Quantum critical itinerant ferromagnetism

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Belitz et al., PRL 2005

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Two types of ferromagnetism

- **Localized ferromagnetism**: moments localised in real space

  - **Ferromagnet**: up arrows
  - **Antiferromagnet**: down arrows

- **Itinerant ferromagnetism**: moments localised in reciprocal space

  - Not magnetised
  - Partially magnetised
Stoner model for itinerant ferromagnetism

- Repulsive interaction energy $U = gn_{\uparrow\downarrow}$
- A $\Delta E$ shift in the Fermi surface causes:
  (i) Kinetic energy increase of $\frac{1}{2}v\Delta E^2$
  (ii) Reduction of repulsion of $-\frac{1}{2}gv^2\Delta E^2$
- Total energy shift is $\frac{1}{2}v\Delta E^2(1-gv)$ so a ferromagnetic transition occurs if $gv > 1$
Ferromagnetism in iron

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- The Stoner model has a second order transition of e.g. iron and nickel which is characterized by:
  - Smoothly varying magnetisation
  - A divergence of length-scales (peaked heat capacity and susceptibility)
Breakdown of Stoner criterion -- ZrZn$_2$

- At low temperature and high pressure ZrZn$_2$ has a first order transition

Uhlarz et al., PRL 2004
Breakdown of Stoner criterion -- MnSi

- MnSi also displays a first order phase transition

Pfleiderer et al., PRB 1997
Breakdown of Stoner criterion

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- At low temperature UGe$_2$, ZrZn$_2$, MnSi, and others are first order

Here I describe two projects that investigate the first order behaviour:

(i) Use atomic gases to probe the first order transition without the lattice

(ii) Motivated by the FFLO phase, apply the formalism to search for a putative textured phase
A gas of Fermionic atoms is prepared by laser and evaporative cooling to $\sim 10^{-8}$K.

Two-body contact collisions are controlled with a Feshbach resonance tuned by an external magnetic field.

Can tune from bound BEC molecules to weakly bound BCS regime\(^1\).

Repulsive interactions might allow us to investigate itinerant ferromagnetism.

**Feshbach resonance**

- Control the relative energy level of states with an external magnetic field

BEC (boson)

Van der Waals

BCS (fermions)

\[ k_Fa > 0 \rightarrow \text{Repulsive} \]
\[ k_Fa < 0 \rightarrow \text{Attractive} \]
Cold atomic gases -- spin

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- Two fermionic atom species have a pseudo-spin:
  
  \[ ^{40}\text{K} \quad m_F = 9/2 \]  
  maps to  
  spin 1/2

  \[ ^{40}\text{K} \quad m_F = 7/2 \]  
  maps to  
  spin -1/2

- The up-and down spin particles cannot interchange -- population imbalance is fixed

- Atomic gases contain no disorder

- Atomic gases provide unprecedented levels of control allowing investigators to probe solid state phenomena e.g. Hubbard model\(^1\), superfluid vortices\(^2\), Josephson effects\(^3\), FFLO\(^4\), and Kosterlitz-Thouless phase transition\(^5\)

A spin up and a spin down particle ($S_z = 0$) in triplet and singlet states:

- $|\uparrow\uparrow\rangle$  $S=1, \ S_z = 1$: State not possible as $S_z$ has changed
- $|\downarrow\downarrow\rangle$  $S=1, \ S_z = -1$: State not possible as $S_z$ has changed

$(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$  $S=1, \ S_z = 0$: Magnetic moment in plane

$(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$  $S=0, \ S_z = 0$: Non-magnetic state

- Ferromagnetism, if favourable, must form in plane
System free energy \( F = -k_B T \ln Z \) is found via the partition function

\[
Z = \sum_{[m(x,t),n(x,t)]} \exp \left( -\frac{E[m(x,t),n(x,t)]}{k_B T} \right)
\]

the summation includes spatial and temporal fluctuations of magnetisation and density

Using only the average magnetisation and density:

\[
m(x,t) = \bar{m}
\]

\[
n(x,t) = \bar{n}
\]

gives

\[
F \propto (1 - g \nu) \bar{m}^2
\]
i.e. the Stoner criterion
Method of steepest descent

• Suppose the partition function takes the form
  \[ Z = \int_0^\infty \exp(-m + s \ln m) \, dm \]

• Expand about the maximum of the function at \( m = s \):
  \[ Z = \int_0^\infty \exp(-s(1 - \ln s) - (m - s)^2 / 2s + O((m - s)^3)) \, dm \]

• Following the Gaussian integral
  \[ Z \approx \sqrt{2\pi s} s^s e^{-s} \]

• This is Stirling's formula
  \[ s! \approx \sqrt{2\pi s} s^s e^{-s} \]
In a similar way we can expand the energy in magnetisation to second order to account for fluctuations

\[ Z = \sum_{\{m(x,t), n(x,t)\}} \exp\left( -E[m, n] / k_B T \right) \]

\[ = \sum_{\{\delta m(x,t), \delta n(x,t)\}} \exp\left( \frac{-1}{k_B T} \left( E[\bar{m}, \bar{n}] + (\delta m \delta n) \begin{pmatrix} E^{(2,0)} \\ E^{(1,1)} \\ E^{(0,2)} \end{pmatrix} \begin{pmatrix} \delta m \\ \delta n \end{pmatrix} \right) \right) \]

Larkin & Pikin [Zh. Eksp. Teor. Fiz. 1969] included auxiliary fluctuations of the lattice which introduced a negative magnetisation term, driving the transition first order

\[ r m^2 + u m^4 + a \phi^2 \pm 2a m^2 \phi = r m^2 + (u - a) m^4 + a (\phi \pm m^2)^2 = r m^2 + (u - a) m^4 \]

Previous work on itinerant ferromagnetism considered a mean field Ginzburg-Landau expansion\(^1\) or non-analyticities to examine the transition\(^2\)

\(^1\)Belitz et al. PRL 2005, \(^2\)Belitz et al. PRL 2002
Fluctuation corrections

- We include corrections due to dynamic quantum fluctuations in x, y, and z directions, and also account for fluctuations in density.

- Similarly here considering the soft transverse magnetic fluctuations drives the transition of the longitudinal first order.

- The results give the following phase diagram.

$M (\mu_B/\text{f.u.})$

$T=2.3K$

Uhlarz et al., PRL 2004
Population imbalanced case

With population imbalance $P$ in the canonical regime we obtain

\[ P = 0 \]

\[ M_{\text{spon}} = M_{\text{perp}} \]

UnM: Unmagnetised
PM: Partially magnetised
FM: Fully magnetised
In the grand canonical ensemble we obtain

\[ \frac{P}{N} = 0.8 \]
\[ \frac{P}{N} = 0.4 \]
\[ \frac{P}{N} = 0 \]
Trap behaviour

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- Trap behaviour corresponds to three trajectories in the phase diagram
QMC calculations

- Fluctuation corrections are not exact and higher order terms might destroy the first order phase transition.
- Exact (except for the fixed node approximation) Quantum Monte Carlo calculations confirmed a first order phase transition.
Wohlfarth Rhodes criterion

Do fluctuations influence the transition through the density of states?

The first order transition could be caused by a peak in the density of states [Sandeman et al. PRL 2003, Pfleiderer et al. PRL 2002]

If the density of states $v(E)$ changes rapidly with energy then a ferromagnetic transition is favourable when [Binz et al. EPL 2004]

$$v v'' > 3 (v')^2$$

Total number of particles is conserved so areas are equal.
Improved Wohlfarth Rhodes criterion

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- Accounting for changes in the energy spectrum $\varepsilon$ gives criterion

$$\int_{0}^{u} \varepsilon^{(0,4)}(w, 0)dw + 4\varepsilon^{(0,3)}(u, 0) + 6\varepsilon^{(1,2)}(u, 0) + 4\varepsilon^{(2,1)}(u, 0) + \varepsilon^{(3,0)}(u, 0) < 0$$

- The terms have magnitude

<table>
<thead>
<tr>
<th>Term</th>
<th>Expansion</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\int_{0}^{u} \varepsilon^{(0,4)}(w, 0)dw$</td>
<td>$0.0k_F a + 0.0086(k_F a)^2$</td>
</tr>
<tr>
<td>$4\varepsilon^{(0,3)}(u, 0)$</td>
<td>$0.0k_F a - 0.04(k_F a)^2$</td>
</tr>
<tr>
<td>$6\varepsilon^{(1,2)}(u, 0)$</td>
<td>$0.024(k_F a)^2$</td>
</tr>
<tr>
<td>$4\varepsilon^{(2,1)}(u, 0)$</td>
<td>$0.0(k_F a)^2$</td>
</tr>
<tr>
<td>$\varepsilon^{(3,0)}(u, 0)$</td>
<td>$2^{-3/2}/27 - 0.0055(k_F a)^2$</td>
</tr>
</tbody>
</table>

Overall change in energy spectrum during the transition

How energy spectrum changes during transition at the Fermi surface

Wohlfarth Rhodes criterion

Differential of energy spectrum curve

Differentiate energy spectrum wrt changing Fermi surface

Transition due to changing energy spectrum at the Fermi surface
Summary of uniform work

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- Consideration of corrections due to fluctuations in magnetisation and density revealed a first order phase transition
- Nature of transition confirmed by Quantum Monte Carlo calculations
- Shed light on relation to features in the density of states
- Motivated by FFLO and experiment now examine a putative textured ferromagnetic phase
• Kink in magnetisation indicative of metamagnetic phase

Uhlarz et al., PRL 2004
Sr$_3$Ru$_2$O$_7$

- Resistance anomaly

Scattering of M fluctuations

Scattering off M crystal?

- Consistent with a new crystalline phase

Grigera et al., Science 2004
• NbFe$_2$ displays antiferromagnetic order where it is expected to be ferromagnetic -- could this be a textured ferromagnetic phase?

Crook & Cywinski, JMMM 1995
MnSi displays non-Fermi liquid behaviour consistent with a spin state (though in a non-centrosymmetric crystal)
Current proposals exploit a quantum critical point:

- Pomeranchuk instability – Grigera et al., Science 2005
- Nanoscale charge instabilities – Honerkamp, PRB 2005
- Electron nematic – Kee & Kim, PRB 2005
- Magnetic mesophase formation – Binz et al., 2005

Here propose a spin-spiral state, previous studies focussed on non-analyticities:

- Rech, Pépin & Chubukov, PRB 74, 195126, (2006) used Eliashberg theory
- Belitz et al., PRB 1997 considered corrections due to magnetisation fluctuations
The Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) phase has a modulated superconducting gap. A Cooper pair has zero momentum, with unequal Fermi surfaces the Cooper pair carries momentum, causing a modulated superconducting gap parameter $\Delta$. The FFLO phase preempts the normal phase-superfluid transition.
Ginzburg-Landau analysis

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- In analogy to FFLO\textsuperscript{1} we can look at a Ginzburg-Landau analysis

\[ \beta H = \int r \, m^2 + u \, m^4 + v \, m^6 + \frac{2}{3} u \left( \nabla m \right)^2 + \frac{3}{5} v \left( \nabla^2 m \right)^2 - hm \]

- The development of the tricritical point is accompanied by sign reversal of the gradient term

- Consider the lowest order term in a Ginzburg-Landau expansion, which is a function of the wave vector \( q \) of the textured phase

\[ \beta H = \sum_q \alpha_q \, m_q^2 \]

- When \( \alpha_q > 0 \) zero magnetisation is favourable, if \( \alpha_q < 0 \) a textured phase preempts the first order ferromagnetic transition

\textsuperscript{1}Saint-James \textit{et al.} 1969, \textsuperscript{2}Buzdin \& Kachkachi 1996
- Textured phase preempted transition with $q=0.1k_F$
Summary
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- Found field theoretic construction to understand population imbalance in atomic gases with a first order transition
- Confirmed with QMC calculations
- Applied improved Wohlfarth Rhodes criterion
- Ginzburg-Landau analysis of textured ferromagnetic phase
- Acknowledgements: Ben Simons & Andrew Green, EPSRC