Myriad Phases of the Checkerboard Hubbard Model

H. Yao and W-F. Tsai

E. Fradkin and E. Arrigoni

Hubbard model is the "simplest" model of interacting fermions

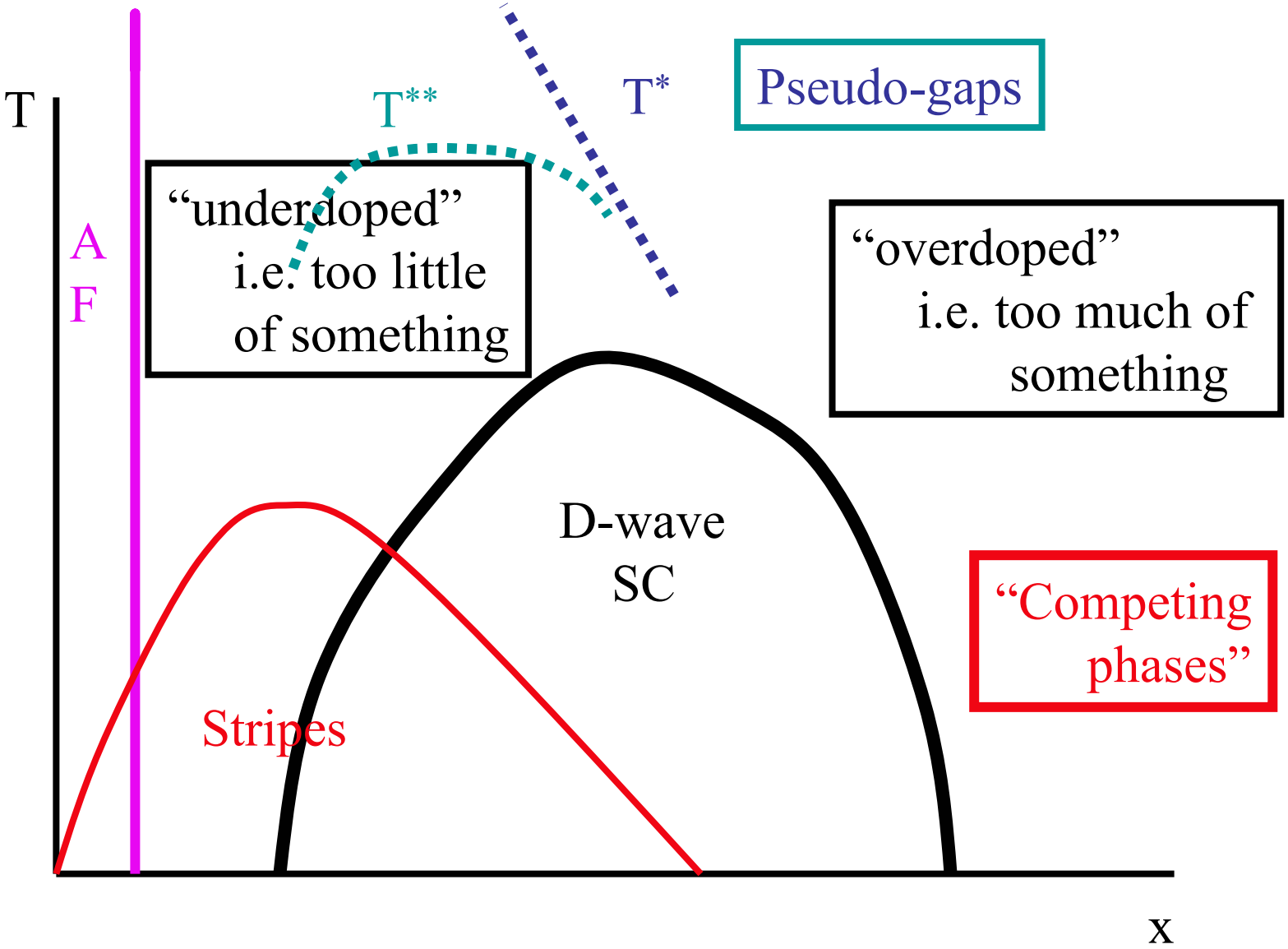
In a literary sense, the Hubbard model is to highly correlated electronic systems as the Ising model is to statistical mechanics.

It has been argued that the Hubbard model holds the secrets of high temperature superconductivity.

The 2D Hubbard model certainly exhibits a remarkably large number of the prominent features of the cuprates: Antiferromagnetism, a tendency to d-wave SC, a tendency to stripe order, pseudo-gaps, …

However, the Hubbard model is not solved in d > 1.

For context, here is the phase diagram of a HTC cuprate



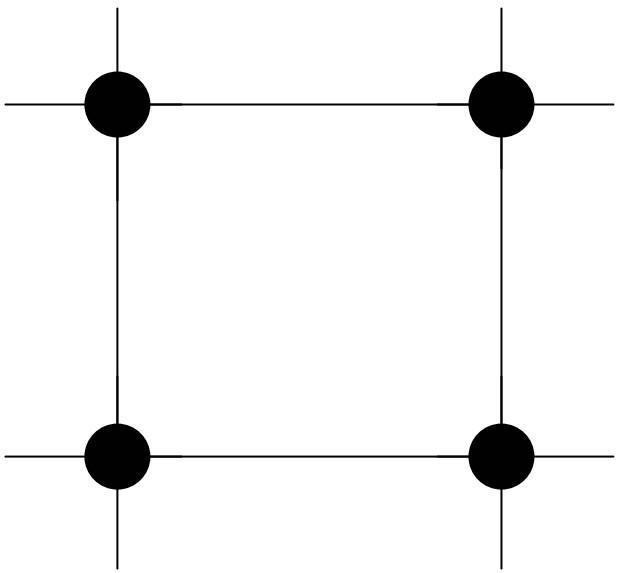
Does d-wave superconductivity occur in the Hubbard model, without any "intermediate bosons" and directly from the repulsive interactions?

(If so, what determines $T_c(x, U, t)$ and is it "high?")

What other phases occur, and where? Are "competing phases" a generic feature of highly correlated electronic systems?

The Hubbard model

$$H = -\sum_{ij,\sigma} t_{ij}\ c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{j}\ \ c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} c_{i,\downarrow} c_{j,\uparrow}$$



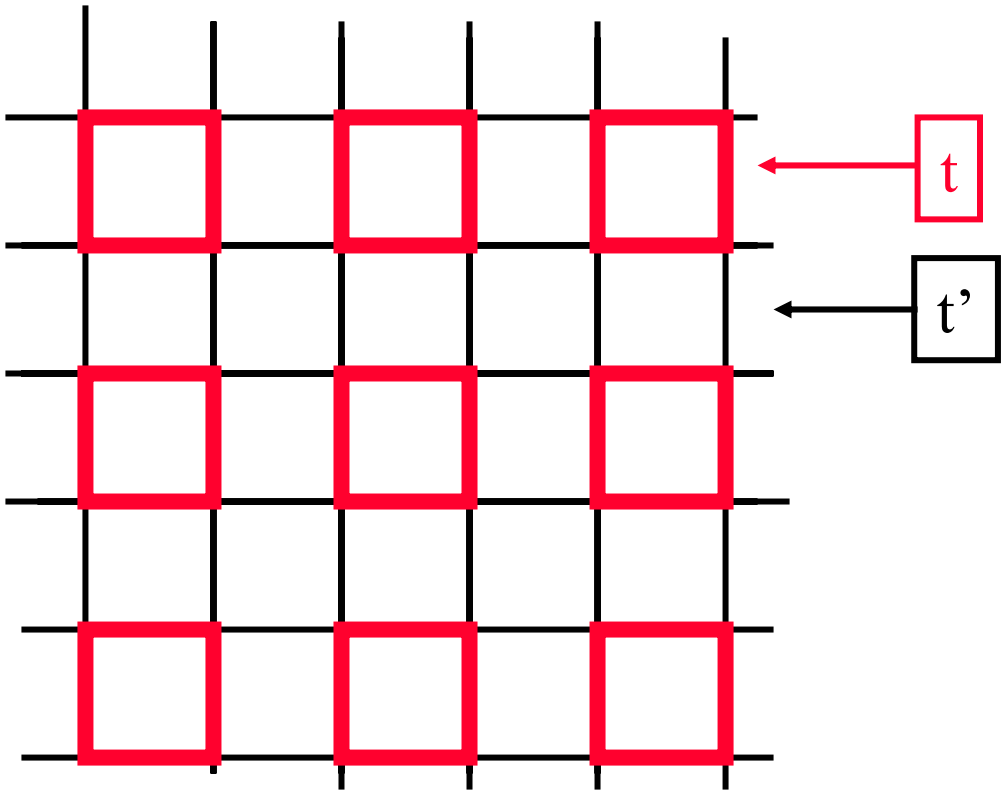
$n_{el} = 1 - x$

x = density of holes
(per site)

Particle-hole symmetry
so we will
take $1 \geq x \geq 0$

Phase diagram of checkerboard Hubbard model

We will solve the model in the "highly inhomogeneous" limit t'/t << 1

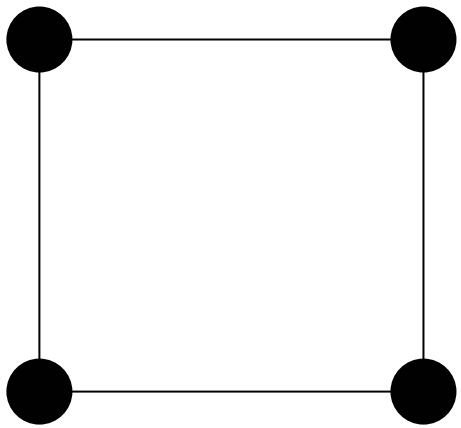


The Hubbard model for t = t'

The Checkerboard Hubbard model for t > t'

Repulsive U Hubbard model on square (4 member ring)

$$H = -\sum_{\langle \mathbf{r},\mathbf{r}' \rangle,\sigma} t_{\mathbf{r},\mathbf{r}'} \left(c^{\dagger}_{\mathbf{r},\sigma} c_{\mathbf{r}',\sigma} + H.c. \right) + U \sum_{\mathbf{r}} n_{\mathbf{r},\uparrow} n_{\mathbf{r},\downarrow},$$

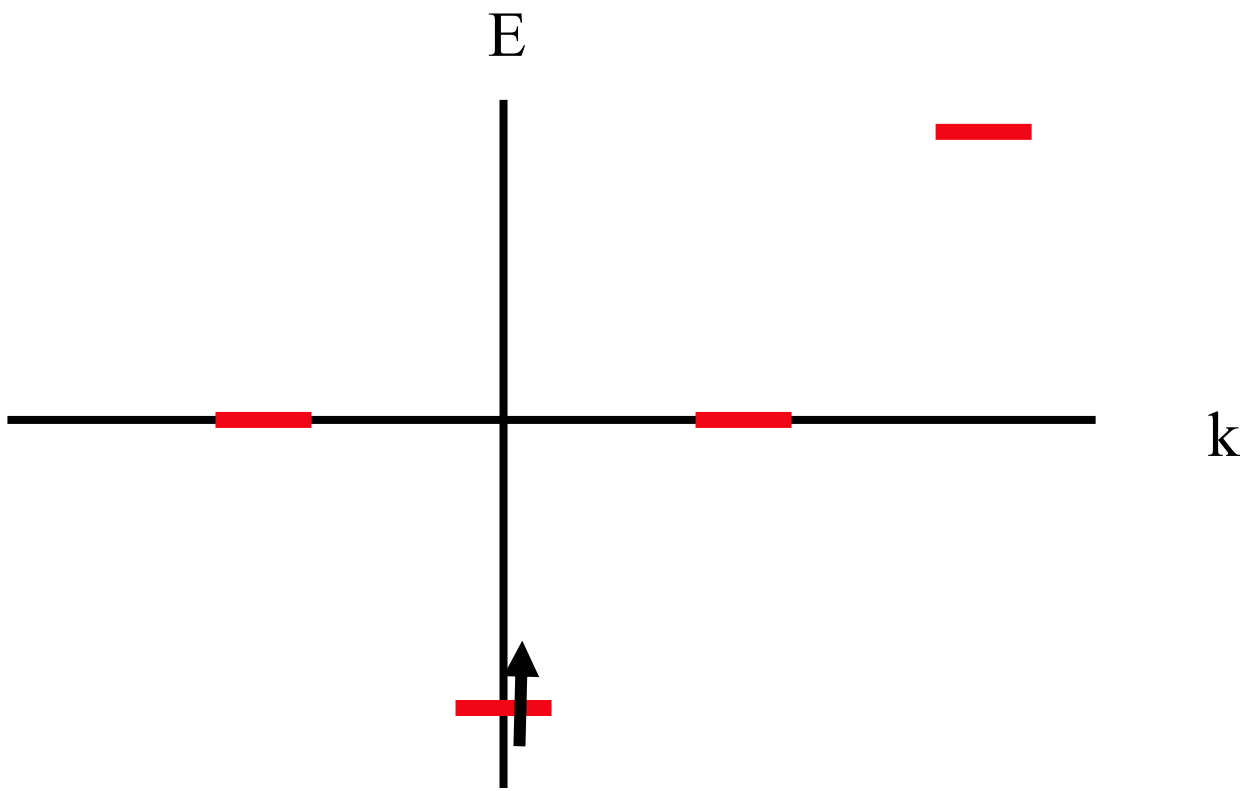


(Solution for t'=0
is direct product
of solutions for
isolated squares.)

4 site Hubbard model (4 member ring)

$N_{el} = 1$

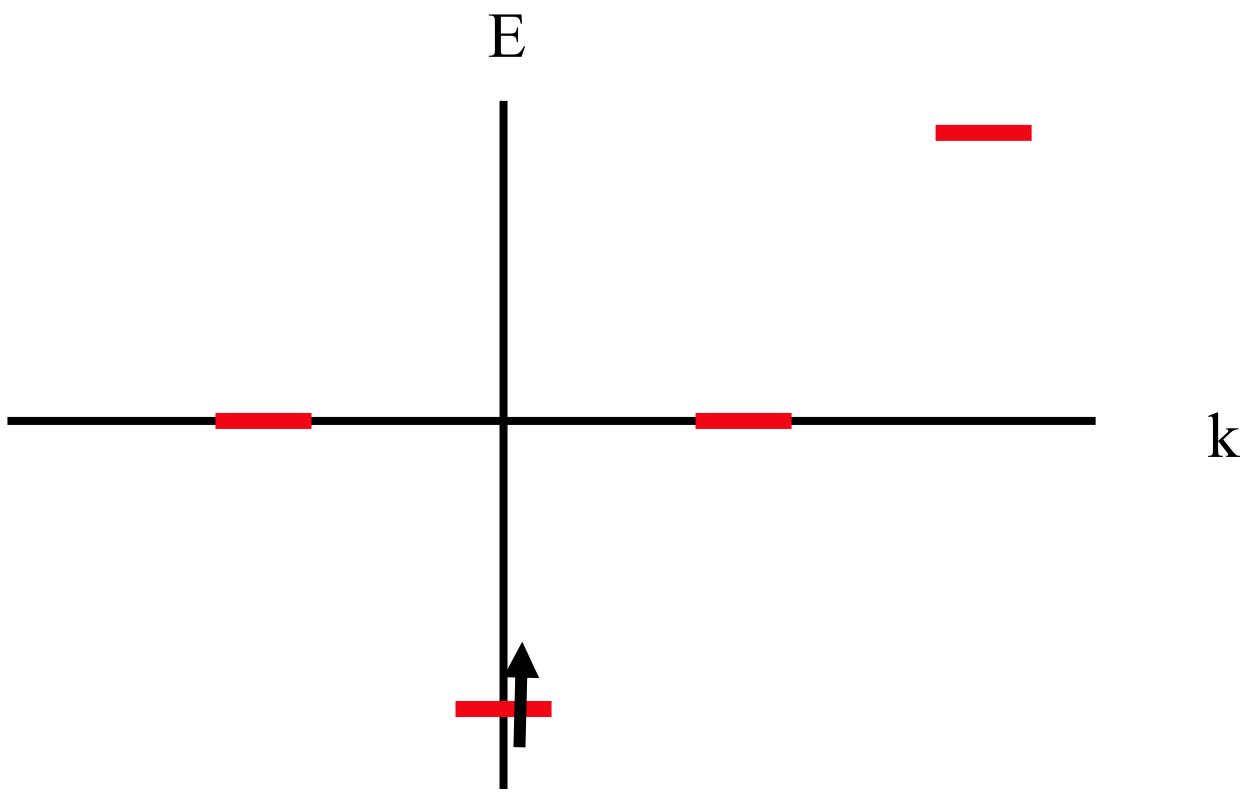
$k = 0, \pm\pi/2, \pi$ $\qquad E = -2t \cos(k)$



4 site Hubbard model (4 member ring)

$N_{el} = 1$

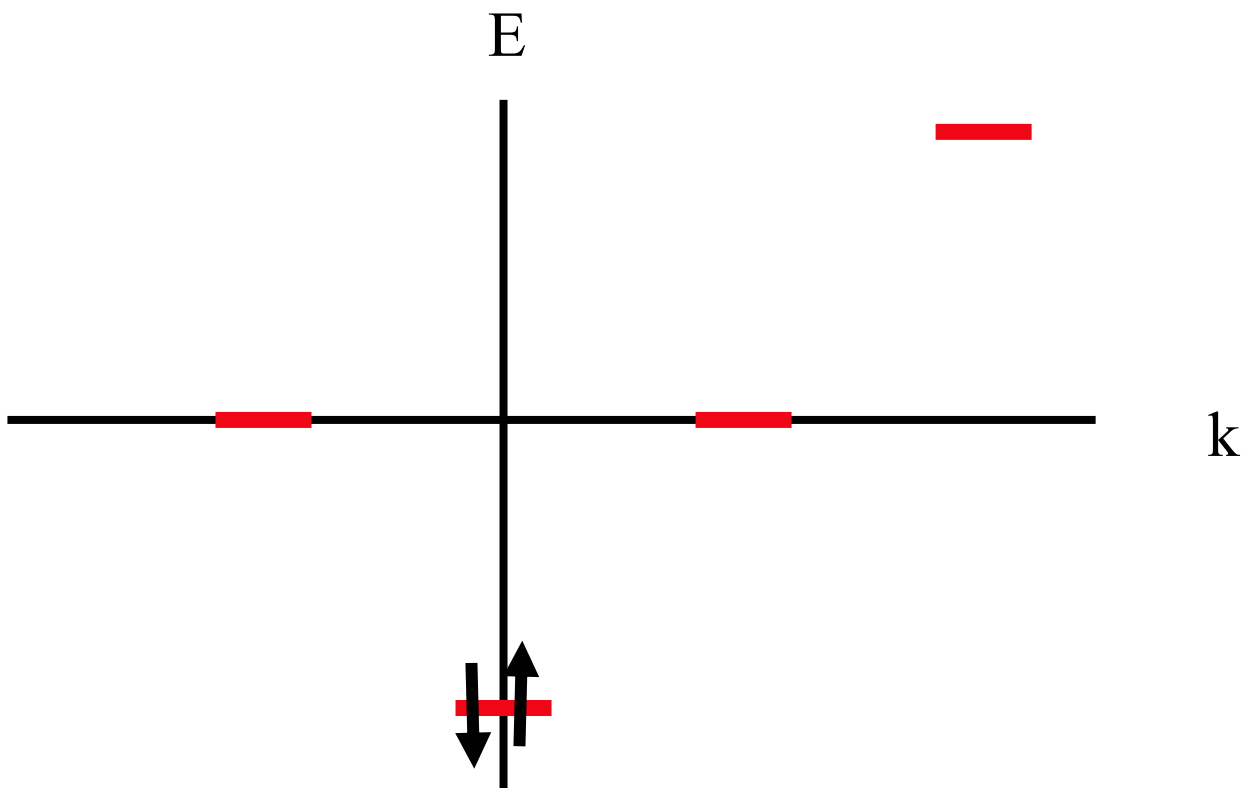
S=1/2 k=0 “s”



4 site Hubbard model (4 member ring)

$N_{el} = 2$

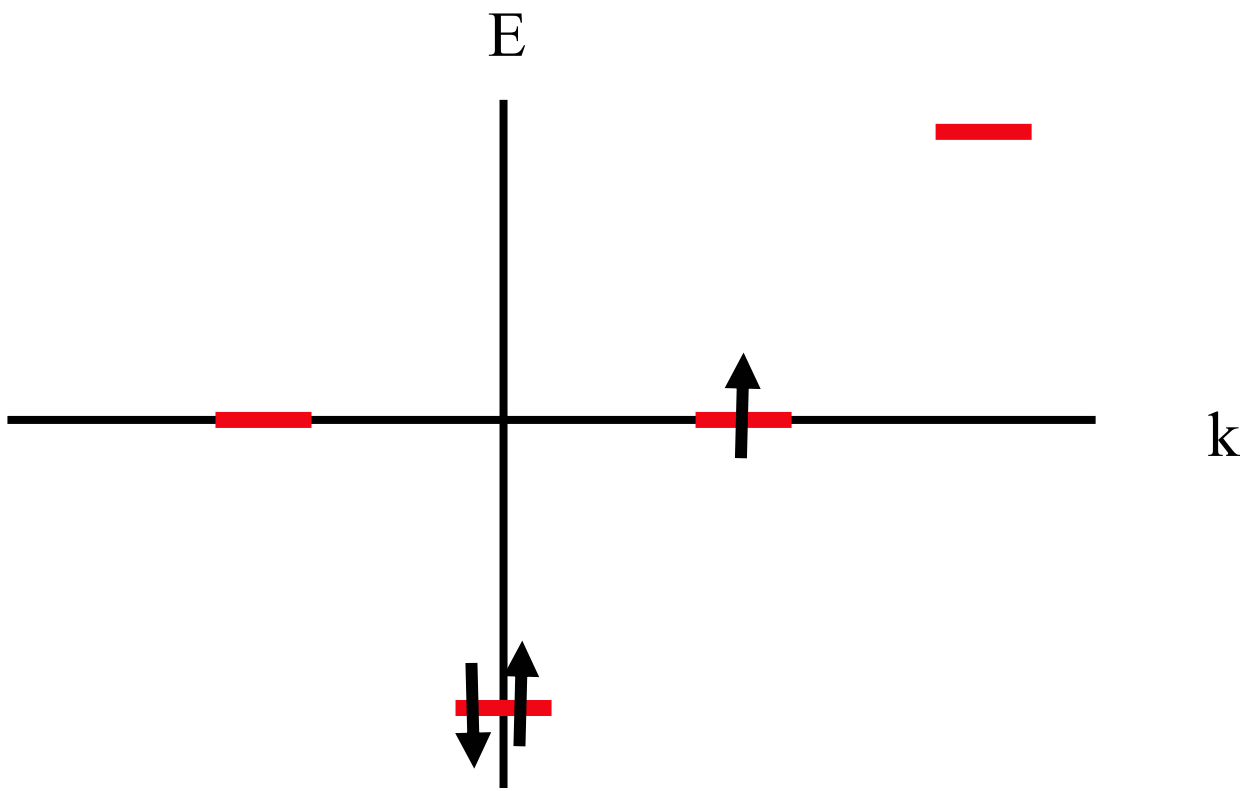
S=0 k=0 “s” for all U



4 site Hubbard model (4 member ring)

$N_{el} = 3$

S=1/2 k=±π/2 "$p_x \pm ip_y$" for $U < U_t$



4 site Hubbard model (4 member ring)

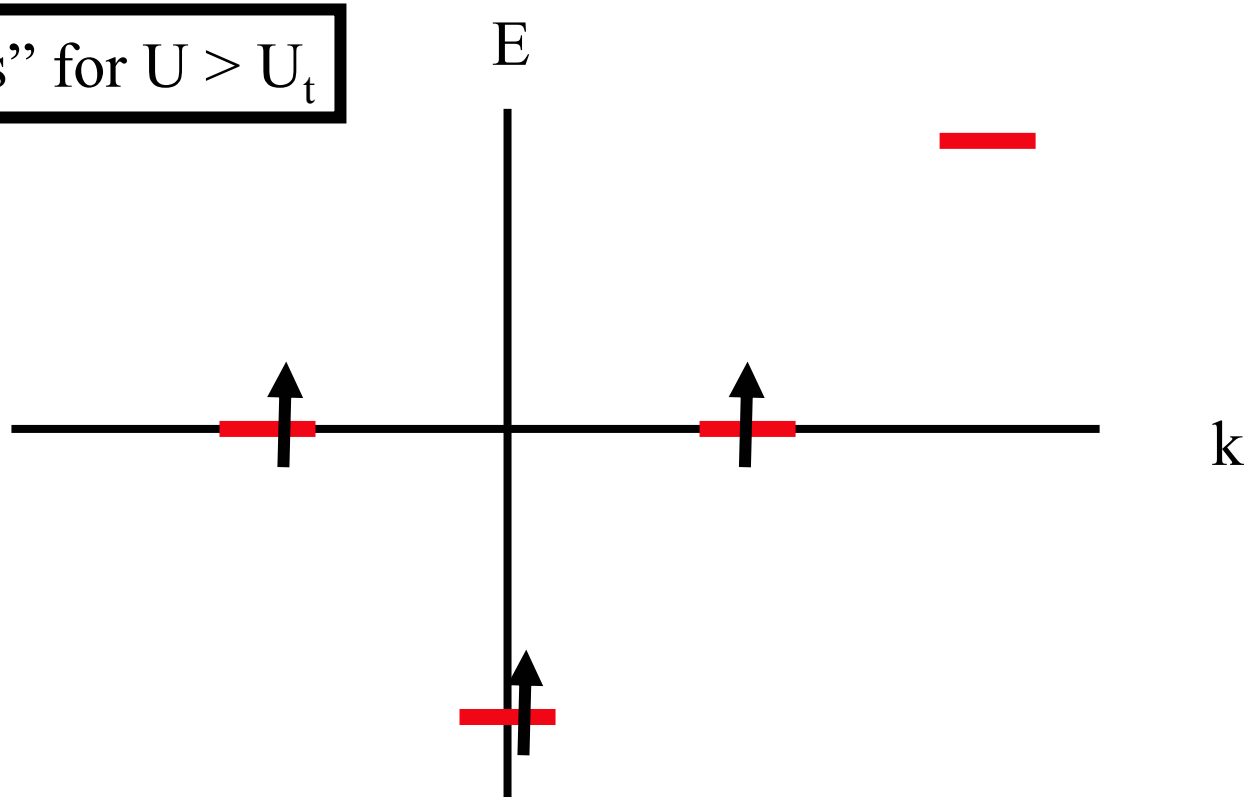
$U_t = 18.6\ t$

$N_{el} = 3$

S=1/2 k=±π/2 "$p_x \pm ip_y$" for $U < U_t$

Nagaoka physics at large U

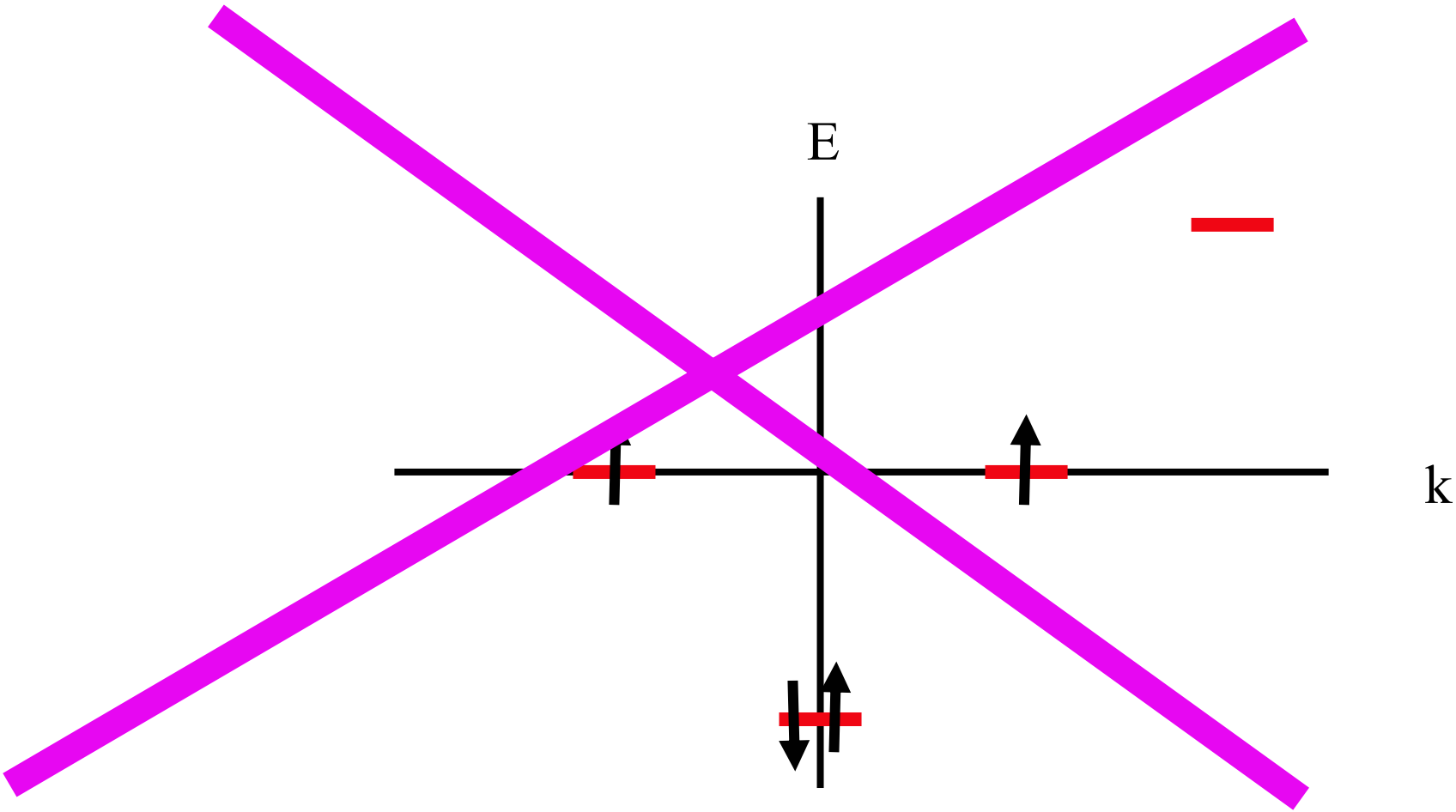
S=3/2 k=0 "s" for $U > U_t$



4 site Hubbard model (4 member ring)

$N_{el} = 4$

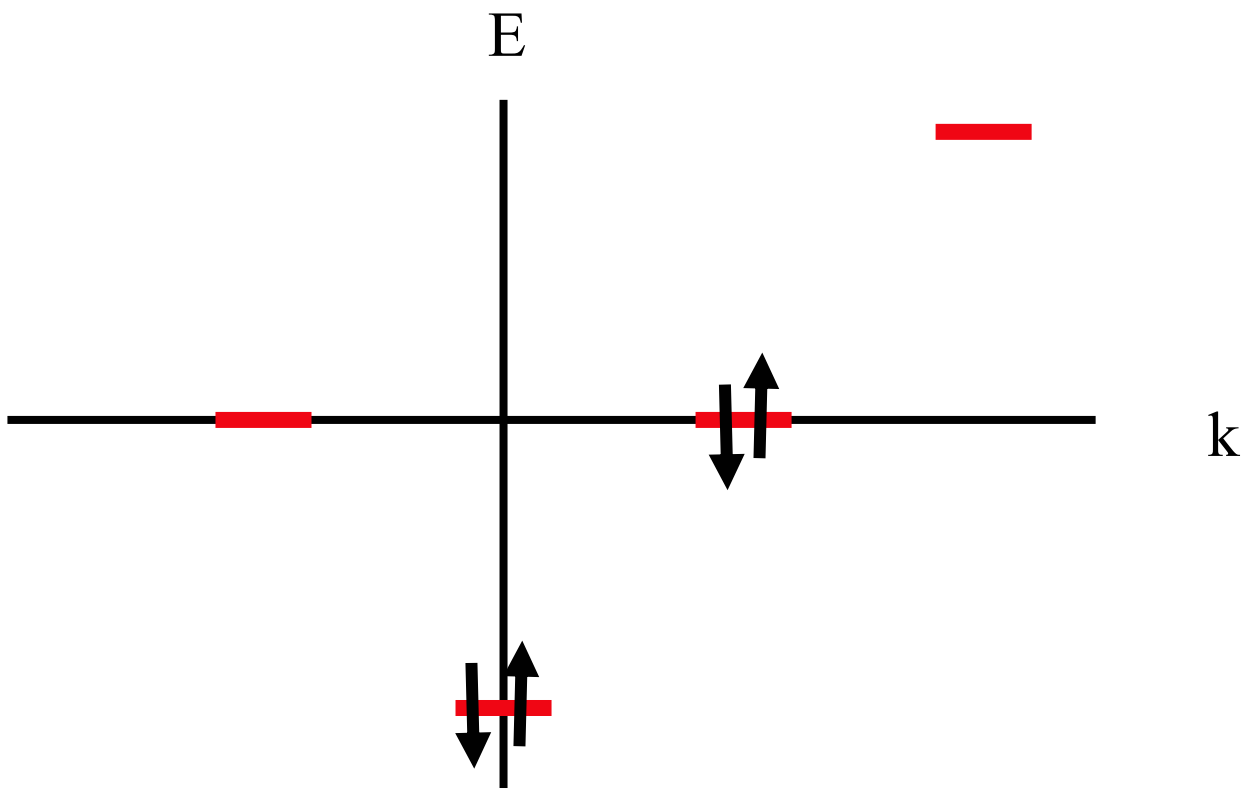
S=1 k=0 “ s” Hund’s rule ???



4 site Hubbard model (4 member ring)

$N_{el} = 4$

S=0	k=±π	“d”	???



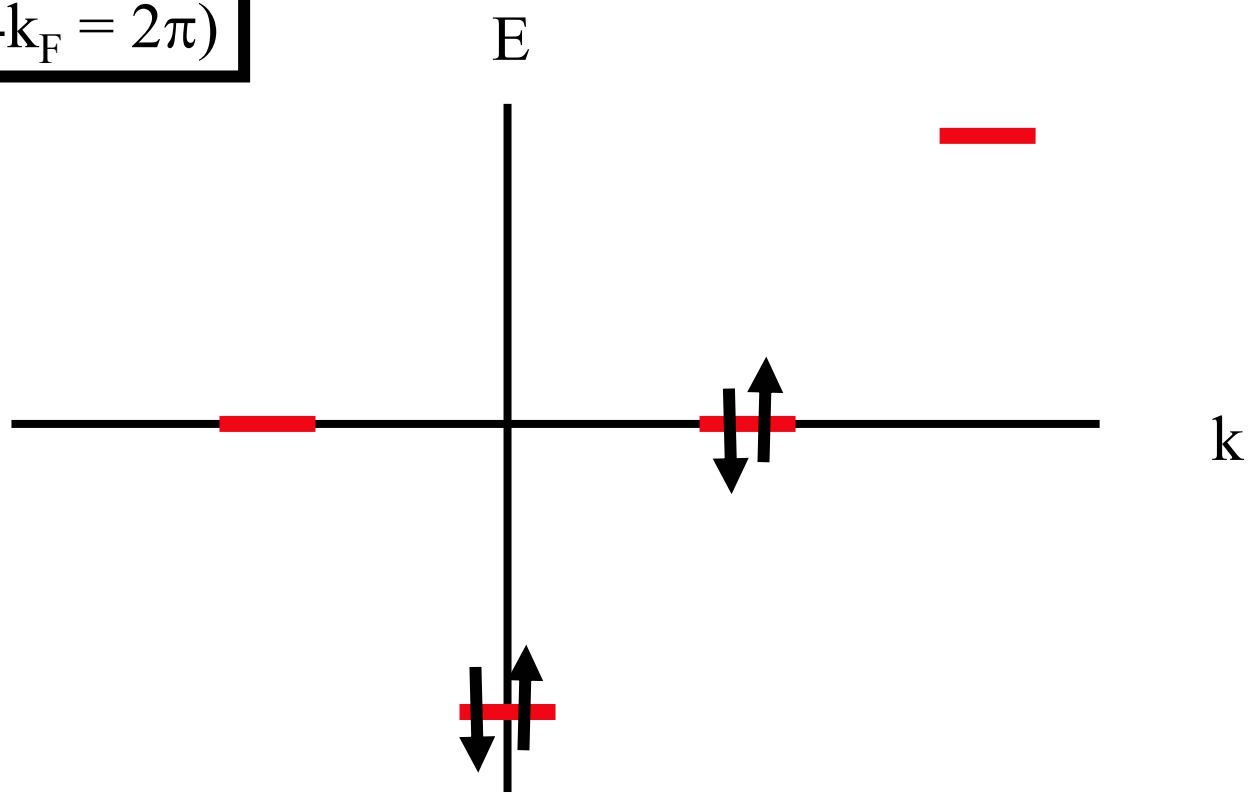
4 site Hubbard model (4 member ring)

$N_{el} = 4$

S=0 k=±π "d"

π= -π

($4k_F = 2\pi$)

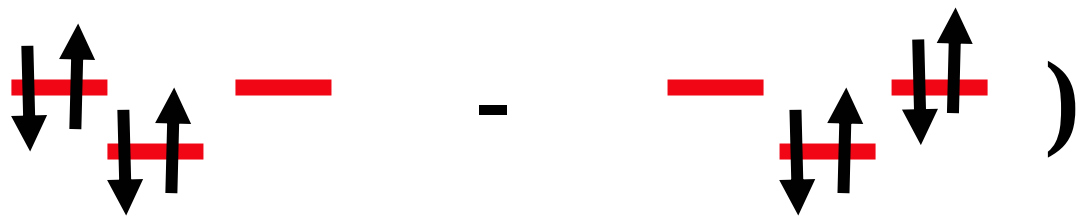


4 site Hubbard model (4 member ring)

$N_{el} = 4$

S=0 k=±π "d" for all U

$\pi = -\pi$

$\Phi =$ 

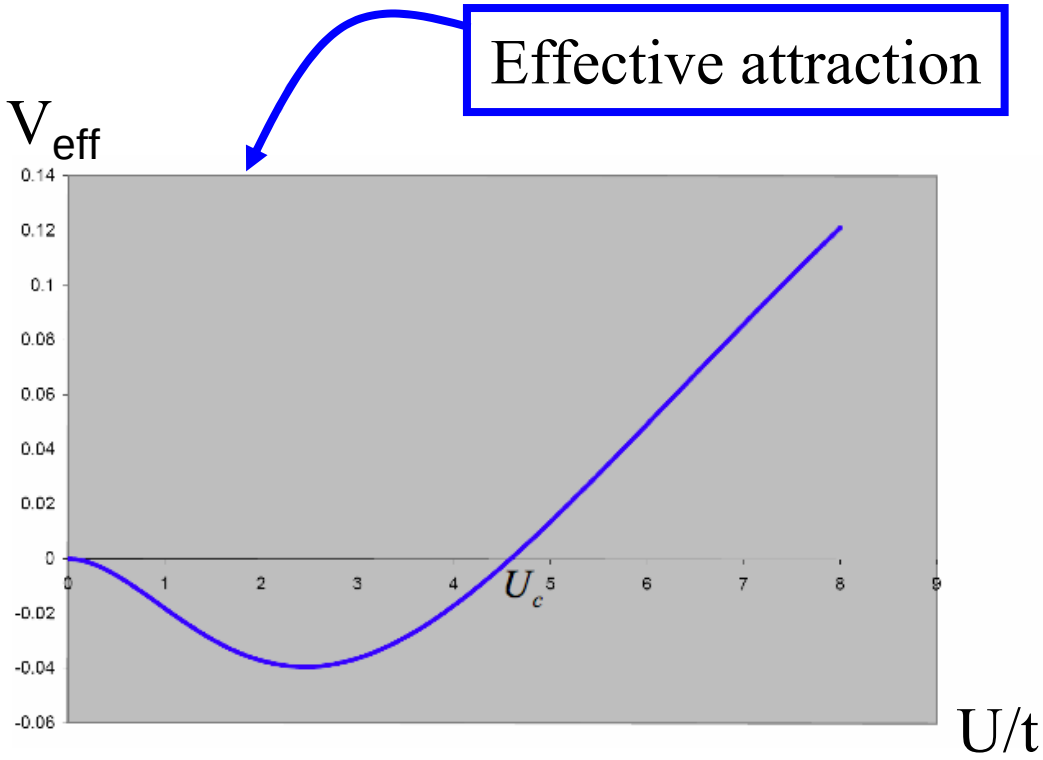
This is a (rare) violation of Hund's first rule.

The ground-state is "entangled" even as U ---> 0.

Sort of a primitive RVB state. (Related to Larkin's work.)

4-site Hubbard model

$V_{eff} = E(4) + E(2) - 2E(3)$



When $V_{eff} < 0$, it is energetically favorable to add two holes to one square rather than one hole to each of two squares. $U_c/t = 4.58 \ldots$

Because the groundstate with N_{el} = 4 is s-wave and the groundstate with N_{el}=2 is d-wave,

the pair creation operator that connects the two states has d-wave symmetry.

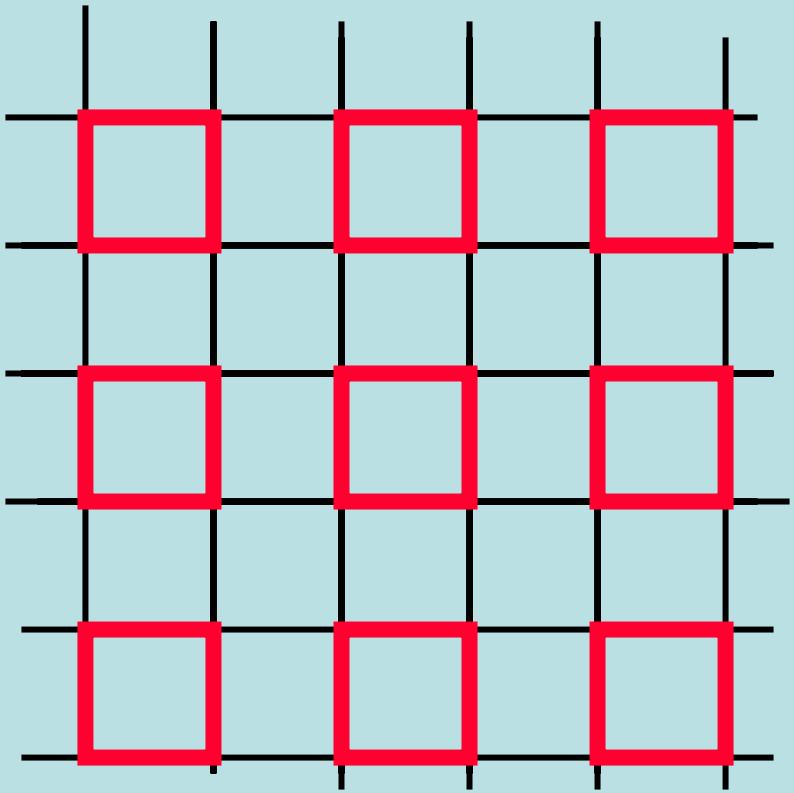
Trugman and Scalapino, 1998*

Now, we study the properties
of the checkerboard Hubbard model
with

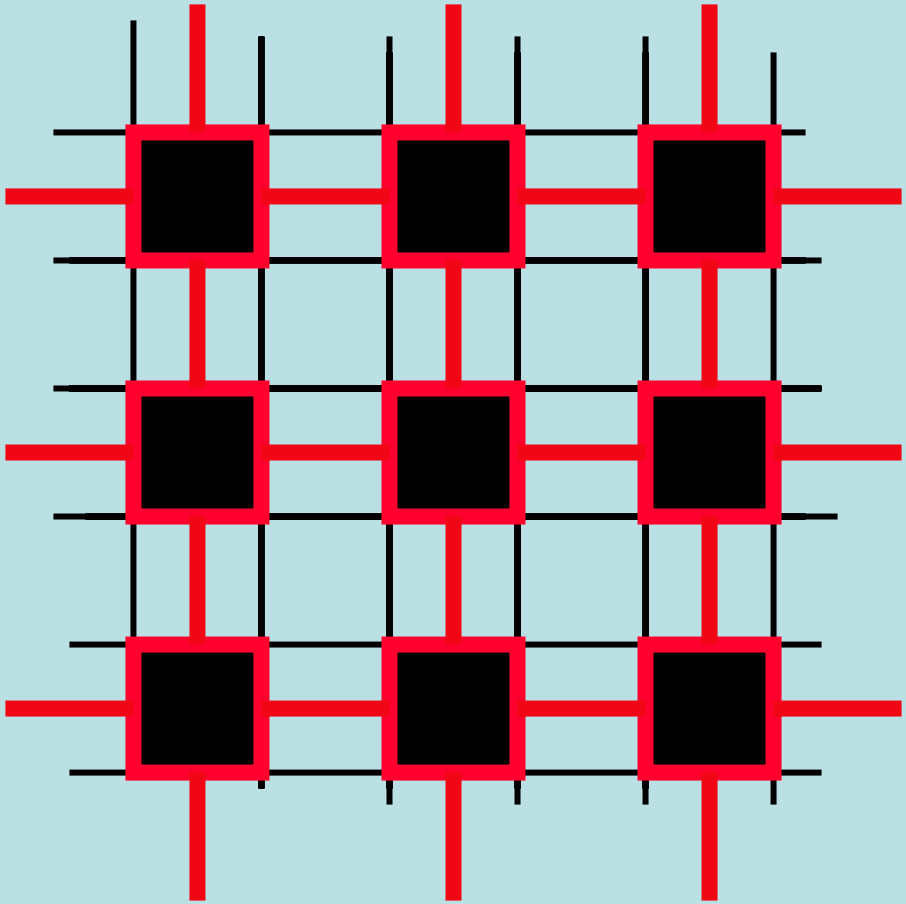
$0 < t'/t << 1$

Gives rise to new manybody problem,
but with a useful small parameter.

New effective models on the “plaquette lattice”

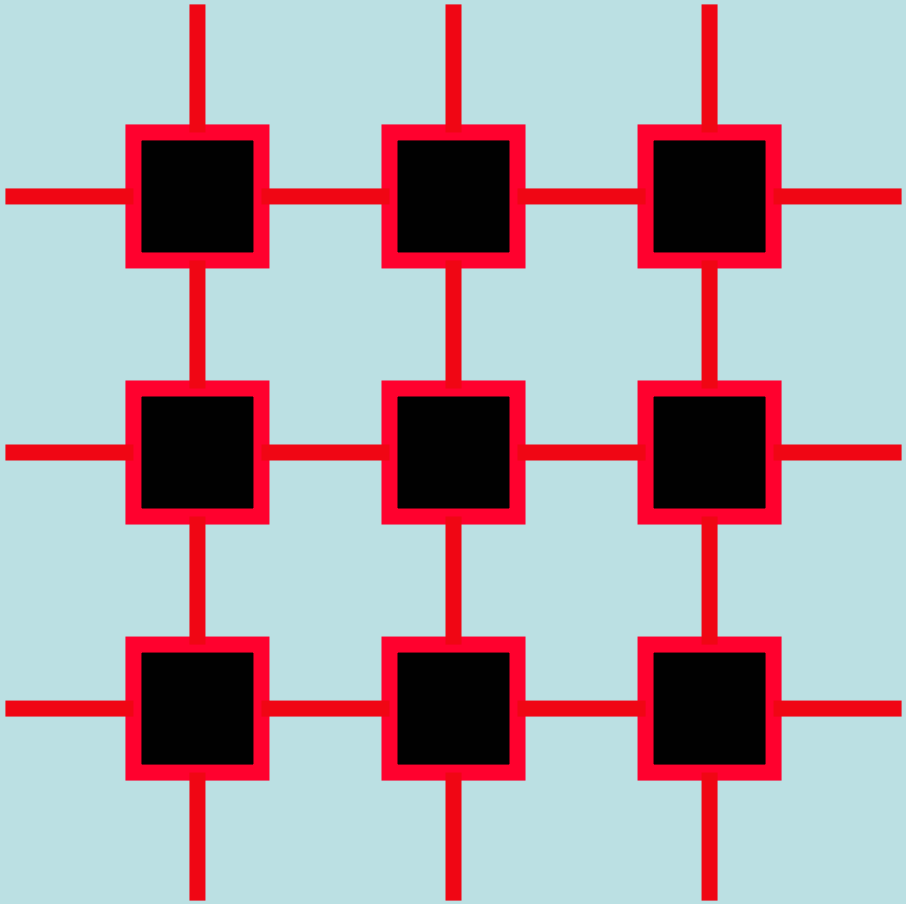


New effective models on the “plaquette lattice”



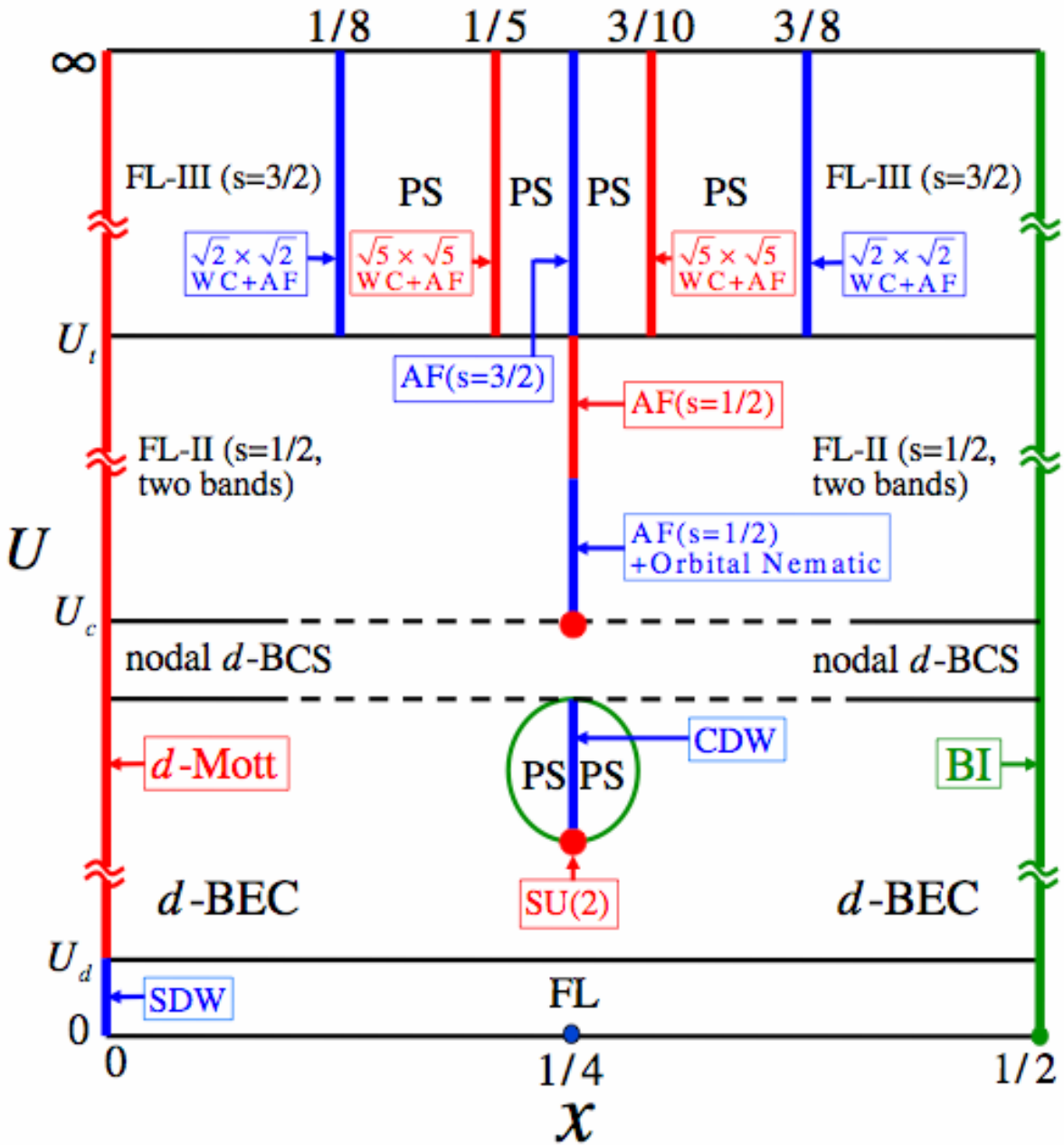
H_{eff} is short-range for $t'/t \ll 1$

New effective models on the "plaquette lattice"
***i.e.* a renormalized square lattice.**

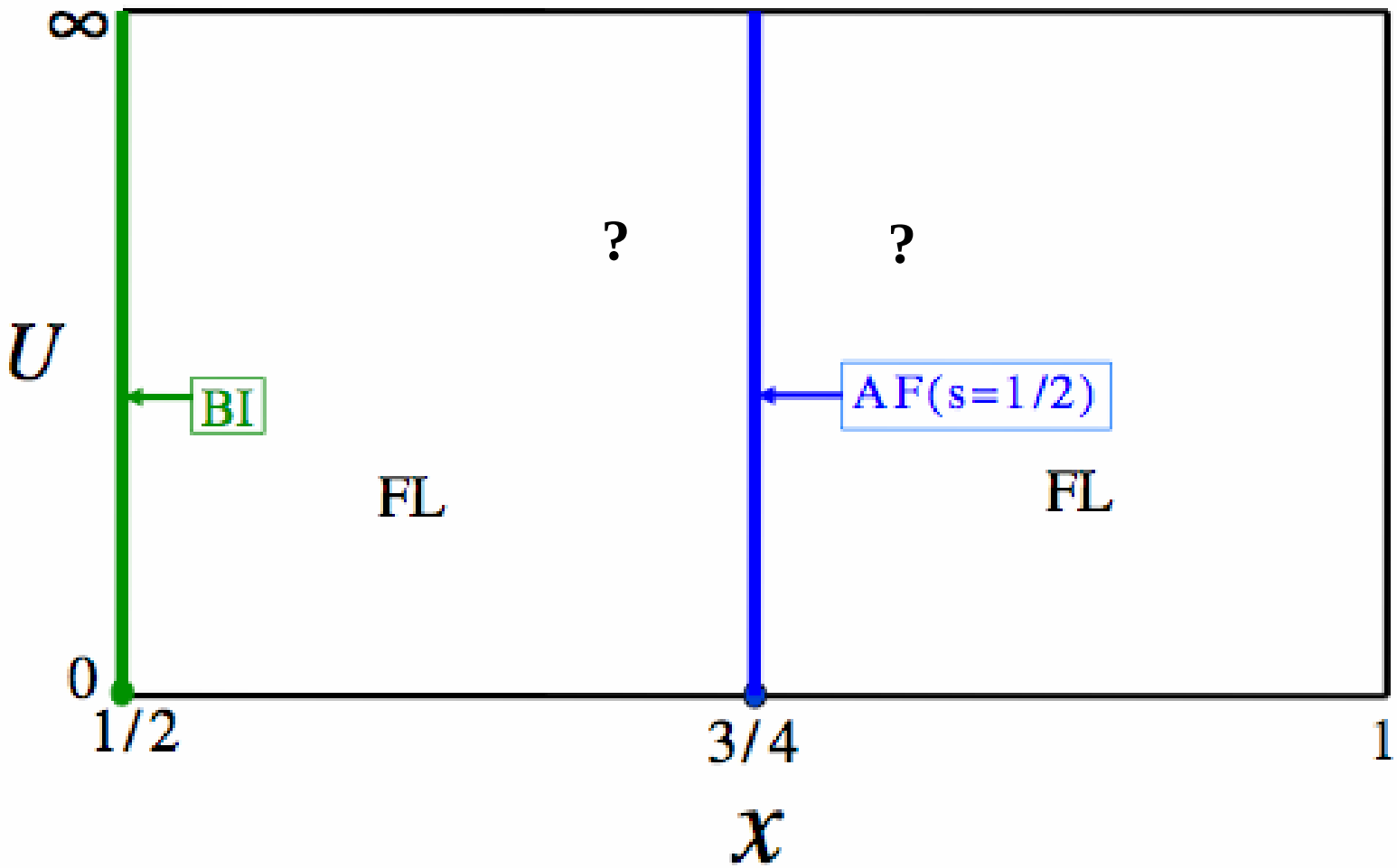


H_{eff} is short-range for $t'/t \ll 1$

Phase diagram at T=0 for checkerboard model with 0 < t' << t.

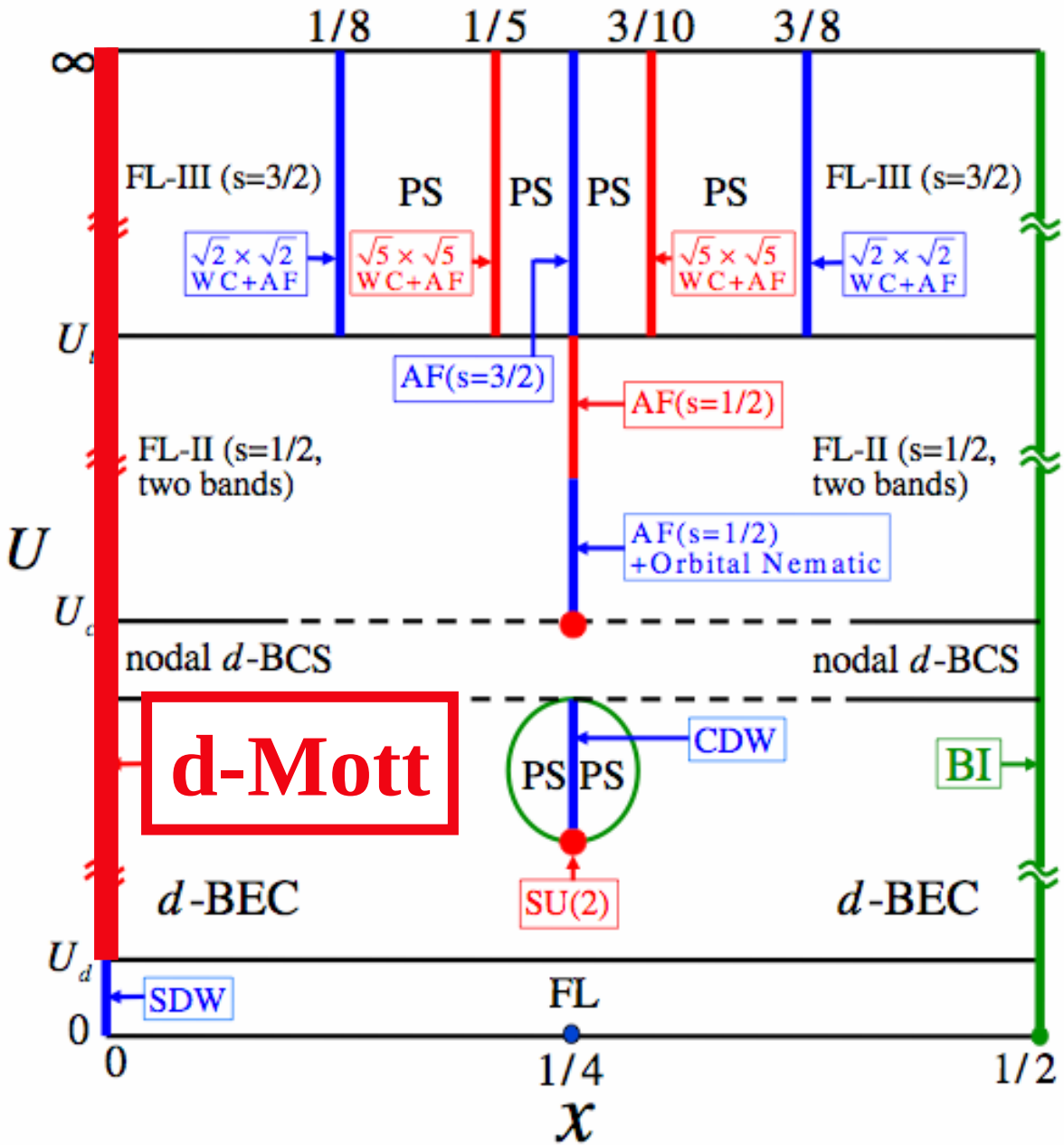


For 1/2 > x > 0 maps onto THE Hubbard model (actually the t-J model) on THE square lattice



Number of electrons per site = 1-x. 4 sites per unit cell.

Phase diagram at T=0 for checkerboard model with 0 < t' << t.



d-Mott phase for x=0 and U > O(t')

Unique ground-state for t'=0

Direct product of ground-states of 4-electrons per plaquette.

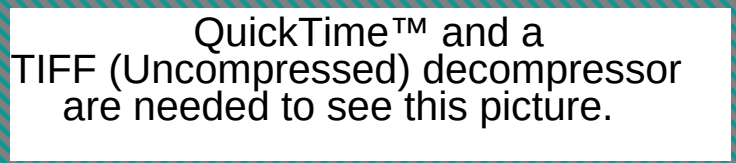
Insulating non-magnetic state with 4 electrons per unit cell, however it is **NOT** adiabatically connected to a band insulator.

Ground-state wave function changes sign (d-wave) under rotation by $\pi/2$.

Behaves like a Bose Mott insulator of d-wave bosons (1 per plaquette).

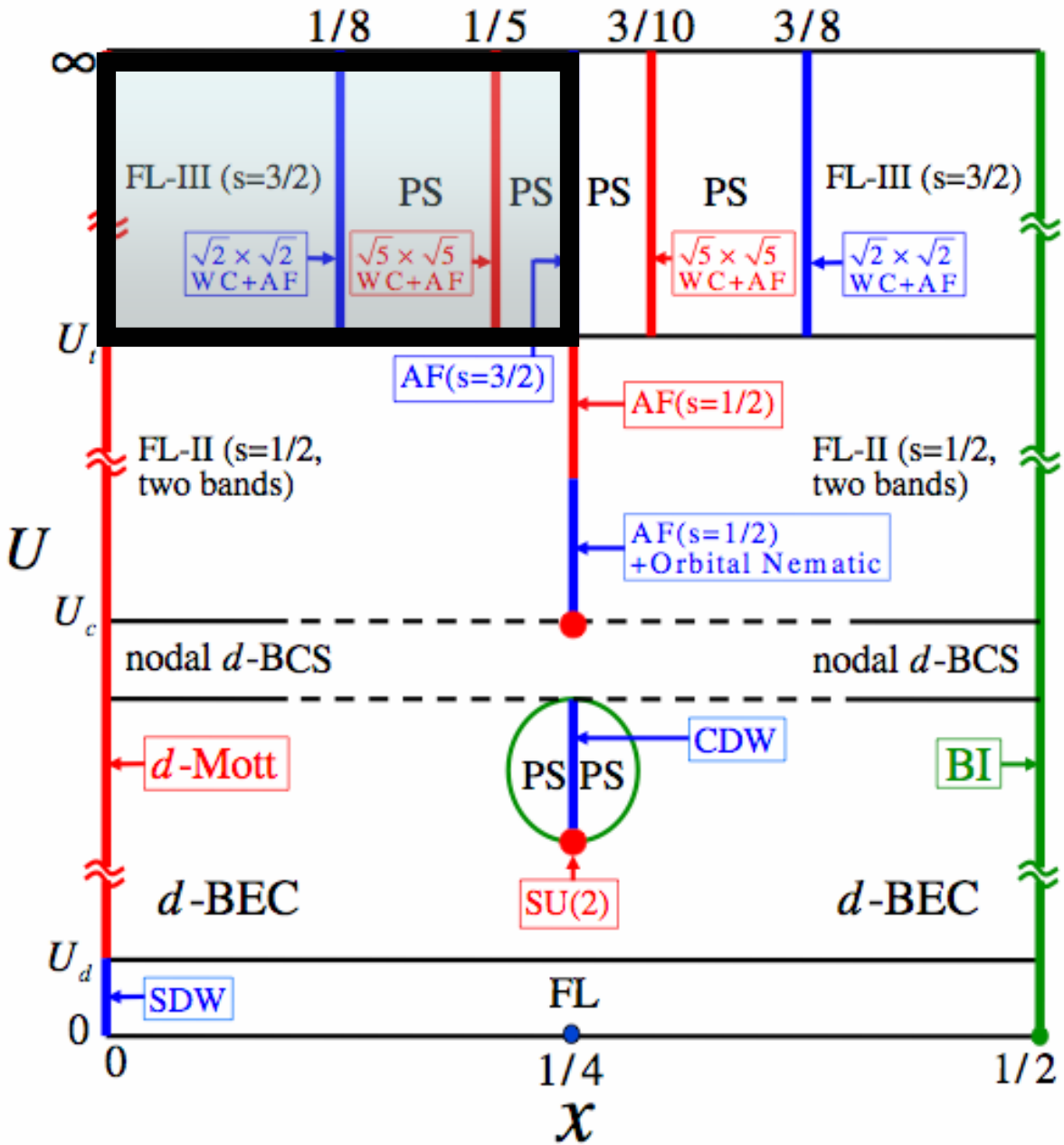
d-Mott phase for x=0 and U > O(t')

where



Also, it is an orbital paramagnet!

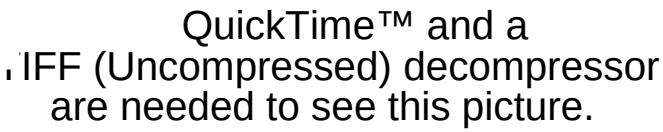
Phase diagram at T=0 for checkerboard model with 0 < t' << t.



Checkerboard Hubbard model with $U > U_t$ and $0 < x < 1/4$

Each plaquette is either "empty" (*i.e.* 4 electrons, s=0)
or occupied by a fermion (*i.e.* 3 electrons, s=3/2)

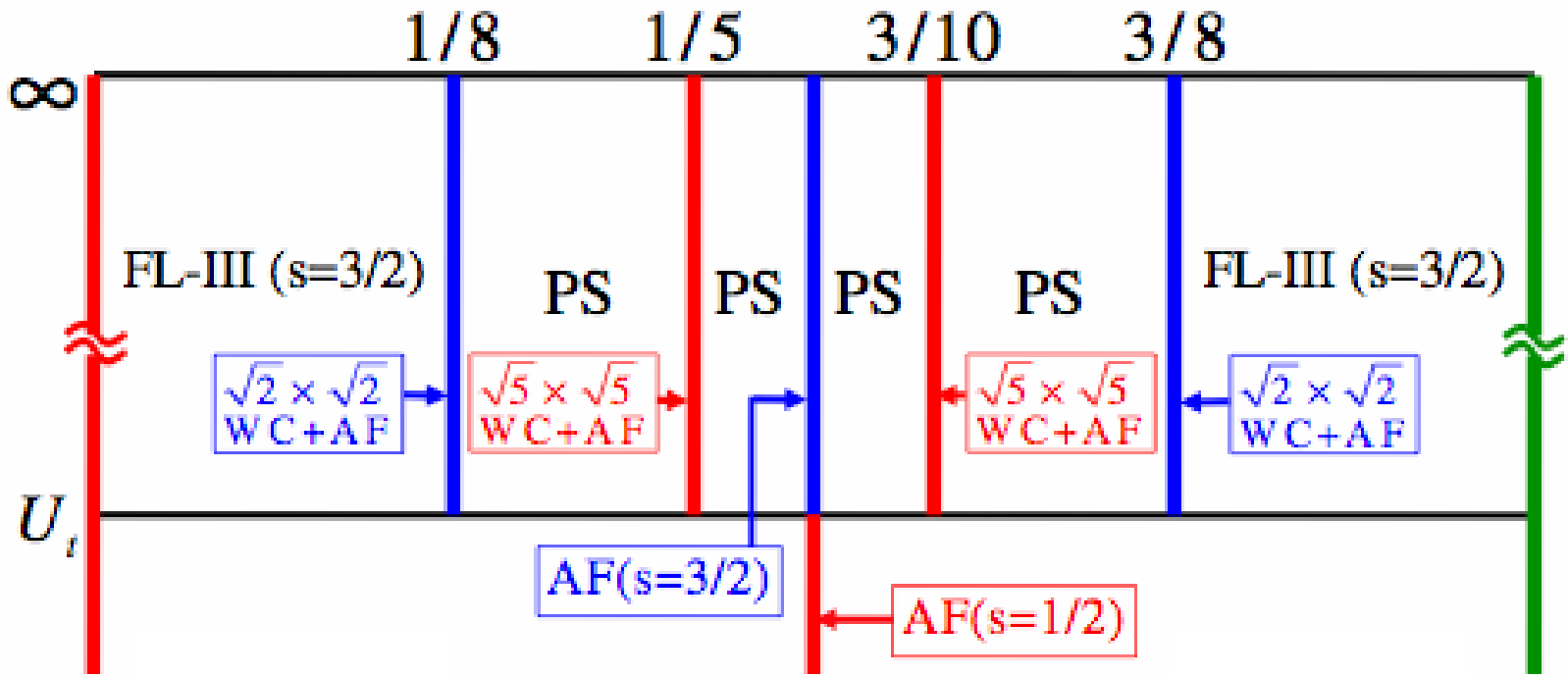
Leads to spin 3/2 t-J-V model:



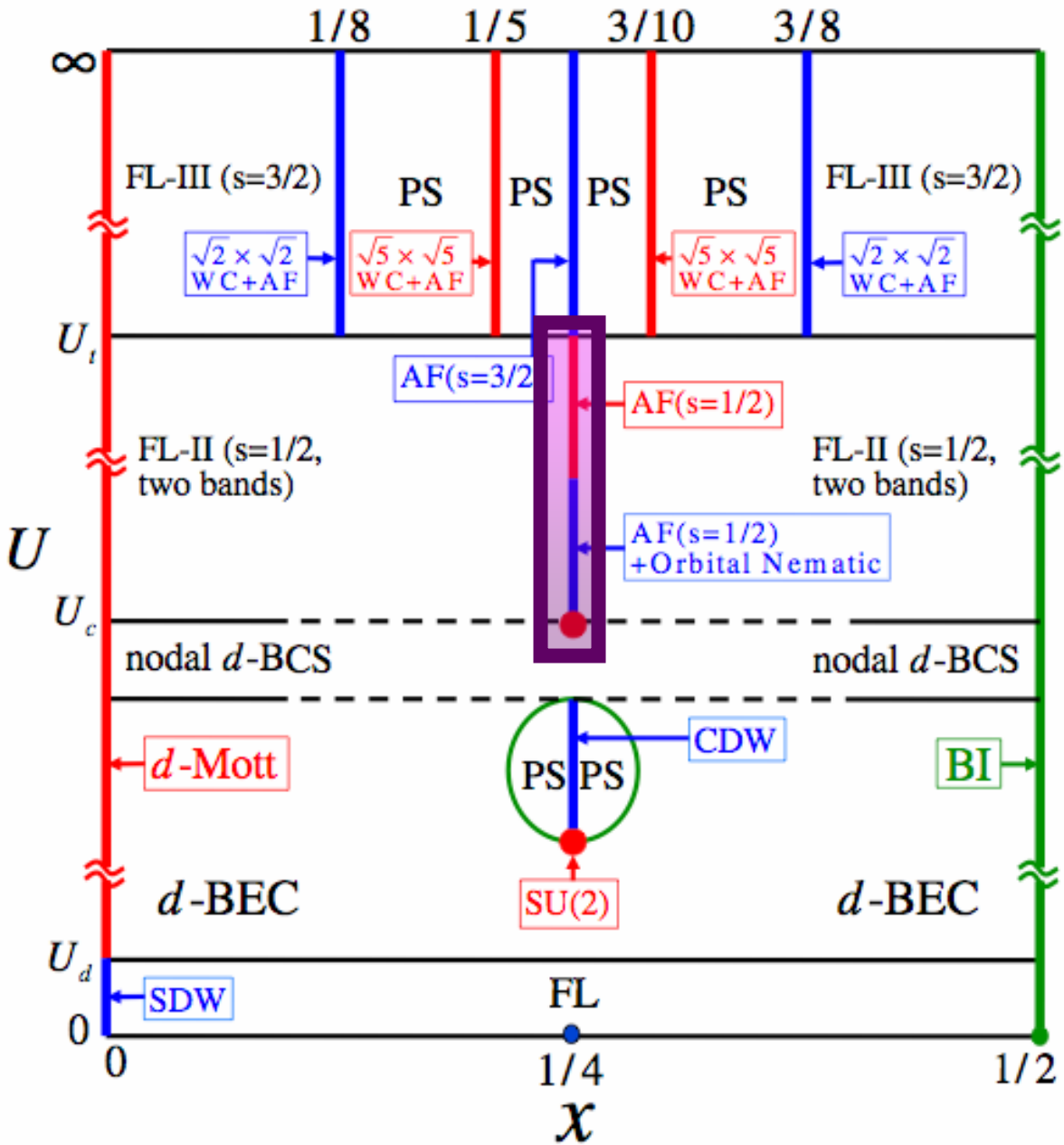
with $t_{eff} \sim (t')^3$ and $J_{eff} \sim (t')^2$

so $t_{eff} << J_{eff}$!!

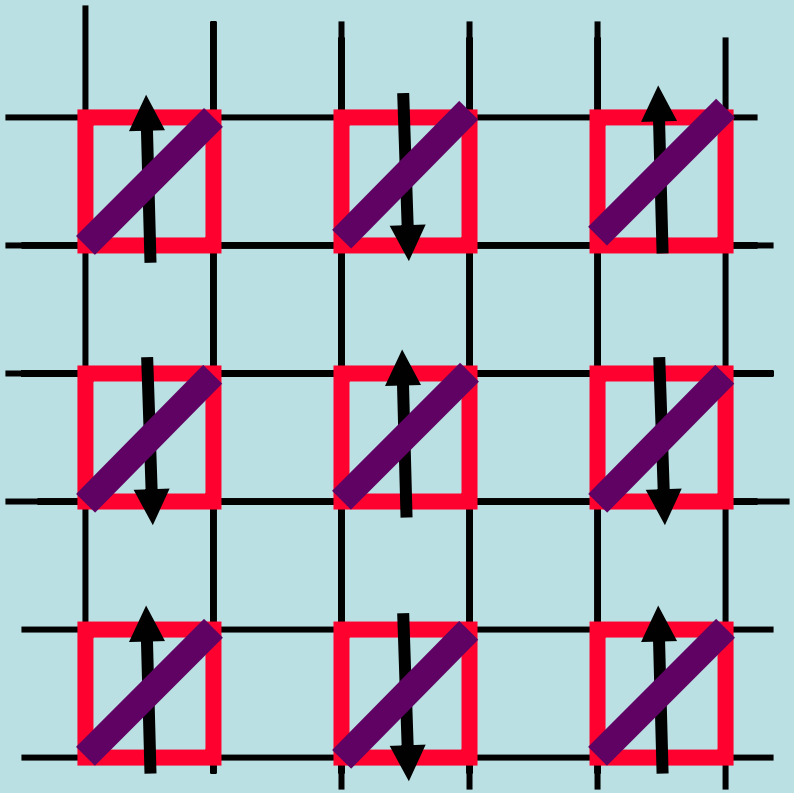
Phase diagram at T=0 for checkerboard model with $0 < t' << t$.



Phase diagram at T=0 for checkerboard model with $0 < t' << t$.

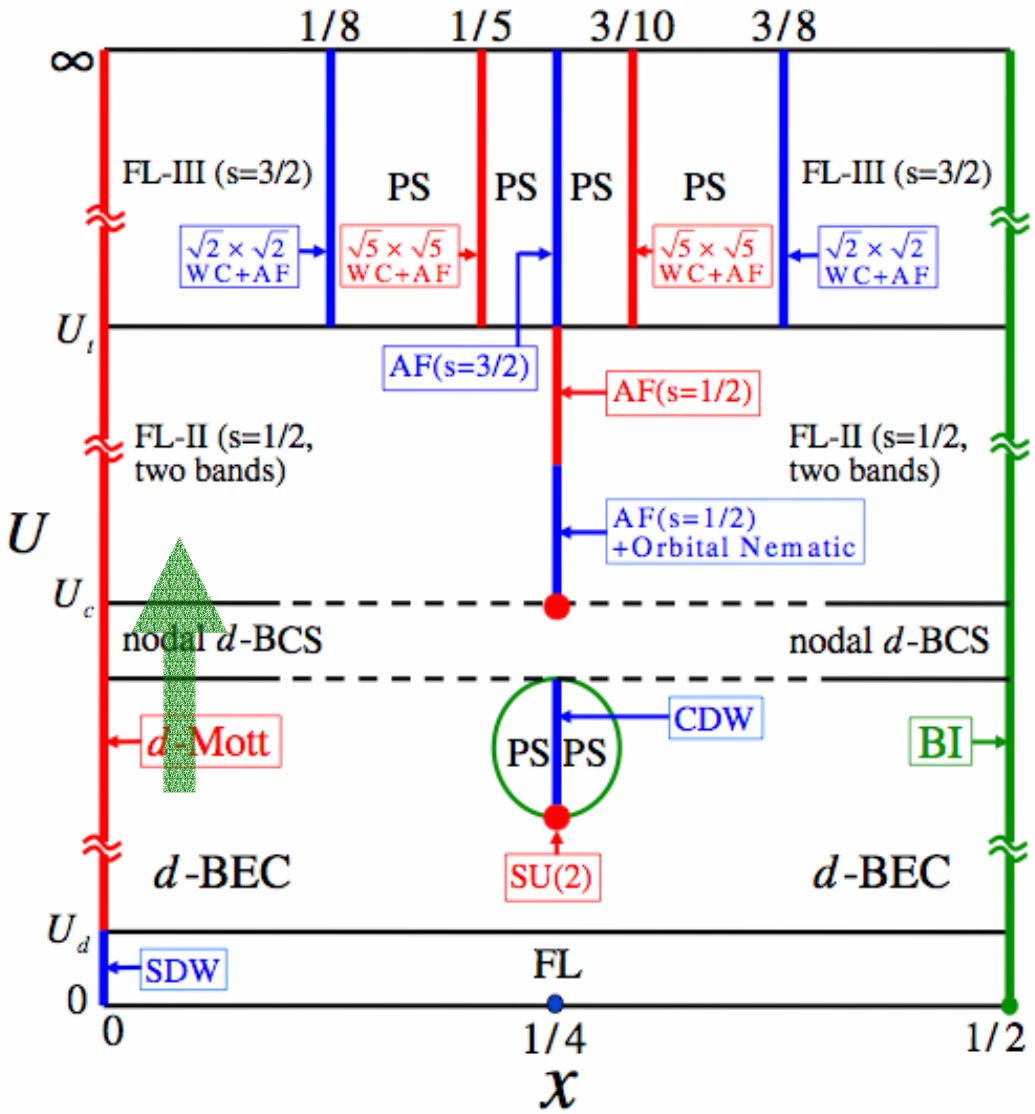


Phases $U_c < U < U_t$ and x = 1/4



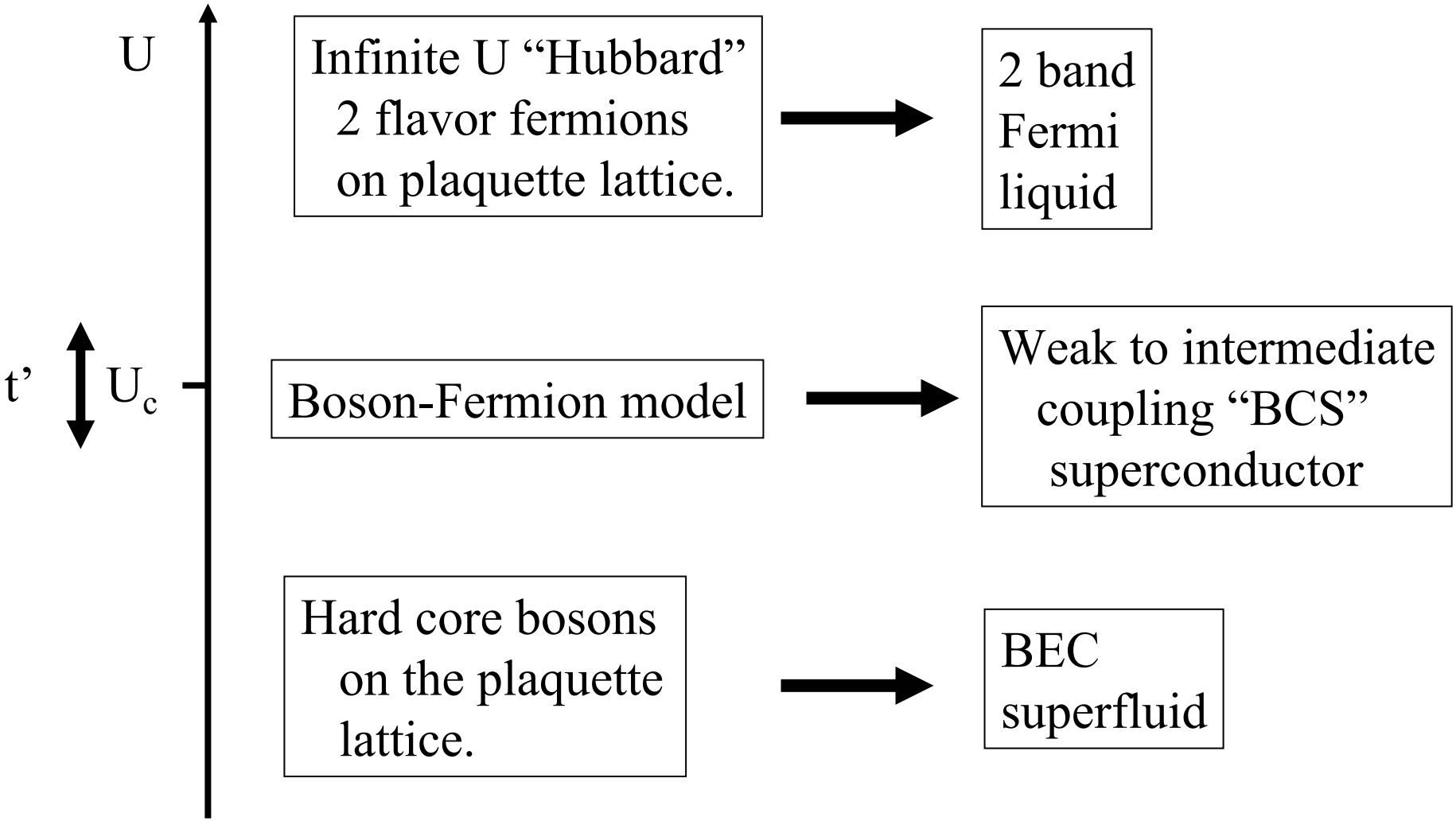
Spin 1/2 Antiferromagnet **with orbital nematic order**

Phase diagram at T=0 for checkerboard model with t' << t.



t'/t << 1 and x << 1 and U near U_c

Checkerboard Hubbard model with $t' \ll t$ and $0 < x \ll 1$



When $0 < U < U_c$ ($|V^{eff}| >> t'$) gas of hard-core bosons*
(d-wave hole pairs)

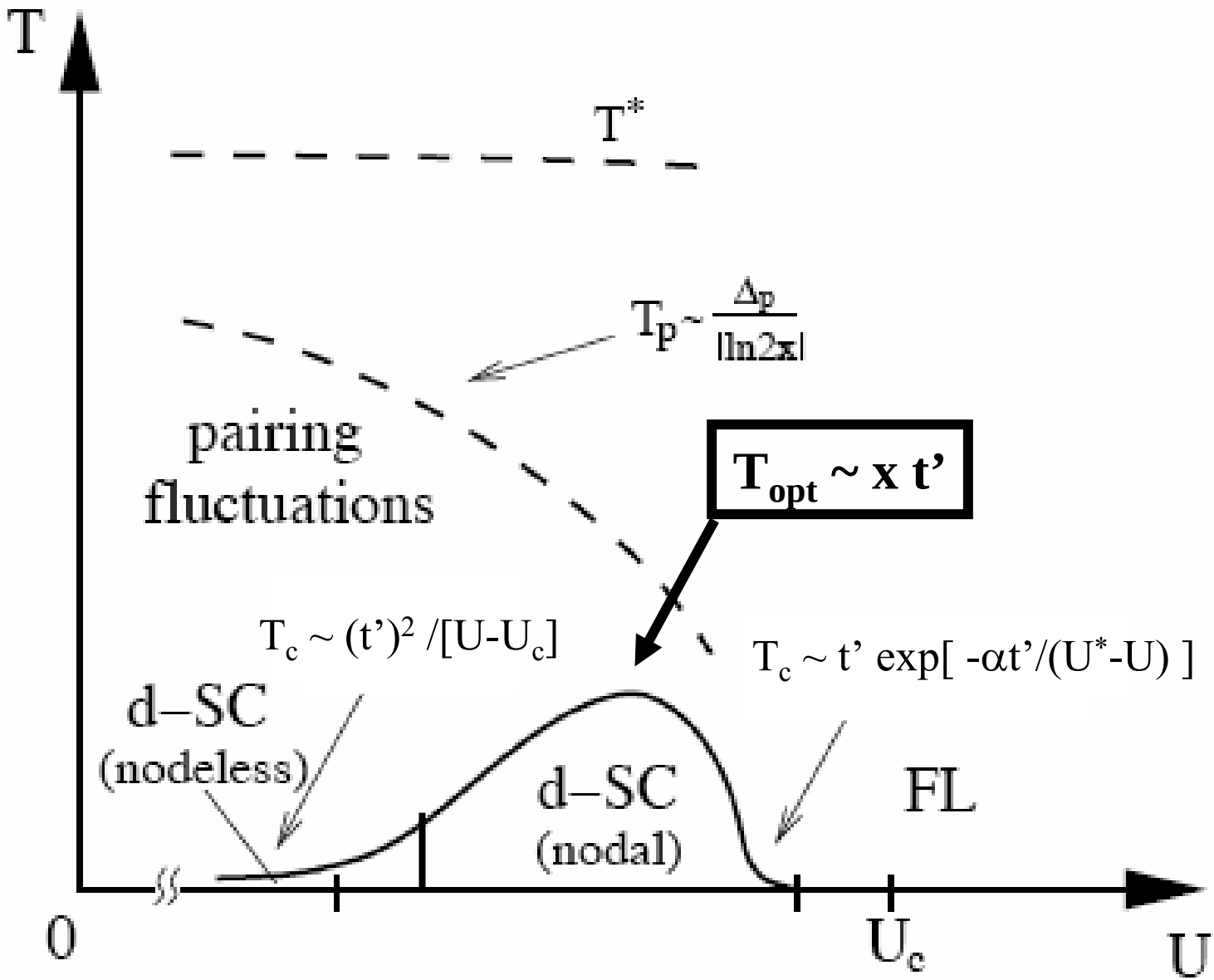
$$t^{eff} \sim \frac{(t')^2}{(U_c - U)}$$

When $U_c < U$ ($V^{eff} << -t'$) gas of interacting fermions

$$T = V^{eff} \sim (\ )t' - \frac{(t')^2}{(U - U_c)}$$

When $| U-U_c | \sim t'$ ($|V^{eff}| \sim t'$) boson-fermion gas.

*Maps onto problem solved by MC by Zimanyi, Scalletar, et al


T
T*
$T_p \sim \frac{\Delta_p}{|\ln 2x|}$
pairing
fluctuations
$T_{opt} \sim x\, t'$
$T_c \sim (t')^2 / [U-U_c]$
$T_c \sim t' \exp[-\alpha t'/(U^*-U)]$
d–SC
(nodeless)
d–SC
(nodal)
FL
0
U_c
U

Checkerboard Hubbard model proves many points of principle.

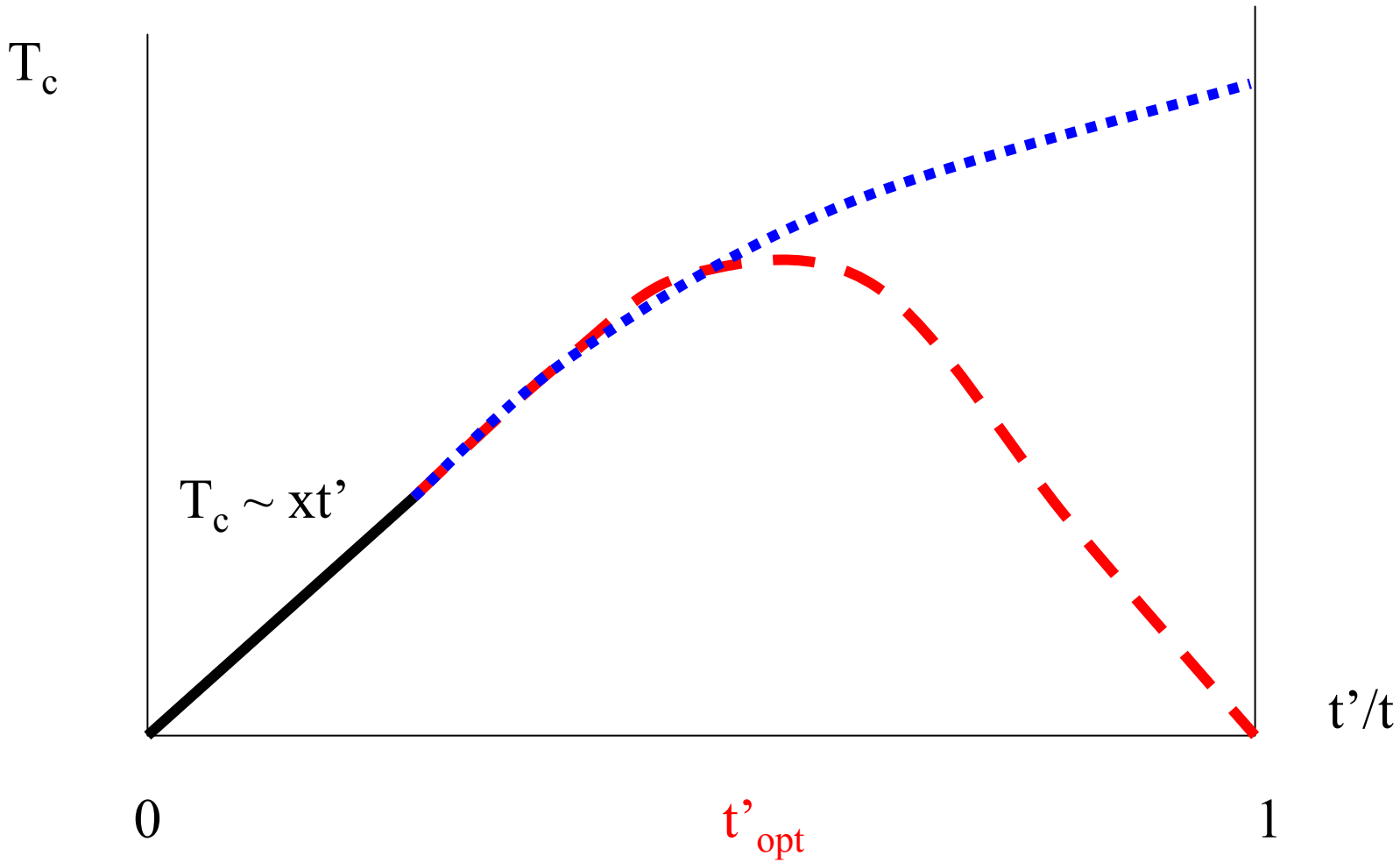
Can get superconductivity directly from strong repulsion between electrons

Highly non-BCS mechanism of SC - no well defined phonon (or any other well defined "boson-glue") exchanged. (More RVB-like: Comes from anomalous stability of undoped square.)

D-wave superconductivity emerges naturally from lattice geometry and strong repulsion.

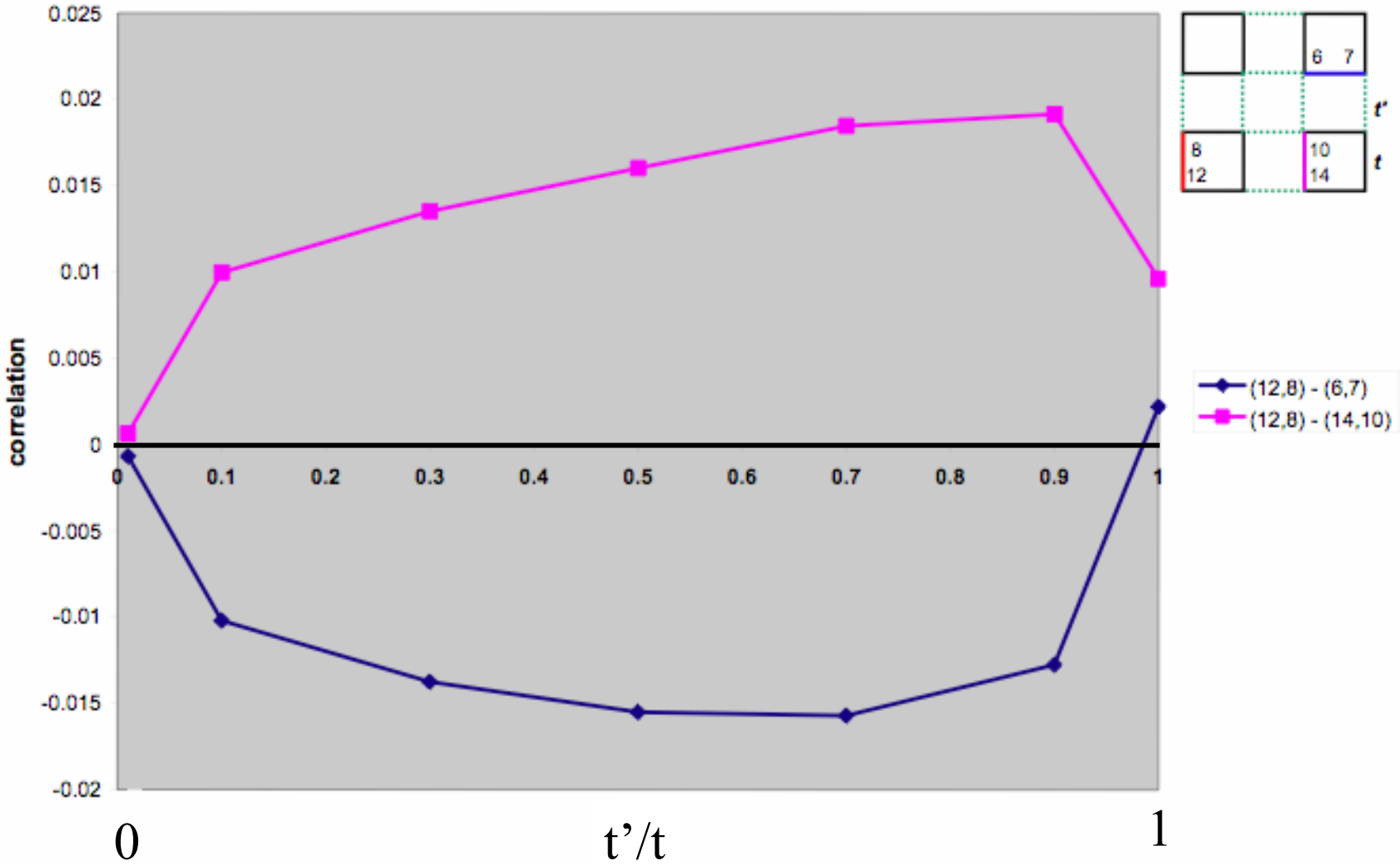
Also has myriad "competing" ordered phases, which may be generic to strongly correlated systems.

Is inhomogeneity essential?

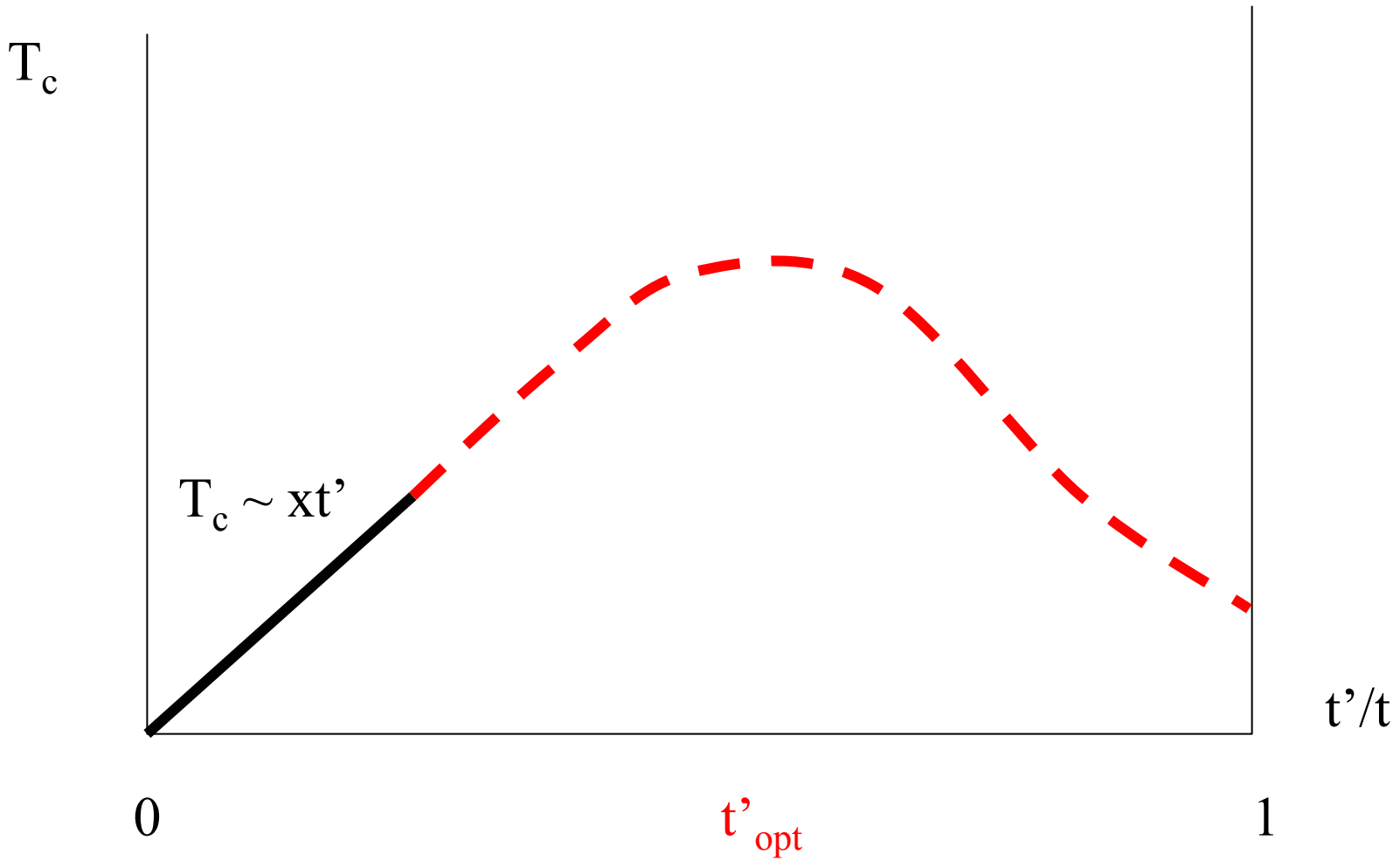


Equal time pairfield-pairfield correlation function on 4x4 checkerboard

14 electrons on 16 sites with U=8t



Probably inhomogeneity essential to optimize T_c!



Optimal Inhomogeneity for High Temperature Superconductivity

The Checkerboard Hubbard model illustrates

a) d-wave superconductivity from purely repulsive interactions
b) large number of competing phases in a strongly correlated electronic system
c) yet another example where maximum T_c occurs at a crossover from pairing to coherence

Suggestive evidence that correct forms of inhomogeneity are essential to high temperature pairing.