Fractional Fermi Liquid from doping spin-triplet doublons

Ya-Hui Zhang (Harvard)

Collaborators:

Ashvin Vishwanath
Harvard

Zheng Zhu
MIT->Harvard->KITS

Ref:

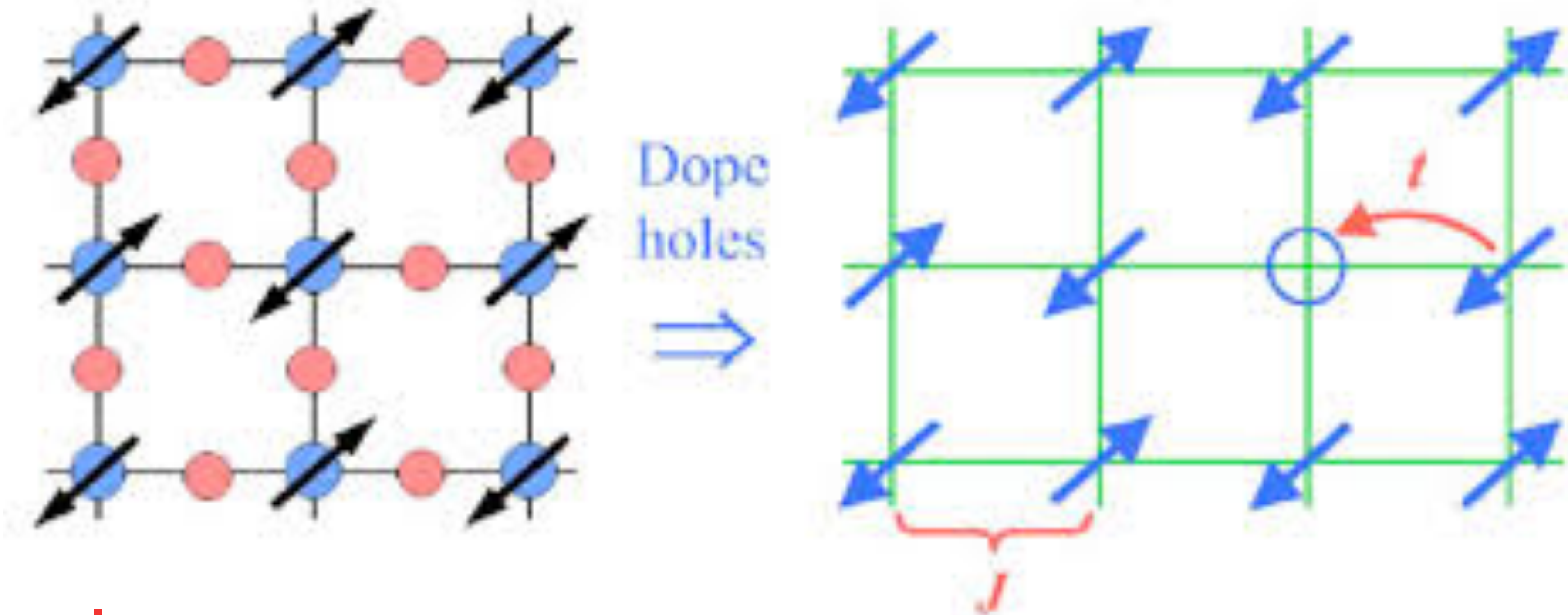
Type II t-J model in superconducting nickelate Nd_xSr_1-xNiO2, **Ya-Hui Zhang** and Ashvin Vishwanath
arxiv: 1909.12865

Symmetric Pseudogap metal in a generalized t-J mdoel, **Ya-Hui Zhang** and Zheng Zhu
arxiv: 2008.11204

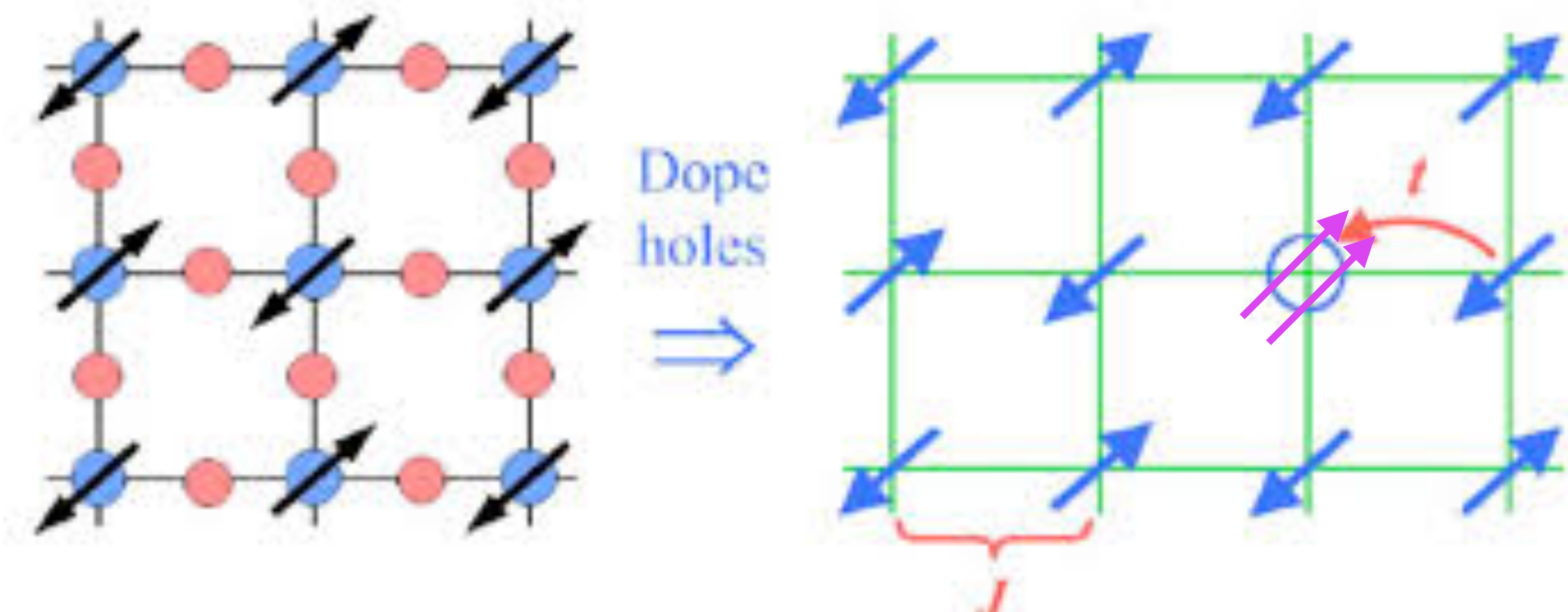
A new t-J model

Conventional t-J model

one hole per site **spin-singlet doublon**

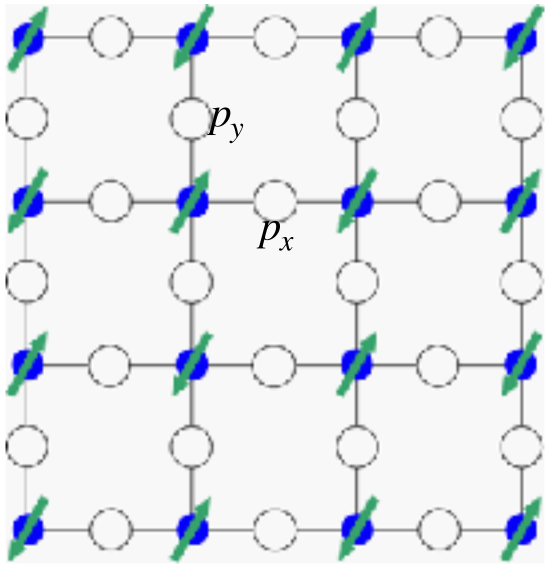


An unusual case:



one hole per site **spin-triplet doublon**

Experimental realization: hole doping a spin 1/2 Mott insulator



$$d_{i;1} : d_{x^2-y^2}$$

$$d_{i;2} : d_{3z^2-r^2}$$

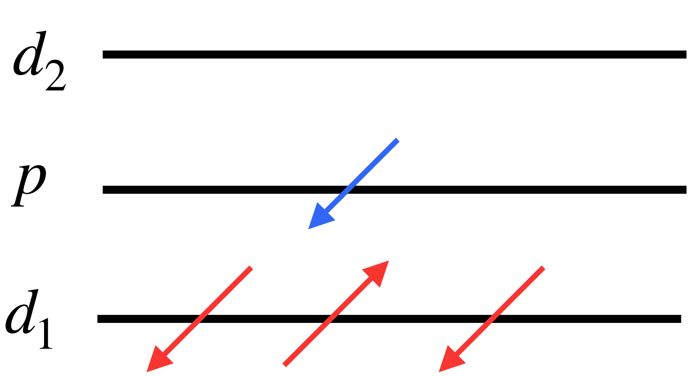
$$p_i \sim p_{i+\frac{1}{2}\hat{x}} + p_{i-\frac{1}{2}\hat{x}} + p_{i+\frac{1}{2}\hat{y}} + p_{i-\frac{1}{2}\hat{y}}$$

Spin Singlet

$$a d^\dagger_{1;\uparrow} d^\dagger_{1;\downarrow} |0> + b \epsilon_{\sigma\sigma'} d^\dagger_{1;\sigma} p^\dagger_{\sigma'} |0>$$

cuprate: $b \approx 1 \ a \approx 0$

$$J_K \overrightarrow{S}_1 \cdot \overrightarrow{S}_p \ \ J_K \sim \frac{t^2_{dp}}{U}$$

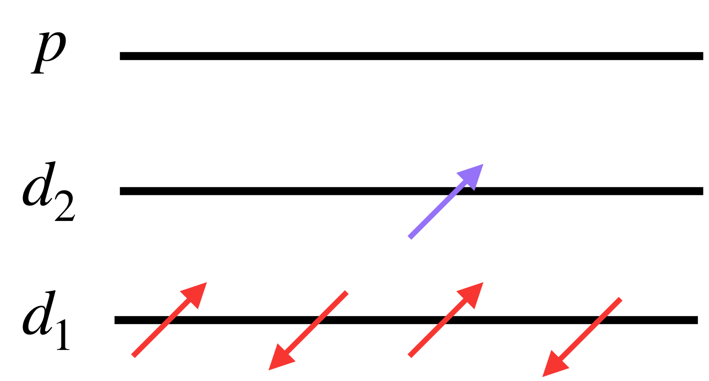


Spin Triplet

$$d^\dagger_{1;\uparrow} d^\dagger_{2;\uparrow} |0> \quad d^\dagger_{1;\downarrow} d^\dagger_{2;\downarrow} |0>$$

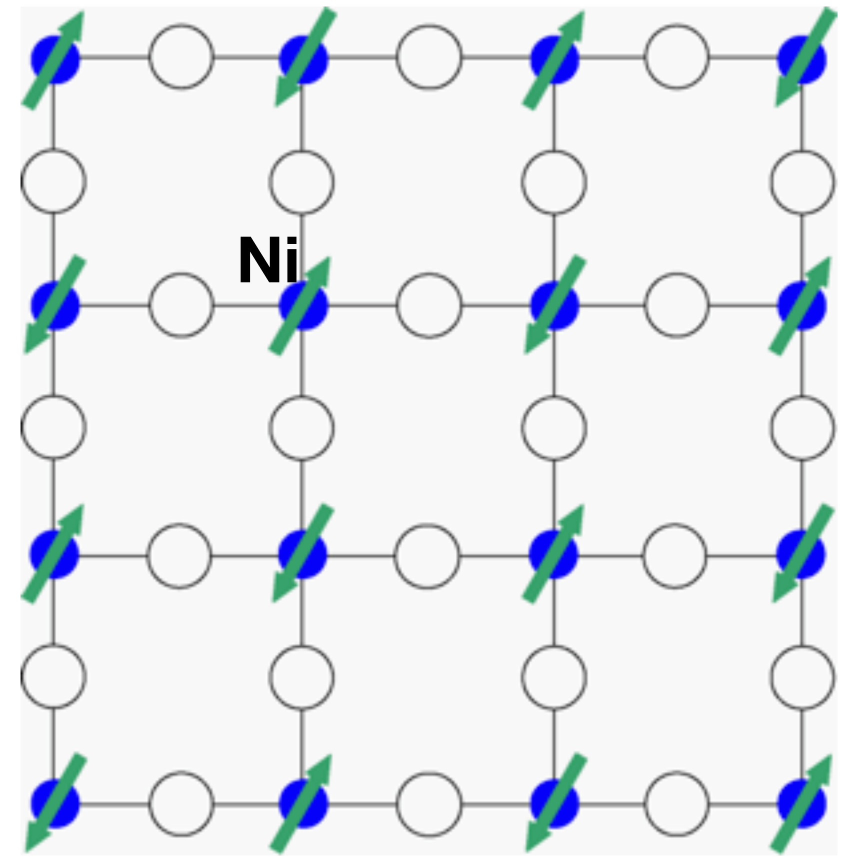
$$\frac{1}{\sqrt{2}} (d^\dagger_{1;\uparrow} d^\dagger_{2;\downarrow} + d^\dagger_{1;\downarrow} d^\dagger_{2;\uparrow}) |0>$$

$$-J_H \overrightarrow{S}_1 \cdot \overrightarrow{S}_2$$



Possible realization in Nickelate

Danfeng Li,…, Harold Y. Hwang, Nature, 572, 624 (2019)



Cuprate-like structure

Undoped site: one hole on d1 orbital Ni^{1+}

T_c around 15 K for hole doping x=0.2

Key difference from cuprate:

Oxygen band is further away from Fermi level

Spin triplet doublon may be favored

Current Status:

It is still not clear whether spin-singlet or spin-triplet doublon wins

Numerical computations (DFT, LDA+U) give opposite results between groups and even within one group.

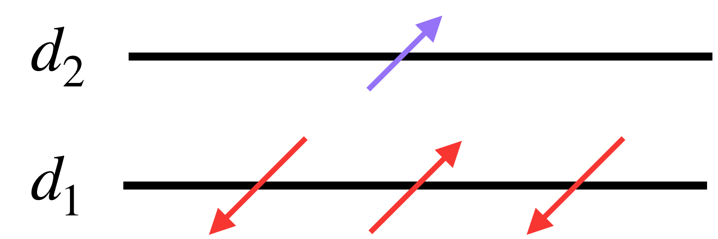
Experimental result (X-ray) is not conclusive

Spin-triplet t-J model

Hilbert Space:

- t-J model Hilbert space (5 dimensional)

$$\{|\uparrow\rangle,\ |\downarrow\rangle,\ |x\rangle,\ |y\rangle,\ |z\rangle\}$$



$$H = H_t + H_J$$

$$H_t = -\sum_{\langle ij\rangle} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \text{h.c.}$$

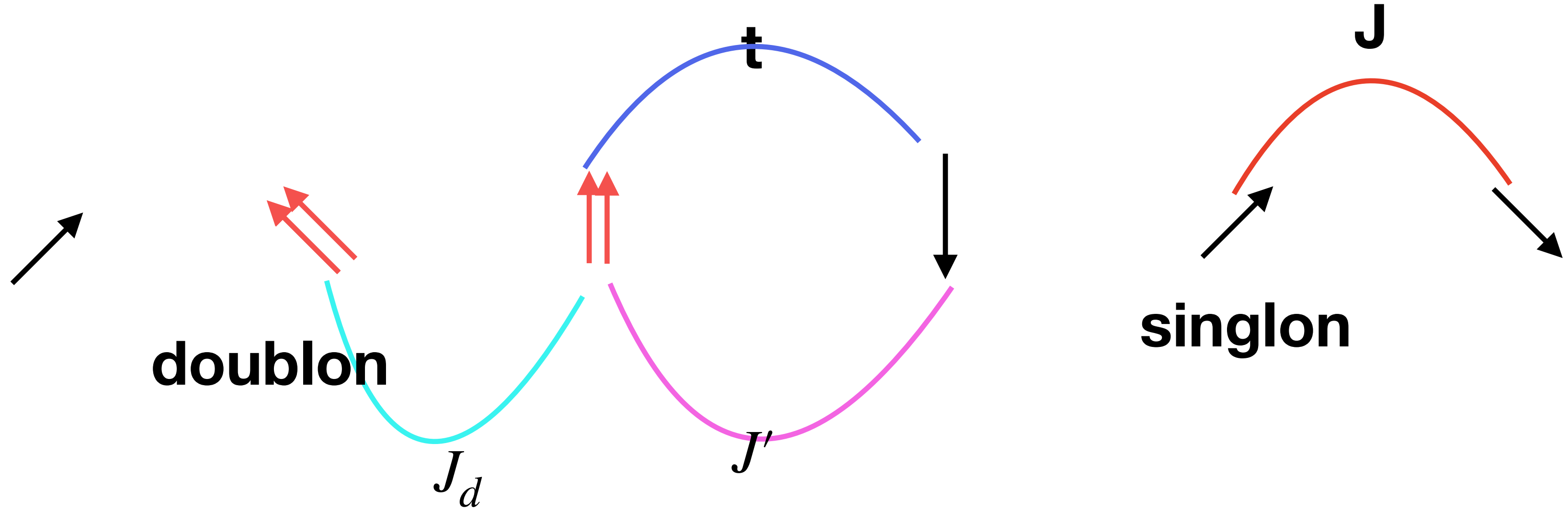
$$H_J = \sum_{\langle ij\rangle} \left(J s_i \cdot s_j + J_d S_i \cdot S_j + \frac{J'}{2}(\mathbf{s}_i \cdot \mathbf{S}_j + \mathbf{S}_i \cdot \mathbf{s}_j)\right)$$

Singlon-doublon coupling

$$d_1 = 0$$

$$c = d_2$$

YH. Zhang and A.V - arXiv:1909.12865

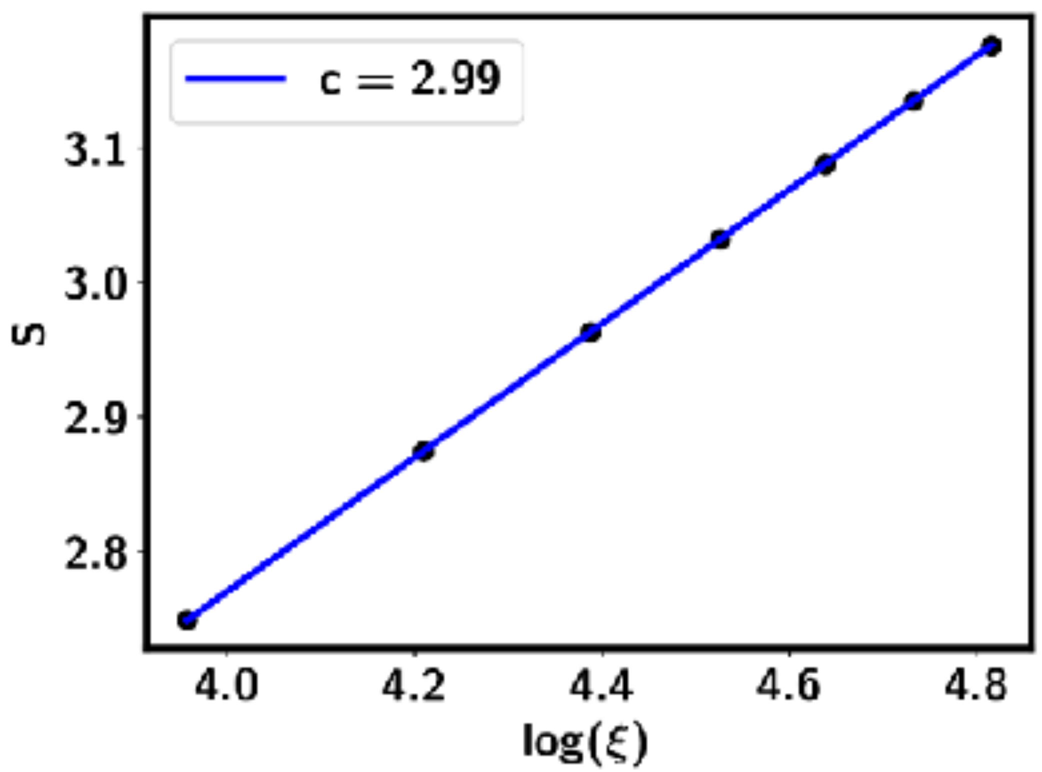


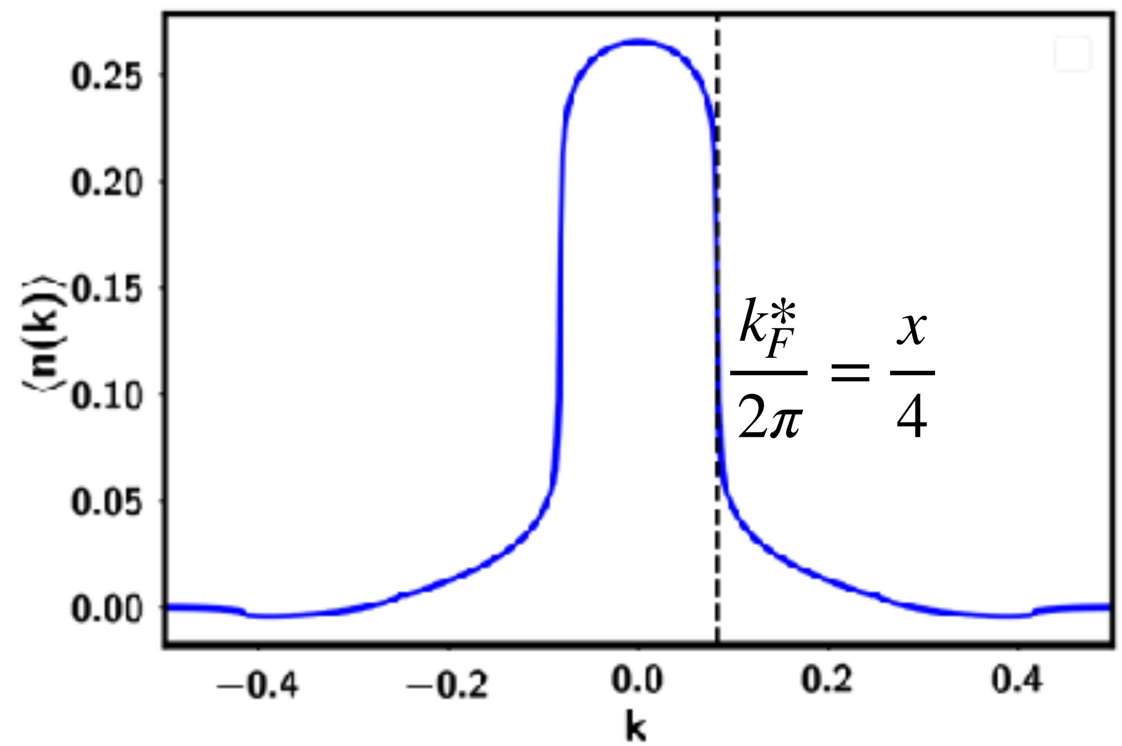
$$J' = J_d = J$$

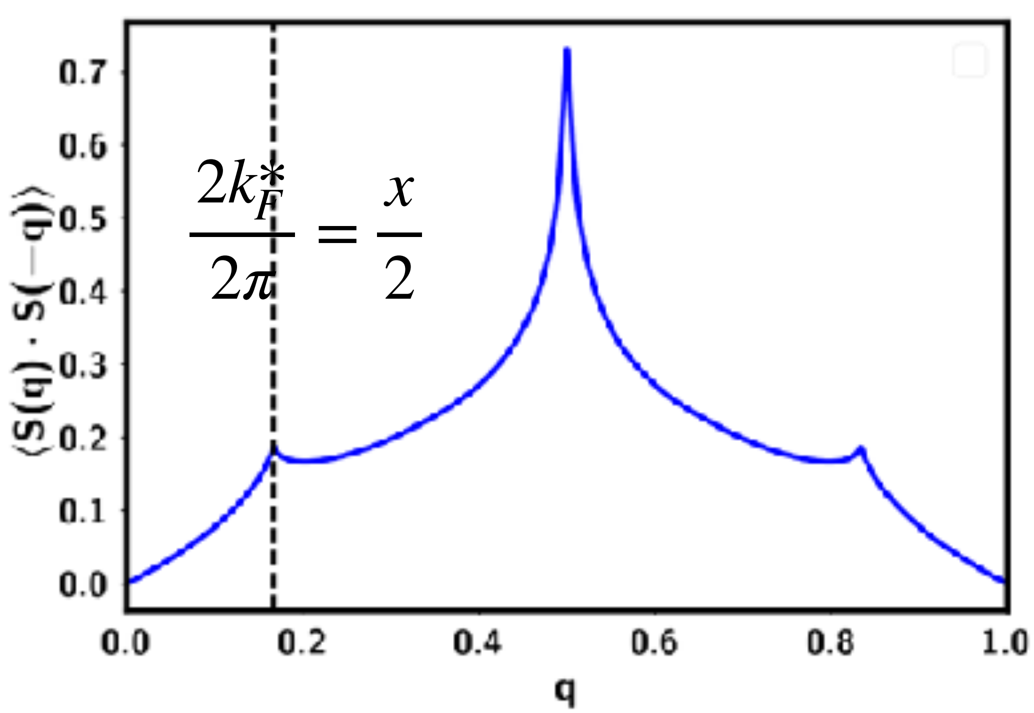
DMRG in 1D

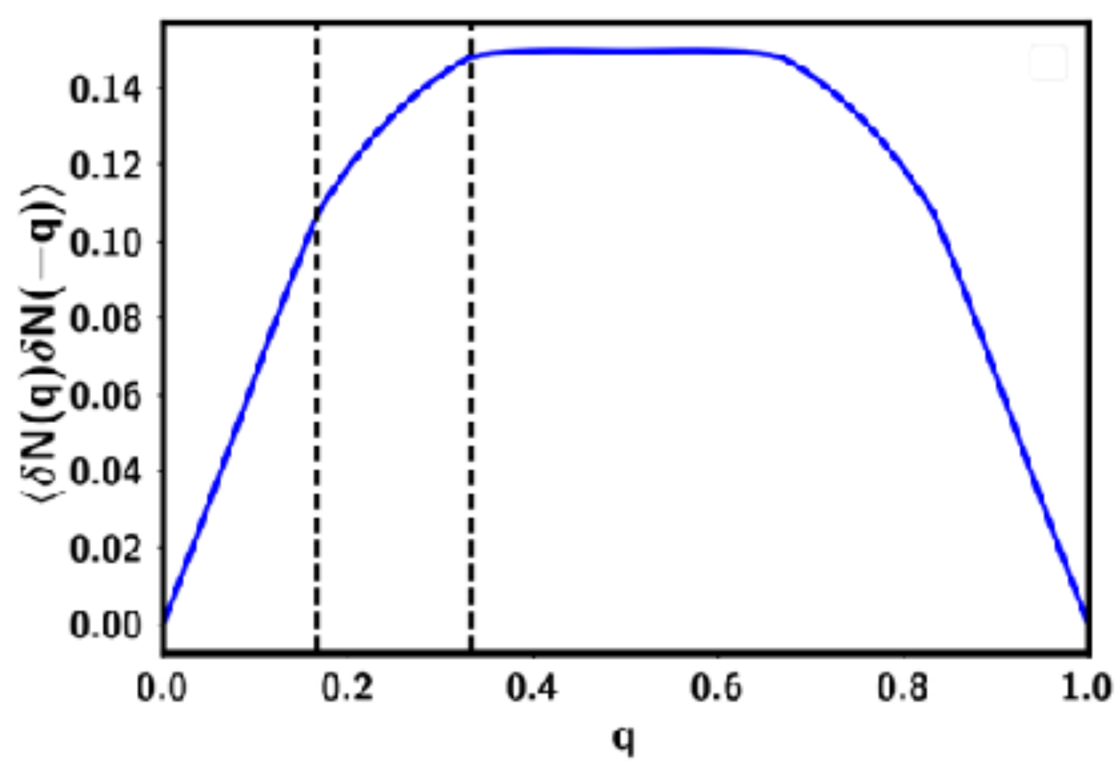
$J/t = 0.5$

x=1/3, infinite DMRG;

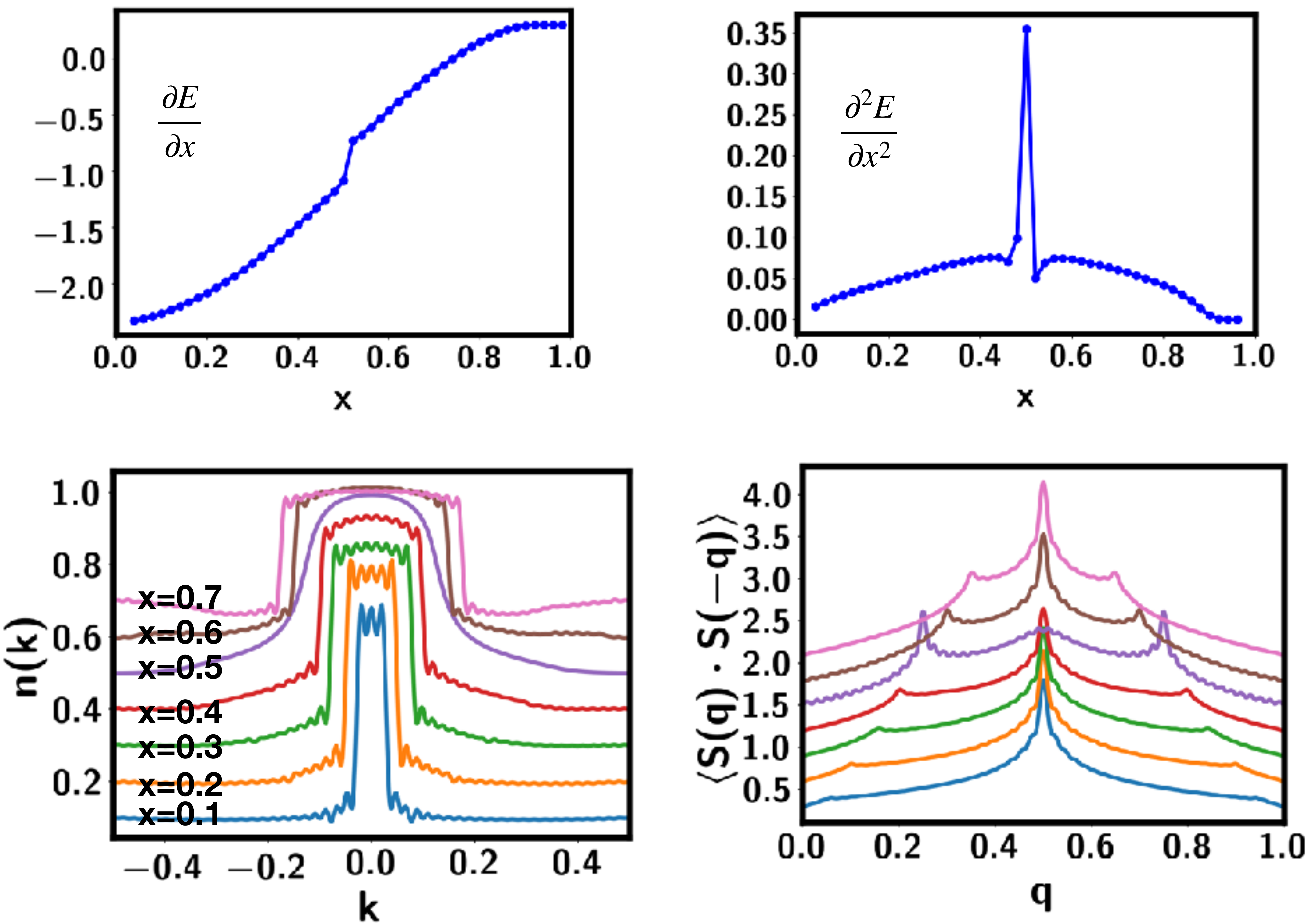








A small pocket+a spin mode at Q=pi



$J/t = 0.5$

x=0.5: CDW/wigner crystal of doublon;

Luttinger Theorem

Masanori Yamanaka, Masaki Oshikawa and Ian Affleck, PRL, 1997

1D LSM theorem:

Consider a Hamiltonian with short-range hopping, and assume it is translationally invariant and also conserves the total particle number (i.e. has charge U(1) symmetry) and parity or time-reversal. In a chain of length L with periodic boundary conditions, there is at least one low-energy (O(1/L)) state above the ground state, if the fermion number per unit cell ν is not an integer. The low-energy state has crystal momentum 2πν relative to the ground state

Gapless state at $$\frac{Q}{2\pi} = \frac{1+x}{2}$$

Conventional Luttinger Liquid (LL) $$\frac{2k_F}{2\pi} = \frac{1+x}{2}$$

Fractional Luttinger Liquid (LL*) $$\frac{Q}{2\pi} = \frac{x}{2} + \frac{1}{2}$$

small pocket **+** "spin liquid"

Emergent quasi-particle

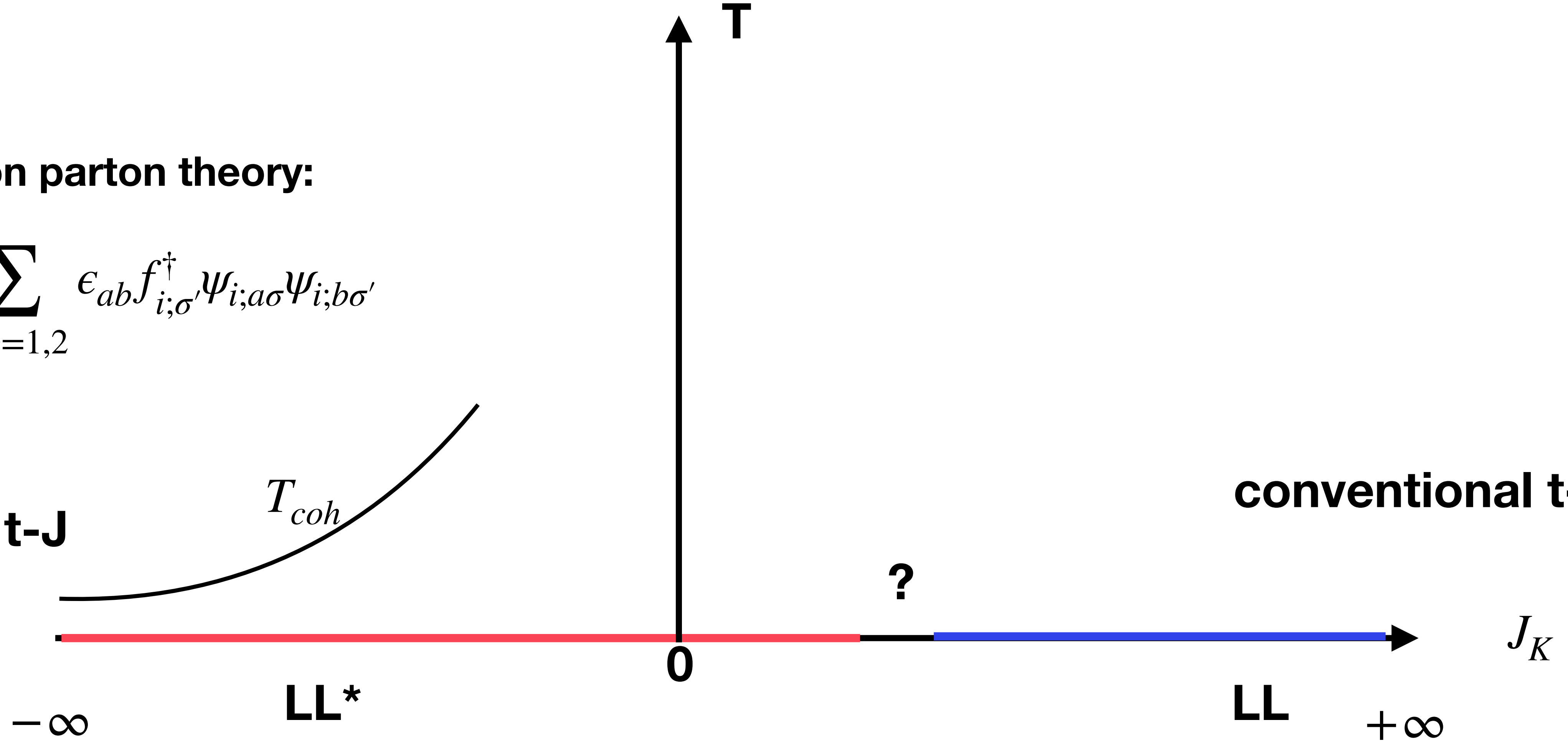
Kondo-Heisenberg model $H = -td^\dagger_{i;2}d_{j;2} + J_K \sum_i (d^\dagger_{i;2}\vec{\sigma}d_{i;2}) \cdot \vec{S}_{i;1} + J\sum_{ij}\vec{S}_{i;1}\cdot\vec{S}_{j;1}$

Three-fermion parton theory:

$$c_{i;\sigma} = \frac{1}{2}\sum_{\sigma'}\sum_{a,b=1,2}\epsilon_{ab}f^\dagger_{i;\sigma'}\psi_{i;a\sigma}\psi_{i;b\sigma'}$$

spin-triplet t-J

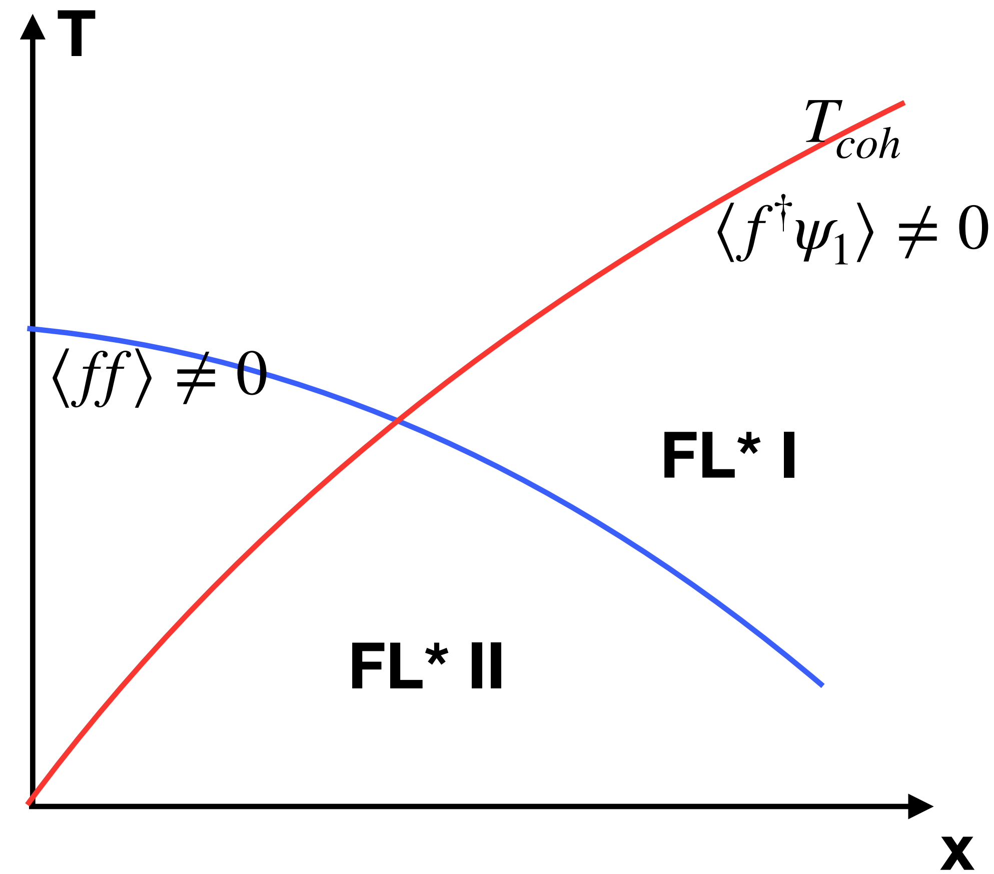
conventional t-J



small pocket	ψ_2	d_2
spinon	f, ψ_1	f

Below a coherent temperature, $\psi_2 = \sqrt{Z}d_2$ $Z \propto x$

Square Lattice



$J' = J = J_d$

FL* I: spin liquid part is a spinon Fermi surface

FL* II: spin liquid part is a Z_2 Dirac fermion SL

Conjecture: **For reasonable value of J'=J,   normal state has a small Fermi surface**

Antiferromagnetic metal is also possible, but still beyond SDW mean field description.

Small to Large Fermi surface transition

FL ? FL*

Two-orbital Hubbard model

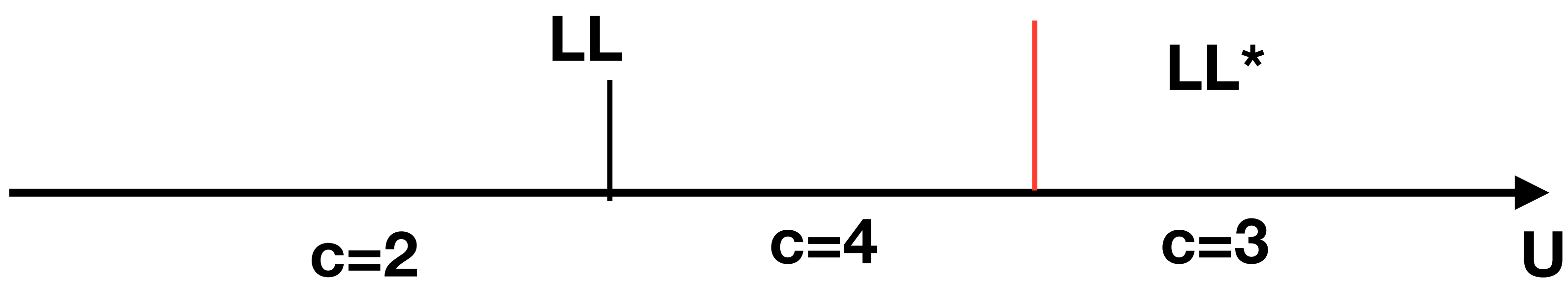
$$H = H_K + \frac{U_1}{2}\sum_i n_{1;i}(n_{1;i}-1) + \frac{U_2}{2}\sum_i n_{2;i}(n_{2;i}-1)$$
$$+ U' \sum_i n_{1;i} n_{2;i} - 2J_H \sum_i (\mathbf{S}_{1;i}\cdot\mathbf{S}_{2;i} + \frac{1}{4} n_{i;1} n_{i;2})$$

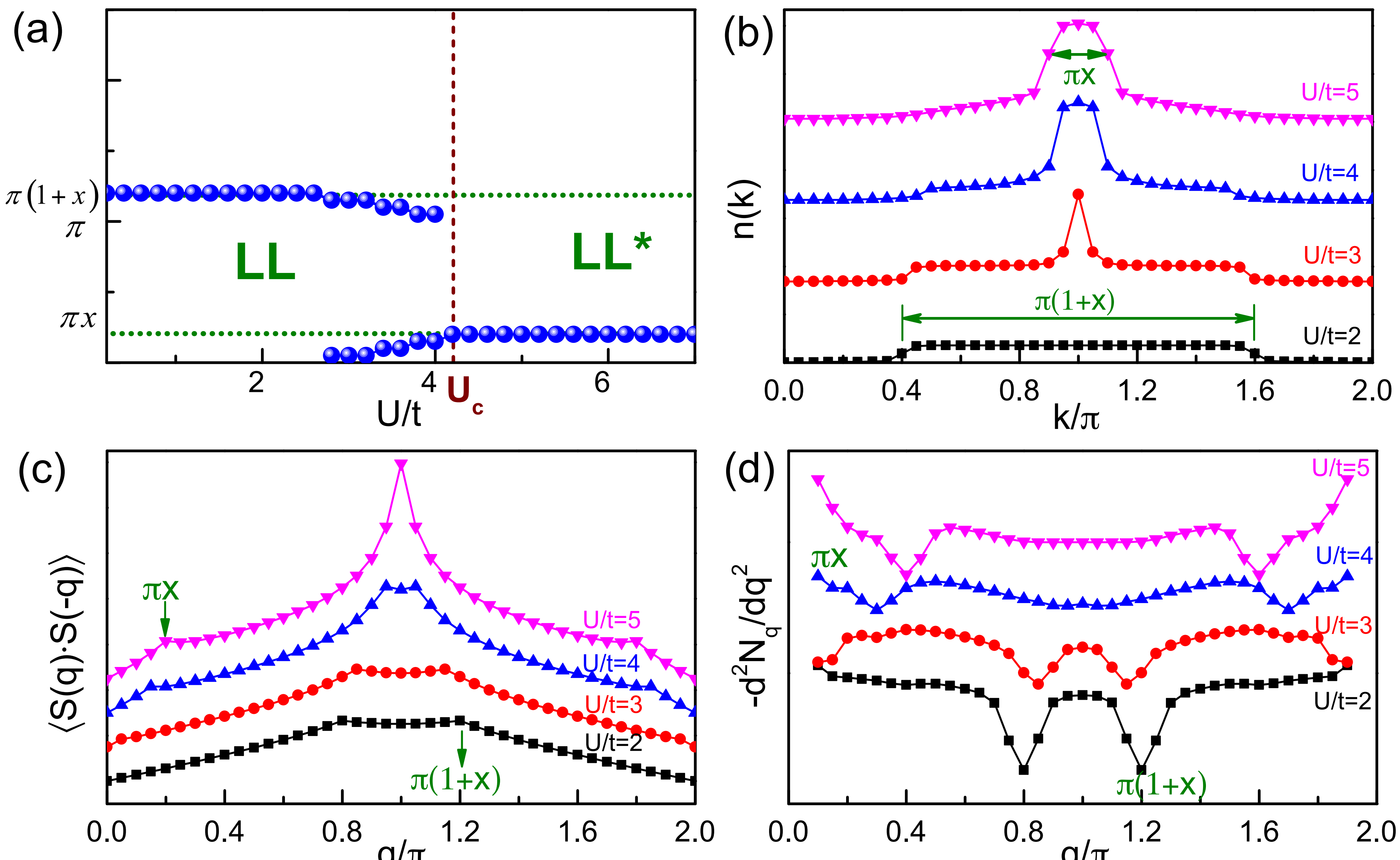
$$H_K = \sum_i \epsilon_{dd} n_{2;i} + V \sum_i (d^\dagger_{i;1} d_{i;2} + h.c.) + \sum_{\langle ij\rangle} t_{1;ij} d^\dagger_{1;i} d_{1;j} + \sum_{\langle ij\rangle} t_{2;ij} d^\dagger_{2;i} d_{2;j}$$
$$+ \sum_{\langle ij\rangle} t_{12;ij} d^\dagger_{1;i} d_{2;j} + h.c.$$

Spin-triplet t-J model: U,J_H large limit

Small to Large Fermi surface transition

$U = 4J_H, U' = 2J_H$



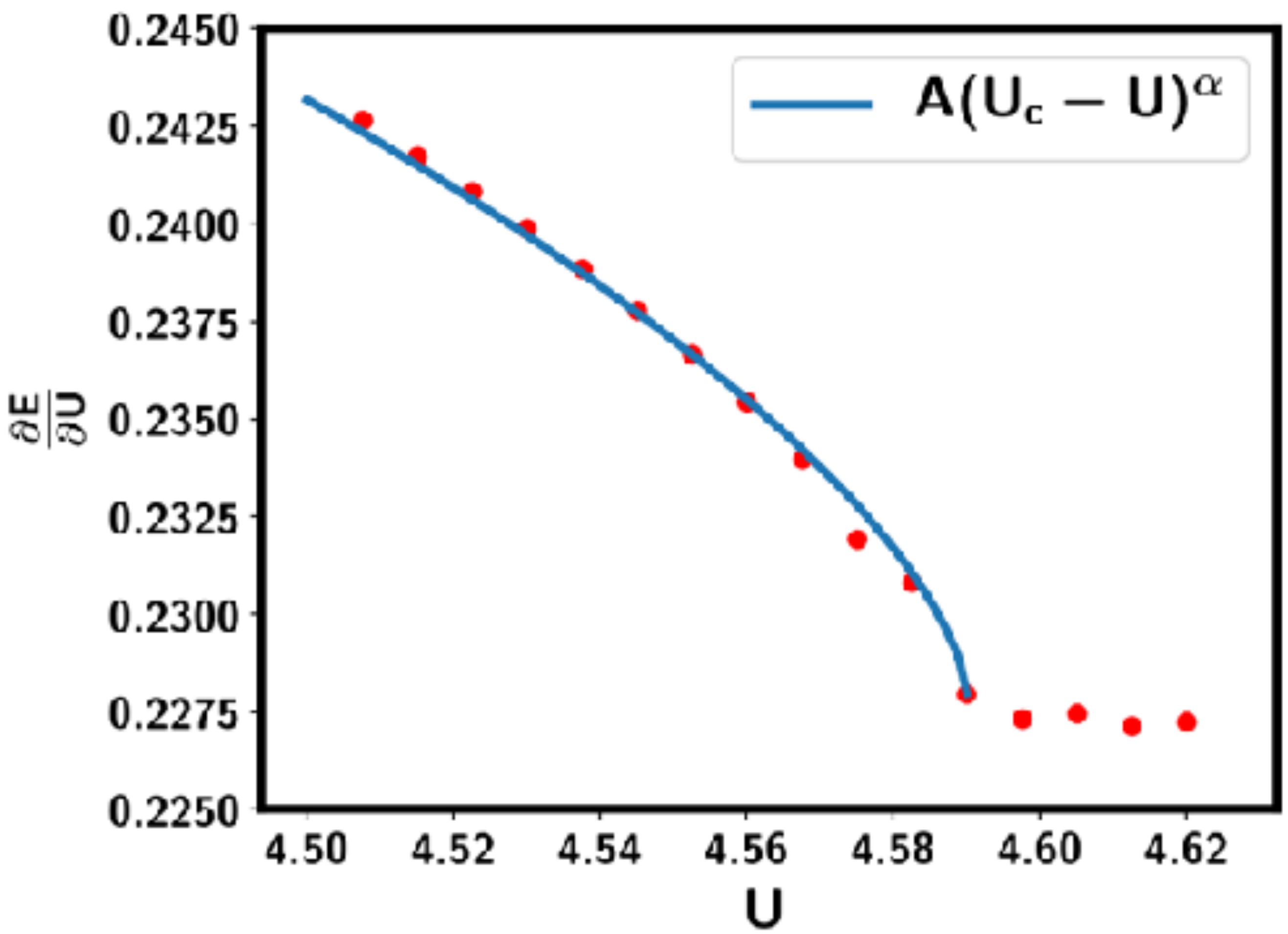


Small to Large Fermi surface transition

A simple picture: chemical potential tuned Mott transition for one Fermi surface

$$U - U_c \propto -(\mu - \mu_c)$$

3D version: T.Senthil, M.Vojta and S.Sachdev (2003)



chemical potential tuned Mott transiton

$$\langle n \rangle = -\frac{\partial E}{\partial \mu} = \begin{cases} A\sqrt{\mu - \mu_c} + 1, & \mu > \mu_c, \\ 1 & \mu < \mu_c \end{cases}$$

Our result:

$$\frac{\partial E}{\partial_U} = \begin{cases} A(U_c - U)^\alpha + C, & U < U_c, \\ C & U > U_c \end{cases}$$

$$\alpha \approx 0.64$$

Two possibilities:

Coupling to the small pocket is relevant and modify the exponent.

It is a numerical error.

Bond dimension: D=5000

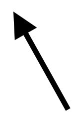
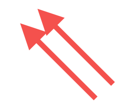
Need a better computer to improve the precision.

Summary

I. A new t-J model when doped doublon is a spin-triplet

II. This t-J model is interesting

A three-fermion Parton theory

Parton theory:  **=** $f^\dagger_\sigma |0>$  **=** $b^\dagger_a |0> \quad a = x, y, z$ **or =** $\psi^\dagger_{1;\sigma}\psi^\dagger_{2;\sigma'}|0>$

SO(3) slave boson theory: $c_i = f^\dagger_i b_i$ symmetric FL is not possible

Three-fermion theory: $c_{i;\sigma} = \frac{1}{2}\sum_{\sigma'}\sum_{a,b=1,2}\epsilon_{ab} f^\dagger_{i;\sigma'}\psi_{i;a\sigma}\psi_{i;b\sigma'}$ U(2) gauge structure

Constraint: $f^\dagger_i f_i + \frac{1}{2}\Psi^\dagger_i \Psi_i = 1 \qquad \Psi^\dagger_i \vec{\tau}\Psi_i = 0$

$$U(1): f_i \to f_i e^{2i\alpha_c(i)}, \Psi_i \to \Psi_i e^{i\alpha_c(i)} \qquad SU(2): f_i \to f_i, \Psi_i \to U_i \Psi_i, \;\; U_i \in SU(2)$$

Coupling:

$$f: 2a_c, \;\; \psi_1: a_c + a_s + \frac{1}{2}A, \;\; \psi_2: a_c - a_s + \frac{1}{2}A$$

Density $n_f = 1 - x \quad n_{\psi_1} = n_{\psi_2} = x$

FL* below coherent temperature

$$
\begin{aligned}
H = &\frac{1}{4} t \sum_{\langle ij\rangle} \epsilon_{ab}\epsilon_{a'b'} \psi^\dagger_{i;b\beta}\psi^\dagger_{i;a\alpha}\psi_{j;a'\alpha}\psi_{j;b'\beta'} f^\dagger_{j;\beta'} f_{i;\beta} + h.c. \\
&- \frac{1}{2} J \sum_{\langle ij\rangle} f^\dagger_{i;\alpha} f_{j;\alpha} f^\dagger_{j;\beta} f_{i;\beta} \\
&- \frac{1}{2} J_d \sum_{\langle ij\rangle} \psi^\dagger_{i;a\alpha}\psi_{j;b\alpha}\psi^\dagger_{j;b\beta}\psi_{i;a\beta} \\
&- \frac{1}{4} J' \sum_{\langle ij\rangle} (f^\dagger_{i;\alpha}\psi_{j;a\alpha}\psi^\dagger_{j;a\beta} f_{i;\beta} + \psi^\dagger_{i;a\alpha} f_{j;\alpha} f^\dagger_{j;\beta}\psi_{i;a\beta})
\end{aligned}
$$

a,b=1,2

$\alpha, \beta = \uparrow, \downarrow$

Mean field: $\Phi_{i;a} f_i^\dagger \psi_{i;a}$ $\quad \Phi = (\Phi_1, \Phi_2)^T$ transforms as fundamentla rep of SU(2)

Fix gauge: $\Phi_{i;1} \neq 0, \Phi_{i;2} = 0$ $\quad f: 2a_c,\ \ \psi_1 : a_c + a_s + \frac{1}{2}A,\ \ \psi_2 : a_c - a_s + \frac{1}{2}A$

Higgs $a_c = a_s + \frac{1}{2}A$ $\quad f: \alpha,\ \ \psi_1 : \alpha,\ \ \psi_2 : A;\ \ \ \alpha = 2a_s + A$

Neutral spinon at total filling 1: f, ψ_1 **Electron:** $c \sim \langle f^\dagger \psi_1 \rangle \psi_2$

FL* phase if f,\psi_1 forms a spin liquid $\quad n_f = 1 - x \ \ \ n_{\psi_1} = n_{\psi_2} = x$