ATOMS IN OPTICAL LATTICES II : SPIN-1/2 LATTICE GASES

* Up to now we have discussed only about Bose gases in optical lattices. Using a similar reasoning as in p. (24) we may introduce the Fermi-Hubbard Hamiltonian for spin-1/2 fermions:

$$\hat{H} = -t \sum_{\langle ij \rangle} \sum_{s=\uparrow\downarrow} c_{is}^{+} c_{js} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

← where now the c_{is} operators obey anticommutation rules.

* The discussion of the fermionic case is complicated by the spin degrees of freedom. What we mean here by spin-1/2 is actually a two-component Fermi gas formed by fermions in two different hyperfine states.

* As for the bosonic case, we still consider that we limit ourselves to the lowest band physics. If we had a single-component Fermi gas, this would mean that we wouldn't be able to put more than 1 fermion per site (Pauli exclusivity). Actually a state with 1 fermion in all sites is a band-insulator → i.e. the lowest band would be completely filled in that case.

[Note: Actually the Pauli exclusion makes the lowest-band approximation more tricky for fermions, since e.g. a too-dense Fermi gas cannot live in a single band if the average filling surpasses 1 (for a single-component Fermi gas).]

* On the contrary, if we have a 2-component Fermi gas, then we may have up to two particles per site, one ↑ and one ↓. This two particles may interact, and this amounts for the interaction term, with the coupling constant U.

[Note: A single-component Fermi gas do not present s-wave interactions due to Pauli exclusion. Hence at very low temperatures we may consider such a gas as ideal. A different situation occurs when the system presents long-range interactions, which allow for inter-site interactions. In that case, single-component Fermi gases may present also a Mott physics as that discussed below. We'll see later long-range interactions.)

* In a two-component Fermi gas we will have a band insulator if we have a filling factor 2 per site. In addition we may have, as for the bosonic case, a Mott-insulator with one fermion per site if the strong on-site repulsion (U) overcomes the kinetic energy (i.e. the hopping) and makes it unfavourable for the particles to form an itinerant (metallic) state.

* From the point of view of band theory, we would have a metal, with one atom per unit cell and a half-filled band. Instead for large-enough values of U/t, a Mott-insulating state with a charge (i.e. density) gap develops. Up to now this is similar as the bosonic case, i.e. it is purely charge (i.e. density) physics, and the spin degree of freedom does not play a major role (apart from allowing for 2 particles per site).

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* Before going into spin, let's point out that the Mott-metal transition has been already observed experimentally some years ago, in the group of T. Esslinger at ETH [R. Jördens et al., Nature 455, 204 (2008)] and in the group of I. Bloch at Mainz [U. Schneider et al., Science 322, 1520 (2008).] [see (37), (39) and (39'')] ←

* The group of Bloch measured directly the compressibility of the gas (recall that a Mott-insulator is incompressible), whereas Esslinger's group studied double-occupancy in the lattice.

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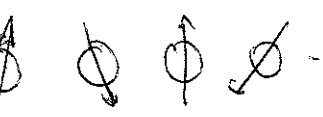
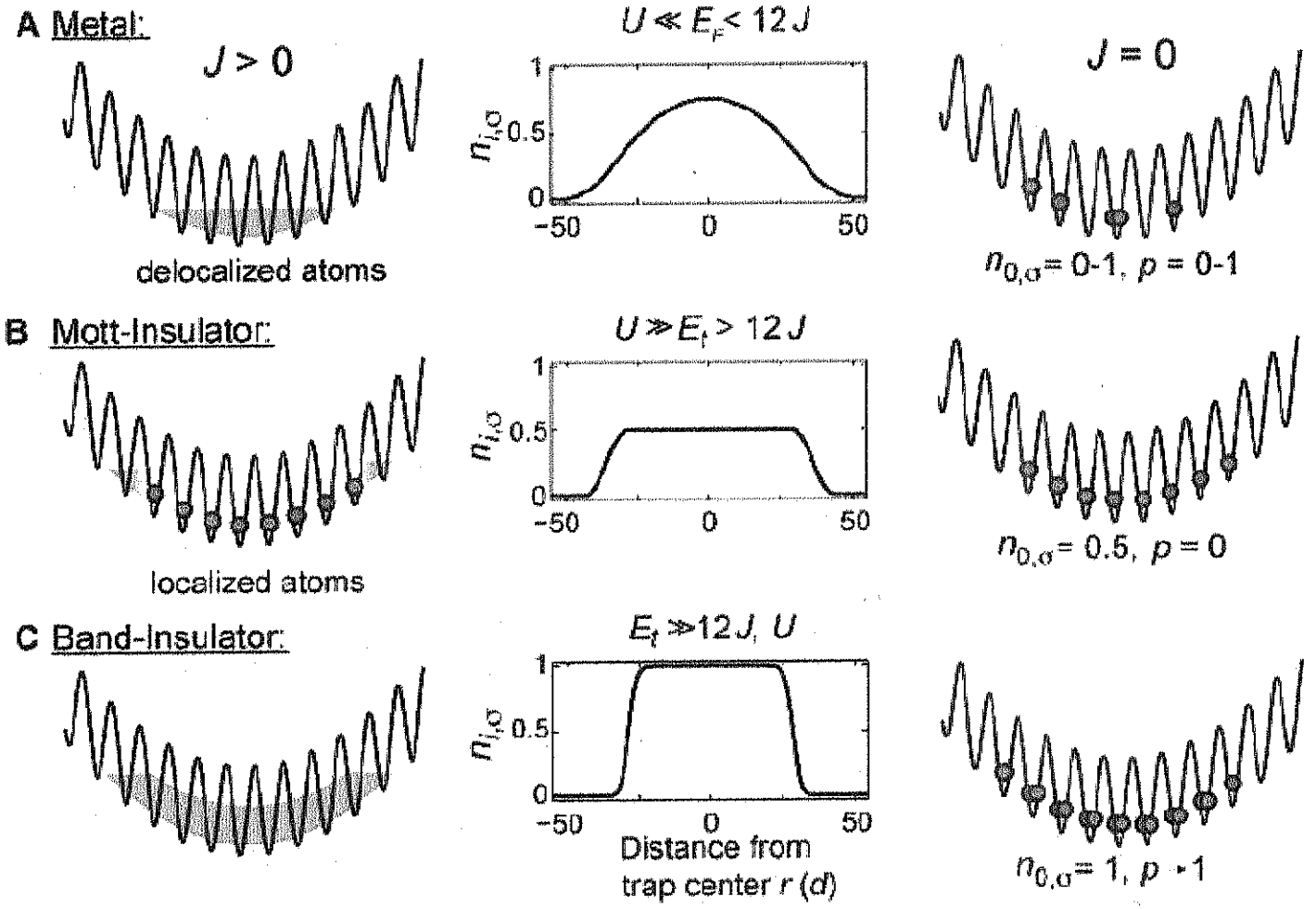
* But, as mentioned above, the charge (i.e. density) physics is just one half of the problem. The "naive" Mott insulating state has in principle a huge spin entropy, being a paramagnet in which the spin of the atom located at a given site can point in either direction. This huge degeneracy must be lifted as one cools down the system (recall the 3rd principle of thermodynamics!)



Mott-Metal transition [Schneider et al., Science 322, 1520 (2008)]



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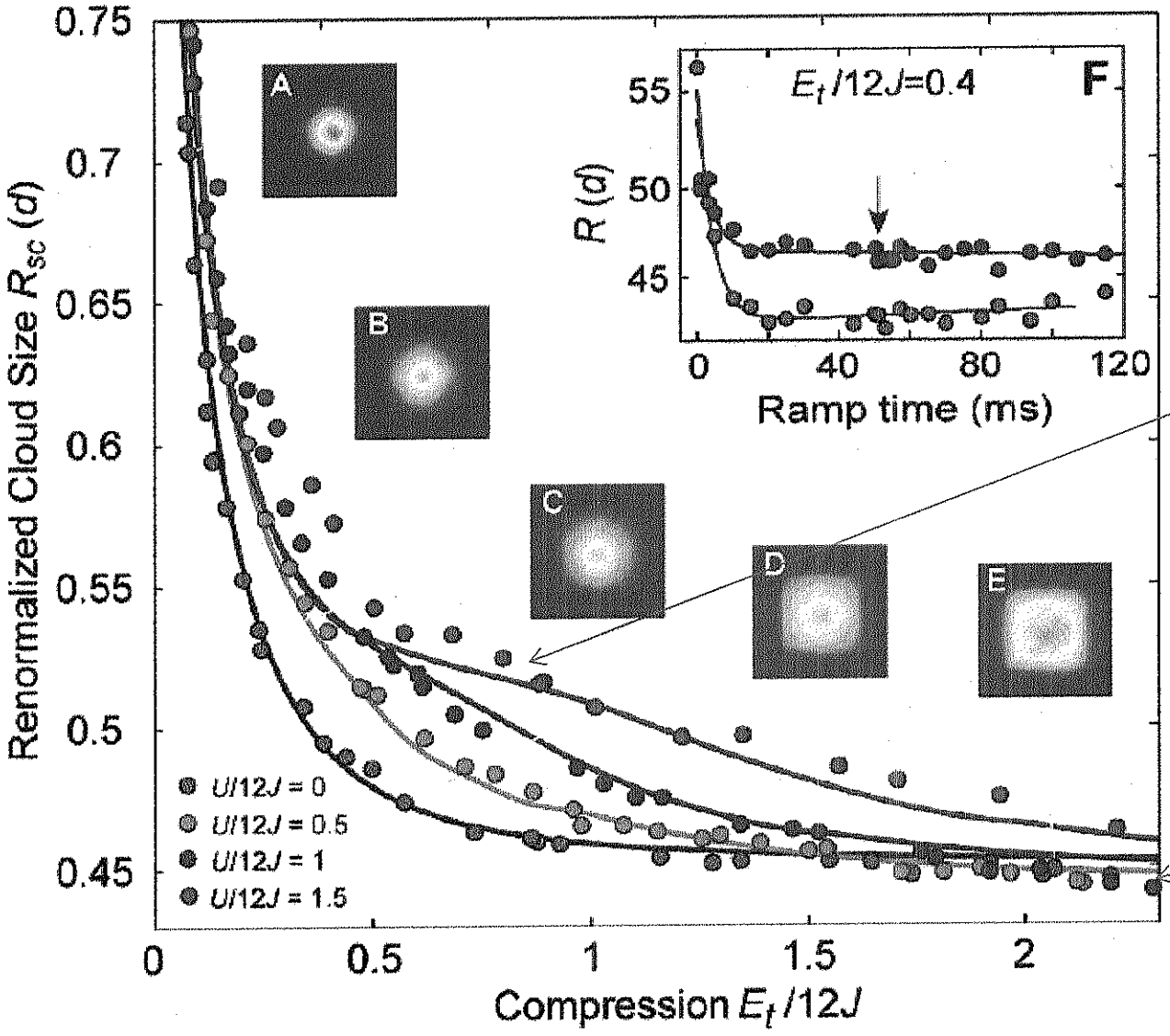
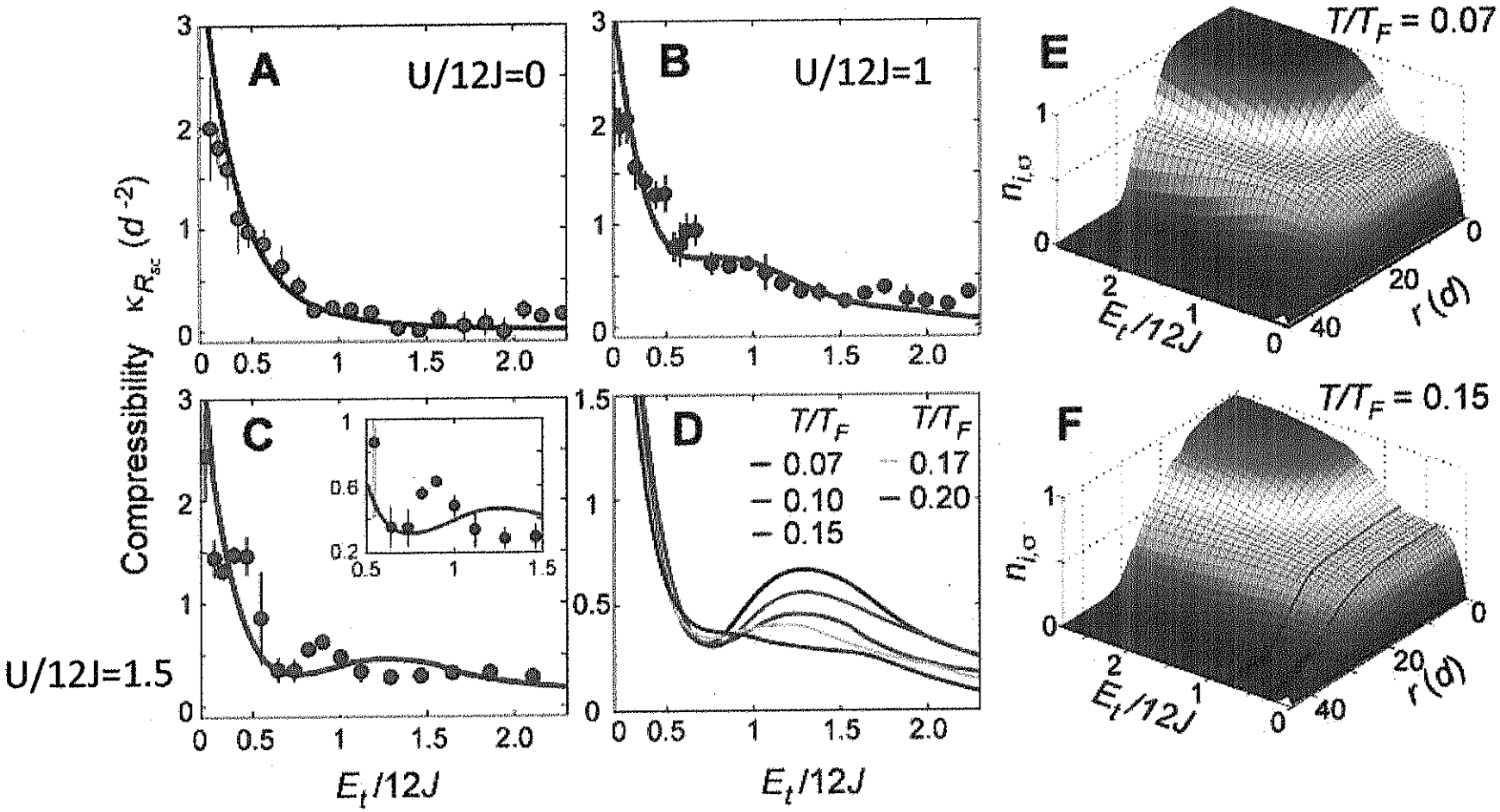


Mott-Metal transition [Schneider et al., Science 322, 1520 (2008)]



* SUPER-EXCHANGE : HEISENBERG HAMILTONIAN

* What happens with the spin degree of freedom depends on the details of the model and of the residual interactions between the spin degrees of freedom. As we will see now, in the simplest case of a 2-component Fermi gas in a bipartite lattice, the spins order into an anti-ferromagnetic state (Néel state).

* This is easily understood in strong coupling $U \gg t$ by introducing Anderson's superexchange mechanism.

Let's consider two sites $i = 1, 2$. The Fermi-Hubbard Hamiltonian is of the form:

$$H = H_0 + H_1$$

with $H_0 = U \sum_i n_{i\uparrow} n_{i\downarrow}$

and $H_1 = -t \sum_s (c_{1s}^\dagger c_{2s} + c_{2s}^\dagger c_{1s})$

For large U/t, we choose H_0 to be our zeroth-order Hamiltonian, whose ground-state manifold is four-fold degenerate:

$$|0\rangle = |s_1, s_2\rangle \; ; \quad s_i = \uparrow, \downarrow \; ; \quad i = 1, 2$$

The energies of the doubly occupied orbitals are higher by U than the multiplet $|0\rangle$. For all states in $|0\rangle \rightarrow \langle H_0 \rangle = 0$ of course

. The hopping Hamiltonian, H_1, acts as a perturbation. We perform hence perturbation theory. It's clear that 1st order perturbation theory in H_1 takes us out of the ground-state manifold, since it puts one fermion on top of other (double occupancy). We need to go to 2nd order in perturbation theory, which can take us from a state $|b\rangle$ in $|0\rangle$ to another state $|a\rangle$ in $|0\rangle$:

$$\langle a|H^{(2)}|b\rangle = \sum_{|n\rangle \notin |0\rangle} \langle a|H_1|n\rangle \frac{1}{[-\langle n|H_0|n\rangle]} \langle n|H_1|b\rangle$$

* Each term in this sum can be represented by an "exchange path".

For example:

$$|\uparrow,\downarrow\rangle \xrightarrow{H_1} |\uparrow\downarrow,0\rangle \xrightarrow{H_1} |\downarrow,\uparrow\rangle$$
$$\longrightarrow |0,\uparrow\downarrow\rangle \longrightarrow |\downarrow,\uparrow\rangle$$

[This process of virtual double occupation is called "super-exchange".]

* When dealing with fermions we must be particularly careful with the ordering, due to the anticommutation rules. Let's use the following ordering:

$$(C_{1\uparrow}^+)^{n_{1\uparrow}} (C_{1\downarrow}^+)^{n_{1\downarrow}} (C_{2\uparrow}^+)^{n_{2\uparrow}} (C_{2\downarrow}^+)^{n_{2\downarrow}} |VAC\rangle = |\{n_{1\uparrow}, n_{1\downarrow}\}, \{n_{2\uparrow}, n_{2\downarrow}\}\rangle$$

e.g. $|\uparrow,\downarrow\rangle \equiv |\{1,0\},\{0,1\}\rangle = C_{1\uparrow}^+ C_{2\downarrow}^+ |VAC\rangle$

$|\uparrow\downarrow,0\rangle \equiv |\{1,1\},\{0,0\}\rangle = C_{1\uparrow}^+ C_{1\downarrow}^+ |VAC\rangle$

* Then:

$$H_1|\uparrow,\downarrow\rangle = -t\left[C_{1\downarrow}^+ C_{2\downarrow} + C_{2\uparrow}^+ C_{1\uparrow}\right] C_{1\uparrow}^+ C_{2\downarrow}^+ |VAC\rangle$$
$$= -t\left[-C_{1\downarrow}^+ C_{1\uparrow}^+ + C_{2\uparrow}^+ C_{2\downarrow}^+\right]|VAC\rangle = -t\left[C_{1\uparrow}^+ C_{1\downarrow}^+ + C_{2\uparrow}^+ C_{2\downarrow}^+\right)|VAC\rangle$$
$$= -t\left[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right]$$

$$H_1|\uparrow\downarrow,0\rangle = -t\left[C_{2\uparrow}^+ C_{1\uparrow} + C_{2\downarrow}^+ C_{1\downarrow}\right]|\uparrow\downarrow,0\rangle = -t\left[C_{2\uparrow}^+ C_{1\downarrow} - C_{2\downarrow}^+ C_{1\uparrow}^+\right]|VAC\rangle$$
$$= -t\left[-C_{1\downarrow}^+ C_{2\uparrow}^+ + C_{1\uparrow}^+ C_{2\downarrow}^+\right]|VAC\rangle$$
$$= -t\left[-|\downarrow,\uparrow\rangle + |\uparrow,\downarrow\rangle\right]$$

Similarly $H_1|0,\uparrow\downarrow\rangle = -t\left[|\uparrow\downarrow\rangle - |\downarrow,\uparrow\rangle\right]$

Hence $\langle\uparrow,\downarrow|H^{(2)}|\uparrow,\downarrow\rangle = -\frac{2t^2}{U}$

$\langle\downarrow,\uparrow|H^{(2)}|\downarrow,\uparrow\rangle = 2t^2/U$

Similarly $\langle\downarrow,\uparrow|H^{(2)}|\downarrow,\uparrow\rangle = -2t^2/U$

$\langle\uparrow,\downarrow|H^{(2)}|\uparrow,\downarrow\rangle = +2t^2/U$

* Note, however, that there are paths which are blocked by the Pauli exclusion:

$|\uparrow,\uparrow\rangle \xrightarrow{H_1} 0$
$|\downarrow,\downarrow\rangle \xrightarrow{H_1} 0$
} the triplet states do not gain 2nd order energy by virtual double occupation.

* Hence

$$H^{(2)} = -\frac{2t^2}{U}\left[-|\uparrow,\downarrow\rangle\langle\downarrow,\uparrow| - |\downarrow,\uparrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow| + |\uparrow\downarrow\rangle\langle\uparrow\downarrow|\right]$$

* Let's add a constant energy $\frac{+2}{U}\hat{1} = \frac{+2}{U}\left[|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow| + |\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\right]$

Then:

$$H^{(2)} = \frac{2t^2}{U}\left[|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow|\right] + \frac{+2}{U}\left[|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow| - |\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\right]$$

$$= \frac{2t^2}{U}\left[(c_{1\uparrow}^+ c_{2\downarrow}^+)(c_{2\uparrow}c_{1\downarrow}) + (c_{1\downarrow}^+ c_{2\uparrow}^+)(c_{2\downarrow}c_{1\uparrow})\right]$$

$$+ \frac{+2}{U}\left[(c_{1\uparrow}^+ c_{2\uparrow}^+)(c_{2\uparrow}c_{1\uparrow}) + (c_{1\downarrow}^+ c_{2\downarrow}^+)(c_{2\downarrow}c_{1\downarrow}) - (c_{1\uparrow}^+ c_{2\downarrow}^+)(c_{2\downarrow}c_{1\uparrow}) - (c_{1\downarrow}^+ c_{2\uparrow}^+)(c_{2\uparrow}c_{1\downarrow})\right]$$

$$= \frac{2t^2}{U}\left\{\left[c_{1\uparrow}^+ c_{1\downarrow}\right]\left[c_{2\downarrow}^+ c_{2\uparrow}\right] + \left[c_{1\downarrow}^+ c_{1\uparrow}\right]\left[c_{2\uparrow}^+ c_{2\downarrow}\right]\right\}$$

$$+ \frac{+2}{U}\left\{\left[c_{1\uparrow}^+ c_{1\uparrow} - c_{1\downarrow}^+ c_{1\downarrow}\right]\left[c_{2\uparrow}^+ c_{2\uparrow} - c_{2\downarrow}^+ c_{2\downarrow}\right]\right\}$$

* Let $\boxed{\vec{S}_i = \frac{1}{2}\sum_{s,s'} c_{is}^+ \vec{\sigma}_{ss'} c_{is'}}$ → Spin operator ($S = 1/2$)
with $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ the Pauli matrices.

Hence:
$$S_i^{(+)} = c_{i\uparrow}^+ c_{i\downarrow}$$
$$S_i^{(-)} = c_{i\downarrow}^+ c_{i\uparrow}$$
$$S_i^{(z)} = \frac{1}{2}\left(c_{i\uparrow}^+ c_{i\uparrow} - c_{i\downarrow}^+ c_{i\downarrow}\right)$$

* Then: $H^{(2)} = \frac{2t^2}{U}\left[S_1^{(+)}S_2^{(-)} + S_1^{(-)}S_2^{(+)}\right) + \frac{4t^2}{U} S_1^{(z)} S_2^{(z)}$

Hence $\boxed{H^{(2)} = \frac{4t^2}{U}\vec{S}_1 \cdot \vec{S}_2}$ → isotropic antiferromagnetic Heisenberg exchange

* This discussion is easily generalized to a multi-site system. The antiferromagnetic coupling will be generated between any two spins that are coupled by a hopping $H_1 \Rightarrow \boxed{\hat{H} = \frac{4t^2}{U} \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j}$

* It's quite instructive to see what happens if we have a two-component Bose gas. We consider again 2 sites and assume $U/t \gg 1$.

$H_1 |\uparrow\uparrow\rangle = -t\sqrt{2}\,[|\uparrow\uparrow,0\rangle + |0,\uparrow\uparrow\rangle]$ ← now we may have 2 bosons ↑ in the same site!

$H_1 |0,\uparrow\uparrow\rangle = -t\sqrt{2}\,|\uparrow,\uparrow\rangle = H_1 |\uparrow\uparrow,0\rangle$

Hence $\langle\uparrow\uparrow|H^{(2)}|\uparrow\uparrow\rangle = -\frac{4t^2}{U} = \langle\downarrow\downarrow|H^{(2)}|\downarrow\downarrow\rangle$

$H_1 |\uparrow\downarrow\rangle = -t\,[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle] = H_1 |\downarrow,\uparrow\rangle$

$H_1 |\uparrow\downarrow,0\rangle = -t\,[|\uparrow\downarrow\rangle + t\,|\downarrow,\uparrow\rangle] = H_1 |0,\uparrow\downarrow\rangle$

Hence $\langle\uparrow\downarrow|H^{(2)}|\uparrow\downarrow\rangle = -\frac{2t^2}{U} = \langle\downarrow\uparrow|H^{(2)}|\uparrow,\downarrow\rangle$

* Hence:

$$H^{(2)} = -4\frac{t^2}{U}\left[|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|\right] - 2\frac{t^2}{U}\left[|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\right]$$
$$- 2\frac{t^2}{U}\left[|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow|\right]$$

Adding $3t^2/U\,\hat{\mathbb{1}}$, we obtain (using the definition of $S=1/2$-operators as before)

$$\boxed{H^{(2)} = -4\frac{t^2}{U}\,\vec{S}_1 \cdot \vec{S}_2}$$ ↝ isotropic ferromagnetic Heisenberg Hamiltonian

* Hence 2-component bosons are characterized by a ferromagnetic superexchange interaction, contrary to 2-component fermions, which are characterized by an anti-ferromagnetic coupling.

* Note that there is a clear separation of energy scales at strong-coupling $U/t \gg 1$.

* Mott insulator → Here we are talking about an energy scale given by U. For temperatures $T \lesssim U$ density fluctuations are suppressed and one has a paramagnetic Mott insulator with large spin entropy.

* Quantum magnetism → Here the energy scale is given by $4t^2/U$, which is (by far) a much lower energy scale. For $T \lesssim 4t^2/U$, the residual spin interactions set-in and the ground state is eventually reached, corresponding, in the simplest case, to an ordered antiferromagnetic state (for 2-component fermions) or a ferromagnetic state (for bosons).

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* Superexchange for bosons in optical lattices has been experimentally observed in the group of I. Bloch [S. Trotzky et al., Science 319, 295 (2007)]. They used optical lattices with different wavelengths to create a set of isolated double wells, and observed spin oscillations within individual wells.

* Let's see briefly how this experiment works. Suppose 2 atoms in 2 sites with zero total magnetization (i.e. equal number of ↑ and ↓ spins). One has hence 4 possibilities:

$$(\uparrow)(\downarrow) \to |\uparrow,\downarrow\rangle \qquad (\uparrow\downarrow)\,\cup \to |\uparrow\downarrow,0\rangle$$
$$(\downarrow)(\uparrow) \to |\downarrow,\downarrow\rangle \qquad \cup\,(\uparrow\downarrow) \to |0,\uparrow\downarrow\rangle$$

The Bose-Hubbard Hamiltonian for the 2 sites is:

$$\hat{H} = -t\sum_{S=\uparrow,\downarrow}\left(c^{+}_{LS}c_{RS} + c^{+}_{RS}c_{LS}\right) + U\left[\hat{n}_{L\uparrow}\hat{n}_{L\downarrow} + \hat{n}_{R\uparrow}\hat{n}_{R\downarrow}\right]$$

Hence $\hat{H}|\uparrow,\downarrow\rangle = -t\left[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right]$

$\hat{H}|\downarrow,\uparrow\rangle = -t\left[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right]$

$\hat{H}|\uparrow\downarrow,0\rangle = -t\left[|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right] + U|\uparrow\downarrow,0\rangle$

$\hat{H}|0,\uparrow\downarrow\rangle = -t\left[|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right] + U|0,\uparrow\downarrow\rangle$

- Let's introduce

$$|S\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right] \quad \| \quad |+\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right]$$

$$|t\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right] \quad \| \quad |-\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle\right]$$

- Then: $\hat{H}|S\rangle = 0$
  $\hat{H}|-\rangle = U|-\rangle$
  $\hat{H}|t\rangle = -2t|+\rangle$
  $\hat{H}|+\rangle = -2t|t\rangle + U|+\rangle$

Four eigenstates:

$|S\rangle \longrightarrow E_S = 0$
$|-\rangle \longrightarrow E_- = U$
$|A\rangle \equiv \cos\phi|t\rangle + \sin\phi|+\rangle$
$|B\rangle \equiv -\sin\phi|t\rangle + \cos\phi|+\rangle$

with $E_{A,B} = \frac{U}{2}\left\{1 \pm \sqrt{1+(4t/U)^2}\right\}$

$$\tan\phi = \frac{-U}{4t}\left[1 + \sqrt{1+(4t/U)^2}\right]$$

* Note that if $\frac{U}{4t} \gg 1$
  ↳ $\tan\phi \longrightarrow -\infty \Rightarrow \phi = -\pi/2 \longrightarrow$ $|A\rangle \cong -|+\rangle$; $E_A \simeq U + 4t^2/U$
  $|B\rangle \cong |t\rangle$; $E_B \simeq -4t^2/U$

* In the experiment they prepare the initial state in the $|\uparrow\downarrow\rangle = \frac{1}{2}\left[|S\rangle + |t\rangle\right]$ state. We rewrite this state in the form:

$$|\psi(0)\rangle = \frac{1}{2}\left[|S\rangle + \cos\phi|A\rangle - \sin\phi|B\rangle\right]$$

We can now calculate easily the time evolution:

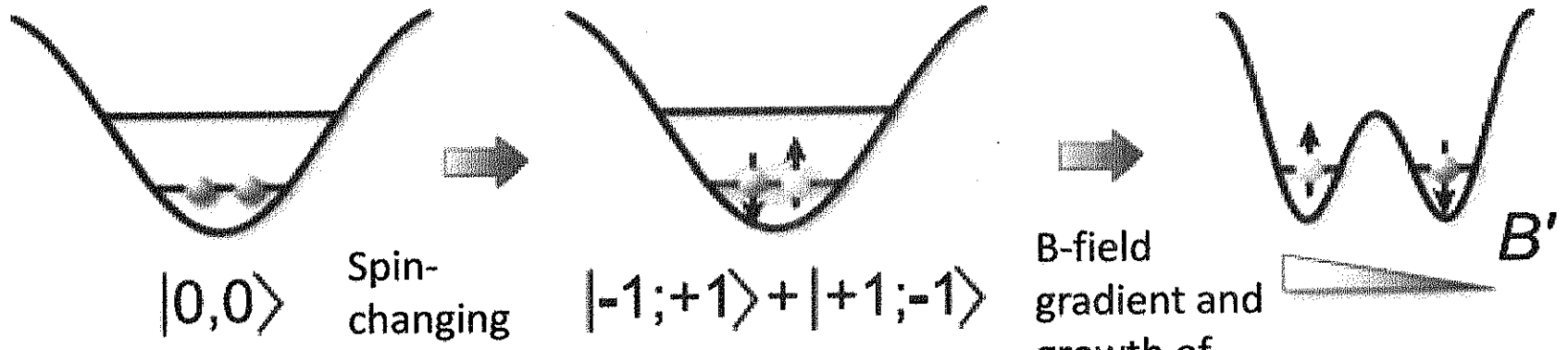
$$|\psi(\tau)\rangle = \frac{1}{2}\left[|S\rangle + \cos\phi\, e^{-iE_A\tau/\hbar}|A\rangle - \sin\phi\, e^{-iE_B\tau/\hbar}|B\rangle\right]$$

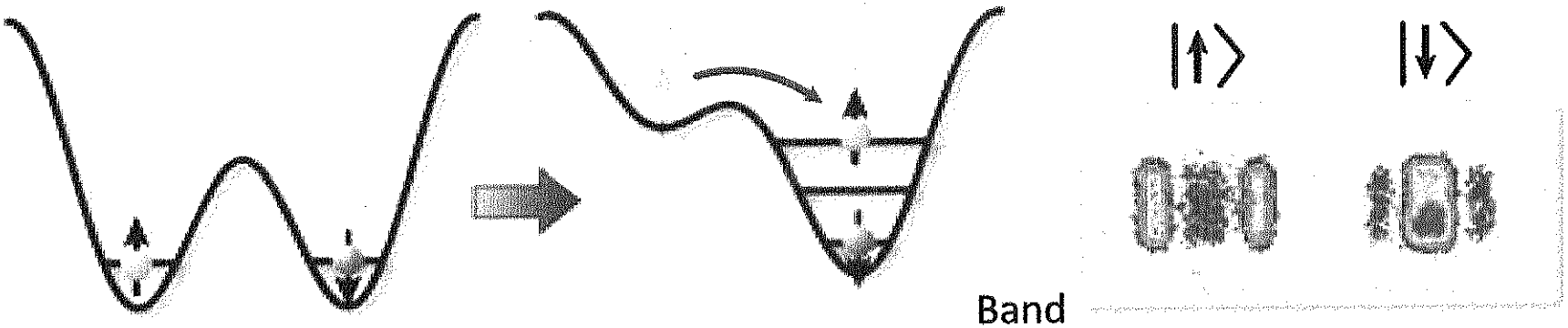
(Note: I employ τ for the time to avoid confusion)

* In the experiment they can evaluate
  * Population imbalance: $\chi(\tau) = \langle\psi(\tau)|\left[(\hat{n}_{\uparrow L} + \hat{n}_{\downarrow L}) - (\hat{n}_{\uparrow R} + \hat{n}_{\downarrow R})\right]|\psi(\tau)\rangle$
  * Spin imbalance: $N_2(\tau) = \langle\psi(\tau)|\frac{1}{2}\left[(\hat{n}_{\uparrow L} - \hat{n}_{\downarrow L}) - (\hat{n}_{\uparrow R} - \hat{n}_{\downarrow R})\right]|\psi(\tau)\rangle$
* A simple calculation shows that $\chi(\tau) = 0$, and that

$$\boxed{N_2(\tau) = \cos^2\phi\,\cos\left(E_A\tau/\hbar\right) + \sin^2\phi\,\cos\left(E_B\tau/\hbar\right)}$$

Super-exchange experiment of I. Bloch [Trotzky et al., Science 319, 295 (2007)]

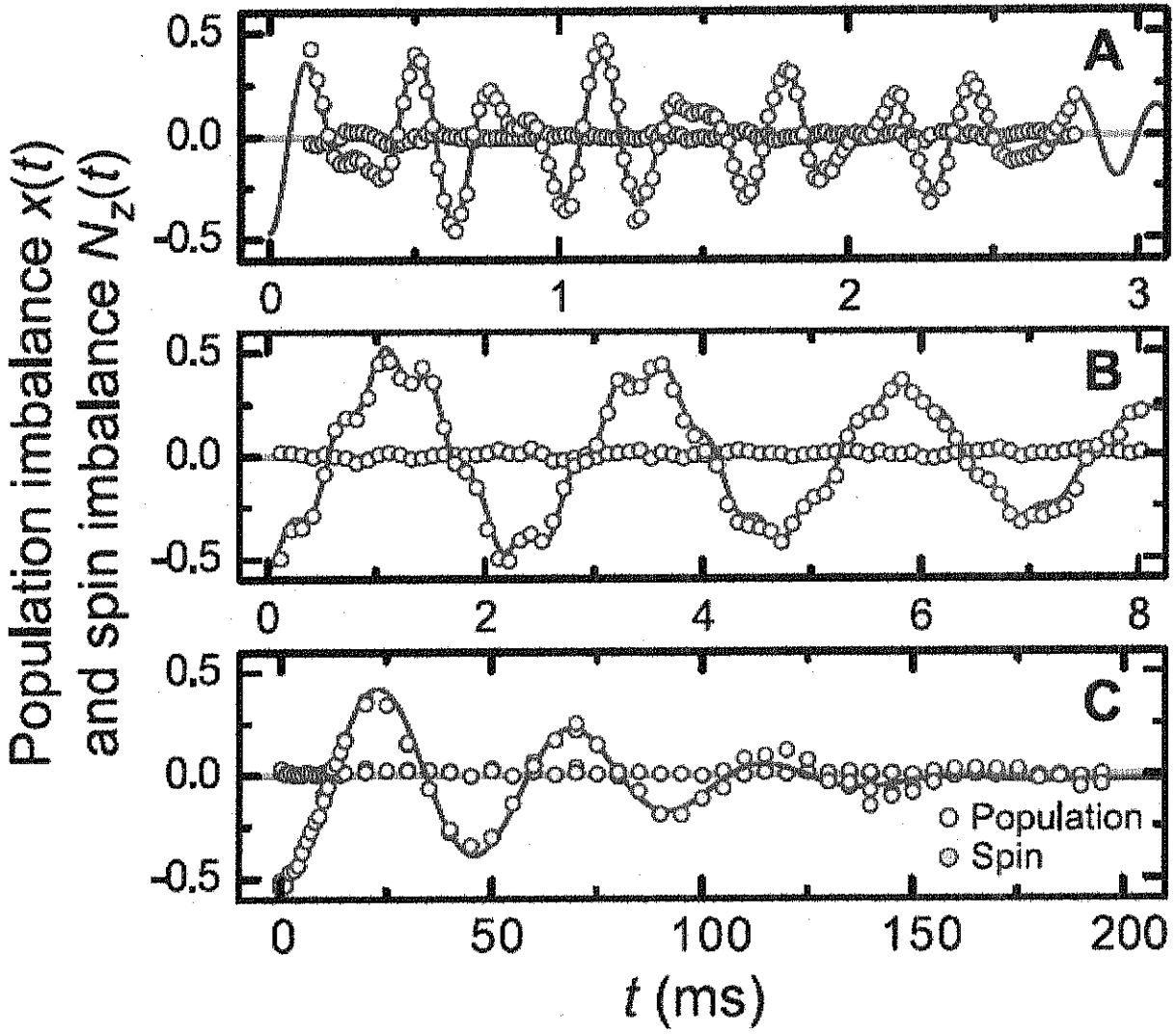




The population of the left well is transferred to a higher vibrational level of the underlying long-lattice

Band mapping and a Stern-Gerlach filter

Super-exchange experiment of I. Bloch [Trotzky et al., Science 319, 295 (2007)]



t/U=1.26

Beating of 2 freqs.

t/U=0.26

t/U=0.048

Only one freq.

The damping resulted mainly from the statistics of many double sites with different potential barriers

* The spin imbalance presents hence oscillations with two beating frequencies $E_{A,B}/\hbar$.

However when $\frac{U}{4t} \gg 1 \rightarrow N_2(t) \simeq \cos\left[\frac{4t^2/U}{\hbar}\tau\right]$

because in this regime $\Phi \simeq -\pi/2$ and $E_B \simeq -4t^2/U$.

- Hence in the regime of strong interite barrier, and hence low hopping, the oscillation of the population imbalance is given by the superexchange energy $4t^2/U$

(Note: From the point of view of spins

$|\uparrow,\downarrow\rangle \xrightarrow{S_L^{(+)} S_R^{(-)}} |\downarrow,\uparrow\rangle \rightarrow$ it's clear that the spin oscillation in the strong U/t regime is given by the superexchange.)

* This is exactly what they observed in their experiment.
For $t/U \sim 1$ they found a beating of 2 frequencies.
For $t/U \ll 1$ they found a single oscillation frequency given by the superexchange $4t^2/U$.

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* WEAK-COUPLING REGIME. PHASE DIAGRAM

- Up to now we have had only a look to the strong U/t regime. However the antiferromagnetism is also relevant at low U/t. Let's have a brief look to that.
- We consider in the following two-component fermions with one atom per site in average in a bipartite lattice (e.g. a cubic lattice).

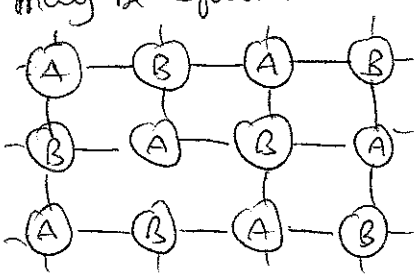
As before we consider the Hubbard Hamiltonian:

$$\hat{H} = \hat{H}_{TUN} + \hat{H}_{INT}$$

$$\hat{H}_{TUN} = -t \sum_{\langle ij \rangle} \sum_{s} \hat{c}_{is}^{+} \hat{c}_{js}$$

$$\hat{H}_{INT} = U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

* Note: recall that a bipartite lattice may be split into two sublattices



* Let's have a look to the interacting term

$$\hat{H}_{INT} \underset{\uparrow}{\simeq} U \sum_i \left[\langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \langle \hat{n}_{i\downarrow} \rangle \hat{n}_{i\uparrow} - \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle \right]$$

decoupling (Hartree-Fock)

- Let $\langle \hat{n}_i \rangle = \langle \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \rangle = 1$ ← average filling 1

$$\langle \delta_i^z \rangle = \frac{1}{2} \langle \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} \rangle = \frac{1}{2} (-1)^i m_S$$

staggered magnetization (this is our order parameter)

→ This means that in our bipartite lattice, sites Ⓐ get + and Ⓑ −.

Then:

$$\langle \hat{n}_{i\uparrow} \rangle = \frac{1}{2} \left[1 + (-1)^i m_S \right]$$

$$\langle \hat{n}_{i\downarrow} \rangle = \frac{1}{2} \left[1 - (-1)^i m_S \right]$$

Hence:

$$\hat{H}_{INT} \cong U \sum_i \left\{ \frac{1}{2} (1 + (-1)^i) m_S \hat{n}_{i\downarrow} + \frac{1}{2} (1 - (-1)^i m_S) \hat{n}_{i\uparrow} - \frac{1}{4} (1 - m_S^2) \right\}$$

$$= U \sum_i \left\{ \frac{1}{2} (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) - \frac{1}{2} (-1)^i m_S (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}) - \frac{1}{4} (1 - m_S^2) \right\}$$

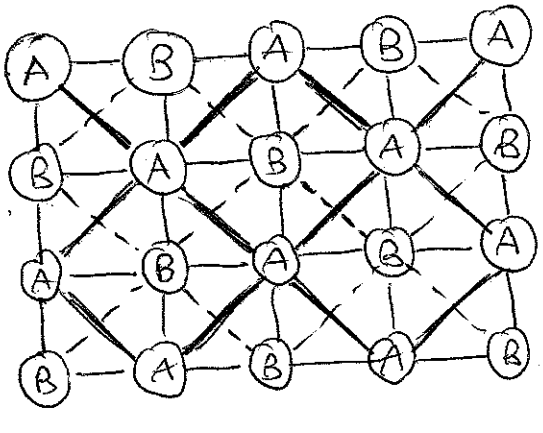
$$= \frac{U}{4} N (1 + m_S^2) - \frac{U m_S}{2} \sum_i (-1)^i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$$

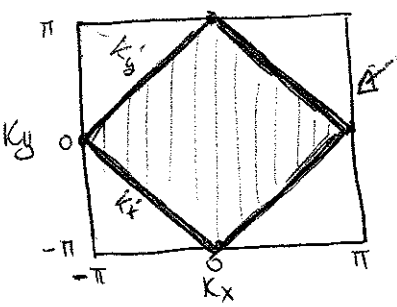
↑ number of sites (= number of particles)

We can then write:

$$\hat{H}_{INT} = \frac{U}{4} N (1 + m_S^2) - \frac{U m_S}{2} \left\{ \sum_{i \in A} (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}) - \sum_{i \in B} (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}) \right\}$$

- Let's have a look to the two sublattices A and B:
  - They build clearly two equal square lattices (in 2D)
  - The new Brillouin zone (for each sublattice) is hence of the form





We will call this Brillouin zone the reduced Brillouin zone

(RBZ) $-\frac{\pi}{\sqrt{2}} \leq k'_{x,y} \leq \frac{\pi}{\sqrt{2}}$

* We will treat hence both sublattices independently.
Note that RBZ is 1/2 of the original Brillouin zone.

* We may then introduce the discrete Fourier transform:

• Sublattice (A): $\hat{C}_{\vec{j}s} = \frac{1}{\sqrt{N/2}} \sum_{\vec{k}\in RBZ} e^{+i\vec{k}\cdot\vec{j}}\, \hat{a}_{\vec{k}s}$ — The sublattices have 1/2 of the total number of sites.

• Sublattice (B): $\hat{C}_{\vec{j}s} = \frac{1}{\sqrt{N/2}} \sum_{\vec{k}\in RBZ} e^{+i\vec{k}\cdot\vec{j}}\, \hat{b}_{\vec{k}s}$

* Then for (A)

$$\hat{n}_{\vec{j}s} = \frac{1}{(N/2)} \sum_{\vec{k},\vec{k}'\in RBZ} e^{+i(\vec{k}-\vec{k}')\vec{j}}\, \hat{a}^{+}_{\vec{k}'s}\, \hat{a}_{\vec{k}'s}$$

and for (B) the same but with $\hat{b}^{+}_{\vec{k}s}\, \hat{b}_{\vec{k}'s}$.

• Then:

$$\sum_{\vec{j}\in A} \hat{n}_{\vec{j}s} = \sum_{\vec{k},\vec{k}'\in RBZ} \hat{a}^{+}_{\vec{k}s}\, \hat{a}_{\vec{k}'s} \underbrace{\frac{1}{(N/2)} \sum_{\vec{j}\in A} e^{i(\vec{k}-\vec{k}')\vec{j}}}_{\delta_{\vec{k},\vec{k}'}} = \sum_{\vec{k}\in RBZ} \hat{a}^{+}_{\vec{k}s}\, \hat{a}_{\vec{k}s}$$

and the same for $\vec{j}\in B$.

• Hence:

$$\hat{H}_{INT} \simeq \frac{UN}{4}(1+m_s^2) - \frac{Um_s}{2} \sum_{\vec{k}\in RBZ} \left[(\hat{a}^{+}_{\vec{k}\uparrow}\hat{a}_{\vec{k}\uparrow} - \hat{a}^{+}_{\vec{k}\downarrow}\hat{a}_{\vec{k}\downarrow}) - (\hat{b}^{+}_{\vec{k}\uparrow}\hat{b}_{\vec{k}\uparrow} - \hat{b}^{+}_{\vec{k}\downarrow}\hat{b}_{\vec{k}\downarrow}) \right]$$

• Let's consider now the hopping term

$$\hat{H}_{TUN} = -t \sum_{\vec{j}\in A} \sum_{\vec{\delta}} \sum_{s} \hat{C}^{+}_{\vec{j}s}\, C_{\vec{j}+\vec{\delta},s} - t \sum_{\vec{j}\in B} \sum_{\vec{\delta}} \sum_{s} C^{+}_{\vec{j}s}\, C_{\vec{j}+\vec{\delta},s}$$

↖ nearest neighbors: $\vec{\delta} = \pm\vec{e}_x, \pm\vec{e}_y, \pm\vec{e}_z$

$$= -t \sum_{\vec{k},\vec{k}'\in RBZ} \sum_{s} \sum_{\vec{\delta}} \left(\hat{a}^{+}_{\vec{k}s}\, \hat{b}_{\vec{k}'s} + \hat{b}^{+}_{\vec{k}'s}\, \hat{a}_{\vec{k}s} \right) e^{-i\vec{k}'\cdot\vec{\delta}} \underbrace{\frac{1}{N/2} \sum_{\vec{j}} e^{i(\vec{k}-\vec{k}')\cdot\vec{j}}}_{\delta_{\vec{k}\vec{k}'}}$$

$$= -t \sum_{\vec{k}\in RBZ} \sum_{s} \left[\sum_{\vec{\delta}} e^{-i\vec{k}\cdot\vec{\delta}} \right] \left(\hat{a}^{+}_{\vec{k}s}\, \hat{b}_{\vec{k}s} + \hat{b}^{+}_{\vec{k}s}\, \hat{a}_{\vec{k}s} \right)$$

• Let $\epsilon_{\vec{k}} = -t \sum_{\vec{\delta}} e^{-i\vec{k}\cdot\vec{\delta}}$ (29) since $\vec{k} = k_x \vec{e}_x' + k_y \vec{e}_y'$ with $-\frac{\pi}{\sqrt{2}} \le k_{x,y} \le \pi/\sqrt{2}$ but $\vec{\delta} = \pm\vec{e}_x, \pm\vec{e}_y$ with $\vec{e}_x' = (\vec{e}_x + \vec{e}_y)/\sqrt{2}$, $\vec{e}_y' = (-\vec{e}_x + \vec{e}_y)/\sqrt{2}$

Then $\epsilon_{\vec{k}} = -t\left[\cos\left(\frac{k_x - k_y}{\sqrt{2}}\right) + \cos\left(\frac{k_x + k_y}{\sqrt{2}}\right)\right] = -2t \cos\left(\frac{k_x}{\sqrt{2}}\right)\cos\left(\frac{k_y}{\sqrt{2}}\right)$

* Hence: $\hat{H}_{TUN} = \sum_{\vec{k}\in RBZ} \sum_{s} \epsilon_{\vec{k}} \left(\hat{a}^+_{\vec{k}s} \hat{b}_{\vec{k}s} + \hat{b}^+_{\vec{k}s} \hat{a}_{\vec{k}s}\right)$

[Note: as expected, of course, the hopping term connects both sublattices.]

• The total Hamiltonian is hence:

$$\hat{H} = \frac{UN}{4}(1+m_s^2) + \sum_{\vec{k}\in RBZ} \sum_{s} \left\{ -(-1)^s \left(\frac{Um_s}{2}\right)\left(\hat{a}^+_{\vec{k}s}\hat{a}_{\vec{k}s} - \hat{b}^+_{\vec{k}s}\hat{b}_{\vec{k}s}\right) + \epsilon_{\vec{k}}\left(\hat{a}^+_{\vec{k}s}\hat{b}_{\vec{k}s} + \hat{b}^+_{\vec{k}s}\hat{a}_{\vec{k}s}\right) \right\}$$

$$= \frac{UN}{4}(1+m_s)^2 + \sum_{\vec{k}\in RBZ} \sum_{s} \left(\hat{a}^+_{\vec{k}s}, \hat{b}^+_{\vec{k}s}\right) \begin{pmatrix} -(-1)^s \frac{Um_s}{2} & \epsilon_{\vec{k}} \\ \epsilon_{\vec{k}} & (-1)^s \frac{Um_s}{2} \end{pmatrix} \begin{pmatrix} \hat{a}_{\vec{k}s} \\ \hat{b}_{\vec{k}s} \end{pmatrix}$$

$$= \frac{UN}{4}(1+m_s)^2 + \sum_{\vec{k}\in RBZ} \sum_{s} \left[\xi^{(+)}_{\vec{k}} \hat{\alpha}^{(+)+}_{\vec{k}s} \hat{\alpha}_{\vec{k}s} + \xi^{(-)}_{\vec{k}} \hat{\alpha}^{(-)+}_{\vec{k}s} \hat{\alpha}^{(-)}_{\vec{k}s} \right]$$

where we have diagonalized for each $\vec{k}\in RBZ$ the matrix above to get two bands:

$$\xi^{(\pm)}_{\vec{k}} = \pm\sqrt{\epsilon^2_{\vec{k}} + \left(\frac{Um_s}{2}\right)^2}$$

→ • Note that the 2 bands are separated by a gap $\Delta = Um_s$
→ Δ is actually the Mott-gap here.

Above $\alpha^{(\pm)}_{\vec{k}s}$ are the corresponding operators for the upper and lower branch.

* At zero temperature the ground state for an average $\langle n_i \rangle = 1$ is given by a filled lower band and an empty upper band.

(Note: $\langle n \rangle = 1$ means a half-filled original band. However the RBZ is half of the original BZ and hence $\langle n \rangle = 1$ means full filling of the lowest band)

Hence $\sum_s \langle \alpha^{(-)+}_{\vec{k}s} \alpha^{(-)}_{\vec{k}s} \rangle_0 = 2$ and $\sum_s \langle \alpha^{(+)+}_{\vec{k}s} \alpha^{(+)}_{\vec{k}s} \rangle_0 = 0$

* Hence at $T=0$:

$$E_0 = \frac{UN}{4}(1+m_s^2) + 2\sum_{k\in RBZ} \varepsilon_k^{(-)}$$

$$= \frac{UN}{4}(1+m_s^2) - 2\sum_{k\in RBZ} \sqrt{\varepsilon_k^2 + \left(\frac{U^2 m_s^2}{4}\right)}$$

* We minimize the energy with respect to m_s to get a self-consistent equation for m_s:

$$\frac{\partial E_0}{\partial m_s} = \frac{UN}{2} m_s - 2\sum_{k\in RBZ} \frac{\frac{1}{2}\frac{U^2 \cdot 2m_s}{4}}{\sqrt{\varepsilon_k^2 + U^2 m_s^2/4}} = 0$$

Hence:

$$\boxed{\Delta = \frac{U}{2(N/2)} \sum_{k\in RBZ} \frac{1}{\sqrt{\varepsilon_k^2 + U^2 m_s^2/4}}}$$

in 2D $\rightarrow$ $\Delta \simeq \frac{U}{2t}\frac{1}{2\pi^2}\int_{-\pi/\sqrt{2}}^{\pi/\sqrt{2}} d^2k \frac{1}{\sqrt{4\cos^2\left(\frac{k_x}{\sqrt{2}}\right)\cos^2\left(\frac{k_y}{\sqrt{2}}\right) + \left(\frac{U}{2t}\right)^2 m_s^2}}$ see p. (48')

Note that due to the contribution of the borders of RBZ one has a solution for $m_s \neq 0$ even for $\frac{U}{2t}$ very small

* At weak coupling, where the Hartree approximation is a reasonable starting point, the antiferromagnetic instability (i.e. the tendency to have $m_s > 0$) occurs for an arbitrarily small U/t (at $T=0$). In this regime, the antiferromagnetism is a spin density wave with wavevector $\vec{Q} = (\pi,\pi)$ and a very weak modulation.

. At finite T one needs a finite U/t to get ~~AF~~ antiferromagnetism. Conversely, for a given U/t there's a critical $T \rightarrow T_{NÉEL}$ (so-called Néel Temperature) below which one has antiferromagnetism.

Note: In 2D square lattice: $T_{NÉEL} \propto t\, e^{-\sqrt{4/U}}$)

---

* In the opposite regime ($U \gg t$) we have already seen that the Hubbard model reduces to the Heisenberg model at low energy. Hence, in this regime $T_{NÉEL} \propto 4t^2/U$ $\left(= 0.957\left(\frac{4t^2}{U}\right)\right.$ in a cubic lattice). Hence $\frac{T_{NEEL}}{t} \sim \frac{t}{U}$ and hence decreases with U/t.

(98)

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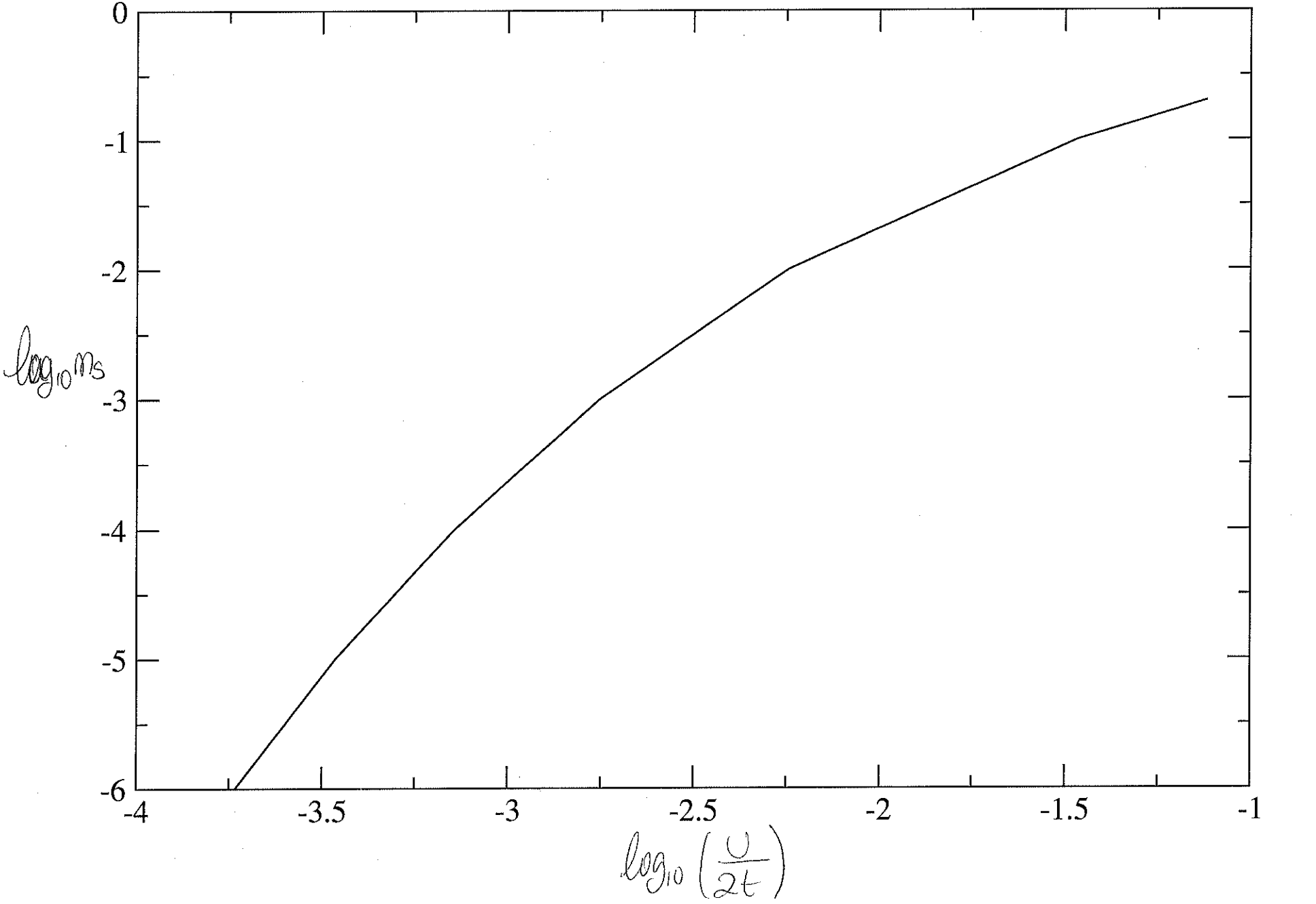
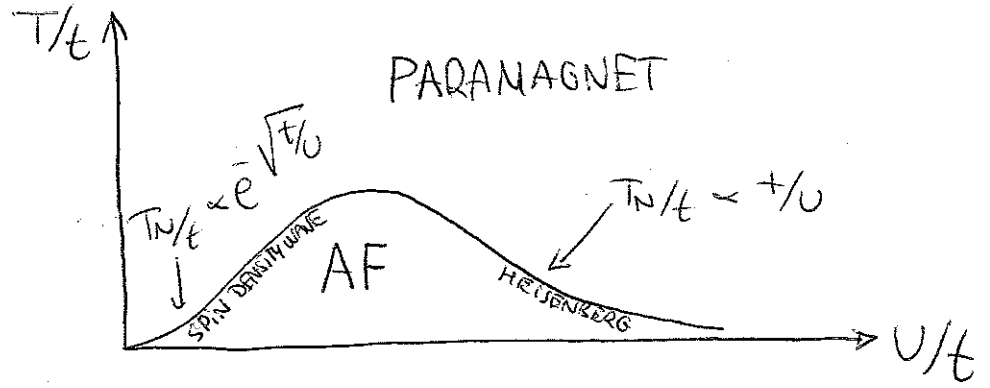


* In between the two regimes T_N/t reaches a maximum value



* The phase diagram presents hence 2 phases:
  - A high-T paramagnetic phase
  - A low-T antiferromagnetic phase

Of course, within the high-T phase there's a gradual crossover from itinerant (paramagnetic metal) to Mott localized as U/t increases, or as T is decreased below the Mott gap. ($\sim U$ at large U/t).

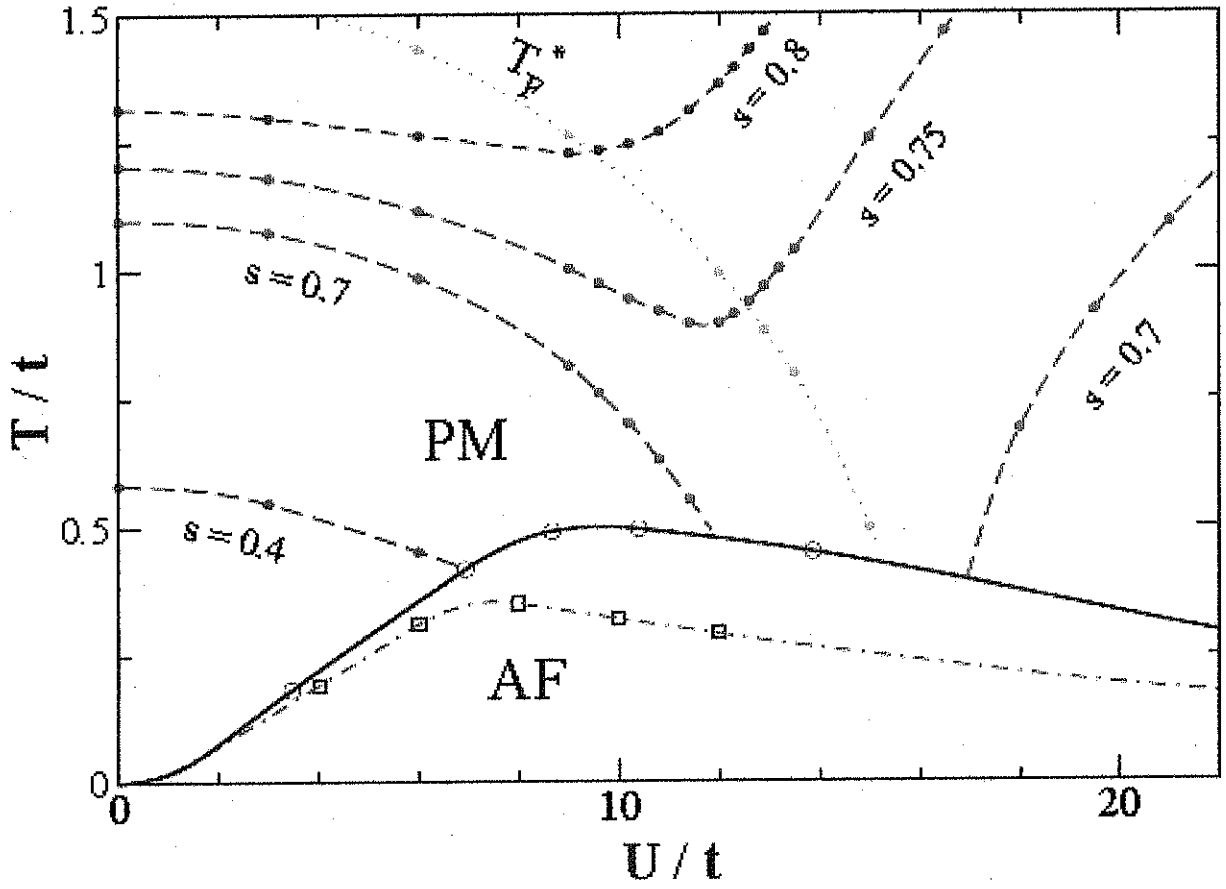
---

* ENTROPY

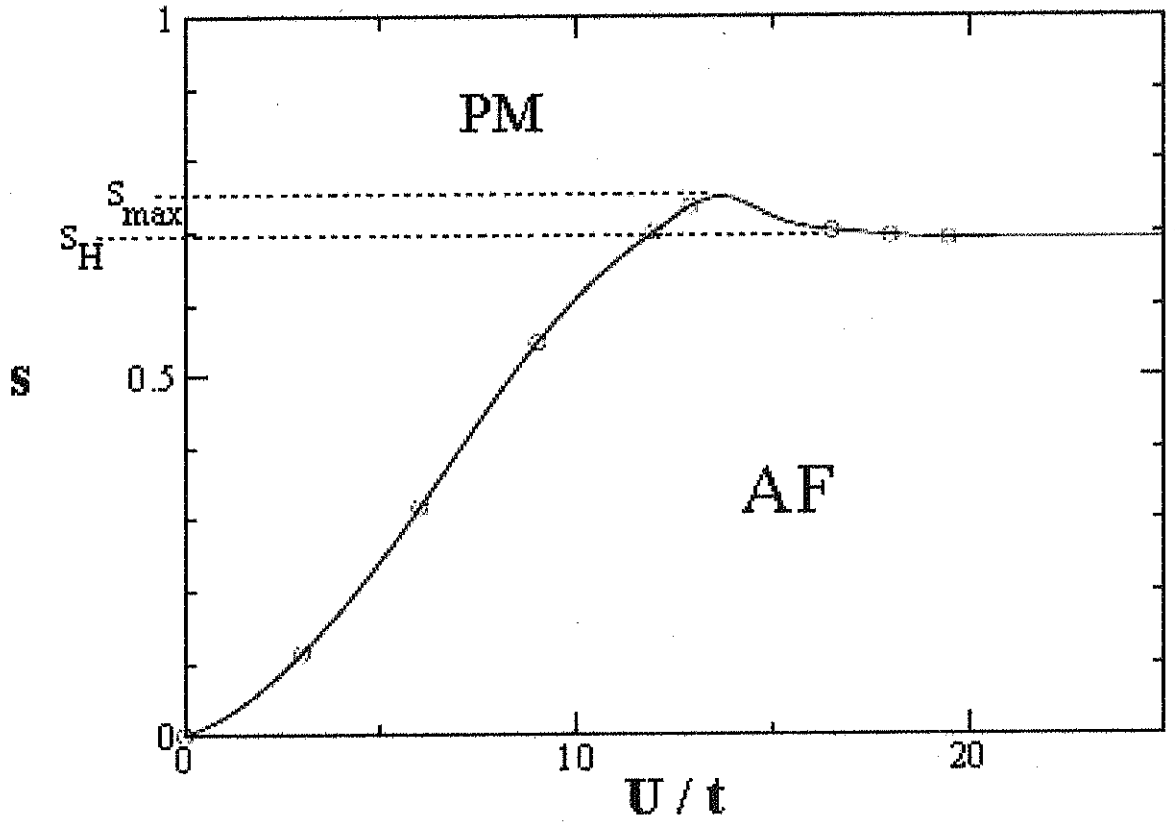
- The Néel temperature T_N is a rather low scale. Even at its maximum $T_N \sim 0.3t$ for a cubic lattice, i.e. much less than the band width ($\sim 12t$). Actually, considering the value of T_N at maximum and falling into account the constraints (especially of V_0/E_{rec}) for the validity of the Hubbard description, one would estimate $T_N \sim 10^{-2} E_R$. One may then conclude that the prospects for cooling down to such T are quite challenging.
- One should think however rather in terms of entropy per particle $S = S/N$. Indeed quantum phase transitions are controlled by entropy because it measures the number of accessible quantum states.

* In the homogeneous half-filled Hubbard model the entropy per particle is a function $S(T/t, U/t)$. The entropy itself is a good thermometer, since $\partial S/\partial T > 0$.

Phase diagram of the half-filled HM [Werner et al., PRL 95, 056401 (2005)]



Phase diagram of the half-filled HM [Werner et al., PRL 95, 056401 (2005)]



* DMFT results

ln 2

(actually $S_H \simeq \ln 2/2$ due to quantum fluctuations)

* Assuming that an adiabatic process is possible, the key point to reach the AF phase is to be able to prepare the system in a state with a lower entropy than that of the Neel transition, i.e. below the critical boundary

$$S_N(U) = S_N(T_N(U), U)$$

[see the curve in p. 42 for $T_N(U)$, and of $S_N(U)$ in p. 48]

* At weak coupling (spin-density wave regime), $S_N(U)$ is expected to be exponentially small.

* A strong coupling (Heisenberg regime), S_N will reach a finite value S_H, which is the entropy of the quantum Heisenberg model at its critical point.

* Mean-field theory of the Heisenberg model yields $S_H = k_B \ln 2$. This is somehow the naive expectation. Note that a paramagnet with the same probability to be ↑ or ↓ in each site will have $S/k_B = \ln 2$.

* Quantum fluctuations reduce the value of S_H down to a value $S_N \sim k_B (\ln 2)/2 \sim 0.35 k_B$ on the cubic lattice (Quantum Monte Carlo results)

* In the intermediate regime S_N goes through a maximum $S_{max} > S_H$.

In order to see this, we take the derivative:

$$\frac{\partial S}{\partial U} = -\frac{\partial p_2}{\partial T}$$

where $p_2 = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ is the probability of double occupation. This is so because of the relation between free energy f and entropy: $s = -\partial f/\partial T$. On the other hand $p_2 = \partial f/\partial U$ (recall that $H \sim U \sum_i n_{i\uparrow} n_{i\downarrow}$). Hence $\frac{\partial S}{\partial U} = -\frac{\partial p_2}{\partial T} = -\frac{\partial^2 f}{\partial U \partial T}$

* Since $S_N(U) = S(T_N(U), U)$ then:

$$\frac{dS_N}{dU} = \frac{\partial S_N}{\partial T_N}\frac{dT_N}{dU} + \frac{\partial S_N}{\partial U} = \frac{C(T_N)}{T_N}\frac{dT_N}{dU} - \left.\frac{\partial p_2}{\partial T}\right|_{T=T_N}$$

where $C(T_N)$ is the specific heat per particle ($C = T\,\partial S/\partial T$).

- If only the first term were present in the r.h.s., it would obviously imply that S_N would be maximum exactly when T_N is maximum
- let's have a look now to the T-dependence of the probability P_2 of double occupancy. When U/t is not too large, P_2 decreases as T is increased from $T=0$ (indicating a higher degree of localization), then turns around and grows again.

This bizarre behavior is similar to the so-called Pomeranchuk effect (known from liquid ^3He). The entropy (spin entropy) is larger in a localized state than when the fermions form a Fermi liquid (for which $S \propto T$).

For large-enough U/t, Mott localization dominates for all $T < U$ suppressing the Pomeranchuk effect.

- In the figure of p. (49') you can see the behavior of the isentropes. You see that there's a temperature $T_F^*(U)$ which splits the regimes $\partial P_2/\partial T < 0$ ($T < T_F^*(U)$) from $\partial P_2/\partial T > 0$ ($T > T_F^*(U)$).
- Hence along the $T_N(U)$ curve, one has a point such that $\partial P_2/\partial T = 0$.
- Hence $S_N(U)$ does reach a maximum $S_{max} > S_H$ (see p. (49''))
- Hence the figure of p. (49') may be understood as a phase diagram of the half-filled Hubbard model, in which entropy itself is used as a thermometer, which is a very natural representation when addressing adiabatic cooling.

* COOLING IN OPTICAL LATTICES

* As we just saw it is necessary to reach very low entropies per particle to be able to observe AF ordering in lattice gases. This is indeed a formidable task, whose difficulty has prevented so far the realization of Neel ordering, in spite of the realization of Mott-insulators of two-component lattice fermions (p. (37)) and the observation of super-exchange (p. (42)).

* In current optical lattice experiments, the lattice potential is slowly superimposed on the atom gas after it is first cooled (via laser + evaporative cooling) to as low T as possible in a parabolic potential. The goal is to make the lattice turn-on as adiabatic as possible so that S/N is preserved

The lowest attainable S/N in the harmonic trap sets hence a lower limit to what will be achievable in the lattice.

[Note: The entropy of a 2-component Fermi gas in a harmonic trap of frequency ω is given by

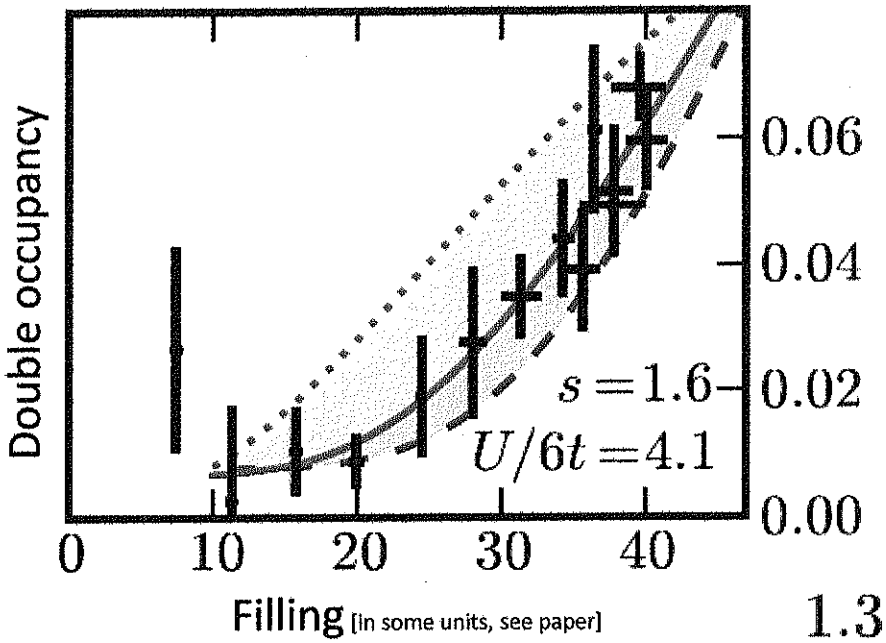
$$\frac{S}{N} \cong k_B \pi^2 T/T_F \quad \text{where } T_F = (3N)^{1/3}\hbar\omega \text{ is the Fermi Temperature of the non-interacting gas.}$$

* For the weakly-interacting regime relevant to lattice-experiments the lowest reported temperatures for fermions (in a harmonic trap before transferring into the lattice) are $\sim 0.13\ T/T_F$, which amounts for $S/N \sim 1.3 k_B$, far too high compared to $S_H \sim 0.35\ k_B$. The study of quantum magnetism demands hence a yet lower S, and hence further cooling.

[a group of T. Esslinger [R. Jördens et al., PRL 104, 180401 (2010)] Theoretical models show however that the central entropy may reach lower values $S \sim 0.77 k_B$] → see p. (52')

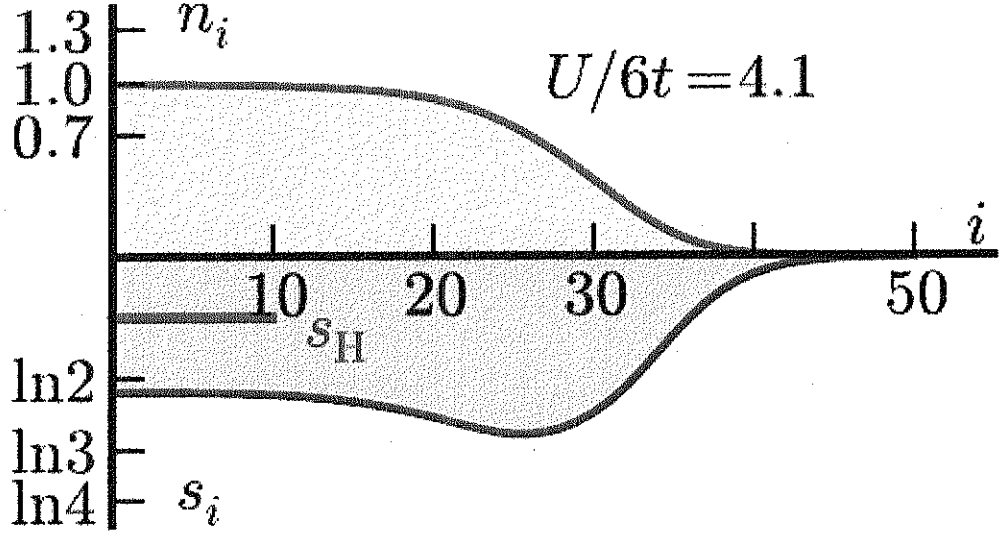
* In principle one could start with even lower T/T_F in the trap (which is already a challenge in itself!). However, methods for cooling to very low S in the harmonic potential may be impaired, mostly due to non-adiabaticity during the lattice turn-on and heating from the lattice.

Cooling in optical lattices [Jördens et al., PRL 104, 180401 (2010)]



- A theory fit of the experimental data for double occupancy provides for U/6t=4.1 a value s=1.6, close to the value s=1.3 that one expects with adiabatic evolution

- The central entropy may be however lower, due to the presence of a Mott plateau at the center surrounded by a metallic region at the borders. The metal may act as an entropy absorber, reducing the central entropy down to ln2, i.e. $2s_H$



(This is already an example of immersion cooling as that discussed in p. (59))

* The challenge is hence to develop methods to cool atoms in a lattice below $S \sim 0.35\, k_B$.

* In the last years there has been a series of proposals on how this may be achieved, which may be roughly grouped into two groups:

  • Filter cooling: takes advantage of entropy residing in certain modes of the system which can then be filtered.

  • Immersion cooling: based on immersing the system in a reservoir that carries away the entropy.

* Here we will just comment on some examples of proposals. For a very good review of cooling (and thermometry) in optical lattices have a look to the review of McKay and DeMarco [Rep. Prog. Phys. 74, 054401 (2011)].

* An example of filter cooling is provided by what one may call spatial filtering, in which one uses the external confinement to create high entropy regions which can be then removed from the system.

With appropriate tuning of the confinement, a gapped phase occurs in the center of trap (i.e. a band insulator for fermions) and the majority of the entropy will reside at the edge. This high entropy region can be filtered from the system (e.g. by adding a potential barrier).

In page (53') you can see a sketch of the method proposed by Bernier et al. [PRA 79, 061601 (2009)]. Their simulations show that entropies $S \sim 0.2\, k_B$ may be achieved in this way.

An advantage of spatial filtering schemes is that they require little changes to be implemented in current experiments.

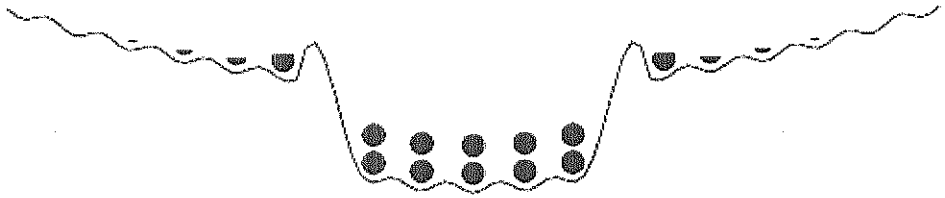
The main limitation of the method of Bernier et al. may be the ability to create effective barrier potentials, although the recent progress in single site addressing at Greiner's and Bloch's group may solve that problem. (recall p. (35))

Spatial filtering [Bernier et al., PRA 79, 061601 (2009)]

(a)

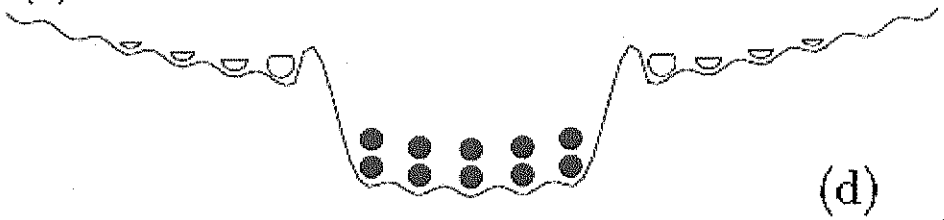
The atoms trapped in a parabolic trap are loaded into an optical lattice

(b)



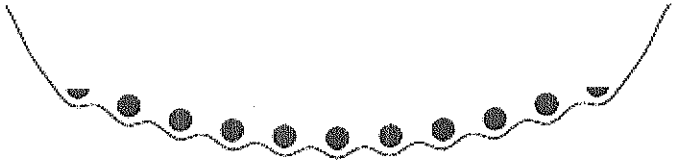
A band insulator is created in a dimple at the trap center. The core is isolated from the rest (storage region) by rising barriers

(c)



The storage region is removed

(d)



The band insulator is relaxed to the desired quantum phase by flatterning the dimple and removing the barriers

* Immersion cooling proposals are based on immersing the system to be cooled (the "sample") in a "reservoir" system that can carry away the entropy. There are different ideas on how this entropy redistribution may be achieved.

For example, Ho and Zhou [PNAS 106, 6916 (2009)] considered a fermionic system in a lattice (+trap) as the sample, and a harmonically trapped BEC as the reservoir. The method goes as follows:

(i) The fermionic harmonic trap is adiabatically compressed turning the fermions at the center into a band insulator. During this process a substantial amount of the original fermion entropy is pushed into the bosons. The entire system has little change of T due to the large heat capacity of the BEC compared to the lattice fermions. Actually, for the fermions one has an isothermal compression.

(ii) The bosons are evaporated, leaving the remaining fermions to equilibrate

(iii) The fermion harmonic trap is adiabatically opened.

Calculations show a decrease to $S \simeq 0.02\, k_B$, well below the $0.35\, k_B$ limit.

• The primary remaining issue is to understand the thermalization rate in these systems, since if thermalization is not efficient, then the intrinsic heating/loss processes will dominate.

* Demagnetization cooling

• An interesting variation of the idea of immersion cooling is to use two degrees of freedom of the same gas to play the role of system/reservoir. For example, in a 2-component system, the spin degree of freedom can be used as a reservoir for the motional degrees of freedom.

• Such a cooling scheme is well-known in condensed-matter physics and is known as adiabatic demagnetization cooling: the sample is prepared in a high magnetic field, and as the field is lowered, the spins disorder and absorb entropy.

* Typically a cold atom system preserves magnetization. Only collisions may lead to a transfer of population between spin components (i.e. to spin flipping). However short-range interactions preserve magnetization. Dipolar interactions may however allow for spin relaxation, and as a matter of fact demagnetization cooling was already observed in Chromium (Pfau's group), which presents a high magnetic moment and therefore a high dipolar relaxation rate [Fattori et al. Nat. Phys. 2, 765 (2006)]

* A related technique, the so-called spin-gradient demagnetization cooling, has been recently demonstrated in cold atoms in Ketterle's group [Medley et al., PRL 106, 195301 (2011)].

A two-component Bose gas is prepared in a magnetic-field gradient, which segregates the components to opposite sites of the trap. As the gradient is lowered the two species mix and ideally entropy from particle-hole excitations is transferred into the spin mixing entropy. Note that the method is very similar to demagnetization cooling but now magnetic field $\longrightarrow$ magnetic field gradient
spin flip $\longrightarrow$ spin transport.

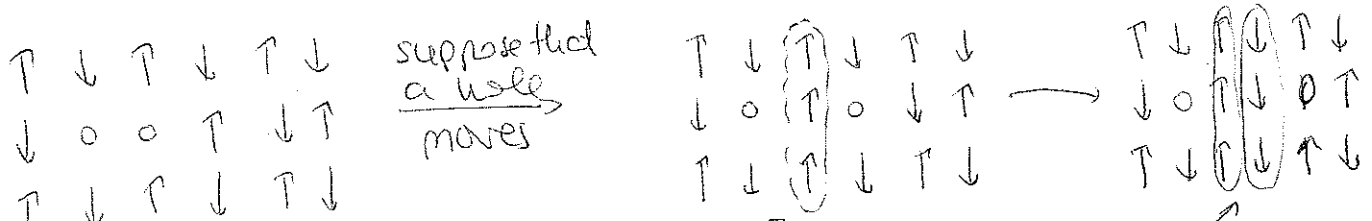
* This type of cooling, however, will be limited by magnetic correlations when T approaches the superexchange energy, and hence may be of limited use for accessing the Néel state when applied to two component fermions.

[* Note: one may use Fermi gases with more than 2 internal states, e.g. a spin-3/2 system, and employ a spatially-dependent quadratic Zeeman effect. This can create an effective spin-1/2 region at the trap center surrounded by a spin-3/2 region at the borders. Entropy of the core may be then transfered to the borders. Here: magnetic field $\rightarrow$ quadratic Zeeman effect
spin-flip $\longrightarrow$ spin-changing collisions
This idea may allow to cool directly the spin degree of freedom [Colomé-Tatché et al. NJP (2011)]

* AWAY FROM HALF-FILLING: D-WAVE SUPERFLUIDITY

* Up to now we have considered just the case of half-filling, showing that at sufficiently low T the system enters an antiferromagnetic phase. Let's see what happens if there are holes in such system.

* Let's consider 2 neighboring holes like in the figure



The motion of a hole in an AF background creates a string of flipped spins

The further the hole moves the more strings are created.

Separating the holes is energetically costly, i.e. there's an effective attraction between holes

(Note: This resembles to some extent the attractive interaction between electrons due to lattice distortions, which is behind conventional BCS superconductors.)

* The effective attraction between holes suggest the possibility of pairing. The orbital symmetry of such hole pairs is rather unconventional. The doped holes form pairs with $d_{x^2-y^2}$ symmetry for which the gap presents a momentum dependence:

$$\Delta_p = \Delta_0 (\cos p_x - \cos p_y)$$

[Note: S-wave symmetry would be $\cos p_x + \cos p_y$]

The operator for adding a pair of holes has the form:

$$\Delta_d = \frac{1}{N} \sum_p \Delta_p c_{p\uparrow} c_{-p\downarrow} \quad \Longleftarrow \text{Fourier transform}$$

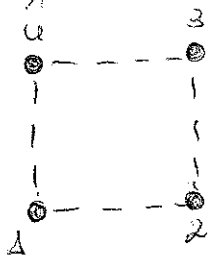
$$= \frac{1}{N} \sum_{\substack{i \\ \text{sites}}} \frac{\Delta_0}{2} \Big[\underbrace{(c_{i+x,\uparrow} c_{i\downarrow} - c_{i+x,\downarrow} c_{i\uparrow})}_{\text{next neighbor along } x} - \underbrace{(c_{i+y\uparrow} c_{i\downarrow} - c_{i+y\downarrow} c_{i\uparrow})}_{\text{next neighbor along } y} + (c_{i-x\uparrow} c_{i\downarrow} - c_{i-x\downarrow} c_{i\uparrow}) - (c_{i-y,\uparrow} c_{i\downarrow} - c_{i-y\downarrow} c_{i\uparrow}) \Big]$$

$\rightarrow$ singlet hole pairs

* This operator creates a superposition of these singlets around each site, giving a state with zero center-of-mass momentum.

* The key feature associated with the $d_{x^2-y^2}$ symmetry is the relative phasing $(+-+-)$ of these singlet pairs.

* To understand the character of the pairing we consider a single square plaquette [This simple argument stems from Scalapino and Trugman, cond-mat/9604008 (1996)]



* For large U the largest real space amplitude in the 4-particle ground state are for the Neel configuration

$$|\phi_a\rangle = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger c_{3\uparrow}^\dagger c_{4\downarrow}^\dagger |0\rangle$$

$$|\phi_b\rangle = c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger c_{3\downarrow}^\dagger c_{4\uparrow}^\dagger |0\rangle$$

* The 2-particle ground state on this 4-site cluster is for $U=0$ of the form:

$$|\tilde{\Psi}_2\rangle = [c_{1\uparrow}^\dagger + c_{2\uparrow}^\dagger + c_{3\uparrow}^\dagger + c_{4\uparrow}^\dagger][c_{1\downarrow}^\dagger + c_{2\downarrow}^\dagger + c_{3\downarrow}^\dagger + c_{4\downarrow}^\dagger]|VAC\rangle$$

one up and on down fermion, each with momentum $K=0$

For large U we need to eliminate double occupancy at a given site, and hence the true ground state is obtained after multiplying $|\tilde{\Psi}_2\rangle$ by a projection operator (which project out double occupancy):

$$|\Psi_2\rangle = (c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger + c_{1\uparrow}^\dagger c_{3\downarrow}^\dagger + \dots)|VAC\rangle$$

• The interesting point is how $|\Psi_2\rangle$ can be created out of $|\phi_{a,b}\rangle$, i.e. which operator creates holes.

One may consider:

• <u>S-wave operator</u>:

$$\begin{aligned}\Delta_S = &(c_{1\uparrow}c_{2\downarrow} - c_{1\downarrow}c_{2\uparrow}) \\ &+ (c_{1\uparrow}c_{4\downarrow} - c_{1\downarrow}c_{4\uparrow}) \\ &+ (c_{2\uparrow}c_{3\downarrow} - c_{2\downarrow}c_{3\uparrow}) \\ &+ (c_{3\uparrow}c_{4\downarrow} - c_{3\downarrow}c_{4\uparrow})\end{aligned}$$

• <u>d-wave operator</u> (as in p. 50):

$$\begin{aligned}\Delta_d = &(c_{1\uparrow}c_{2\downarrow} - c_{1\downarrow}c_{2\uparrow}) \\ &- (c_{1\uparrow}c_{4\downarrow} - c_{1\downarrow}c_{4\uparrow}) \\ &+ (c_{2\uparrow}c_{3\downarrow} - c_{2\downarrow}c_{3\uparrow}) \\ &- (c_{3\uparrow}c_{4\downarrow} - c_{3\downarrow}c_{4\uparrow})\end{aligned}$$

* It's quite easy to see that $\langle \Psi_2 | \Delta_s | \Phi_{a/b} \rangle = 0$

e.g. $\Delta_s |\Phi_a\rangle = -[c_{3\uparrow}^\dagger c_{4\downarrow}^\dagger + c_{2\downarrow}^\dagger c_{3\uparrow}^\dagger + c_{1\uparrow}^\dagger c_{4\downarrow}^\dagger + c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger]|VAC\rangle$

$\langle \Psi_2 | \Delta_s | \Phi_a \rangle = -1 + 1 - 1 + 1 = 0$

* On the other hand $\langle \Psi_2 | \Delta_d | \Phi_{a/b} \rangle \neq 0$ as one may easily check as above.

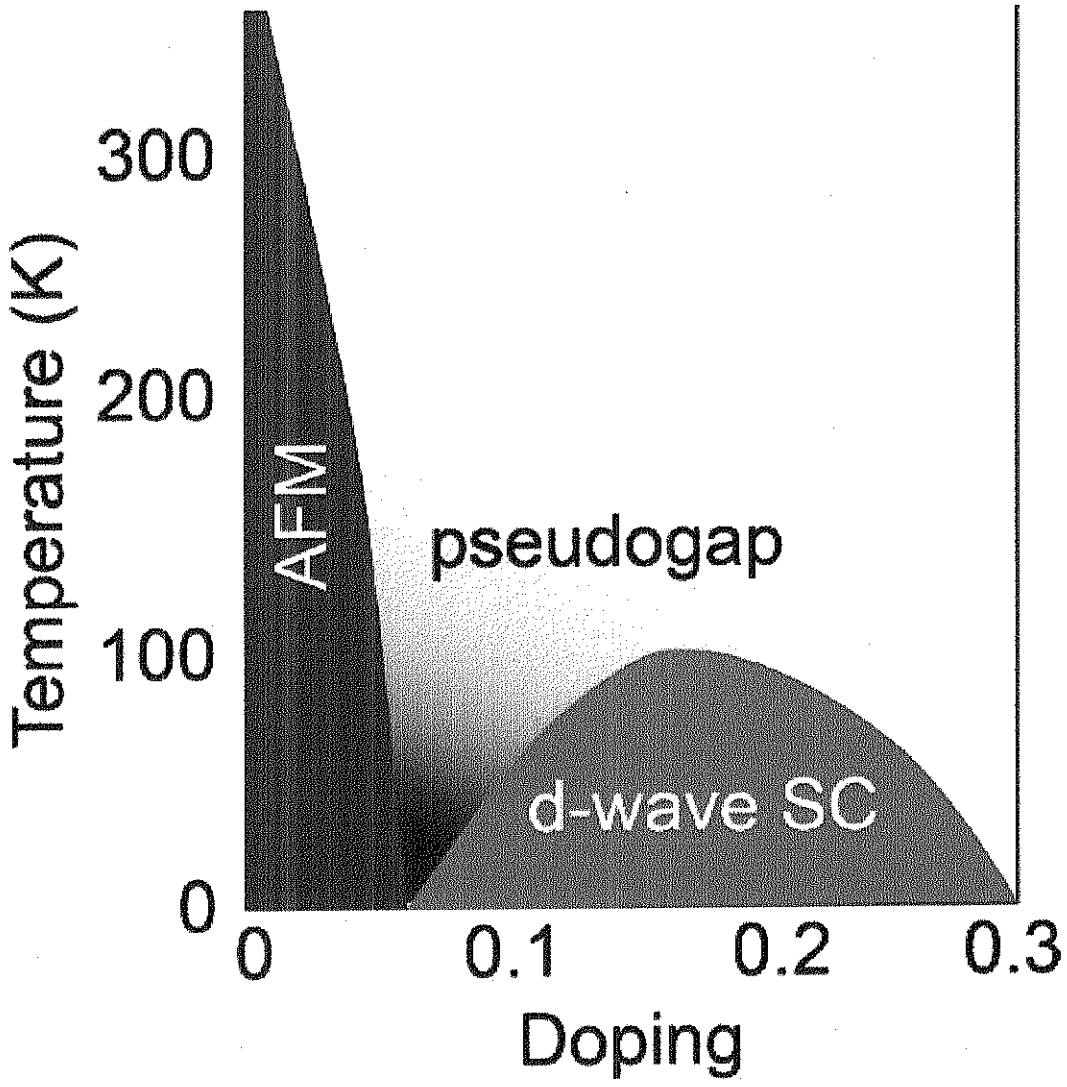
* Thus sugsest that holes pair in d-wave.

* d-wave pairing plays a crucial role in <u>high-temperature superconductivity</u> cuprates. A simplied phase diagram for cuprates is shown in p. (58), where we see the AF phase (at low or zero dopings) and a d-wave superconductor at sufficient doping.

* A grand challenge for the field of ultracold gases in optical lattices is to determine <u>the conditions necessary for d-wave superfluidity in the Hubbard model</u>. Note however that even <u>lower S/N is necessary</u> (compared to s_N) to reach the d-wave superfluid regime.

* If the cooling issue is settled, then ultracold gases in lattices may allow for an interesting insight into the physics of high-T_c superconductors!

High-Tc cuprate superconductors



Simplified cuprate phase diagram