What is Optimal for High Temperature Superconductivity?

(What are the key features for **a** mechanism of HTC?)

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E.Arrigoni, I.Martin, D. Poldolsky
V.J.Emery and S. Chakravarty

A distant fjord in Norway, 2007

Hamiltonian engineering:

What Hamiltonian would give the highest possible superconducting T_c?

Problem #1: We can't solve most strongly interacting electronic models in $d > 1$.

Problem #2: The question is not well defined unless we specify constraints on what we can vary.

What is needed for a large T_c?

A high pairing scale Δ_0

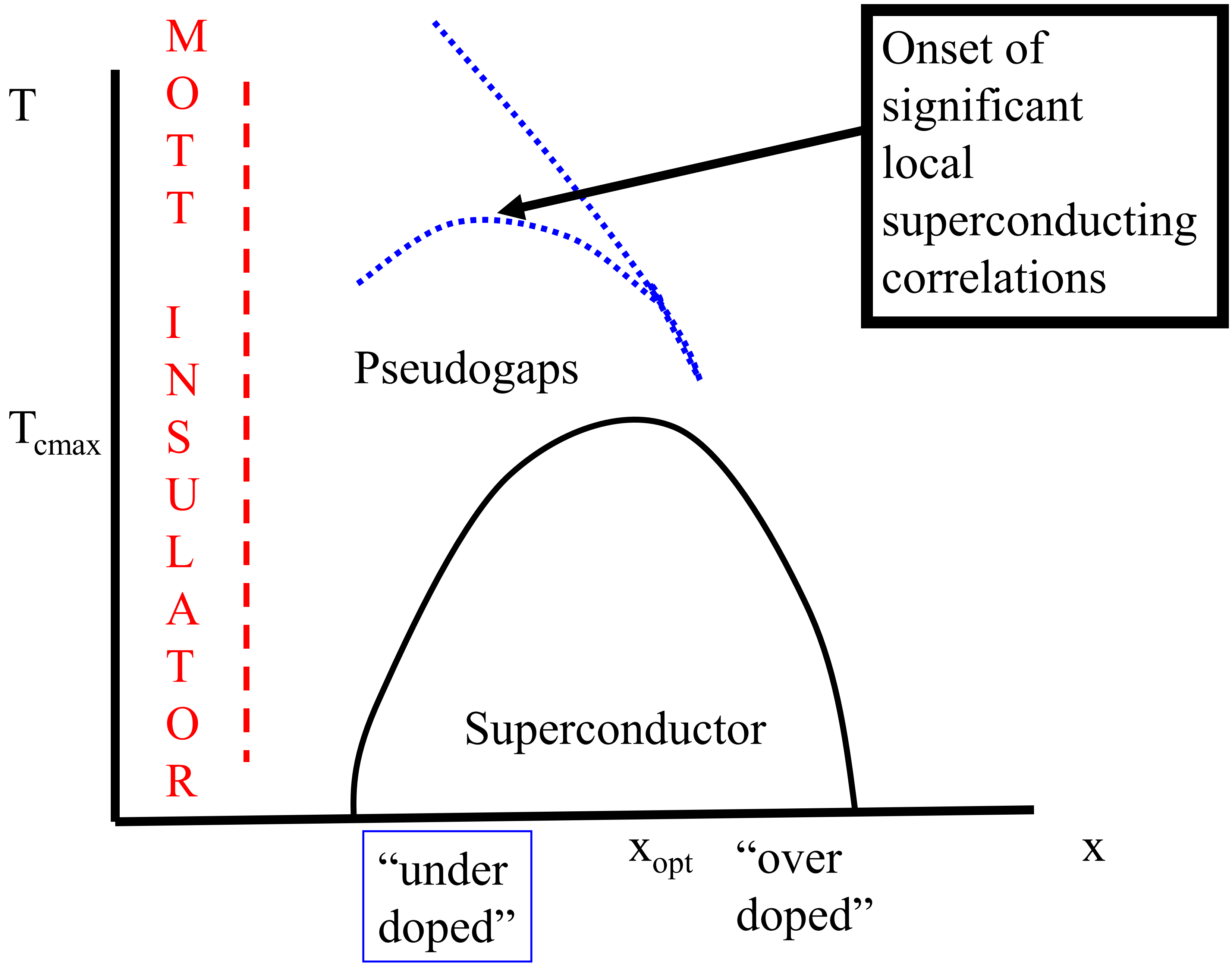
A large phase coherence (condensation) temperature $T_\theta \sim \rho_s$

No "competing" instability to ruin things.

Unless the superconducting phase is cut off by
a (first order) transition to a competing phase,
optimal T_c occurs at a crossover from
a pairing dominated regime - $\mathbf{T_c \sim \Delta_0}$
to a condensation regime - $\mathbf{T_c \sim T_\theta}$

Breaking a system into meso-scale "clusters"
can, under special circumstances, produce
enormous enhancement of Δ_0 but always
at the expense of reduced T_θ, so optimal T_c
occurs at an "optimal inhomogeneity."

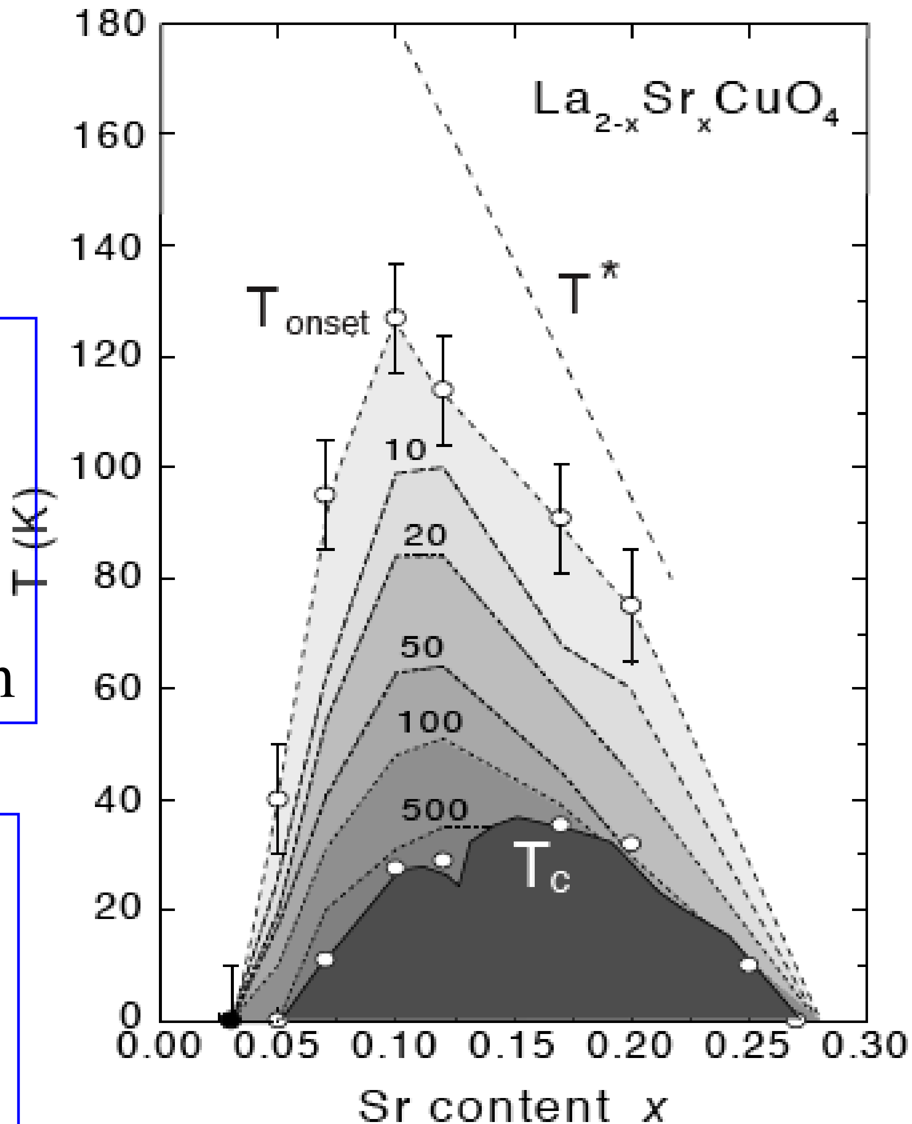
One can use these principles to develop strategies for
making high T_c higher.



T
MOTT INSULATOR
Onset of significant local superconducting correlations
Pseudogaps
T_{cmax}
Superconductor
"under doped"
x_{opt}
"over doped"
x

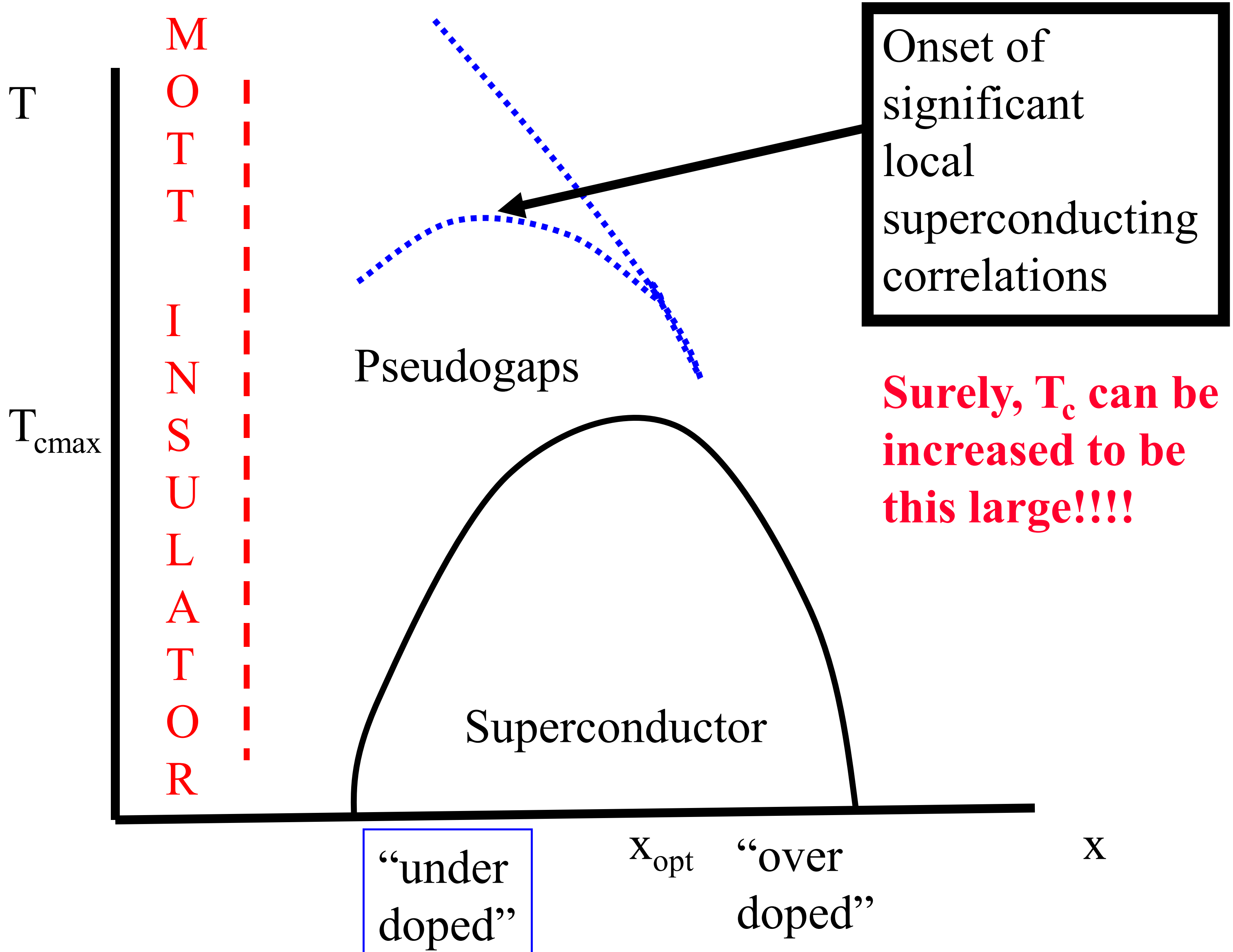
Pseudo-gap phenomena

From Wang et al cond-mat/0510470



T_{onset} is onset of fluctuation diamagnetism

T* is onset of supression of spin susceptibility


T
T_{cmax}
MOTT INSULATOR
Onset of significant local superconducting correlations
Pseudogaps
Surely, T_c can be increased to be this large!!!!
Superconductor
“under doped”
x_{opt}
“over doped”
x

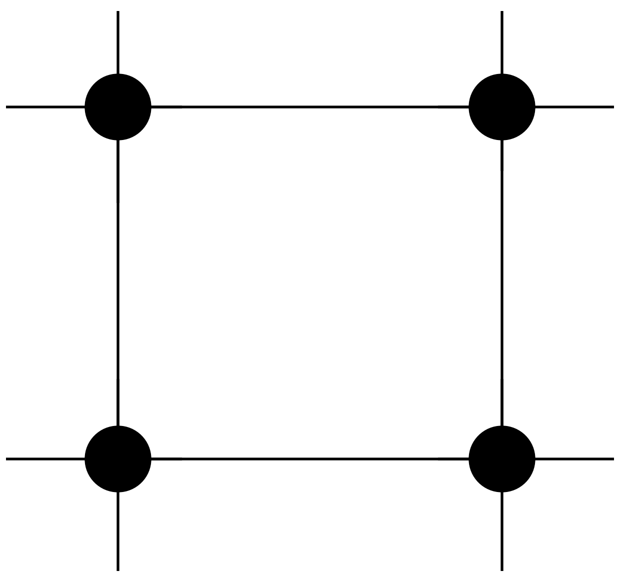
Some solutions of model problems:

1) The negative U Hubbard model

(Following on talk of DJS)

The Hubbard model

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



U > 0 Repulsive
U < 0 Attractive

$|U| << t$ BCS superconductivity

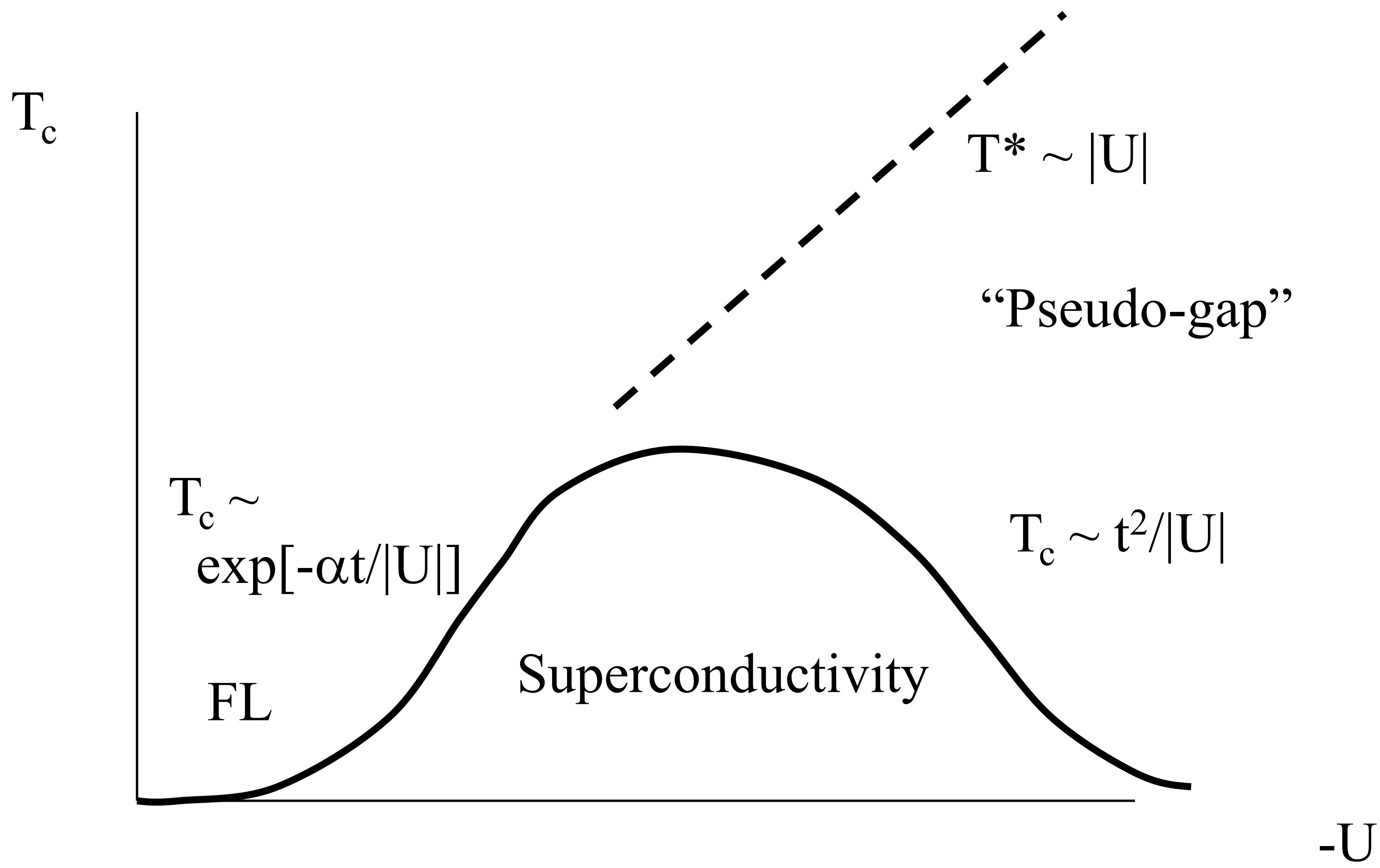
$$T_c \sim t \exp[- \alpha\, t/|U|]$$

very mean-field like transition.

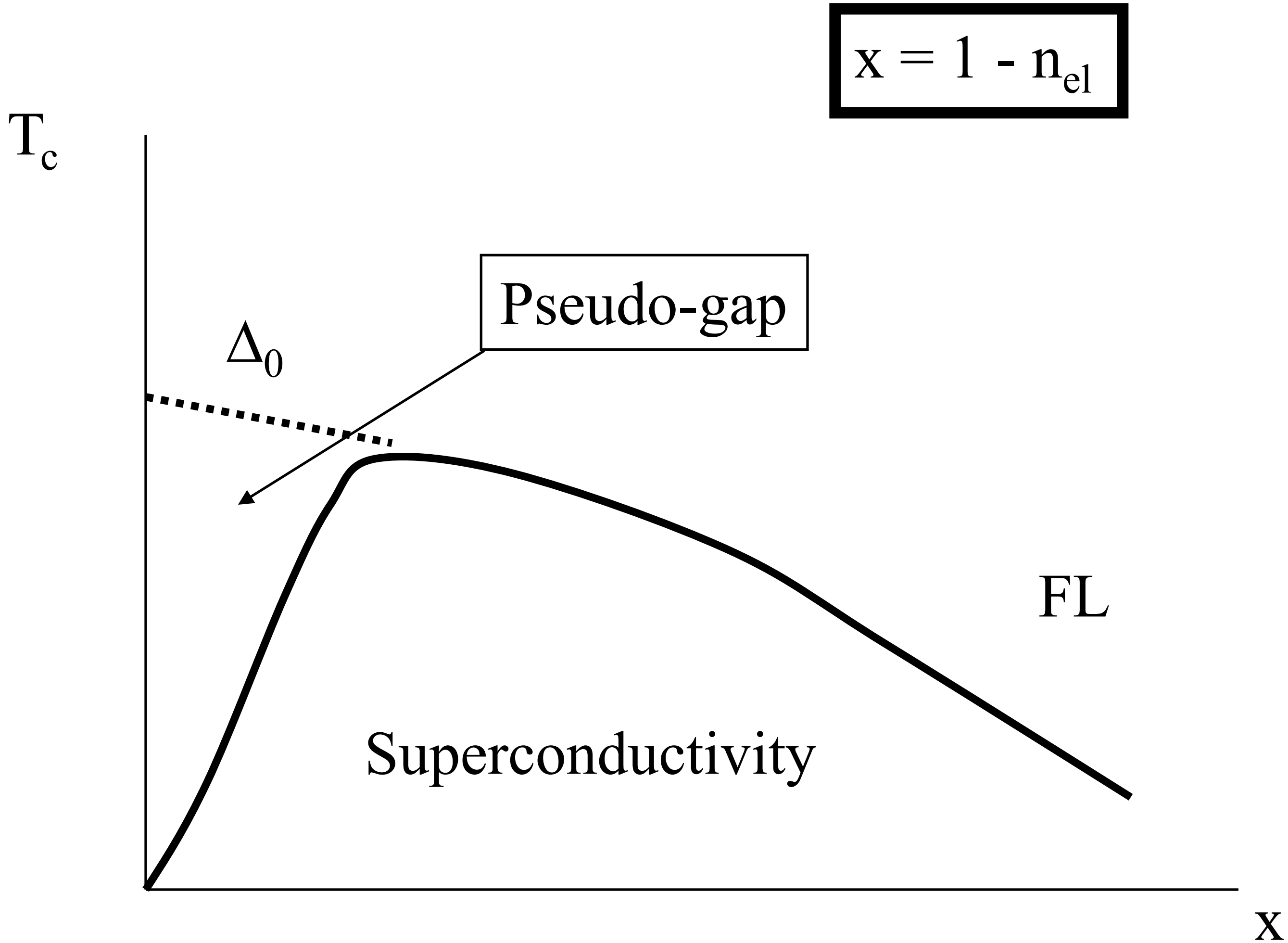
$|U| >> t$ BEC superconductivity

pairs form at $T \sim |U|$ (pseudo-gap)

$$T_c \sim \rho_s \sim t^2 / |U|$$



Maximal T_c occurs at a point of crossover in the physics



For x small, $T_c \sim \rho_s \sim$ condensation (phase coherence) scale.
For x large, $T_c \sim \Delta_o \sim$ pairing scale.

For small x, ρ_s is supressed due to “competing” CDW order.

Some solutions of model problems:

1) The negative U Hubbard model

2) The Holstein model (electron-phonon problem).

(Also discussed by DJS.)

Holstein model

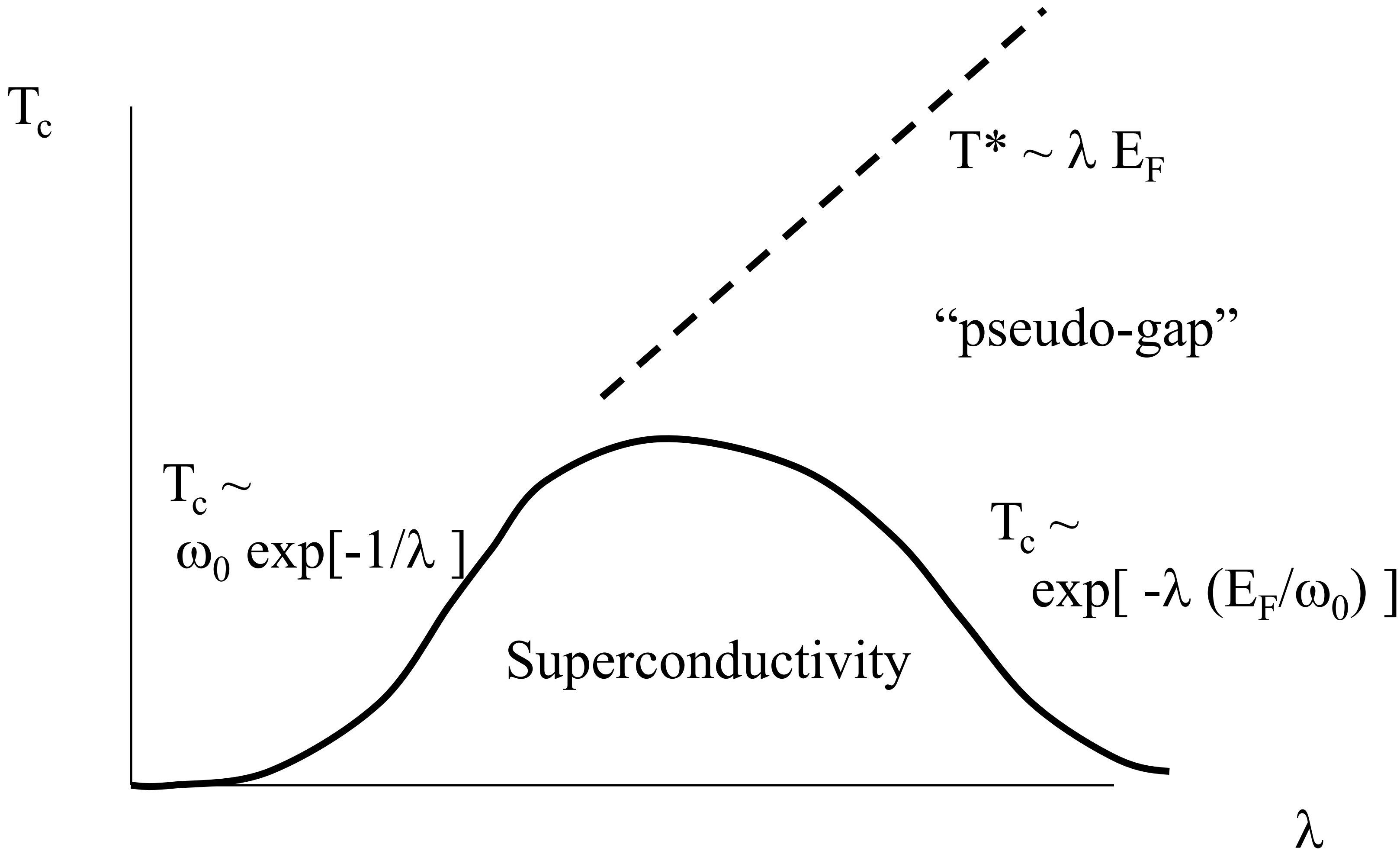
Small $\lambda << 1$ $T_c \sim \omega_0 \exp[-1/\lambda]$

Large $\lambda >> 1$ $T_c \sim \exp[-\lambda (E_F/\omega_0)]$

$\Delta_0 \sim E_F \lambda$

"small bipolarons"

This is a breakdown of
Eliashberg theory!!!



Again, optimal T_c occurs at the crossover from a pairing dominated to a condensation dominated regime.

Some solutions of model problems:

1) The negative U Hubbard model

2) The Holstein model (electron-phonon problem).

3) The inhomogeneous negative U Hubbard model
(in the weak coupling limit).

Suppose you have some (weak) attractive U's
of concentration $x < 1$
to distribute in some way on the lattice.

If they are distributed uniformly,
$T_c \sim \exp[-\alpha t / |U_{av}|]$ $|U_{av}| = x|U| < |U|$

If they are macroscopically phase separated,
$T_c \sim \exp[-\alpha t / |U|]$ and $T_c = 0$

With appropriate distribution can make a spatially
structured phase with "uniform"
$T_c \sim \exp[-\alpha t / |U|]$

Some solutions of model problems:

1) The negative U Hubbard model

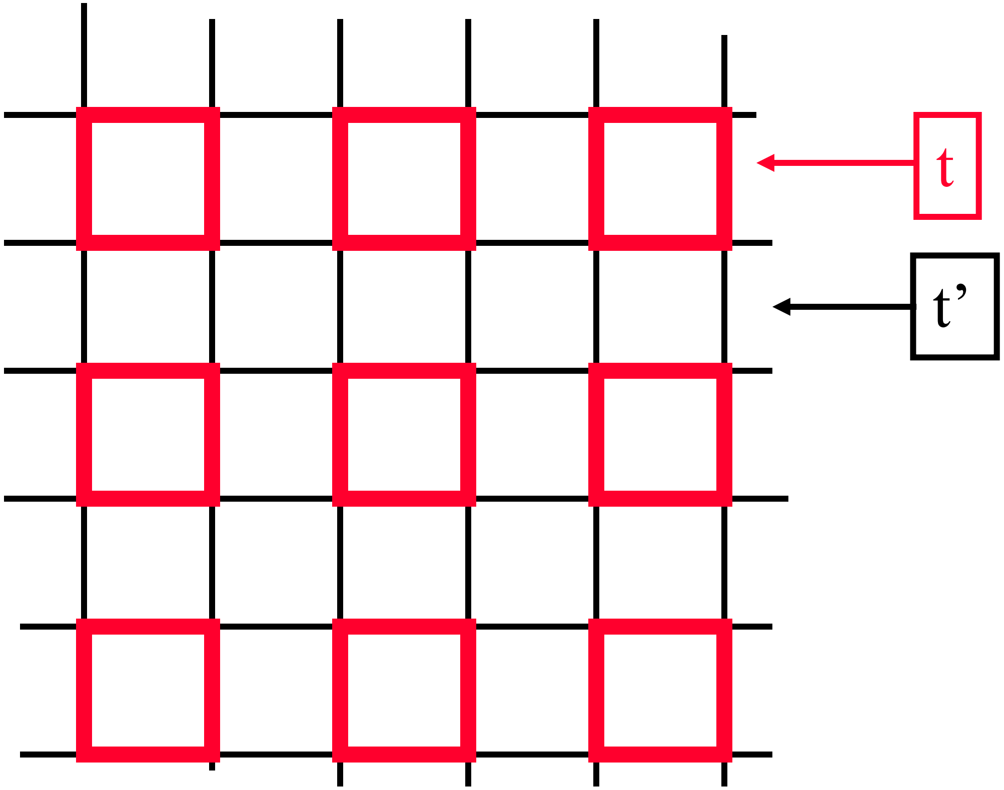
2) The Holstein model (electron-phonon problem).

3) The inhomogeneous negative U Hubbard model
(in the weak coupling limit).

4) The "Checkerboard Hubbard model."
(Similar, although not as complete, results pertain to the "Striped Hubbard model.")

Phase diagram of checkerboard Hubbard model

"Homogeneous" (t'/t=1) to "highly inhomogeneous" (t'/t << 1)

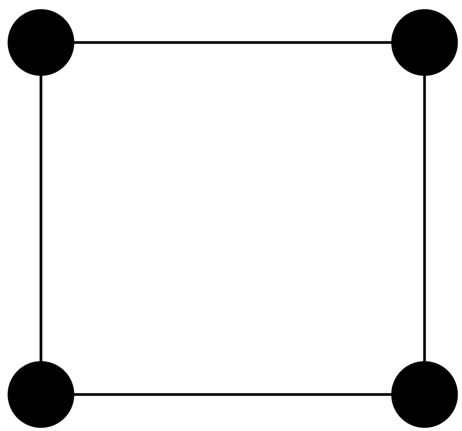


The Hubbard model for t = t'

The Checkerboard Hubbard model for t > t'

Repulsive U Hubbard model on 4 sites

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



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

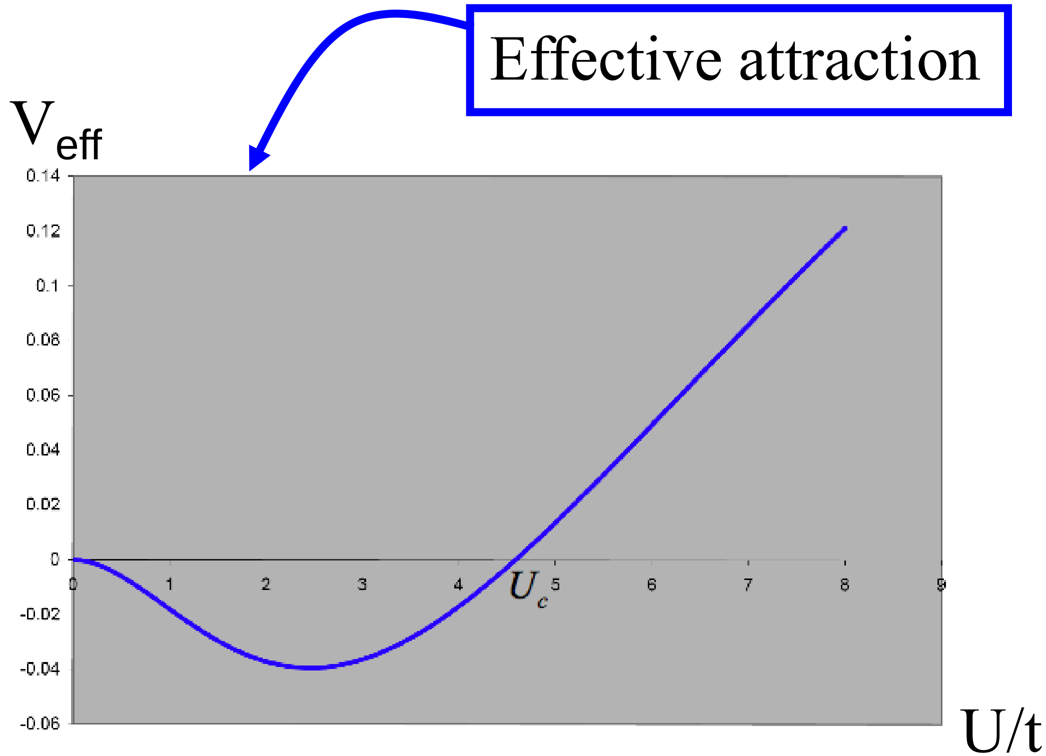
4 site Hubbard model

$Q = 4 - N_{electrons} = N_{holes}$ E(Q) = Ground-state energy

Q	E(Q)	S	S_z	symmetry	eigenstate
0	$\frac{\sqrt{3}U-2\sqrt{16t^2+U^2}\cos(\frac{\beta}{3})}{\sqrt{3}}$	0	0	d-wave	Ψ_{111}
1	$\frac{U-\sqrt{32t^2+U^2+4\sqrt{64t^4+3t^2U^2}}}{2}$	$\frac{1}{2}$	$\pm\frac{1}{2}$	$p_x \pm ip_y$	Ψ_{46},Ψ_{70} Ψ_{50},Ψ_{74}
2	$\frac{U-2\sqrt{48t^2+U^2}\cos(\frac{\alpha}{3})}{3}$	0	0	s-wave	Ψ_{22}

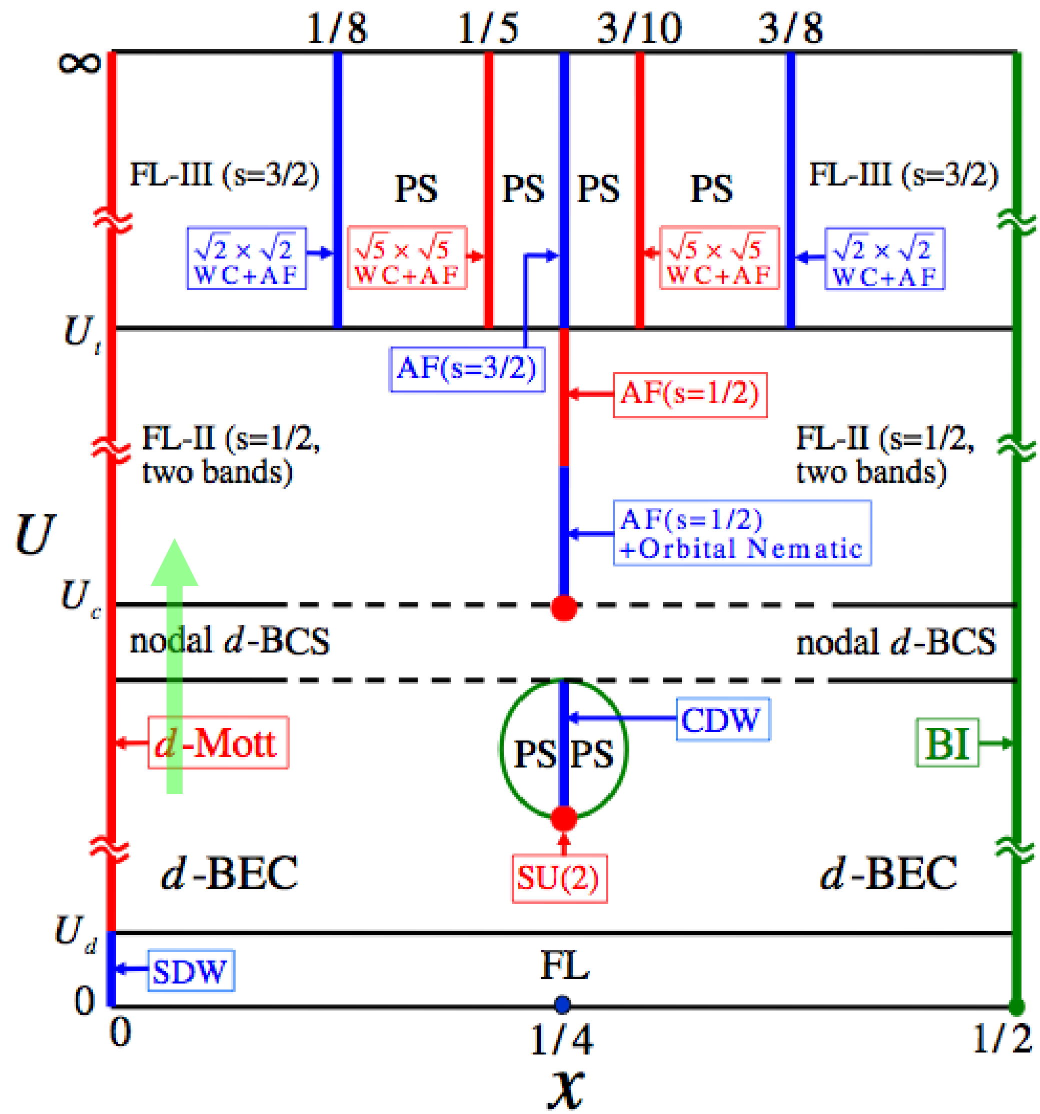
4-site Hubbard model

$$V_{eff} = E(2) + E(0) - 2E(1)$$

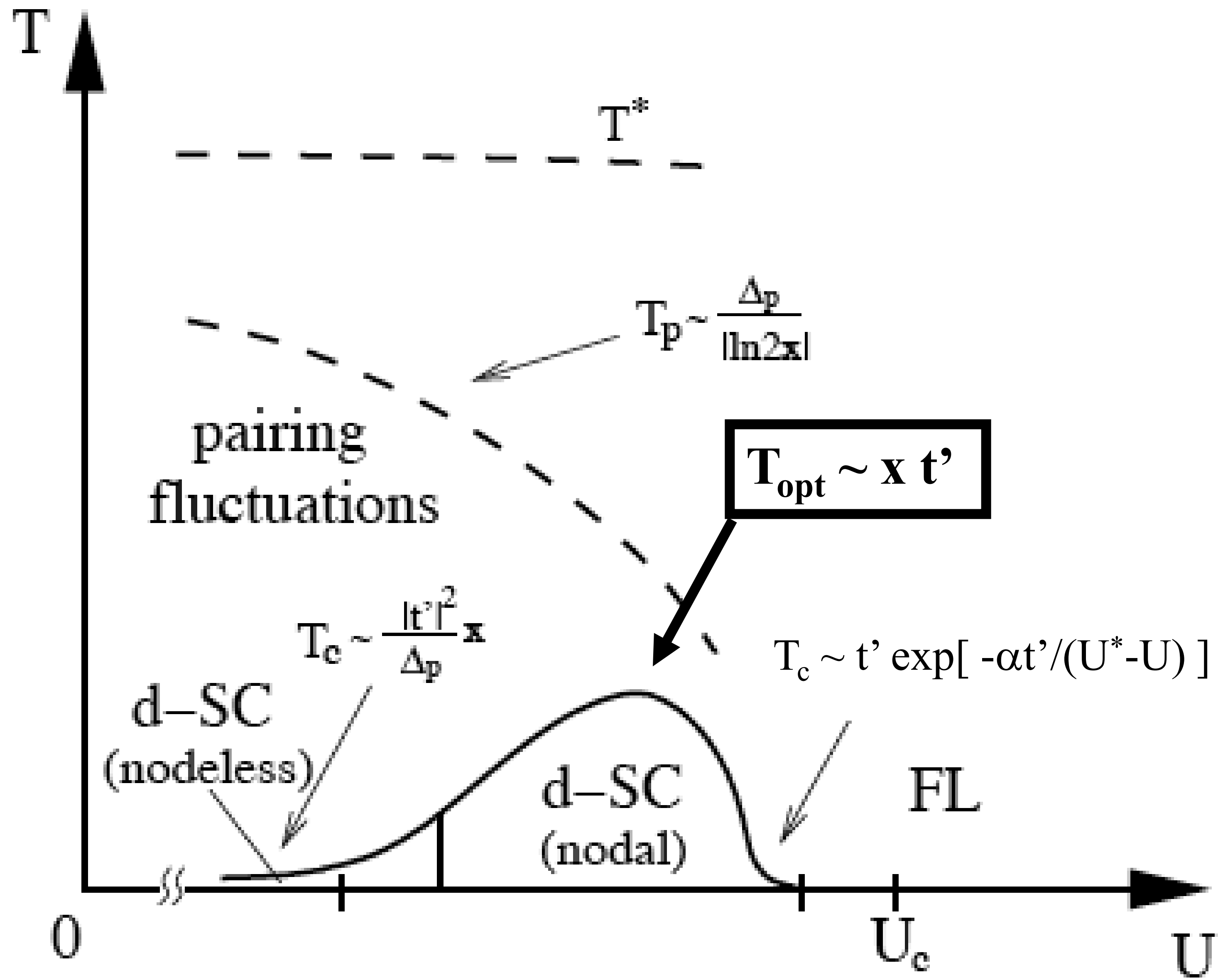


When $V_{eff} < 0$, it is energetically favorable to add two holes to one square rather than one hole to each of two squares. $U_c/t = 4.58 \ldots$

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



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



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

Checkerboard Hubbard model proves many points of principle.

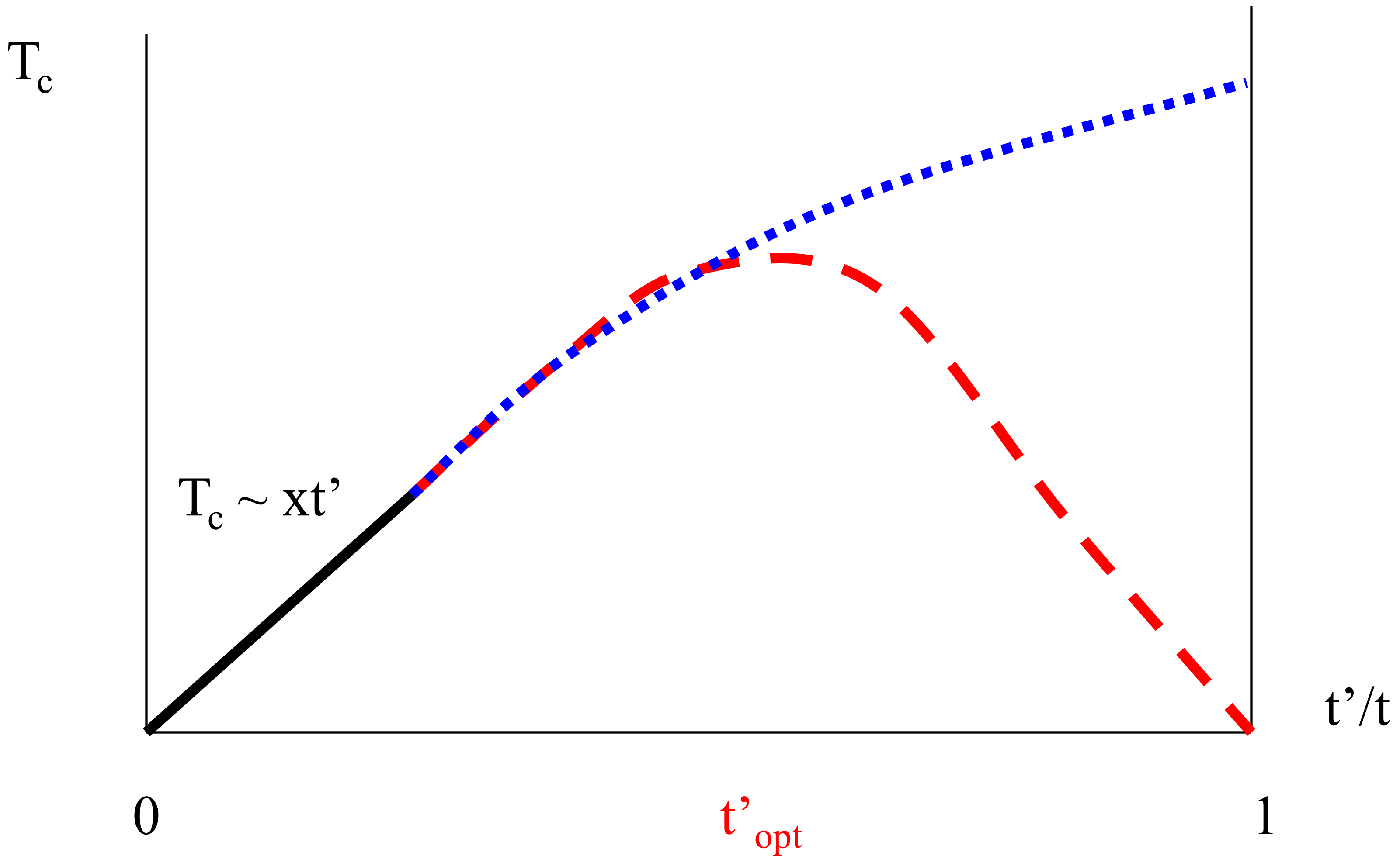
Can get superconductivity directly from strong repulsion between electrons

Highly non-BCS **mechanism** of SC - no well defined phonon (or any other well defined boson) exchanged, and no FL “normal” state.

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

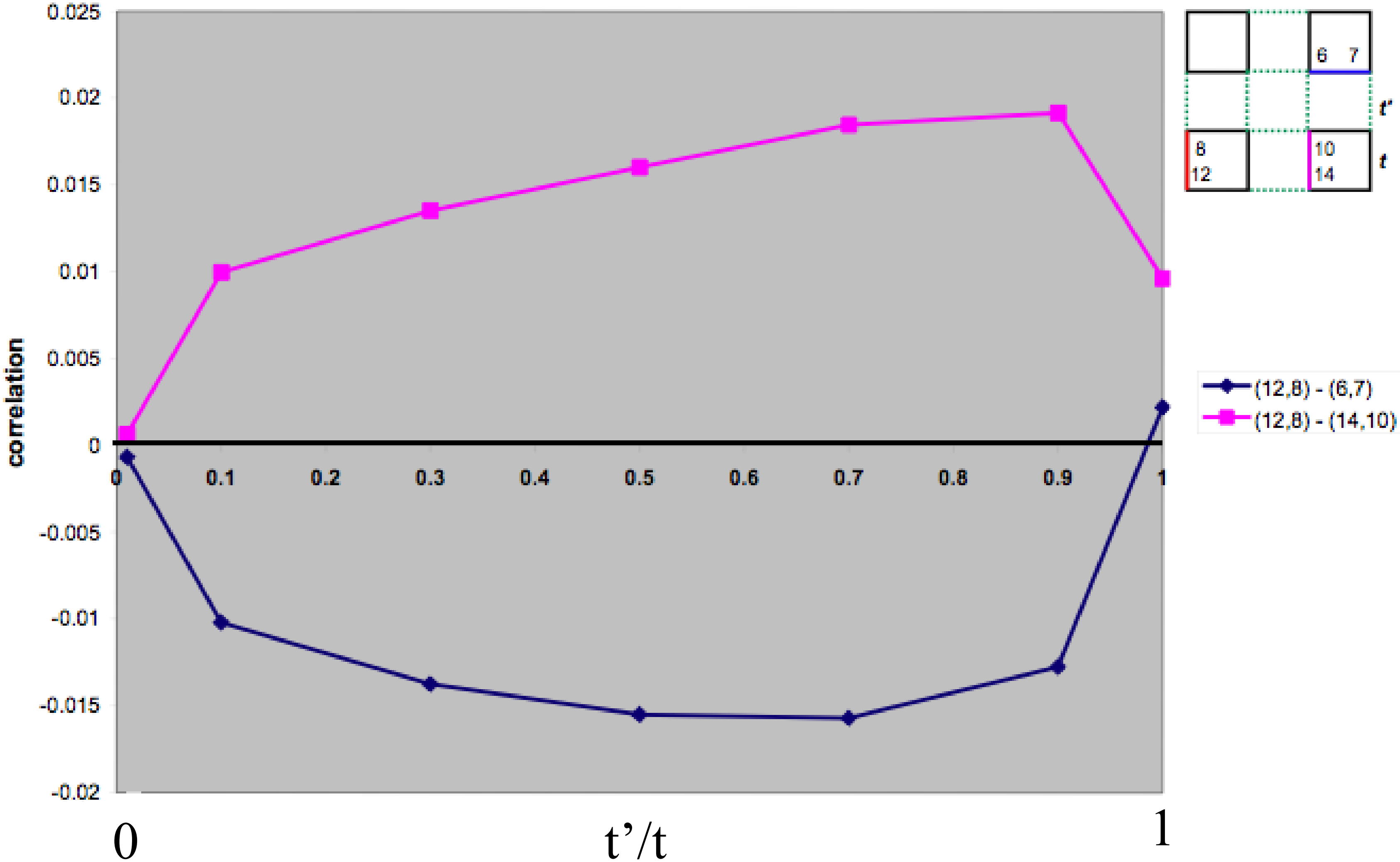
Also has a crossover from pairing to coherence at roughly T_{opt}

Is inhomogeneity essential?

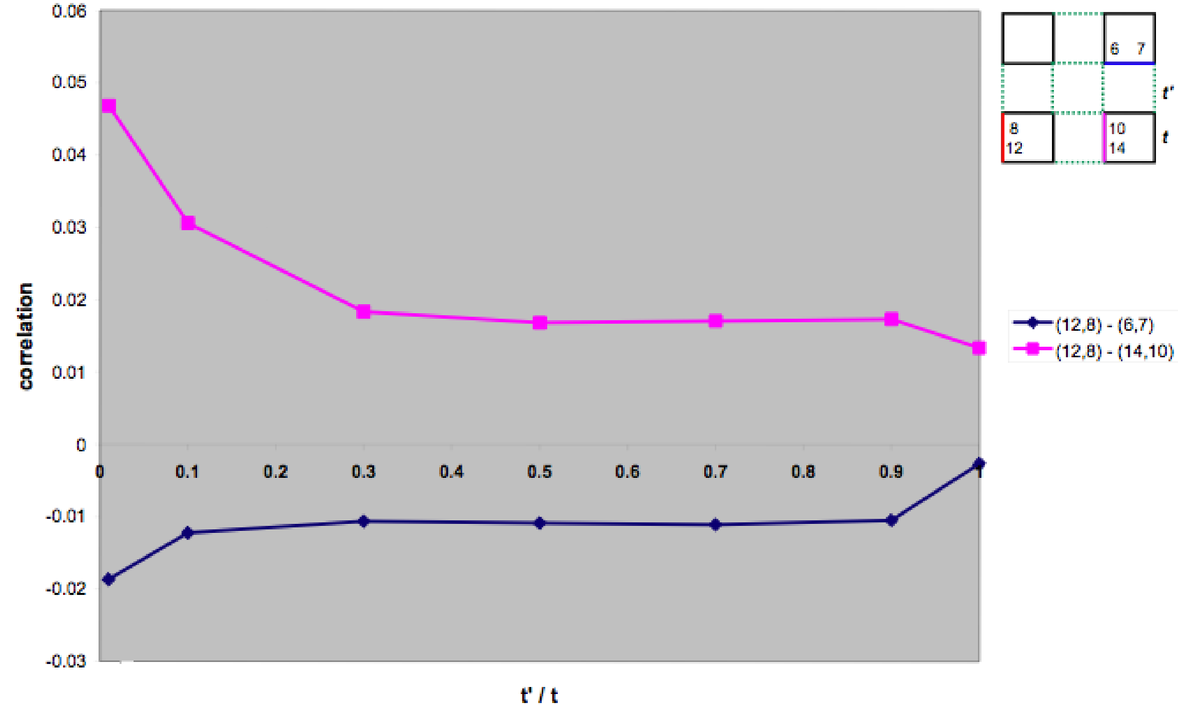


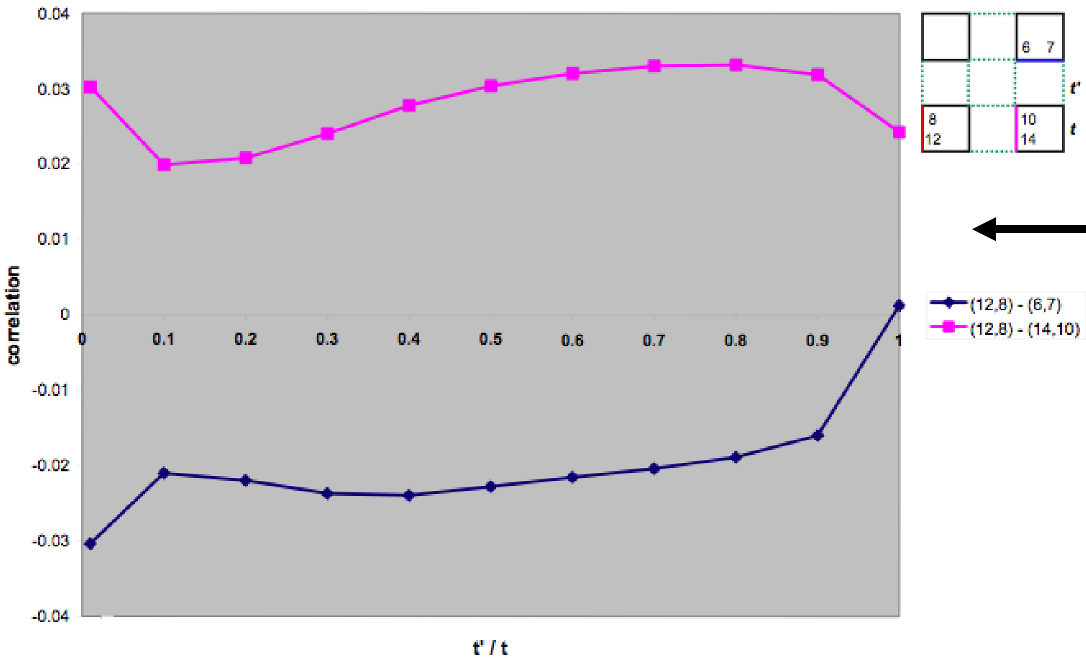
Equal time Pairfield-pairfield correlation function on 4x4 checkerboard

14 electrons on 16 sites with U=8t



12 electrons
U=4

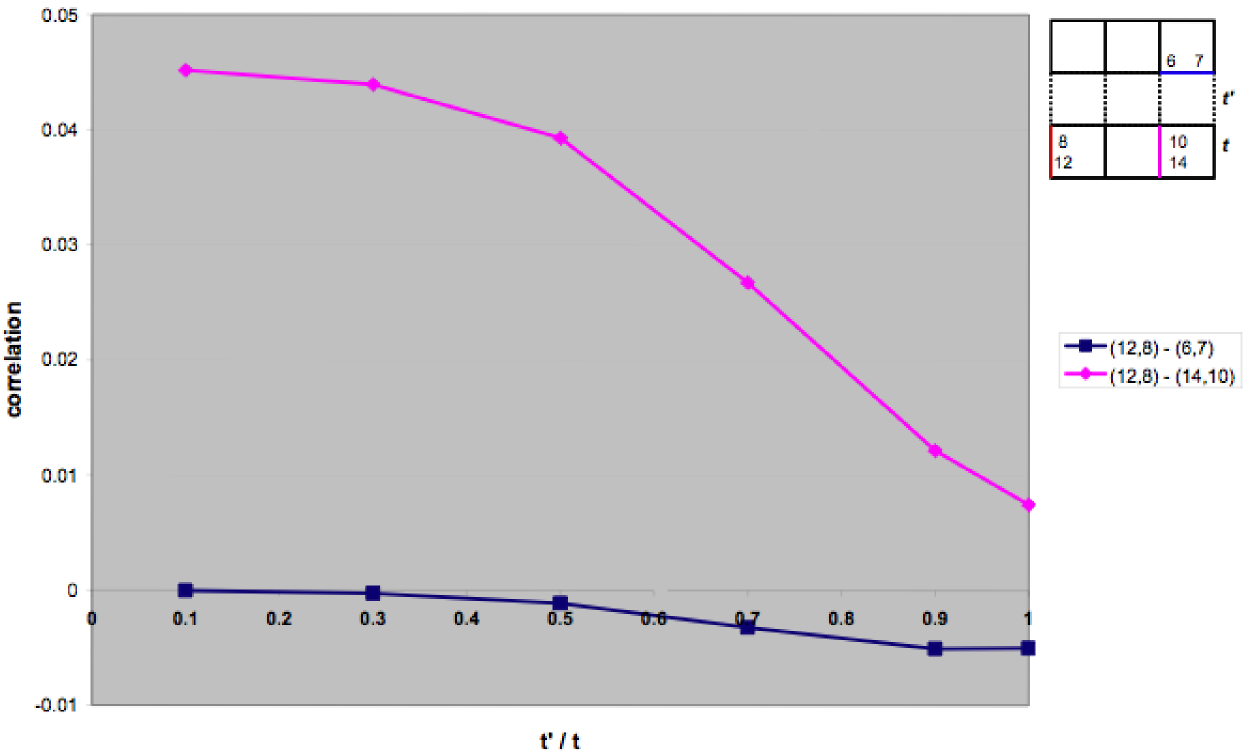




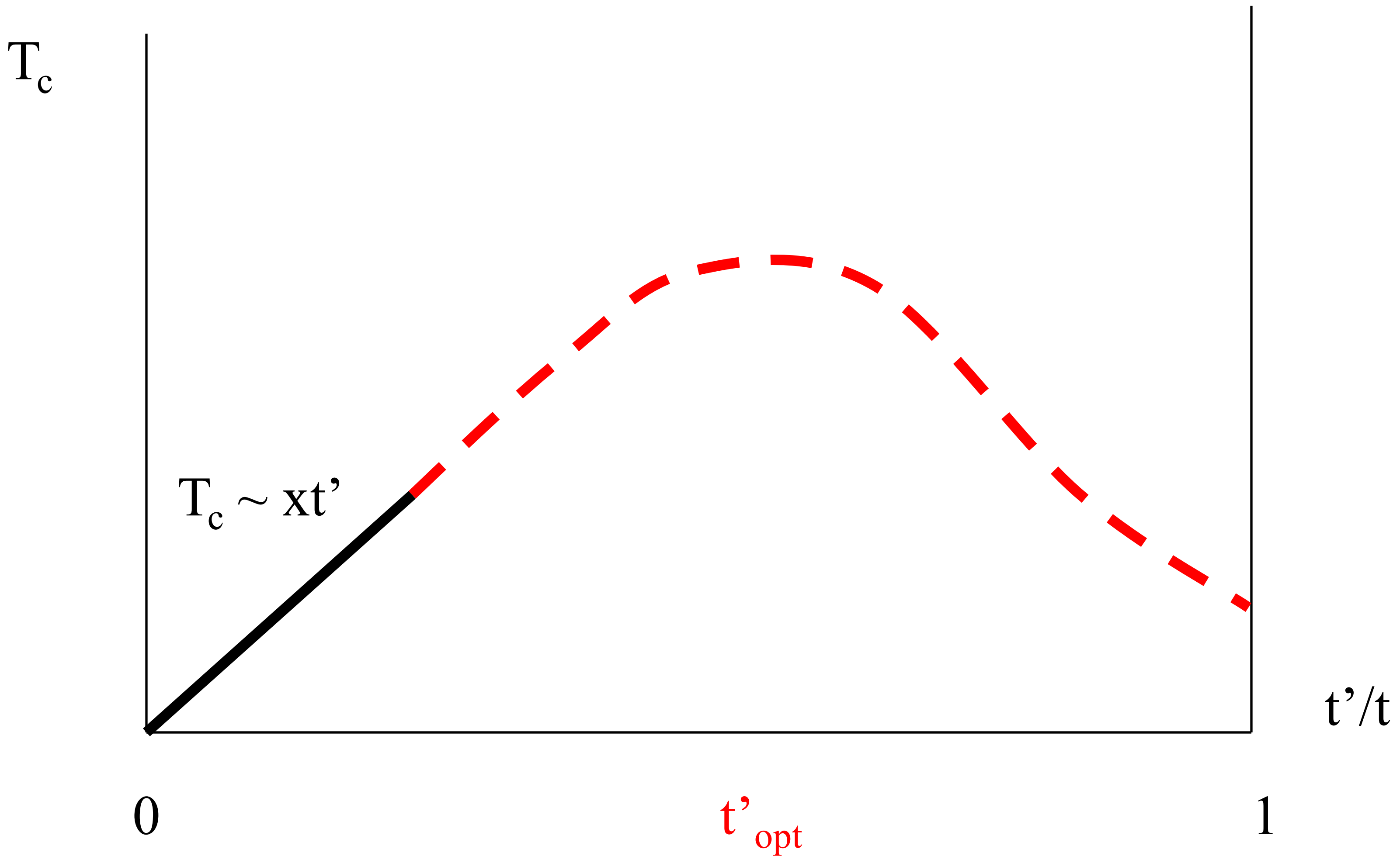
14 electrons
U=4

Two “coupled two leg ladders”

U=4t 16 electrons in 16 sites



Probably inhomogeneity essential to optimize T_c!



Maybe there is an "optimal inhomogeneity" for HTC.

Then "stripes" may be essential - a form of self-organized inhomogeneity.

Mesoscale structure of another kind is demonstrably important T_c rises for n=1 to 2 to 3, then drops for n=4 to 5 … (n=number of layers)

Search for ways of making inhomogeneous systems with high pairing regions and highly coherent (itinerant) regions.

How to make High T_c higher - a theoretical proposal

Physica **B 318**, 61-67 (2002).

Suppose it is true that in underdoped cuprates, $T_{pair} >> T_c$.

Then, to enhance T_c, we need to enhance T_θ.

$x_2 \geq x_{opt}$ — T_θ large

$x_1 < x_{opt}$ — Δ_0 large

$x_2 \geq x_{opt}$ — T_θ large

$T_{pair} \sim T_{BCS} \sim \Delta_0/2$

$T_\theta \sim \rho_s/m^*$

Consider a bilayer cuprate with two inequivalent layers
vary, separately, x_1 and x_2 to optimize T_c

Maybe this already occurs in $Y_2Ba_4Cu_7O_{15}$

Y Y Y Y Y Y Y Y Y Y

double chain double chain double chain

Y Y Y Y Y Y Y Y Y

chain chain chain chain chain chain chain

$T_c = 95K$ = 3 K enhancement over $YBa_2Cu_3O_7$

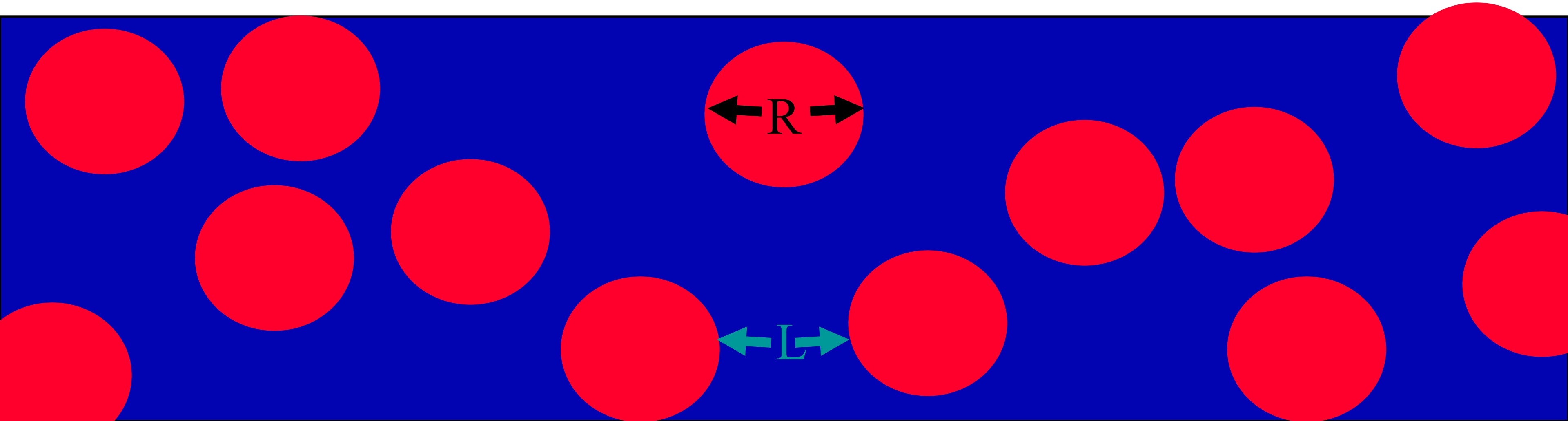
Making an optimal high temperature superconductor from a mixture of two phases

A= strong pairing but small superfluid density (possibly both deriving from stripe order).

B= large Drude weight, but little or no pairing (possibly an overdoped metal).

$R \sim \xi_0$

$L \sim L_T \sim v_F/T$



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a pairing dominated regime - $\mathbf{T_c \sim \Delta_0}$
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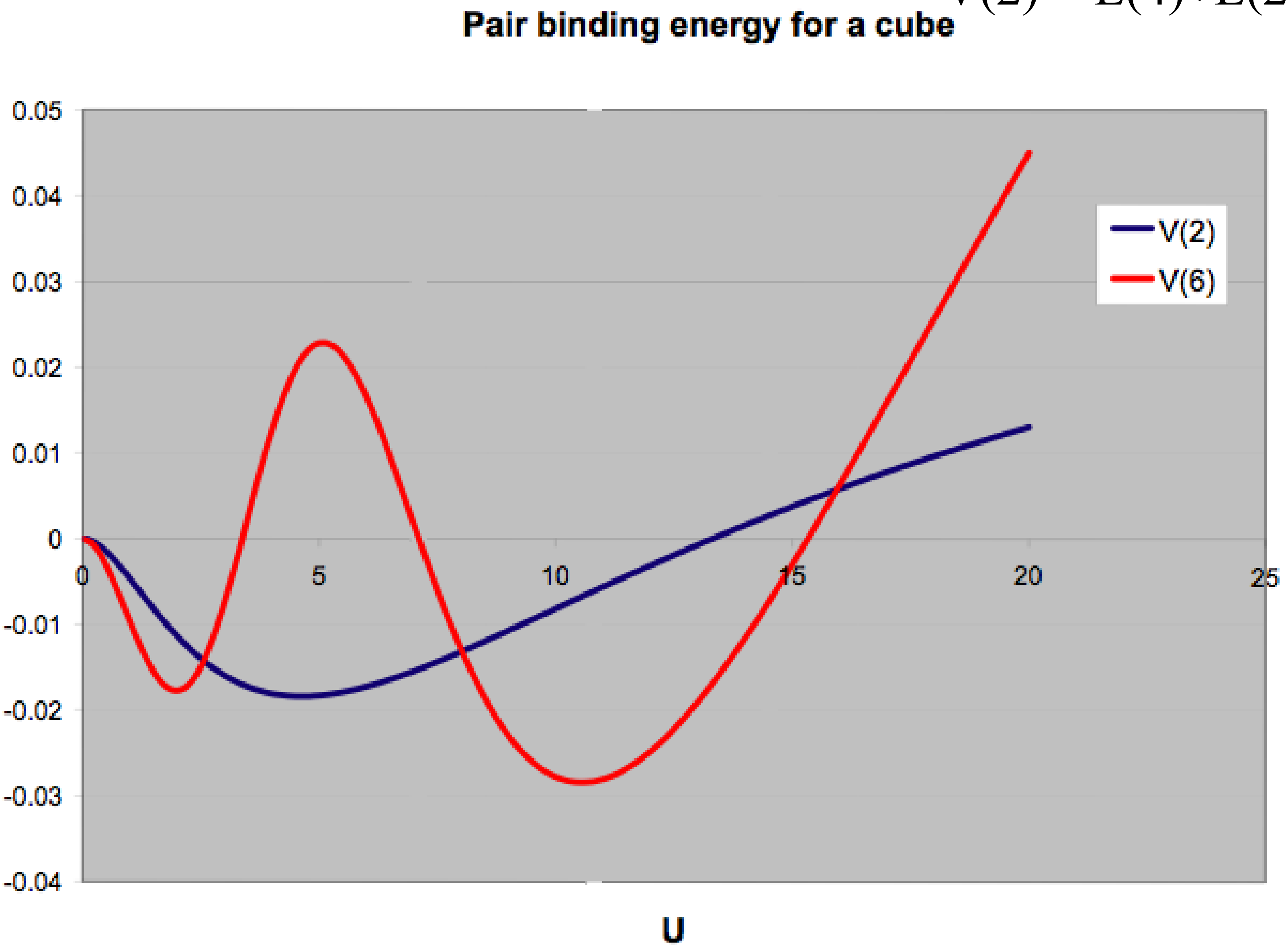
Breaking a system into intermediate scale "clusters" can, under special circumstances, produce enormous enhancement of Δ_0 but always at the expense of reduced T_θ, so optimal T_c occurs at an "optimal inhomogeneity."

One can use these principles to develop strategies for making high T_c higher.

The end

$$V(6) = E(8)+E(6) - 2E(7)$$
$$V(2) = E(4)+E(2) - 2E(3)$$



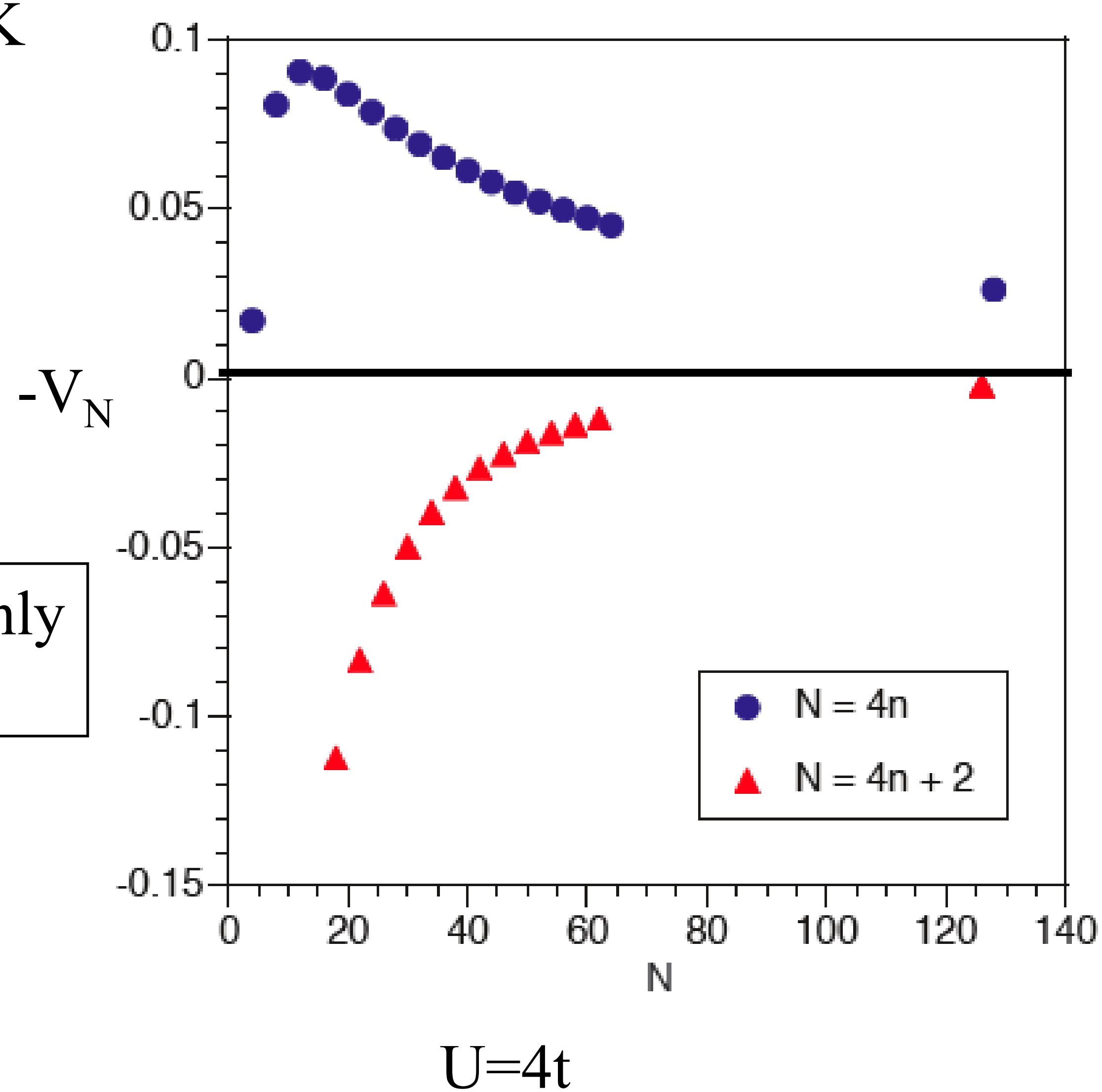
Pair binding energy on N membered Hubbard ring

S.Chakravarty and SAK
PRB (2001)

Pair-attraction occurs preferentially for intermediate sizes

Pair-attraction occurs only for intermediate U/t.

Pair-attraction occurs only on special clusters

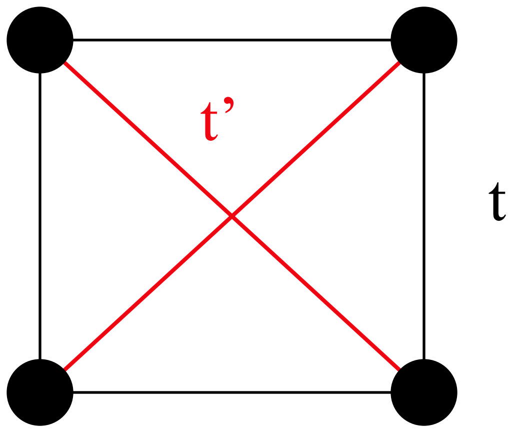


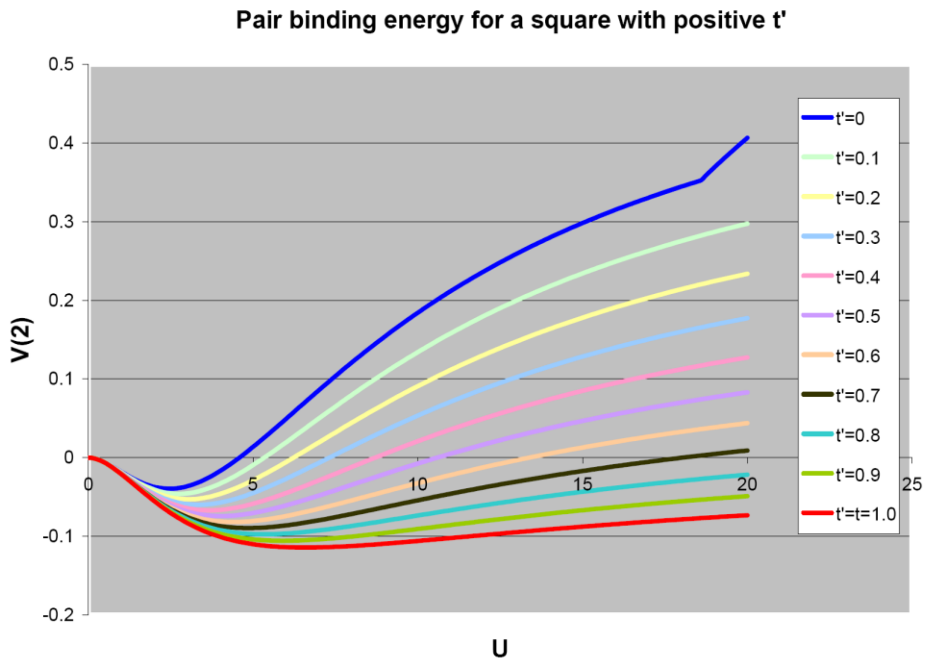
$CuO_2/_c$	n=1		n=2		n3	
	T_c(K)	Separations (Å)	T_c(K)	Separations (Å)	T_c(K)	Separations (Å)
LSCO-214	40	6.6	-	-	-	-
Hg-12(n-1)n	98	9.5	127	9.5	134	9.5
Tl-12(n-1)n	-		103	-	133	-
Tl-22(n-1)n	95	11.5	118	11.5	125	11.5
Bi-22(n-1)n	38	-	96	-	120	-
Y123 (6 GPa)	-	-	95	7.9	-	-
Y124 (6 GPa)	-	-	105	9.8	-	-

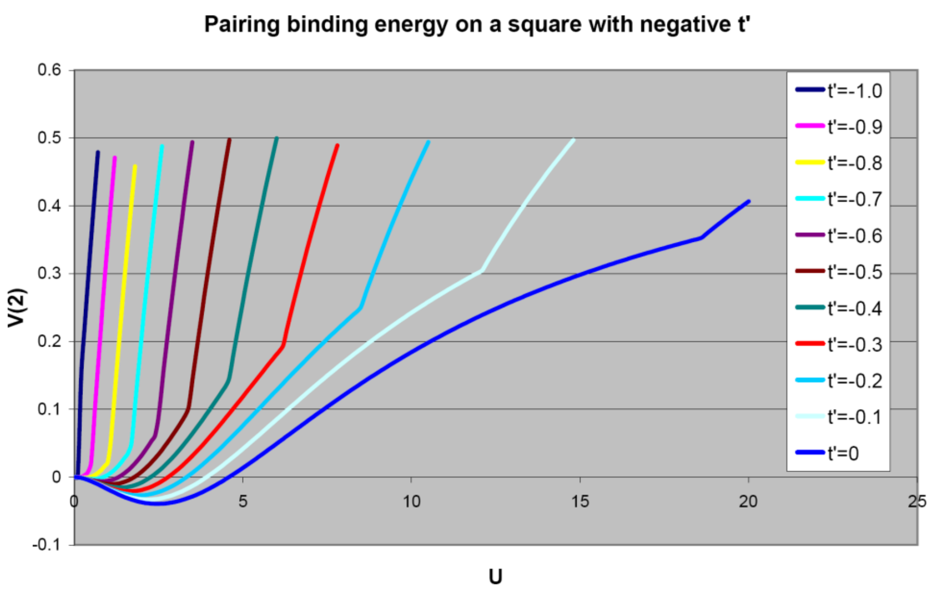
From “What can Tc teach about superconductivity?”
by Geballe and Koster, cond-mat/0604026

More about the Hubbard square

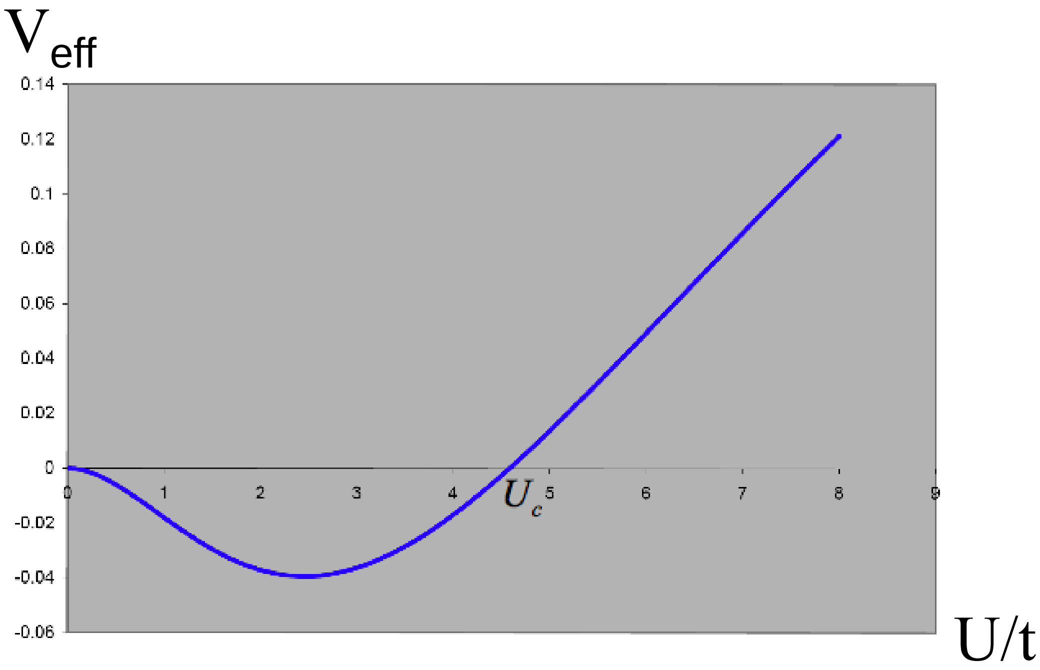
t’=t is the tetrahedron - the “best” cluster we have found yet.







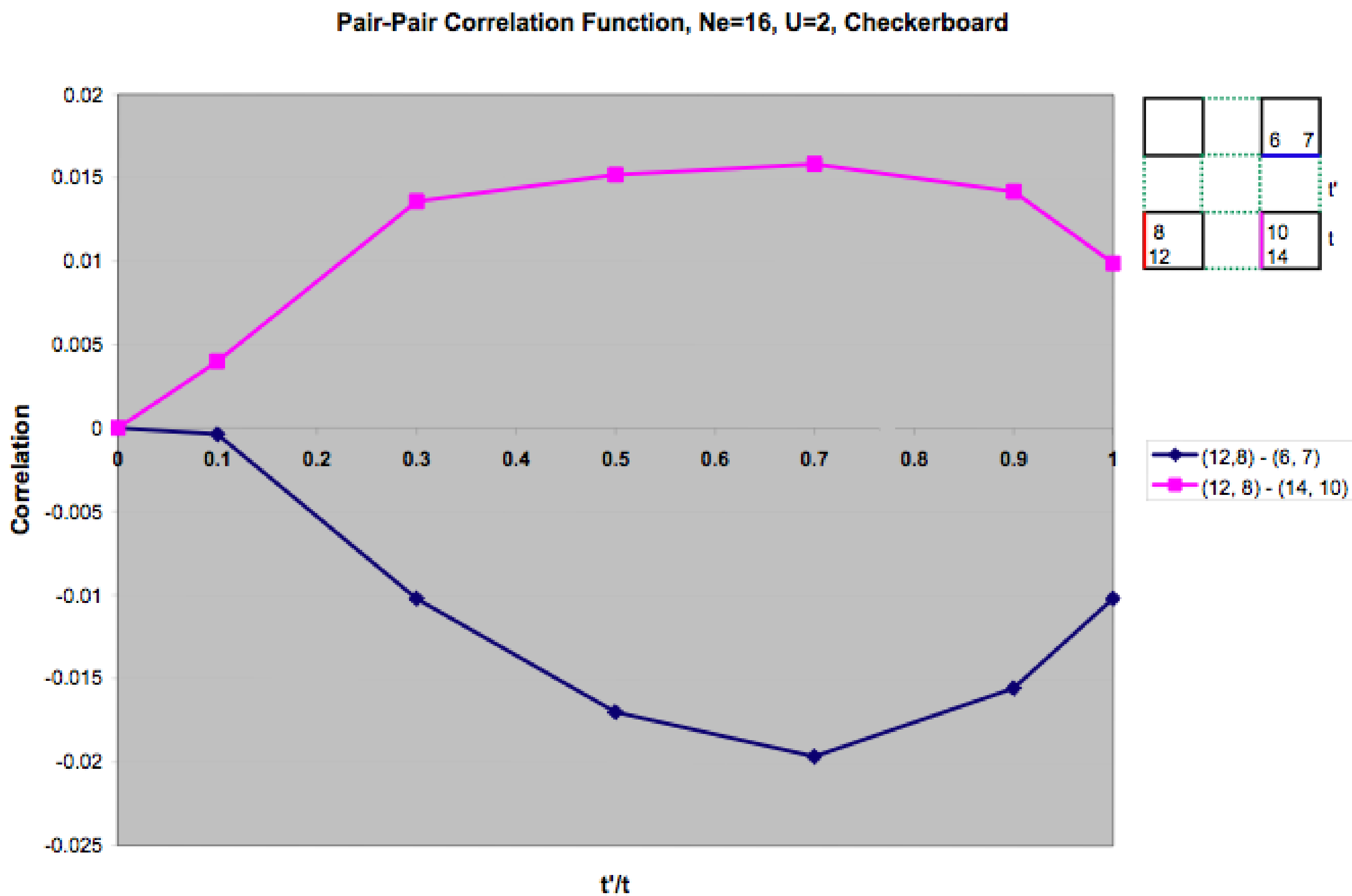
Four-site Hubbard



We can understand the onset of the effect using perturbation theory.

$V_{eff} = A\,U - B\,U^2 + \ldots \qquad A \geq 0 \qquad B > 0$

Under what circumstances is A=0?



Pair-Pair Correlation Function, Ne=16, U=2, Checkerboard
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
-0.025
Correlation
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
t'/t
6 7
t'
8
12
10
14
t
(12,8) - (6, 7)
(12, 8) - (14, 10)