• BOSE GASES IN OPTICAL LATTICES

In the previous lecture we have analyzed the rich physics of a two-well system. We have seen that the GP-formalism is for many situations not applicable. In this lecture we will consider the case of a Bose gas in a multi-well system, i.e. a periodic sinusoidal potential, a so-called optical lattice.

Let's recall that for a sufficiently large detuning (δ) we may write the dipole potential exerted by a laser on an atom in the form (p. 11)

$$V_D(x) = \frac{\hbar}{4\delta}\Omega_1^2(x)$$

where $\Omega_1^2(x)$ is related to the laser intensity. Already in p. 13 we mentioned that by employing two counterpropagating lasers, we can build an standing wave, and hence $\Omega_1^2(x) = \Omega_0^2 \sin^2 qx$

Then the atom experiences an external potential

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

with periodicity $d = \pi/q$

(Note: q is the wavenumber of the lasers ($e^{\pm iqx}$) but note that the potential doubles the periodicity. Hence, if the laser have wavelength λ, the potential shows an inter-well spacing $\lambda/2$.)

Let's consider first the non-interacting case. This will allow us to re-call some ideas of solid-state physics, because as you have probably noticed, the cold atoms loaded in such a periodic potential behave in a <u>similar fashion as electrons in a crystal</u>

(Note: an important difference, however, is that the optical crystal is not formed by ions, and hence the crystal shows no phonons. The crystal is also, in principle, perfect, showing no defects.)

The atoms in the optical lattice obey in absence of interactions the Schrödinger equation (we keep the discussion 1D for simplicity)

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

* From the Bloch theorem we know that the stationary solutions of this Schrödinger equation are of the form

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

where p is the so-called quasimomentum and $u_p(x)$ is a periodic function of period a [$u_p(x) = u_p(x+a)$]. Note that values of p differing by $2\pi n\hbar/a$ (with n integer) are physically equivalent. This means that we can restrict the value of p to the First Brillouin zone: $-\pi\hbar/a \le p \le \pi\hbar/a$ (i.e. $-\hbar q \le p \le \hbar q$)

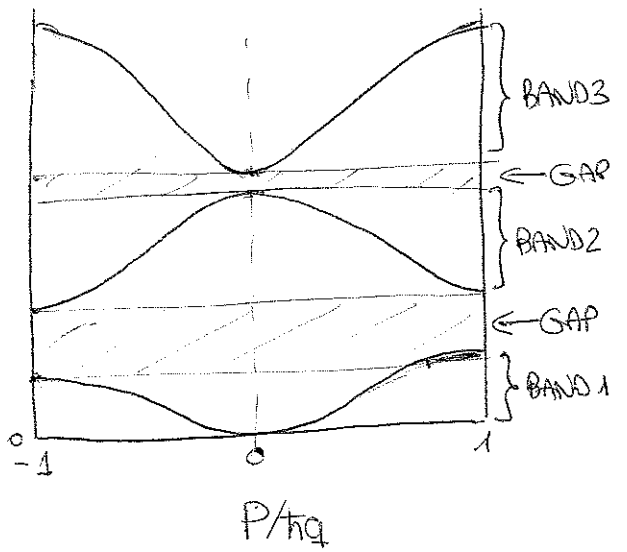
* We obtain then the equation for the functions $u_{pn}(x)$:

$$E_{pn}\, u_{pn}(x) = \frac{-\hbar^2}{2m}\left(\frac{d}{dx} - i\,p/\hbar\right)^2 u_{pn}(x) + V_0 \sin^2 qx\; u_{pn}(x)$$

This equation can be easily solved numerically.

Note: Actually the Schrödinger equation at the bottom of page (179) is a Mathieu equation, and hence the Bloch functions may be expressed as a function of Mathieu functions. More about Mathieu functions can be found in Abramowicz - Stegun, "Handbook of mathematical functions".)

* For a given value of the quasimomentum p we have different eigenenergies E_{pn}. These solutions give rise to the typical band structure for the energies of particles in periodic potentials.



- As expected the spectrum presents allowed bands, and forbidden gaps.
- In the figure we have set the bottom of the lowest band to zero energy.

* Note that each band is characterized by a dispersion law

$$\epsilon_n(p) \equiv E_{np}$$

* The dispersion law can be calculated analytically in the so-called tight-binding approximation (very deep lattices).
We can introduce at this point the Wannier functions, which we can form for each band n from the corresponding Bloch functions

$$\psi_{np}(x) = e^{ipx/\hbar} u_{np}(x)$$

The Wannier function at the site j is of the form:

$$W_j^{(n)}(x) \equiv w^{(n)}(x - jd) = \frac{1}{\sqrt{N}} \sum_p e^{-ipjd/\hbar} \psi_n(x)$$ where N = number of sites

These functions form a complete set of orthogonal functions. They are particularly suited for the description of the tight-binding regime, because the $W_j^{(n)}(x)$ function is localized at site j.

* We concentrate in the following on the lowest band (n = 0) and hence we remove for simplicity the band index.

We may express the Bloch functions as a function of the Wannier functions: $$\psi_p(x) = \frac{1}{\sqrt{N}} \sum_j e^{ipjd/\hbar} w(x - jd)$$

* From the Schrödinger equation

$$\psi_0^*(x) \left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2}\right] \psi_p(x) + V_{ext}(x) \psi_0^* \psi_p = E_p \psi_0^* \psi_p$$

$$\psi_p(x) \left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2}\right] \psi_0^*(x) + V_{ext}(x) \psi_0^* \psi_p = E_0 \psi_0^* \psi_p$$

Then: $$+\frac{\hbar^2}{2m} \left\{ \psi_0^* \left(-\frac{d^2}{dx^2} \psi_p\right) - \psi_p \left(\frac{-d^2}{dx^2} \psi_0^*\right) \right\} = (E_p - E_0) \psi_0^* \psi_p$$

We integrate now in the interval $z \in (-d/2, d/2)$

Note that $\int_{-d/2}^{d/2} dx\, \psi_0^*(x)\psi_p(x) = \frac{1}{N}\sum_{j,j'} e^{ipjd/\hbar} \underbrace{\int_{-d/2}^{d/2} w(x-jd)\, w(x-j'd)\, dx}_{\delta_{j,0}\,\delta_{j',0}}$

$\cong 1$

(the Wannier wavefunctions are very localized)

Integrating by parts we obtain

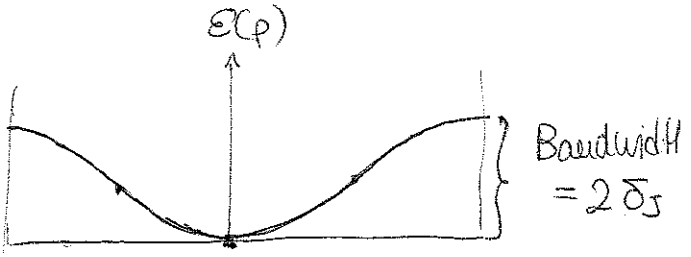
$$\epsilon(p) = E_p - E_0 = \frac{\hbar^2}{2m}\frac{d}{dx}\left[\psi_p \frac{d}{dz}\psi_0^* - \psi_0^* \frac{d}{dz}\psi_p\right]_{-d/2}^{d/2}$$

* Note that at $d/2$ only $w_0(x)$ and $w_1(x)$ contribute, and at $-d/2$ only $w_0(x)$ and $w_1(x)$ contribute. Then for the purpose of the previous sum we may use

$$\psi_p(x) \simeq w(z) + e^{ipd/\hbar} w(z-d) + e^{-ipd/\hbar} w(z+d) + \dots$$

* We get the final expression:

$$\epsilon(p) = \delta_J\left(1 - \cos\frac{pd}{\hbar}\right)$$



with $\delta_J = -2\frac{\hbar^2}{m}\left[w(z)\frac{d}{dz}w(z)\right]_{z=d/2}$

which coincides with the tunneling energy introduced in p. 179.

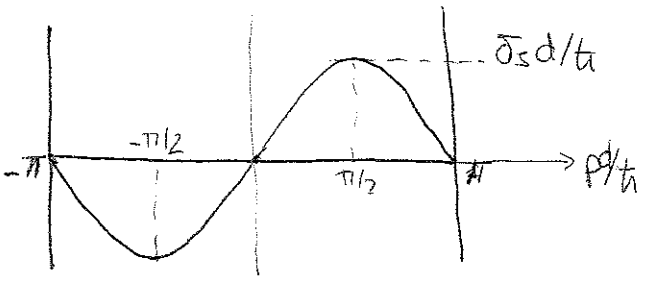
* Note that the bandwidth of the first band corresponds to twice δ_J. Hence the deeper is the lattice the flatter is the band. This has of course important consequences for the mobility of the particles. This is easier to see from the idea of effective mass and group velocity.

* Remember from quantum mechanics that the group velocity is defined from the dispersion law as

$$v_g = \frac{\partial}{\partial p}\epsilon(p)$$

In the tight binding regime

$$v_g(p) = \left[\frac{\delta_J}{\hbar} d\right] \sin pd/\hbar$$



The group velocity has hence a non-trivial dependence with p.

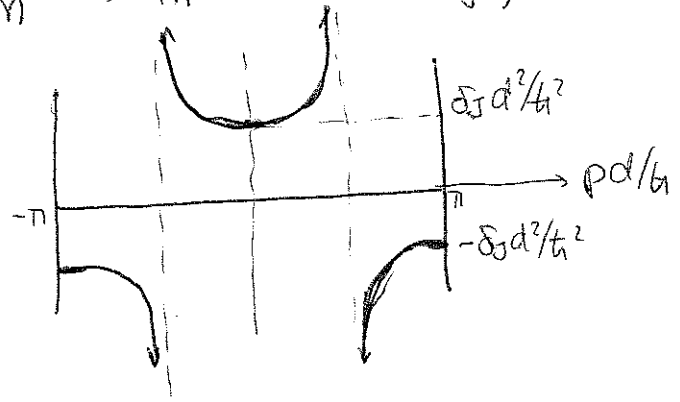
* The effective mass m^* is defined as

$$m^* = \left[\frac{d^2}{dp^2}\epsilon(p)\right]^{-1}$$ → hence $m^*(p)$ is given by the inverse of the curvature of the dispersion law.

(Note: for usual dispersion $\epsilon(p) = p^2/2m \longrightarrow m^* = m$ clearly)

In the tight-binding regime

$$\frac{1}{m^*} = \left[\delta_J \frac{d^2}{\hbar^2}\right] \cos pd/\hbar$$



Note that for $pd/\hbar \in (-\pi, -\pi/2)$ and $pd/\hbar \in (\pi/2, \pi)$ the effective mass m^* is negative!

This has of course very remarkable consequences.

* For small p, $m^* \simeq \frac{\hbar^2}{\delta_J d^2}$, and hence m^* is directly related to the tunneling energy. When the lattice gets very deep, δ_J gets very small, and hence $m^* \gg m$. The inertia is hence large, i.e. the mobility is largely handicapped.

* As mentioned above, the special dispersion law of the atoms loaded in the optical lattice may have quite remarkable consequences. One of them is the so-called Bloch osaillations.

The idea is rather simple, and it is perhaps best understood in the semiclassical picture. We assume the quasi-momentum spreading (of the corresponding atomic wavepackets) as much smaller than the width of the 1st Brillouin zone (i.e. $\Delta K \ll q$), which in turn means that the wavepacket is delocalized over many lattice sites. Let $X \equiv$ position of the wavepacket center.

Then $\frac{dX}{dt} = v_g = \frac{\delta_J d}{\hbar} \sin(pd/\hbar)$

Let's assume that the system is under the influence of a constant force [it may be gravity for atoms (or alternatively it may be induced by a slight detuning between the lasers forming the lattice) or it may be a constant electric field for electrons].

Then $\frac{dp}{dt} = F \longrightarrow p = Ft$ (let $p(t=0)=0$)

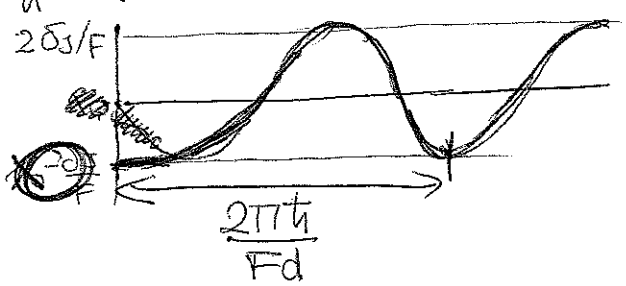
($p \equiv$ central quasimomentum of the wavepacket).

Naively you would expect that the wavepacket accelerates, beyond the Brillouin limits, but this is NOT what happens, and the reason is the dispersion law.

Since $p = Ft \longrightarrow \frac{dx}{dt} = \frac{\delta_J d}{\hbar} \sin\left[\frac{Fd}{\hbar} t\right]$

Then $X(t) = \text{const} - \frac{\delta_J}{F} \cos\left[\frac{Fd}{\hbar} t\right]$

For $X(0)=0 \longrightarrow X(t) = \frac{\delta_J}{F}\left[1 - \cos\left(\frac{Fd}{\hbar} t\right)\right]$



* This oscillatory motion is the so-called Bloch-oscillations. As you see the oscillations have

  - Amplitude → $2\delta_J/F$
  - Period: $\frac{2\pi\hbar}{Fd}$

* Note that the period just depends on the applied force (and d), but not on the tunneling. The amplitude on the contrary depends on δ_J/F.

* Bloch oscillations were observed in cold gases already many years ago (1996), at that time in non-condensed gases. Actually the phenomenon of Bloch oscillations doesn't demand condensation, but merely that the momentum width $< \hbar q$.

* Bloch oscillations have been also observed in condensates more recently (Armando, 2001). Interactions do play an important role in the Bloch oscillations (especially in the damping of the oscillations) but we won't describe it here.

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* Before leaving the discussion on the band dispersion law let me point that there are other important consequences, in particular of the fact that the effective mass m^* may be negative. More remarkably one may have BEC (bright) solitons with $a > 0$. These are the so-called gap solitons. The idea is simple. If the typical length of variation of the wavefunction is much larger than the inter-site spacing d, we may substitute

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{lattice}(x) \simeq -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}$$

* The corresponding 1D GPE will be

$$\frac{-\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}\psi(x,t) + g|\psi(x,t)|^2\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

(Note: actually g must be also regularized due to the presence of the lattice but I won't enter in these details here.)

* If $m^*<0$, then contrary to the usual wavepacket dispersion, now the kinetic energy tends to compress the wavepacket. If $g>0$ the interactions tend to expand the wavepacket. The gap soliton results from the balance between these two tendencies.

* Gap solitons were observed recently in BECs (Oberthaler, 2005).

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* More information about gap solitons may be found in the book of P. Meystre, "Atom optics".

More details about the role of m^*, the regularization of g, and more, may be found in the Stringari-Pitaevskii book.

* BEC IN AN OPTICAL LATTICE

* After discussing some general ideas related to optical lattices, let's analyze now the particular case of a BEC in an optical lattice. We shall first consider the case in which actually there's condensation, and we may employ a GPE formalism.

* We hence consider the GPE (time independent) (we reduce the discussion to 1D in order to keep as simple as possible)

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

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

* The ground state solution of the GPE is the Bloch function with $p=0$ (this is true obviously without interactions, but the interactions don't change this fact).

We may hence express the ground-state wavefunction as

* Linear combination of Wannier functions (p. 81)

$$\psi_0(x) = \frac{1}{\sqrt{N}}\sum_j w(x-jd)$$

Let's calculate the Fourier-transform:

$$\tilde{\psi}_0(p) = \int dx\, \psi_0(x) e^{-ipx/\hbar} = \frac{1}{\sqrt{N}}\sum_j \int dx\, w(x-jd) e^{-ipx/\hbar}$$

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

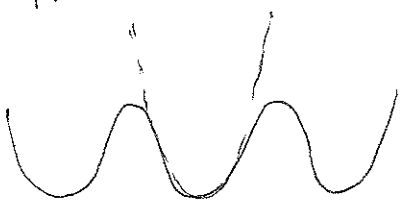
Hence $$\tilde{\psi}_0(p) = \tilde{w}(p)\underbrace{\sum_n \delta\left[p - 2\pi\frac{\hbar}{d}n\right]}$$

$\tilde{w}(p)$: Fourier transform of the on-site (Wannier) function

delta comb with peaks at $0, \pm 2\hbar q, \pm 4\hbar q, \dots$

* Although we may calculate exactly the Wannier function from the Bloch functions (p. 187) we may obtain a good approximation for the Wannier function associated to the lowest band, for the case in which the lattice is very deep.

In that case, close to a lattice minimum we may approximate $V_0 \sin^2 qx \simeq V_0 q^2 x^2 = \frac{1}{2} m \omega_{eff}^2 x^2$



Hence at the minima we have like an on-site harmonic oscillator of frequency

$$\omega_{eff} = \sqrt{\frac{2V_0 q^2}{m}}$$

Let $\ell_{HO} = \sqrt{\frac{\hbar}{m\omega_{eff}}}$.

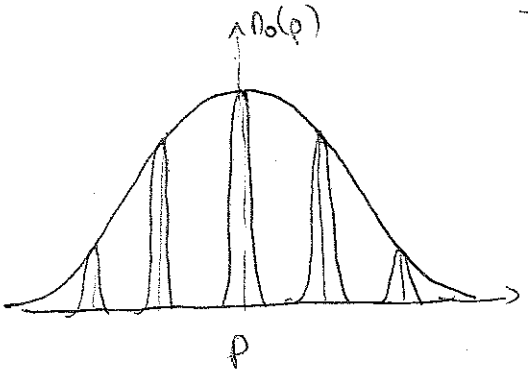
We may then approximate the Wannier function as the ground-state of the harmonic oscillator:

$$w(x) \simeq \frac{1}{\sqrt{\pi}\,\ell_{HO}} e^{-x^2/2\ell_{HO}^2}$$

Hence $\tilde{w}(p) = e^{-p^2 \ell_{HO}^2/2}$

* The momentum distribution is hence

$$n_0(p) = |\psi_0(p)|^2 \propto \sum_n e^{-4\pi^2 n^2 \ell_{HO}^2/d^2}\, \delta\left[p_z - \frac{2\pi\hbar n}{d}\right]$$



The momentum distribution is hence given by a series of peaks with a gaussian envelope. In reality the condensate has a finite size L, and hence the δ-peaks aren't infinitely narrow, but with a finite width $\sim 1/L$

* 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 real density distribution (remember our discussion on expansion in p. 150)

(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. As mentioned in p. 105 for a pure BEC the coherence length ($l_{coherence}$) is 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 $l_{coherence} \leq d$, then $\Delta K \sim q$, and the peaks merge.

(Note: in other words when the quasimomentum distribution $\Delta K \approx q$, 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 BECs.

* 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:

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

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

Hence:

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

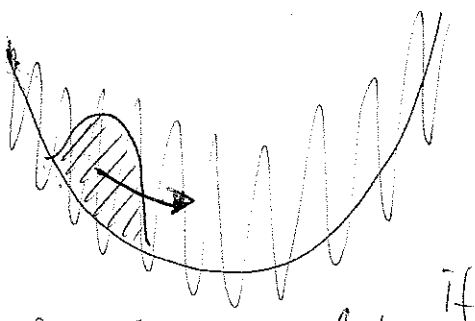
This is the discrete NLSE

* This equation is very helpful to describe the physics of BEC in optical lattices

(Note: This type of discrete nonlinear equation is also well-known in nonlinear optics, in particular in the context of the so-called discrete solitons.)

. Although we can approximate the condensates in each lattice site as having their own wave functions, tunneling between adjacent wells locks all the different condensates in phase (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 (remember our discussion on the dipole mode (p. 151)).
In the presence of the lattice they observed a substantially lower oscillation frequency.

The reason for this is because, as we already know (p. 171), 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. (191) in the form:

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

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

(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 derivation of the Thomas-Fermi regime in p. (115)).

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

pendular 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. (172) 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 (p. (173)) 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 <u>classical insulator regime</u> (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. Smirnov-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. 174) 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 p (189) concerning the interference fringes after switching-off the lattice. There we already mentioned that the recoil 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

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

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

Then the momentum distribution is

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

(we have employed translational invariance)

where $n_0(p) = |\tilde{w}(p)|^2 \simeq e^{-p^2 \ell_{ho}^2/2}$ (see p. (188)) and $\langle \ldots \rangle$ means the average over the phase fluctuations.

Note: 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. (175).

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. (188). 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 $\sum_j e^{-ipjd/\hbar} e^{-|j|/\Delta_j} \propto \frac{\Delta_j}{1+\left(\frac{pd}{\hbar}\Delta_j\right)^2}$, i.e. every

δ-peak is substituted by a Gaussian of width $\frac{t_c}{\Delta_j}$. Here we reason on discussion of p. 189. It's clear that if coherence $\equiv \Delta_j$ is $\ll d$, then $\Delta p \sim t_c q$, and as discussed in p. 189 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 assuming individual BECs at each lattice sites.

* We shall rather employ the Bose-Hubbard Hamiltonian which we already introduced in p. 177 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 $V_{ext}(\vec{r}) = V_0 \left(\sin^2 q_x + \sin^2 q_y + \sin^2 q_z \right)$

is a cubic optical lattice.

* 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

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

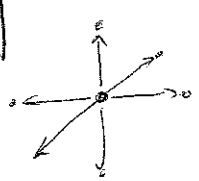
(Note: This is similar as what we did in the derivation of the DNLSE in p. 150)

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

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

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

where $\vec{j}+\vec{\delta}$ 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:

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

where μ is the chemical potential

Bose-Hubbard Hamiltonian

* 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 fix 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 we shall mention below it isn't so good in 1D lattices.

* Analogous to our discussion of the Bogoliubov approach (p. 108) we introduce the superfluid order parameter

$$\psi = \langle a_i^\dagger \rangle = \langle a_i \rangle$$

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!

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

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

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

$$= \frac{z}{2} t \sum_{\vec{j}} \left[\psi^2 - \psi\left(\hat{a}_{\vec{j}}^\dagger + \hat{a}_{\vec{j}}\right)\right]$$

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 $\hat{H}_j^{(0)} = \frac{1}{2}\tilde{U}\hat{n}_j(\hat{n}_j - 1) - \tilde{\mu}\hat{n}_j + \psi^2$ $\quad \tilde{U} = U/2t$, $\tilde{\mu} = \mu/2t$

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

As for the case with $t=0$ the eigenstates of $\hat{H}_j^{(0)}$ are Fock states $|n\rangle$. 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 interest in the correction of the energy of the ground state $|\bar{n}\rangle$, where $\bar{n}$ was introduced in p. (198). We clearly need to go to second-order perturbation theory:

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

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

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

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

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

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

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

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

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

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:

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

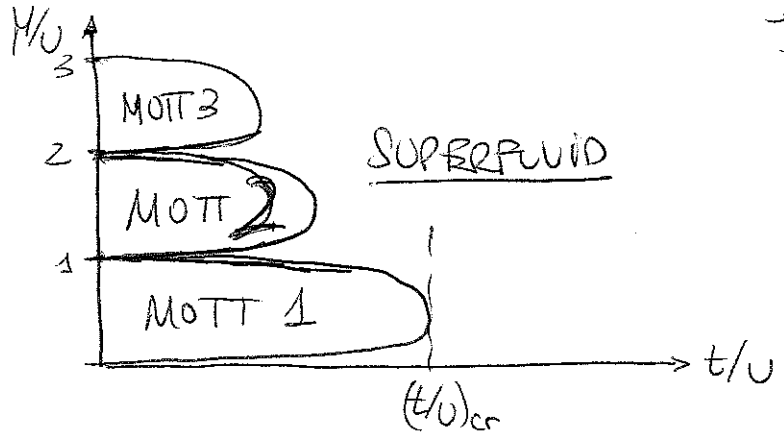
Note that for $t = 0$

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

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

$\Rightarrow$ <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 $\bar{n}$) 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 $$\frac{U}{2t} = (1+2\bar{n}) + \sqrt{(1+2\bar{n})^2 - 1}$$

For $\bar{n} = 1$ one gets $\left(\frac{U}{2t}\right)_{\text{critic}} \simeq 5.83$

* 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 here 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.

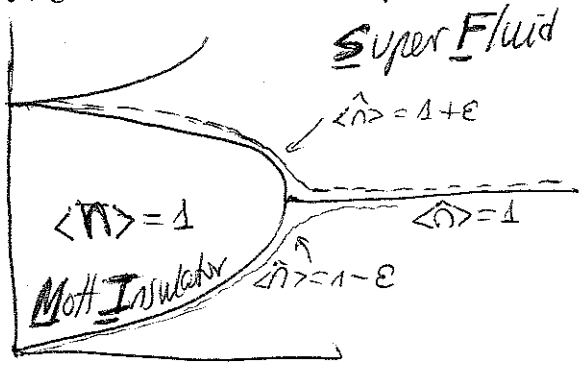
* let's consider the case of unit filling, i.e. the number of atoms (N) is precisely equal to the number of sites (M). In the limit of deep optical lattices ($V_0 \to \infty$) there isn't hopping ($J = 0$) and the ground state is a product state of Fock states of $\bar{n} = 1$ per site

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

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 J in kinetic energy due to the hopping is sufficiently smaller than U, the atoms remain localized, although the ground state of the system is not any more the product state above. Once J/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 $J \gg U$ the ground state of the system becomes

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

So when $U \to 0$ we recover a BEC with all atoms in the zero-momentum state (as we showed in p. (187)), 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 $\langle \hat{n} \rangle = 1 + \epsilon$ slightly larger than 1.

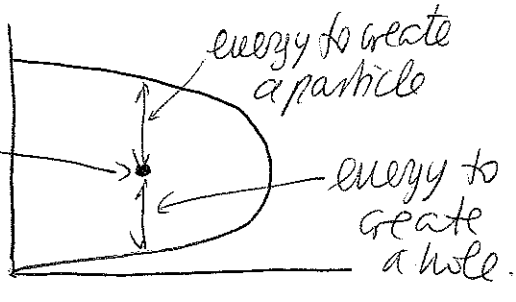
* For large J/U the ground state has all atoms delocalized over all the lattice and the structure is indistinguishable from that of $\langle \hat{n} \rangle = 1$. However when J/U lowers, the line of constant density $\langle \hat{n} \rangle = 1+\epsilon$ cannot enter the Mott phase. For any non-integer filling, the ground state remains superfluid as long as the atoms can hop at all, i.e. all the way till $J=0$. In other words, even for $J \ll U$ 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 $\langle \hat{n} \rangle = 1-\epsilon$ 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 $\rightarrow$ incompressibility.

- 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

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

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

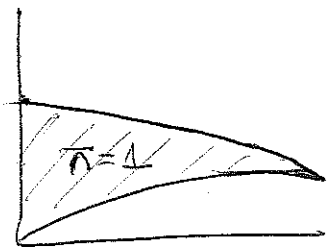
$(t/U) \to (t/U)_{cr}$, $E_{gap} \to 0$

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

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

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 "spiky", 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! Let's see why an overall potential helps us in this sense.

An harmonic confinement leads to an extra term

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

in the Bose-Hubbard Hamiltonian of p. (197), 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 Floquet experiments at p. (193)).

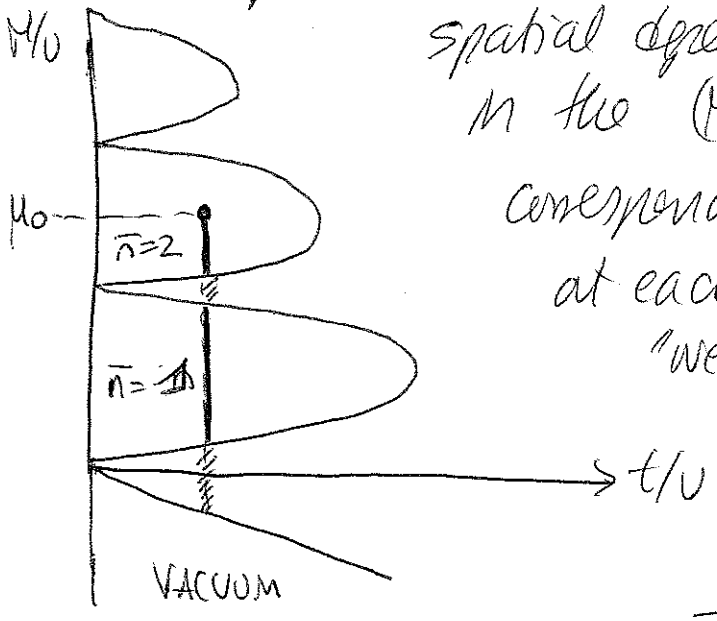
Then, whereas in p. (19) we had the same chemical potential μ at every site, now we have a local chemical potential

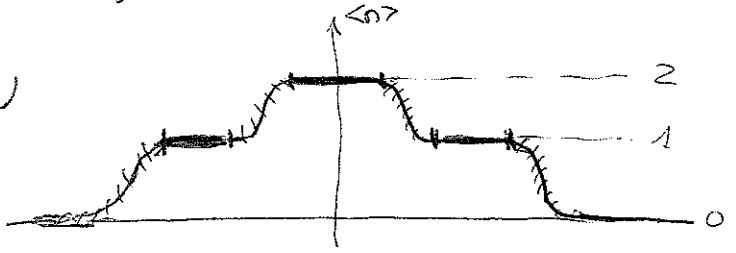
$$\mu \longrightarrow \mu_{\vec{j}} = \mu_0 - \frac{m\omega^2 d^2}{2} |\vec{j}|^2$$

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 looking in the $(\mu/U)-(t/U)$ 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. 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. 208 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 observes 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, ~~and~~ 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 thermalized 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. Simply beautiful!

- The above mentioned experiment led to an incredible amount of experimental and theoretical activities in strongly correlated systems in optical lattices, which I unfortunately cannot review in detail here.
- For reviews on this topic (and also other strongly correlated atomic systems) see e.g.
  - I. Bloch, J. Dalibard and W. Zwerger, Reviews of modern Physics 80, 885 (2008)
  - M. Lewenstein et al., cond-mat/0606771