Probing the physics of strong correlations with cold fermions in optical lattices

(A condensed matter physicist viewpoint)

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http://www.cpht.polytechnique.fr/cpht/correl/mainpage.htm
A new condensed matter physics, with light and atoms?

- "Quantum simulations" of models of interest in condensed matter physics
  >> help answer some of the outstanding open questions on strongly correlated materials?

- New physical regimes, level of controllability, etc… unreachable in traditional solid-state physics
OUTLINE

- General notions on Mott insulator of fermions w/ spin: magnetic ground-state

- Adiabatic cooling using interactions and Pauli blocking
  [F.Werner, O.Parcollet, A.G & S.R.Hassan, condmat/0504003]
  Thanks to: C.Salomon, F.Chevy (LKB-ENS)

- Exotic quantum magnetism in optical lattices?

- The Mott transition in frustrated systems as a liquid-gas transition

- When the quasiparticle concept breaks down:
  ``hot'' and ``cold'' regions on the Fermi surface
Strongly correlated materials in solid-state physics: who are the suspects?

Localized orbitals (close enough to nuclei): 3d, 4f
[Materials with transition metals or rare-earth ions]

>> Strong screening: on-site matrix element of Coulomb interaction plays the dominant role

\[ U \sim \int dr dr'|W_i(r)|^2 V_{\text{screened}}^{\text{int}}(r - r')|W_i(r')|^2 \]

>> Narrow bandwidths (small kinetic energy)
Minimal model: 
the Hubbard hamiltonian

\[ H = -t \sum_{<ij>} \sum_{\sigma=\uparrow, \downarrow} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

t : hopping amplitude between lattice sites
U: on-site repulsive interaction

This model plays in this field a role similar to that of the Ising model in classical statmech/magnetism

NOTE: Fermi statistics (Pauli blocking) and spin degrees of freedom yields richer physics than bosonic case...
The Mott phenomenon is a key to the properties of correlated materials.

Consider, for simplicity, one particle per site.

When $U=0$: half-filled band $\rightarrow$ METAL

\[ \epsilon_k = -2t \cos k \]

Fermi level
Metallic (conducting) state:

* **Real-space** picture is complicated!
  (Many holes and double occupancies)

* **k-space** description is simpler: extended wave-function
  (simple Slater determinant of Bloch eigenstates for $U=0$)

“snapshot” of one component of the wave function
Large U/t: Mott insulator

Intersite hopping is blocked if:

- tunneling amplitude \( (t) \) is small enough compared to
- \( U = \) on-site repulsive interaction

Real-space picture is simple: mostly singly-occupied sites

**NOTE:** At large \( U \), Mott localisation has nothing to do with spin ordering. Gap for charge motion \( \sim U \).

However, at low-\( T \), long-range spin order will (in most cases...) set in, at a critical temperature \( T_c \).

For \( T_c < T < U \): \( \sim \) random mixture of spins (paramagnet)
What are the residual spin-spin interactions (at large U)?

The inter-site magnetic exchange

>> Virtual hopping is blocked (Pauli principle)

>> Virtual hopping is allowed

Inter-site antiferromagnetic exchange:

\[
J_{AF} = \frac{4t^2}{U}
\]
What does the Mott insulating ground-state look like?

Above cartoon of Mott insulator was a random spin configuration \(\rightarrow\) cannot be the ground-state!

* Simplest possibility is a Néel-like antiferromagnet:

(Note: this is a semi-classical picture. Quantum wave function is more complicated…)

* Other more exotic possibilities exist, depending e.g. on the lattice: will come back to this later …
Atoms in an optical lattice: when does the Hubbard model apply?

3D lattice:

\[ V(\vec{r}) = V_0 \sum_{i=1}^{3} \sin^2(k_L x_i) \]

\[ k_L = \frac{2\pi}{\lambda} \quad (\lambda \text{ wavelength of Laser}) \]

\[ a = \frac{\lambda}{2} \text{ lattice spacing} \]

\[ E_R = \frac{\hbar^2 k_L^2}{2m} \quad \text{recoil energy} \]

Typical orders of magnitude \((^6\text{Li})\)

\[ \lambda = 1.06 \mu m, \quad E_R = 1.4 \mu K \]
Free-particle bands: from Bloch waves to Wannier functions

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

\[ H_x |\psi_{nk}\rangle = \epsilon_{nk} |\psi_{nk}\rangle \]

\[ \psi_{nk}(x) = e^{ikx} u_{nk}(x) \]

Wannier function localised on lattice site \( R \):

\[ |W_{\bar{n},\bar{R}}\rangle = \frac{1}{\sqrt{N}} \sum_{\bar{k}} e^{-i\bar{k} \cdot \bar{R}} |\Psi_{\bar{n},\bar{k}}\rangle \]

\( V_0 = E_R \): 1\textsuperscript{st} and 2\textsuperscript{nd} band (1D)

Contour plot of 2D Wannier function \( V0=10\) ER
Interacting part of Hamiltonian:

Consider e.g. \(^6\)Li atoms in the 2 lowest hyperfine states

Pseudopotential approximation:

\[
V = g \int d^3 \mathbf{r} \Psi_\uparrow^*(\mathbf{r}) \Psi_\uparrow(\mathbf{r}) \Psi_\downarrow^*(\mathbf{r}) \Psi_\downarrow(\mathbf{r})
\]

\[
g = \frac{4\pi \hbar^2 a_s}{m}
\]

\(a_s\): scattering length
Interaction in Wannier basis set:

\[ V = g \int d^3 \vec{r} \Psi_{\uparrow}^\dagger(\vec{r}) \Psi_{\uparrow}(\vec{r}) \Psi_{\downarrow}^\dagger(\vec{r}) \Psi_{\downarrow}(\vec{r}) \]

\[ = g \sum_{\vec{R}_i, n_i} c_{\vec{R}_1, n_1, \uparrow}^\dagger c_{\vec{R}_2, n_2, \uparrow} c_{\vec{R}_3, n_3, \downarrow}^\dagger c_{\vec{R}_4, n_4, \downarrow} \int d^3 \vec{r} W_{\vec{R}_1, n_1} W_{\vec{R}_2, n_2} W_{\vec{R}_3, n_3} W_{\vec{R}_4, n_4} \]

\[ = U \sum_{\vec{R}} n_{\vec{R}, 1, \uparrow} n_{\vec{R}, 1, \downarrow} + U_2 \sum_{\vec{R}, \alpha} n_{\vec{R}, 2\alpha, \uparrow} n_{\vec{R}, 2\alpha, \downarrow} \]

\[ + \sum_{l, l'} V_{l, l'} (n_{l, \uparrow} n_{l', \downarrow} + c_{l, \uparrow}^\dagger c_{l', \downarrow} c_{l, \downarrow} c_{l', \uparrow} - c_{l, \uparrow}^\dagger c_{l, \downarrow} c_{l', \uparrow} c_{l', \downarrow}) \]

\[ + V_{\text{vois}} \sum_{\vec{R}, \vec{R}', \sigma} n_{\vec{R}, -\sigma} (c_{\vec{R}', \sigma}^\dagger c_{\vec{R}, \sigma} + \text{h.c.}) \]

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

\[ U_2 = g \left( \int w_2(x)^4 dx \right) \left( \int w_1(x)^4 dx \right)^2 \]

\[ V_{\text{vois}} = g \left( \int w_1(x)^3 w_1(x + a) dx \right) \left( \int w_1(x)^4 dx \right)^2 \]
Region of validity of controlled 1-band Hubbard:

Hopping-like interactions set in

Pseudo-potential fails $a_s \sim l_{h.o}$

2nd band
Well-separated
(U>$\Delta$)

Spin-density wave
Heisenberg

cf. F.Werner, O.Parcollet, A.G and S.R. Hassan cond-mat/0504003
The phase diagram at $\frac{1}{2}$-filling (3D case)

Coherence scale (effective Fermi energy)

ITINERANT (CORRELATED) ~FERMI LIQUID

MOTT-LOCALIZED

ANTIFERROMAGNET

[Calculations using dynamical mean-field theory]

F. Werner, O. Parcollet, A. G and S. R. Hassan cond-mat/0504003
Cooling using the combined effect of interactions and Pauli blocking: an analogue of the Pomeranchuk effect in He3

In a strongly correlated Fermi-liquid, one can INCREASE LOCALIZATION (∼solidify) by HEATING

Indeed spin entropy in localised regime (∼ln2/particle) Is bigger than entropy in itinerant state (∼T)
In the Hubbard model context, this is seen from the T-dependence of the probability of double occupancy:

\[ d = \langle n_\uparrow n_\downarrow \rangle \]

This effect is seen throughout the itinerant regime, i.e. \( T < T_F^* \).

FIG. 2: Double occupancy \( d = \langle n_\uparrow n_\downarrow \rangle \) as a function of temperature, for several values of \( U/t \), calculated within DMFT(IPT). The initial decrease is the Pomeranchuk effect responsible for adiabatic cooling.

cf. A.G& W.Krauth, PRL 1992
Shape of the isentropic curves:

Thermodynamic relation:
\[
\frac{\partial s}{\partial U} = - \frac{\partial d}{\partial T}
\]

implies that isentropics \( T_i(U) \) obey:

\[
c(T_i) \frac{\partial T_i}{\partial U} = T_i \frac{\partial d}{\partial T} |_{T=T_i}
\]
Using entropy as a thermometer:

Reach the antiferromagnetic phase by adiabatic cooling?

Note: for typical parameters $\frac{\hbar}{t} \simeq 0.5\text{ms}$, $\frac{\hbar}{J_{AF}} \simeq 2\text{ms}$
Effect of the non-uniform trapping potential:

Mott state is incompressible:

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

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

Rigol and Muramatsu, Phys Rev A 2004
A technical remark: mean-field theories of the Mott phenomenon are easier for bosons than for fermions!

Bosons:

\[-t \sum_{ij} b_i^\dagger b_j + U \sum_i n_i (n_i - 1)\]
\[\rightarrow \sum_i [\lambda_i b_i^\dagger + h.c + U n_i (n_i - 1)] \text{ with: } \lambda_i = t \langle b_i \rangle\]

Krauth et al., Ramakrishnan et al, Fisher et al., 90’s

Not a viable route for fermions! (\langle c \rangle not an order parameter of Either metal or superconductor)
II. Possible “exotic” ground-states of the Mott insulator

How can one avoid conventional antiferromagnetic long-range order?

>>> Strong quantum fluctuations
>>> Many classically degenerate ground-states
>>> Frustration
>>> Low dimensionality
Valence bond states

\[ \frac{1}{\sqrt{2}} \left( \begin{array}{c} \uparrow \\ \downarrow \end{array} - \begin{array}{c} \downarrow \\ \uparrow \end{array} \right) \]

- Valence bond CRYSTALS:
  - columnar
  - staggered

Symmetry breaking: spins = NO
translation = YES
Resonating valence bond states (RVB)

Wave function = superposition of many dimer coverings by singlets

NO SYMMETRY BREAKING AT ALL (spin or translation): “SPIN LIQUID”

+ ... (many)

~ Giant benzene molecule
Example of RVB state: The Kagome quantum antiferromagnet

NO GAP IN $S=0$ SECTOR!
NO TRANSLATION STRY BREAKING
GAP TO $S=1$ SECTOR

Lecheminant et al.- C.Lhuillier’s group

See also: recent work on Moessner and Sondhi on quantum dimer models.
Kagome optical lattice


FIG. 1. (a) Ideal Kagomé lattice for $\phi = \pi/2$. (b) TKL using $\phi = \pi/4$. This lattice can be generated using three SWs with a $\pi/3$ angle between themselves. Each SW is generated by three lasers with a configuration shown in (c). (d) Enumeration of spins in a trimer and of neighboring trimers.
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:

\[ S^+ \sim b^\dagger, \quad S^- \sim b, \quad S^z \sim b^\dagger b - \frac{1}{2} \]

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?
III. An open question:

Is there indeed, as suggested by this theory, a first order, finite-T, Mott transition even in the absence of lattice degrees of freedom? (Frustration is almost certainly necessary)

In solid-state context: the crystal lattice reacts to the electronic instability e.g. lattice spacing is discontinuous through the transition (but same crystal symmetry)
Critical behaviour at the Mott critical endpoint

A liquid-gas transition? Simple picture:

**Insulator:** low-density of doubly occupied sites

![GAS]

**Metal:** High-density

![LIQUID]

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<th>Liquid-gas</th>
<th>Ising model</th>
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<td>(p - p_c)</td>
<td>(p - p_c)</td>
<td>Field (h)</td>
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<td>(T - T_c)</td>
<td>(T - T_c)</td>
<td>(T - T_c)</td>
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<td>id.</td>
<td>(v_g - v_L)</td>
<td>Order parameter (scalar)</td>
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What do real (strongly correlated) solids do?

A material poised close to the Mott instability: $V_2O_3$

Note: slope of $T_c$ vs. $p$ again the Pomeranchuk effect!

Recent experiments (Limelette et al, Science 2003) show that critical Endpoint is indeed Ising-like

![Phase diagram for doped $V_2O_3$ systems, $(V_{1-x}Cr_x)_2O_3$ and $(V_{1-x}Ti_x)_2O_3$. From McWhan et al., 1971, 1973.](image)
IV. From Fermi surface imaging to measuring quasiparticle properties?

Very recent experiments in Esslinger’s group [PRL 94 (2005) 080403] have succeeded in imaging the Fermi surface of $^{40}$K atoms in an optical lattice.

A key measurement would be to characterize the spectrum of quasiparticle excitations at each k-point on the Fermi surface:

- Dispersion relation (Fermi velocity)
- Lifetime
- Spectral weight $Z(k)$
This would have bearing on crucial current issue in the physics of strongly correlated materials, particularly low-dimensional.

Indeed, in cuprate superconductors, the quasiparticle concept seems to break down on some sections of the Fermi surface (i.e. lifetimes are very short, a pseudo-gap appears) while retaining some validity close to the ``nodal” directions.

« Hot » regions (no quasiparticles)

« Cold » spots (nodal ~ quasiparticles)
In solids: angle-resolved photoemission experiments

- Remove (or add) an electron at time \( t=0 \): \( d_k^\dagger |\psi_0\rangle \)
- Evolve the state up to time \( t \)
- Measure overlap with original state \( \langle \psi(r',t')\psi^+(r,t) \rangle \)

Spectral density (~ 1-particle Green’s function):

\[
A(k, \omega) = \sum_A |\langle \Psi_A |d_{k\sigma}^\dagger |\Psi_0\rangle|^2 \delta(\omega + E_0 - E_A) \quad (\omega > 0)
\]

\[
A(k, \omega) = \sum_B |\langle \Psi_B |d_{k\sigma} |\Psi_0\rangle|^2 \delta(\omega + E_B - E_0) \quad (\omega)
\]
A new condensed matter physics, with light and atoms?

[Several things I have not talked about]

- "Quantum simulations" of models of interest in condensed matter physics
- New physical regimes, level of controllability, etc... unreachable in traditional solid-state physics

Optical lattice "engineering": state-selective lattice, low -dimensional Lattices, random potentials, etc...

Time-dependent phenomenon (strongly out of equilibrium), Manipulation of individual atoms in the optical lattice, etc...
I have tried to raise several questions that have been discussed in a condensed matter context:

- Finite-T (liquid-gas) Mott transition
- Exotic Mott insulating ground-states
- Nature of strongly correlated conducting states
- etc... (e.g. disorder + interactions)

>>> Hopes & challenges for
   ‘’Condensed matter of cold atoms ‘’