⊙ 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 :

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

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

* 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 exclusion) 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 ↓. These two particles may interact, and this accounts 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 Fermigas we will have a <u>band insulator</u> if we have a filling factor 2 per site. In addition we may have, as for the bosonic case, a <u>Mott-insulator</u> 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 (<u>metallic</u>) 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).

---

* Before going into spin, let's point out that the Mott-metal transition has been <u>already observed experimentally</u> 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 (25), (26) and (27)]

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

---

* 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 <u>huge spin entropy</u>, being a paramagnet in which the spin of the atom localized 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!)
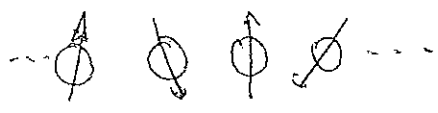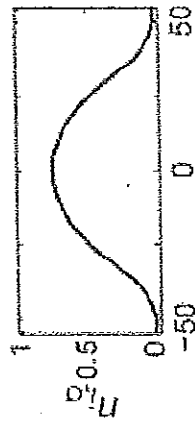
$$\cdots \uparrow \quad \downarrow \quad \uparrow \quad \downarrow \cdots$$
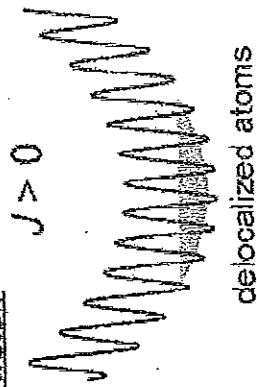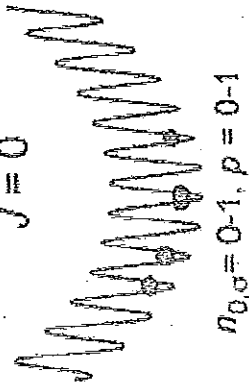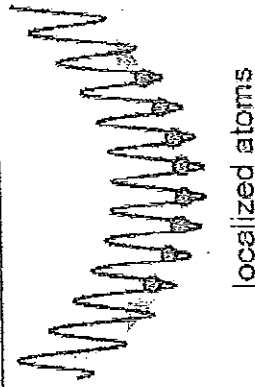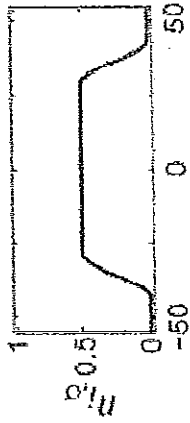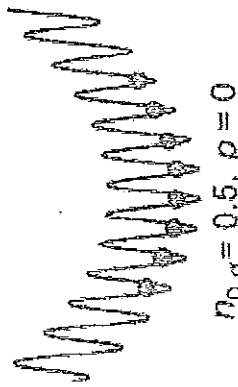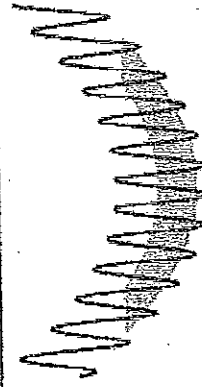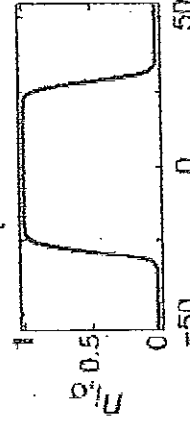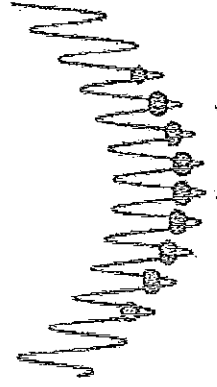
Mott-Metal transition [Schneider et al., Science 322, 1520 (2008)]

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

Mott-
insulator
at the
trap
center

Band-
insulator

F

$E_t/12J=0.4$

R (d)

55

50

45

0   40   80   120

Ramp time (ms)

A

B

C

D

E

Renormalized Cloud Size R_{sc} (d)

0.75

0.7

0.65

0.6

0.55

0.5

0.45

0   0.5   1   1.5   2

Compression $E_t/12J$

$U/12J = 0$
$U/12J = 0.5$
$U/12J = 1$
$U/12J = 1.5$
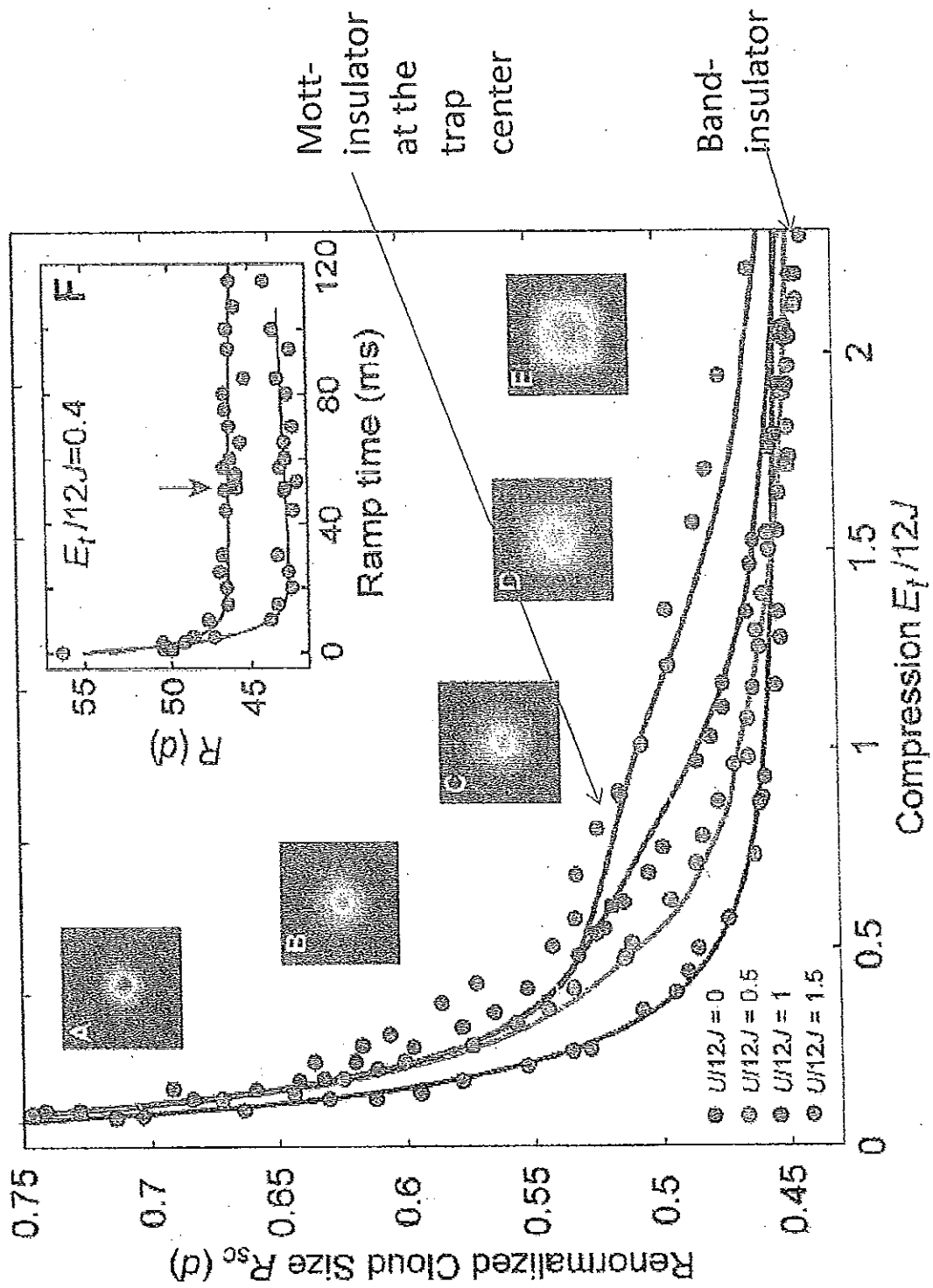
Mott-Metal transition [Schneider et al., Science 322, 1520 (2008)]
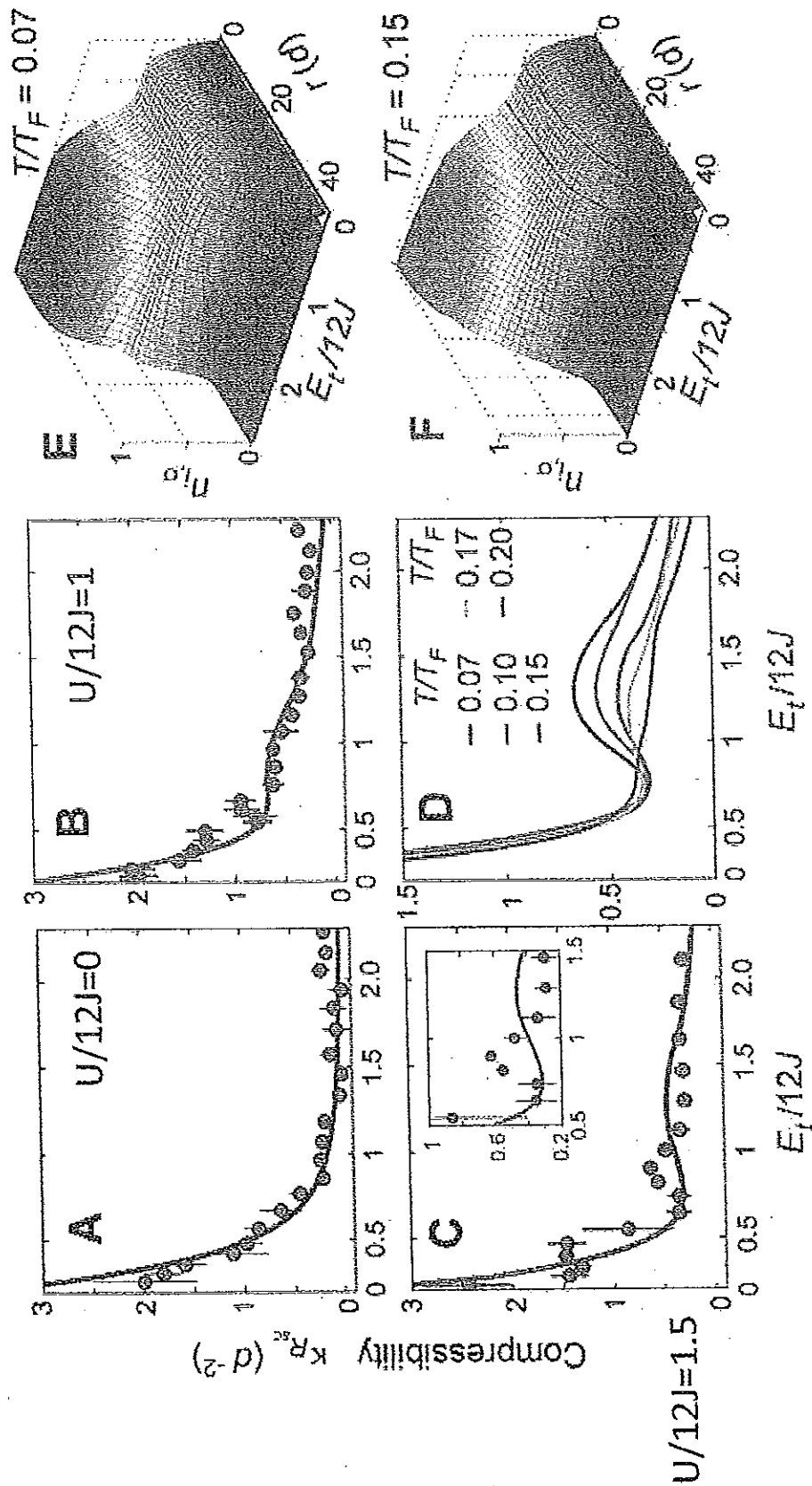
* SUPER-EXCHANGE : HEISENBERG HAMILTONIAN

* 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:

$$\{0\} = |S_1, S_2\rangle \quad ; \quad S_i = \uparrow, \downarrow \quad ; \quad i = 1, 2$$

The energies of the doubly occupied orbitals are higher by U than the multiplet $\{0\}$. For all states in $\{0\} \rightarrow \langle H_0 \rangle = 0$ 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 $\{0\}$ to another state $|a\rangle$ in $\{0\}$:

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

* 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 occupancy is called "super-exchange". (Anderson)

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

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

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

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

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 $\frac{t^2}{U}\hat{1} = \frac{t^2}{U}\left[\begin{array}{c}|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow| \\ + |\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\end{array}\right]$

then:

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

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

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

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

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

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

$\hookrightarrow$ Spinoperator $(S = \frac{1}{2})$

Hence: $S_i^{(+)} = C_{i\uparrow}^+ C_{i\downarrow}$

$S_i^{(-)} = C_{i\downarrow}^+ C_{i\uparrow}$

$S_i^{(z)} = \frac{1}{2}(C_{i\uparrow}^+ C_{i\uparrow} - C_{i\downarrow}^+ C_{i\downarrow})$

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

Thus your 1st spin model

We'll be more in the future...

* 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 $U/t \gg 1$.

now we may have 2 bosons $\uparrow$ in the same site!

$$H_1 |\uparrow \uparrow\rangle = -t\sqrt{2} \left[|\uparrow\uparrow, 0\rangle + |0, \uparrow\uparrow\rangle \right]$$

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

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

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

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

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

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

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

— This makes the physics of 2-comp. bosons very different (within the Mott state) compared to 2-comp. fermions!

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

    * <u>Mott insulator</u> → 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.

    * <u>Quantum magnetism</u> → 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).

_____

* <u>Superexchange</u> for bosons in optical lattices has been <u>experimentally observed</u> 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:

$(↑)(↓) \rightarrow |↑,↓\rangle \quad\quad (↑↓)(\;) \rightarrow |↑↓,0\rangle$

$(↓)(↑) \rightarrow |↓,↑\rangle \quad\quad (\;)(↑↓) \rightarrow |0,↑↓\rangle$

The Bose-Hubbard Hamiltonian for the 2 sites is:

$$\hat{H} = -t \sum_{S=↑,↓}(C^\dagger_{LS}C_{RS} + C^\dagger_{RS}C_{LS}) + U[\hat{n}_{L↑}\hat{n}_{L↓} + \hat{n}_{R↑}\hat{n}_{R↓}]$$

Hence $\hat{H}|↑,↓\rangle = -t[|↑↓,0\rangle + |0,↑↓\rangle]$

    $\hat{H}|↓,↑\rangle = -t[|↑↓,0\rangle + |0,↑↓\rangle]$

    $\hat{H}|↑↓,0\rangle = -t[|↑,↓\rangle + |↓,↑\rangle] + U|↑↓,0\rangle$

    $\hat{H}|0,↑↓\rangle = -t[|↑,↓\rangle + |↓,↑\rangle] + U|0,↑↓\rangle$

- Let's introduce

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

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

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

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

* Note that if $\dfrac{U}{4t} \gg 1$

  $\hookrightarrow \tan\phi \longrightarrow -\infty \Rightarrow \phi = -\pi/2 \longrightarrow$

  $|A\rangle \cong -|+\rangle \; ; \; E_A \simeq U + 4t^2/U$

  $|B\rangle \cong |t\rangle \; ; \; E_B \simeq -4t^2/U$

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

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

We can now calculate easily the time evolution:

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

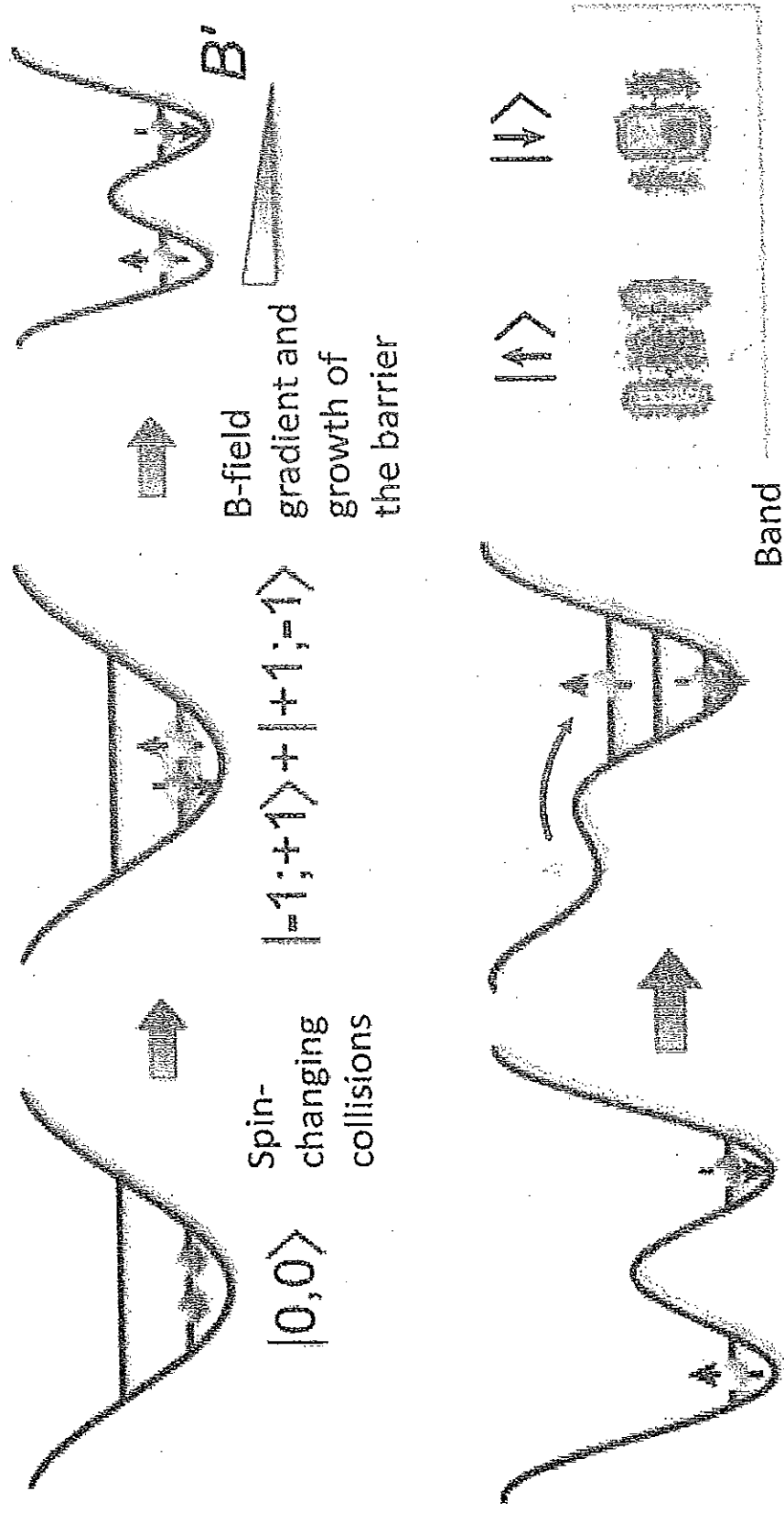(Note: I employ τ for the time to avoid confusion)

* 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: $N_z(\tau) = \langle\psi(\tau)|\frac{1}{2}\left[(\hat{n}_{\uparrow L} - \hat{n}_{\downarrow L}) - (\hat{n}_{\uparrow R} - \hat{n}_{\downarrow R})\right]|\psi(\tau)\rangle$

* A simple calculation shows that $\chi(\tau) = 0$, and that

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

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

$|0,0\rangle$

Spin-changing collisions

$|{-}1;{+}1\rangle\rangle + |{+}1;{-}1\rangle$

B'

B-field gradient and growth of the barrier

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

$|\Uparrow\rangle$ $|\Downarrow\rangle$

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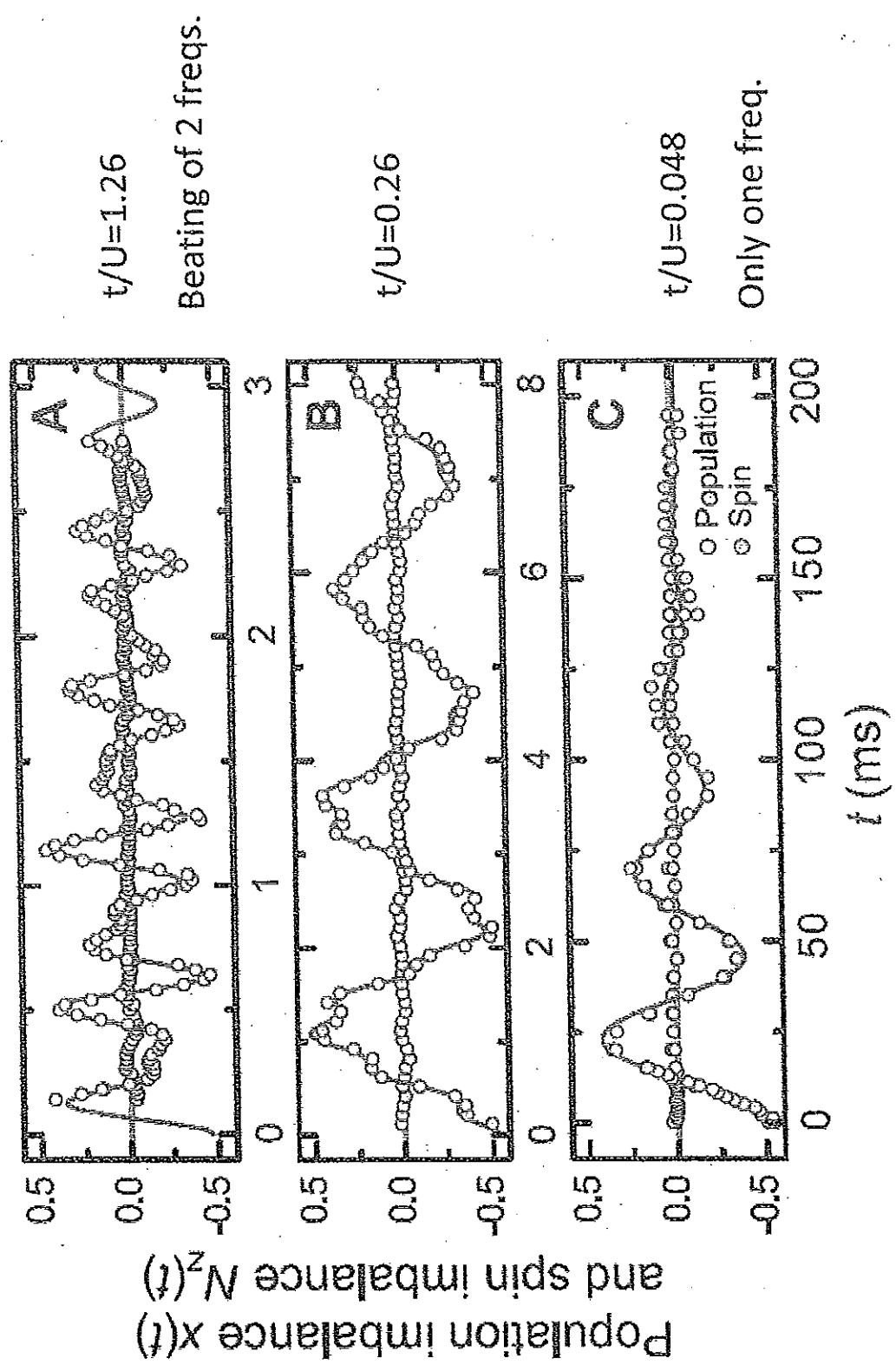
The damping resulted mainly from the statistics of many double sites with different potential barriers

* 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 $\phi = -\pi/2$ and $E_B \simeq -4t^2/U$.

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

(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 $4t^2/U$.

---

* <u>WEAK-COUPLING REGIME. PHASE DIAGRAM</u>
. 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 <u>bipartite</u> 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

$$\langle \hat{s}_i^z \rangle = \frac{1}{2} \langle \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} \rangle = \frac{1}{2} (-1)^i m_s$$ ← 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:
$$\hat{H}_{INT} \cong U \sum_i \left\{ \frac{1}{2} (1 + (-1)^i) m_s \hat{n}_{i\downarrow} + \frac{1}{2} (1 - (-1)^i m_s) \hat{n}_{i\uparrow} - \frac{1}{4} (1 - m_s^2) \right\}$$

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

$$= \frac{U}{4} N (1 + m_s^2) - \frac{U m_s}{2} \sum_i (-1)^i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$$
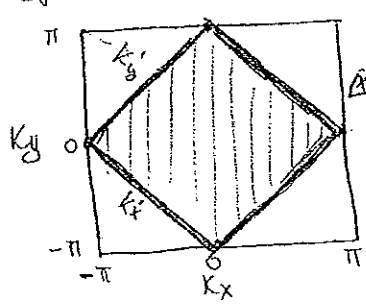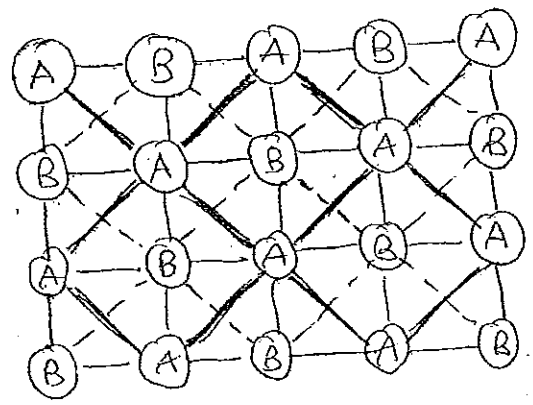
number of sites
(= number of particles)

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 two sublattices A and B:
  • They build clearly two equal square lattices (in 2D)
  • The new Brillouin zone is hence of the form (for each sublattice)

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 $\frac{1}{2}$ of the original Brillouin zone.

* We may then introduce the discrete Fourier transform:

  • Sublattice $\textcircled{A}$: $\hat{C}_{\vec{j}s} = \frac{1}{\sqrt{N/2}} \sum_{\vec{k}\in RBZ} e^{+i\vec{k}\cdot\vec{j}} \hat{a}_{\vec{k}s}$

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

The sublattices have $\frac{1}{2}$ of the total number of sites.

* Then for $\textcircled{A}$

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

and for $\textcircled{B}$ 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:

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

• Let's consider now <u>the hopping term</u>

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

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

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

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

- Let $\epsilon_{\vec{K}} = -t \sum_{\vec{\delta}} e^{-i\vec{K}\vec{\delta}}$ [2D]

$\left[\begin{array}{l} \text{since } \vec{R} = K_x \vec{e}_x' + K_y \vec{e}_y' \text{ with } -\frac{\pi}{\sqrt{2}} \leq K_{x,y} \leq \pi/\sqrt{2} \\ \text{but } \vec{\delta} = \pm\vec{e}_x, \pm\vec{e}_y \text{ with } \vec{e}_x' = (\vec{e}_x + \vec{e}_y)/\sqrt{2}, \vec{e}_y' = (-\vec{e}_x + \vec{e}_y)/\sqrt{2} \\ \text{Then } \epsilon_{\vec{K}} = -t\left[\cos\left(\frac{K_x - K_y}{\sqrt{2}}\right) + \cos\left(\frac{K_x + K_y}{\sqrt{2}}\right)\right] = -2t\cos\left(\frac{K_x}{\sqrt{2}}\right)\cos\left(\frac{K_y}{\sqrt{2}}\right) \end{array} \right]$

* 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:

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

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

$= \frac{UN}{4}(1+m_s)^2 + \sum_{\vec{K}\in RBZ} \sum_{S} \left[\epsilon_{\vec{K}}^{(+)} \hat{\alpha}_{\vec{K}S}^{(+)+} \alpha_{\vec{K}S}^{(+)} + \epsilon_{\vec{K}}^{(-)} \hat{\alpha}_{\vec{K}S}^{(-)+} \alpha_{\vec{K}S}^{(-)} \right]$

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

$$\boxed{\epsilon_{\vec{K}}^{(\pm)} = \pm\sqrt{\epsilon_{\vec{K}}^2 + \left(\frac{Um_s}{2}\right)^2}}$$

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

Above $\alpha_{\vec{K}S}^{(\pm)}$ are the corresponding operators for the upper and lower branch.

* At zero temperature the ground state for an average $\langle n \rangle = 1$ 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 $T=0$:

$$E_0 = \frac{UN}{4}(1+m_s^2) + 2\sum_{\vec{K}\in RBZ} \mathcal{E}_{\vec{K}}^{(-)}$$

$$= \frac{UN}{4}(1+m_s^2) - 2\sum_{\vec{K}\in RBZ} \sqrt{\mathcal{E}_{\vec{K}}^2 + \left(\frac{U^2 m_s^2}{4}\right)}$$

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

$$\frac{\partial E_0}{\partial m_s} = \frac{UN}{2} m_s - 2\sum_{\vec{K}\in RBZ} \frac{\frac{1}{2}\frac{U^2 \cdot 2m_s}{4}}{\sqrt{\mathcal{E}_{\vec{K}}^2 + U^2 m_s^2/4}} = 0$$

Hence: $$\boxed{1 = \frac{U}{2(N/2)} \sum_{\vec{K}\in RBZ} \frac{1}{\sqrt{\mathcal{E}_{\vec{K}}^2 + U^2 m_s^2/4}}}$$

in 2D, $1 \simeq \frac{U}{2t}\frac{1}{2\pi^2}\iint_{-\pi/\sqrt{2}}^{\pi/\sqrt{2}} d^2 K \frac{1}{\sqrt{4\cos^2\left(\frac{K_x}{\sqrt{2}}\right)\cos^2\left(\frac{K_y}{\sqrt{2}}\right) + \frac{U^2}{2t^2}m_s^2}}$

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

* At weak coupling, where the Hartree approximation is a reasonable $\uparrow$ 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 <u>spin density wave</u> with wavevector $\vec{Q} = (\pi,\pi)$ and a very weak modulation.

. At finite T one needs a finite U/t to get AntiFerromagnetism. Conversely, for a given U/t there's a critical $T \rightarrow T_{NÉEL}$ (so-called <u>Neel Temperature</u>) 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).

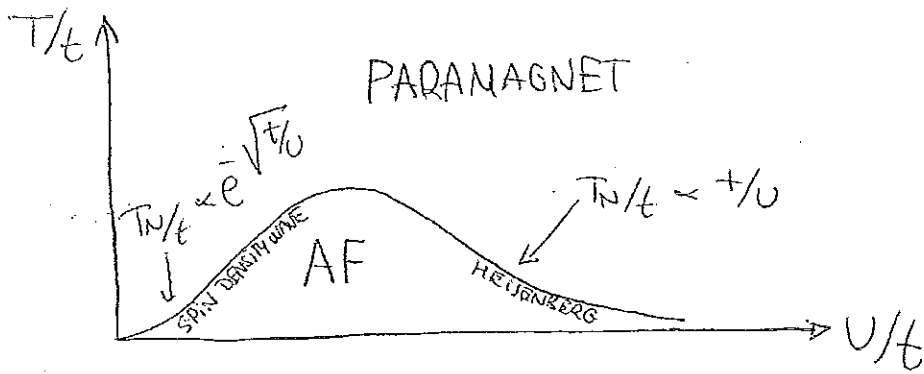Hence $\frac{T_{NÉEL}}{t} \sim \frac{t}{U}$ and hence decreases with U/t.
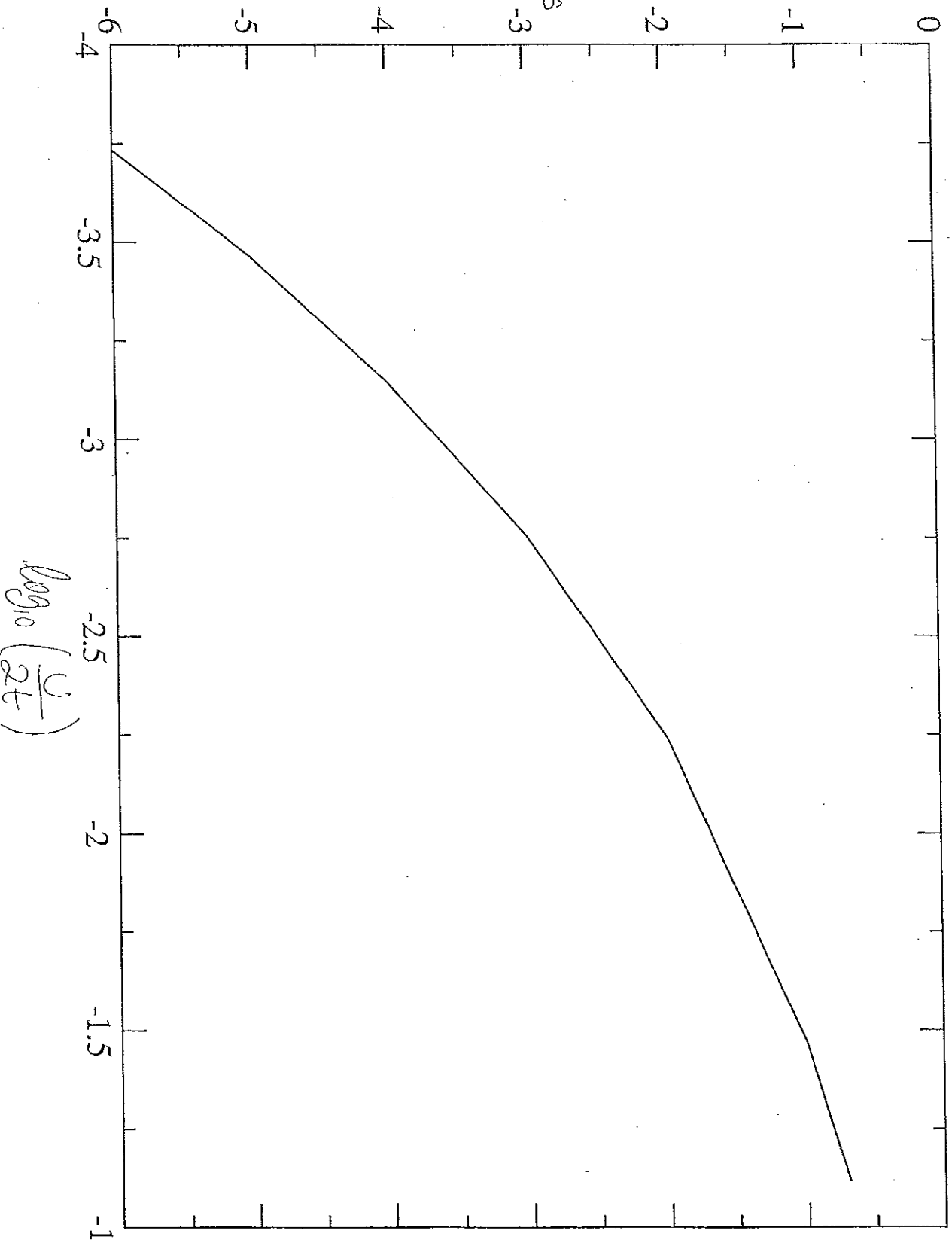
* In between the two regimes T_N/t reaches a maximum value (4)

T/t ↑

PARAMAGNET

$T_N/t \propto e^{-\sqrt{t/U}}$

$T_N/t \sim t/U$

SPIN DENSITY WAVE

AF

HEISENBERG

→ U/t

* 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 (paramagnetic metal) from itinerant to Mott localized as U/t increases, or as T is decreased below the Mott gap. ($\sim U$ at large U/t).
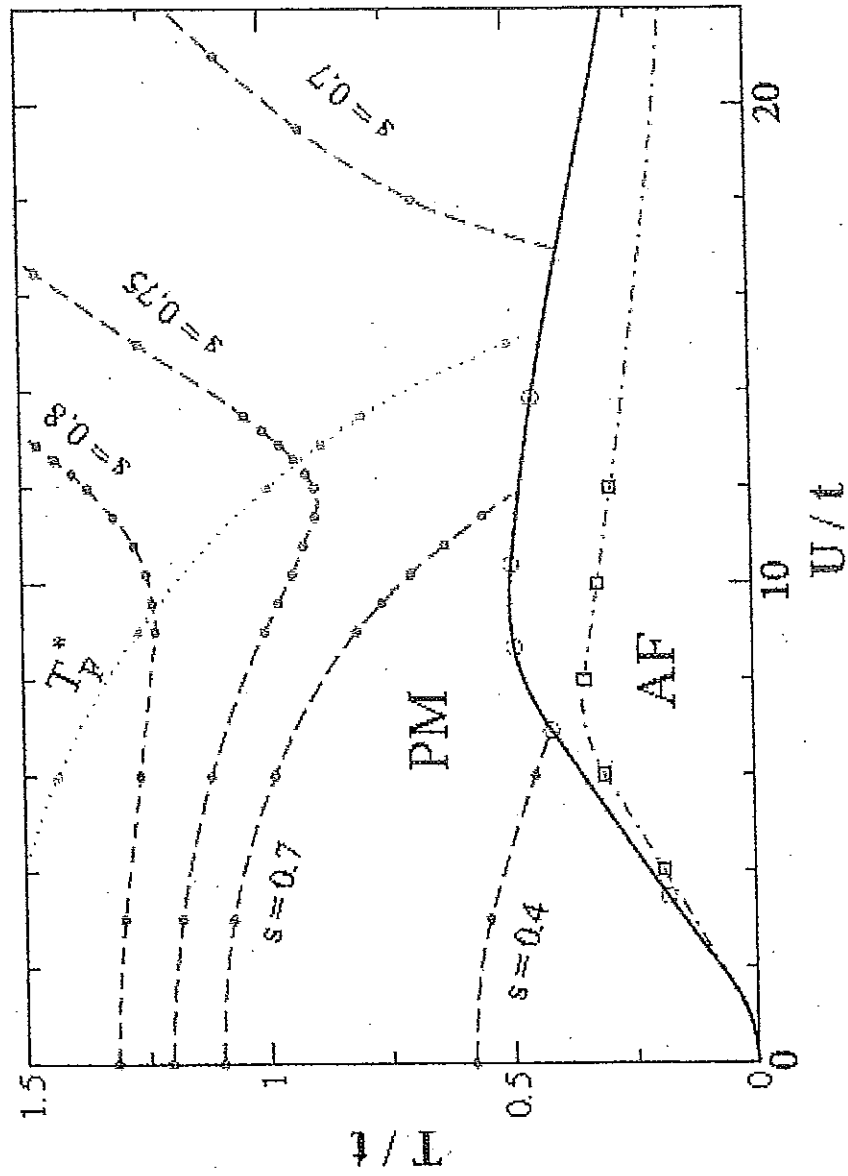

✳ ENTROPY

- The Néel temperature T_N is a rather low scale. Even at its maximum $T_N \sim 0.3 t$ 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.
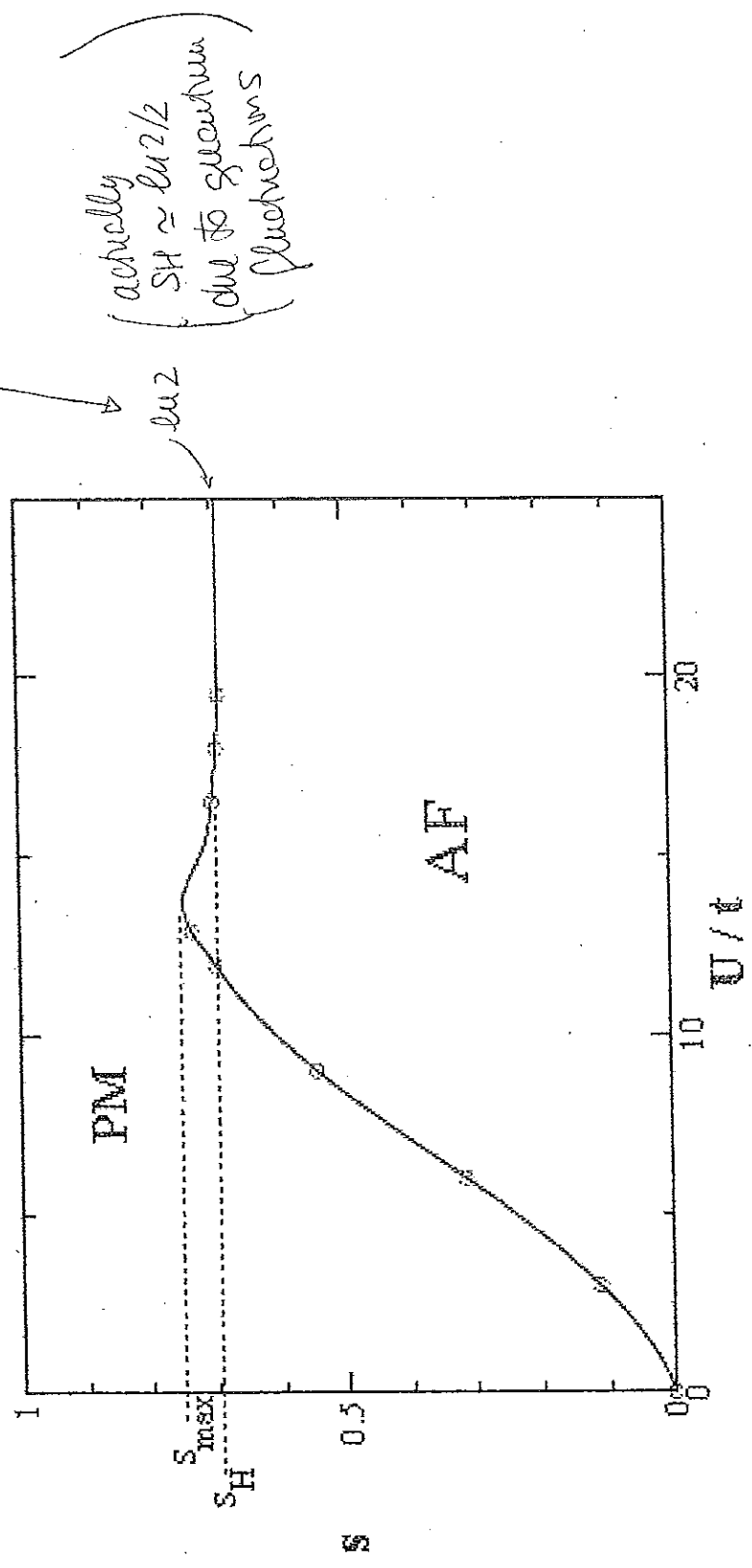
* In the homogeneous half-filled Hubbard model, the entropy per particle is a function $S(T/t, U/t)$. The entropy itself is a good thermometer, since $\partial S/\partial T > 0$.

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

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

* DMFT result

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

$\ln 2$

PM

AF

S_{max}

S_H

S

U / t

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

$$S_N(U) = S_N(T_N(U), U) \qquad \left[\begin{array}{l} \text{see the curve in p. } \textcircled{23} \\ \text{for } T_N(U), \text{ and of } S_N(U) \text{ in p. } \textcircled{44} \end{array} \right]$$

* 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 $S_H = k \ln 2$. This is somehow the naive expectation. Note that a paramagnet with the same probability to be $\uparrow$ or $\downarrow$ M 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 result).

* 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 $H \sim U n_{i\uparrow} n_{i\downarrow}$). 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:

$$\frac{dS_N}{du} = \frac{\partial S_N}{\partial T_N}\frac{dT_N}{du} + \frac{\partial S_N}{\partial U} = \frac{C(T_N)}{T_N}\frac{dT_N}{du} - \frac{\partial P_2}{\partial T}\bigg|_{T=T_N}$$

where $C(T,N)$ is the <u>specific heat per particle</u> ($C = T \partial S/\partial T$).

• 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 <u>Pomeranchuk</u> <u>Effect</u> (known from liquid ^{3}He). 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.⑲ 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.㊹)

The figure of p.㊹ 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.

* First experiments on short-range antiferromagnetic correlations have been recently performed at T. Esslinger's group. Let's have a brief look to them.
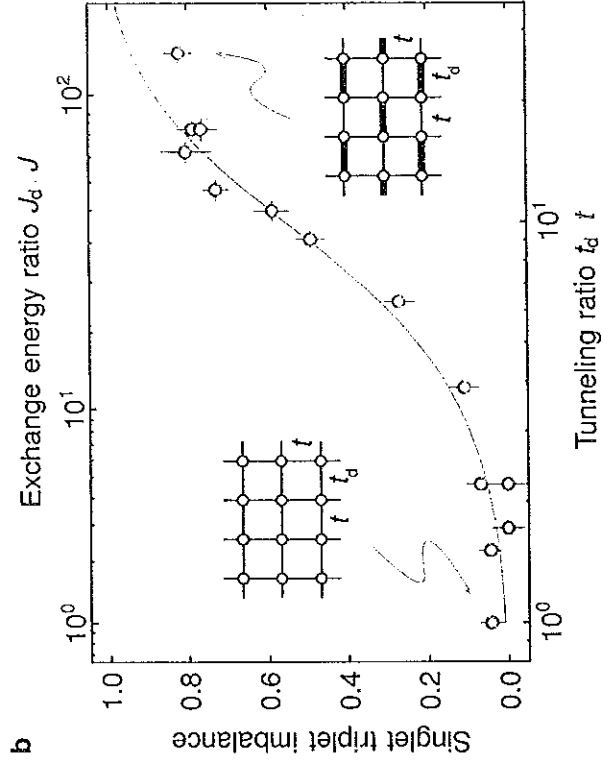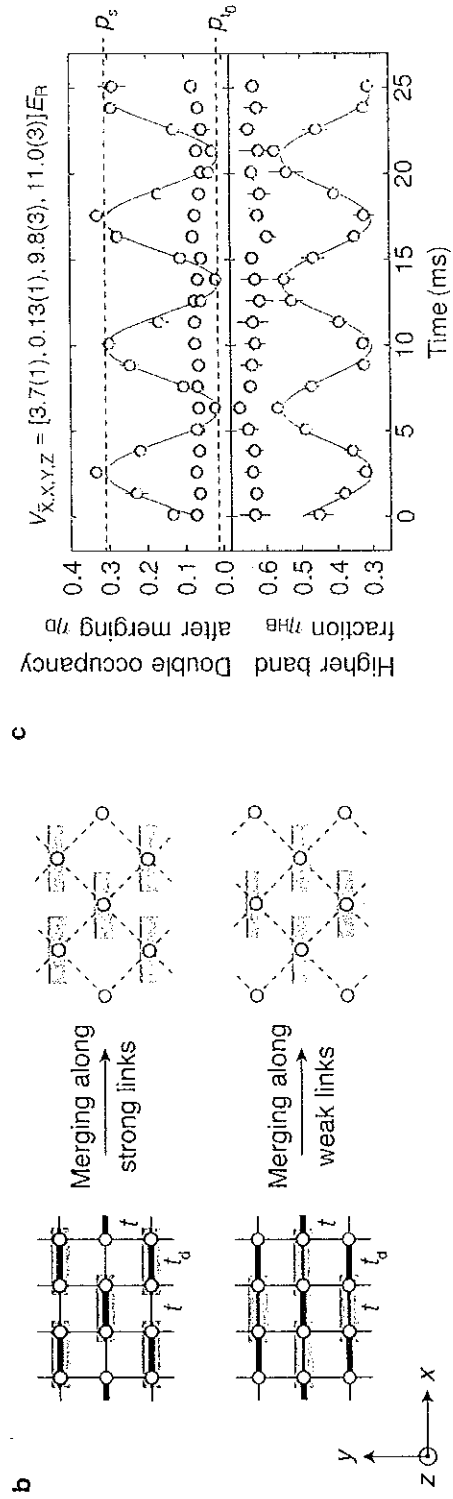
Short-range AF correlations [Greif et al., Science **340**, 1307 (2013)]
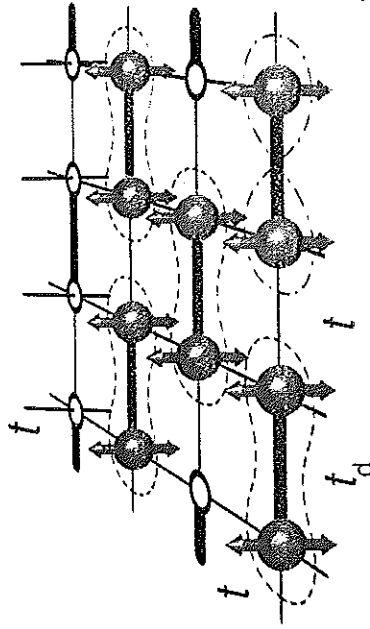
Observation of short-range AFM in dimerized lattices
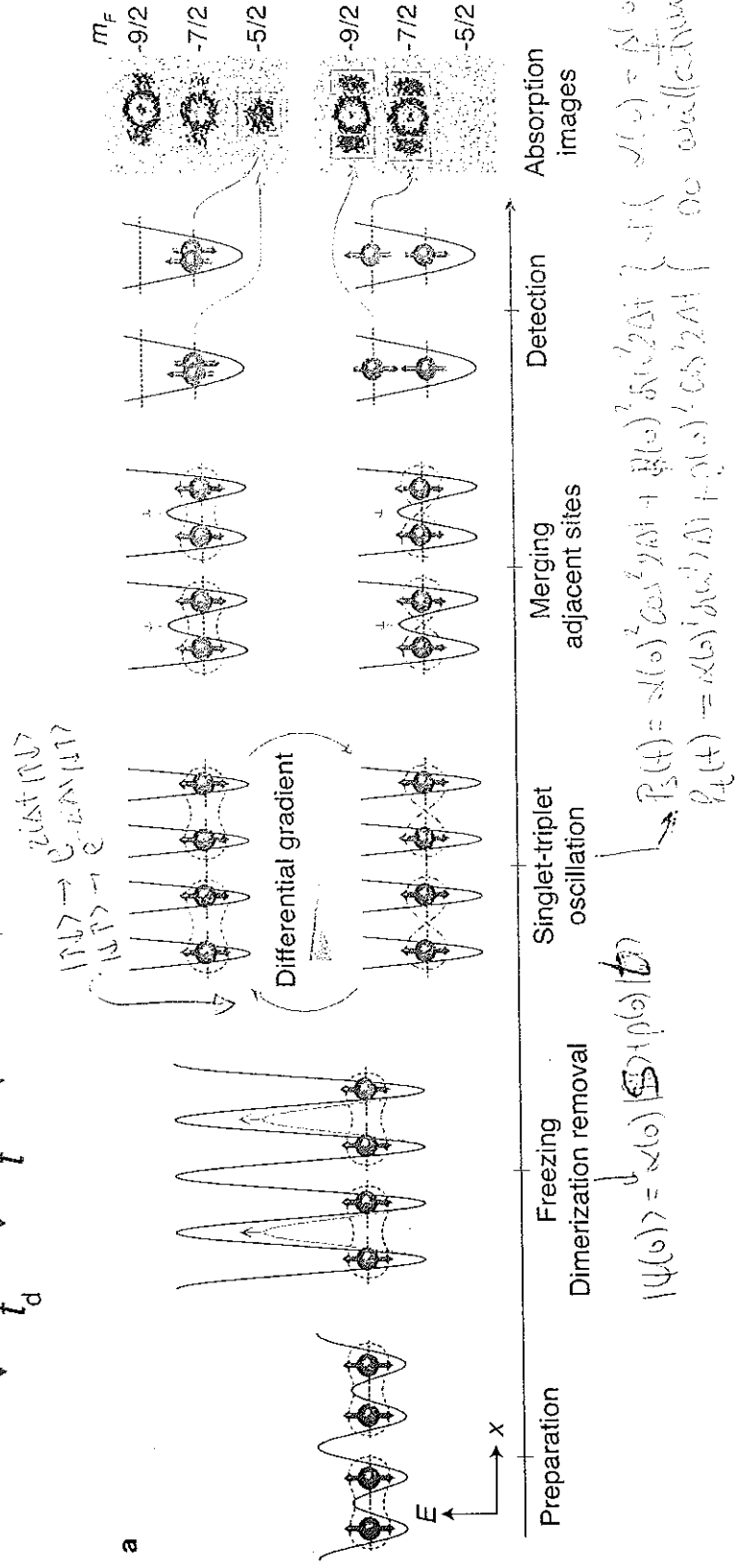
# Short-range AF correlations [Greif et al., Science **340**, 1307 (2013)]

Singlet vs triplet imbalance

$$\mathcal{I} = \frac{p_s - p_t}{p_s + p_t}$$

* 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 <u>holes</u> in such system.

* Let's consider 2 neighbouring holes like in the figure
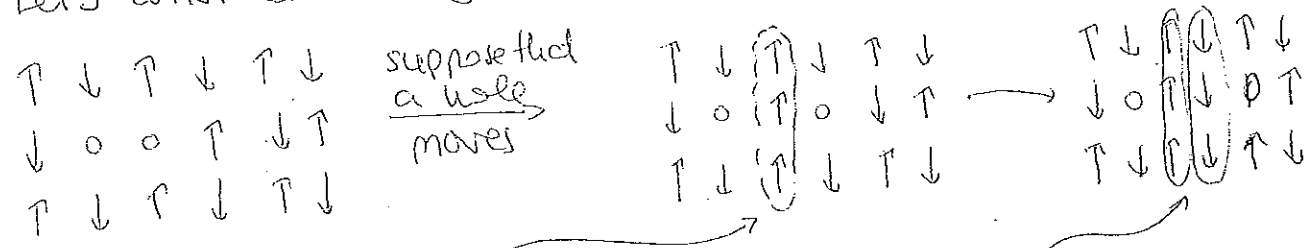
The motion of a hole in an AF background creates a string of flipped spins

The further the hole moves the more strings are created.

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

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

* <u>The effective attraction between holes suggest the possibility of pairing</u>: 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:

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

$\left[\begin{array}{l}\text{Note: s-wave symmetry would be}\\ \cos p_x + \cos p_y\end{array}\right]$

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

$$\Delta_d = \frac{1}{N} \sum_p \Delta_p \, C_{p\uparrow} C_{-p\downarrow} \overset{\text{Fourier transform}}{=\!=\!=\!=}$$

$$= \frac{1}{N} \sum_\ell \frac{\Delta_0}{2} \left[(C_{\ell+x,\uparrow} C_{\ell\downarrow} - C_{\ell+x,\downarrow} C_{\ell\uparrow}) - (C_{\ell+y\uparrow} C_{\ell\downarrow} - C_{\ell+y\downarrow} C_{\ell\uparrow}) \right.$$
$$\left. + (C_{\ell-x\uparrow} C_{\ell\downarrow} - C_{\ell-x\downarrow} C_{\ell\uparrow}) - (C_{\ell-y\uparrow} C_{\ell\downarrow} - C_{\ell-y\downarrow} C_{\ell\uparrow}) \right]$$

next neighbor along x / next neighbor along y / sites / 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)]
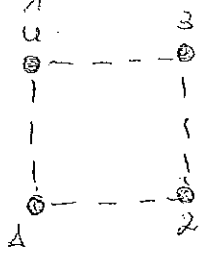
* For large U the largest real space amplitude in the 4-particle ground state are for the Neel configuration

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

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

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

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

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 projects out double occupancy):

$$|\psi_2\rangle = (C_{1\uparrow}^+ C_{2\downarrow}^+ + C_{1\uparrow}^+ C_{3\downarrow}^+ + \dots)|VAC\rangle$$

• 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:

- S-wave operator:
$$\begin{aligned} A_s = &(C_{1\uparrow} C_{2\downarrow} - C_{1\downarrow} C_{2\uparrow}) \\ &+ (C_{1\uparrow} C_{4\downarrow} - C_{1\downarrow} C_{4\uparrow}) \\ &+ (C_{2\uparrow} C_{3\downarrow} - C_{2\downarrow} C_{3\uparrow}) \\ &+ (C_{3\uparrow} C_{4\downarrow} - C_{3\downarrow} C_{4\uparrow}) \end{aligned}$$

- d-wave operator:
$$\begin{aligned} A_d = &(C_{1\uparrow} C_{2\downarrow} - C_{1\downarrow} C_{2\uparrow}) \\ &- (C_{1\uparrow} C_{4\downarrow} - C_{1\downarrow} C_{4\uparrow}) \\ &+ (C_{2\uparrow} C_{3\downarrow} - C_{2\downarrow} C_{3\uparrow}) \\ &- (C_{3\uparrow} C_{4\downarrow} - C_{3\downarrow} C_{4\uparrow}) \end{aligned}$$

* It's quite easy to see that $\langle \Psi_2 | \Delta_S | \Phi_{ab} \rangle = 0$

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

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

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

* This suggest that holes pair in d-wave.

* d-wave pairing plays a crucial role in <u>high-temperature superconductg</u> cuprates. A simplied phase diagram for cuprates is shown in p. (S2) where we see the AF phase (at low or zero doping) 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 superfluiding 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-Tc superconductors!

High-Tc cuprate superconductors
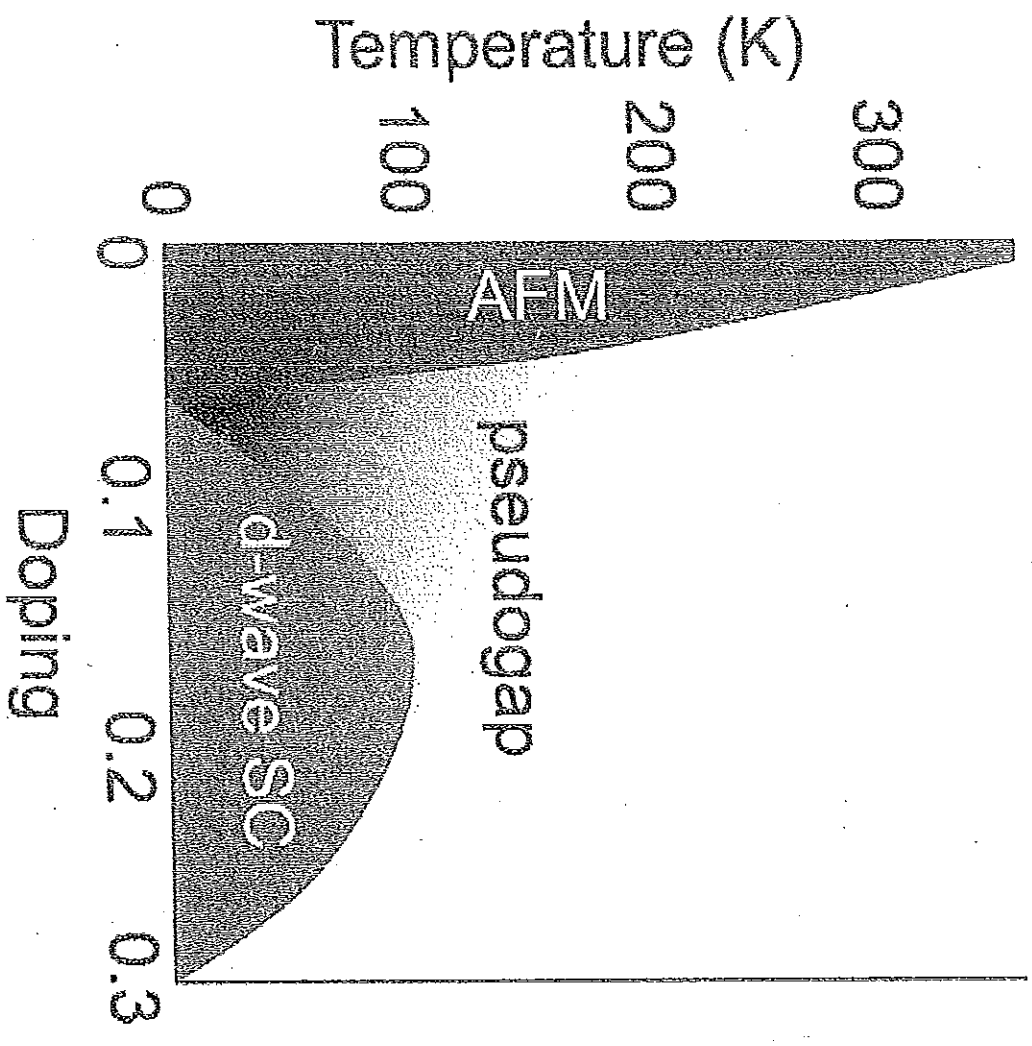
Simplified cuprate
phase diagram