_j)$$

* For a large number of atoms we may neglect the J-dependent terms in the eq. of $\dot{\phi}_j$ (this is equivalent as neglecting the quantum pressure in the discussion of the Thomas-Fermi regime in p. (5)).
In the Thomas-Fermi regime $U n_j = \mu - \Omega (j - \xi)^2$

Hence $\hbar \dot{\phi}_j \simeq -\mu + \Omega (j-\xi)^2 - \Omega j^2$

Also $\hbar \dot{\phi}_{j+1} \simeq -\mu + \Omega[(j+1) - \xi]^2 - \Omega (j+1)^2$

Hence $\hbar(\dot{\phi}_{j+1} - \dot{\phi}_j) \simeq -2\Omega\xi$

* Assuming that the inter-site relative phase remains locked (but time dependent): $\phi_{j+1} - \phi_j = \Delta\phi(t)$, we arrive to the

pendulum equations:

$$\begin{cases} \hbar \frac{d}{dt} \xi(t) = 2J \sin \Delta\phi(t) \\ \hbar \frac{d}{dt} \Delta\phi(t) = -2\Omega\, \xi(t) \end{cases}$$

These are indeed very similar eqs. as those of p. (8) for a single Josephson junction.

* For small amplitude oscillations, $\sin\Delta\phi \simeq \Delta\phi$, and we obtain $\frac{d^2}{dt^2}\xi(t) = -\frac{4}{\hbar^2}\Omega J \xi$

Hence the oscillatory motion is with a frequency

$$\omega_{osc} = \frac{2}{\hbar}\sqrt{\Omega J} = \frac{2}{\hbar}\sqrt{\frac{m\omega^2}{2}d^2 J} = \omega\left[J/E_{REC}\right]^{1/2}$$

where we have introduced the (important) recoil energy

$$E_{rec} = \frac{\hbar^2}{2md^2}$$

• For very small tunneling $J \ll E_{rec}$, $\omega_{osc} \ll \omega$ as observed.

• As a final remark, note that (as for the Josephson junction) larger displacements lead to anharmonic motion (recall p. (8)) and $\Delta\phi$ may reach $\pi/2$. The system then becomes unstable (dynamically) and phase coherence is lost after a transient time. One gets into the so-called classical insulator regime (which is the Josephson junction array equivalent of the already mentioned self-trapping in individual Josephson junctions.)

• The BEC in an optical lattice has a very rich physics which we can't discuss in detail here. For more details see e.g. Stringari–Pitaevskii book. We will now move to the very interesting case in which the GPE formalism fails.

• BOSE GASES IN A LATTICE (BEYOND MEAN FIELD)

* Recall from our discussion of the Josephson effect (p. (10)) that for sufficiently large E_C/E_J (i.e. interaction energy vs. tunneling energy) the coherent state (for which the mean-field GPE formalism applies) doesn't any more describe the two-well system, which is rather described by a number-squeezed (and eventually a Fock-) state for which the coherence factor vanishes.

* We will extend now this discussion to the case of bosons in an optical lattice. Recall our discussion of pgs (15)-(16) concerning the <u>interference fringes</u> after switching-off the lattice. There we already mentioned that the peak width is a measurement of coherence. Let's see this in some more detail. As in the previous case we reduce to 1D.

Let's assume that each condensate at each site is characterized by its own phase S_K. Then

$$\psi_0(z) = \frac{1}{\sqrt{N}}\sum_j w(x-jd)\, e^{iS_j}$$

$$\tilde{\psi}_0(p) = \frac{1}{\sqrt{N}}\sum_j \int dx\, w(x-jd)\, e^{-ipx/\hbar} e^{iS_j} = \tilde{w}(p)\,\frac{1}{\sqrt{N}}\sum_j e^{-ipjd/\hbar} e^{iS_j}$$

Then the momentum distribution is

$$\langle n_0(p)\rangle = n_0(p)\sum_j e^{-ijpd/\hbar}\langle\cos[S_j-S_0]\rangle$$

(we have employed translational invariance)

where $n_0(p)=|\tilde{w}(p)|^2 \simeq e^{-p^2 l_{ho}^2/2}$ (see p. (15)) and $\langle..\rangle$ means the average over the phase fluctuations.

(<u>Note</u>: we recover the factor $\langle\cos(S_j-S_0)\rangle$ similar to that of the coherence factor that we saw already in the Josephson junction in p. (9)).

• In the absence of phase fluctuations one has $\langle\cos[S_j-S_0]\rangle = 1$ and one recovers the δ-peaked structure introduced in p. (15). On the contrary, phase fluctuations tend to destroy the interference picture. Note that if the coherence factor decays exponentially (and this is what happens in an insulator) $\sim e^{-|j|/\Delta_j}$, then $\sum_j e^{-ijpd/\hbar} e^{-|j|/\Delta_j} \propto \frac{\Delta_j}{1+\left(\frac{pd}{\hbar}\Delta_j\right)^2}$, i.e. every

δ-peak is substituted by a Lorentzian of width $\frac{\hbar}{\Delta_j}$. Here we recover our discussion of p. (16). It's clear that if $l_{coherence} \equiv \Delta_j$ is $\lll d$, then $\Delta p \sim \hbar q$, and as discussed in p. (16) the interference fringes disappear.

• The full disappearance of the fringes tell us, hence, that the system is basically incoherent from site to site. This is particularly important in the following discussion.

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* BOSE-HUBBARD HAMILTONIAN: THE SUPERFLUID TO MOTT INSULATOR TRANSITION

* In the case in which the mean atom number occupation per site is quite small (of the order of 1) and the lattice is deep (this is particularly true for strong 3D optical lattices induced by 3 pairs of counterpropagating lasers) then we can't treat any longer the problem with a DNLSE, which was assumming individual BECs at each lattice sites.

* We shall rather employ the Bose-Hubbard Hamiltonian which we already introduced in p. (11) in our discussion of the Josephson effect. As for that case our starting point is the second-quantized Hamiltonian

$$\hat{H} = \int d^3r\, \hat{\psi}^+(\vec{r}) \left[\frac{-\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) \right] \hat{\psi}(\vec{r}) + \frac{g}{2}\int d^3r\, \hat{\psi}^+(\vec{r})\hat{\psi}^+(\vec{r})\hat{\psi}(\vec{r})\hat{\psi}(\vec{r})$$

where $V_{ext}(\vec{r}) = V_0 \left(\sin^2 qx + \sin^2 qy + \sin^2 qz \right)$

is a cubic optical lattice (we consider such a lattice for simplicity of the discussion)

* We will restrict our discussion to the lowest energy band, which as for previous discussions means that all other energies of the problem are much lower than the gap to the second band.

* Associated to the lowest band we have the Wannier functions. Due to the easy separability of the cubic potential, the Wannier function at the site $\vec{j} = (j_x\, j_y\, j_z)$ is simply

$$W_{\vec{j}}(\vec{r}) = w(x - j_x d)\, w(y - j_y d)\, w(z - j_z d)$$

where w is the Wannier function associated to each one of the 1D potentials in each direction.

* We may then expand

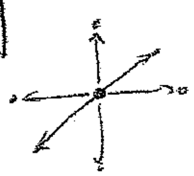
$$\hat{\Psi}(\vec{r}) = \sum_{\vec{j}} W_{\vec{j}}(\vec{r})\, \hat{a}_{\vec{j}}$$

(Note: This is similar as what we did in the derivation of the DNLSE in p. (18))

Introducing this expansion into the original $\hat{H}$, and in the tight-binding approximation (very localized $W_{\vec{j}}(\vec{r})$ that very poorly overlap), we obtain

$$\hat{H}_{BH} = -t \sum_{\vec{j},\vec{\sigma}} \hat{a}^{+}_{\vec{j}}\, \hat{a}_{\vec{j}+\vec{\sigma}} + \frac{U}{2} \sum_{\vec{j}} \hat{n}_{\vec{j}} (\hat{n}_{\vec{j}} - 1)$$

where $\boxed{t = -\int d^3r\; W_{\vec{j}}(\vec{r}) \left[\frac{-\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r})\right] W_{\vec{j}+\vec{\sigma}}(\vec{r})}$ ← hopping energy



where $\vec{j}+\vec{\sigma}$ are the nearest neighbors of the site $\vec{j}$

and $\boxed{U = g\int d^3r\; |W_{\vec{j}}(\vec{r})|^4}$ ← interaction energy and $\hat{n}_{\vec{j}} = \hat{a}^{+}_{\vec{j}} \hat{a}_{\vec{j}}$

* The actual relevant energy is the grand-canonical energy, and hence we redefine:

$$\boxed{\hat{H}_{BH} = -t \sum_{\vec{j},\vec{\sigma}} \hat{a}^{+}_{\vec{j}}\, \hat{a}_{\vec{j}+\vec{\sigma}} + \frac{U}{2} \sum_{\vec{j}} \hat{n}_{\vec{j}} (\hat{n}_{\vec{j}} - 1) - \mu \sum_{\vec{j}} \hat{n}_{\vec{j}}}$$

↓ Bose-Hubbard Hamiltonian

where μ is the chemical potential

[* Note: If we evaluate the Heisenberg eqs. for $\hat{a}_j$, and take the mean-field: $\psi_j = \langle \hat{a}_j \rangle$, we recover the DNLSE of p. (18).]

* In the following we will be particularly interested in the ground-state properties of this Hamiltonian. We will see that depending on the physical parameters two ground-state phases may be attained: a superfluid phase and a gapped insulator phase known as Mott insulator.

* Let's first consider the case without tunneling.

$$\hat{H}_{BH} \simeq \sum_j \hat{H}_j^{(0)}$$

where $\hat{H}_j^{(0)} = \frac{U}{2} \hat{n}_j (\hat{n}_j - 1) - \mu \hat{n}_j$

Very clearly the eigenstates of $\hat{H}_j^{(0)}$ are Fock states $|n\rangle$ with a definite atom number per site. These states have then an energy $E_n^{(0)} = \frac{U}{2} n(n-1) - \mu n$

The ground state is given by the lowest energy:

$$\frac{dE_n^{(0)}}{dn} = \frac{U}{2}(2n-1) - \mu = 0 \longrightarrow n = \frac{\mu}{U} + 1/2$$

Since n must be an integer $\longrightarrow n = \left[\frac{\mu}{U} + 1/2\right]$ ← this means the closest integer.

It's easy to see that for $\mu/U < 0 \rightarrow n = 0$

and that for $\bar{n} - 1 < \mu/U < \bar{n} \longrightarrow n = \bar{n}$

· Hence in absence of tunneling the ground state is provided by a fixed number of atoms per site $\bar{n}$, where this number changes at $\mu/U = \bar{n}$ from $\bar{n}$ to $\bar{n}+1$ abruptly.

Note that within $\bar{n} - 1 < \mu/U < \bar{n}$ the number of atoms doesn't change $\longrightarrow \partial n/\partial\mu = 0 \longrightarrow$ This means that this phase is actually incompressible.

* Let's see now what happens at finite tunneling.
We shall employ a mean-field formalism (based on a decoupling approximation introduced below). This treatment is rather OK in 2D and 3D, although as we shall mention below it isn't so good in 1D lattices.

* Analogous to our discussion of the Bogoliubov approach (p. ④) we introduce the superfluid order parameter

$$\psi = \langle a_i^\dagger \rangle = \langle a_i \rangle \qquad [\hat{a}_i = \psi + \delta\hat{a}_i] \sim \text{fluctuations}$$

We will now find the conditions at which $\psi \neq 0$ in the ground state. When $\psi \neq 0$ the system will be in a superfluid phase.

* We now perform a decoupling approximation for the tunneling part of the Hamiltonian:

$$\hat{H}_{TUNNEL} = -t \sum_{\vec{j},\vec{\delta}} \hat{a}_{\vec{j}}^\dagger \hat{a}_{\vec{j}+\vec{\delta}}$$

here's the decoupling!

$$\hat{a}_j^\dagger \hat{a}_{\vec{j}+\vec{\delta}} = [\psi + \delta\hat{a}_{\vec{j}}^\dagger][\psi + \delta\hat{a}_{\vec{j}+\vec{\delta}}] \cong \psi^2 + \psi(\delta\hat{a}_{\vec{j}}^\dagger + \delta\hat{a}_{\vec{j}+\vec{\delta}})$$

$$= \psi^2 + \psi[\hat{a}_{\vec{j}}^\dagger - \psi + \hat{a}_{\vec{j}+\vec{\delta}} - \psi] = -\psi^2 + \psi(\hat{a}_{\vec{j}}^\dagger + \hat{a}_{\vec{j}+\vec{\delta}})$$

Then

$$\hat{H}_{TUNNEL} = -t \sum_{\vec{j}} \sum_{\vec{\delta}} (-\psi^2 + \psi(\hat{a}_{\vec{j}}^\dagger + \hat{a}_{\vec{j}+\vec{\delta}}))$$

$$= zt \sum_{\vec{j}} [\psi^2 - \psi(\hat{a}_{\vec{j}}^\dagger + \hat{a}_{\vec{j}})]$$

where z is the so-called coordination number, i.e. the number of nearest neighbors ($z=2$ in 1D, 4 in 2D, 6 in 3D for a cubic lattice).

* We may then write the decoupled Hamiltonian

$$\frac{\hat{H}_{BH}}{zt} \cong \sum_{\vec{j}} \hat{H}_{\vec{j}}$$

where $\hat{H}_j = \hat{H}_j^{(0)} + \hat{V}_j$

with $\hat{H}_j^{(0)} = \frac{1}{2}\tilde{U}\,\hat{n}_j(\hat{n}_j-1) - \tilde{\mu}\,\hat{n}_j + \psi^2$ with $\left\{\begin{array}{l}\tilde{U} = U/zt \\ \tilde{\mu} = \mu/zt\end{array}\right\}$

$\hat{V}_j = -\psi(\hat{a}_j^+ + \hat{a}_j)$

* As for the case with $t=0$ the eigenstates of $\hat{H}_j^{(0)}$ are Fock states. These Fock states have an energy

$$E_n^{(0)} = \frac{\tilde{U}}{2}\,n(n-1) - \tilde{\mu}\,n + \psi^2$$

* We will consider $\hat{V}$ as a perturbation of $\hat{H}_0$ (I forget from now on the subindex j)

Clearly $\hat{V}\,|n\rangle = -\psi\left[\sqrt{n+1}\,|n+1\rangle + \sqrt{n}\,|n-1\rangle\right]$

* We are interested in the correction of the energy of the ground state $|\bar{n}\rangle$, where $\bar{n}$ was introduced in p. 25. We clearly need to go to second-order perturbation theory:

$$E_{\bar{n}}^{(2)} = \sum_n \frac{\langle\bar{n}|V|n\rangle\langle n|V|\bar{n}\rangle}{E_{\bar{n}}^0 - E_n^0}$$

$$E_{\bar{n}+1}^{(0)} = \frac{\tilde{U}}{2}(\bar{n}+1)\bar{n} - \tilde{\mu}(\bar{n}+1) + \psi^2 = \tilde{U}\bar{n} - \mu + E_{\bar{n}}^0$$

$$E_{\bar{n}-1}^{(0)} = -\tilde{U}(\bar{n}-1) + \mu + E_{\bar{n}}^0$$

$$= \psi^2\left\{\frac{\bar{n}+1}{E_{\bar{n}}^0 - E_{\bar{n}+1}^0} + \frac{\bar{n}}{E_{\bar{n}}^0 - E_{\bar{n}-1}^0}\right\}$$

$$= \psi^2\left\{\frac{\bar{n}+1}{\tilde{\mu} - \tilde{U}\bar{n}} + \frac{\bar{n}}{-\tilde{\mu} + \tilde{U}(\bar{n}-1)}\right\}$$

Then, up to second order in ψ^2:

$$E_{\bar{n}} \simeq \frac{\tilde{U}}{2}\,\bar{n}(\bar{n}-1) - \tilde{\mu}\,\bar{n} + \psi^2\left\{1 + \frac{(\bar{n}+1)}{\tilde{\mu} - \tilde{U}\bar{n}} + \frac{\bar{n}}{\tilde{U}(\bar{n}-1) - \tilde{\mu}}\right\}$$

$$= E_{\bar{n}}(\psi=0) + r_{\bar{n}}\psi^2 + \mathcal{O}(\psi^4)$$

where $r_{\bar{n}} = 1 + \frac{\bar{n}+1}{\tilde{\mu} - \tilde{U}\bar{n}} + \frac{\bar{n}}{\tilde{U}(\bar{n}-1) - \tilde{\mu}}$

* Clearly $\psi \neq 0$ minimizes the energy only if $r_{\bar{n}} < 0$ whereas $\psi = 0$ would do the job for $r_{\bar{n}} > 0$

(Note: this is the usual Landau procedure for 2nd order phase transitions)

* Then for $r_{\bar{n}} < 0$ the system will be in a superfluid phase with $\psi \neq 0$. The separatrix between $\psi \neq 0$ and $\psi = 0$ is hence at

$$0 = r_{\bar{n}} = 1 + \frac{\bar{n}+1}{\tilde{\mu} - \tilde{U}\bar{n}} + \frac{\bar{n}}{\tilde{U}(\bar{n}-1) - \tilde{\mu}}$$

$$\Longrightarrow \mu^2 + \mu\left[\tilde{U}(1-2\bar{n}) + 1\right] + \tilde{U}^2\bar{n}(\bar{n}-1) + \tilde{U} = 0$$

$$\tilde{\mu}_\pm = \frac{1}{2}\left[\tilde{U}(2\bar{n}-1) - 1\right] \pm \frac{1}{2}\sqrt{\tilde{U}^2 - 2\tilde{U}(1+2\bar{n}) + 1}$$

Coming back to the original units

$$\mu_\pm = \frac{1}{2}\left[U(2\bar{n}-1) - zt\right] \pm \frac{1}{2}\sqrt{U^2 - 2Uzt(1+2\bar{n}) + (zt)^2}$$

To compare with the $t=0$ case it's perhaps better to make the discussion in units of U:

$$\boxed{\frac{\mu_\pm}{U} = \frac{1}{2}\left[(2\bar{n}-1) - \frac{zt}{U}\right] \pm \frac{1}{2}\sqrt{1 - 2\frac{zt}{U}(1+2\bar{n}) + \left(\frac{zt}{U}\right)^2}}$$

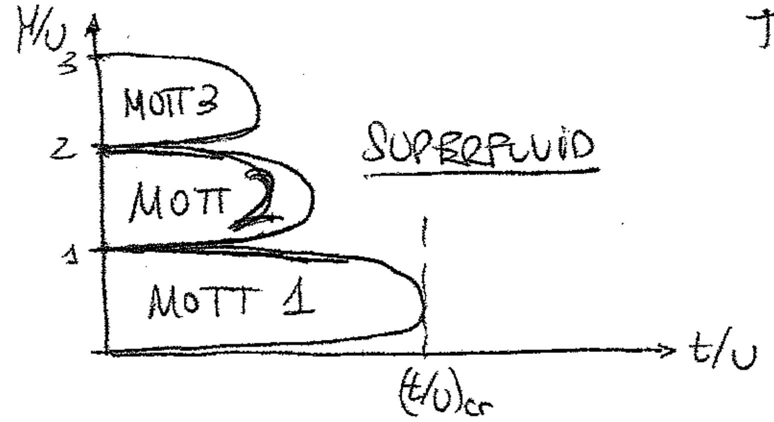
Note that for $t=0$

$$\frac{\mu_\pm}{U} = \bar{n} - 1/2 \pm 1/2 \begin{cases} \nearrow \bar{n} \\ \searrow \bar{n}-1 \end{cases} \longrightarrow \bar{n} - 1 \leq \frac{\mu_\pm}{U} \leq \bar{n}$$

Hence for $t=0$ we have no superfluid phase but just the incompressible phase with a fix $\bar{n}$ number we saw before

$\Longrightarrow$ <u>MOTT-INSULATOR PHASE</u>

* For growing t/U one obtains a phase diagram of the form:



The boundaries of the Mott-insulator phases (with fix $\bar{n}$) are given by the expressions of $\frac{\mu_\pm}{U}(t/U)$ calculated before.

* By imposing $\mu_+ = \mu_-$ we may calculate the tip of the lobes of the previous graph.

$$\mu_+ = \mu_- \quad \text{for} \quad \tilde{U}^2 - 2\tilde{U}(1+2\bar{n}) + 1 = 0$$

This gives
$$\frac{U}{zt} = (1+2\bar{n}) + \sqrt{(1+2\bar{n})^2 - 1}$$

For $\bar{n} = 1$ one gets $\left(\frac{U}{zt}\right)_{critic} \cong 5.83$

* This critical value for the Mott-insulator to superfluid transition is reasonably well described by this mean field approximation. In 1D there are strong deviations ($\left(\frac{U}{t}\right)_{cr} = 3.84$, hence much lower than the mean-field result).

* We have hence seen that the phase diagramm is characterized by a peculiar lobe structure. Let's try now to get a quick understanding of the physics behind this structure.

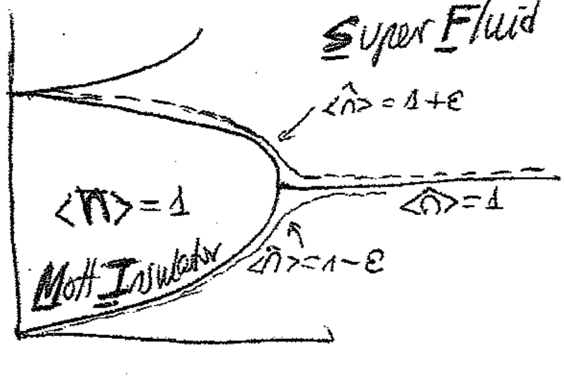
* let's consider the case of <u>unit filling</u>, i.e. the number of atoms (N) is precisely equal to the number of sites (M). In the limit of deep optical lattices ($V_0 \to \infty$) there isn't hopping ($t=0$) and the ground state is a <u>product state of Fock states</u> of $\bar{n}=1$ per site

$$|\psi\rangle = \prod_{\ell=1}^{M} |\bar{n}=1\rangle_\ell$$

When V_0 decreases the atoms start to hop around, which necessarily involves double occupancy, increasing the energy by U. Now as long as the gain t in kinetic energy due to the hopping is sufficiently smaller than U, the atoms <u>remain localized</u>, although the ground state of the system is <u>not any more the product state</u> above. Once t/U becomes large-enough, the gain in kinetic energy outweights the repulsion due to the double occupancies and the atom will delocalize over the whole lattice (superfluid phase). In the limit $t \gg U$ the ground state of the system becomes

$$|\psi\rangle = \Big(\underbrace{\frac{1}{\sqrt{M}} \sum_{\ell=1}^{M} \hat{a}_\ell^{\dagger}}_{\hat{a}^{\dagger}_{\vec{k}=0}}\Big)^{\otimes N} |VACUUM\rangle$$

So when $U \to 0$ we recover a BEC with all atoms in the zero-momentum state (as we showed on p. (14)), i.e. we recover the GPE formalism.



* Up to now we have considered a filling one, and hence always $\langle\hat{n}\rangle = 1$ for both MI and SF regimes.
* let's consider now what happens for a filling $\langle\hat{n}\rangle = 1+\varepsilon$ slightly larger than 1.

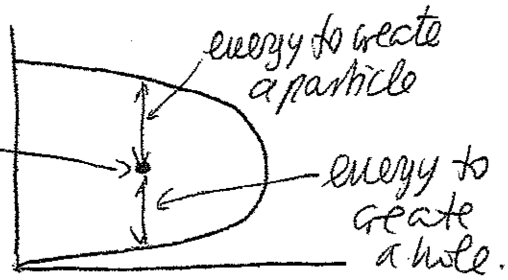
• For large t/U the ground state has all atoms delocalized over all the lattice and the situation is indistinguishable from that of $\langle \hat{n} \rangle = 1$. However when t/U lowers, the line of constant density $\langle \hat{n} \rangle = 1+\varepsilon$ cannot enter the Mott phase. For any non-integer filling, <u>the ground state remains superfluid</u> as long as the atoms can hop at all, i.e. all the way till $t=0$.
In other words, even for $t \ll U$ there's a small fraction ε of atoms (on top of a "frozen" Mott-insulator with $\bar{n}=1$) that remain superfluid. Indeed this fraction can still gain kinetic energy by delocalizing over the whole lattice without being blocked by U because 2 extra particles are never at the same site.

• You can easily see that the same is true for $\langle \hat{n} \rangle = 1-\varepsilon$ but now with holes instead than particles.

• From the previous discussion you can understand two crucial (and related) features of the Mott-insulator phase

• As mentioned above, inside of the Mott-lobe $\langle n \rangle$ is constant. In particular $\frac{\partial \langle n \rangle}{\partial \mu} = 0$ inside the lobe. This is a quite remarkable property → <u>incompressibility</u>.

• The lowest-lying excitations on top of the Mott-insulator that conserve particle number must be particle-hole like. But from the previous discussion, you see that if the system is inside the MI lobe



* Then, inside the Mott-insulator phase, there's a gap (given by the width of the lobe) to the lowest-lying excitations. Hence the Mott-insulator is a gapped phase.

Note: in our previous mean-field calculation

$$E_{GAP}(\bar{n}) = U\sqrt{1-2\frac{2t}{U}(1+2\bar{n})+\left(\frac{2t}{U}\right)^2}$$

For $t/U \to 0$, $E_{gap} \to U$

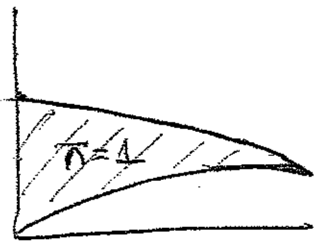
$(t/U) \to (t/U)_{cr}$, $E_{gap} \to 0$

Note that close to $\left(\frac{2t}{U}\right)_{cr} \longrightarrow \left(\frac{2t}{U}\right) = \left(\frac{2t}{U}\right)_{cr}(1-\epsilon)$

$$E_{GAP}(\epsilon) = \left[2\left(\frac{2t}{U}\right)_{cr}(1+2\bar{n}) - 2\left(\frac{2t}{U}\right)_{cr}^2\right]^{1/2}\sqrt{\epsilon} \sim \epsilon^{1/2}$$

i.e. the gap opens with a critical exponent 1/2. This is typical of mean field theories and gives the rounded form of the lobe tips.

For 1D systems the "lobes" are actually "spicky", more like this



* Up to now in our discussions we have not taken into account an overall harmonic confinement on top of the lattice, as it is actually the case experimentally. This extra potential is actually very important. Probably you have already noticed that the Mott-insulator demands an exact filling factor 1, i.e. as many atoms as sites. You have probably thought that this must be quite hard in practice, and (in absence of an overall harmonic confinement) you would be certainly right! Overall potential helps us in this sense.

* let's see why an overall potential helps us in this sense. An harmonic confinement leads to an extra term

$$\sum_{\vec{j}} \epsilon_{\vec{j}} \hat{a}^{+}_{\vec{j}} \hat{a}_{\vec{j}}$$

in the Bose-Hubbard Hamiltonian of p. (24), where $\epsilon_{\vec{j}} = \frac{1}{2} m \omega^2 d^2 |\vec{j}|^2$ (we consider an isotropic oscillator)

(Note: we employed a similar term in our DNLSE discussion of Florence experiments at p. (20)).

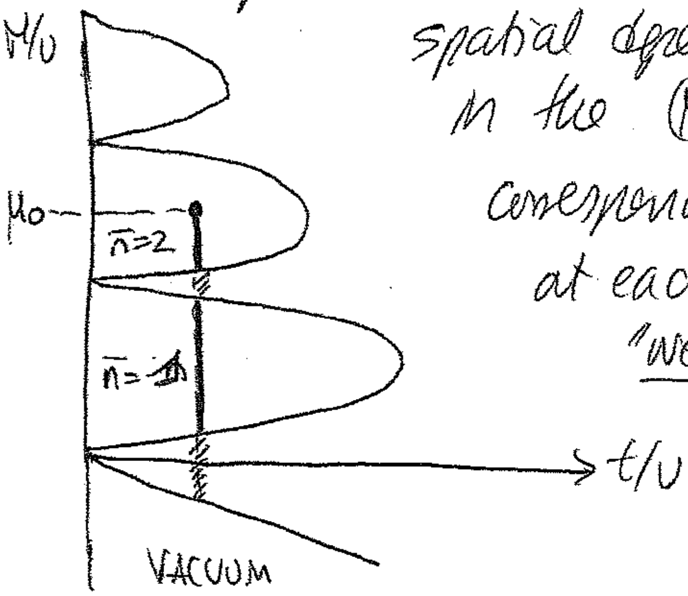
* Then, whereas in p. (24) we had the same chemical potential μ at every site, now we have a local chemical potential

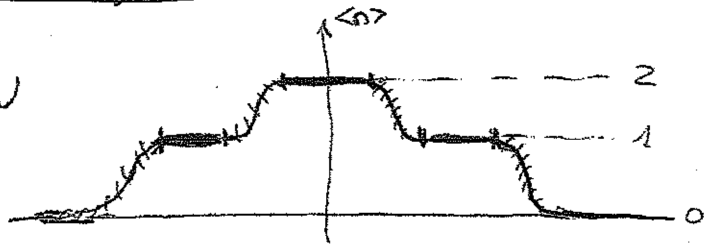
$$\mu \longrightarrow \mu_{\vec{j}} = \mu_0 - \frac{m\omega^2 d^2}{2} |\vec{j}|^2$$

where $\mu_0 \equiv$ chemical potential at the center.

* It's very easy to see what happens if we employ the so-called local density approximation, i.e. we assume that locally we can assume an homogeneous system with the local

chemical potential. We can then simply read out the spatial dependence of the forces by cutting in the (μ/U)-(t/U) diagram which phase corresponds to the local chemical potential at each point. This gives a typical "wedding cake" structure





* Note that the local chemical potential allows now for regions with an exact $\langle n \rangle = 1$, circumventing the problem we spotted before.

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* The Mott-insulator to superfluid transition was experimentally observed in cold atoms in optical lattices by Greiner et al. in 2002. [M. Greiner et al. Nature 415, 39 (2002)]
In that experiment, they probe the Mott-insulator - Superfluid transition in two ways:

1) The trapping potential was suddenly switched-off. As mentioned in p. 15 in the superfluid phase (where coherence is large) nice interference fringes were observed. However when V_0 surpassed a given value, the interference fringes are washed out and one recovers an incoherent gaussian-like background (indicating the onset of the insulating regime).

2) In that experiment they measured as well the excitation gap. They did it in a very clever way. In the MI regime they tilted the lattice, then went back quickly to the SF regime, and then expand. If the tilting was large enough, excitations are produced in the MI, that are translated after the quench into the SF regime, and result in a peak broadening in the interference pattern. Hence by measurement the peak broadening as a function of the tilting they were able to probe the gap.

• More recent experiments have allowed for a direct probing of the wedding-cake structure (Bloch's group and Ketterle's group, 2006)

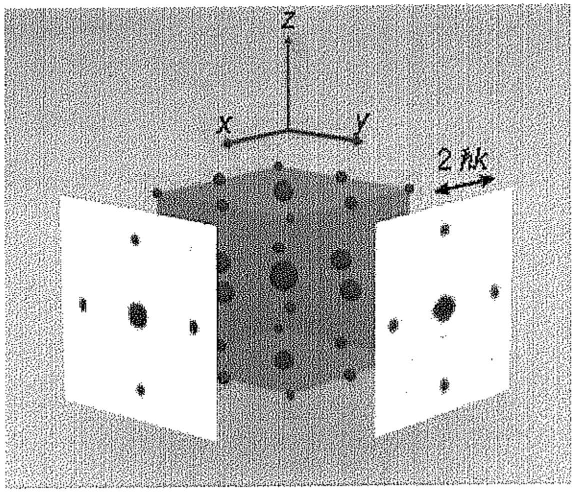
Bloch's group: using spatially-selective microwave transitions and spin-changing collisions [Fölling et al., PRL 97, 060403 (2006)]

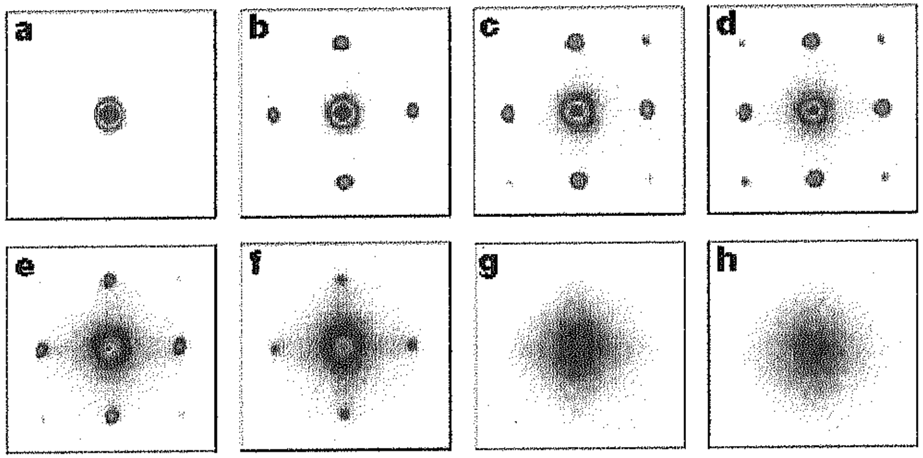
Ketterle's group: using microwave spectroscopy [Campbell et al., Science 313, 649 (2006)]

• Even more recently, the Mott shells have been observed by M. Greiner's group [Bakr et al., Science 329, 547 (2010)] and I. Bloch's group [Sherson et al., Nature 467, 68 (2010)] by means of single-atom-resolved fluorescence imaging.

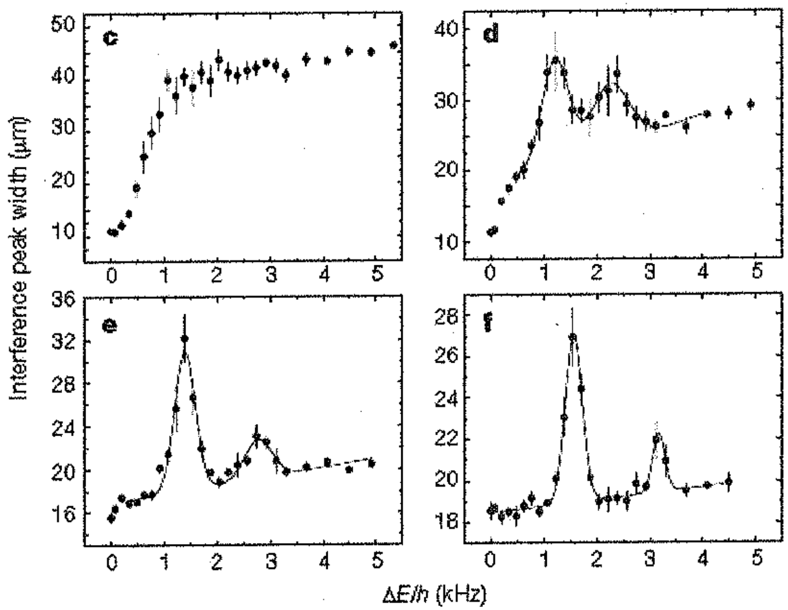
(Note: What these experiments actually do is a parity measurement. This is because the fluorescence technique leads to photoassociation, which blows particles in pairs. Hence 1, 3, 5, ... particles will be detected as 1 particle per site, whereas 0, 2, 4, ... will be detected as zero.

Superfluid-to-Mott transition [Greiner et al., Nature 415, 39 (2002)]



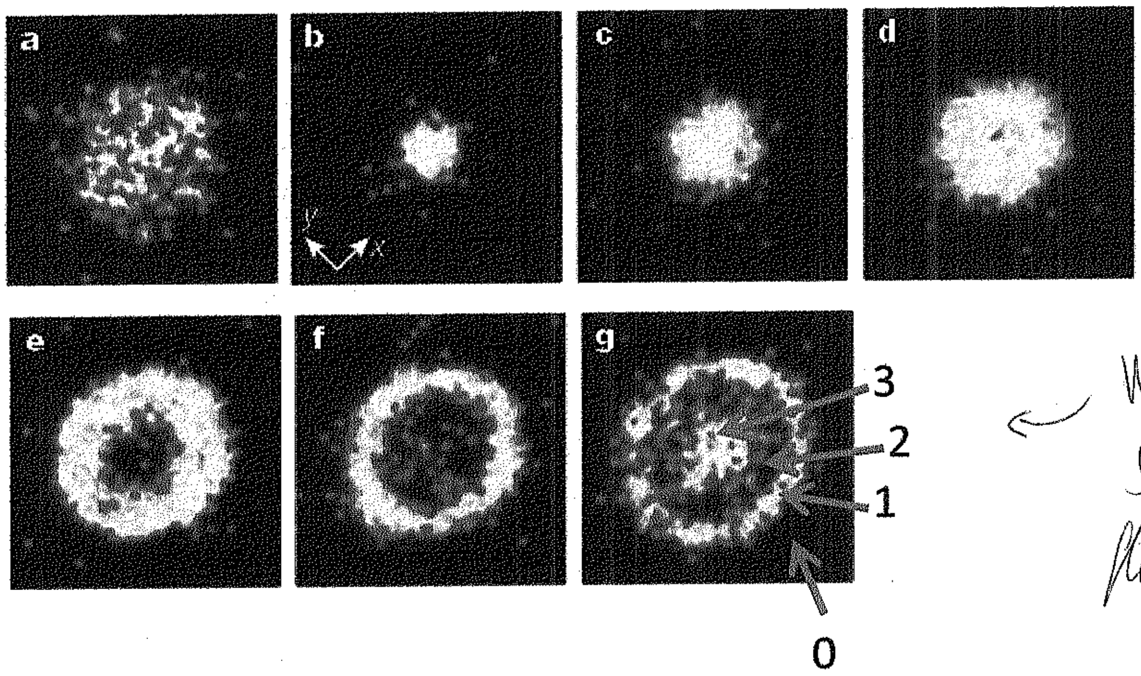


Interference fringes



gapped excitations

Mott shells [Sherson et al., Nature 467, 68 (2010)]



← Wedding cake structure in fluorescence images