Small and large Fermi surfaces in metals with local moments

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Transparencies online at http://pantheon.yale.edu/~subir
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

$$2 \times \frac{v_0}{(2\pi)^d} \left( \text{Volume enclosed by Fermi surface} \right) = (n_T - 1) \pmod{2}$$

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, $f_{i\sigma}$

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

$$n_{f_i\sigma} = f_{i\sigma}^\dagger f_{i\sigma} ; \quad n_{c_i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$$

$$n_T = n_f + n_c$$

For small $U$, we obtain a Fermi liquid ground state, with a Fermi surface volume determined by $n_T \pmod 2$

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

$$n_T \pmod 2 = (1 + n_c) \pmod 2$$
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.

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

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

We will show that for small $J_K$, a ground state with a “small” electron-like Fermi surface enclosing a volume determined by $n_c \text{ (mod 2)}$ 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

\[ \langle \vec{S}(r) \rangle \propto \vec{N} \cos(Q \cdot r) \]
\[ Q = (\pi, \pi); \quad \vec{N}^2 = 1 \]

(B) Non-collinear spins

\[ \langle \vec{S}(r) \rangle \propto \vec{N}_1 \cos(Q \cdot r) + \vec{N}_2 \sin(Q \cdot r) \]
\[ Q = \left( \frac{4\pi}{3}, \frac{4\pi}{\sqrt{3}} \right); \quad \vec{N}_1^2 = \vec{N}_2^2 = 1; \quad \vec{N}_1 \cdot \vec{N}_2 = 0 \]
(A) Collinear spins, bond order, and confinement

\[
\langle \vec{S}(r) \rangle \propto N \cos(\vec{Q} \cdot r)
\]

\[Q = (\pi, \pi); \quad \bar{N}^2 = 1\]

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

Bond-ordered state

Excitations of bond-ordered paramagnet

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

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

$\Delta \to$ Spin gap

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

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

\[
H = 2J \sum_{\langle ij \rangle} \left( S_i^x S_j^x + S_i^y S_j^y \right) - K \sum_{\langle ijk \rangle \subset \square} \left( S_i^+ S_j^- S_k^- S_l^- + S_i^- S_j^+ S_k^- S_l^- \right)
\]
(B) Non-collinear spins, deconfined spinons, $\mathbb{Z}_2$ gauge theory, and topological order

\[ \langle S(r) \rangle \propto N_1 \cos(Q \cdot r) + N_2 \sin(Q \cdot r) \]
\[ Q = \left( \frac{4\pi}{3}, \frac{4\pi}{\sqrt{3}} \right); \quad N_1^2 = N_2^2 = 1; \quad N_1 \cdot N_2 = 0 \]

RVB state with free spinons


\[ \langle \bar{S}(r) \rangle \propto \bar{N}_1 \cos(Q \cdot r) + \bar{N}_2 \sin(Q \cdot r) \]
\[ Q = \left( \frac{4\pi}{3}, \frac{4\pi}{3\sqrt{3}} \right); \quad \bar{N}_1^2 = \bar{N}_2^2 = 1; \quad \bar{N}_1 \cdot \bar{N}_2 = 0 \]

Solve constraints by writing:
\[ \bar{N}_1 + i\bar{N}_2 = \varepsilon_{ac} z_c \bar{\sigma}_{ab} z_b \]
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:
Vortices associated with $\pi_1(S^3/Z_2) = Z_2$

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

A paramagnetic phase with vison excitations suppressed has topological order
Model effective action and phase diagram

\[ S = -J \sum_{\langle ij \rangle} \sigma_{ij} z_{\alpha i}^* z_{\alpha j} + \text{h.c.} - K \prod \sigma_{ij} \]

\[ \sigma_{ij} \rightarrow Z_2 \text{ gauge field} \]

First order transition

Magnetically ordered

Confined spinons

Free spinons and topological order

Impose boundary conditions inducing single vortex on walls of cylinder


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

Vison present or absent

III. “Small” Fermi surfaces in Kondo lattices

Kondo lattice model:

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

Consider, first the case \( J_K = 0 \) and \( J_H \) chosen so that the spins form a \textit{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)

\[ n_T = n_f^+ + n_c = n_c \text{ (mod 2)}, \text{ and} \]

\textbf{“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:

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

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)

\[ n_T = n_f + n_c \neq n_c \text{ (mod 2)} \]

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.
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.
Adiabatically insert flux $\Phi = 2\pi$ (units $\hbar = c = e = 1$) acting on $\uparrow$ electrons. State changes from $|\Psi\rangle$ to $|\Psi'\rangle$, and $U H(0) U^{-1} = H(\Phi)$, where

$$U = \exp\left[\frac{2\pi i}{L_x} \sum_r x \hat{n}_{tr\uparrow}\right].$$

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

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

so shift in momentum $\Delta P_x$ between states $U|\Psi \rangle$ and $|\Psi \rangle$ is

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

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

$$\Delta P_x = \frac{2\pi}{L_x} \left( \text{Volume enclosed by Fermi surface} \right) \left( \text{mod} \frac{2\pi}{a_x} \right) \quad (2).$$

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

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

Effect of flux-piercing on a topologically ordered quantum paramagnet

N. E. Bonesteel,
G. Misguich, C. Lhuillier, M. Mambrini, and P. Sindzingre,

\[ |D\rangle = \sum_D a_D |D\rangle \]
Effect of flux-piercing on a topologically ordered quantum paramagnet

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\[ |D\rangle = \sum_D a_D |D\rangle \]

After flux insertion \( |D\rangle \Rightarrow (-1)^{\text{Number of bonds cutting dashed line}} |D\rangle \); 

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?