# Inhomogeneous phase formation on the border of itinerant ferromagnetism



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# **Breakdown of Stoner criterion — ZrZn<sub>2</sub>**

• At low temperature and high pressure ZrZn<sub>2</sub> has a first order transition



Uhlarz *et al.*, PRL 2004

# **Breakdown of Stoner criterion**

• Generic phase diagram of the itinerant ferromagnet



- Two explanations of first order phase behaviour:
  - (1) Lattice-driven peak in the density of states (Pfleiderer *et al.* PRL 2002, Sandeman *et al.* PRL 2003)

(2) Transverse quantum fluctuations (Belitz et al. Z. Phys. B 1997)

# **Fluctuation corrections**

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

Integrate over fluctuations in magnetization and density and develop a perturbation theory in interaction strength

$$F = F_0 + \frac{1 - gv}{2v}m^2 + um^4 + vm^6 + g^2 (rm^2 + wm^4 \ln|m|) \qquad k_F a_{crit} = 1.05$$

• First order transition<sup>1</sup>

#### Results

• First order ferromagnetic phase transition



#### **Quantum Monte Carlo verification**



# **Textured order parameter**

1/q

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

- Gauge transformation brings textured phase to uniform order parameter
- Coefficient of m<sup>4</sup> has the same form as q<sup>2</sup>m<sup>2</sup>  $F = F_0 + rm^2 + um^4 + vm^6 + \frac{uk_F^2}{24\pi^2 a^2} q^2 m^2$
- Tricritical point accompanied by textured phase

Belitz *et al*. Rev. Mod. Phys. (2005) Betouras *et al*. PRB (2005)

#### Results

Textured phase preempts transition



## **Quantum Monte Carlo: textured phase**

• QMC verifies presence of textured phase

0

0.8



 $k_{\rm F}a$ 

0.9

0.85

# Summary

- Soft transverse magnetic fluctuations drive the ferromagnetic transition first order
- Textured phase preempts ferromagnetic transition
- Verification with Quantum Monte Carlo
- First observation of itinerant ferromagnetism in ultracold atom gases [Jo *et al.* Science **325**, 1521 (2009), Conduit & Simons, Phys. Rev. Lett. **103**, 200403 (2009)] – see session Y31

# **Condensation of topological defects**

 Defects freeze out from disordered state

- Defect annihilation hinders the formation of the ferromagnetic phase thus raising the required interaction strength
- Defect radius L ~ t<sup>1/2</sup> [Bray, Adv. Phys. 43, 357 (1994)]



# **Condensation of topological defects**

Condensation of defects inhibits the transition



Conduit & Simons, Phys. Rev. Lett. 103, 200403 (2009)

#### First order phase transition and Quantum Monte Carlo verification

First order transition into uniform phase with TCP



• QMC also sees first order transition



#### Summary of equilibrium results



#### **Momentum distribution**



# 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 order5) Integrate out density and magnetisation fluctuations
- Aim to uncover connection to second order perturbation theory
- Unravel origin of logarithmic divergence in energy and relation to tricritical point structure

## **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  $m = \overline{\psi}_{\downarrow} \psi_{\uparrow} \overline{\psi}_{\uparrow} \psi_{\downarrow}$ gives  $F \propto (1 - g \nu) m^2$  i.e. the Stoner criterion

#### **Quantum Monte Carlo verification**

• First order transition into uniform phase with TCP



QMC also sees first order transition



# Cold atomic gases — spin

- Two fermionic atom species have a *pseudo-spin*:
  - <sup>6</sup>Li  $m_{\rm F}=1/2$  maps to spin 1/2
  - <sup>6</sup>Li  $m_{\rm F} = -1/2$  maps to spin -1/2
- The up-and down spin particles *cannot* interchange population imbalance is fixed. Possible spin states are:
  - $$\begin{split} |\uparrow\uparrow\rangle & S=1, S_z=1 & \text{State not possible as } S_z \text{ has changed} \\ |\downarrow\downarrow\rangle & S=1, S_z=-1 & \text{State not possible as } S_z \text{ has changed} \\ (|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle)/\sqrt{2} & S=1, S_z=0 & \text{Magnetic moment in plane} \\ (|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)/\sqrt{2} & S=0, S_z=0 & \text{Non-magnetic state} \end{split}$$
- Ferromagnetism, if favourable, must form in-plane

# **Particle-hole perspective**

To second order in g the free energy is  $F = \sum_{\sigma,k} \epsilon_k^{\sigma} n(\epsilon_k^{\sigma}) + g N^{\uparrow} N^{\downarrow}$   $- \frac{2g^2}{V^3} \sum_p \int \int \frac{\rho^{\uparrow}(p,\epsilon_{\uparrow})\rho^{\downarrow}(-p,\epsilon_{\downarrow})}{\epsilon_{\uparrow} + \epsilon_{\downarrow}} d\epsilon_{\uparrow} d\epsilon_{\downarrow}$   $+ \frac{2g^2}{V^3} \sum_{k_{1,2,3,4}} \frac{n(\epsilon_{k_1}^{\uparrow})n(\epsilon_{k_2}^{\downarrow})}{\epsilon_{k_1}^{\uparrow} + \epsilon_{k_2}^{\downarrow} - \epsilon_{k_3}^{\downarrow}} \delta(k_1 + k_2 - k_3 - k_3)$ 



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

$$\rho^{\sigma}(\boldsymbol{p},\boldsymbol{\epsilon}) = \sum_{\boldsymbol{k}} n(\boldsymbol{\epsilon}_{\boldsymbol{k}+\boldsymbol{p}/2}^{\sigma}) \Big[ 1 - n(\boldsymbol{\epsilon}_{\boldsymbol{k}-\boldsymbol{p}/2}^{\sigma}) \Big] \delta \Big[ \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{k}+\boldsymbol{p}/2}^{\sigma} + \boldsymbol{\epsilon}_{\boldsymbol{k}-\boldsymbol{p}/2}^{\sigma} \Big]$$

- Enhanced particle-hole phase space at zero magnetisation drives transition first order
- Recover  $m^4 \ln m^2$  at T=0
- Links quantum fluctuation to second order perturbation approach<sup>1</sup>
  <sup>1</sup>Abrikosov 1958 & Duine & MacDonald 2005

# **Quantum Monte Carlo: Textured phase**

• Textured phase preempted transition with  $q=0.2k_{\text{F}}$ 

**T=0** 

#### **Modified collective modes**

Collective mode dispersion

$$\Omega = \frac{q^2}{2} \left( 1 - \frac{2^{5/3} 3}{5k_{\rm F}a} \frac{1}{1 + \tilde{\lambda}^2/(k_{\rm F}a)^2} \right)$$

Collective mode damping

$$\Gamma = \frac{q^2}{2} \frac{2^{5/3} 3\tilde{\lambda}}{5(k_{\rm F}a)^2} \frac{1}{1 + \tilde{\lambda}^2/(k_{\rm F}a)^2}$$