

DEMOCRITOS
DEmocritos MOdeling Center for
Research In aTOMistic Simulation **INFM**



Ground-state properties of the disordered Hubbard model in 2D

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OUTLINE

- AIM: studying the **INTERPLAY** of **DISORDER** and **INTERACTION** within the 2d Hubbard with disorder
- METHOD: Variational Monte Carlo
- RESULTS (1): the transition from an Anderson Insulator to Mott insulator with a paramagnetic solution
- RESULTS (2): phase diagram for the magnetic solution

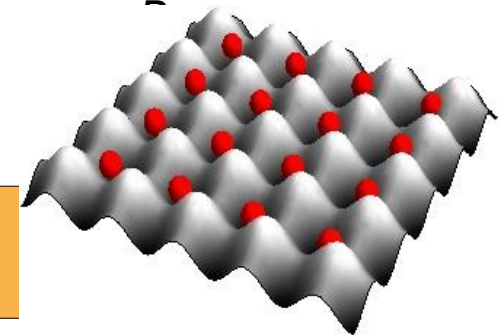
DISORDERED HUBBARD MODEL

2 dimensions

• # sites = # electrons

$$H = - \sum_{\langle RR' \rangle, \sigma} t_{R,R'} c_{R,\sigma}^\dagger c_{R',\sigma} + U \sum_R n_{R,\uparrow} n_{R,\downarrow} + \sum_R \epsilon_R n_R$$

$$\epsilon_R \in [-D, D]$$

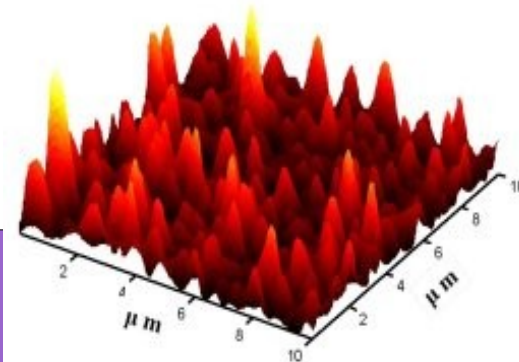


$D=0$



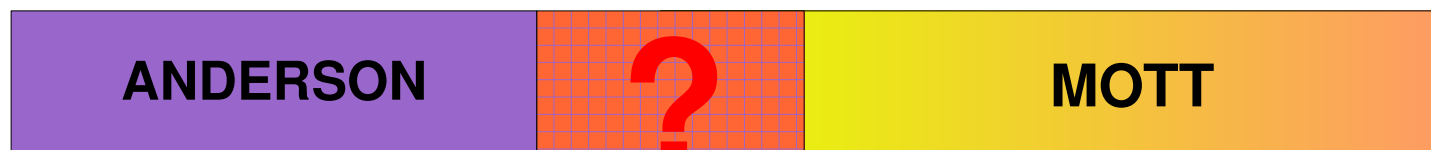
U

$U=0$



D

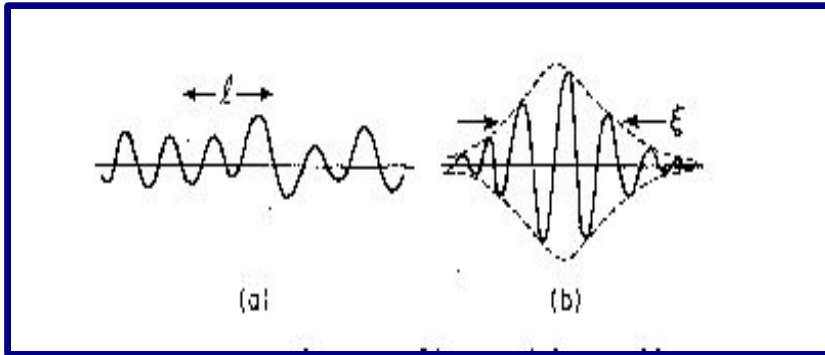
$D \neq 0$



U

MIT in 2 DIMENSIONS

- EXPERIMENTS ON Si Mosfets



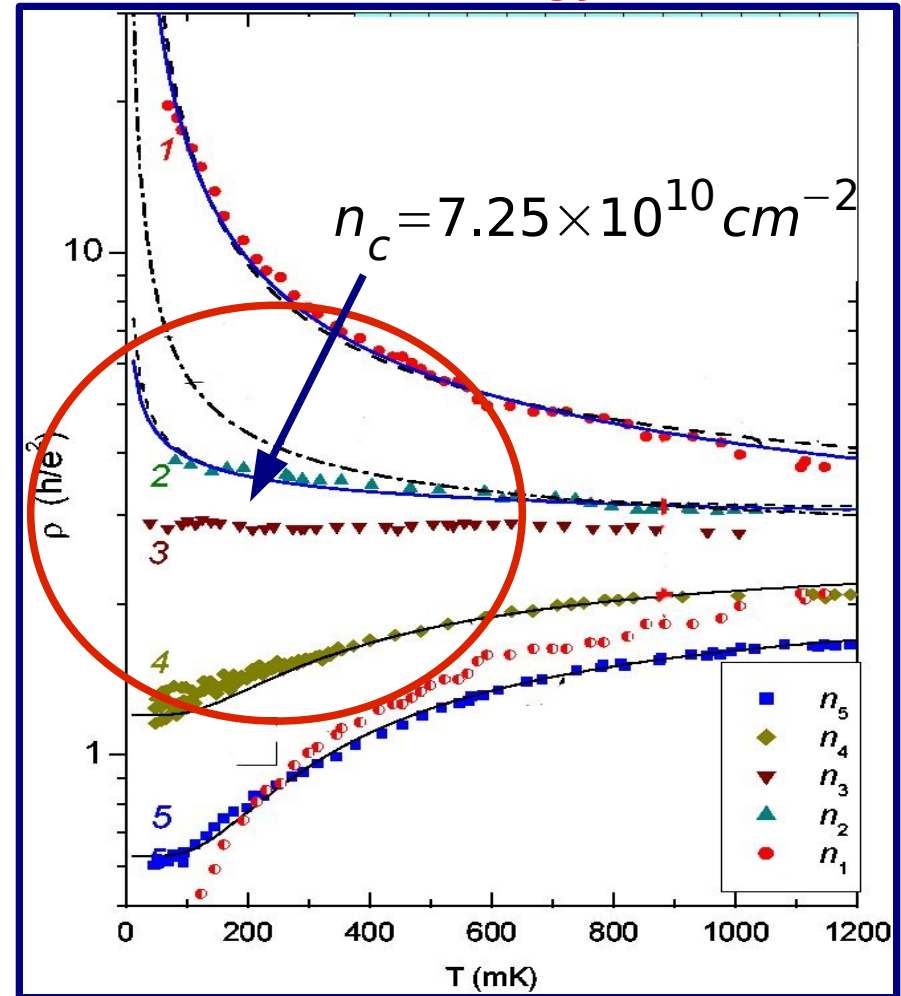
E_{e-e} is the dominant energy scale.

SCALING THEORY OF LOCALIZATION:

IN 2 dimensions

FOR ANY FINITE AMOUNT OF
DISORDER
THERE ARE NO EXTENDED STATES

T=0 INSULATOR

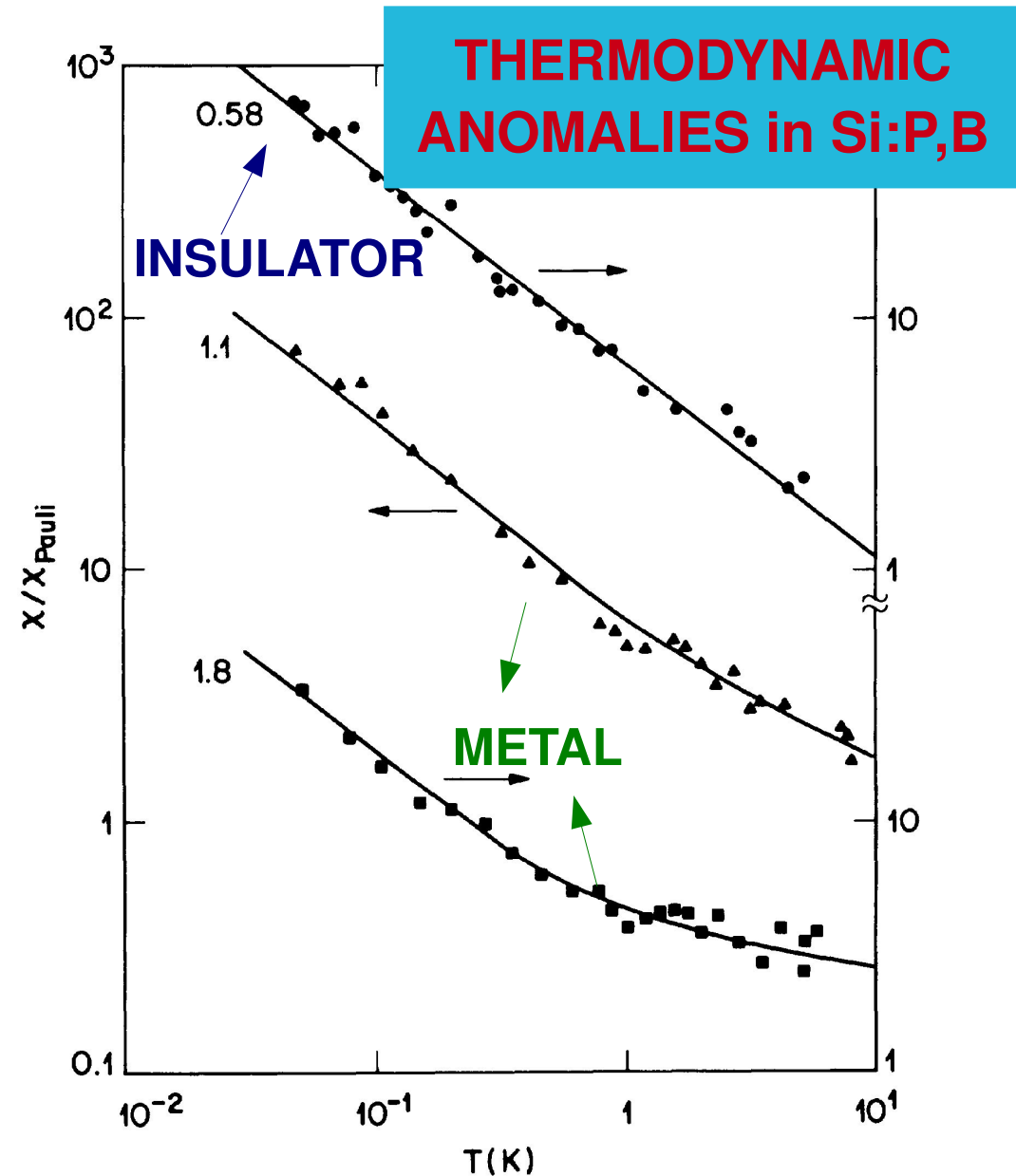
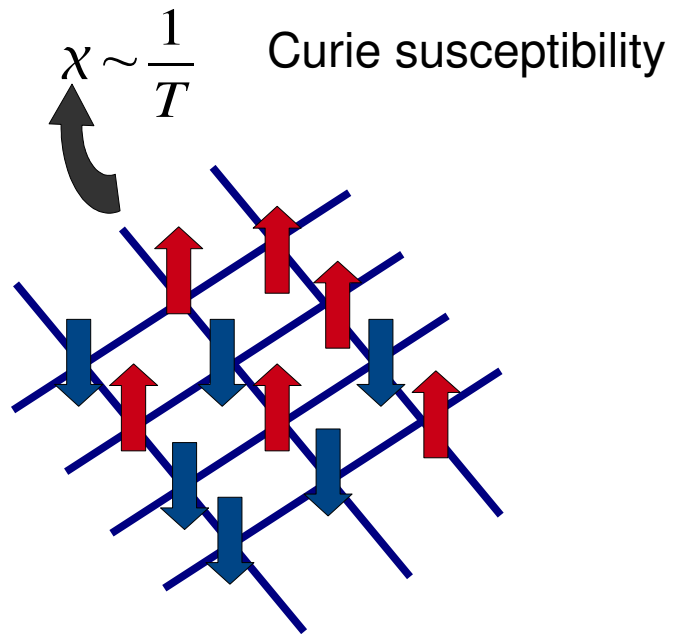


Abrahams, Anderson,
Licciardiello, Ramakrishnan

(Phys Rev Lett 42, 673) (1979)

Kravchenko et al., Phys. Rev. Lett. **84**, 2909
Punnoose et al. Science **310**, 289 (2005)

EFFECTS of the COMPETITION between DISORDER and INTERACTION



Hirsch et al., Phys. Rev. Lett. 68, 1418

METHOD

- Variational MC**

$$E_0(\alpha) = \langle \psi_T(\alpha) | H_{HUB} | \psi_T(\alpha) \rangle$$

$$H_{HUB} = - \sum_{\langle RR' \rangle, \sigma} t_{R,R'} c_{R,\sigma}^\dagger c_{R',\sigma} + U \sum_R n_{R,\uparrow} n_{R,\downarrow} + \sum_R \epsilon_R n_R$$

- Trial wave function**

$$|\psi_T\rangle = P_G P_J |\psi_0\rangle$$

$|\psi_0\rangle$ **INCLUDES DISORDER BUT NO CORRELATION**

$$H_{MF} = -t \sum_{\langle RR' \rangle, \sigma} c_{R,\sigma}^\dagger c_{R',\sigma} + \sum_R \tilde{\epsilon}_{R,\uparrow} n_{R,\uparrow} + \sum_R \tilde{\epsilon}_{R,\downarrow} n_{R,\downarrow}$$



+ CORRELATIONS

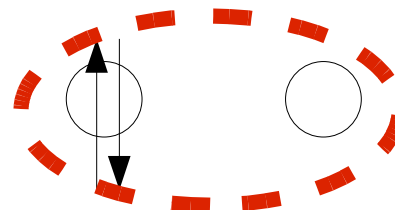
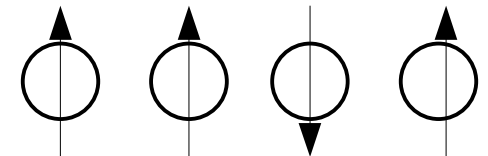
$$P_G = e^{\sum_R g_R n_R^2}$$

It describes a non realistic Mott insulator

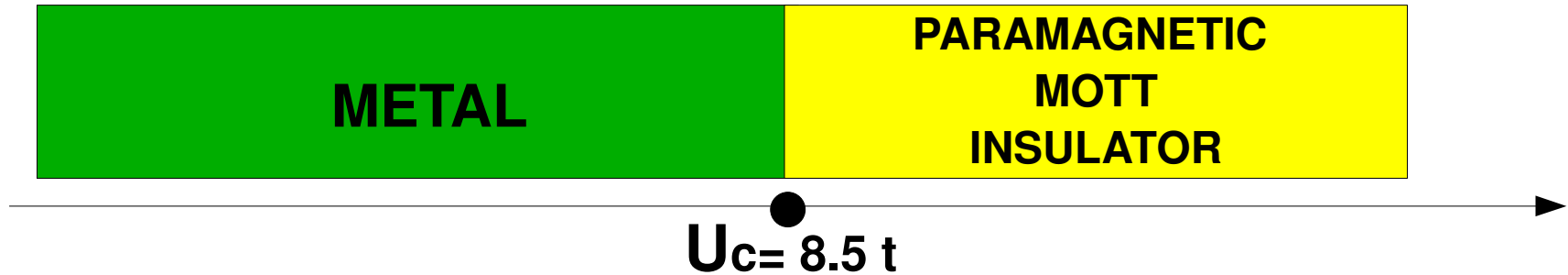


+ LONG RANGE CORRELATIONS

$$P_J = e^{-\frac{1}{2} \sum_{\langle RR' \rangle} v_{RR'} (n_R - 1)(n_{R'} - 1)}$$



The limit $D=0$: the Hubbard model



M. Capello, et al. Phys. Rev. Lett **94**, 026406 (2005)

How to detect a metal insulator transition?

- Static structure factor

$$N_q = \langle n_q n_{-q} \rangle \quad n_q = \frac{1}{L} \sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}} n(\mathbf{R})$$

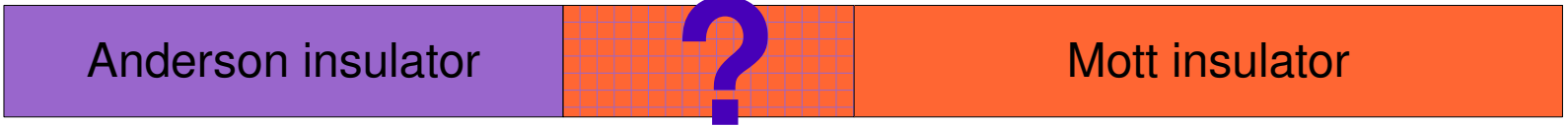
f-sum rule $\Delta_q \sim \lim_{q \rightarrow 0} \frac{q^2}{N_q}$ **average energy of an excitation**

$$N_q \underset{q \rightarrow 0}{\sim} q \quad \text{charge gap} = 0$$

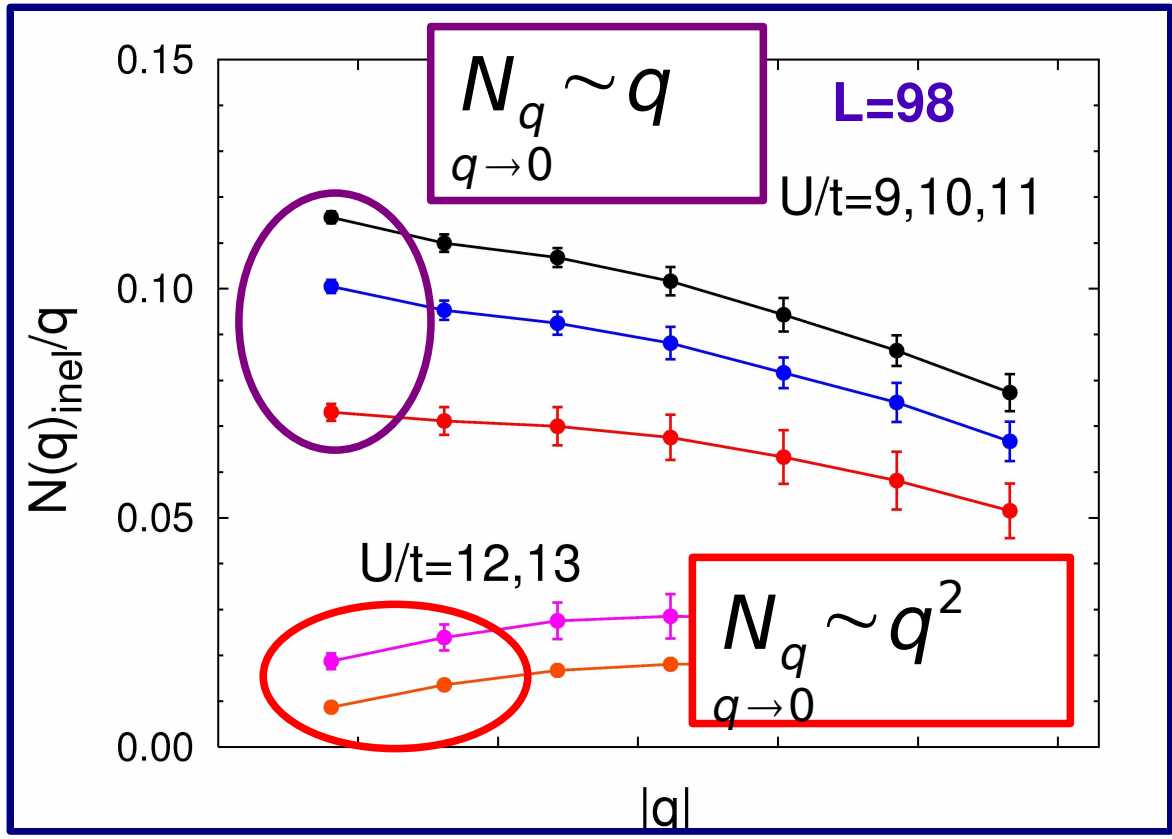
$$N_q \underset{q \rightarrow 0}{\sim} q^r \quad \text{charge gap} \neq 0$$

The paramagnetic wave function

$D = 5$

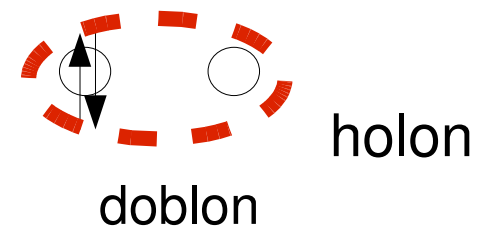


$$|\psi_G\rangle = P_J |\psi_0\rangle \quad H_{MF} = -t \sum_{\langle RR'\rangle, \sigma} c_{R, \sigma}^\dagger c_{R', \sigma} + \sum_R \tilde{\epsilon}_R n_R$$



$U_c = (11.5 \pm 0.5)t$

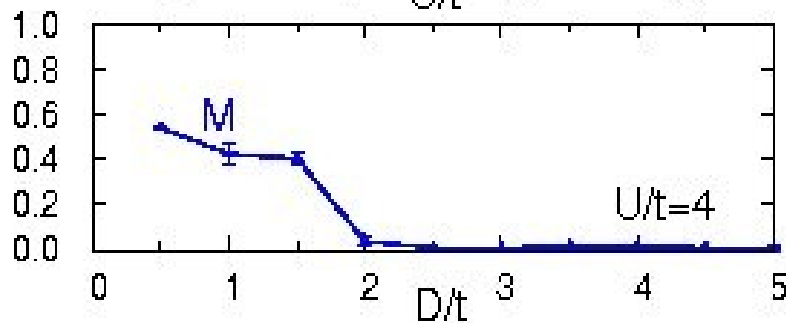
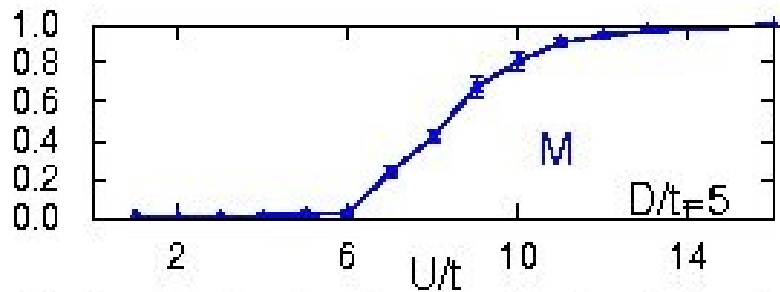
a charge gap opens !!



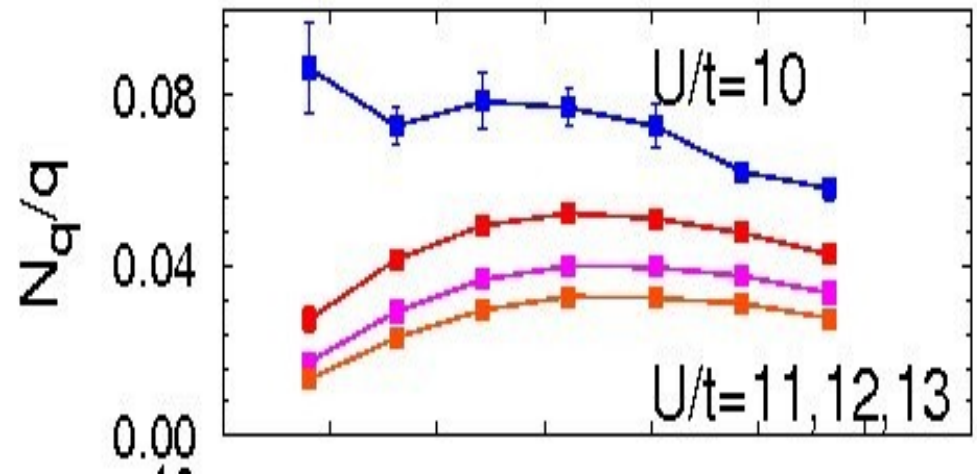
The "MAGNETIC" wave function

$$|\psi_G\rangle = P_J |\psi.\rangle \quad H_{MF} = -t \sum_{\langle RR'\rangle, \sigma} c_{R,\sigma}^+ c_{R',\sigma} + \sum_R \tilde{\epsilon}_{R,\uparrow} n_{R,\uparrow} + \sum_R \tilde{\epsilon}_{R,\downarrow} n_{R,\downarrow}$$

$$M = \frac{1}{L} (-1)^{(i)} \sum_i \langle n_{\uparrow} - n_{\downarrow} \rangle_i$$



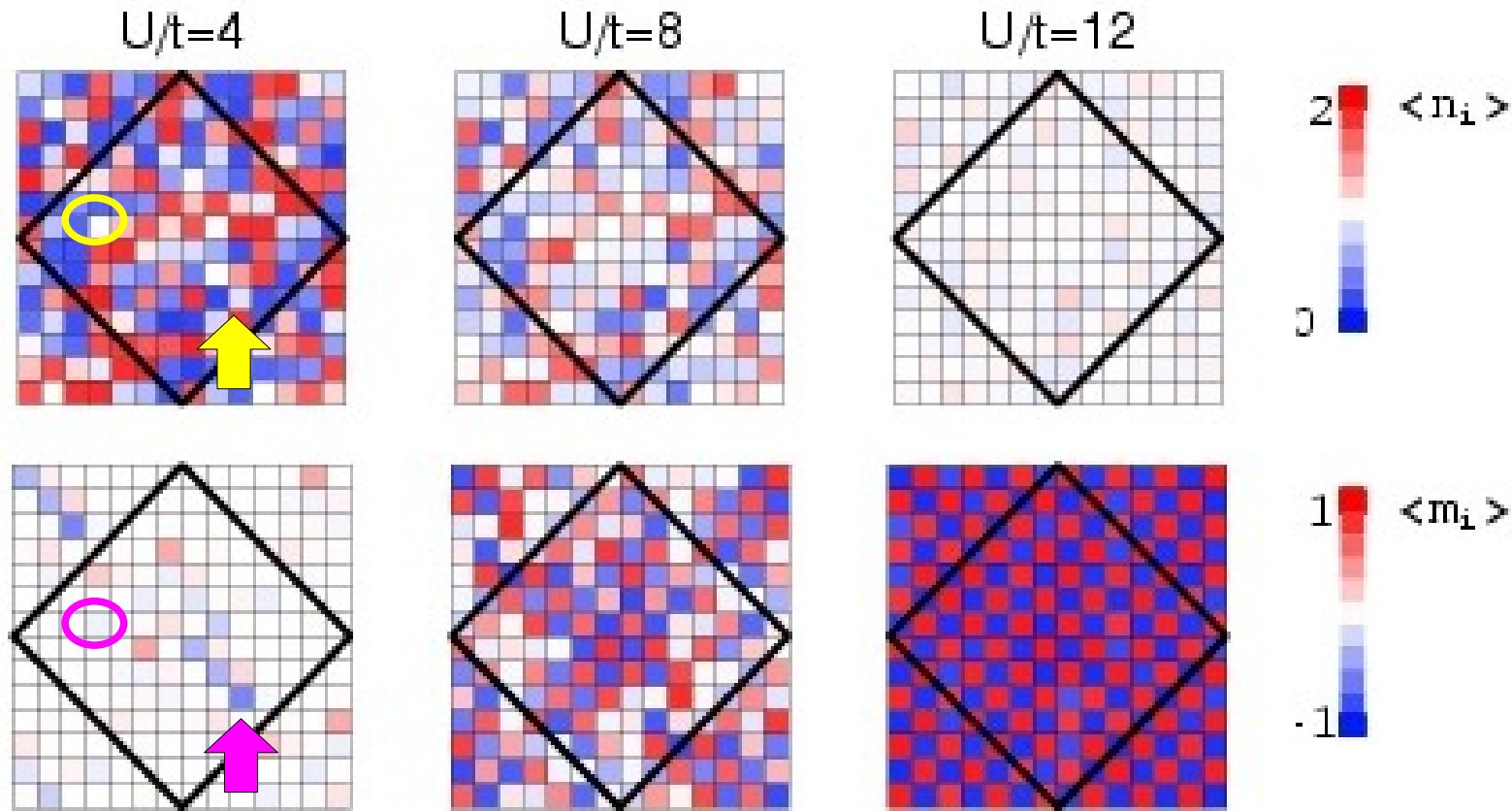
$$N_q = \langle n_q n_{-q} \rangle$$



INTERMEDIATE PHASE

- localized states
- gap = 0
- AF order

LOCAL MAGNETIC MOMENTS



- Presence of local magnetic moments at $T=0$
- Local magnetic moments appear before the onset of long-range order
- Two different "types of electrons"

CONCLUSIONS

- Variational wave function which well describes both an Anderson insulator and a Mott insulator
- INTERMEDIATE PHASE with antiferromagnetic order and finite compressibility
- FORMATION OF LOCAL MOMENTS

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PERSPECTIVES

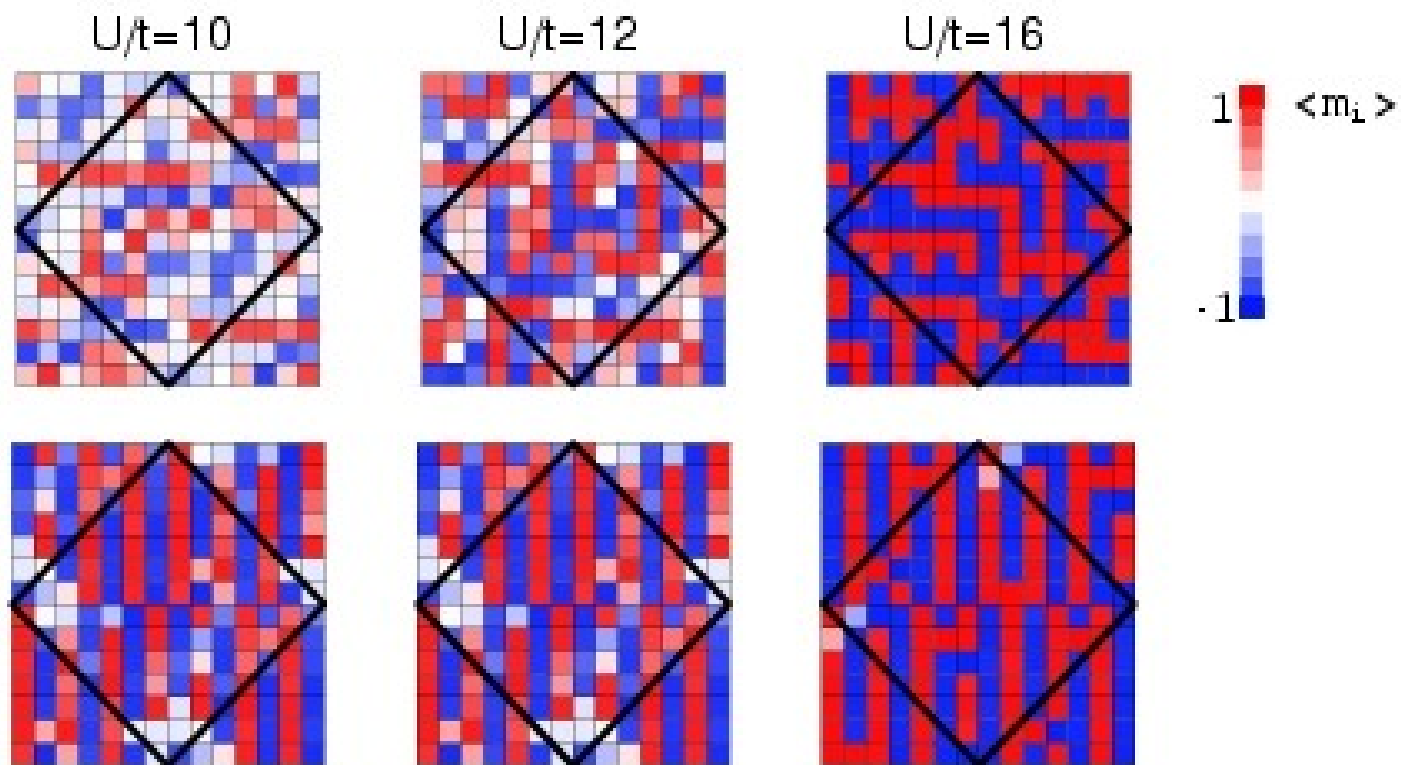
- EXTENSION TO THE THREE DIMENSIONAL CASE
- STUDY OF THE MODEL WITH OFF DIAGONAL DISORDER

Thank you



LOCAL MINIMA

- $t' = 1$



Temperature $\neq 0$ **possible glassy behavior**