Small and large Fermi surfaces in metals with local moments

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Luttinger's theorem on a d-dimensional lattice

For simplicity, we consider systems with SU(2) spin rotation invariance, which is preserved in the ground state.

Let v_0 be the volume of the unit cell of the ground state, n_T be the total number of electrons per volume v_0.

Then, in a metallic Fermi liquid state with a sharp electron-like Fermi surface:

$$2 \times \frac{v_0}{(2\pi)^d}\left(\text{Volume enclosed by Fermi surface}\right)$$

$$= n_T \left(\text{mod } 2\right)$$

A "large" Fermi surface

Our claim

There exist "topologically ordered" ground states in dimensions $d > 1$ with a Fermi surface of **sharp** electron-like quasiparticles for which

$$2 \times \frac{v_0}{(2\pi)^d} \left(\text{Volume enclosed by Fermi surface} \right)$$

$$= \left(n_T - 1 \right) \left(\text{mod } 2 \right)$$

A "small" Fermi surface

Outline

I. Kondo lattice models

II. Topologically ordered states of quantum antiferromagnets
    "Quantum-disordering" transitions of magnetically ordered states with non-collinear spin correlations

III. Models with "small" Fermi surfaces.

IV. Lieb-Schultz-Mattis-Laughlin-Bonesteel-Affleck-Yamanaka-Oshikawa flux-piercing arguments

V. Conclusions

I. Kondo lattice models

Model Hamiltonian for intermetallic compound with conduction electrons, $c_{i\sigma}$, and localized orbitals, $f_{i\sigma}$

$$H = \sum_{i<j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} \left(V c_{i\sigma}^{\dagger} f_{i\sigma} + V f_{i\sigma}^{\dagger} c_{i\sigma} + \varepsilon_f \left(n_{fi\uparrow} + n_{fi\downarrow} \right) + U n_{fi\uparrow} n_{fi\downarrow} \right) + \cdots$$

$$n_{fi\sigma} = f_{i\sigma}^{\dagger} f_{i\sigma} \quad ; \quad n_{ci\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$$

$$n_T = n_f + n_c$$

For small U, we obtain a Fermi liquid ground state, with a Fermi surface volume determined by n_T (mod 2)

This is adiabatically connected to a Fermi liquid ground state at large U, where n_f=1, and whose Fermi surface volume must also be determined by

$$n_T \text{ (mod 2)} = (1 + n_c) \text{ (mod 2)}$$

The large U limit is also described (after a Schrieffer-Wolf transformation) by a Kondo lattice model of conduction electrons $c_{i\sigma}$ and S=1/2 spins on f orbitals

$$H = \sum_{i<j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} \left(J_K c_{i\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} c_{i\sigma} \cdot \vec{S}_{fi} \right) + \sum_{i<j} J_H \left(i, j \right) \vec{S}_{fi} \cdot \vec{S}_{fj}$$

This can have a Fermi liquid ground state whose Fermi surface volume is determined by (1+ n_c)(mod 2)

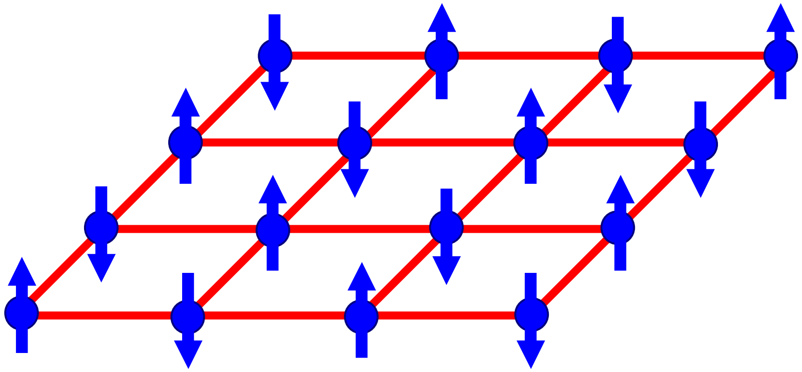
We will show that for small J_K, a ground state with a "small" electron-like Fermi surface enclosing a volume determined by n_c (mod 2) is also possible.

II. Topologically ordered states of quantum antiferromagnets

Begin with magnetically ordered states, and consider quantum transitions which restore spin rotation invariance

Two classes of ordered states:

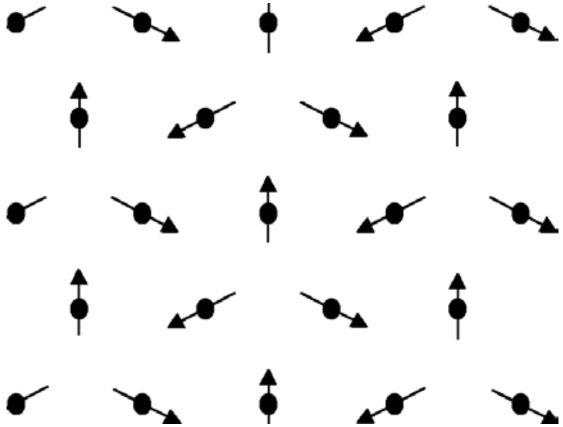
(A) Collinear spins



$$\left\langle \vec{S}(\boldsymbol{r}) \right\rangle \propto \vec{N} \cos(\boldsymbol{Q} \bullet \boldsymbol{r})$$

$$\boldsymbol{Q} = (\pi, \pi); \ \vec{N}^2 = 1$$

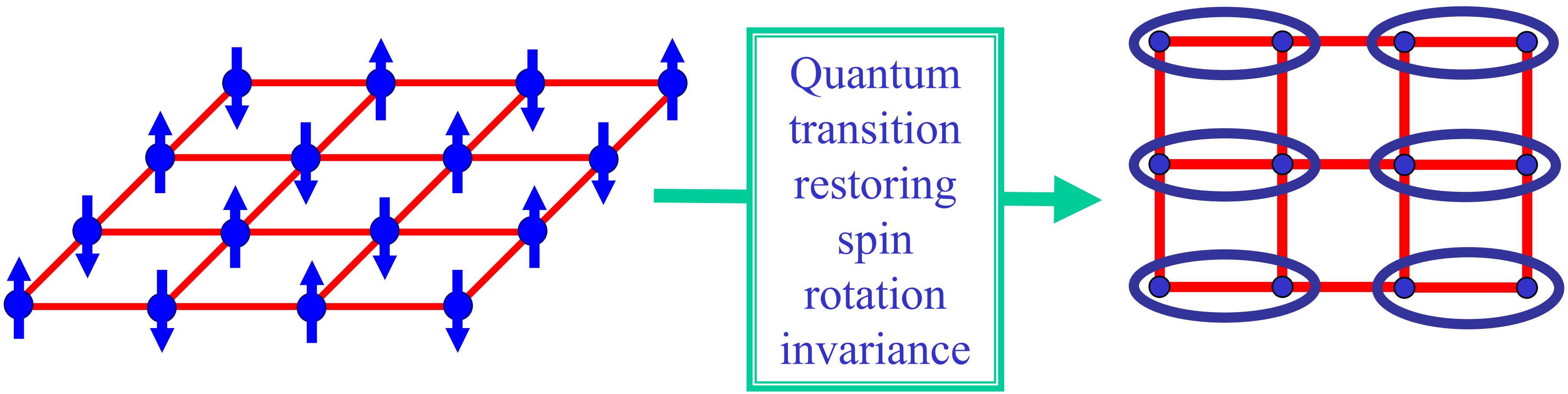
(B) Non-collinear spins



$$\left\langle \vec{S}(\boldsymbol{r}) \right\rangle \propto \vec{N}_1 \cos(\boldsymbol{Q} \bullet \boldsymbol{r}) + \vec{N}_2 \sin(\boldsymbol{Q} \bullet \boldsymbol{r})$$

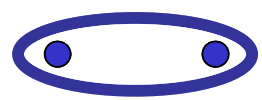
$$\boldsymbol{Q} = \left(\frac{4\pi}{3}, \frac{4\pi}{\sqrt{3}} \right); \ \vec{N}_1^2 = \vec{N}_2^2 = 1; \ \vec{N}_1 \bullet \vec{N}_2 = 0$$

(A) Collinear spins, bond order, and confinement



$$\left\langle \vec{S}(\boldsymbol{r}) \right\rangle \propto \vec{N} \cos(\boldsymbol{Q} \bullet \boldsymbol{r})$$

$$\boldsymbol{Q} = (\pi, \pi); \; \vec{N}^2 = 1$$

 $= \frac{1}{\sqrt{2}}\left(\left| \uparrow\downarrow \right\rangle - \left| \downarrow\uparrow \right\rangle \right)$

Bond-ordered state

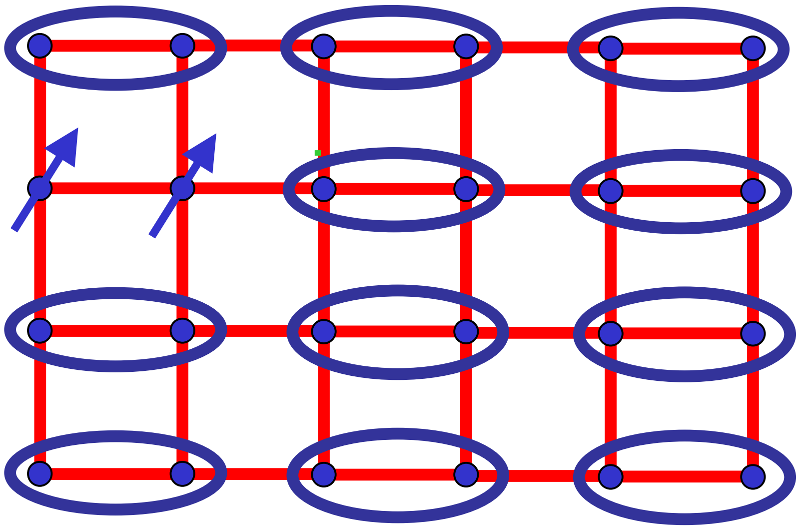
N. Read and S. Sachdev, *Phys. Rev. Lett*. **62**, 1694 (1989).

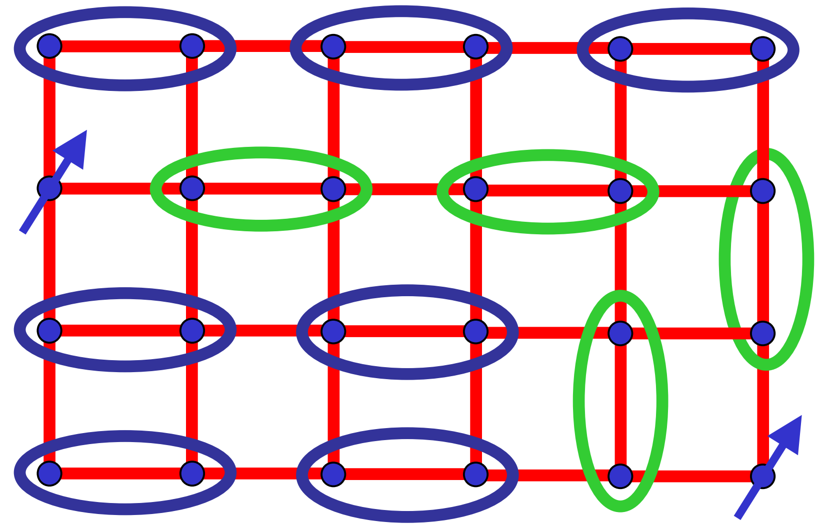
Excitations of bond-ordered paramagnet

Stable S=1 spin exciton – quanta of 3-component vector particle $\vec{N}$

$$\varepsilon_k = \Delta + \frac{c_x^2 k_x^2 + c_y^2 k_y^2}{2\Delta}$$

$\Delta \rightarrow$ Spin gap





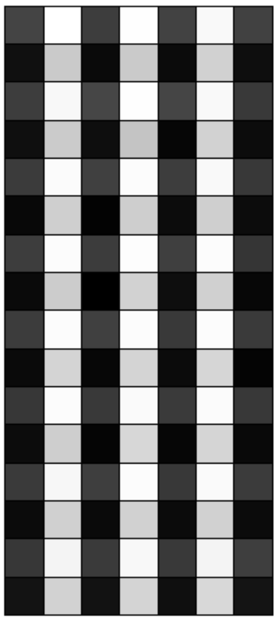
S=1/2 spinons are ***confined*** by a linear potential.

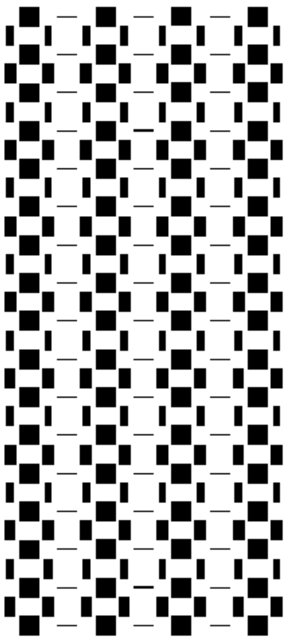
Transition to Neel state $\Rightarrow$ Bose condensation of $\vec{N}$

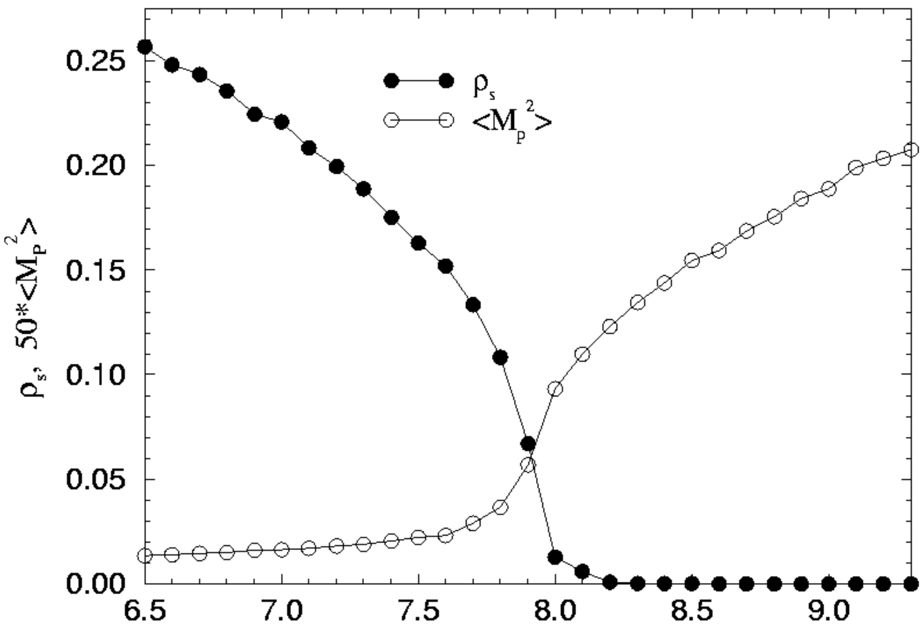
Bond order wave in a frustrated $S=1/2$ XY magnet

A. W. Sandvik, S. Daul, R. R. P. Singh, and D. J. Scalapino, cond-mat/0205270

First large scale numerical study of the destruction of Neel order in $S=1/2$ antiferromagnet with full square lattice symmetry



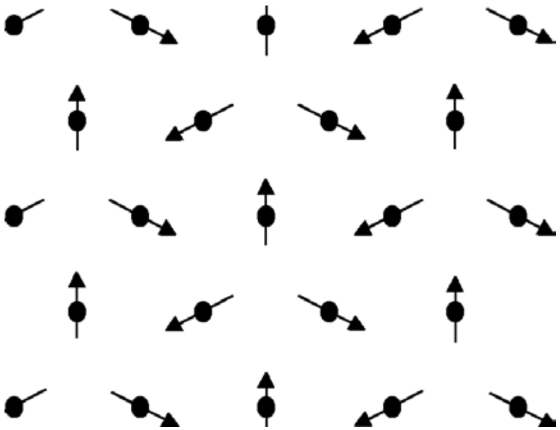




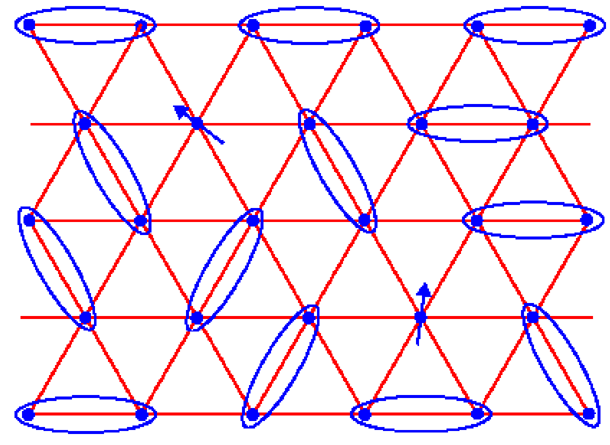
$g=$

$$H = 2J\sum_{\langle ij\rangle}\left(S_i^x S_j^x + S_i^y S_j^y\right) - K\sum_{\langle ijkl\rangle\subset\square}\left(S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+\right)$$

(B) Non-collinear spins, deconfined spinons, Z_2 gauge theory, and topological order



Quantum transition restoring spin rotation invariance



$$\left\langle \vec{S}(\boldsymbol{r}) \right\rangle \propto \vec{N}_1 \cos(\boldsymbol{Q}\cdot\boldsymbol{r}) + \vec{N}_2 \sin(\boldsymbol{Q}\cdot\boldsymbol{r})$$

$$\boldsymbol{Q} = \left(\frac{4\pi}{3}, \frac{4\pi}{\sqrt{3}} \right); \; \vec{N}_1^2 = \vec{N}_2^2 = 1 \, ; \; \vec{N}_1 \bullet \vec{N}_2 = 0$$

RVB state with free spinons

P. Fazekas and P.W. Anderson, *Phil Mag* **30**, 23 (1974).

N. Read and S. Sachdev, *Phys. Rev. Lett*. **66**, 1773 (1991) –<u>first</u> discussion of Z_2 gauge theory

A.V. Chubukov, T. Senthil and S. Sachdev, *Phys. Rev. Lett.* **72**, 2089 (1994).

$$\left\langle \vec{S}(\boldsymbol{r}) \right\rangle \propto \vec{N}_1 \cos(\boldsymbol{Q} \bullet \boldsymbol{r}) + \vec{N}_2 \sin(\boldsymbol{Q} \bullet \boldsymbol{r})$$

$$\boldsymbol{Q} = \left(\frac{4\pi}{3}, \frac{4\pi}{\sqrt{3}} \right); \; \vec{N}_1^2 = \vec{N}_2^2 = 1 \,; \; \vec{N}_1 \bullet \vec{N}_2 = 0$$

Solve constraints by writing:

$$\vec{N}_1 + i \vec{N}_2 = \varepsilon_{ac} z_c \vec{\sigma}_{ab} z_b$$

where $z_{1,2}$ are two complex numbers with

$$|z_1|^2 + |z_2|^2 = 1$$

Order parameter space: S_3 / Z_2

Physical observables are invariant under the Z_2 gauge transformation $z_a \to \pm z_a$

Other approaches to a Z_2 gauge theory:

R. Jalabert and S. Sachdev, *Phys. Rev.* B **44**, 686 (1991); S. Sachdev and M. Vojta, *J. Phys. Soc. Jpn* **69,** Suppl. B, 1 (2000).

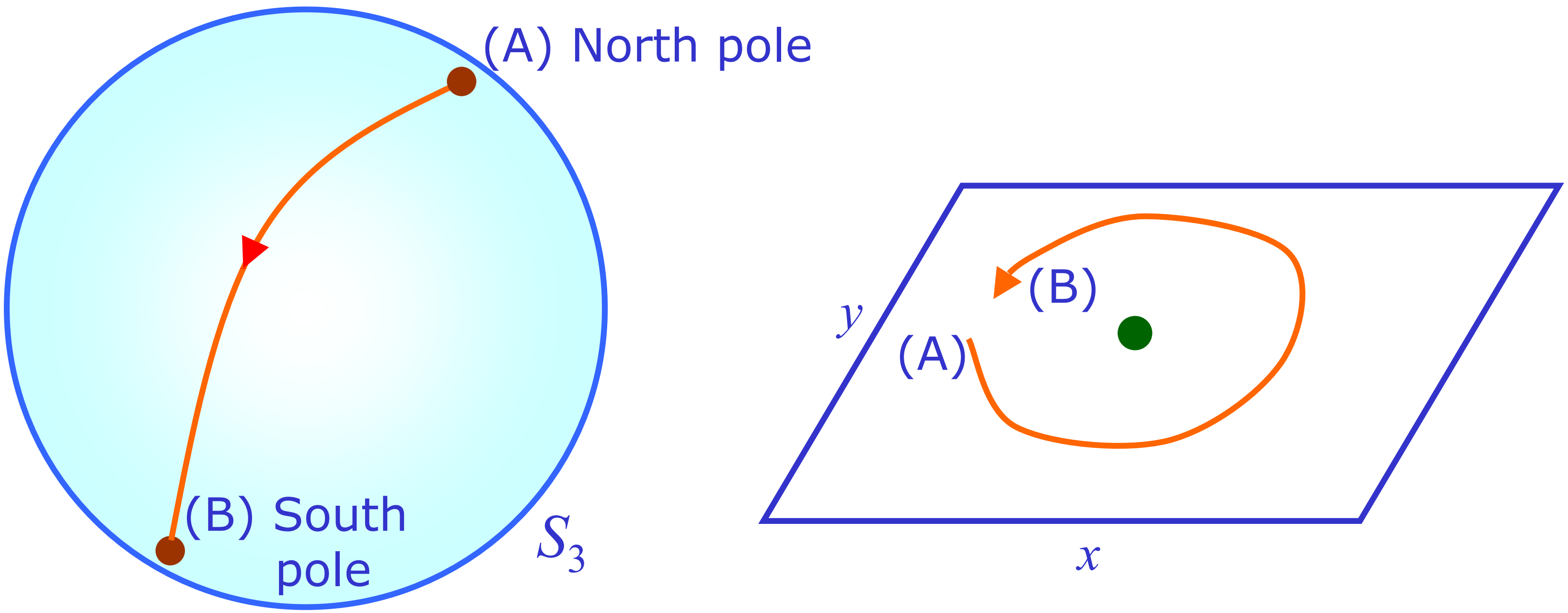
X. G. Wen, *Phys. Rev.* B **44**, 2664 (1991).

T. Senthil and M.P.A. Fisher, *Phys. Rev.* B **62**, 7850 (2000).

R. Moessner, S. L. Sondhi, and E. Fradkin, *Phys. Rev.* B **65**, 024504 (2002).

L. B. Ioffe, M.V. Feigel'man, A. Ioselevich, D. Ivanov, M. Troyer and G. Blatter, *Nature* **415**, 503 (2002).

Vortices associated with $\pi_1(S_3/Z_2)=Z_2$



Can also consider vortex excitation in phase without magnetic order, $\left\langle \vec{S}(r) \right\rangle = 0$: **vison**

A paramagnetic phase with vison excitations suppressed has topological order

Model effective action and phase diagram

$$\mathcal{S} = -J \sum_{\langle ij \rangle} \sigma_{ij} z^*_{\alpha i} z_{\alpha j} + \text{h.c.} - K \sum_{\square} \prod_{\square} \sigma_{ij}$$

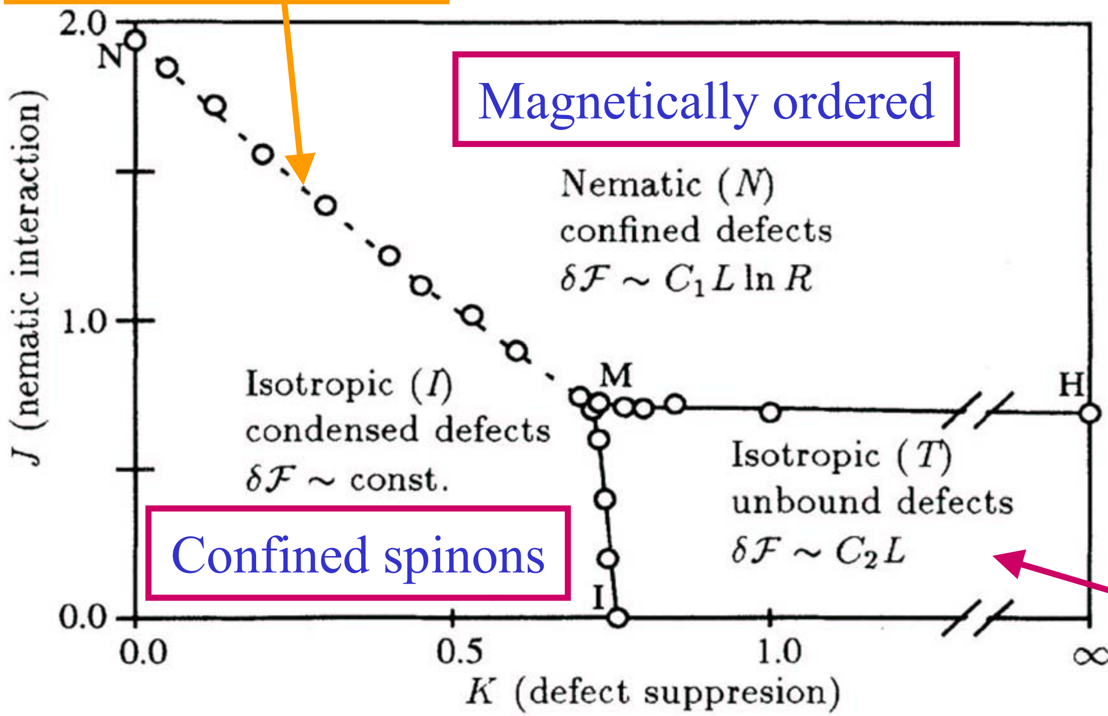
(Derivation using Schwinger bosons on a quantum antiferromagnet: S. Sachdev and N. Read, *Int. J. Mod. Phys*. B **5**, 219 (1991)).

$\sigma_{ij} \rightarrow Z_2$ gauge field

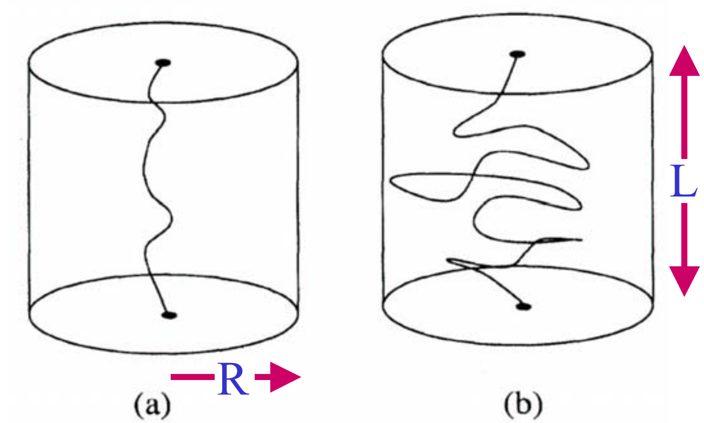
First order transition

Magnetically ordered

Confined spinons



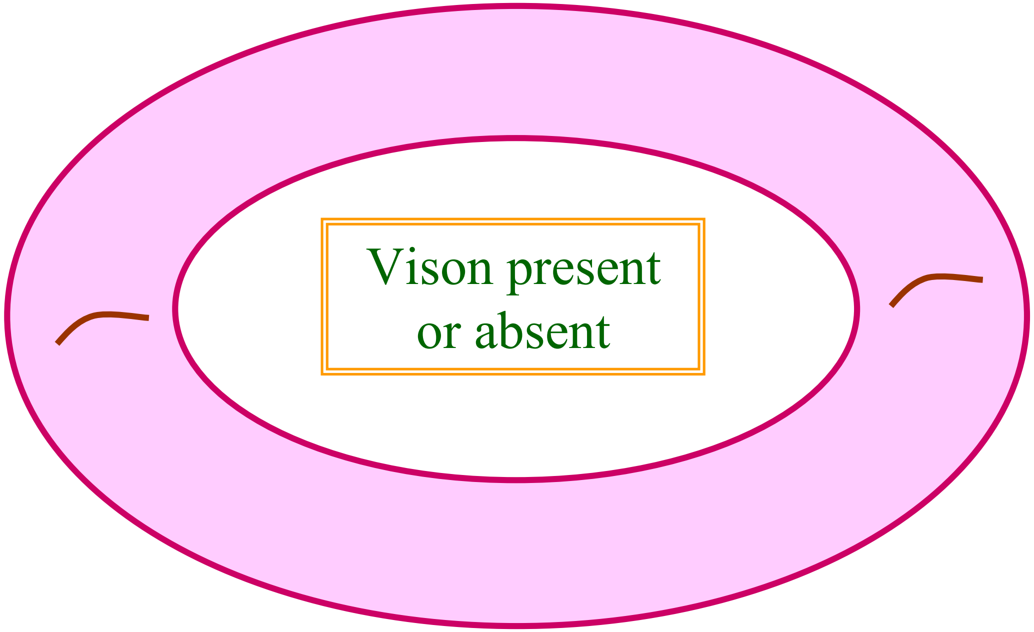
Free spinons and topological order



Impose boundary conditions inducing single vortex on walls of cylinder

P. E. Lammert, D. S. Rokhsar, and J. Toner, *Phys. Rev. Lett*. **70**, 1650 (1993) ; *Phys. Rev.* E **52**, 1778 (1995). (For nematic liquid crystals)

Topologically ordered state has a 2^d-fold degeneracy on a d-dimensional torus



S. Kivelson, *Phys. Rev.* B **39**, 259 (1989);
N. Read and B. Chakraborty, *Phys. Rev.* B **40**, 7133 (1989).
N. E. Bonesteel, *Phys. Rev.* B **40**, 8954 (1989).
G. Misguich, C. Lhuillier, M. Mambrini, and P. Sindzingre, *Eur. Phys. J.* B **26**, 167 (2002).

III. "Small" Fermi surfaces in Kondo lattices

Kondo lattice model:

$$H = \sum_{i<j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} \left(J_K c_{i\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} c_{i\sigma} \cdot \vec{S}_{fi} \right) + \sum_{i<j} J_H \left(i, j\right) \vec{S}_{fi} \cdot \vec{S}_{fj}$$

Consider, first the case J_K=0 and J_H chosen so that the spins form a *bond ordered* paramagnet

This system has a Fermi surface of conduction electrons with volume n_c (mod 2)

However, because n_f=2 (per unit cell of ground state)
$\boldsymbol{n_T = n_f + n_c = n_c}$ **(mod 2)**, and
"small" Fermi volume="large" Fermi volume
(mod Brillouin zone volume)

These statements apply also for a finite range of J_K

Conventional Luttinger Theorem holds

III. "Small" Fermi surfaces in Kondo lattices

Kondo lattice model:

$$H = \sum_{i<j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} \left(J_K c_{i\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} c_{i\sigma} \cdot \vec{S}_{fi} \right) + \sum_{i<j} J_H \left(i, j\right) \vec{S}_{fi} \cdot \vec{S}_{fj}$$

Consider, first the case J_K=0 and J_H chosen so that the spins form a *topologically ordered* paramagnet

This system has a Fermi surface of conduction electrons with volume n_c (mod 2)

Now n_f=1 (per unit cell of ground state)

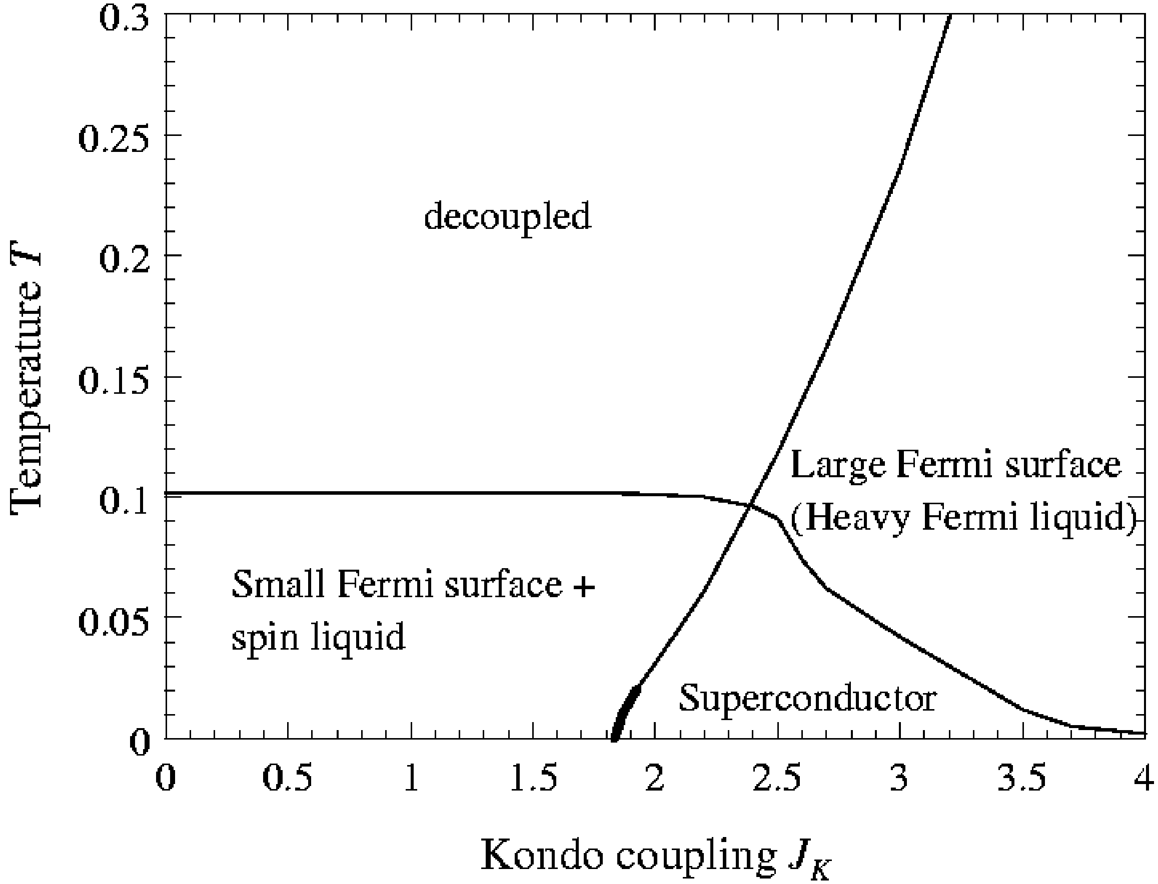
$$n_T = n_f + n_c \neq n_c \left(\text{mod } 2\right)$$

This state, and its Fermi volume, survive for a finite range of J_K

Perturbation theory is J_K is free of infrared divergences, and the topological ground state degeneracy is protected.

A "small" Fermi surface which violates conventional Luttinger theorem

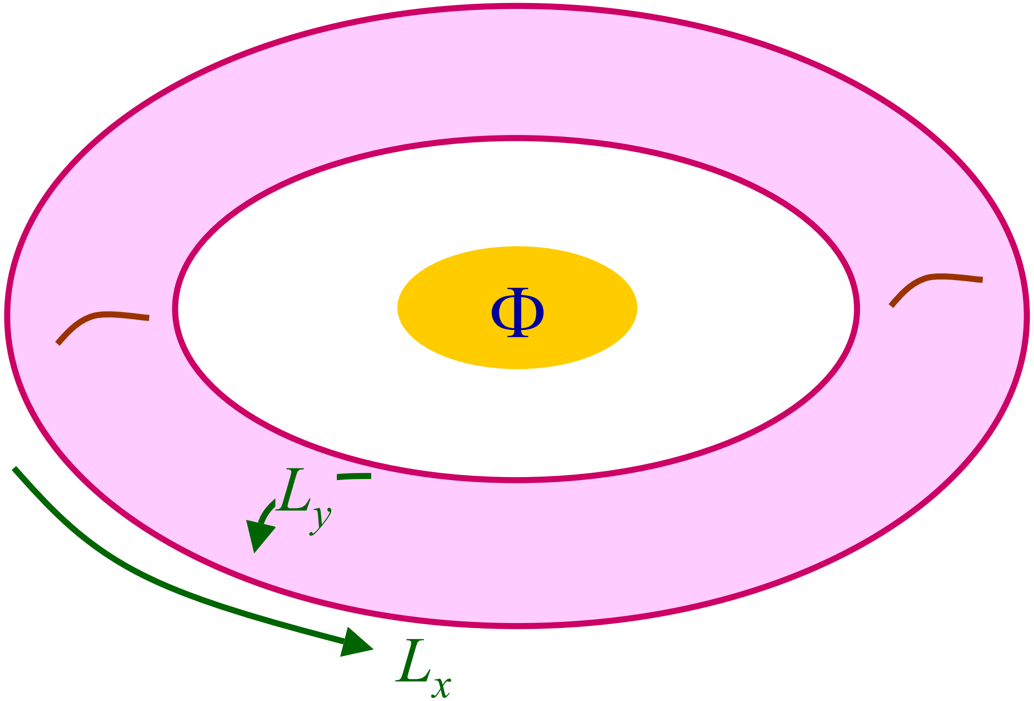
Mean-field phase diagram (Sp(N), large N theory)



Pairing of spinons in small Fermi surface state induces superconductivity at the confinement transition

Small Fermi surface state can also exhibit a second-order metamagnetic transition in an applied magnetic field, associated with vanishing of a spinon gap.

IV. Lieb-Schultz-Mattis-Laughlin-Bonesteel-Affleck-Yamanaka-Oshikawa flux-piercing arguments



Unit cell a_x, a_y.
L_x/a_x, L_y/a_y
coprime integers

Adiabatically insert flux $\Phi = 2\pi$ (units $\hbar$=c=e=1) acting on $\uparrow$ electrons.

State changes from $|\Psi\rangle$ to $|\Psi'\rangle$, and $UH(0)U^{-1} = H(\Phi)$, where

$$U = \exp\left[\frac{2\pi i}{L_x}\sum_{\boldsymbol{r}} x\,\hat{n}_{\boldsymbol{r}\uparrow}\right].$$

M. Oshikawa, *Phys. Rev. Lett.* **84**, 3370 (2000).

Adiabatic process commutes with the translation operator T_x, so momentum P_x is conserved.

$$\text{However } U^{-1} T_x U = T_x \exp\left[\frac{2\pi i}{L_x} \sum_{\boldsymbol{r}} \hat{n}_{\boldsymbol{Tr}\uparrow}\right];$$

so shift in momentum ΔP_x between states $U|\Psi'\rangle$ and $|\Psi\rangle$ is

$$\Delta P_x = \frac{\pi L_y}{v_0} n_T \left(\bmod \frac{2\pi}{a_x}\right) \qquad (1).$$

Alternatively, we can compute ΔP_x by assuming it is absorbed by quasiparticles of a Fermi liquid. Each quasiparticle has its momentum shifted by $2\pi/L_x$, and so

$$\Delta P_x = \frac{2\pi}{L_x} \frac{(\text{Volume enclosed by Fermi surface})}{(2\pi)^2/(L_x L_y)} \left(\bmod \frac{2\pi}{a_x}\right) \qquad (2).$$

From (1) and (2), same argument in y direction, using coprime $L_x/a_x, L_y/a_y$:

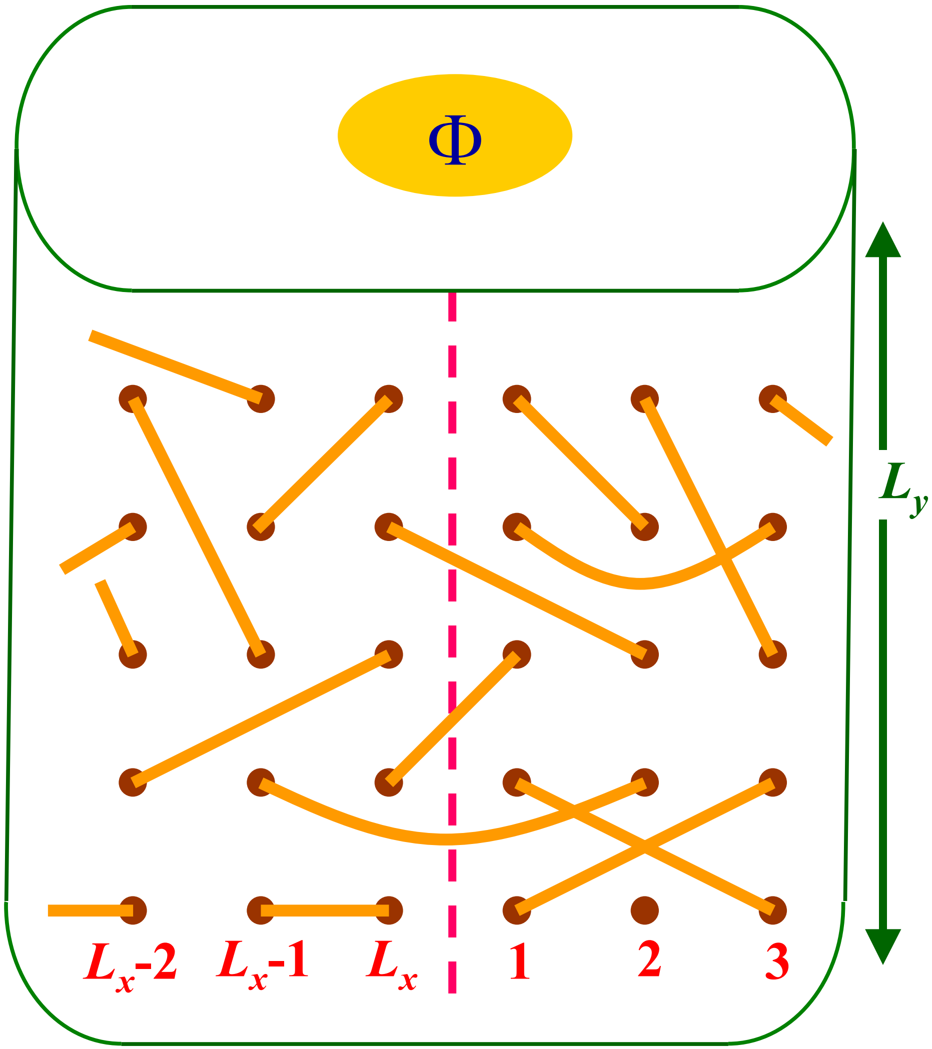
$$2 \times \frac{v_0}{(2\pi)^2} (\text{Volume enclosed by Fermi surface}) = n_T \ (\bmod 2)$$

M. Oshikawa, *Phys. Rev. Lett.* **84**, 3370 (2000).

Effect of flux-piercing on a topologically ordered quantum paramagnet

N. E. Bonesteel, *Phys. Rev.* B **40**, 8954 (1989).
G. Misguich, C. Lhuillier, M. Mambrini, and P. Sindzingre, *Eur. Phys. J.* B **26**, 167 (2002).

$$|D\rangle =$$



$$|\Psi\rangle = \sum_D a_D |D\rangle$$

Effect of flux-piercing on a topologically ordered quantum paramagnet

N. E. Bonesteel, *Phys. Rev.* B **40**, 8954 (1989).
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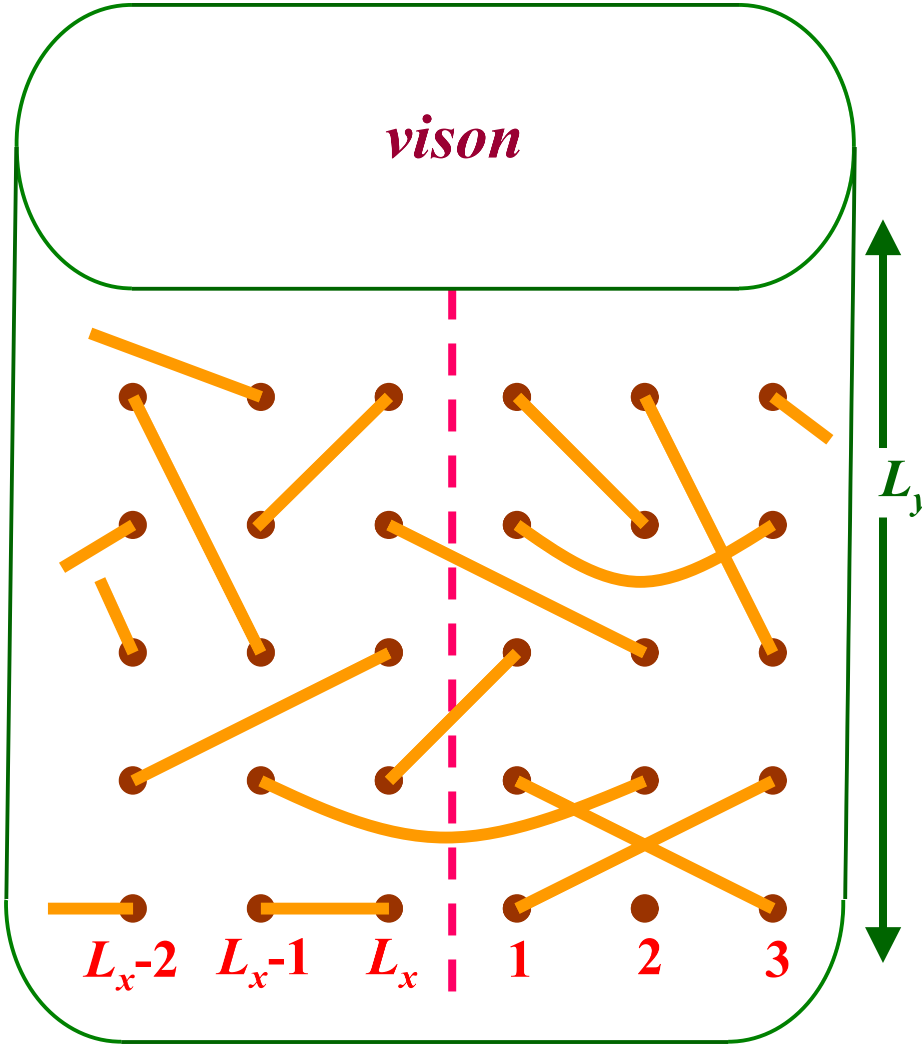
$$\left|D\right\rangle =$$



$$\left|\Psi\right\rangle = \sum_D a_D \left|D\right\rangle$$

After flux insertion $\left|D\right\rangle \Rightarrow$

$$\left(-1\right)^{\substack{\text{Number of bonds} \\ \text{cutting dashed line}}} \left|D\right\rangle;$$

Equivalent to inserting a ***vison*** inside hole of the torus.

Vison carries momentum $\pi L_y / v_0$

Flux piercing argument in Kondo lattice

Shift in momentum is carried by n_T electrons, where

$$n_T = n_f + n_c$$

In topologically ordered, state, momentum associated with n_f=1 electron is absorbed by creation of vison. The remaining momentum is absorbed by Fermi surface quasiparticles, which enclose a volume associated with n_c electrons.

A small Fermi surface.

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Conclusions

I. Orders characterizing ground states of regular Kondo lattices:

(A) Spin density wave.

(B) Superconductivity.

(C) Topological order – small Fermi surface,

(D) Large Fermi surface.

II. Some orders can co-exist, and this permits a plethora of phase diagrams and quantum critical points.

(A) $\leftrightarrow$ (D) Hertz theory

(C) $\leftrightarrow$ (D) "Local" quantum criticality ?

(Small Fermi surfaces in extended DMFT:
S. Burdin, D. R. Grempel, and A. Georges,
Phys. Rev. B **66**, 045111 (2002)).