

Happy Nth Birthday Michael Freedman

“Exact results concerning the
phase diagram of the
Hubbard Model

S.Raghu, D.J. Scalapin, J. Liu, E. Berg

H. Yao, W-F. Tsai, S. Chakraborty

G. Karakonstantakis, S. Whitehead, S. Cho

Exact:

Not approximate.

**Involving precise statements that
are either exactly right or simply wrong.**

I will present evidence that they are right.

The Hubbard Model

- The paradigmatic model of strongly correlated electron systems

The Hubbard model is to correlated electron systems as the Ising model is to statistical mechanics

except that the phase diagram of the Ising model is well understood, while almost everything about the Hubbard model is subject to controversy.

The Hubbard Model

- The paradigmatic model of strongly correlated electron systems
- The most studied model of high temperature superconductivity
- The principle model of metallic ferromagnetism
- The fundamental model of quantum (insulating) antiferromagnetism

The Hubbard model

$$H = - \sum_{i,j,\sigma} t_{ij} [c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.C.}] + U \sum_j c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger c_{j,\downarrow} c_{j,\uparrow}$$

$U > 0$ Repulsive

Parameters:

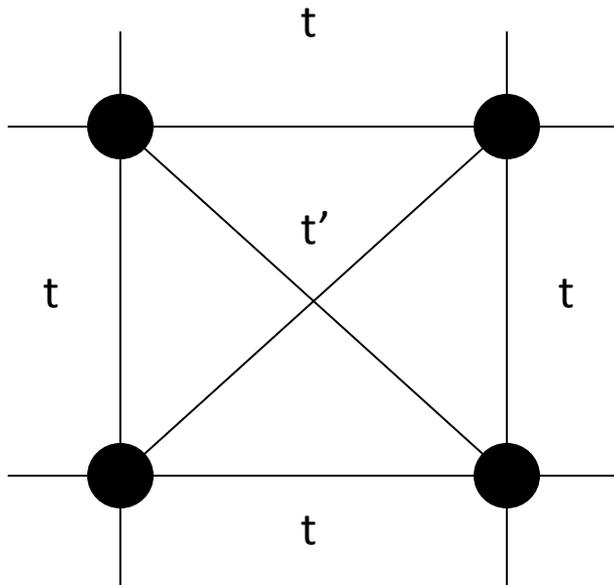
U/t = “strength” of coupling

$n = (1-x) =$

number of electrons
per site

Dimensionality and
lattice structure

t'/t = “band-structure”



In Someone's Theory of the Hubbard Model:

Ferromagnetic metal

Fermi liquid

Antiferromagnetic insulator

Spin 3/2 Fermi liquid

Antiferromagnetic metal

Charge density wave

Electronic Phase Separation

Unconventional Superconductivity:

d-wave, p-wave, f-wave, and s_{\pm} superconductivity

Intertwined spin and charge density wave order:

"Stripes" and bubbles and checkerboards

Electron nematic and other electronic liquid crystalline phases

Spin liquid ground-states of various sorts:

Fully gapped Z_2 , Nodal, pseudo-Fermi surface

Spatially oscillatory superconductivity:

Striped superconductor or PDW

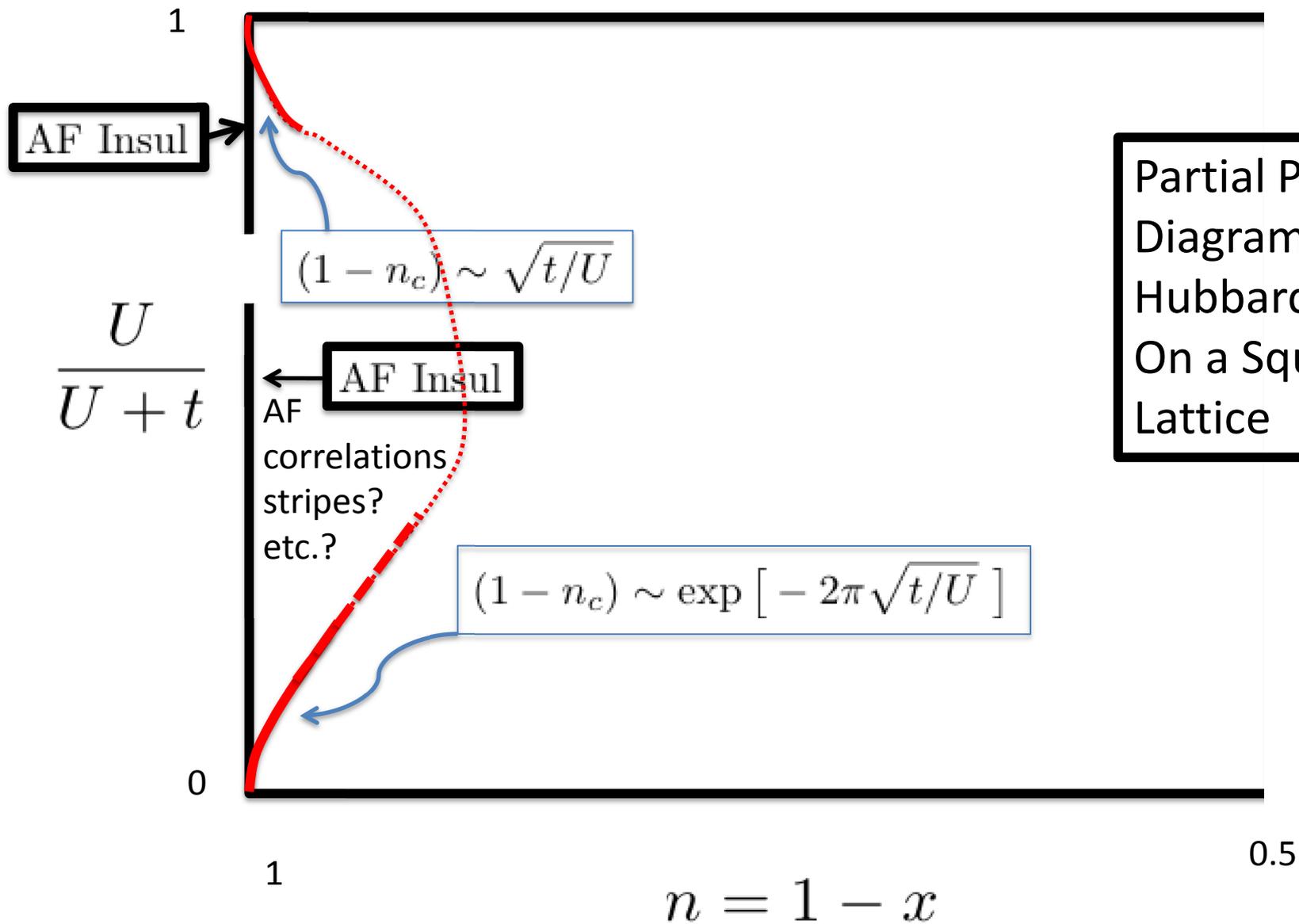
Non-Fermi liquid or "hidden Fermi liquid" or RVB

There is a large, and vocal community that holds that superconductivity is impossible without attractive (electron-phonon) interactions.

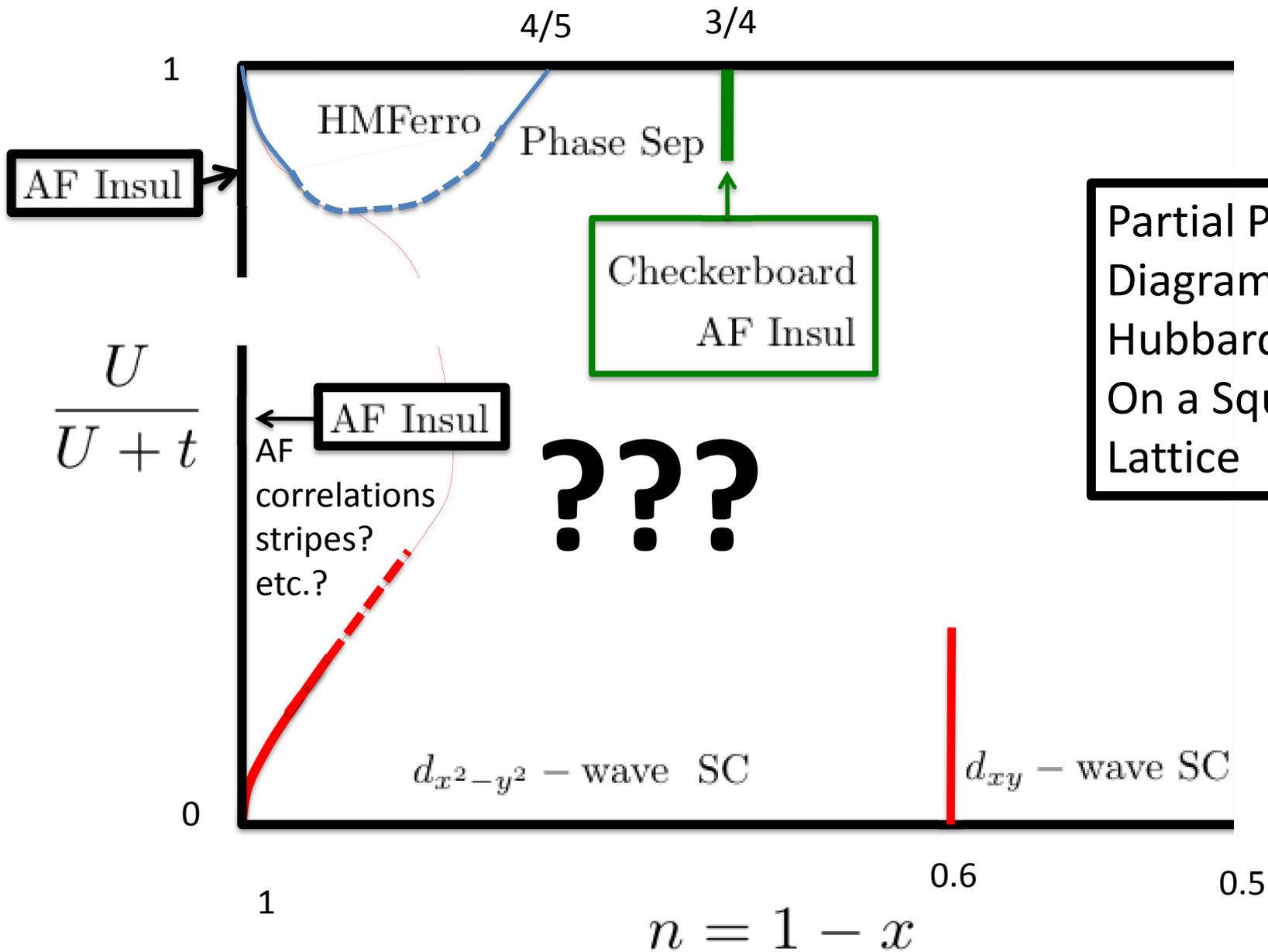
“No wonder American taxpayers are upset! They could well wonder what they are paying for. One way of looking at this is that we are relatively well off: Steve could have been selling subprime mortgages instead.”

- a very distinguished condensed matter theorist presenting a reasoned argument against superconductivity in the positive U Hubbard model

However, they are wrong.



Partial Phase Diagram of the Hubbard Model On a Square Lattice



Partial Phase Diagram of the Hubbard Model On a Square Lattice

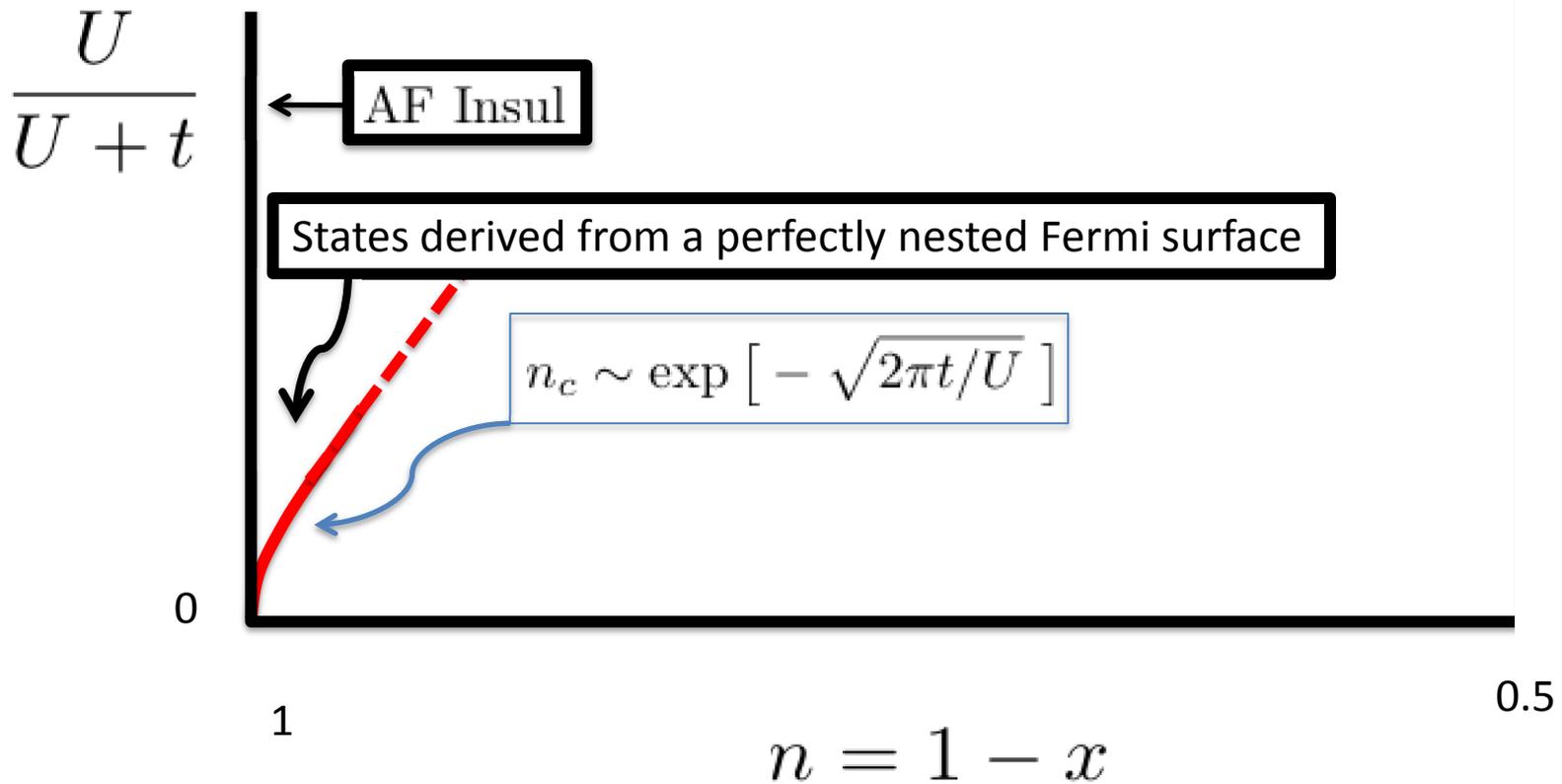
Small U/t limit of the Hubbard Model:

S. Raghu, SAK, and D. J. Scalapino - *PRB* **81**, 224505 (2010)

Draws on work of Kohn and Luttinger, Shankar and Polchinski, Chubukov and Kagan, and many others

- 1) The only infinitesimal instabilities of a Fermi gas are the superconducting (Cooper) instability, except under fine-tuned circumstances (e.g. conditions of perfect nesting).

Small U/t limit of the Hubbard Model:



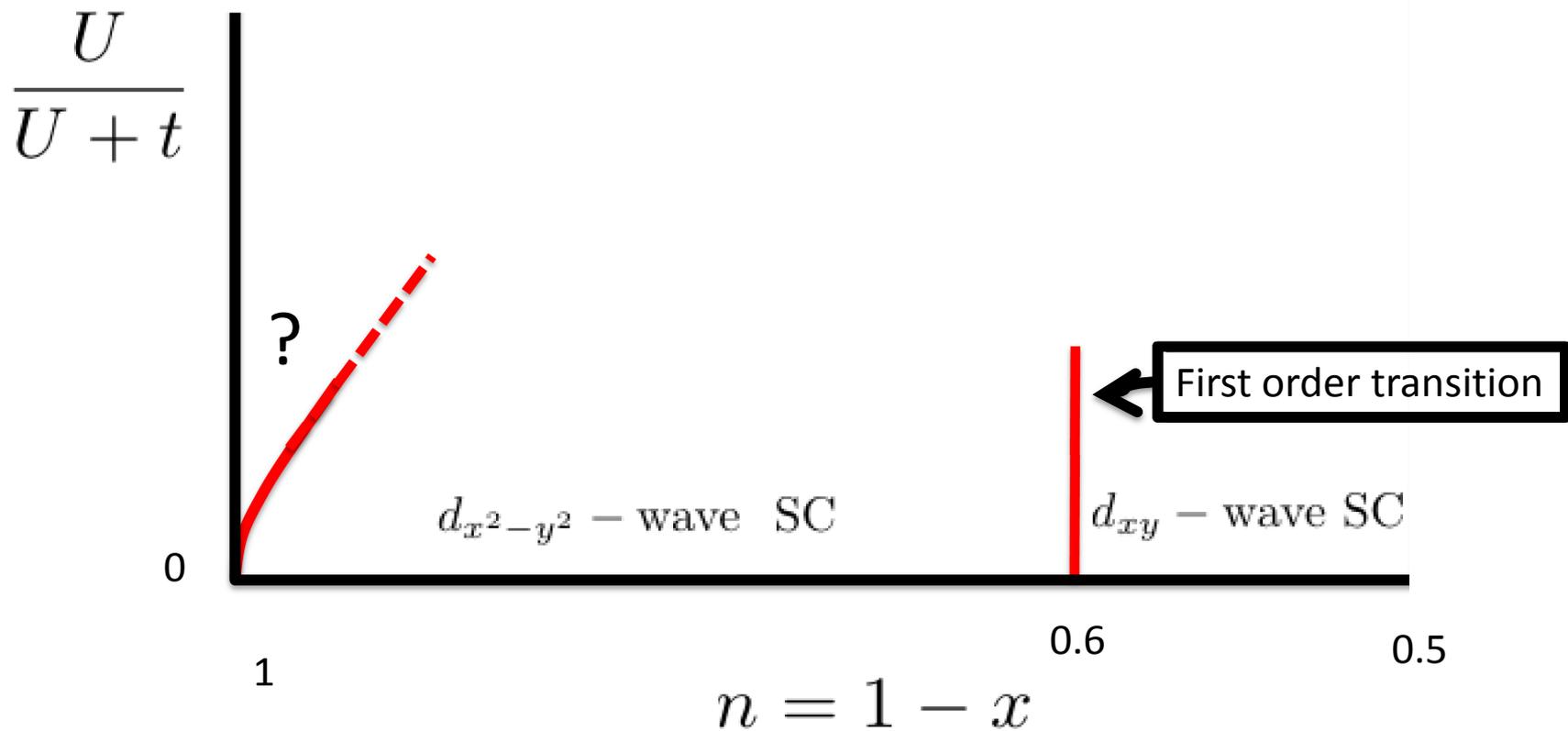
Small U/t limit of the Hubbard Model:

- 1) The only infinitesimal instabilities of a Fermi gas are the superconducting (Cooper) instability, except under fine-tuned circumstances (e.g. conditions of perfect nesting).
- 2) Effective attraction for unconventional pairing is generated by transient flows as irrelevant operators scale to 0.

“Unconventional superconductivity” means that the gap averaged over the Fermi surface vanishes (or approximately vanishes).

$$\left| \langle c_{\vec{R},\uparrow}^\dagger c_{\vec{R},\downarrow}^\dagger \rangle \right| \ll \text{Max} \left\{ \left| \langle c_{\vec{R},\sigma}^\dagger c_{\vec{R}',\sigma'}^\dagger \rangle \right| \right\}$$

Small U/t limit of the Hubbard Model:



Small U/t limit of the Hubbard Model:

Generic “unconventional” superconducting ground-state with low T_c .

Asymptotic expansion:

$$T_c \sim 4t \exp\{-1/\lambda\}$$

$$\lambda = (U/t)^2 [A + B(U/t) + C(U/t)^2 + \dots]$$

Can calculate **A** and **B** exactly from band-structure properties of non-interacting system

Can calculate symmetry and structure of the gap and the pair wave-function.

Small U/t limit of the Hubbard Model:

Generic “unconventional” superconducting ground-state with low T_c .

Asymptotic expansion:

$$T_c \sim 4t \exp\{-1/\lambda\}$$

$$\lambda = (U/t)^2 [A + B(U/t) + C(U/t)^2 + \dots]$$

Note that this is not a theory of a high superconducting T_c .

The normal state is, with high precision, a Fermi liquid.

There is no significant regime of superconducting fluctuations above T_c .

There are no competing orders.

There are no exotic phases or phase transitions.

However, if extrapolated to intermediate coupling ...

Infinite U Hubbard model

New paper by Li, Yao, Berg, and Kivelson – arxiv:1103.3305

$$H = - \sum_{\langle i,j \rangle, \sigma} \mathcal{P} [c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.C.}] \mathcal{P}$$

\mathcal{P} is the projection operator onto the space of no-double occupancy

$$n_i = \sum_{\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} = 0 \text{ or } 1 \quad \text{for all } i$$

All there is the lattice structure and the mean electron density.

Infinite U Hubbard model

New paper by Li, Yao, Berg, and Kivelson – arxiv:1103.3305

We have studied this model by DMRG on 2, 3, 4, 5, and 6 leg ladders.

2-leg ladders up to length $N=50$

4-leg ladders up to length $N=20$

6-leg ladders up to length $N=8$

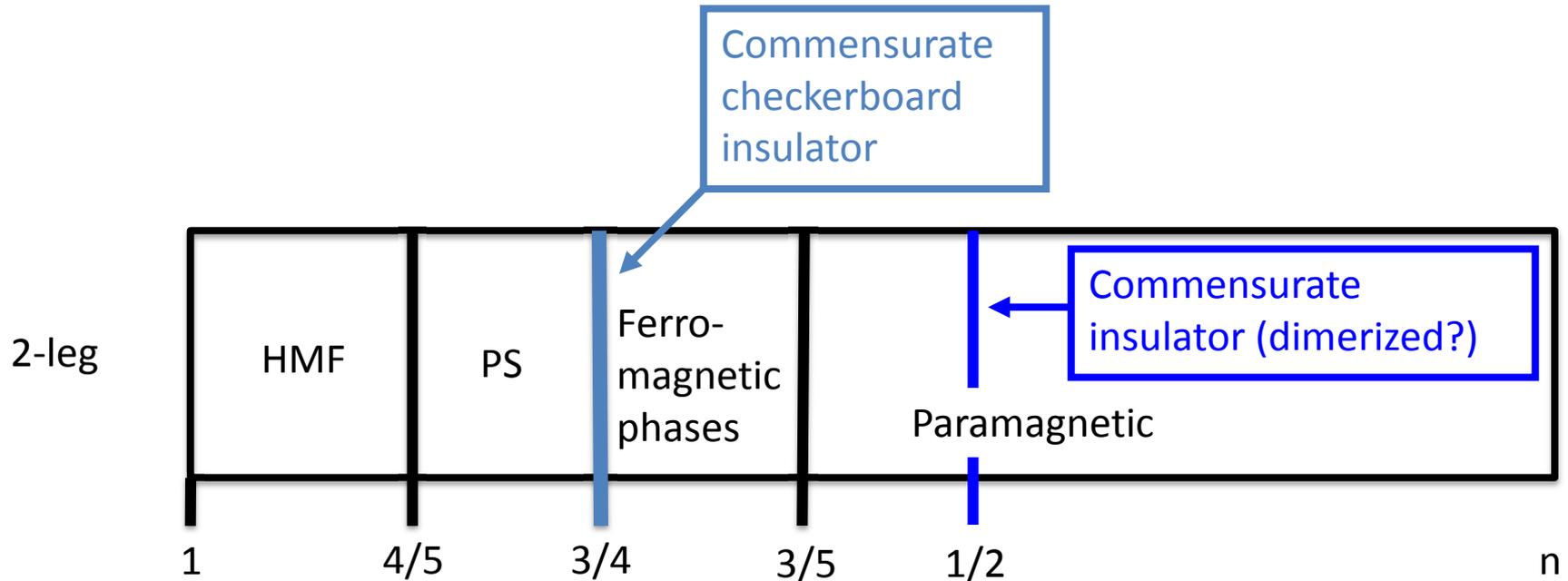
2-leg Infinite U Hubbard ladder

HMF= “Half metallic ferromagnet” = fully spin polarized Fermi liquid

PS = phase separation = regime of 2-phase coexistence

Ferromagnetic phases = partially spin polarized electron fluids

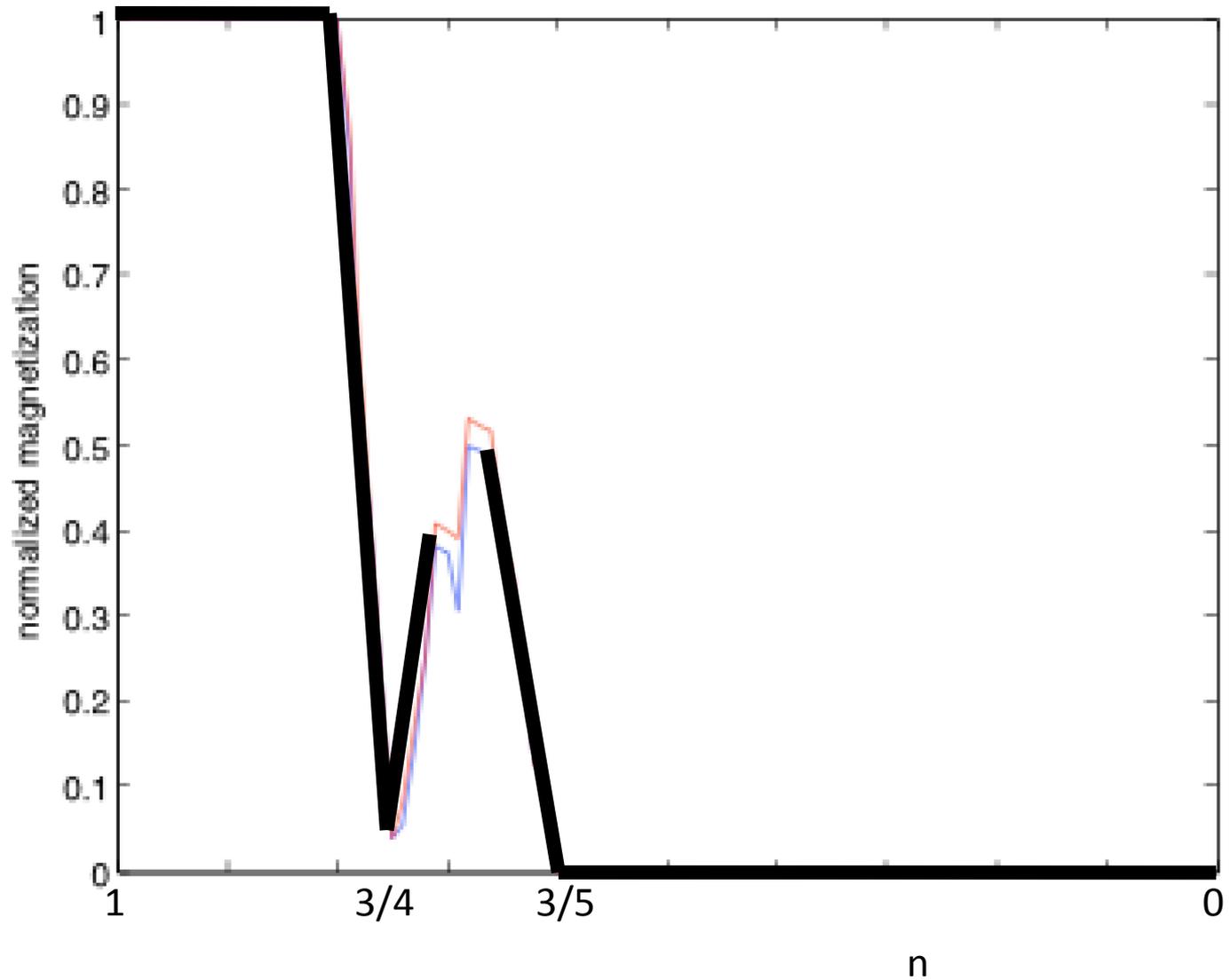
Paramagnetic = spin unpolarized = magnetization-density vanishes as $N \rightarrow \infty$



$$m = M/M_{\max}$$

2 leg ladder at infinite U

2*50lattice



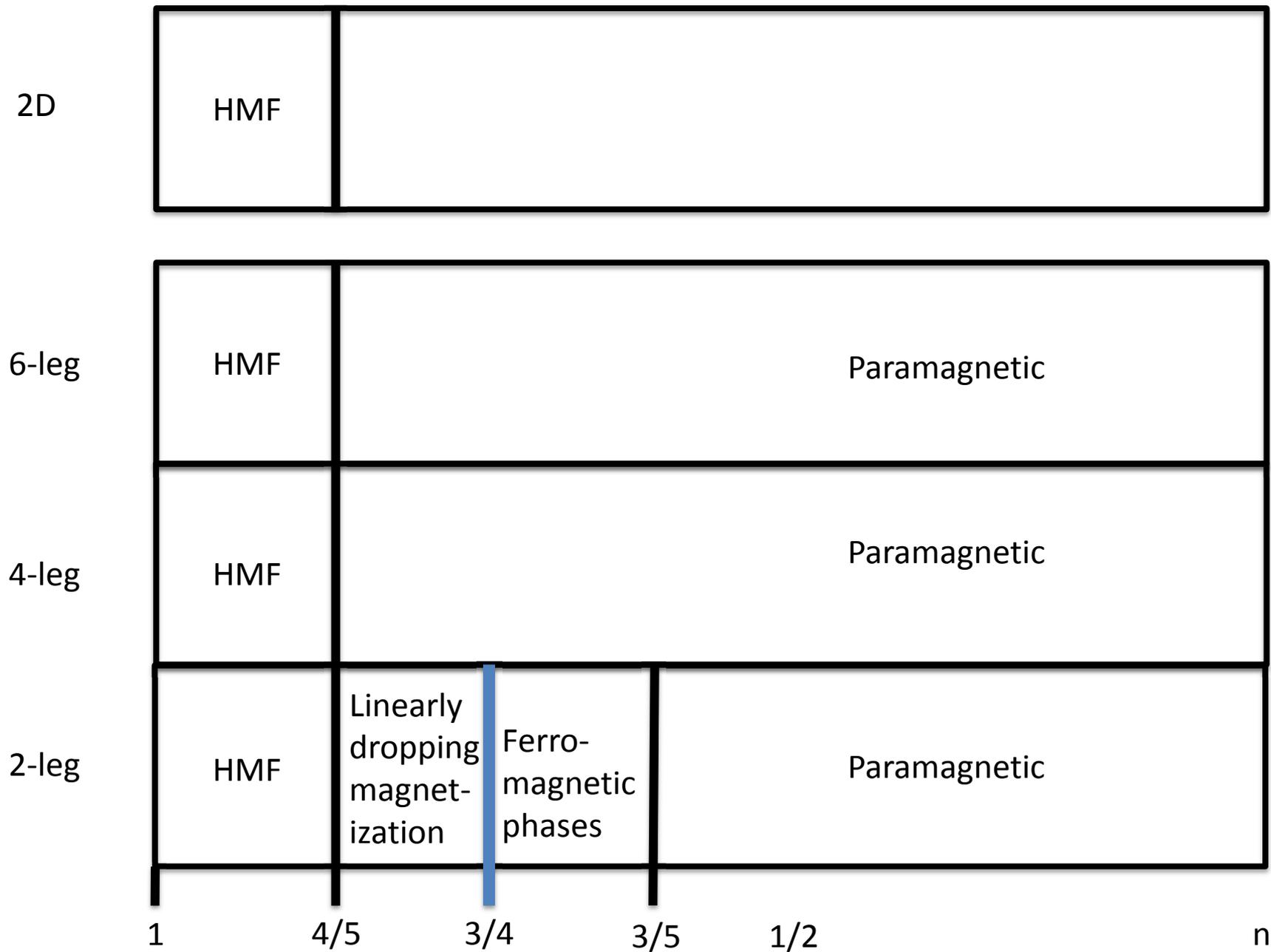
HMF & Paramagnetic Phases

lattice size	n_F
2×20	0.800
2×30	0.800
2×40	0.800
2×50	0.800
4×10	0.800
4×15	0.817
4×20	0.800
6×10	0.817
6×15	0.800

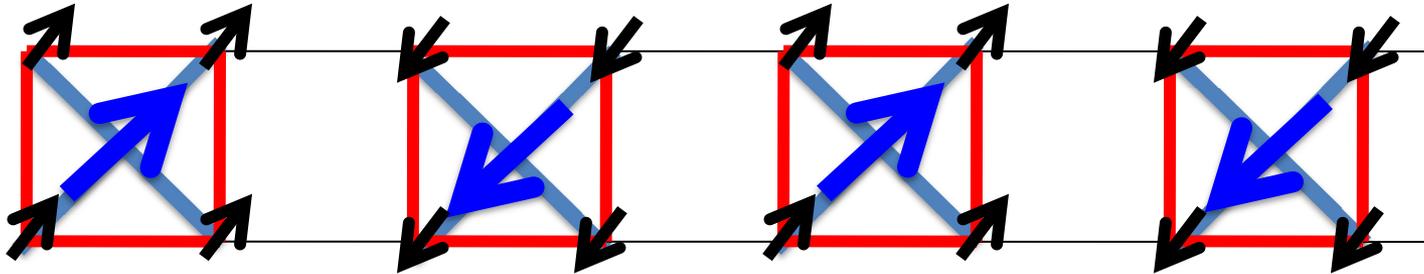
For all n such that
 $1 > n \geq n_F$
the groundstate is
fully polarized.

For all n such that
 $n_F > n$
the groundstate is
incompletely or
unpolarized.

Note that in the fully polarized sector of Hilbert space, the electrons are non-interacting.



Insulating phase at $n=3/4$ for two leg ladder with infinite U



$$K_{ij} = \sum_{\sigma} \langle [c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{H.C.}] \rangle = \text{bond charge density}$$

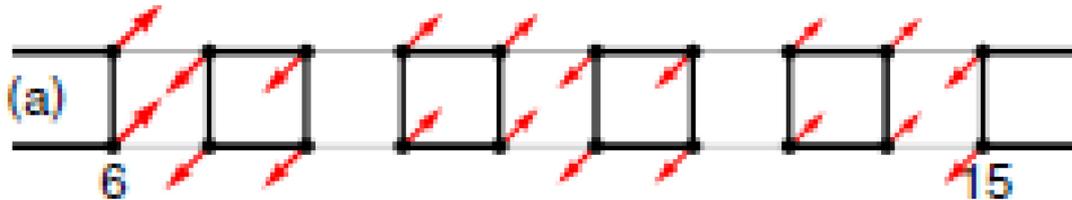
Breaks discrete symmetries

$$\vec{S}_j = \sum_{\sigma, \sigma'} \langle c_{j,\sigma}^{\dagger} \vec{\tau}_{\sigma, \sigma'} c_{j,\sigma'} \rangle = \text{spin density}$$

Continuous spin rotational symmetry so at most power law order

Equivalent to an effective spin 3/2 Heisenberg chain

Checkerboard AF Insulator at $n=3/4$



A Zeeman field of strength 1 has been applied to the lower left site, (0,0)

Bond density ranges from $K_{ij}=0.3$ to $K_{ij} = 0.45$

The magnitude of the spin density decays from 0.21 at the left to 0.19 at the right

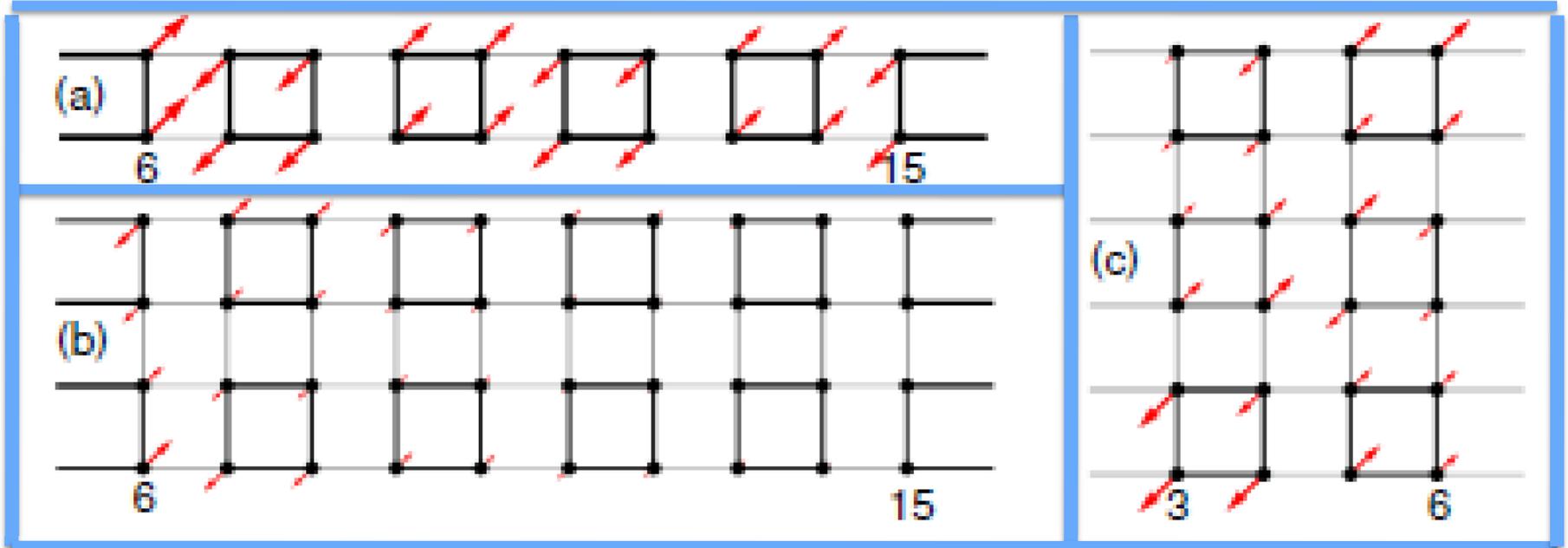
Checkerboard AF Insulator with $n=3/4$

$$\Delta_c \equiv [E(N_{el} + 2) + E(N_{el} - 2) - 2E(N_{el})]/2$$

$$\Delta_s \equiv [E(S = 1; N_{el}) - E(S = 0; N_{el})]$$

	Δ_c	Δ_s
2x20 lattice	~ 0.286	~ 0.0003
2xN leg ladder $N \rightarrow \infty$	~ 0.245	< 0.0003

Checkerboard AF Insulator at $n=3/4$



2-leg ladder \square — \square spin 3/2 chain with quasi LRO

4-leg ladder \square — \square spin 3/2 2-leg ladder with SRO

6-leg ladder \square — \square spin 3/2 3-leg ladder with quasi LRO

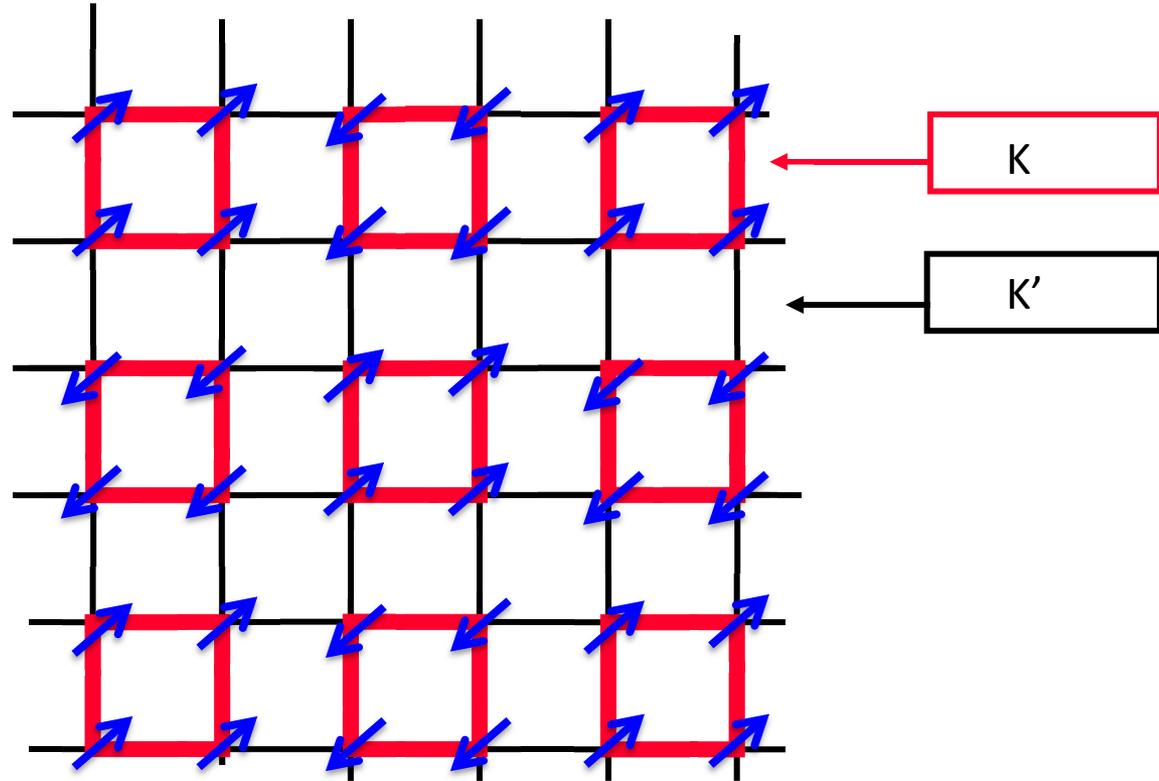
Plaquette Checkerboard AF Insulator

$$\Delta_c \equiv [E(N_{el} + 2) + E(N_{el} - 2) - 2E(N_{el})]/2$$

$$\Delta_s \equiv [E(S = 1; N_{el}) - E(S = 0; N_{el})]$$

	Δ_c	Δ_s
2x20 lattice	$\sim 0.286t$	$\sim 0.0003t$
4x20 lattice	$\sim 0.23t$	$\sim 0.008t$
2xN leg ladder $N \rightarrow \infty$	$\sim 0.245t$	$< 0.0003t$

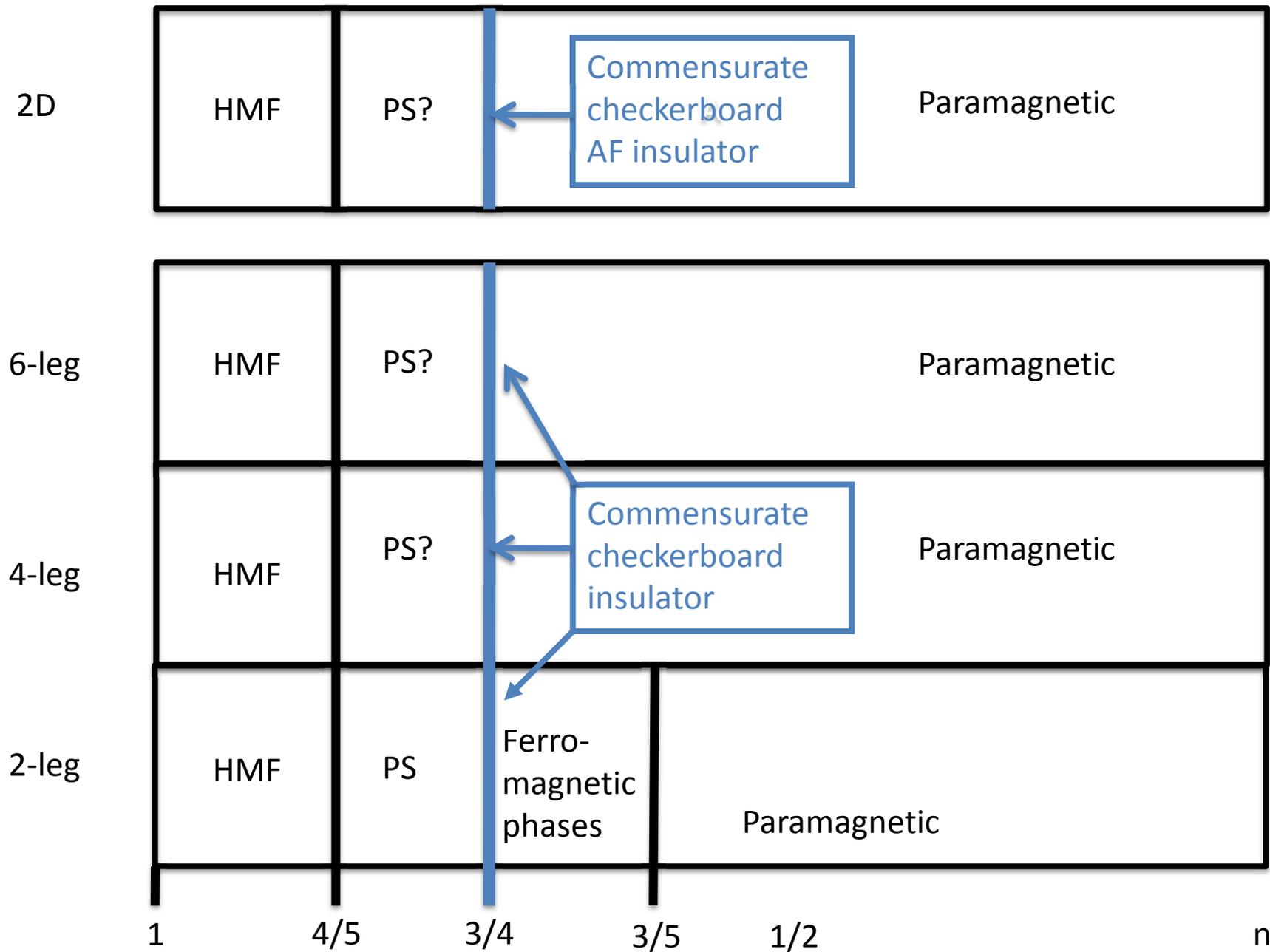
Checkerboard antiferromagnetic phase of the infinite U Hubbard model with $n=3/4$

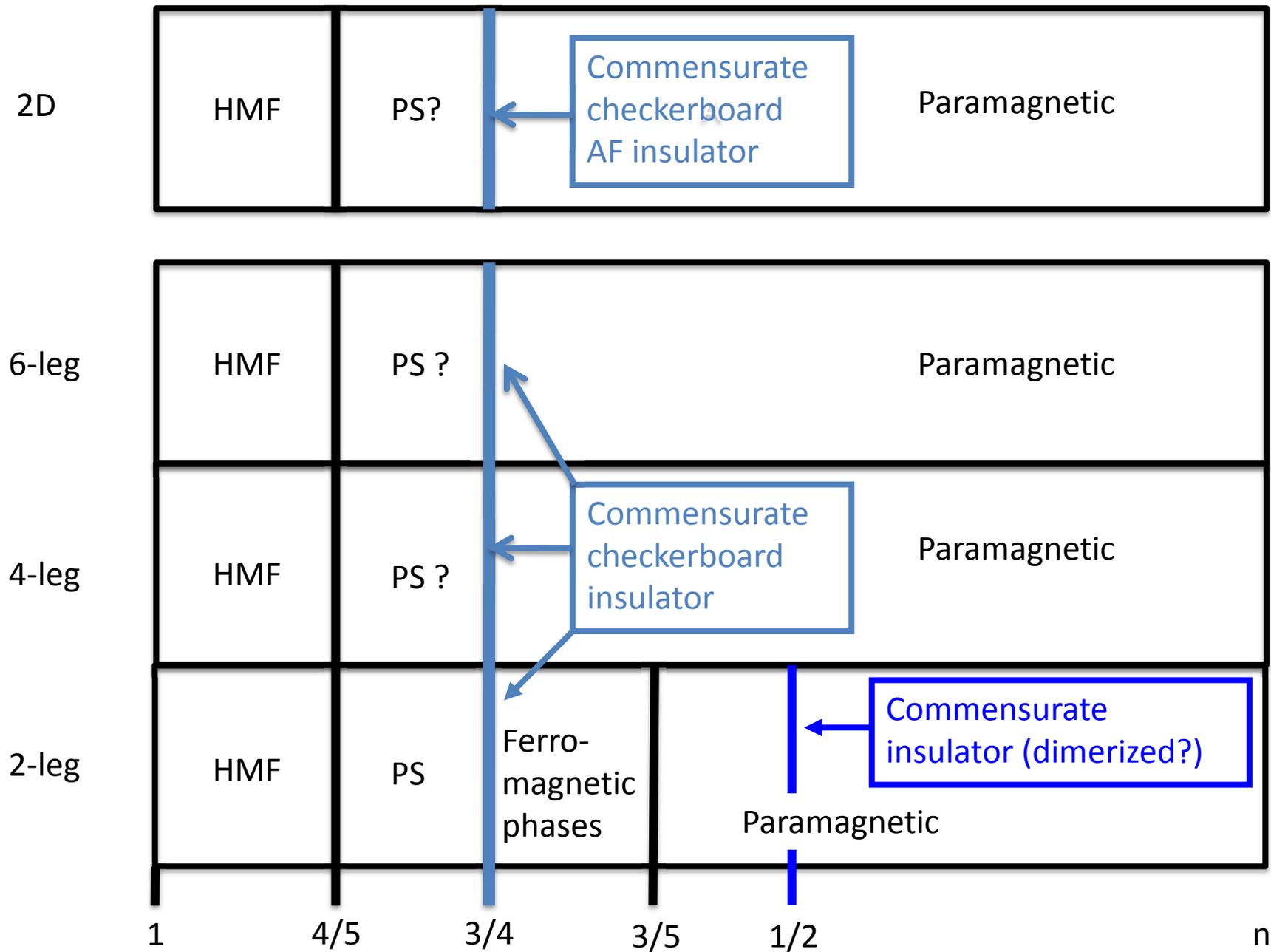


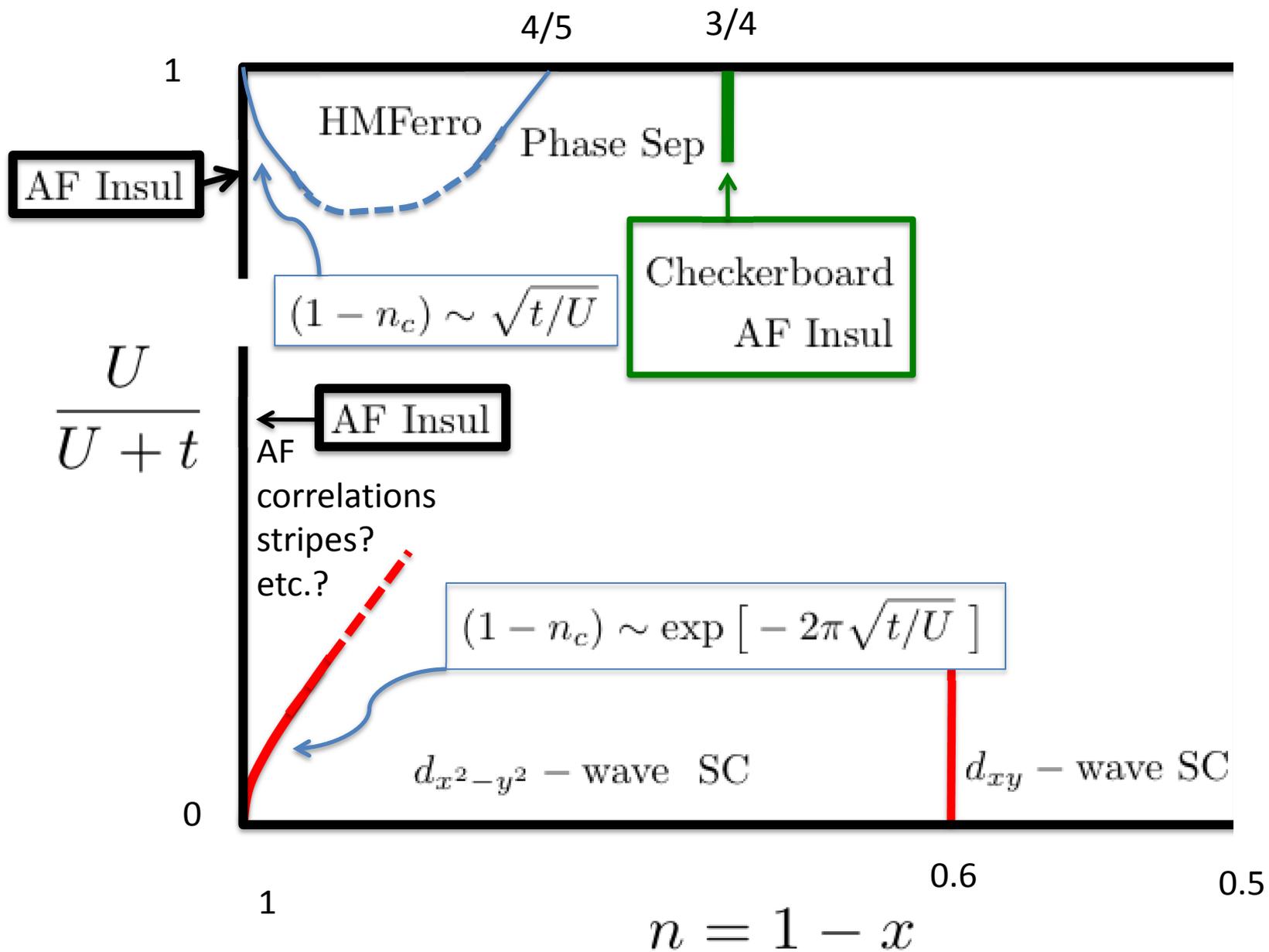
$$K = \sum_{\sigma} \langle [c_{0,\sigma}^{\dagger} c_{\hat{x},\sigma} + \text{H.C.}] \rangle$$

$$K' = \sum_{\sigma} \langle [c_{\hat{x},\sigma}^{\dagger} c_{2\hat{x},\sigma} + \text{H.C.}] \rangle$$

Purely kinetic energy driven insulating density wave order!



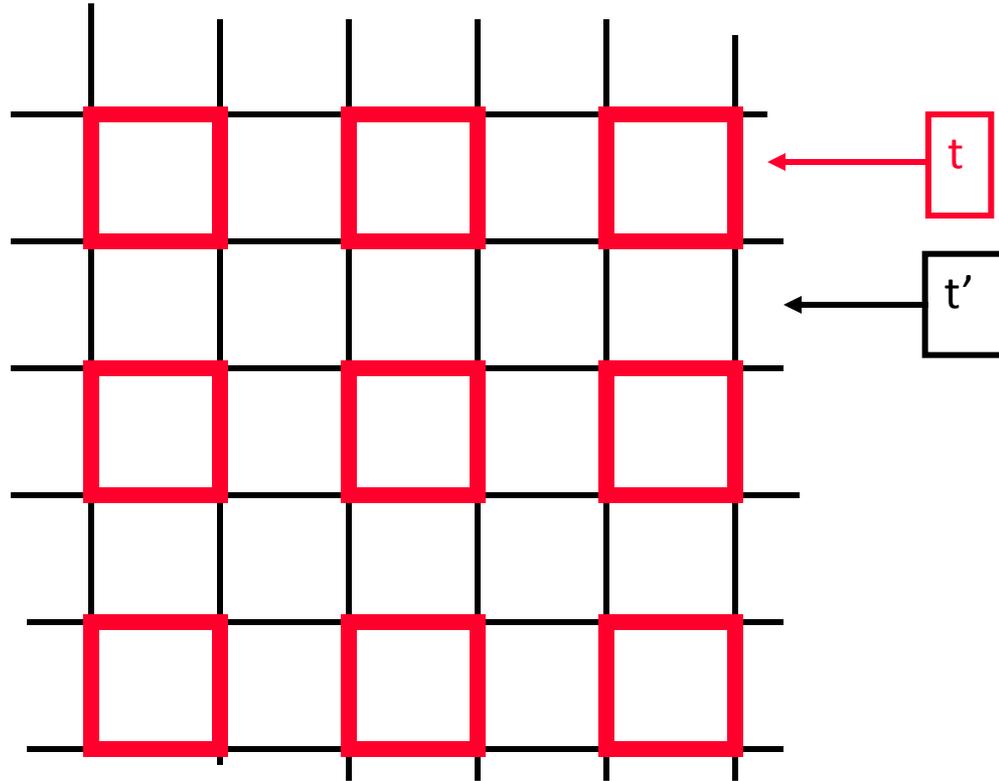




Phase diagram of checkerboard Hubbard model

– a route to the physics of intermediate coupling, $U/8t \sim 1$

“Homogeneous” ($t'/t=1$) to “highly inhomogeneous” ($t'/t \ll 1$)

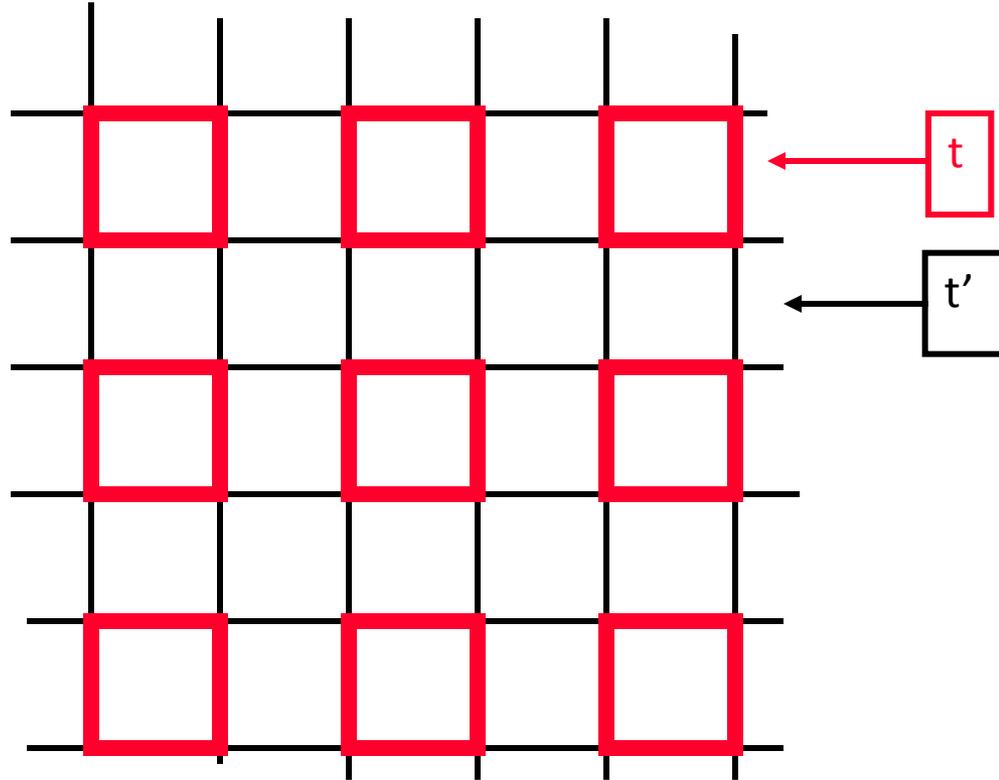


Phase diagram of checkerboard Hubbard model

– a route to the physics of intermediate coupling, $U/8t \sim 1$

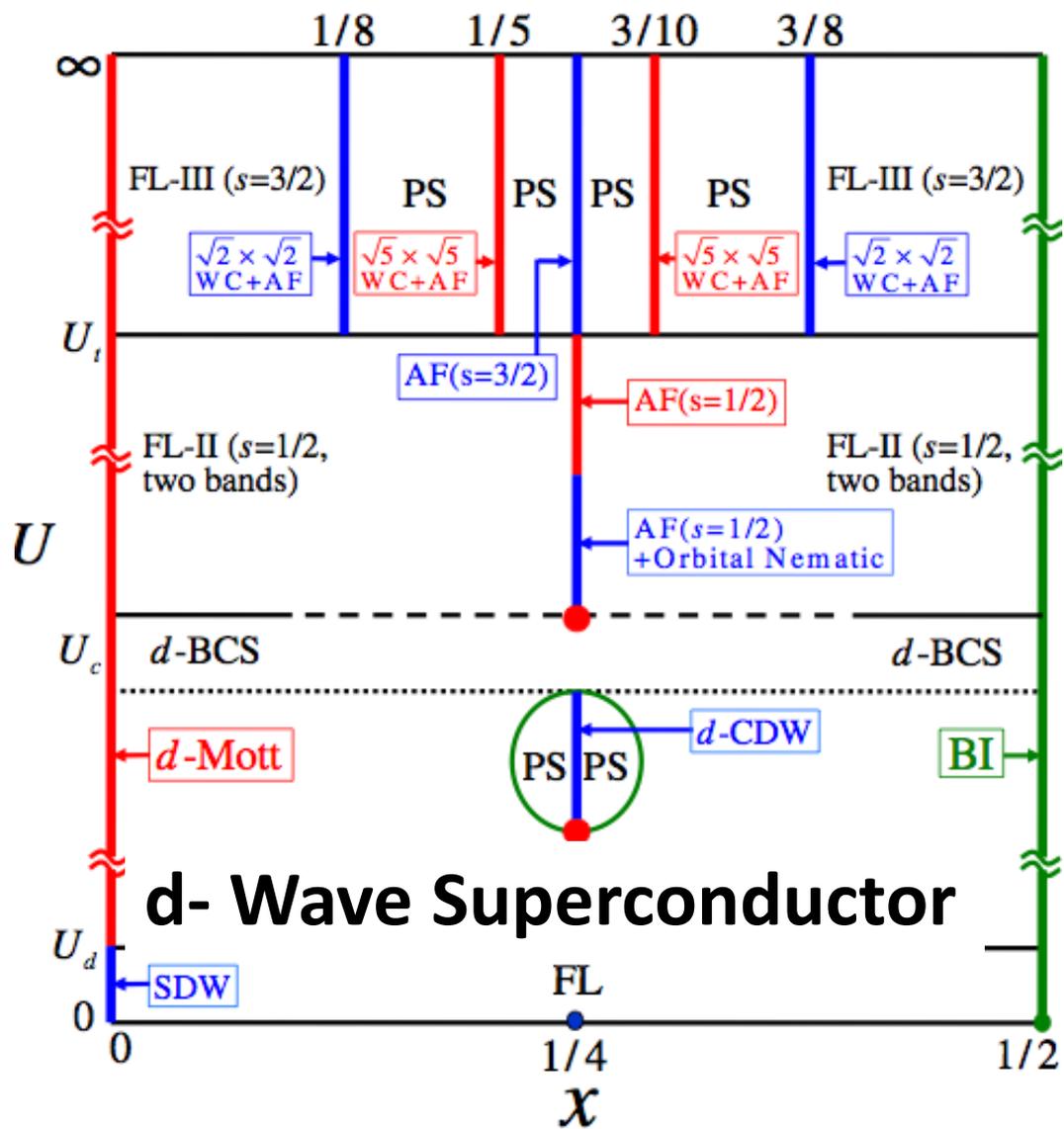
Asymptotic solution exists for arbitrary U/t

in the limit $t'/t \ll 1$. *H.Yao et al, PRB 2007*



Myriad phases including d-wave superconducting,
spin 3/2 Fermi liquid, electron nematic, AFI, ...

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



d- Wave Superconductor

Physics stories

- There are unconventional superconducting phases in the Hubbard model with purely repulsive interactions.
- For intermediate to strong interactions, there are myriad other ordered phases which “compete” or “intertwine” with superconductivity.
- For large enough U there is a half metallic ferromagnetic phase. (There probably are also partially polarized metallic phases.)

Open Questions

- Is superconductivity sufficiently strong, and T_c sufficiently high, that this plausibly captures (in essence) the mechanism of high temperature superconductivity?
- How robust is the superconductivity to inclusion of longer-range Coulomb repulsion and pair-breaking effects of phonons?
- What are the optimal conditions for high temperature superconductivity? How can one make high T_c higher?

Stay tuned

Stay tuned

Phase Separation

Evidence:

1 linear S
dependence

2 linear
energy
dependence

3 potential induced
phase separation

