

Chaire de Physique de la Matière Condensée

Des oxydes supraconducteurs aux atomes froids - la matière à fortes corrélations quantiques -

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Cours 3: Transition de Mott et modèle de Hubbard bosonique, atomes froids

<u>Séminaire :</u>



Matthias TROYER ETH-Zurich

Superfluidity near the Mott transition of cold bosonic atoms:

validating a quantum simulator.

OUTLINE OF LECTURE 3:

- 1- The bosonic Hubbard model: meanfield theory
- 2- Relevance to cold atoms in optical lattices
- 3- Experimental observation of the superfluid to Mott insulator transition
- 4- Beyond mean-field: critical behavior, universality class, field theory

1- The bosonic Hubbard model

$$H = -\sum_{ij} t_{ij} b_i^{\dagger} b_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$

- Bosons on a lattice
- Hopping amplitude t_{ii} between sites i,j
- e.g. t_{ii} = t for nearest-neighbor sites
- (w/ apology to the cold atom community where t \rightarrow J !)
- U on-site interaction (repulsive U>0 otherwise unstable)
- µ chemical potential controls average number of bosons per site n= <n_i>

Why study this model in lecture 3?

We have seen in lectures 1-2 the effect of `Coulomb blockade' in the context of one site coupled to a bath (Kondo impurity models)

The bosonic Hubbard model is the simplest model in which we can study the effect of on-site repulsion in an extended lattice model and explore the Mott phenomenon (free of the `complications' of fermionic statistics and spin degrees of freedom) Experimental motivations (just a list, some details later on some of them)

- Cold atoms in an optical lattice*
- Array of coupled Josephson junctions
- ⁴He adsorbed on graphite
- Vortex lines in superconductors w/ pinning
- Bose condensation of magnons in some magnetic insulators*
- Others ?

Which phases do we expect, at T=0 ?

- A <u>superfluid phase</u>, in which bosons condense into a k=0 state
- A <u>Mott insulating state</u> in which the repulsive interaction blocks the coherent motion of bosons
- We expect the MI phase to exist when the average number of bosons per site is integer and U/t is large enough

1.1 The `atomic' limit t=0

Eigenstates on each site are the states of definite particle number: |n>

with energies:

$$E_n = \frac{U}{2}n(n-1) - \mu n$$

T T

e.g.:
$$E_{n=0} = 0, E_{n=1} = -\mu, E_{n=2} = U - 2\mu, \text{ etc...}$$

Ground-state is |n> provided:

$$\mu \in](n-1)U, nU[.$$



"Coulomb blockade staircase"

Ground-state is:

- Non-degenerate (|n> on each lattice site) for µ within each charge plateau
- Macroscopically degenerate (2^{Nsites}) at degeneracy points μ_n =nU

The non-degenerate ground-state is protected by a gap:

$$\Delta_g = E_{n+1} + E_{n-1} - 2E_n = U$$

process: $(n,n) \rightarrow (n-1,n+1)$ Creating hole + double occupancy on pair of sites

Note, in `chemical' terms: $\Delta_g = (E_{n+1} - E_n) + (E_{n-1} - E_n)$ ``affinity'' ``ionization''

Gap \rightarrow ``incompressibility'': finite energy to add an extra particle

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Compressibility:

$$\kappa \sim \left(\frac{\partial^2 E}{\partial n^2}\right)^{-1} = \frac{\partial n}{\partial \mu} = 0$$

What happens when turning on a finite hopping t?

General quantum-mechanical wisdom:

- Non-degenerate ground-state protected by a gap: Robust to perturbation <u>if t/U small enough</u> Remains incompressible → Mott insulator for t/U < (t/U)_c
- i) Degenerate case: the system will find a way to lift degeneracy
 → Superfluid as soon as t is turned on



1.2 A Mean-Field Theory (substantiating and quantifying this expectation)

4 references, slightly different points of view, ~ identical results:

- MPA Fisher et al. Phys Rev B 40 (1989) 546
- D.Rokhsar and G.Kotliar Phys Rev B 44 (1991) 10328
- W. Krauth et al. Phys Rev B 45 (1992) 3137
- K. Seshadri et al. Europhysics Lett. 22 (1993) 257

- Decouple the hopping term, neglect fluctuations:

$$b_i^{\dagger} b_j \rightarrow \text{const.} + \langle b_i^{\dagger} \rangle b_j + b_i^{\dagger} \langle b_j \rangle + \text{fluct}$$

- Maps the lattice model onto <u>a single-site problem</u> in a self-consistent field (which creates or destroys bosons):

$$h_{\text{eff}}^{(i)} = -\lambda_i b^{\dagger} - \lambda_i b + \frac{U}{2}\hat{n}(\hat{n} - 1) - \mu\hat{n}$$

 $\lambda_i = \sum_{\mathbf{j}} \mathbf{t}_{\mathbf{ij}} \left< \mathbf{b}_{\mathbf{j}} \right>$: self-consistency condition

Translational invariance:

$$\lambda = z \, {\rm t} \, \langle {\rm b} \rangle$$

z: lattice connectivity

 : order parameter for the superfluid phase

- Easy to solve numerically, using |n>-basis \rightarrow phase diagram
- Analytical study, close to MI/SF transition points:

Consider plateau $\mu \in [(n-1)U, nU]$

Expand for small λ :

$$\begin{aligned} |\psi_0\rangle &= |n\rangle - \lambda \left[\frac{\sqrt{n}}{U(n-1) - \mu} |n-1\rangle + \frac{\sqrt{n+1}}{\mu - Un} |n+1\rangle \right] \\ \overline{\langle\psi_0|b|\psi_0\rangle} &= -\lambda \left[\frac{n}{U(n-1) - \mu} + \frac{n+1}{\mu - Un} \right] \end{aligned}$$

Inserting into self-consistency condition:

$$\lambda = -z \operatorname{t} \lambda \left[\frac{\mathrm{n}}{\mathrm{U}(\mathrm{n}-1) - \mu} + \frac{\mathrm{n}+1}{\mu - \mathrm{Un}} \right] + \cdots$$

Vanishing of coefficient linear in λ (i.e quadratic term in energy functional, cf. Landau) yields critical boundary:

$$\frac{zt}{U} = \frac{(n - \mu/U)(\mu/U - n + 1)}{1 + \mu/U}$$

- Tip of the Mott lobe (critical coupling):

$$\frac{zt}{U}|_{c,n} = \operatorname{Max}_{x \in [n-1,n]} \frac{(n-x)[x-n+1]}{1+x} = \frac{1}{2n+1+2\sqrt{n(n+1)}}$$

$$(U/zt)_{c} \simeq 5.8 \text{ for } n = 1 \quad ((U/zt)_{c} \sim 4n \text{ for large } n)$$
- Gap in the Mott insulating phase: $\Delta_{g}(n) = \mu_{+}(n) - \mu_{-}(n)$

$$(\mu/U)^{2} - [2n-1-(zt/U)](\mu/U) + n(n-1) + (zt/U) = 0$$

$$\Delta_{g}(n) = U \left[(\frac{zt}{U})^{2} - 2(2n+1)\frac{zt}{U} + 1 \right]^{1/2} \qquad \propto \sqrt{U-U_{c}}$$

$$\sim U \text{ at large } U$$



Note: Mott phase can be approached in 2 ways



1.3 Three viewpoints on the Mean-Field Theory

Viewpoint 1: The limit of infinite lattice connectivity



The `local field' $\frac{1}{z} \sum_{j; < j, i >} b_j^{\dagger}$ has no fluctuations as $z \rightarrow$ infinity

Hence, neglecting fluctuations becomes exact, provided the hopping is scaled appropriately as: $t \rightarrow t / z$

In fact, this is very familiar from statistical mechanics, and clear in the large-U limit where we keep only n=0,1 (``hard-core bosons'')

Digression: the Bose Hubbard model and quantum magnets Bose-condensing magnons...

- Hard-core boson = a spin-1/2 operator

Matsubara and Matsuda, Prog Theor Phys 16 (1956) 416

$$S_i^+ = b_i^{\dagger} , \ S_i^- = b_i , \ S_i^z = b_i^{\dagger} b_i - \frac{1}{2}$$

- Bose Hubbard = Quantum XY model in applied field along z-axis:

$$H = J_{\perp} \sum_{\langle ij \rangle} [S_i^+ S_j^- + \text{h.c.}] - H \sum_i S_i^z \qquad J_{\perp} = -t \ , \ H = \mu$$

 $M_z = \langle S^z \rangle = \langle n \rangle - \frac{1}{2}$

Mott plateau = magnetization plateau
→ Magnon density can be controlled

- Mean-field above is the usual statmech mean-field for XY model

- Additional nearest-neighbor interaction V yields XXZ model:

$$H = J_{\perp} \sum_{\langle ij \rangle} [S_i^+ S_j^- + \text{h.c.}] + J_z \sum_{\langle ij \rangle} S_i^z S_j^z - H \sum_i S_i^z$$
$$J_{\perp} = -t \ , \ J_z = V \ , \ H = \mu$$

Table 1 Correspondence between a Bose gas and a quantum antiferromagnet.

Bose gas	Antiferromagnet
Particles	Spin excitations ($S = 1$ quasiparticles)
Boson number N	Spin component S^z
Charge conservation $U(1)$	Rotational invariance $O(2)$
Condensate wavefunction $\langle \psi(\mathbf{r}) \rangle$	Transverse magnetic order $\langle S_i^x + iS_j^y \rangle$
Chemical potential μ	Magnetic field H
Superfluid density ρ_s	Transverse spin stiffness
Mott insulating state	Magnetization plateau

REVIEW ARTICLE | FOCUS

Bose–Einstein condensation in magnetic insulators

THIERRY GIAMARCHI¹*, CHRISTIAN RÜEGG²* AND OLEG TCHERNYSHYOV³*

nature physics | VOL 4 | MARCH 2008





→Beautiful recent experiments and theory/experiment comparisons

A spin-liquid ground-state is analogous to a NORMAL (=non superfluid) Bose liquid at T=0 Anisotropic Heisenberg model:

$$H = J_{\perp} \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + J_z \sum_{\langle ij \rangle} S_i^z S_j^z$$

Hard-core boson representation:

$$S^+ \sim b^{\dagger}, \ S^- \sim b, \ S^z \sim b^{\dagger}b - \frac{1}{2}$$

XY order = superfluid phase Antiferromagnet w/ Ising anisotropy = Checkerboard crystal phase

Spin-liquid (NO symmetry breaking) = NORMAL Bose liquid

Can one design interactions such that Bose condensation is suppressed?

Viewpoint 2: wave-functions

The exact wave-function is a product over sites in both t=0 and U=0 limit (at least for a large system) :

t=0: Fock state

$$\prod_i |n\rangle_i = \prod_i \frac{1}{\sqrt{n!}} (b_i^\dagger)^n |0\rangle$$

U=0: Bose condensed state can be seen as coherent state with a definite phase:

$$\frac{1}{\sqrt{N!}} [b_{\mathbf{k}=0}^{\dagger}]^{N} |0\rangle = \frac{1}{\sqrt{N!}} \left[\frac{1}{\sqrt{N_{s}}} \sum_{i} b_{i}^{\dagger} \right]^{N} |0\rangle$$

or large N, N_s ~
$$\prod_{i} |\alpha\rangle_{i} \quad |\alpha\rangle = e^{-|\alpha|^{2}/2} \sum_{n=0}^{\infty} \frac{\alpha^{n}}{\sqrt{n!}} |n\rangle$$
$$|\alpha|^{2} = \langle n\rangle = \frac{N}{N_{s}}$$

Variational ansatz for ground-state wavefunction: a site-factorized state (~ Gutzwiller)

$$|\Psi\rangle = \prod_{i} \left[\sum_{n=0}^{\infty} c_n |n\rangle_i\right] , \quad \sum_{n} |c_n|^2 = 1$$

Minimizing energy yields same MFT equations as above

This yields a pure Fock state: $c_n = \delta_{n,n0}$ throughout the whole Mott insulating phase, with no fluctuation of the local occupation number: this is of course an approximation.

Number statistics:

- Fock $p(n) = \delta n, n0$ in Mott state
- Poisson at U=0:

$$p(n) = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!} \quad |\alpha|^2 = \langle n \rangle = \langle n^2 \rangle - \langle n \rangle^2$$

Note: p(n) a.k.a `valence histogram'

Note: beware of some apparent paradoxes associated with mean-field theories !

→ Blackboard

Viewpoint 3: field-theory - saddle point and fluctuations -

→ Blackboard

2. Cold atoms in an optical lattice: a controlled experimental realization of the Hubbard Model

D.Jaksch, C.Bruder, J.I. Cirac, C.W.Gardiner and P.Zoller Phys Rev Letters, 81 (1998) 3108

Review articles:

- I.Bloch, J.Dalibard and W.Zwerger Rev Mod Phys 80 (2008) 885

- I. Bloch Nature Physics 1 (2005) 23

Ultra-cold atomic gases :

The temperature scale of these cold gases



-Bosonic atoms, e.g: ⁸⁷Rb, ⁷Li, ⁴¹K, ⁴He, etc... -Fermionic atoms, e.g: ⁶Li, ⁴⁰K, 3He, etc...

The 3 C's: « Cooling, Control, Confine »

• Cooling :

reach quantum degeneracy

• Control :

tuning of system parameters, in particular interaction strength.

• Confine :

Spatial confinement

(in particular via trapping in optical lattices)
 → reach strong interaction regimes and realize

 (artificial solids with atoms and light)



- Typical solid-state physics issues have been investigated long ago even in thermal gases, e.g *pioneering Bloch oscillation experiment (Dahan et al, 1996)*

In the lattice, interaction effects become prominent (spatial confinement)

Atoms in an optical lattice: energy scales



Free-particle bands (neglect trapping potential): Bloch waves

$$H_x = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_0 \sin^2(k_L x).$$

$$H_x |\psi_{nk}\rangle = \epsilon_{nk} |\psi_{nk}\rangle \quad \psi_{nk}(x) = e^{ikx} u_{nk}(x)$$



 $V_0 = E_R$: 1st and 2nd band (1D)

For a deep enough lattice (tight-binding limit), key parameter: tunneling amplitude t between 2 neighbouring wells:



$$\varepsilon_{\mathbf{k}} = -2t\sum_{i=1}^{D}\cos k_{i}$$

Tight-binding limit (deep lattice):

Bandwidth: (W = 4Dt)

 $W \sim E_R$ for shallow lattice $V_0 \ll E_R$

$$t/E_R = 4\pi^{-1/2} (V_0/E_R)^{3/4} e^{-2(V_0/E_R)^{1/2}}$$
, $V_0 \gg E_R$



Natural scale for quantum degeneracy (free particles) \rightarrow Adiabatic cooling – <u>think in terms of entropy</u>: \rightarrow Conserve ~ T/T_F for fermions

<u>What about interactions ?</u>

Consider first the gas, in the absence of the optical lattice :

Very dilute gases: typical density $n \sim 10^{11}$ - 10^{12} cm⁻³

Interparticle distance is thus of order n^{-1/3}~10⁻⁶ m, MUCH bigger than hard-core part of interatomic potential

Hence, naively, interactions are very weak

But in fact, what really matters is the (s-wave) scattering amplitude a_s , which controls the collision cross-section: $\sigma = 4\pi a_s^2$

Effective contact interaction:

 $\frac{g}{2} \int d^3x \psi^{\dagger}(x) \psi^{\dagger}(x) \psi(x) \psi(x) \ , \ g = \frac{4\pi a_s \hbar^2}{m}$

g can be controlled Through Feshbach resonances

Interacting hamiltonian in the lattice: use Wannier functions

$$H_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0 \sin^2(k_L x). \quad H_x \left|\psi_{nk}\right\rangle = \epsilon_{nk} \left|\psi_{nk}\right\rangle \quad \psi_{nk}(x) = e^{ikx}u_{nk}(x)$$

Wannier function localised on lattice site R:

$$\left|W_{\vec{n},\vec{R}}\right\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}} \left|\Psi_{\vec{n},\vec{k}}\right\rangle$$



On-site interaction:

$$U = g \int d^3r \, |W(\vec{r})|^4$$

Deep lattice:

$$\frac{U}{E_R} \simeq \sqrt{\frac{8}{\pi}} a_s k_L \left(\frac{V_0}{E_R}\right)^{3/4}$$

Contour plot of 2D Wannier function $V_0=10 E_R$

Hubbard interaction Interaction in Wannier basis set: In 1st band $V = g \int d^3 \vec{r} \Psi^{\dagger}_{\uparrow}(\vec{r}) \Psi_{\uparrow}(\vec{r}) \Psi^{\dagger}_{\downarrow}(\vec{r}) \Psi_{\downarrow}(\vec{r})$ $= g \sum c^{\dagger}_{\vec{R_1},\vec{n_1},\uparrow} c_{\vec{R_2},\vec{n_2},\uparrow} c^{\dagger}_{\vec{R_2},\vec{n_3},\downarrow} C_{\vec{R_4},\vec{n_4},\downarrow} \int d^3 \vec{r} W_{\vec{R_1},\vec{n_1}} W_{\vec{R_2},\vec{n_2}} W_{\vec{R_3},\vec{n_3}} W_{\vec{R_4},\vec{n_4}}$ \vec{R}_i, \vec{n}_i $U\sum_{\vec{R}} n_{\vec{R},1,\uparrow} n_{\vec{R},1,\downarrow} + U_2 \sum_{\vec{R},\alpha} n_{\vec{R},2\alpha,\uparrow} n_{\vec{R},2\alpha,\downarrow}$ $+\sum V_{l,l'}(n_{l,\uparrow}n_{l',\downarrow}+c^{\dagger}_{l,\uparrow}c^{\dagger}_{l,\downarrow}c_{l',\downarrow}c_{l',\uparrow}-c^{\dagger}_{l,\uparrow}c_{l,\downarrow}c^{\dagger}_{l',\downarrow}c_{l',\uparrow})$

 $+V_{vois} \sum n_{\vec{R},-\sigma} (c^{\dagger}_{\vec{R}',\sigma} c_{\vec{R},\sigma} + \text{h.c.})$

Hopping-like term (small ?)

$$U = g\left(\int w_1(x)^4 dx\right)^3$$

 $\vec{R}.\vec{R'}.\sigma$

$$U_{2} = g\left(\int w_{2}(x)^{4}dx\right)\left(\int w_{1}(x)^{4}dx\right)^{2}$$
$$V_{vois} = g\left(\int w_{1}(x)^{3}w_{1}(x+a)dx\right)\left(\int w_{1}(x)^{4}dx\right)^{2}$$

Region of validity of (controlled) 1-band Hubbard:

Hopping-like interactions set in

.05

Pseudo-potential fails (must have $a_s < l_{ho}$)

30

 $-l_{ho} = typical$ extension of Wannier function - Delta= energy separation between bands

> 2nd band Well-separated (must have U<Delta)

0.01 പ്പ UK 0.001 10 20 V_{o} / E_{p}

cf. F.Werner, O.Parcollet, A.G and S.R. Hassan Phys Rev Lett. 95 (2005) 056401

3. Experimental observation of the Mott insulator to superfluid transition for cold bosonic atoms

Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms NATURE [VOL 4

NATURE VOL 415 3 JANUARY 2002

Markus Greiner*, Olaf Mandel*, Tilman Esslinger†, Theodor W. Hänsch* & Immanuel Bloch*



Phase coherence between wells in superfluid phase >interference pattern





Momentum distribution for different Potential Depths

Time of flight: multiple matter-wave interference patterns in SF phase



Figure 2 Absorption images of multiple matter wave interference patterns. These were obtained after suddenly releasing the atoms from an optical lattice potential with different potential depths V_0 after a time of flight of 15 ms. Values of V_0 were: **a**, 0 E_r ; **b**, 3 E_r ; **c**, 7 E_r ; **d**, 10 E_r ; **e**, 13 E_r ; **f**, 14 E_r ; **g**, 16 E_r ; and **h**, 20 E_r .

Interpretation of these images: \rightarrow blackboard

Detailed analysis of these interferences pattern reveal more precisely the nature of the Mott insulator wave function [F.Gerbier et al., PRL 95, 050404 (2005)]

Doubly occupied/empty sites are present in the finite-U ground-state:

$$|\Psi^{(1)}\rangle \approx |\Psi\rangle_{\mathrm{MI}} + \frac{t}{U} \sum_{\langle i,j \rangle} \hat{a}_{i}^{\dagger} \hat{a}_{j} |\Psi\rangle_{\mathrm{MI}} \quad |\Psi\rangle_{\mathrm{MI}} = \prod_{i} |n_{0}\rangle_{i}$$

$$n(\mathbf{r}) = \left(\frac{m}{\hbar t}\right)^3 \left\| \tilde{w} \left(\mathbf{k} = \frac{m\mathbf{r}}{\hbar t} \right) \right\|^2 S \left(\mathbf{k} = \frac{m\mathbf{r}}{\hbar t} \right)$$
$$|S(\mathbf{k}) = \sum_{i,j} e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle \hat{a}_i^{\dagger} \hat{a}_j \rangle,$$

Visibility of interference pattern:

$$\mathcal{V} = \frac{n_{\max} - n_{\min}}{n_{\max} + n_{\min}} = \frac{S_{\max} - S_{\min}}{S_{\max} + S_{\min}} \approx \frac{4}{3}(n_0 + 1)\frac{zt}{U}.$$



A reversible process: phase coherence can be restored !



The non-uniform trapping potential *helps :* extended regions w/commensurate filling « wedding cake » shape of density profile





FIG. 2. (Color online). Four density profiles (Δ) (cuts across Fig. 1) and their variances (O). The fillings are N_f =50 (a), 68 (b), 94 (c), and 150 (d).

Density profiles for increasing number of trapped atoms: rings/disks w/ commensurate filling

Rigol and Muramatsu, Phys Rev A 2004

Shell structure as a consequence of incompressibility

Local density approximation allows to deduce in-trap density profile from the equation of state computed in the uniform case:

$$\mu(\mathbf{r}) = \mu - V_{\text{ext}}(\mathbf{r})$$



Figures courtesy of M. Niemeyer and H. Monien (Bonn)

Slide courtesy F.Gerbier

Experimental observation of wedding cake:



Fölling et al. PRL 2006

Very recently: direct observation in 2D by single-site imaging Here we report on a direct observation of the in-trap density distribution with a high spatial resolution. This is achieved by locally modifying the spin state using a technique similar to magnetic resonance imaging and to the rf addressing technique in [19]. Spin-changing collisions [20] allow us to independently measure the integrated density profiles of both the total atom distribution and sites with a specific occupation number. From such integrated profiles we obtain clear signatures of the emergence of Mott plateaus with uniform occupation above the MI transition. The measured plateau radii agree well with a simple model assuming a fully incompressible system, zero temperature, and zero tunneling.

FIG. 2 (color). Integrated in-trap density profiles of the atom cloud for different lattice depths and atom numbers: (a) 1.0×10^5 atoms in the superfluid regime ($V_0 = 3E_r$); (b) 1.0×10^5 atoms in the Mott regime ($V_0 = 22E_r$); (c) 2.0×10^5 atoms; (d) 3.5×10^5 atoms. The gray data points denote the total density distribution and the red points the distribution of doubly occupied sites. The blue points show the distribution of sites with occupations other than n = 2. The solid lines are fits to an integrated Thomas-Fermi distribution in (a) and an integrated shell distribution for (b)–(d). The n = 2 data points are offset vertically for clarity.

Many other observations:

- Number statistics
- Gap in MI (modulation spectroscopy, potential gradient)
- Sound mode in SF not (yet) been observed to my knowledge
- FERMIONS: Onset of Mott incompressible regime has now been reached

CONCLUSIONS, PERSPECTIVES...

- Emerging field at the interface between condensed matter physics and quantum optics
- Strongly correlated quantum phases and phase transitions
- Need for imaginative probes
- Unconventional regimes: out of equilibrium, etc...
- Many other exciting topics not covered here