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SCHOOL ON QUANTUM PHASE TRANSITIONS AND NON-EQUILIBRIUM PHENOMENA IN COLD ATOMIC GASES

11 - 22 July 2005

Probing the physics of strong correlations with cold fermions in optical lattices: *adiabatic cooling and quantum magnetism*

Presented by:

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Probing the physics of strong correlations with cold fermions in optical lattices: *adiabatic cooling and quantum magnetism*

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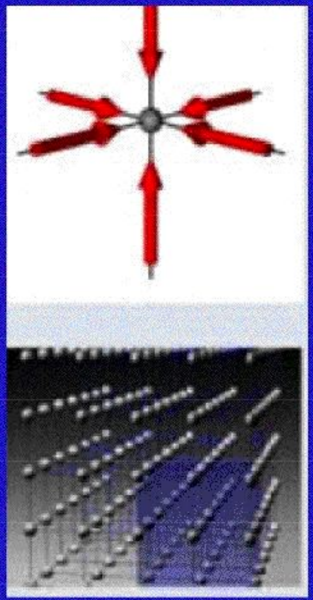
ICTP, July 2005

http://www.cpht.polytechnique.fr/cpht/correl/mainpage.htm



A new condensed matter physics, with light and atoms ?

- Realization 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, Phys. Rev. Lett. (in print)]

Thanks to: C.Salomon, F.Chevy (LKB-ENS)

>> Using entropy as a thermometer !

- 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

Minimal model of relevance to strongly-correlated condensed matter systems: the Hubbard hamiltonian

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

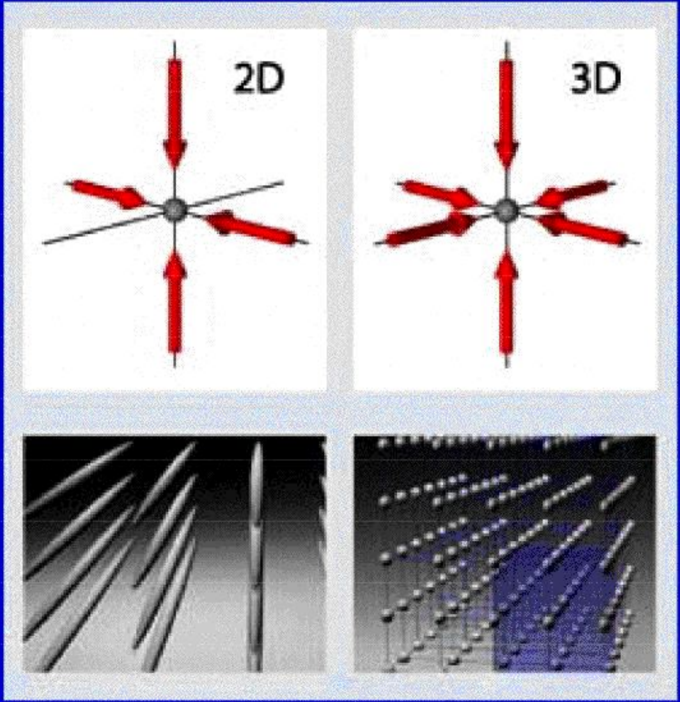
t : hopping amplitude between lattice sites

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…

Atoms in an optical lattice: when does the Hubbard model apply ?



3D lattice:

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

$k_L = 2\pi/\lambda$
(λ wavelength of Laser)

$a = \lambda/2$ lattice spacing

$$E_R = \frac{\hbar^2 k_L^2}{2m}$$ **recoil energy**

Typical orders of magnitude (^{6}Li)

$$\lambda = 1.06\mu m,\ E_R = 1.4\mu K$$

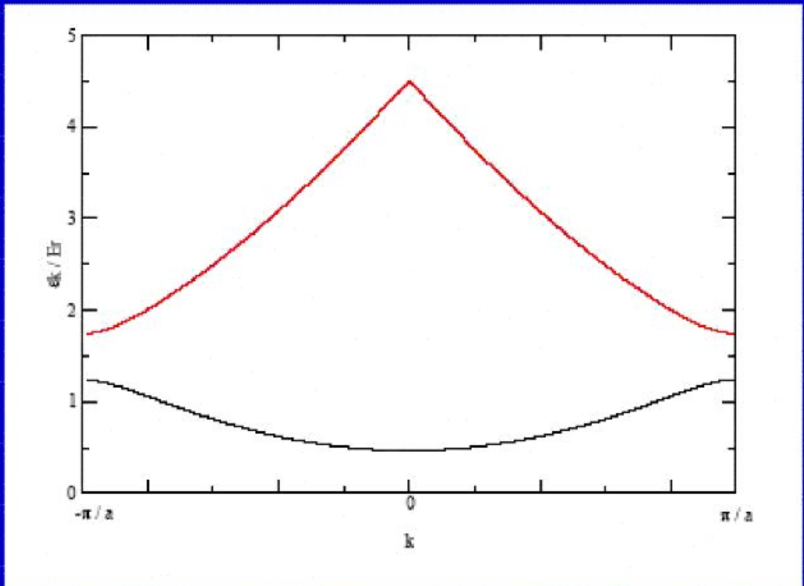
Pioneering article: Jaksch et al, PRL 81 (1998) 3108

Free-particle bands: from Bloch waves to Wannier functions

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

$$H_x \left|\psi_{nk}\right\rangle = \epsilon_{nk}\left|\psi_{nk}\right\rangle$$

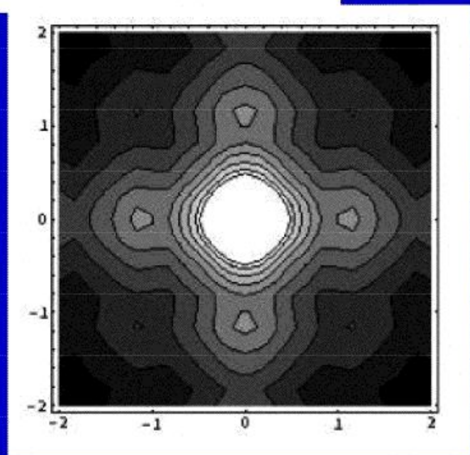
$$\psi_{nk}(x) = e^{ikx} u_{nk}(x)$$



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

Wannier function localised on lattice site R:

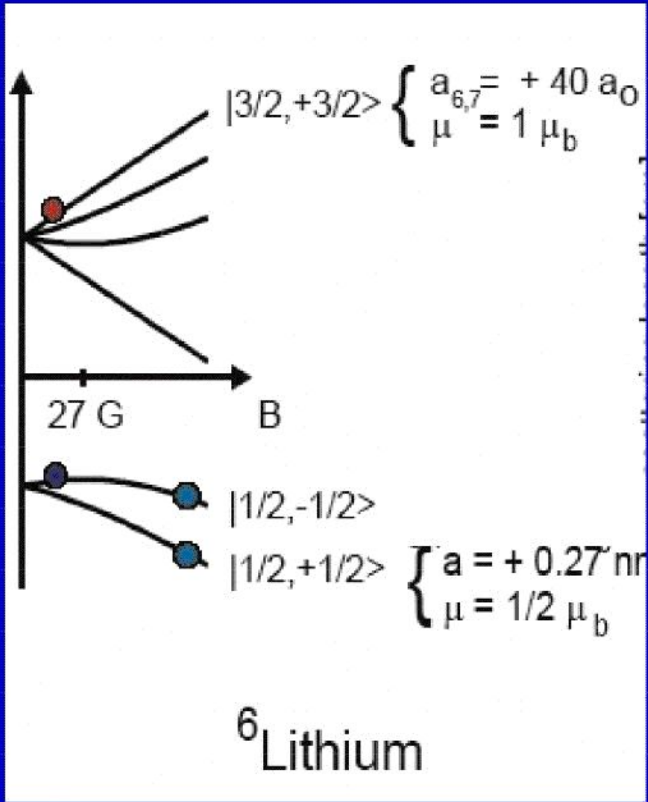
$$\left|W_{\vec{n},\vec{R}}\right\rangle = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}}\left|\Psi_{\vec{n},\vec{k}}\right\rangle$$



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

Interacting part of Hamiltonian:

Consider e.g ^{6}Li atoms in the 2 lowest hyperfine states

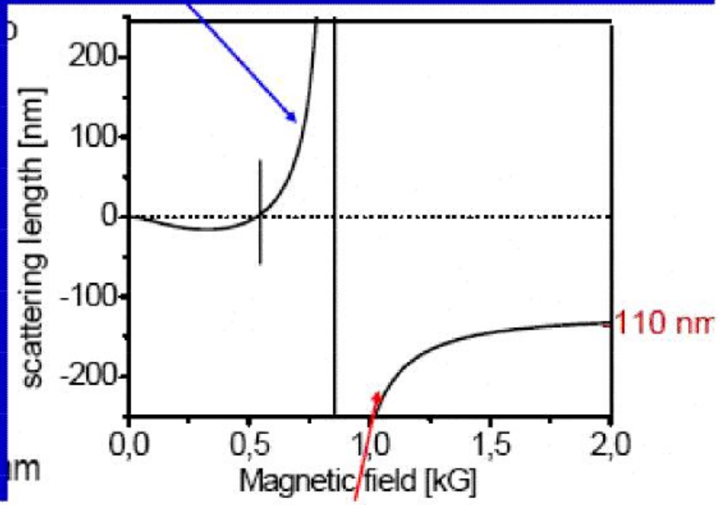


Pseudopotential approximation:

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

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

a_s: scattering length



Interaction in Wannier basis set:

Hubbard interaction
In 1st band

$$
\begin{aligned}
V &= g\int d^3\vec{r}\,\Psi^\dagger_\uparrow(\vec{r})\Psi_\uparrow(\vec{r})\Psi^\dagger_\downarrow(\vec{r})\Psi_\downarrow(\vec{r}) \\
&= g\sum_{\vec{R}_i,\vec{n}_i} c^\dagger_{\vec{R}_1,\vec{n}_1,\uparrow} c_{\vec{R}_2,\vec{n}_2,\uparrow} c^\dagger_{\vec{R}_3,\vec{n}_3,\downarrow} c_{\vec{R}_4,\vec{n}_4,\downarrow} \int d^3\vec{r}\, W_{\vec{R}_1,\vec{n}_1} W_{\vec{R}_2,\vec{n}_2} W_{\vec{R}_3,\vec{n}_3} W_{\vec{R}_4,\vec{n}_4}
\end{aligned}
$$

$$
\begin{aligned}
&= U\sum_{\vec{R}} n_{\vec{R},1,\uparrow} n_{\vec{R},1,\downarrow} + U_2 \sum_{\vec{R},\alpha} n_{\vec{R},2\alpha,\uparrow} n_{\vec{R},2\alpha,\downarrow} \\
&\quad + \sum_{l,l'} V_{l,l'}\left(n_{l,\uparrow} n_{l',\downarrow} + c^\dagger_{l,\uparrow} c^\dagger_{l,\downarrow} c_{l',\downarrow} c_{l',\uparrow} - c^\dagger_{l,\uparrow} c_{l,\downarrow} c^\dagger_{l',\downarrow} c_{l',\uparrow}\right) \\
&\quad + V_{vois} \sum_{\vec{R},\vec{R}',\sigma} n_{\vec{R},-\sigma}\left(c^\dagger_{\vec{R}',\sigma} c_{\vec{R},\sigma} + \text{h.c.}\right)
\end{aligned}
$$

Hopping-like term (small ?)

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

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

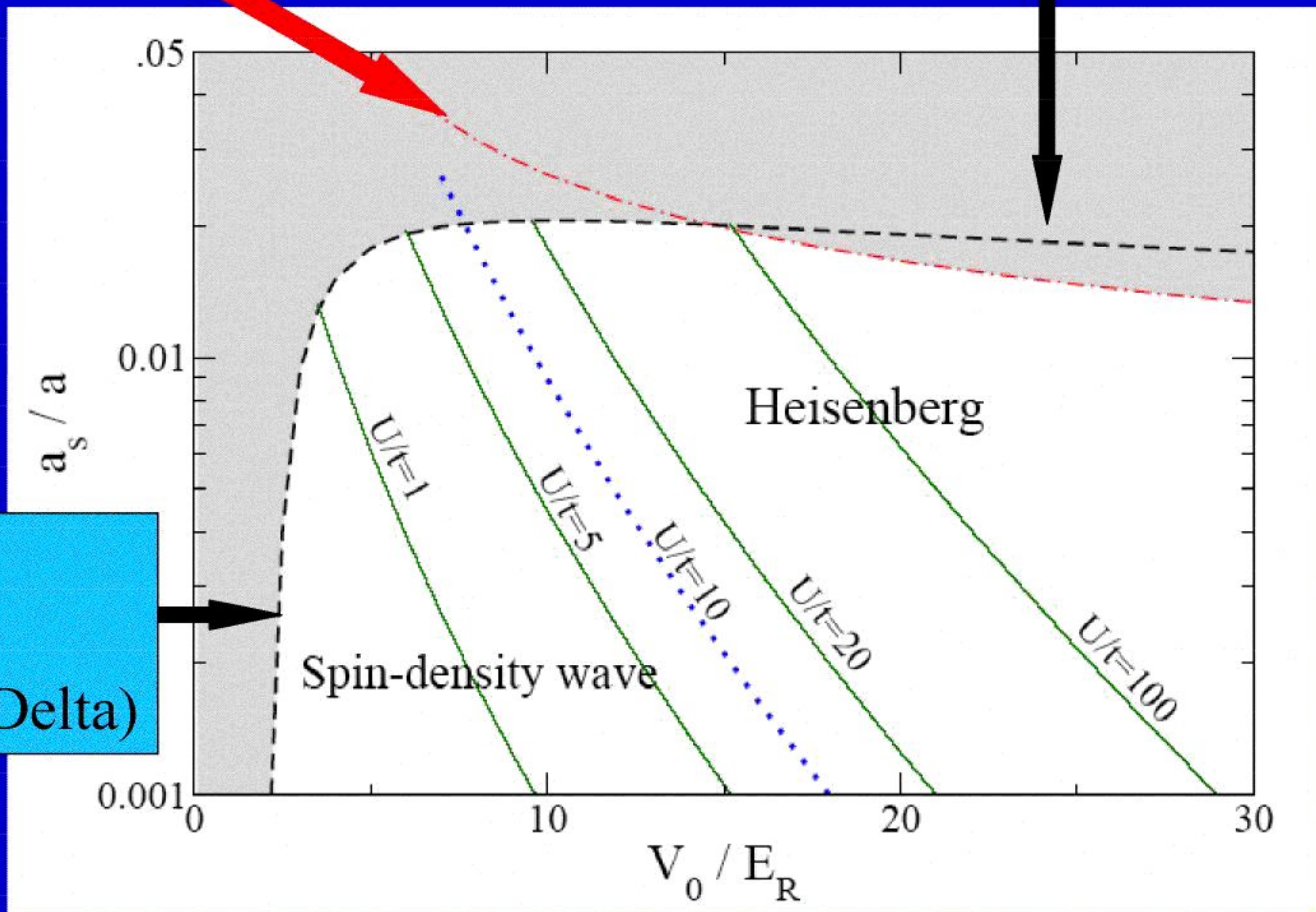
$$V_{vois} = g\left(\int w_1(x)^3 w_1(x+a) dx\right)\left(\int w_1(x)^4 dx\right)^2$$

Region of validity of controlled 1-band Hubbard:

Hopping-like interactions set in

Pseudo-potential fails (must have $a_s < l_{h.o}$)

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



2^{nd} band Well-separated (must have U<Delta)

cf. F.Werner, O.Parcollet, A.G and S.R. Hassan cond-mat/0504003 (PRL in press)

Hoppings and couplings…

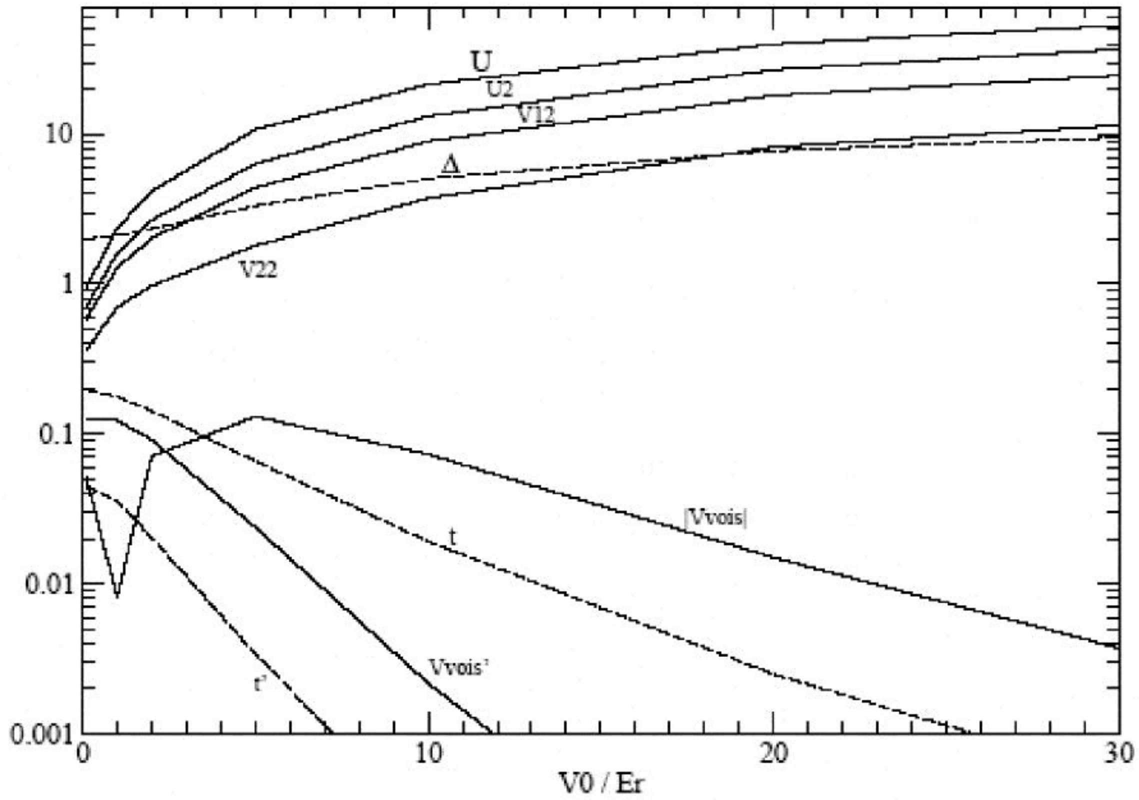
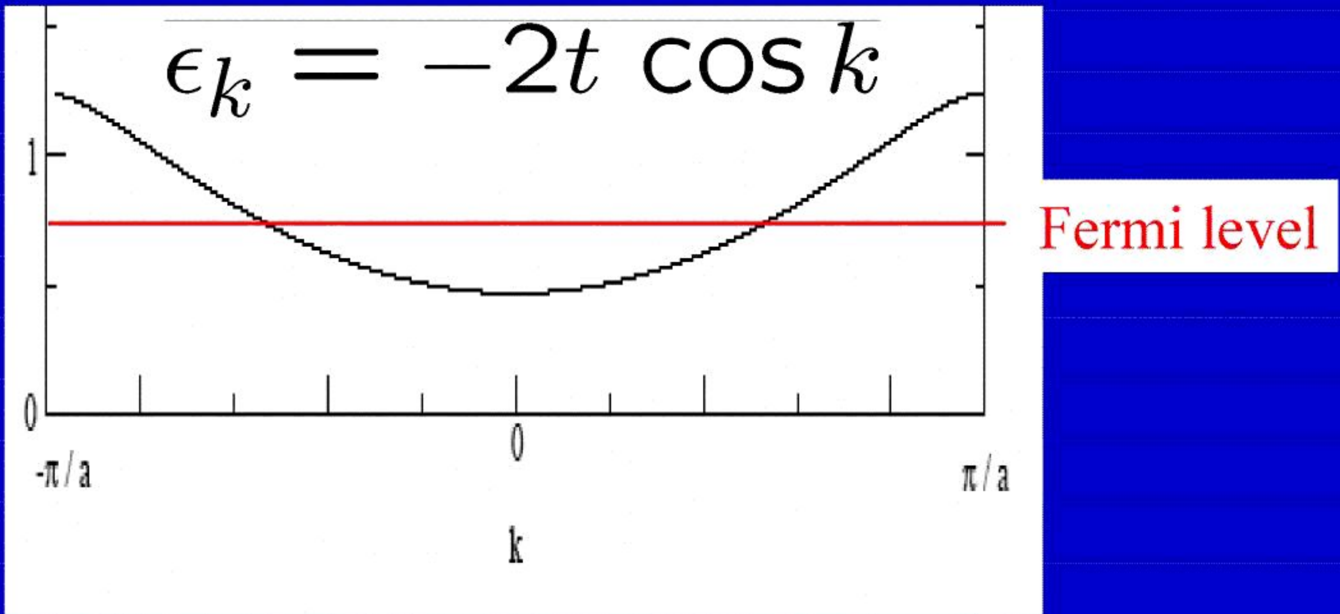


FIG. 13 – Coefficients du Hamiltonien dans la base de Wannier, en fonction de la profondeur du potentiel V_0/Er. Les coefficients t,t' et Δ (traits pointillés) sont expimés en unités de E_r, tandis que les coefficients de l'interaction U,U_2 etc. (traits pleins) sont en unités de $E_r\, a_s/a$.

The **Mott phenomenon** is a key to the properties of correlated materials

Consider, for simplicity, one particle per site

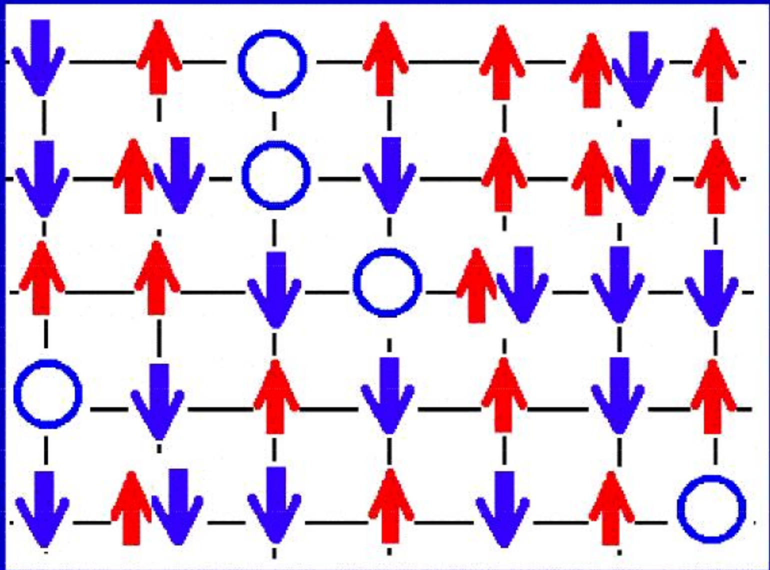
When U=0: half-filled band > METAL



Metallic (conducting) state:

* **Real-space** picture is complicated !

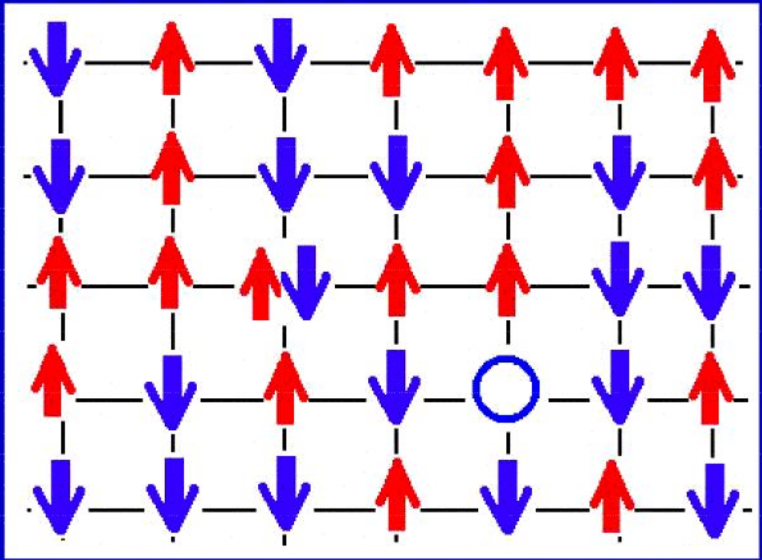
(Many holes and double occupancies)



* **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

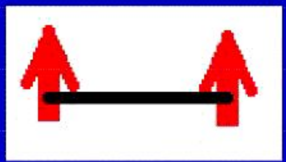
Real-space picture is simple: mostly singly-occupied sites

NOTE: At large U, Mott localisation has nothing to do with spin ordering. Gap for charge motion ~ U.

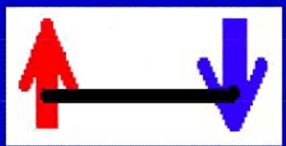
However, at low-T, long-range spin order will (in most cases…) set in, at a critical temperature T_c

For $T_c<T<U$: ~ 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

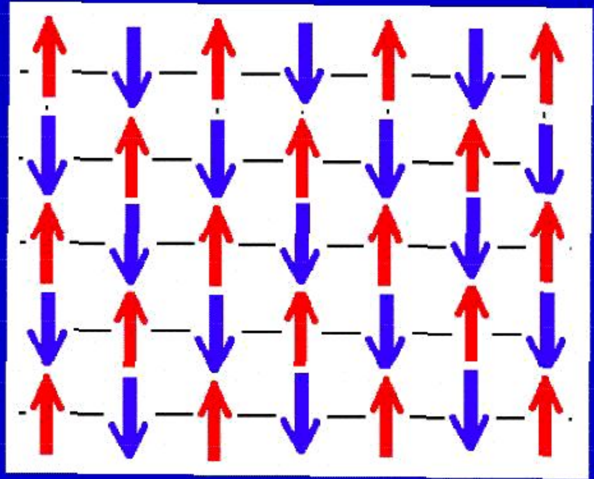
Inter-site **antiferromagnetic** exchange:

$$J_{AF} = \frac{4t^2}{U}$$

What does the Mott insulating **ground-state** look like ?

Above cartoon of Mott insulator was a random spin configuration >> cannot be the ground-state !

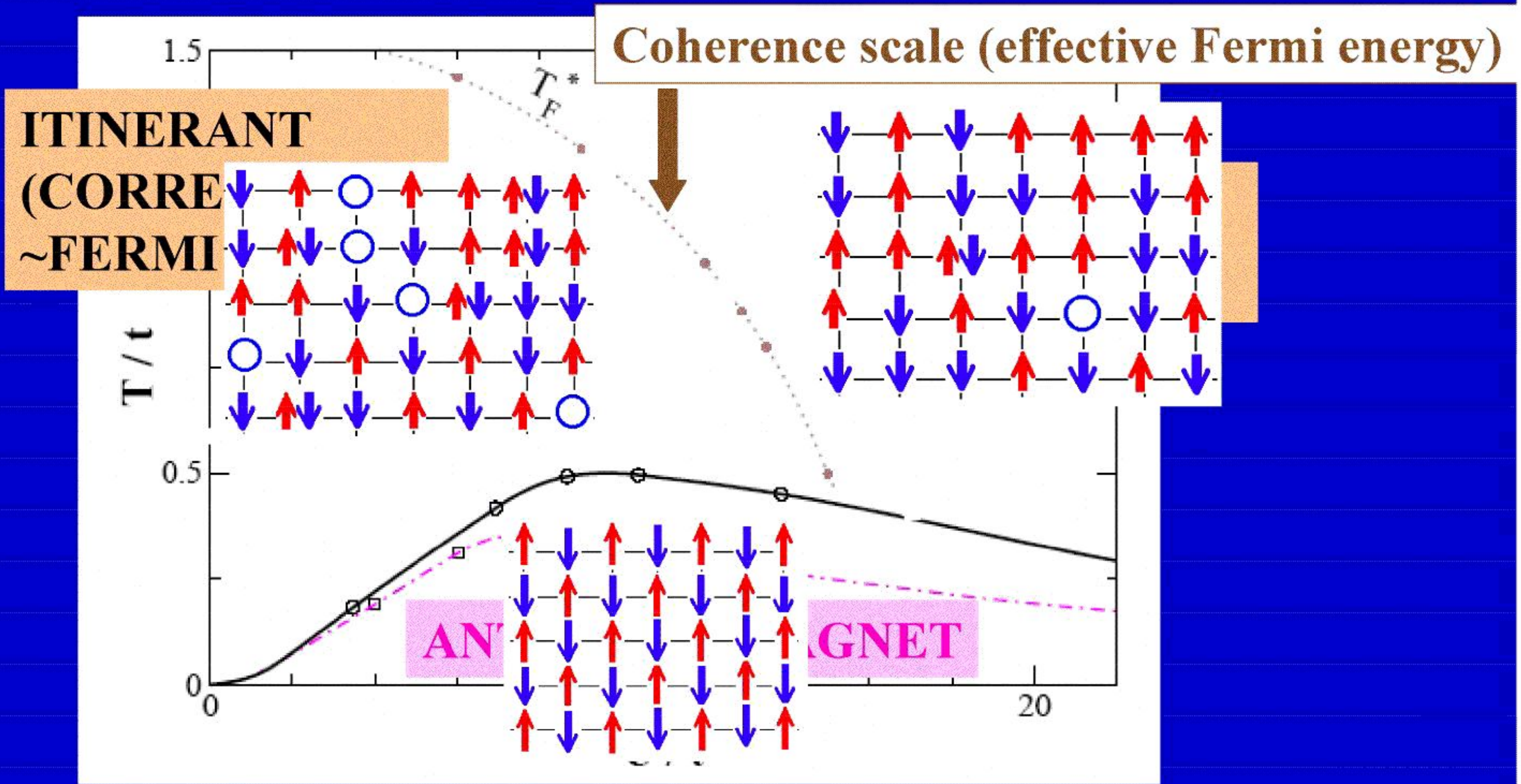
* Simplest possibility is a Néel-like antiferromagnet:



(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 …

The phase diagram at ½-filling (3D case)



Critical boundary calculated for a 3D cubic lattice using:

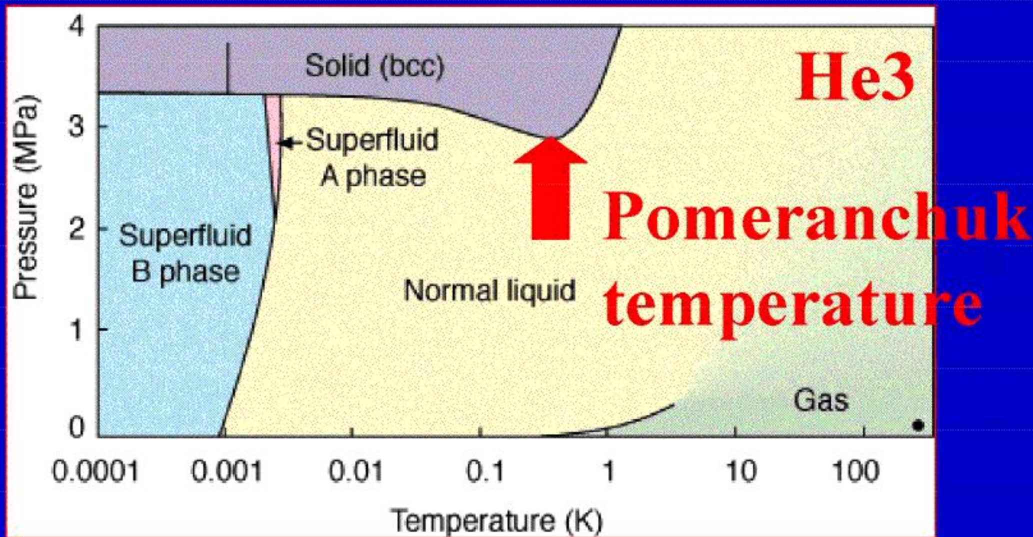
-Quantum Monte Carlo (Staudt et al. Eur. Phys. J. B17 (2000) 411)

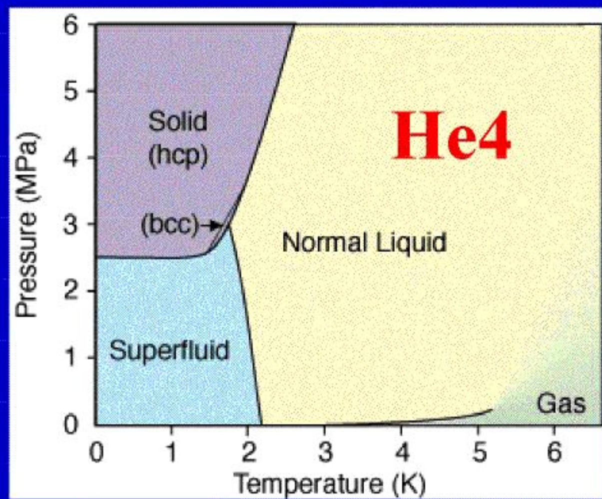
- Dynamical Mean-Field Theory approximation

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:

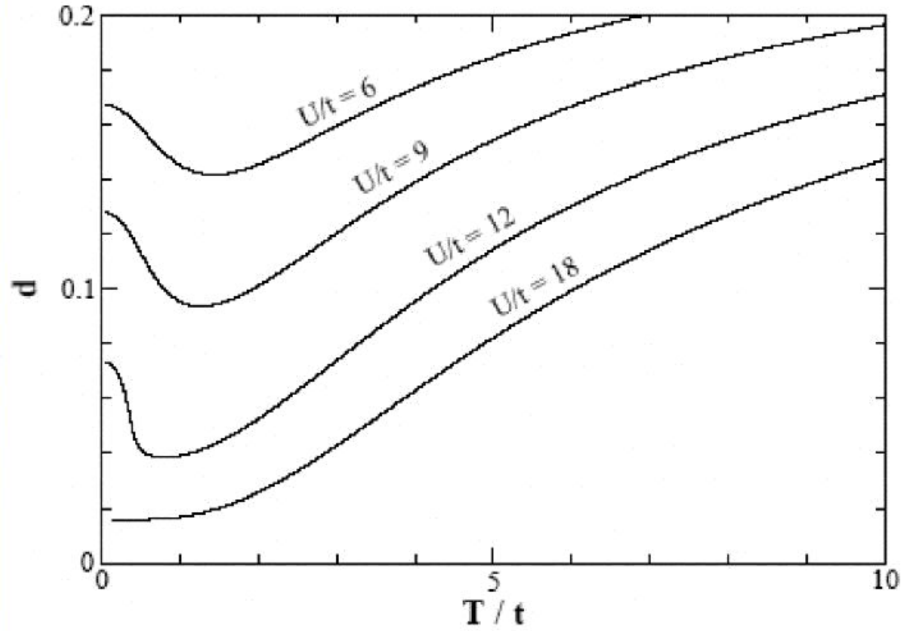


FIG. 2: Double occupancy $d = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ as a function of temperature, for several values of U/t, calculated within DMFT(IPT). The initial decrease is the Pomeranchuk effect responsible for adiabatic cooling.

$$d = \langle n_\uparrow n_\downarrow \rangle$$

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

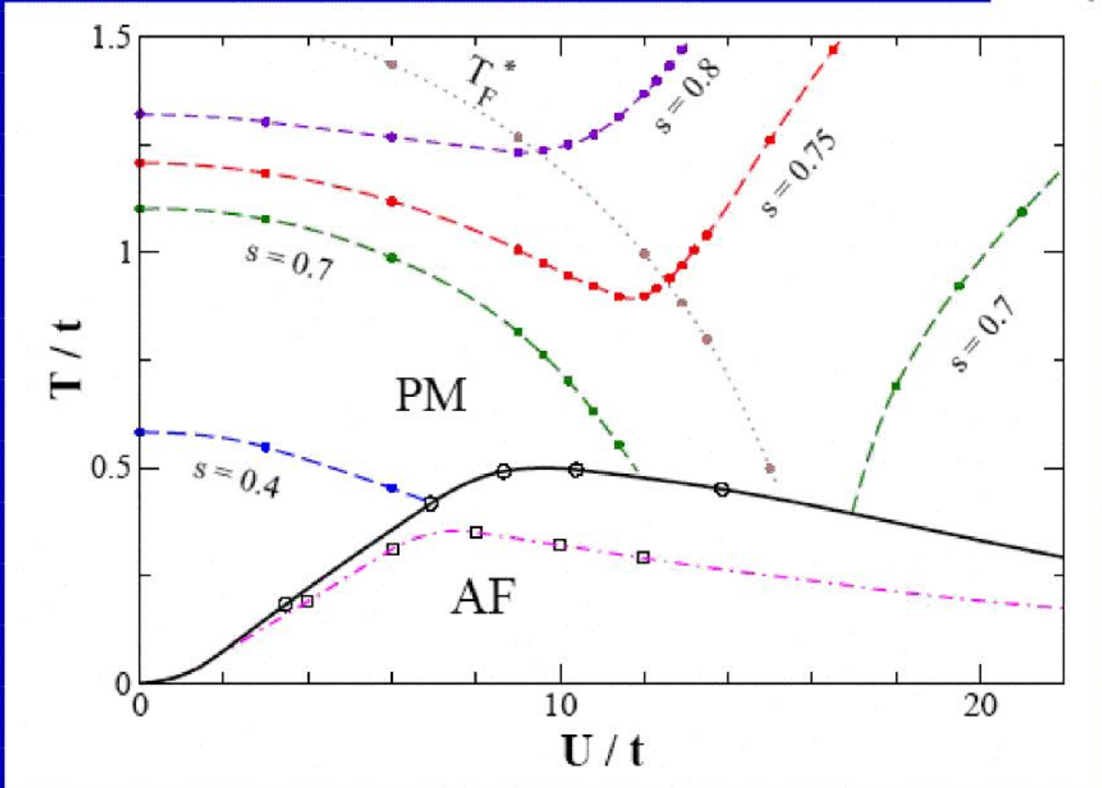
cf. A.G&W.Krauth, PRL 1992

Shape of the isentropic curves:

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

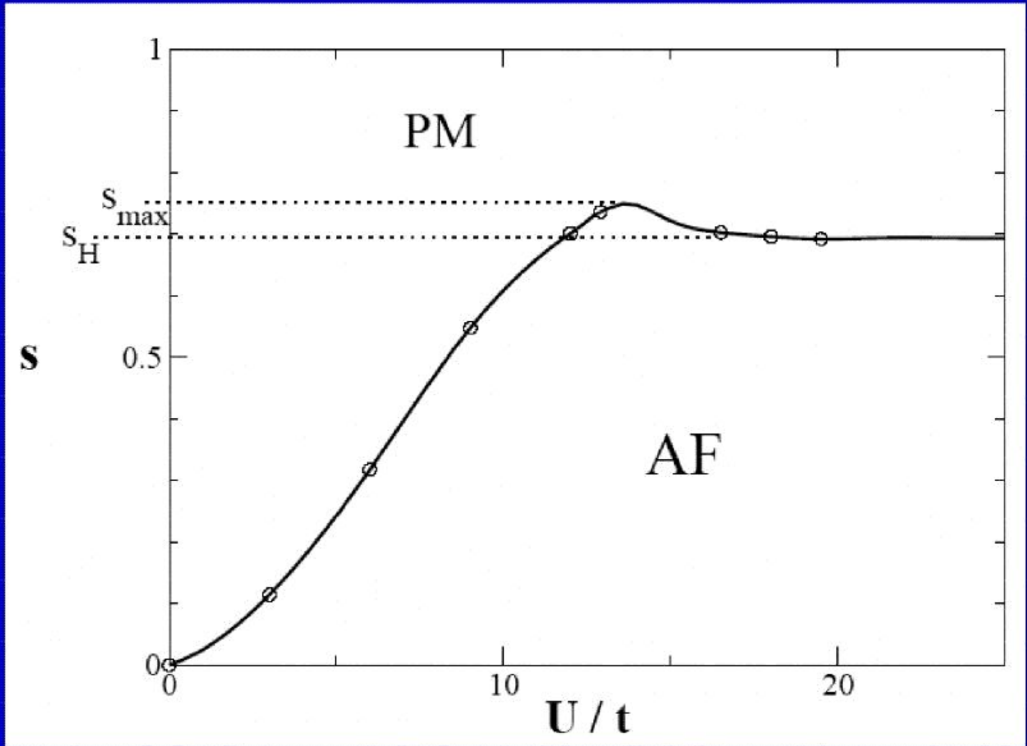
Hence the isentropicsTi(U) obey: $$c(T_i)\,\frac{\partial T_i}{\partial U} = T_i\,\frac{\partial d}{\partial T}\Big|_{T=T_i}$$

< 0 when d(T) decreases



Isentropic curves of the ½-filled Hubbard model (calculated using the dynamical mean-field theory approximation)

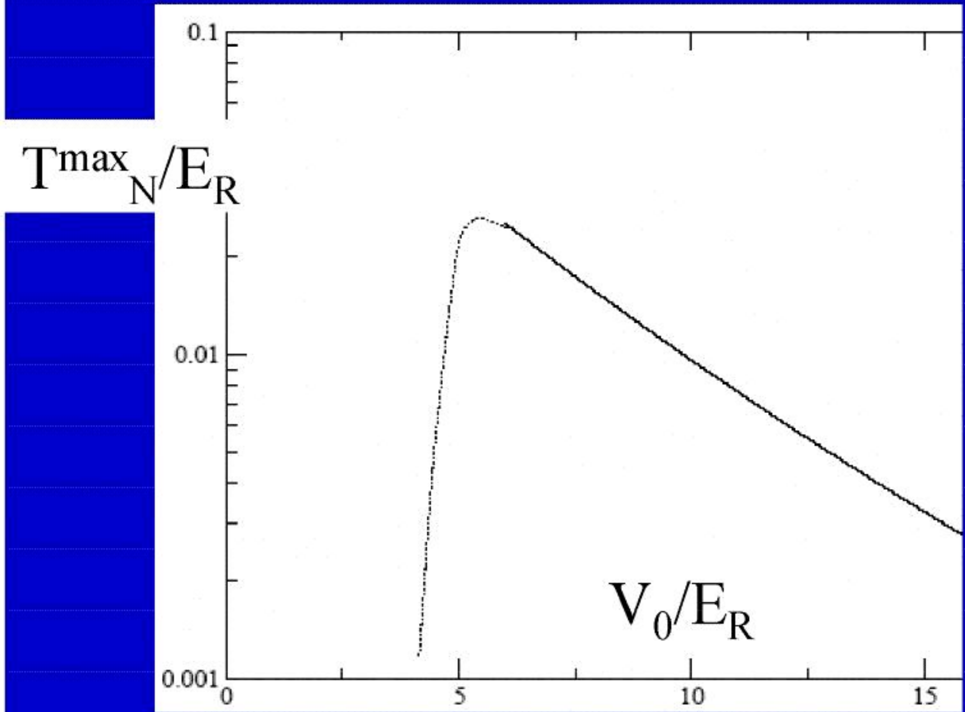
Using entropy as a thermometer:



Reach the antiferromagnetic phase by adiabatic cooling ?

Note: for typical parameters $\hbar/t \simeq .5\text{ms}$, $\hbar/J_{AF} \simeq 2\text{ms}$

Let us put in some numbers…



The Neel temperature in the lattice is never larger than $\sim 0.015\ E_R$, i.e about 10 nK

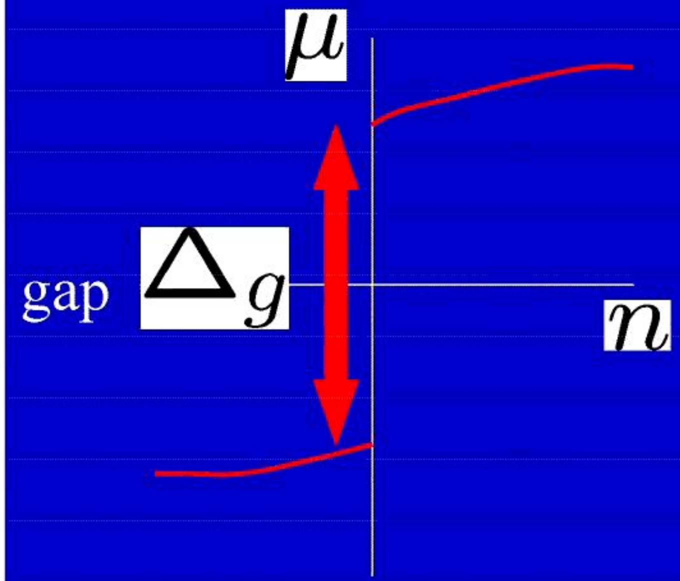
Typical Fermi energy in the ENS 6Li experiment is 10μK,
So it **seems** we would need to reach TF/1000 or so… a daunting task !

However, in fact what we need to achieve is to cool the gas down to a temperature corresponding to an entropy smaller than S_H per particle, i.e down to $s_H{}^*T_F/\pi^2$, i.e of order $T_F/30$, and then turn on lattice adiabatically.

DONT GET TOO CLOSE TO RESONANCE (no longer simple Hubbard)

Effect of the non-uniform trapping potential :

Mott state is **incompressible:**



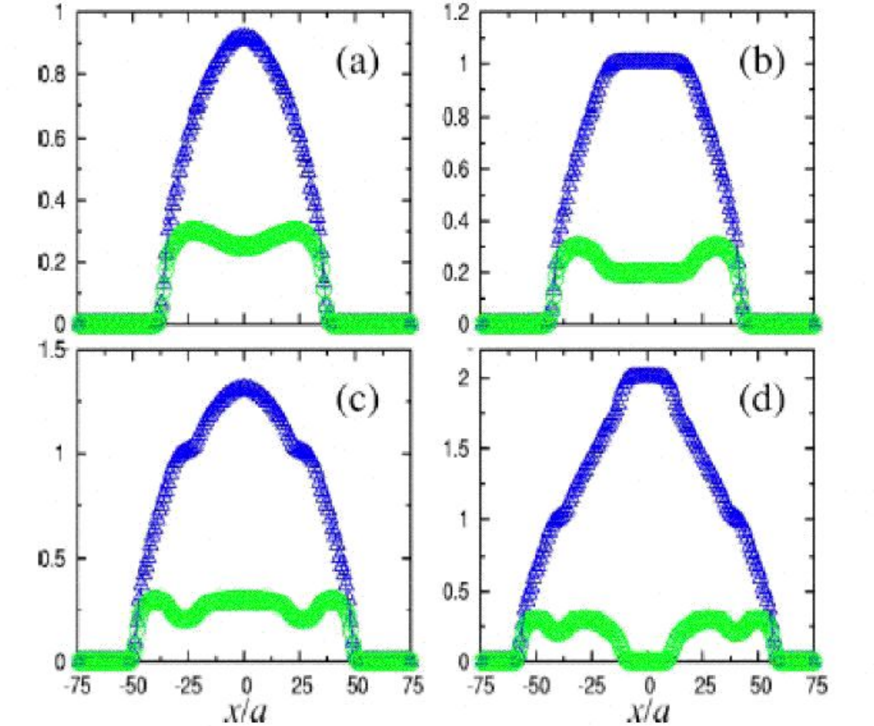


FIG. 2. (Color online). Four density profiles (△) (cuts across Fig. 1) and their variances (○). The fillings are N_f=50 (a), 68 (b), 94 (c), and 150 (d).

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

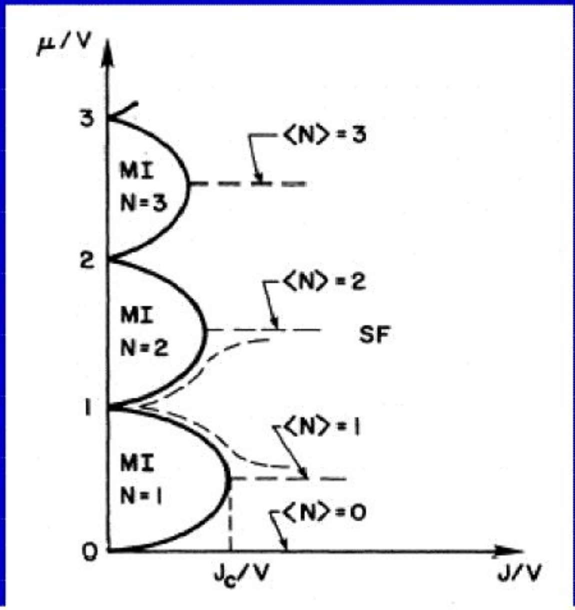
Rigol and Muramatsu, Phys Rev A 2004

A technical remark: mean-field theories of the Mott phenomenon are easier for bosons than for fermions !

Bosons:

$$-t\sum_{ij} b_i^\dagger b_j + U\sum_i n_i(n_i-1)$$

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



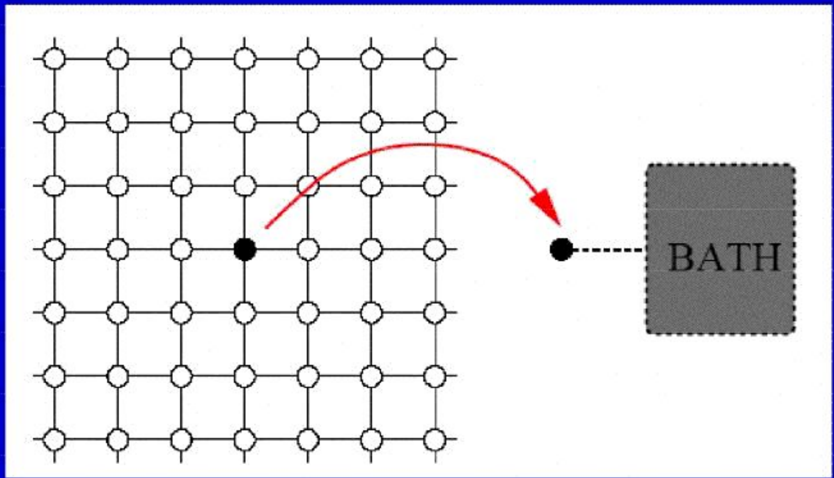
Krauth et al., Ramakrishnan et al, Fisher et al., 90's

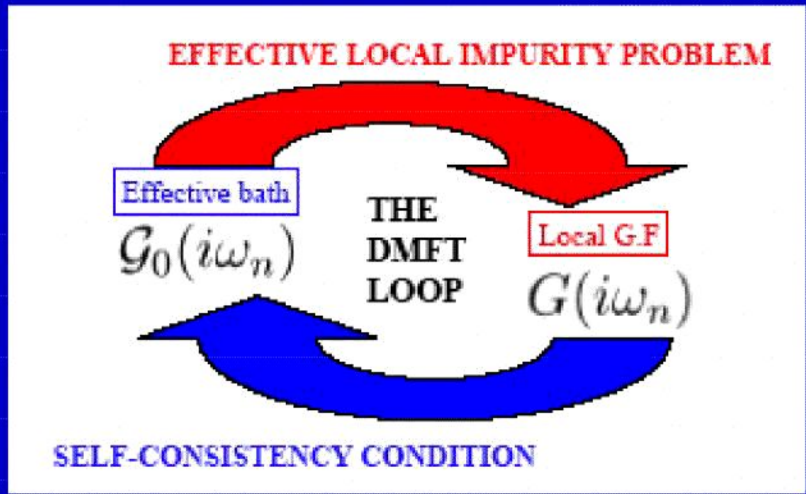
Not a viable route for fermions !
(<c> not an order parameter of
Either metal or superconductor)

Fermions: Dynamical Mean-Field Theory

cf Rev. Mod. Phys. 68 (1996) 13

& Physics Today, 2003

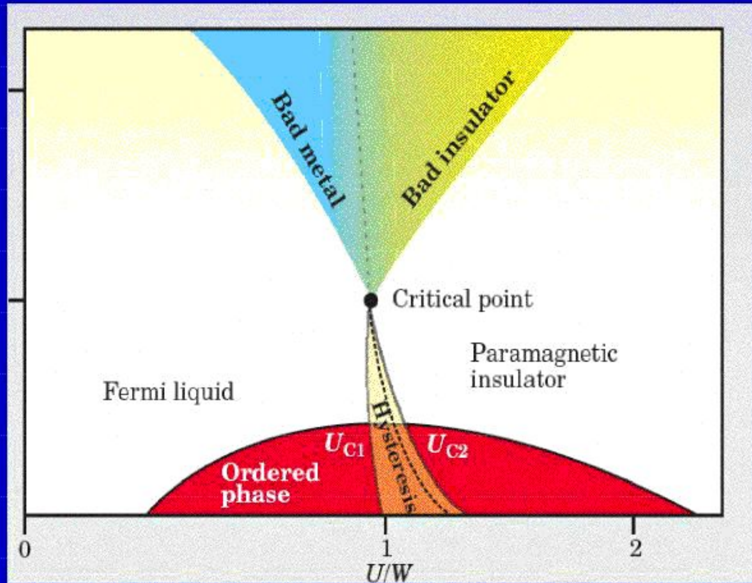




$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^+(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_\sigma(\tau') + U \int_0^\beta d\tau\, n_\uparrow(\tau)n_\downarrow(\tau)$$

II. 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)

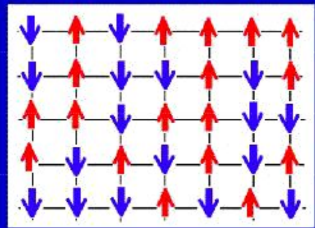


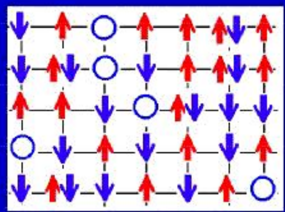
In solid-state context: the crystal lattice reacts to the electronic instability e.g lattice spacing is discontinuous through the transition (but same crystal symmetry)

Critical behaviour at the Mott critical endpoint

A liquid-gas transition ? Simple picture:

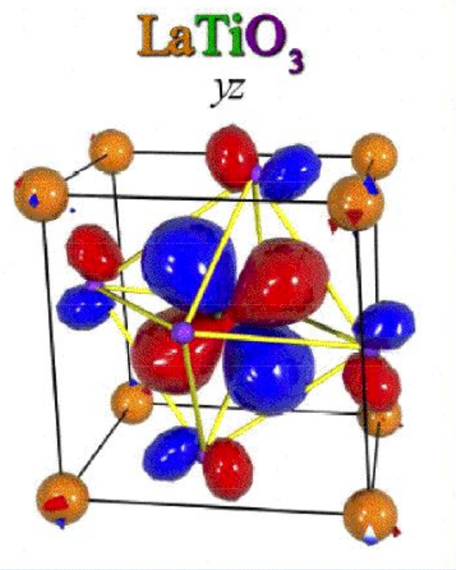
Insulator:
low-density of doubly occupied sites
➡ GAS





Metal:
High-density ➡ LIQUID

Hubbard model	Mott MIT	Liquid-gas	Ising model
$(t/U) - (t/U)_c$	$p - p_c$	$p - p_c$	Field h
$T - T_c$	$T - T_c$	$T - T_c$	Distance to cr. pt.
Low-ω spectral weight	id.	$v_g - v_L$	Order parameter (scalar)



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

$$U \sim \int dr dr' |W_i(r)|^2 V^{int}_{\mathbf{screened}}(r - r')|W_i(r')|^2$$

>> Narrow bandwidths (small kinetic energy)

What do real (strongly correlated) solids do ?

A material poised close to the Mott instability: V_2O_3

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

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

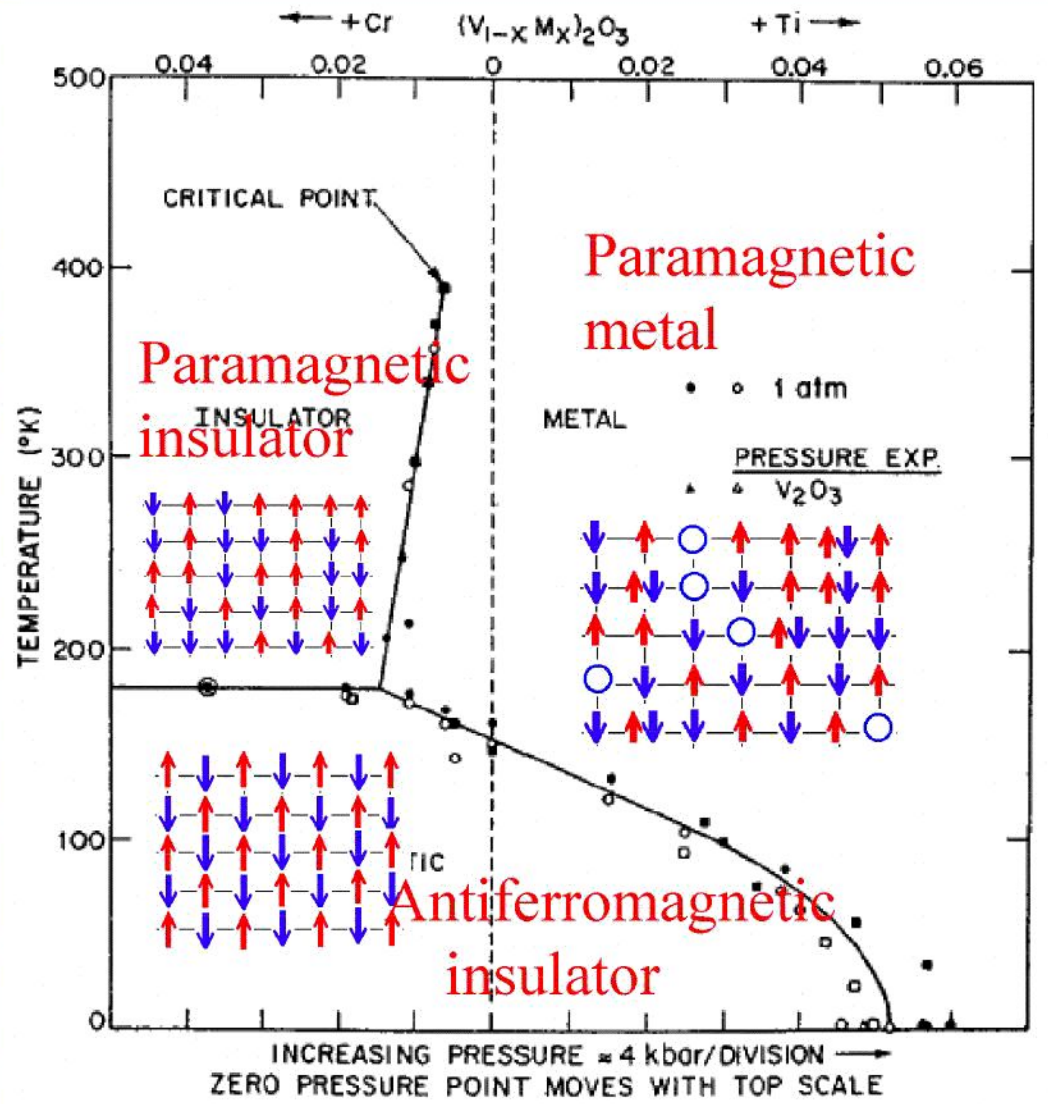
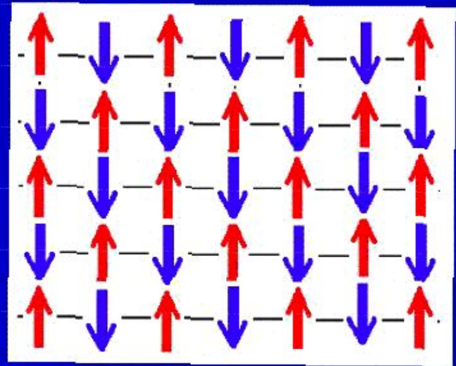


FIG. 70. Phase diagram for doped V_2O_3 systems, $(V_{1-x}Cr_x)_2O_3$ and $(V_{1-x}Ti_x)_2O_3$. From McWhan *et al.*, 1971, 1973.

III. Possible “exotic'' ground-states of the Mott insulator

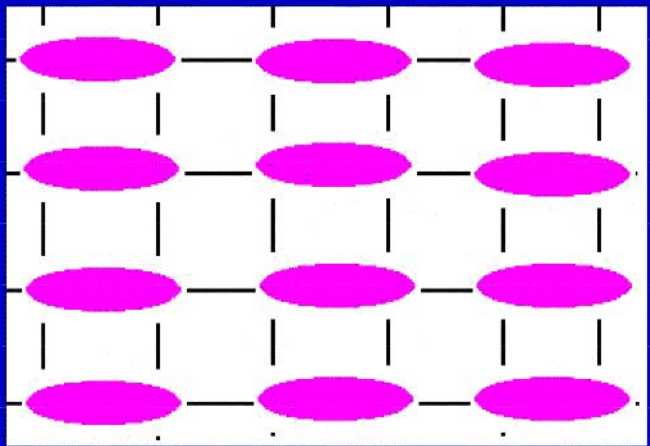
How can one avoid conventional antiferromagnetic long-range order ?



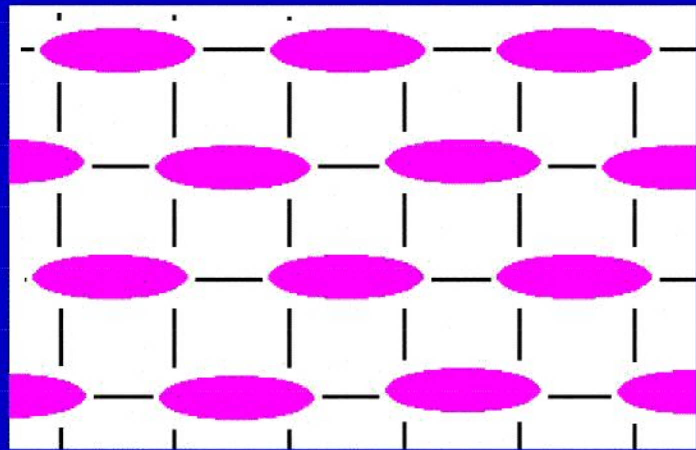
>>> Strong quantum fluctuations
>>> Many classically degenerate ground-states
>>> Frustration
>>> Low dimensionality

Valence bond states

- Valence bond CRYSTALS:



columnar



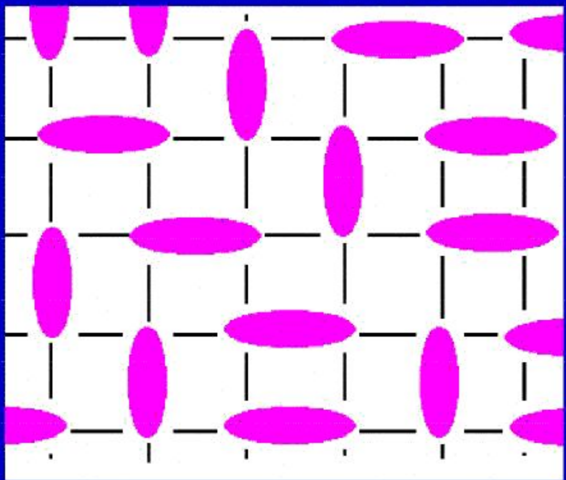
staggered

Symmetry breaking: spins=NO

translation = YES

Resonating valence bond states (RVB)

Wave function= superposition of many dimer coverings by singlets

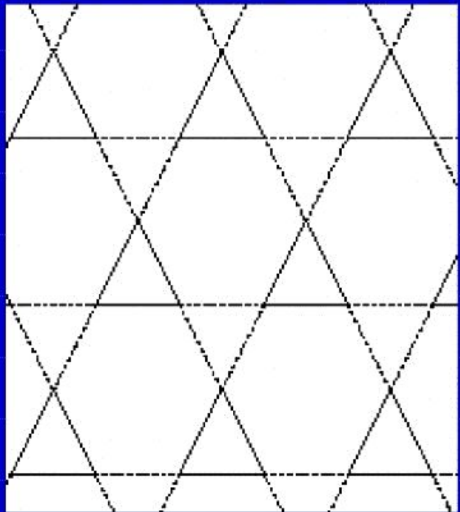


+ … (many)

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

~ Giant benzene molecule

Example of RVB state: The Kagome quantum antiferromagnet



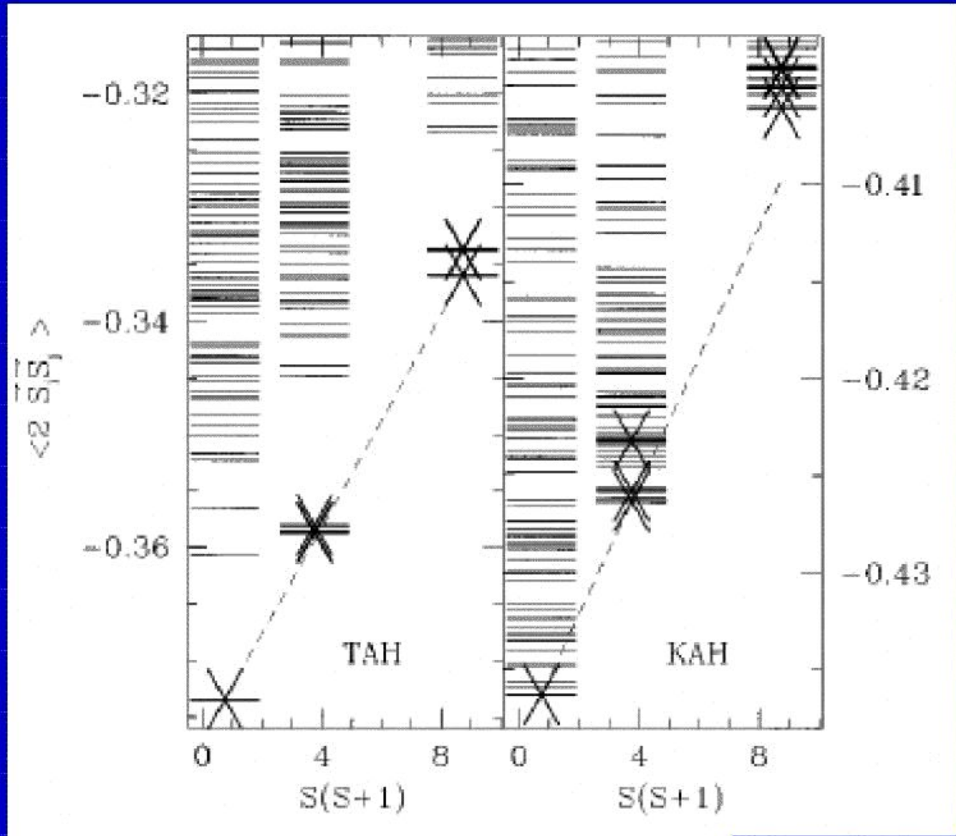


FIG. 2. The low-lying energy levels of the TAH and KAH spectrum of the $N=27$ sample. The levels which possess the symmetry expected for an ordered solution are denoted by a star. The Pisa tower of the TAH is easily seen, quite distinct from the first-magnon excitations. In the KAH, on the contrary, the levels candidate for the building of a tower of states are mixed with other representations in a continuum of excitations.

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

[Santos et al. Phys Rev Lett 93 (2004) 030601]

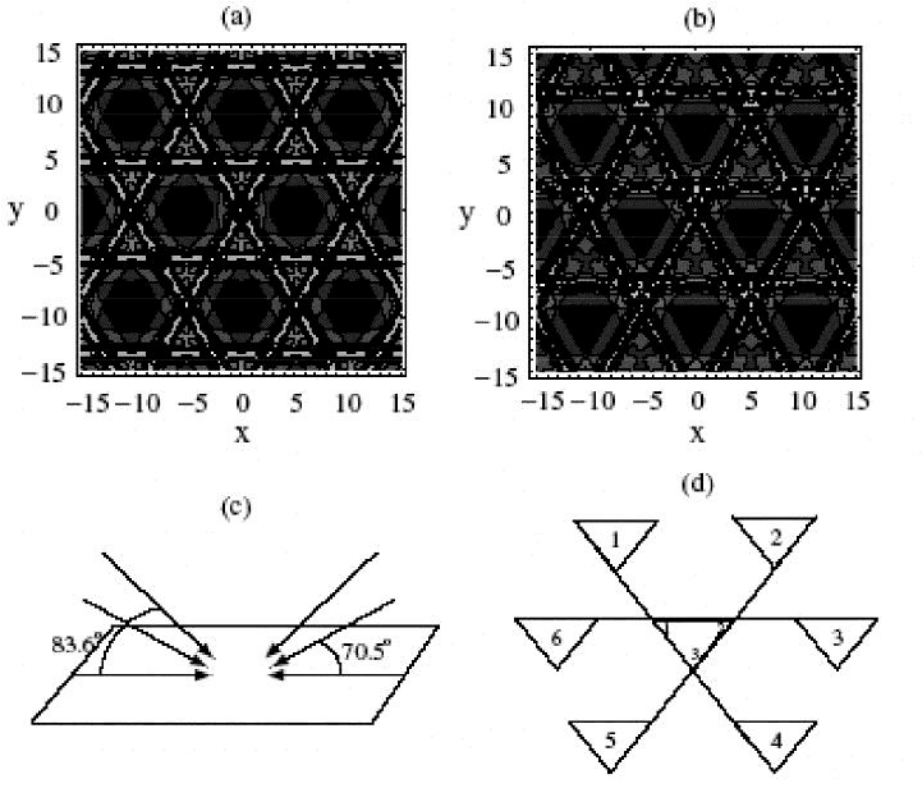


FIG. 1. (a) Ideal Kagomé lattice for $\phi = \pi/2$. (b) TKL using $\phi = \pi/4$. This lattice can be generated using three SWs with a $\pi/3$ angle between themselves. Each SW is generated by three lasers with a configuration shown in (c). (d) Enumeration of spins in a trimer and of neighboring trimers.

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

Anisotropic Heisenberg model:

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

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 ?

Conclusion, **perspectives …**

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 ''