Inhomogeneous phase formation on the border of itinerant ferromagnetism

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Itinerant ferromagnetism in an atomic Fermi gas: Influence of population imbalance

Inhomogeneous phase formation on the border of itinerant ferromagnetism
Two types of ferromagnetism

- **Localised ferromagnetism**: moments confined in real space
  - Ferromagnet
  - Antiferromagnet

- **Itinerant ferromagnetism**: electrons in Bloch wave states
  - Not magnetised
  - Partially magnetised
Stoner model for itinerant ferromagnetism

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

- The Stoner model predicts a second order transition that is characterised by 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

- Generic phase diagram of the first order transition

- Two explanations of first order behaviour:
Feshbach resonance

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

\[ k_F a > 0 \rightarrow \text{Repulsive} \]
\[ k_F a < 0 \rightarrow \text{Attractive} \]
Outline of talk

Part I: Analyse uniform ferromagnetism for atomic gases

• Survey previous analytical work on itinerant ferromagnetism
• Demonstrate physical origin of first order transition
• Analyse population imbalance in cold atom gas
• Review ongoing cold atoms experiments

Part II: Search for inhomogeneous phase

• Survey experimental motivation
• Perform a gauge transformation to study putative textured phase
• Supplementary Quantum Monte Carlo calculations
Analytical method

- System free energy $F=-k_B T \ln Z$ is found via the partition function

$$Z = \int D\psi \exp \left( -\int \sum_\sigma \bar{\psi}_\sigma (-i\omega + \epsilon - \mu) \psi_\sigma - g \int \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right)$$

- Decouple using only the average magnetisation

$$m = \bar{\psi}_\downarrow \psi_\uparrow - \bar{\psi}_\uparrow \psi_\downarrow$$

gives

$$F \propto (1 - g \nu) m^2$$

i.e. the Stoner criterion

- Hertz-Millis (spin triplet channel) [Hertz PRB 1976 & Millis PRB 1993]

$$F = \frac{1}{2} \left( |\omega| / \Gamma_q + r + q^2 \right) m^2 + \frac{u}{4} m^4 + \frac{v}{6} m^6 - hm$$
Extension to Hertz-Millis

- Coupling to auxiliary fields can drive a transition first order [Rice 1954, Garland & Renard 1966]
  \[ rm^2 + um^4 + a \phi^2 \pm 2 am^2 \phi \]
  \[ = rm^2 + (u - a)m^4 + a(\phi \pm m^2)^2 \]
  \[ = rm^2 + (u - a)m^4 \]

  \[ F = \frac{1}{2} \left( |\omega|/\Gamma_q + r + q^2 \right) m^2 + \frac{u}{4} m^4 \ln(m^2 + T^2) + \cdots - hm \]

- Chubukov-Pepin-Rech approach [Rech et al. 2006]
New approach to fluctuation corrections

\[ Z = \int D\psi \exp \left( -\int \sum_\sigma \bar{\psi}_\sigma (-i\omega + \epsilon - \mu) \psi_\sigma - g \int \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right) \]

• Analytic strategy:
  1) Decouple in both the density and spin channels (previous approaches employ only spin)
  2) Integrate out electrons
  3) Expand about uniform magnetisation
  4) Expand density and magnetisation fluctuations to second order
  5) Integrate out density and magnetisation fluctuations
Particle-hole perspective

- To first order in $g$ the free energy is

$$F = \sum_{\sigma, k} \epsilon_k^\sigma n(\epsilon_k^\sigma) + g N^\dagger N^\downarrow + \cdots$$

- To go beyond Stoner model need the next order in perturbation theory that will encompass fluctuation corrections
Particle-hole perspective

- To second order in $g$ the free energy is

$$F = \sum_{\sigma, k} \epsilon_k^\sigma n(\epsilon_k^\sigma) + gN^\uparrow N^\downarrow$$

$$- \frac{2g^2}{V^3} \sum_p \int \int \frac{\rho^\uparrow(p, \epsilon_\uparrow) \rho^\downarrow(-p, \epsilon_\downarrow)}{\epsilon_\uparrow + \epsilon_\downarrow} d\epsilon_\uparrow d\epsilon_\downarrow$$

$$+ \frac{2g^2}{V^3} \sum_{k_{1,2,3,4}} \frac{n(\epsilon_k^\uparrow) n(\epsilon_k^\downarrow)}{\epsilon_k^\uparrow + \epsilon_k^\downarrow - \epsilon_k^\downarrow} \delta(k_1 + k_2 - k_3 - k_3)$$

with $\epsilon_k^\sigma = \epsilon_k + \sigma gm$ and a particle-hole density of states

$$\rho^\sigma(p, \epsilon) = \sum_k n(\epsilon_k^\sigma_{+p/2}) \left[ 1 - n(\epsilon_k^\sigma_{-p/2}) \right] \delta(\epsilon - \epsilon_k^\sigma_{+p/2} + \epsilon_k^\sigma_{-p/2})$$

- Enhanced particle-hole phase space at zero magnetisation drives transition first order and tricritical point emerges

- Recover $m^4 \ln m^2$ at $T=0$

- Links quantum fluctuation to second order perturbation approach

\(^1\)Abrikosov 1958 & Duine & MacDonald 2005
Population imbalanced case

- Phase diagram with population imbalance $P$ in the canonical regime

UnM: Unmagnetised
PM: Partially magnetised
FM: Fully magnetised

Conduit & Simons, PRB 2009
Three body losses inhibit stability of ferromagnetic state.

Pauli exclusion prevents three-body losses in the ferromagnetic state.

Rather than disadvantage, three-body losses can be a detection method of the absence of a ferromagnetic state, $a^6n_\uparrow n_\downarrow$. 
G.-B. Jo and W. Ketterle have recently observed itinerant ferromagnetism in cold atom gases\textsuperscript{1}

- Use $^6\text{Li}$ atoms and short 2.5ms ramp time
- Atom loss rate $a^6n_{\uparrow}n_{\downarrow}$ is peaked at the transition

\textsuperscript{1}Jo \textit{et al}., submitted 2009
Experimental study with cold atom gases

- Repulsive interactions increases the pressure, raising cloud size

- But reducing the kinetic energy $\sim n^{5/3}$ before the transition
Summary of cold atoms work

- Revealed link between nonanalyticities and first order transition
- Motivated by Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) and experiment now examine a putative textured ferromagnetic phase
Outline of textured ferromagnetism

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ZrZn$_2$

- Kink in magnetisation indicative of novel phase behaviour

Uhlarz et al., PRL 2004
Gauge transform analysis

- Gauge transformation $\psi \rightarrow e^{\frac{1}{2} i \mathbf{q} \cdot \mathbf{r} \sigma_z} \psi$ renders magnetisation $m \sigma_x$ uniform and yields a similar expression for the free energy

$$F = \sum_{\sigma, k} \epsilon_k \epsilon_{k,q} n(\epsilon_{k,q}^\sigma) + gN_q^\sigma N_q^\downarrow \frac{2g^2}{V^3} \sum_k \int \int \frac{\rho_q^\uparrow(k, \epsilon^\uparrow) \rho_q^\downarrow(-k, \epsilon^\downarrow)}{\epsilon^\uparrow + \epsilon^\downarrow} d\epsilon^\uparrow d\epsilon^\downarrow$$

$$+ \frac{2g^2}{V^3} \sum_{k_1, k_2, q} \frac{n(\epsilon_{k_1,q}^\uparrow) n_{k_2,q}^\downarrow}{\epsilon_{k_1,q}^\uparrow + \epsilon_{k_2,q}^\downarrow - \epsilon_{k_3,q}^\uparrow - \epsilon_{k_4,q}^\downarrow} \delta(k_1 + k_2 - k_3 - k_4)$$

- Modifies the electron dispersion

$$\epsilon_{p,q}^\pm = \frac{\epsilon_{p+q/2} + \epsilon_{p-q/2}}{2} \pm \frac{\sqrt{(\epsilon_{p+q/2} - \epsilon_{p-q/2})^2 + (2g \epsilon m)^2}}{2}$$

- Coefficient of $m^4$ has the same form as $q^2m^2$

$$\rho^\sigma(\mathbf{p}, \epsilon) = \sum_k n(\epsilon_{k+p/2}^\sigma) \left[ 1 - n(\epsilon_{k-p/2}^\sigma) \right] \delta(\epsilon - \epsilon_{k+p/2}^\sigma + \epsilon_{k-p/2}^\sigma)$$
Results

- Uniform ferromagnetic phase with tricritical point
Results

- Textured phase preempted transition with $q=0.1k_F$
Quantum Monte Carlo: Uniform phase

- First order transition into uniform phase
Quantum Monte Carlo: Textured phase

- Textured phase preempted transition with $q=0.2k_F$
Summary

- Transfer from second to first order ferromagnetic transition at low temperature understood through soft transverse magnetic fluctuations.
- Fluctuations responsible for development of nonanalyticities at zero $T$.
- First indications of ferromagnetism in ultracold atom gas.
- First order transition accompanied by textured ferromagnetic phase.
Breakdown of Stoner criterion — MnSi

- MnSi also displays a first order phase transition

Pfleiderer et al., PRB 1997
Cold atomic gases — interactions

- A gas of Fermionic atoms is laser and evaporatively cooled 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\(^1\)

\[ \text{BEC superfluidity of bound molecules} \quad \text{BCS - BEC crossover} \quad \text{BCS superfluidity of Cooper pairs} \]

- Repulsive interactions allow us to investigate itinerant ferromagnetism

Cold atomic gases — spin

- Two fermionic atom species have a *pseudo-spin*:
  
  \[ ^{6}\text{Li} \quad m_F=1/2 \quad \text{maps to} \quad \text{spin } 1/2 \]
  
  \[ ^{6}\text{Li} \quad m_F=-1/2 \quad \text{maps to} \quad \text{spin } -1/2 \]
  
  \[ ^{40}\text{K} \quad m_F=9/2 \quad \text{maps to} \quad \text{spin } 1/2 \]
  
  \[ ^{40}\text{K} \quad m_F=-7/2 \quad \text{maps to} \quad \text{spin } -1/2 \]

- The up-and down spin particles *cannot* interchange — population imbalance is fixed by \(S_z\)

- Ferromagnetism, if favourable, must form in x-y plane
Cold atomic gases — spin

- Two fermionic atom species have a pseudo-spin:

  \[ ^{40}\text{K} \quad m_F=9/2 \quad \text{maps to} \quad \text{spin 1/2} \]

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

- The up-and-down spin particles cannot interchange — population imbalance is fixed. Possible spin states are:

  \[ |\uparrow\uparrow\rangle \quad S=1, \ S_z=1 \quad \text{State not possible as } S_z \text{ has changed} \]

  \[ |\downarrow\downarrow\rangle \quad S=1, \ S_z=-1 \quad \text{State not possible as } S_z \text{ has changed} \]

  \[ (|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle)/\sqrt{2} \quad S=1, \ S_z=0 \quad \text{Magnetic moment in plane} \]

  \[ (|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)/\sqrt{2} \quad S=0, \ S_z=0 \quad \text{Non-magnetic state} \]

- Ferromagnetism, if favourable, must form in plane
Integrating out electron fluctuations

Partition function:

\[ Z = \int D\psi \exp \left( -\int \sum_\sigma \bar{\psi}_\sigma \left( -i \omega + \epsilon - \mu \right) \psi_\sigma - g \int \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right) \]

1) Decouple in both the density (\( \rho \)) and spin (\( \phi \)) channels

\[ Z = \int D\phi D\rho D\psi \exp \left( -g (\phi^2 - \rho^2) - \int \sum_{\alpha,\beta} \bar{\psi}_\alpha \left[ (G_0^{-1} - g \rho) \delta_{\alpha\beta} - g \sigma_{\alpha\beta} \cdot \phi \right] \psi_\beta \right) \]

2) Integrate out electrons

\[ Z = \int D\phi D\rho \exp \left( -g (\phi^2 - \rho^2) - \text{tr} \ln \left[ G_0^{-1} - g \rho - g \sigma \cdot \phi \right] \right) \]
Integrating out magnetisation fluctuations

\[ Z = \int D\phi D\rho \exp \left( -g (\phi^2 - \rho^2) - \text{tr} \ln \left[ G_0^{-1} - g \rho - g \sigma \cdot \phi \right] \right) \]

3) Expand about uniform magnetisation \( m \)

\[ Z = \int D\phi D\rho \exp \left( -g (m^2 + \phi^2 - \rho^2) - \text{tr} \ln \left[ G_0^{-1} - gm\sigma_z - g \rho - g \sigma \cdot \phi \right] \right) \]

4) Expand density and magnetisation fluctuations to second order

\[ Z = \int D\phi D\rho \exp \left( -gm^2 - \text{tr} \ln G^{-1} - \text{tr} \left[ \rho^2 - \phi^2 + \frac{g}{2} G (\rho - \sigma \cdot \phi) G (\rho - \sigma \cdot \phi) \right] \right) \]

5) Integrate out density and magnetisation fluctuations

\[ Z = \exp \left( -gm^2 - \text{tr} \ln G^{-1} - g \text{tr} \Pi_{\uparrow\downarrow} - \frac{g^2}{2} \text{tr} \left[ \Pi_{\uparrow\uparrow} \Pi_{\downarrow\downarrow} + \Pi_{\uparrow\downarrow} \Pi_{\downarrow\uparrow} \right] \right) \]

where \( \Pi_{\alpha\beta} = G_\alpha G_\beta \)
Final expression for the free energy

\[
F = \sum_{\sigma, k} \epsilon_k n_\sigma(\epsilon_k) + gN_\uparrow N_\downarrow
- \frac{2g^2}{V^3} \sum_{k_{1,2,3,4}} n_\uparrow(\epsilon_{k_1}) n_\downarrow(\epsilon_{k_2}) [n_\uparrow(\epsilon_{k_3}) + n_\downarrow(\epsilon_{k_4})] \frac{\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_3} - \epsilon_{k_4}}{\delta(\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_3} - \epsilon_{k_4})}
\]

is identical to second order perturbation theory [Abrikosov 1958, Lee & Yang 1960, Mohling, 1961, Duine & MacDonald, 2005]
Ferromagnetic transition

- Considering the soft transverse magnetic fluctuations drives the transition first order
- Recover the following phase diagram

Uhlarz et al., PRL 2004
In the grand canonical ensemble we obtain...
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 phase transition.
Consequences of fluctuations

- In a similar way we can expand the energy in magnetisation to second order to account for fluctuations

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

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

- The coupling of fields\(^1\) can drive a transition first order

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

\(^1\)Rice 1954, Garland & Renard 1966, Larkin & Pikin 1969
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.
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 $\nu(E)$ changes rapidly with energy then a ferromagnetic transition is favourable when [Binz et al. EPL 2004]

$$\nu \nu'' > 3(\nu')^2$$
Improved Wohlfarth Rhodes criterion

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

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

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

- 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>$0.0k_Fa + 0.0086(k_Fa)^2$</td>
</tr>
<tr>
<td>$4\varepsilon^{(0,3)}(u, 0)$</td>
<td>$0.0k_Fa - 0.04(k_Fa)^2$</td>
</tr>
<tr>
<td>$6\varepsilon^{(1,2)}(u, 0)$</td>
<td>$0.024(k_Fa)^2$</td>
</tr>
<tr>
<td>$4\varepsilon^{(2,1)}(u, 0)$</td>
<td>$0.0(k_Fa)^2$</td>
</tr>
<tr>
<td>$\varepsilon^{(3,0)}(u, 0)$</td>
<td>$2^{-3/2}/27 - 0.0055(k_Fa)^2$</td>
</tr>
</tbody>
</table>

Transition due to changing energy spectrum at the Fermi surface
**NbFe$_2$**

- NbFe$_2$ displays antiferromagnetic order where it is expected to be ferromagnetic — could this be a textured ferromagnetic phase?

Crook & Cywinski, JMMM 1995
MnSi

• MnSi displays non-Fermi liquid behaviour consistent with a spin state (though in a non-centrosymmetric crystal)

Pfleiderer et al., Nature 2004
MnSi displays non-Fermi liquid behaviour consistent with a spin state (though in a non-centrosymmetric crystal)
**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
Previous analytical work

- 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., PRL 2006
- Previous spin-spiral state studies:
  - Rech et al., PRB 2006, Belitz et al., PRB 1997
  - Lattice driven reconstruction – Berridge et al. PRL 2009
Approach to textured phase

- Homogeneous strategy:
  1) Decouple in both the density and spin channels
  2) Integrate out electrons
  3) Expand about uniform magnetisation
  4) Expand magnetisation and density fluctuations to second order
  5) Integrate out density and magnetisation fluctuations

- Textured strategy:
  1) **Gauge transform electrons**
  2) Decouple in both the density and spin channels
  3) Integrate out electrons
  4) Expand about textured magnetisation to second order
  5) Expand magnetisation and density fluctuations to second order
  6) Integrate out density and magnetisation fluctuations
Gauge transformation

- **Partition function**

\[
Z = \int D\psi \exp\left( -\int \sum_\sigma \bar{\psi}_\sigma (-i\omega + \epsilon - \mu) \psi_\sigma - g \int \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right)
\]

1) **Gauge transform electrons**

- Make the mapping of the fermions
  \[
  \psi \rightarrow e^{\frac{1}{2}i \mathbf{q} \cdot \mathbf{r}_\sigma} \psi
  \]

- Renders magnetisation \( m\sigma_x \) uniform with a spin dependent dispersion

\[
Z = \int D\phi D\rho \exp\left( -g (\phi^2 - \rho^2) - \text{tr} \ln \left[ \begin{pmatrix} i\omega + \epsilon_{p+q/2} - \mu & gm \\ gm & i\omega + \epsilon_{p-q/2} - \mu \end{pmatrix} - g\rho - g\sigma \cdot \phi \right] \right)
\]

- Diagonalisation gives the energies relative to a spiral

\[
\epsilon_{p,q}^\pm = \frac{\epsilon_{p+q/2} + \epsilon_{p-q/2}}{2} \pm \frac{\sqrt{(\epsilon_{p+q/2} + \epsilon_{p-q/2})^2 + (2gm)^2}}{2}
\]

which replaces \( \epsilon_p \pm gm \) in the uniform case

- Analysis then proceeds as before
Quantum Monte Carlo

- Ran \textit{ab initio} Quantum Monte Carlo calculations on the system using the CASINO program

- After a gauge transformation used the non-collinear trial wave function

\[
e^{-J(R)}\det\left( \begin{pmatrix} \psi_{k\in k_{F\uparrow}} & \bar{\psi}_{k\in k_{F\uparrow}} \end{pmatrix} \right)
\]

\[
\psi_{k\in k_{F\uparrow}} = \begin{pmatrix} \cos[\theta/2]\exp[i(k-q/2)\cdot r] \\ \sin[\theta/2]\exp[i(k+q/2)\cdot r] \end{pmatrix} \quad \bar{\psi}_{k\in k_{F\uparrow}} = \begin{pmatrix} -\sin[\theta/2]\exp[-i(k-q/2)\cdot r] \\ \cos[\theta/2]\exp[-i(k+q/2)\cdot r] \end{pmatrix}
\]

- Single determinant not exact spin eigenstate in finite sized system

\[
\langle \hat{S}_\perp, \text{RMS} \rangle \approx \langle \hat{S} \rangle / \sqrt{n_\uparrow + n_\downarrow} \ll \langle \hat{S} \rangle
\]

- Planar spin spiral at $\theta=\pi/2$

- Optimisable Jastrow factor $J(R)$ accounts for electron correlations