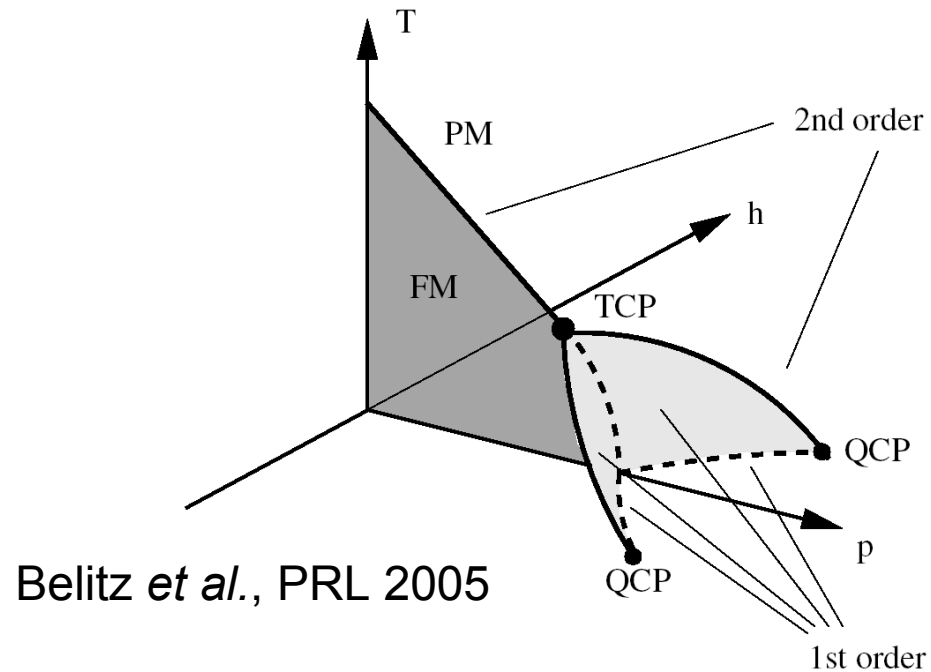


Itinerant ferromagnetism: A quantum fluctuation driven FFLO analogue



Gareth Conduit¹, Andrew Green², Ben Simons¹

1. University of Cambridge

2. University of St Andrews

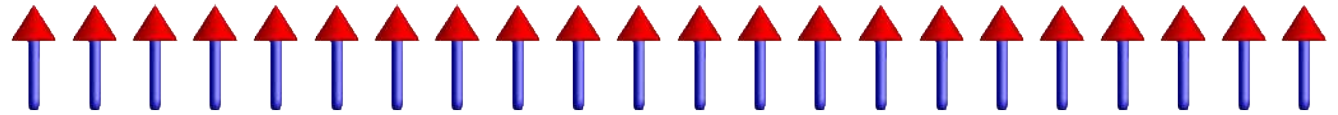
Itinerant ferromagnetism in an atomic Fermi gas: Influence of population imbalance

G.J. Conduit & B.D. Simons, Phys. Rev. A 79, 053606 (2009)

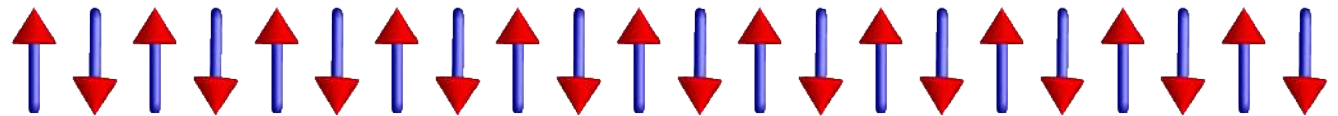
Two types of ferromagnetism

- *Localised ferromagnetism*: moments confined in real space

Ferromagnet

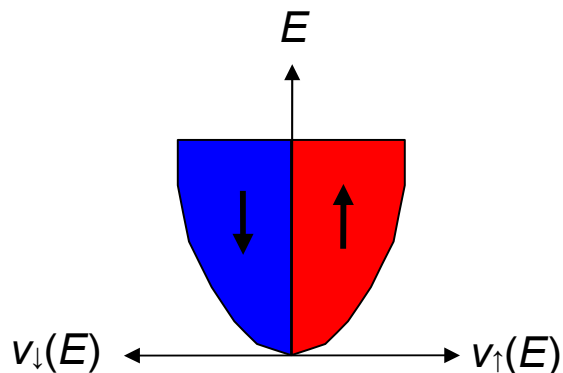


Antiferromagnet

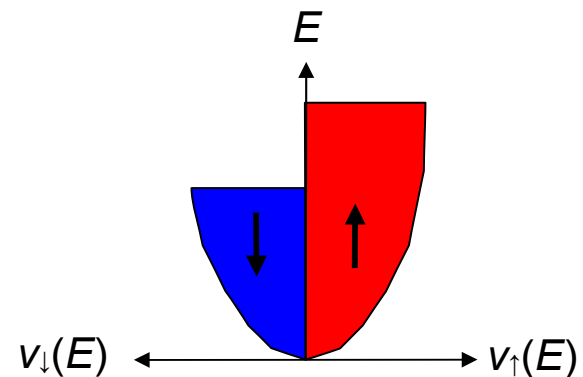


- *Itinerant ferromagnetism*: electrons in Bloch wave states

Not magnetised



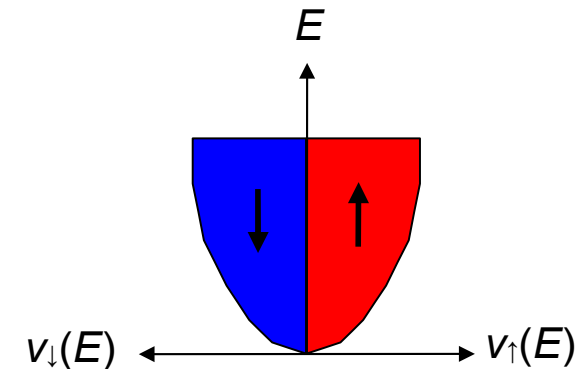
Partially magnetised



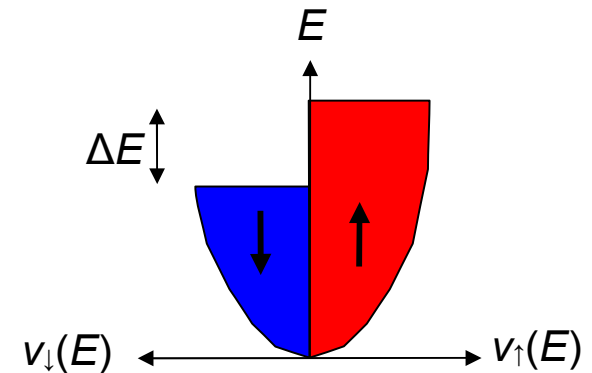
Stoner model for itinerant ferromagnetism

- Repulsive interaction energy $U=gn_{\uparrow}n_{\downarrow}$
- A ΔE shift in the Fermi surface causes:
 - (1) Kinetic energy increase of $\frac{1}{2}v\Delta E^2$
 - (2) 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 $gv>1$

Not magnetised



Partially magnetised



Ferromagnetism in iron and nickel

- The Stoner model predicts a *second order* transition

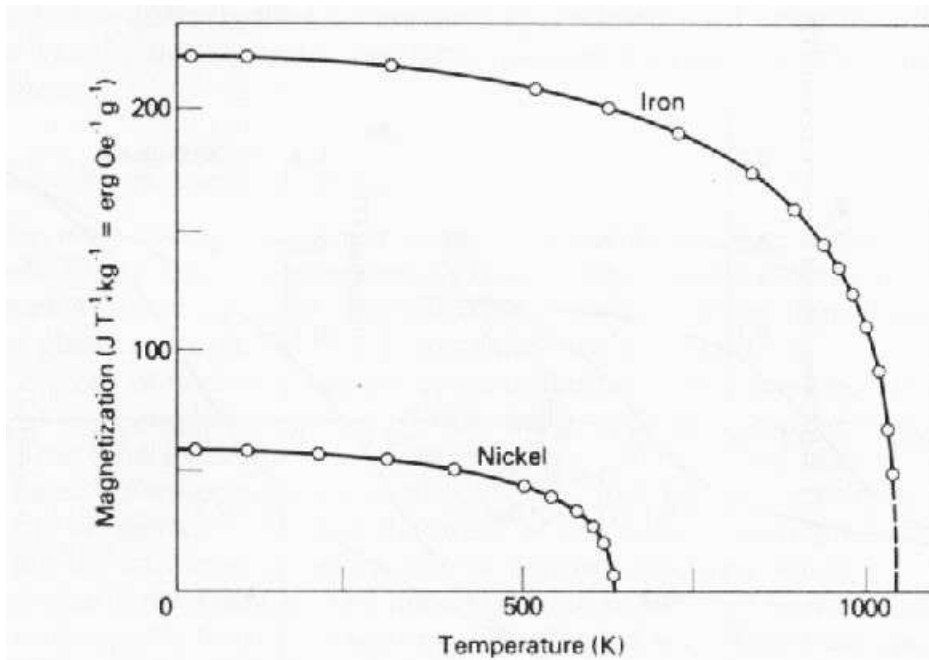


Figure 1.2 Spontaneous magnetization plotted against temperature for iron and nickel.

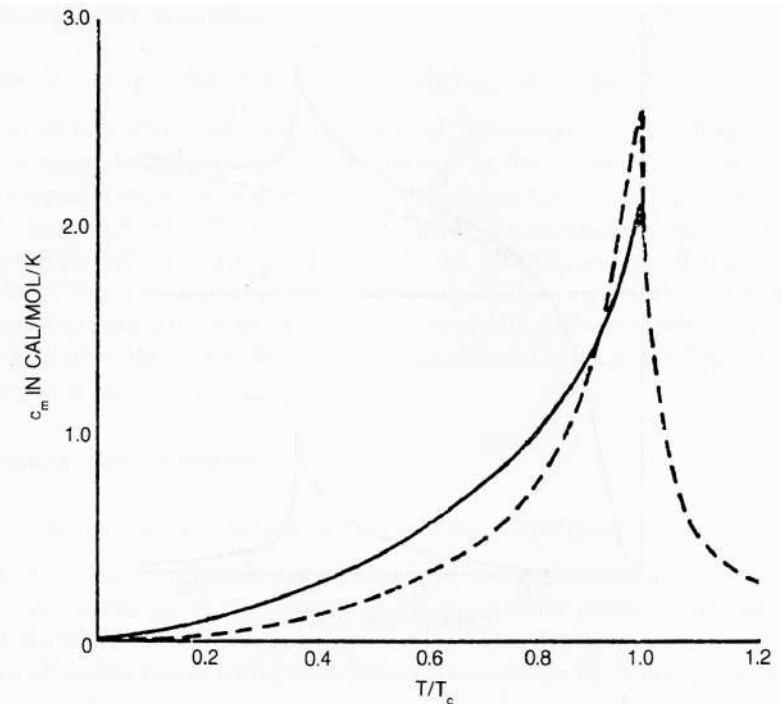
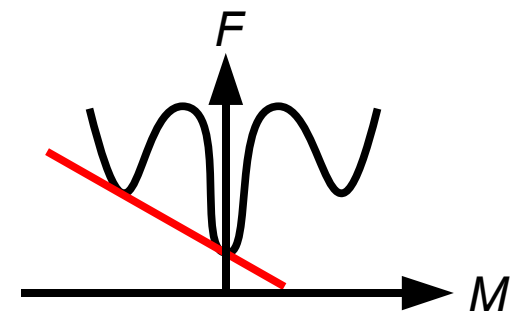
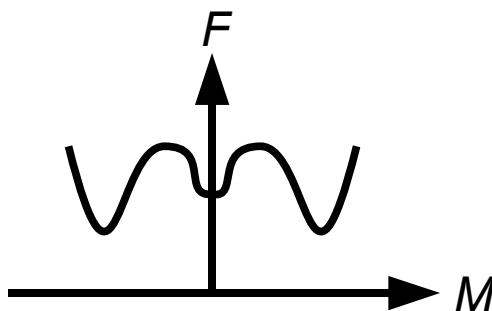
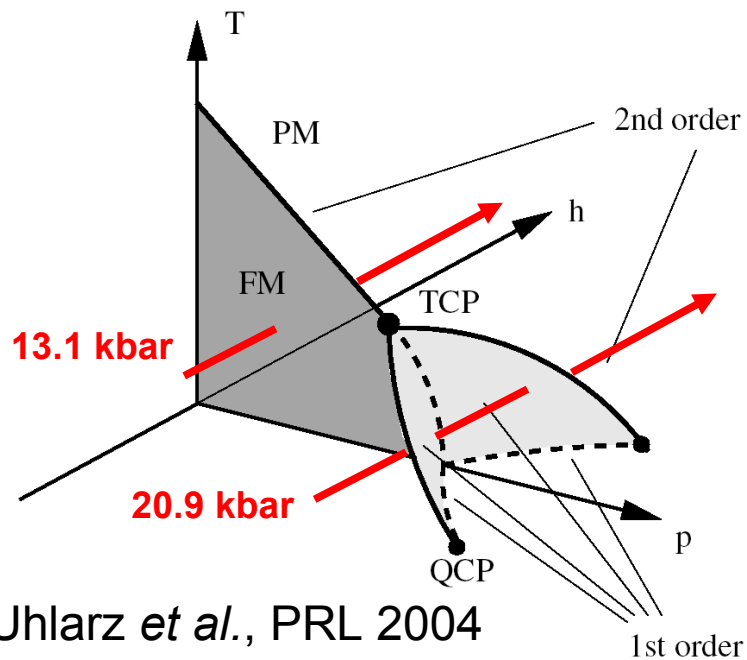
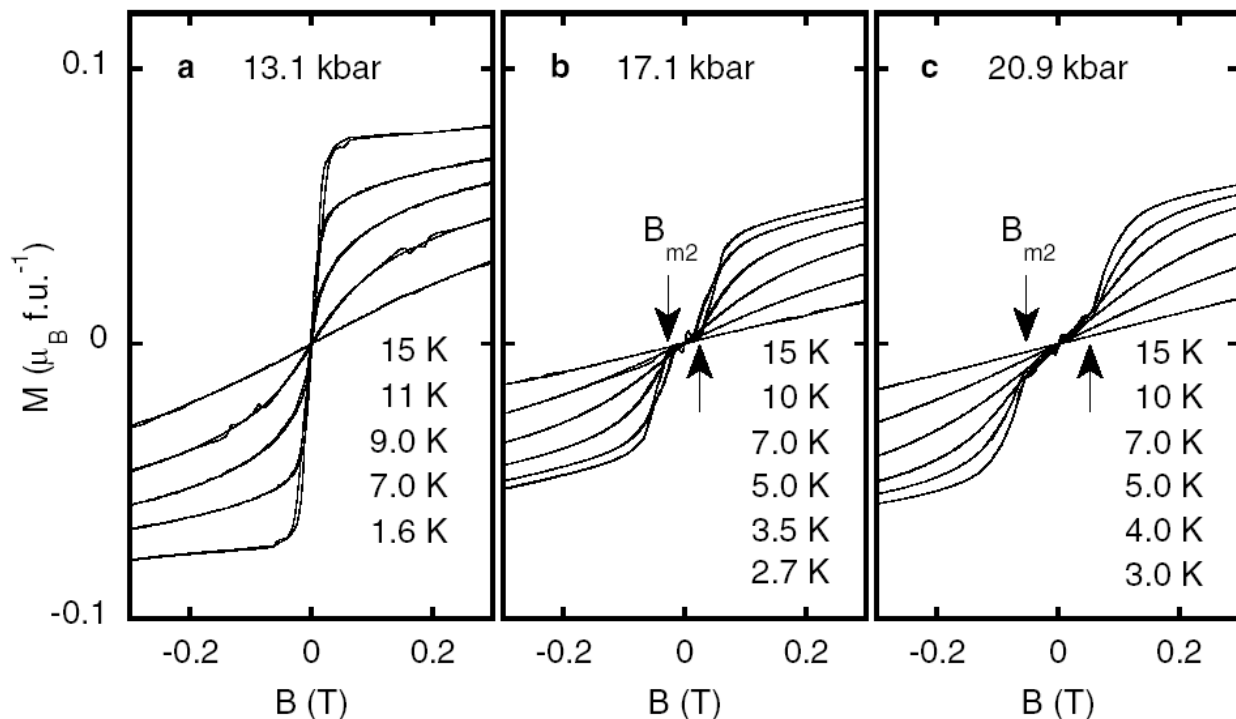
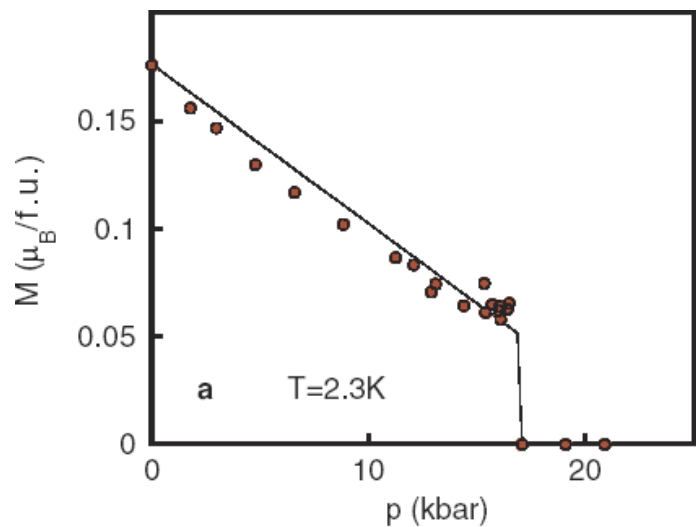


Fig. 9.20 Specific heat anomaly for nickel at its Curie point compared with the theoretical prediction.

that is characterised by a divergence of length-scales (peaked heat capacity and susceptibility)

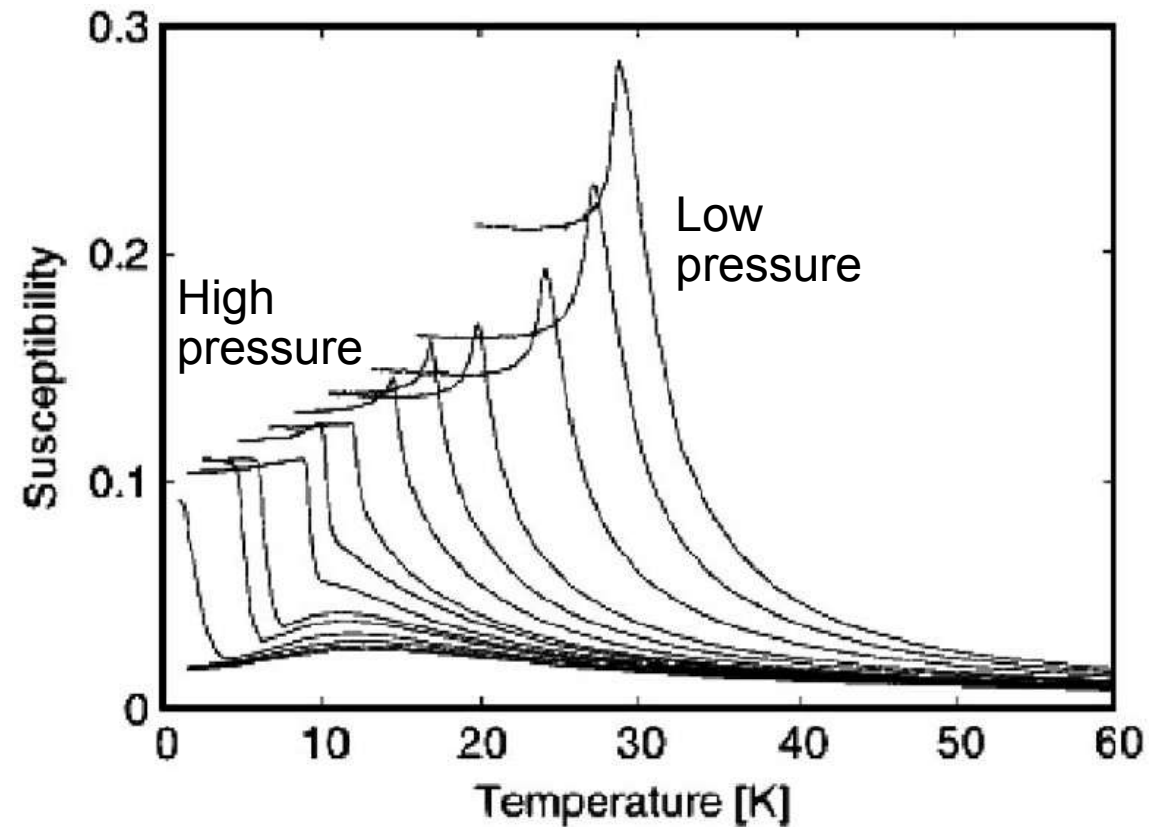
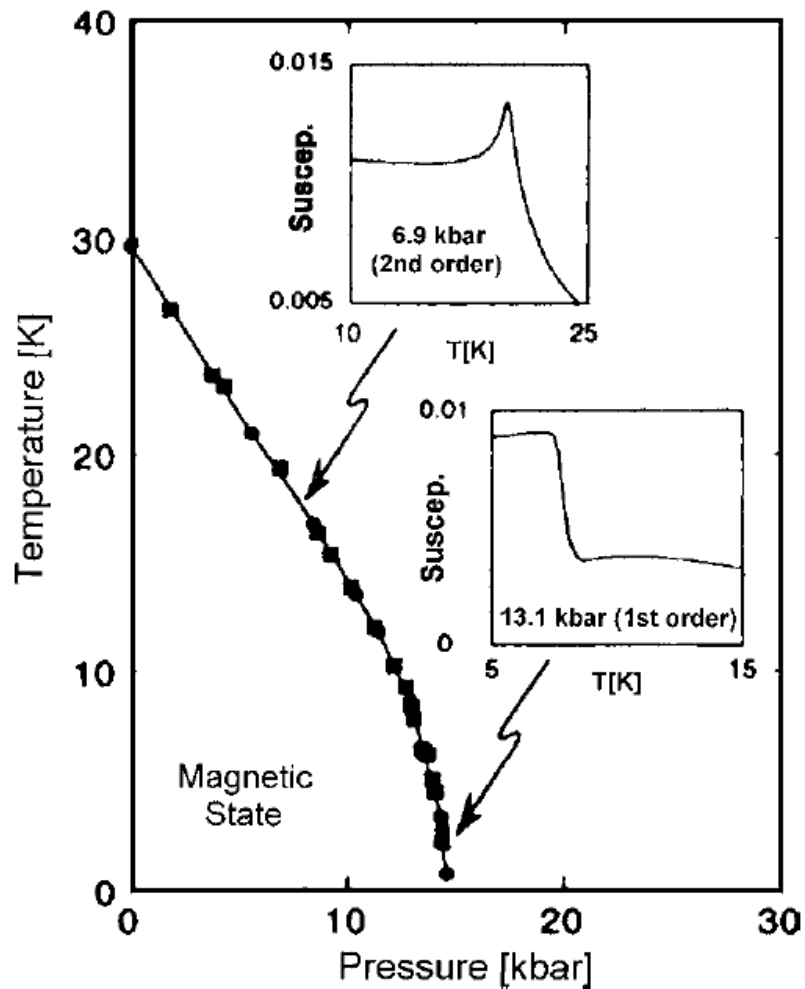
Breakdown of Stoner criterion — ZrZn₂

- At low temperature and high pressure ZrZn₂ has a first order transition



Breakdown of Stoner criterion — MnSi

- MnSi also displays a first order phase transition



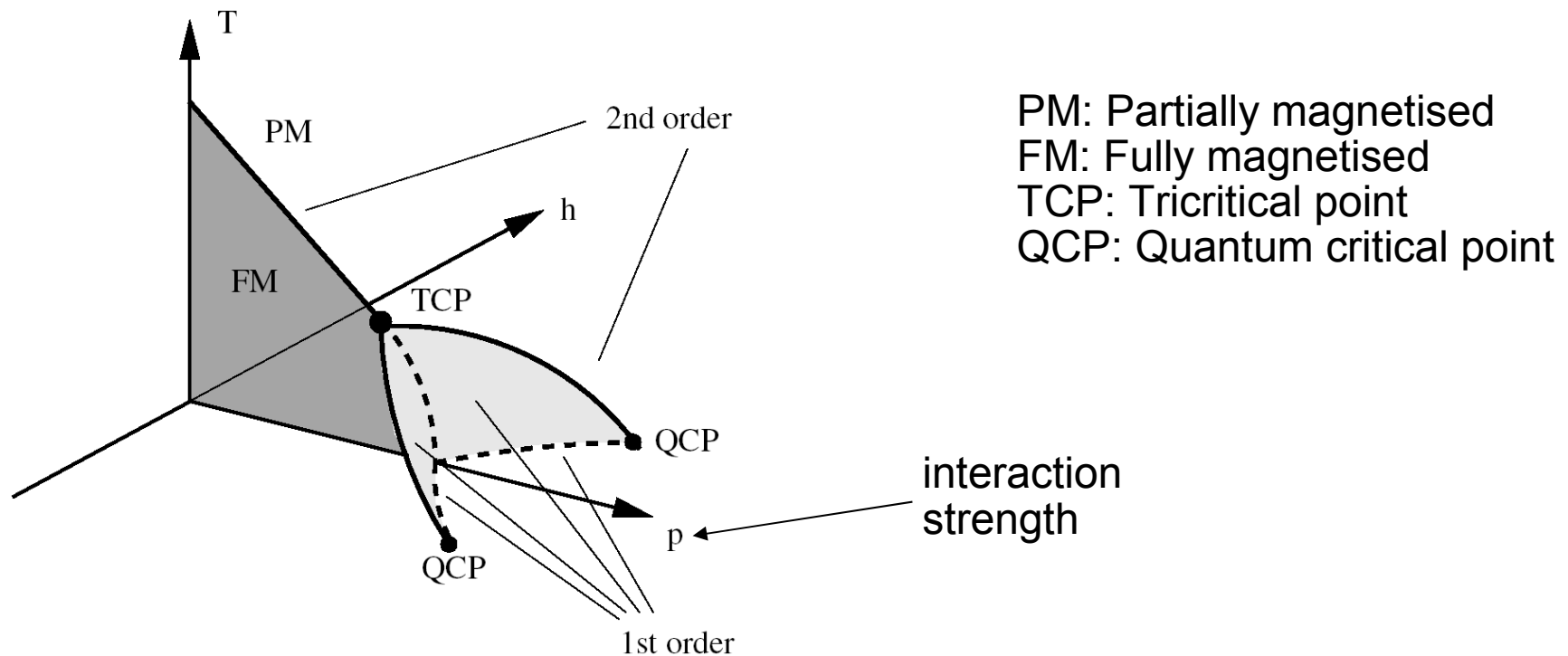
Pfleiderer *et al.*, PRB 1997

Pfleiderer *et al.*, PRB 1997

Vojta *et al.*, 1999 Ann. Phys. 1999

Breakdown of Stoner criterion

- Generic phase diagram of the first order transition



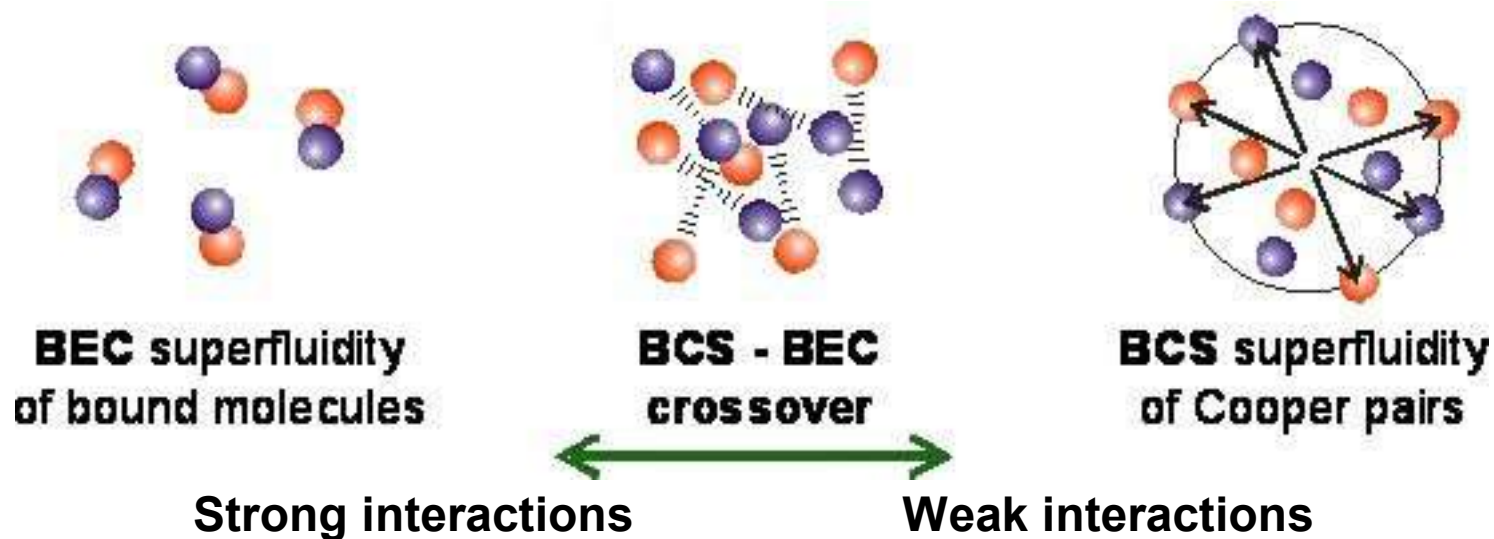
- Two explanations of first order behaviour:

(1) Lattice-driven peak in the density of states
(Pfleiderer *et al.* PRL 2002, Sandeman *et al.* PRL 2003)

(2) Transverse quantum fluctuations

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 regime¹

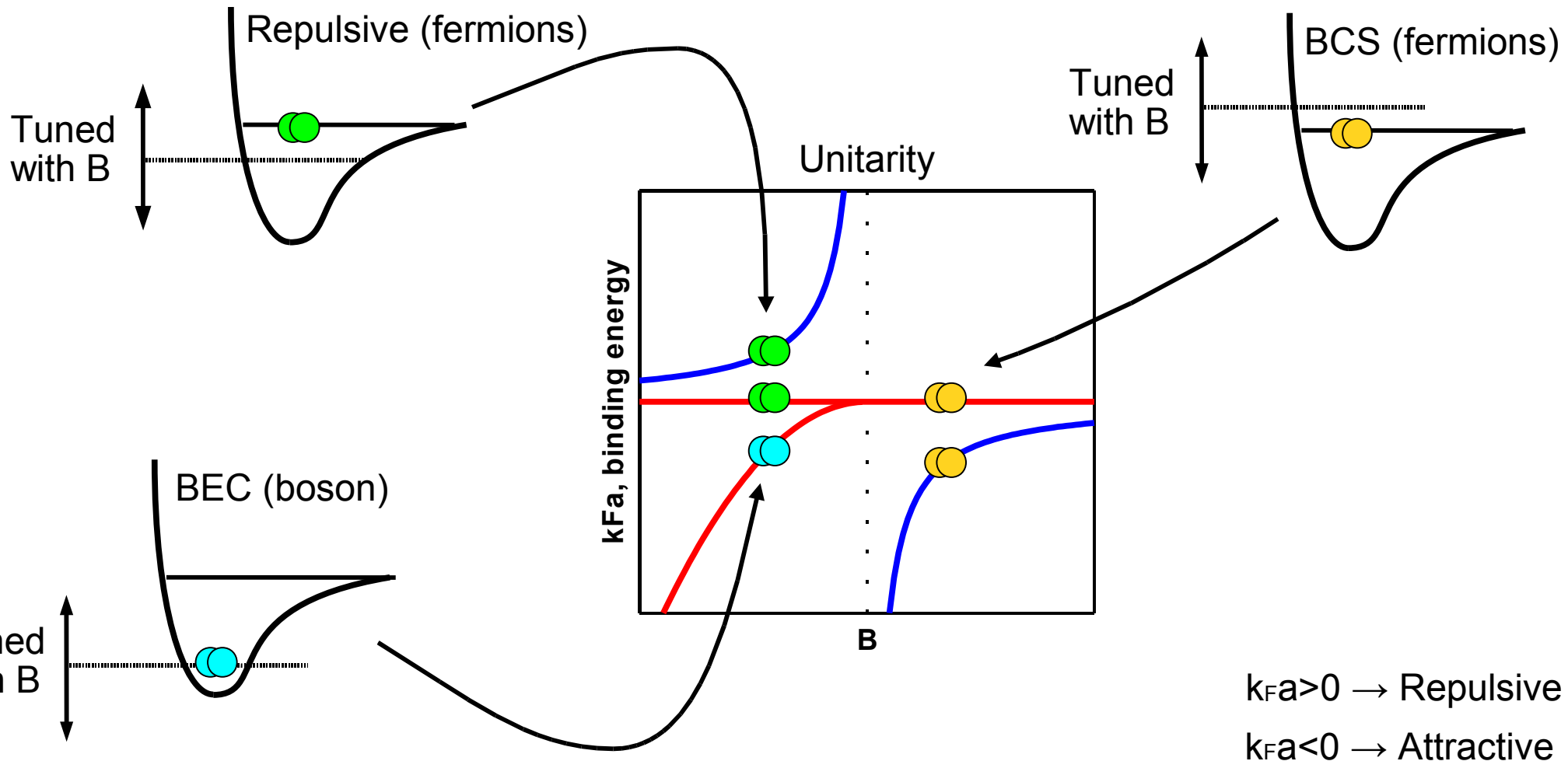


- Repulsive interactions allow us to investigate itinerant ferromagnetism

¹Lofus *et al.* PRL 2002, O'Hara *et al.* Science 2002, Bourdel *et al.* PRL 2003

Feshbach resonance

- Control the relative energy level of the states with a magnetic field



Cold atomic gases — spin

- Two fermionic atom species have a *pseudo-spin*:

^{40}K $m_F=9/2$ maps to spin 1/2

^{40}K $m_F=7/2$ maps to spin -1/2

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

$|\uparrow\uparrow\rangle$ $S=1, S_z=1$ 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

Outline of uniform analysis

- Survey previous analytical work on itinerant ferromagnetism
- Outline how calculation proceeds
- Demonstrate physical origin of first order transition
- Analyse population imbalance in cold atom gas
- Employ phenomenology to study putative textured phase

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

$$F \propto (1 - gv) m^2$$

i.e. the Stoner criterion

- The coupling of fields¹ can drive a transition first order

$$\begin{aligned} & rm^2 + um^4 + a\phi^2 \pm 2am^2\phi \\ &= rm^2 + (u - a)m^4 + a(\phi \pm m^2)^2 \\ &= rm^2 + (u - a)m^4 \end{aligned}$$

¹Rice 1954, Garland & Renard 1966, Larkin & Pikin 1969

Extension to Hertz-Millis

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

$$F = \frac{1}{2} \left(|\omega| / \Gamma_q + r + q^2 \right) \phi^2 + \frac{u}{4} \phi^4 + \frac{v}{6} \phi^6 - h \phi$$

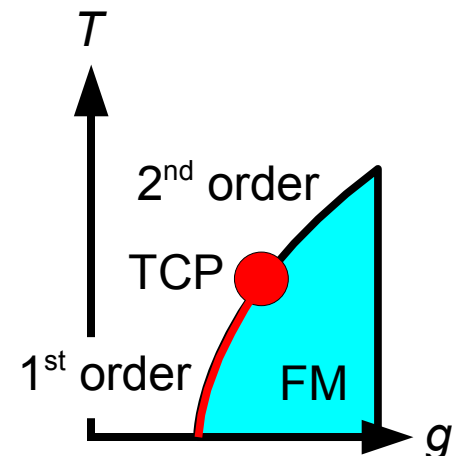
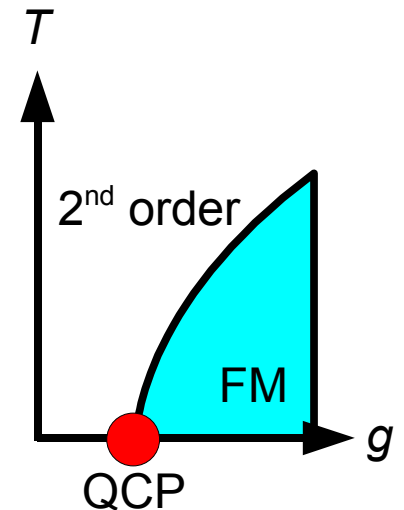
- Belitz-Kirkpatrick-Vojta (soft particle-hole & magnetisation) [Belitz *et al.* Z. Phys. B 1997]

$$F = \frac{1}{2} \left(|\omega| / \Gamma_q + r + q^2 \right) \phi^2 + \frac{u}{4} \phi^4 \ln(\phi^2 + T^2) + \dots - h \phi$$

- Chubukov-Pepin-Rech approach [Rech *et al.* 2006]

- Second order perturbation theory [Abrikosov 1958 & Duine & MacDonald 2005]

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



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
- Aim to uncover connection to second order perturbation theory
- Unravel origin of logarithmic divergence in energy and relation to tricritical point structure
- Examine textured phase

Integrating out electron fluctuations

- Partition function:

$$Z = \int D\psi \exp\left(-\int \sum_{\sigma} \bar{\psi}_{\sigma} \underbrace{(-i\omega + \epsilon - \mu)}_{G_0^{-1}} \psi_{\sigma} - g \int \bar{\psi}_{\uparrow} \bar{\psi}_{\downarrow} \psi_{\downarrow} \psi_{\uparrow}\right)$$

- 1) Decouple in both the density (ρ) and spin (ϕ) channels

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

- 2) Integrate out electrons

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

Integrating out magnetisation fluctuations

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

3) Expand about uniform magnetisation m

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

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

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

where $\Pi_{\alpha\beta} = G_\alpha G_\beta$

Result

- Final expression for the free energy

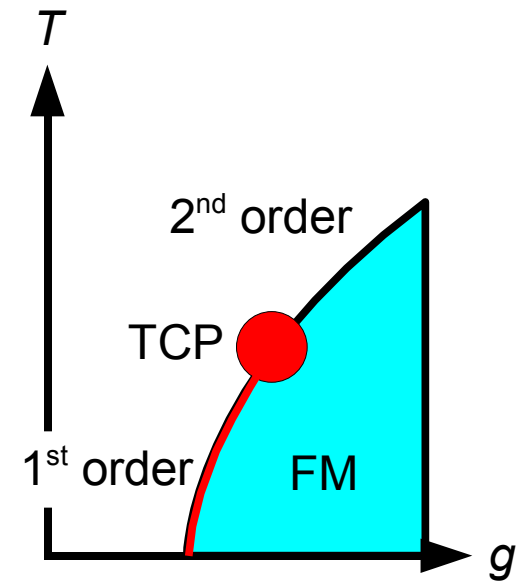
$$F = \sum_{\sigma, k} \epsilon_k n_{\sigma}(\epsilon_k) + gN_{\uparrow}N_{\downarrow} - \frac{2g^2}{V^3} \sum_{k_{1,2,3,4}} \frac{n_{\uparrow}(\epsilon_{k_1})n_{\downarrow}(\epsilon_{k_2})[n_{\uparrow}(\epsilon_{k_3})+n_{\downarrow}(\epsilon_{k_4})]}{\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_3} - \epsilon_{k_4}} \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)$$

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

Particle-hole perspective

- The free energy is

$$\begin{aligned}
 F = & \sum_{\sigma, k} \epsilon_k n_{\sigma}(\epsilon_k) + g N_{\uparrow} N_{\downarrow} \\
 & - \frac{2g^2}{V^3} \sum_q \int \int \frac{\rho_{\uparrow}^{\text{ph}}(\mathbf{q}, \epsilon_{\uparrow}) \rho_{\downarrow}^{\text{ph}}(-\mathbf{q}, \epsilon_{\downarrow})}{\epsilon_{\uparrow} + \epsilon_{\downarrow}} d\epsilon_{\uparrow} d\epsilon_{\downarrow} \\
 & + \frac{2g^2}{V^3} \sum_{k_{1,2,3,4}} \frac{n_{\uparrow}(\epsilon_{k_1}) n_{\downarrow}(\epsilon_{k_2})}{\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_3} - \epsilon_{k_4}} \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)
 \end{aligned}$$



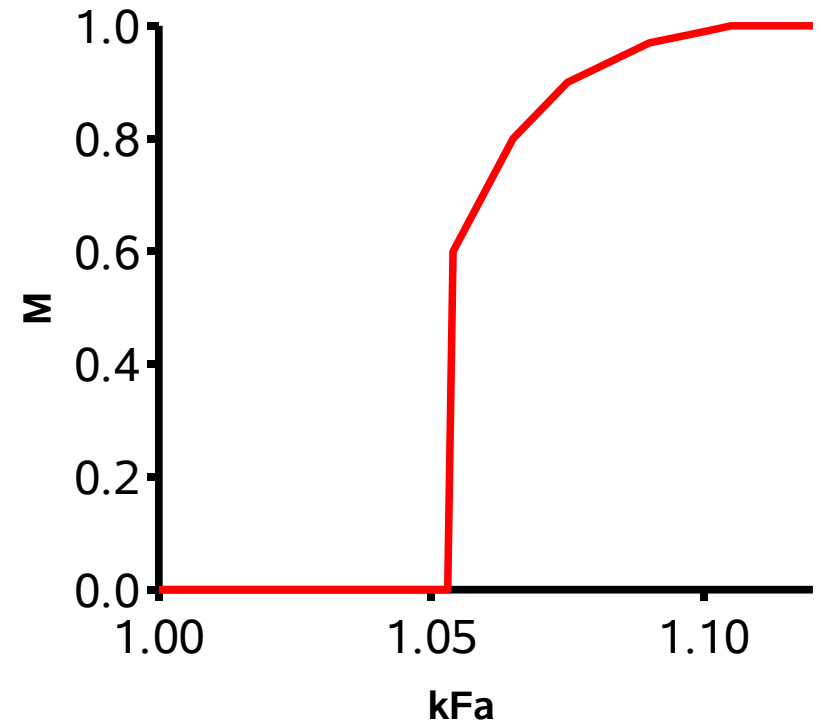
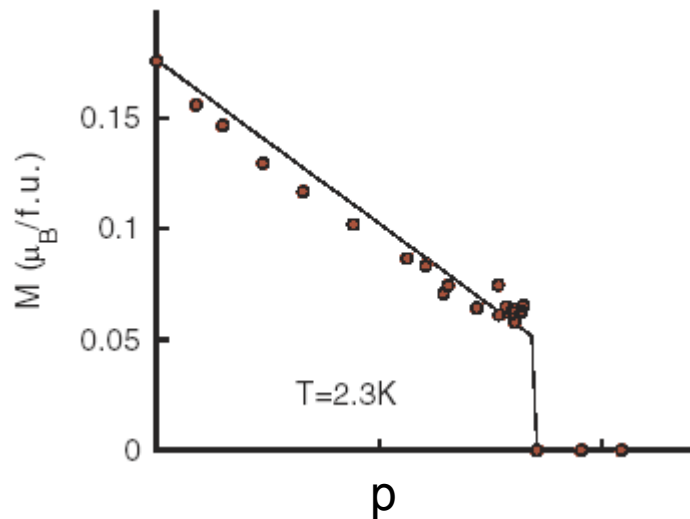
with a particle-hole density of states

$$\rho_{\sigma}^{\text{ph}}(\mathbf{q}, \epsilon) = \sum_k n(\epsilon_{\mathbf{k}+\mathbf{q}/2}^{\sigma}) \left[1 - n(\epsilon_{\mathbf{k}-\mathbf{q}/2}^{\sigma}) \right] \delta(\epsilon - \epsilon_{\mathbf{k}+\mathbf{q}/2}^{\sigma} + \epsilon_{\mathbf{k}-\mathbf{q}/2}^{\sigma})$$

- 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

Ferromagnetic transition

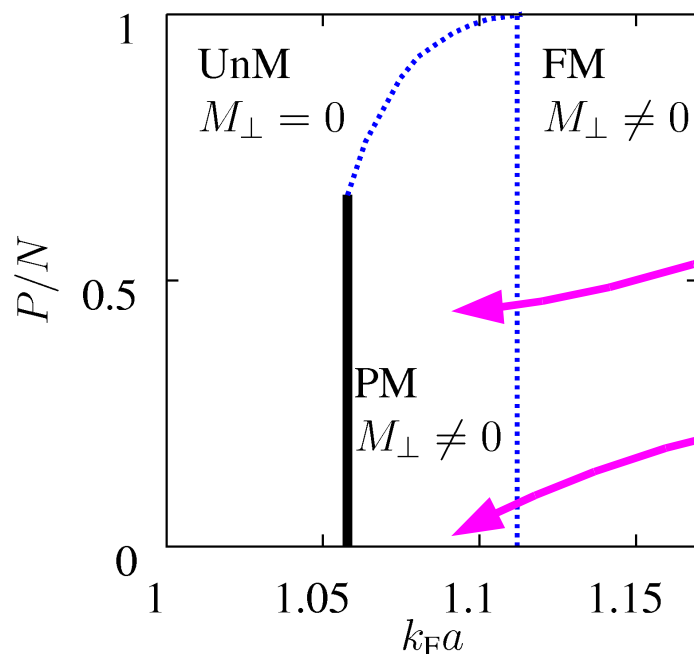
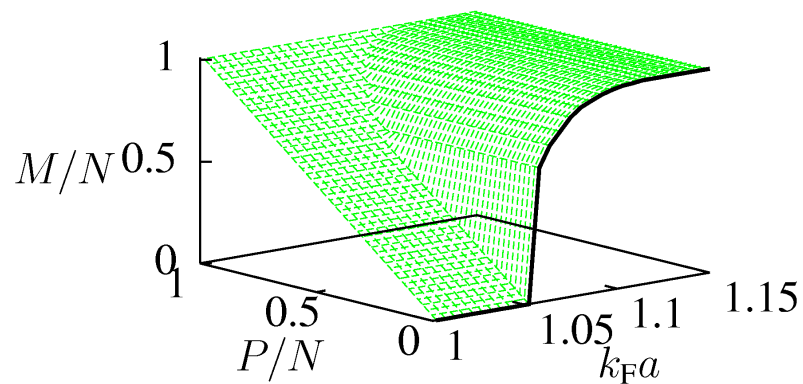
- Considering the soft transverse magnetic fluctuations drives the transition first order
- Recover the following phase diagram



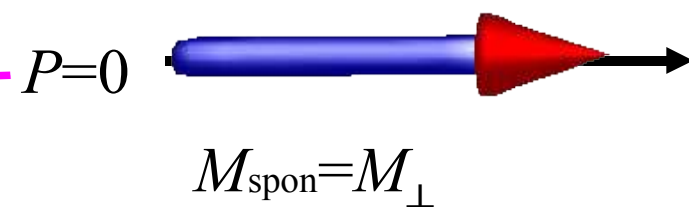
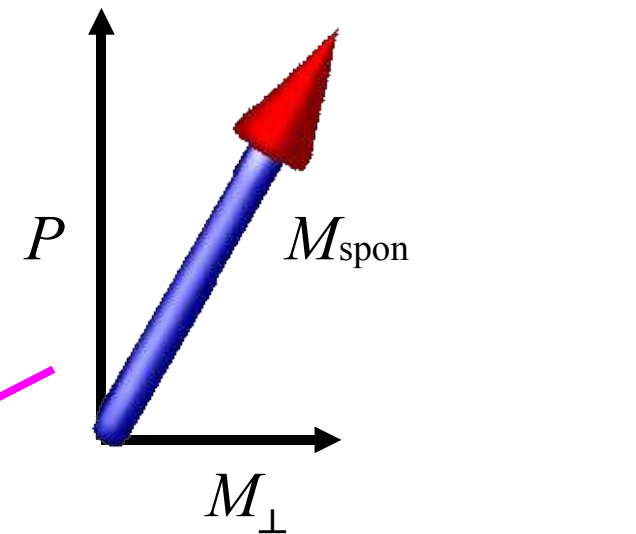
Uhlarz *et al.*, PRL 2004

Population imbalanced case

- Phase diagram with population imbalance P in the canonical regime

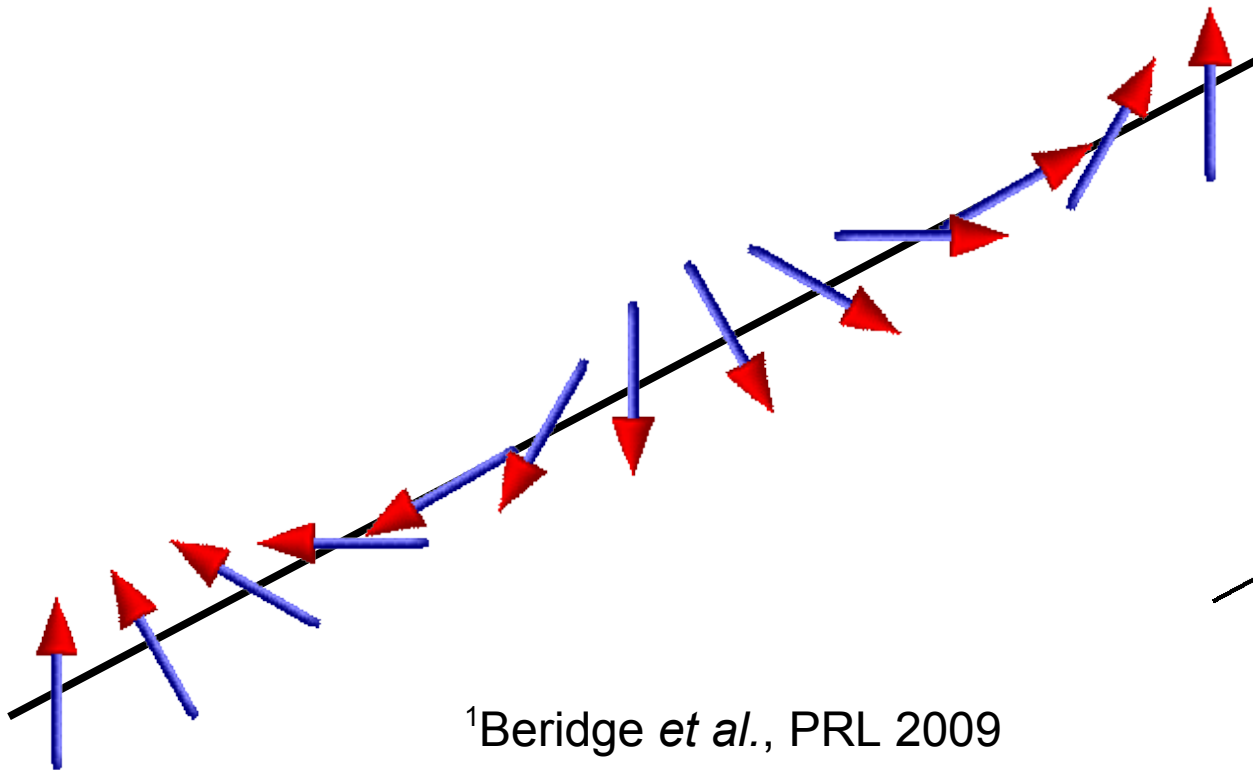


UnM: Unmagnetised
 PM: Partially magnetised
 FM: Fully magnetised

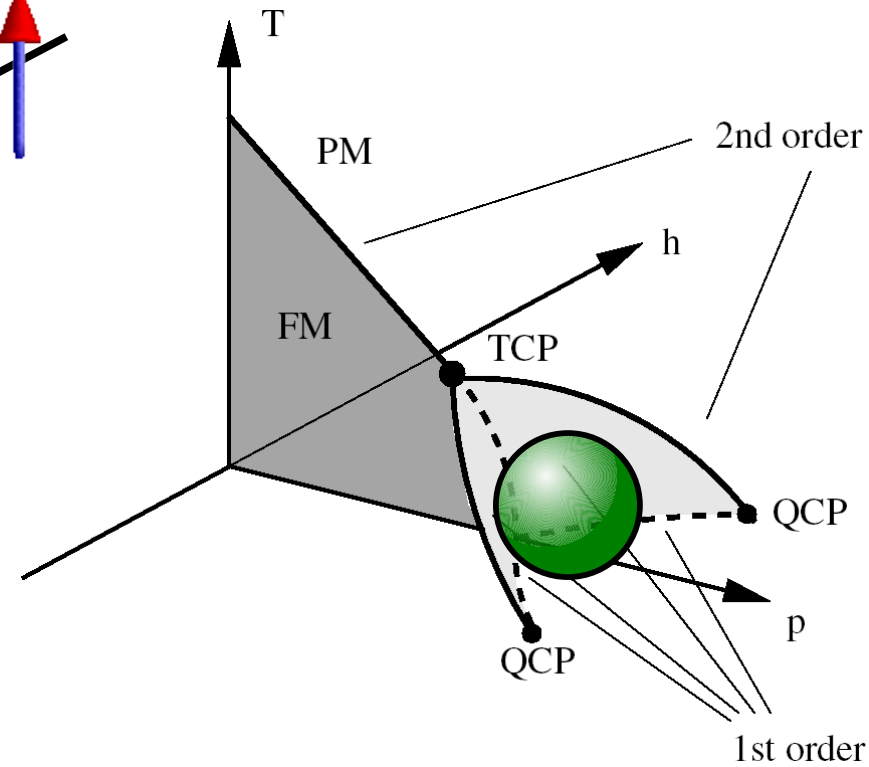


Summary of uniform work

- Extended Hertz-Millis by considering particle-hole, magnetisation and density fluctuations, revealing a first order phase transition
- Motivated by Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) and experiment now examine a putative textured ferromagnetic phase
- Lattice-driven mechanism¹ could give rise to texture, now consider a quantum driven mechanism

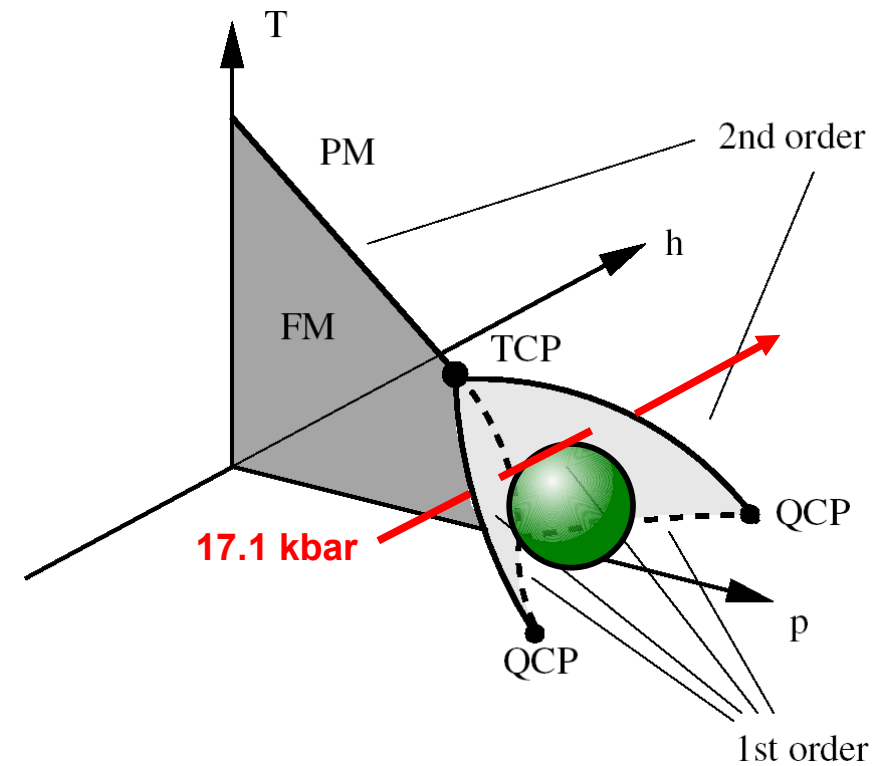
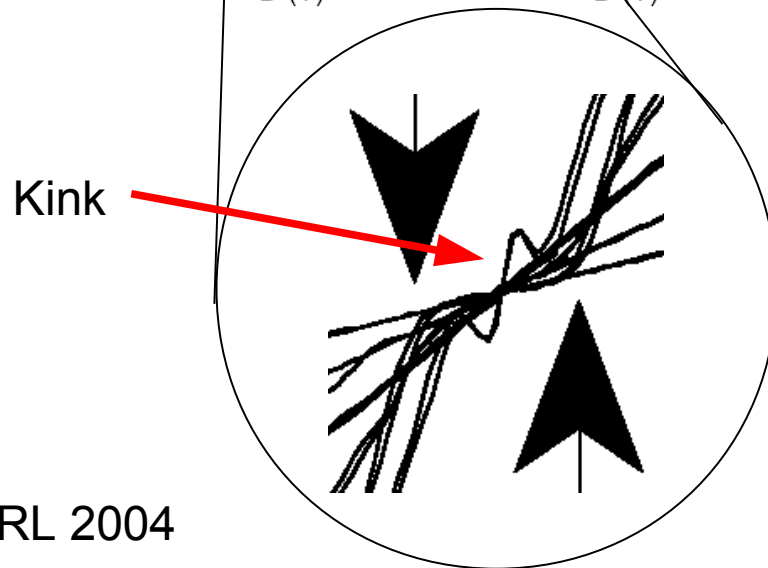
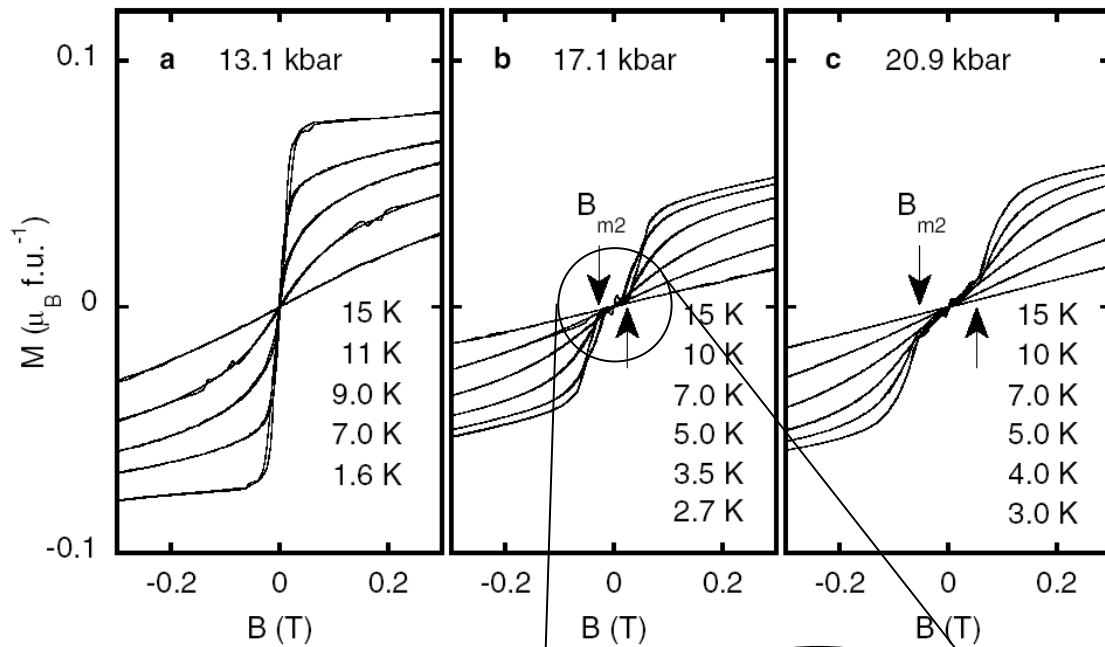


¹Beridge *et al.*, PRL 2009



ZrZn₂

- Kink in magnetisation indicative of novel phase behaviour

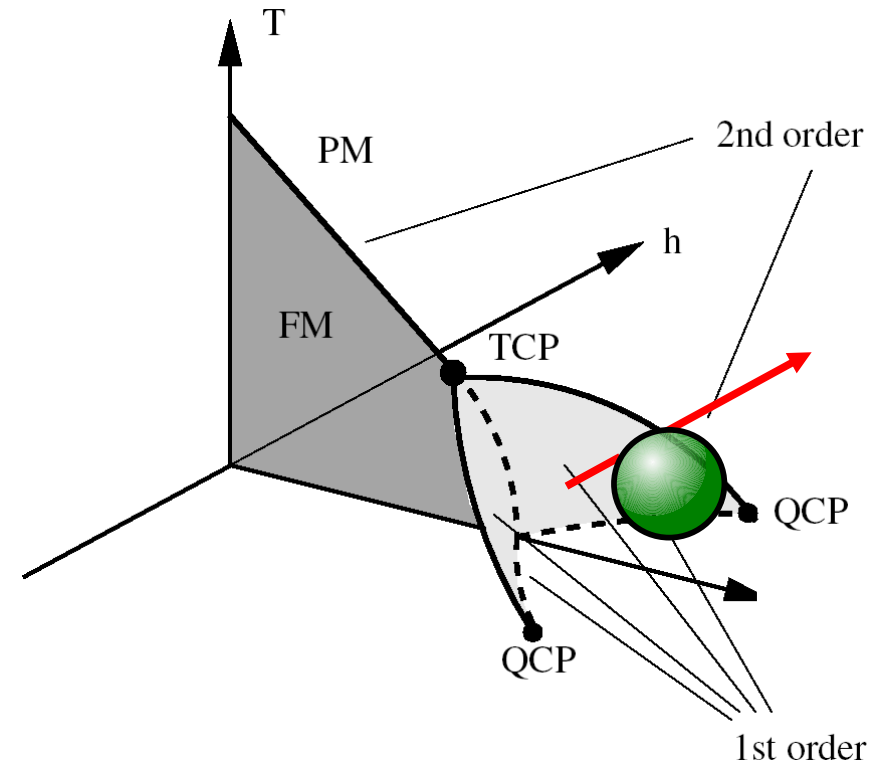
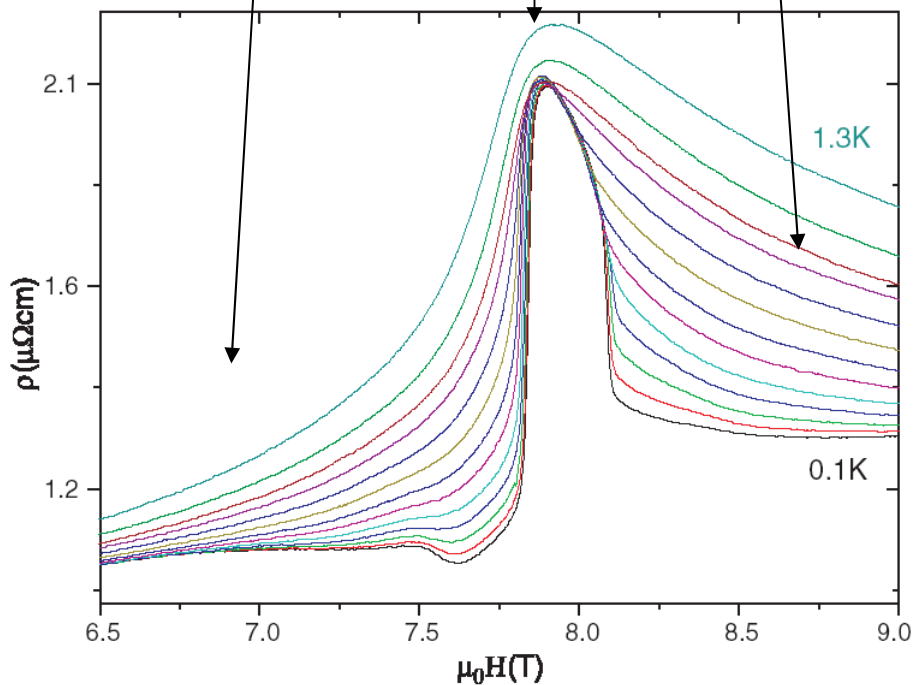


Sr₃Ru₂O₇

- Resistance anomaly

Scattering of M fluctuations

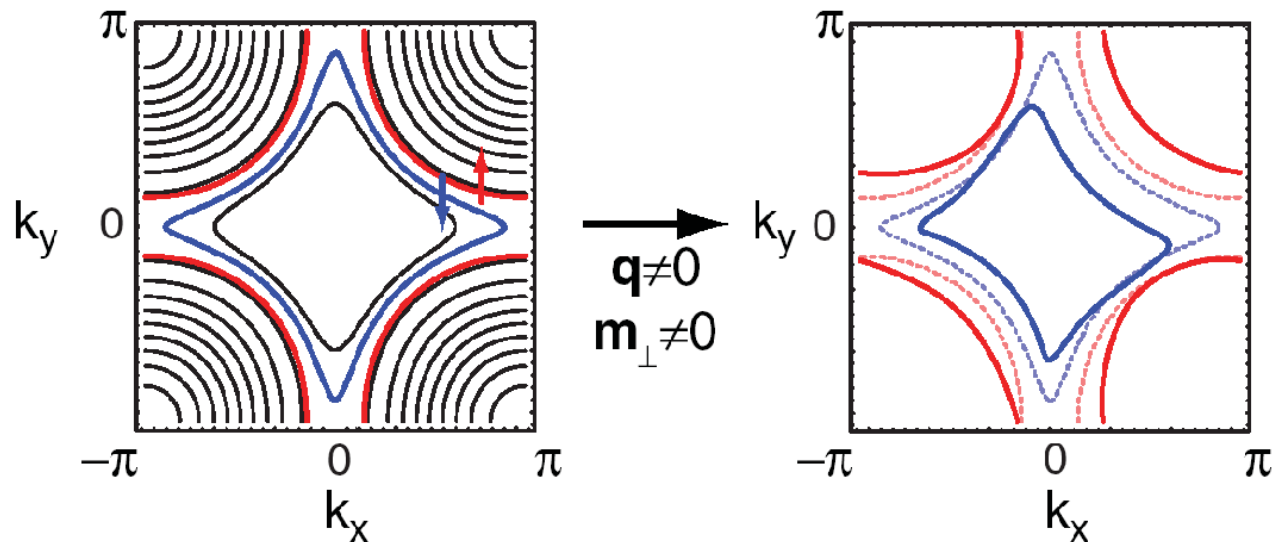
Scattering off M crystal?



- Consistent with a new crystalline phase

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

$$\psi \rightarrow e^{\frac{1}{2}i\mathbf{q}\cdot\mathbf{r}\sigma_z} \psi$$

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

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

- 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

Ginzburg-Landau analysis

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

- Coefficient of m^4 has the same form as q^2m^2
- In analogy to FFLO¹ we can look at a Ginzburg-Landau analysis

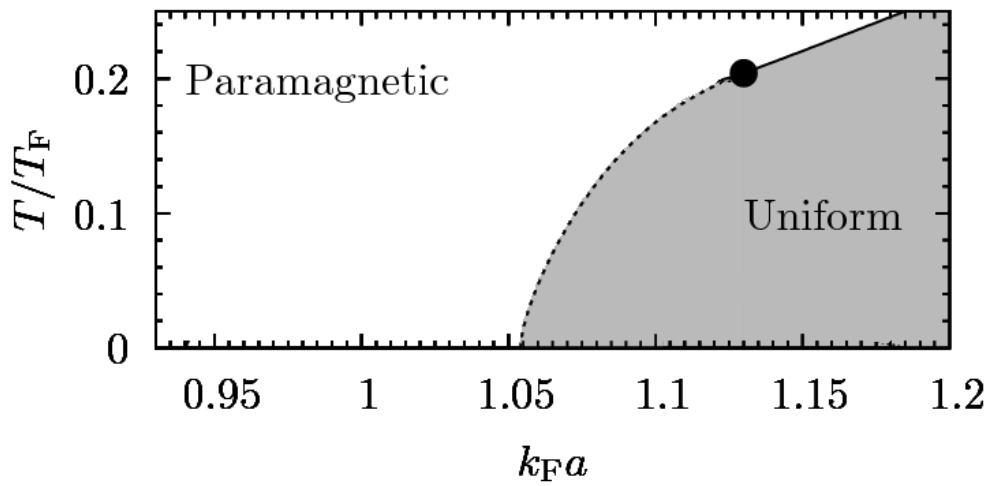
$$\beta H = \int r m^2 + \mathbf{u} m^4 + v m^6 + \frac{2}{3} \mathbf{u} (\nabla m)^2 + \frac{3}{5} v (\nabla^2 m)^2 - hm$$

- Development of the tricritical point is accompanied by sign reversal of the gradient term as both contain G^4

¹Saint-James *et al.* 1969, Buzdin & Kachkachi 1996

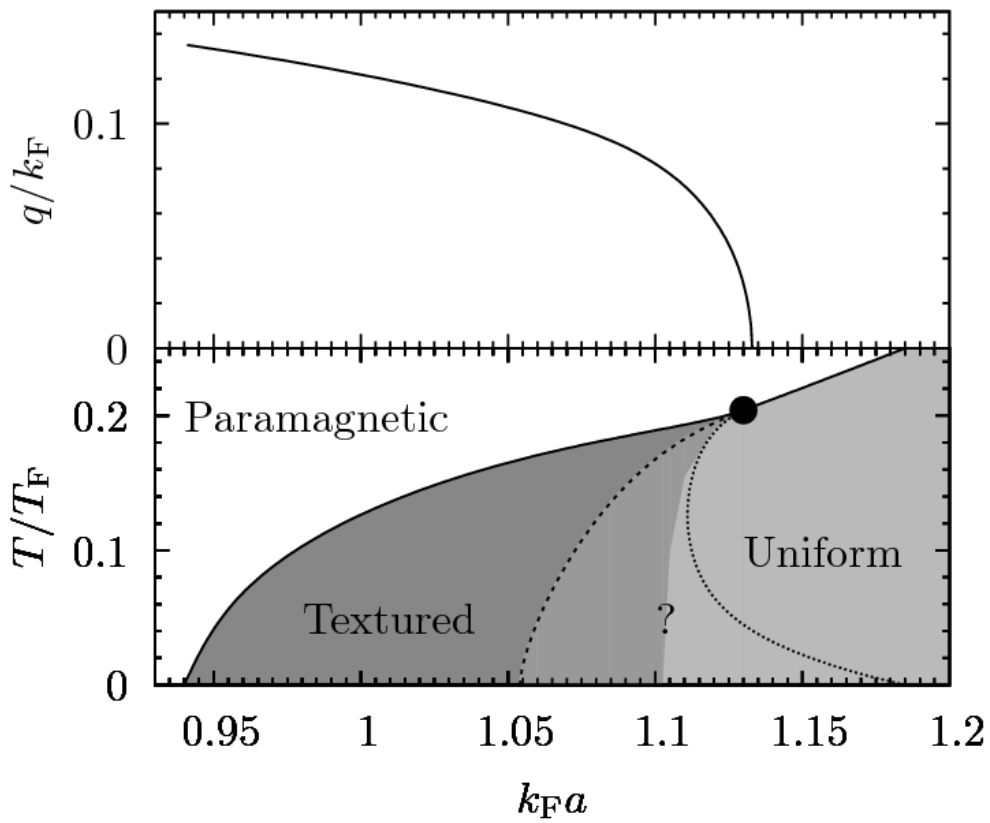
Results

- Uniform ferromagnetic phase with tricritical point



Results

- Textured phase preempted transition with $q=0.1k_F$



Quantum Monte Carlo

- Ran *ab initio* Quantum Monte Carlo calculations on the system using the CASINO program
- After a gauge transformation used the non-collinear trial wave function

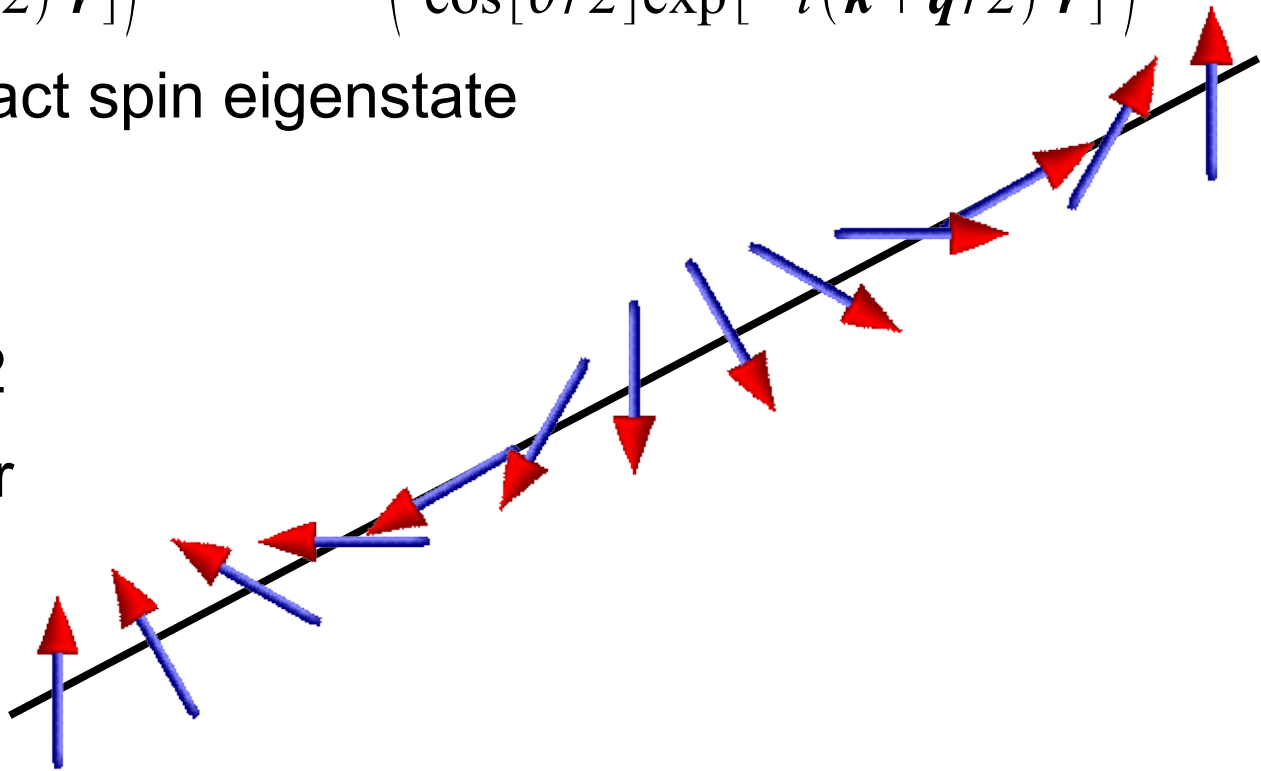
$$e^{-J(\mathbf{R})} \det\left(\{\psi_{\mathbf{k} \in k_{F\uparrow}}, \bar{\psi}_{\mathbf{k} \in k_{F\downarrow}}\}\right)$$

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

- Single determinant not exact spin eigenstate in finite sized system

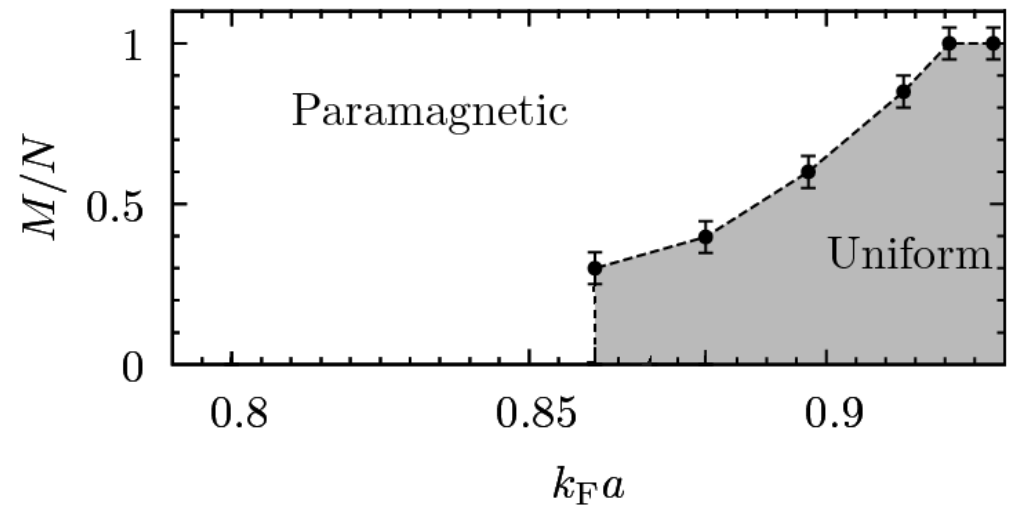
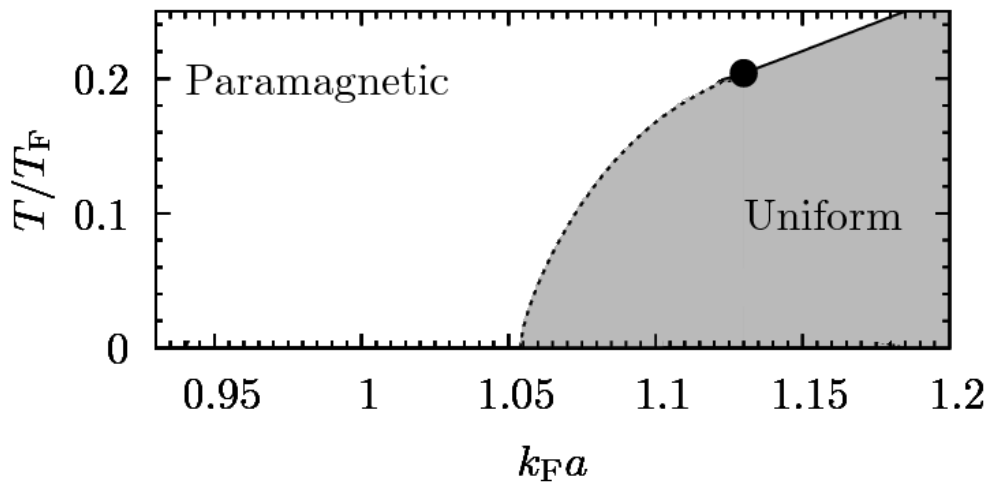
$$\langle \hat{S}_{\perp, \text{RMS}} \rangle \approx \langle \hat{S} \rangle / \sqrt{n_{\uparrow} + n_{\downarrow}} \ll \langle \hat{S} \rangle$$

- Planar spin spiral at $\theta = \pi/2$
- Optimisable Jastrow factor $J(\mathbf{R})$ accounts for electron correlations



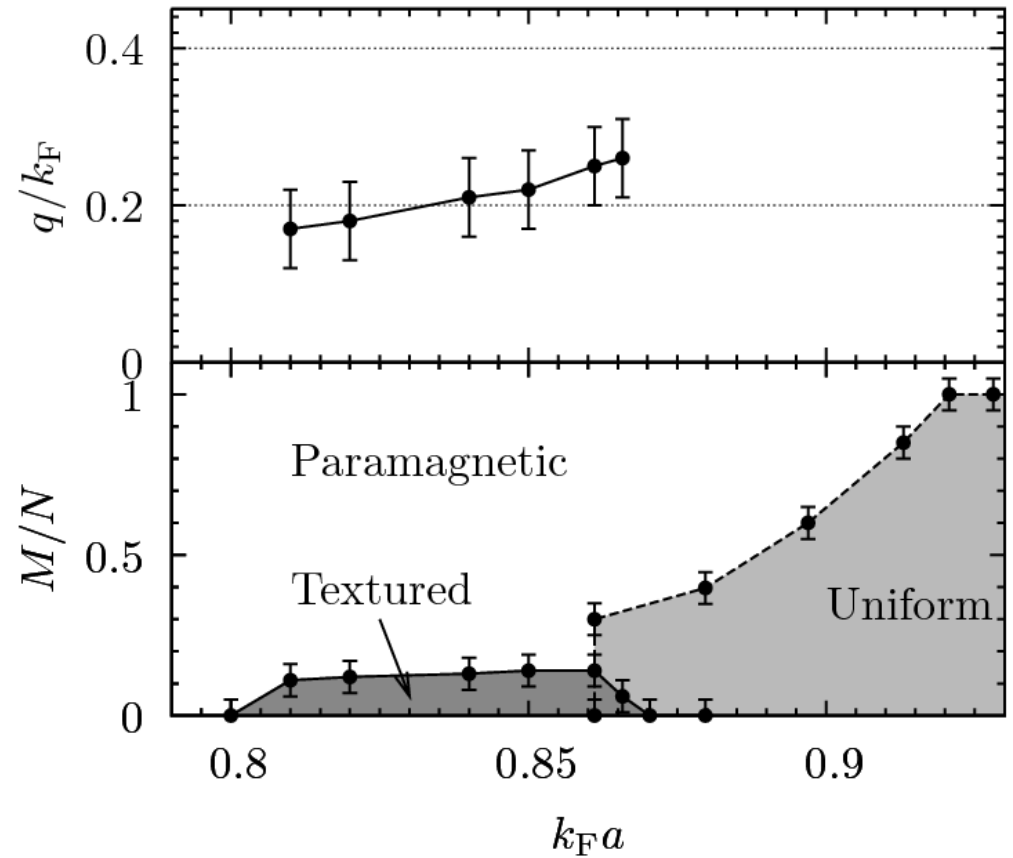
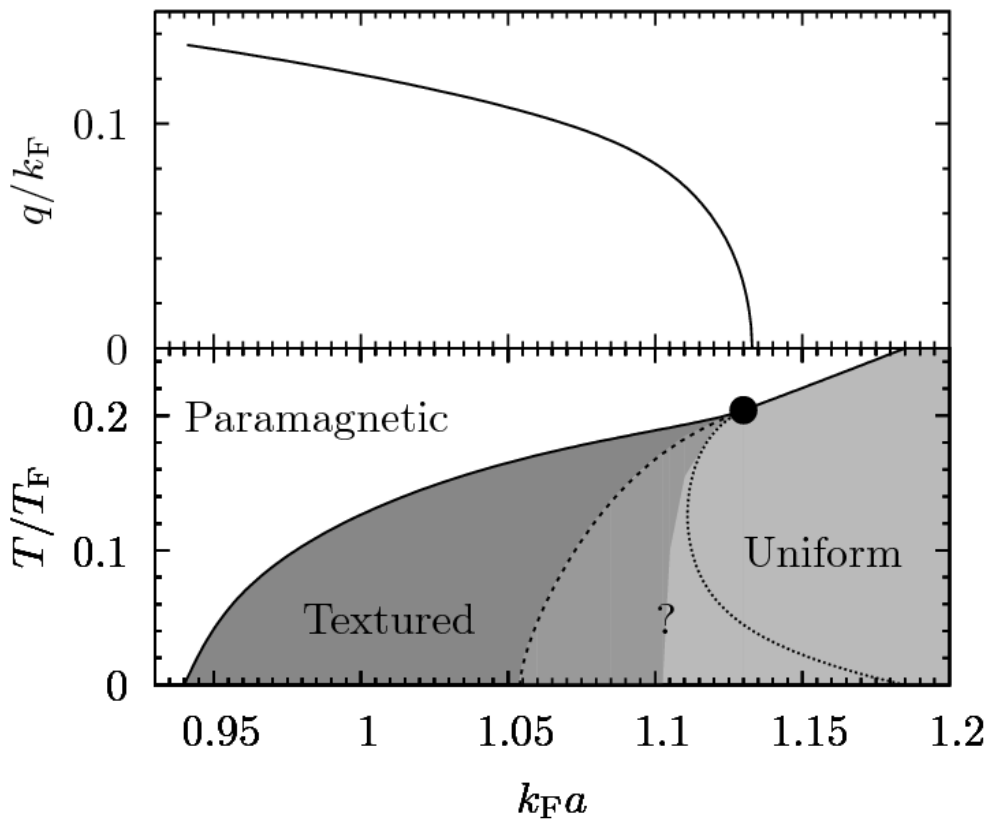
Quantum Monte Carlo: Uniform phase

- First order transition into uniform phase



Quantum Monte Carlo: Textured phase

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

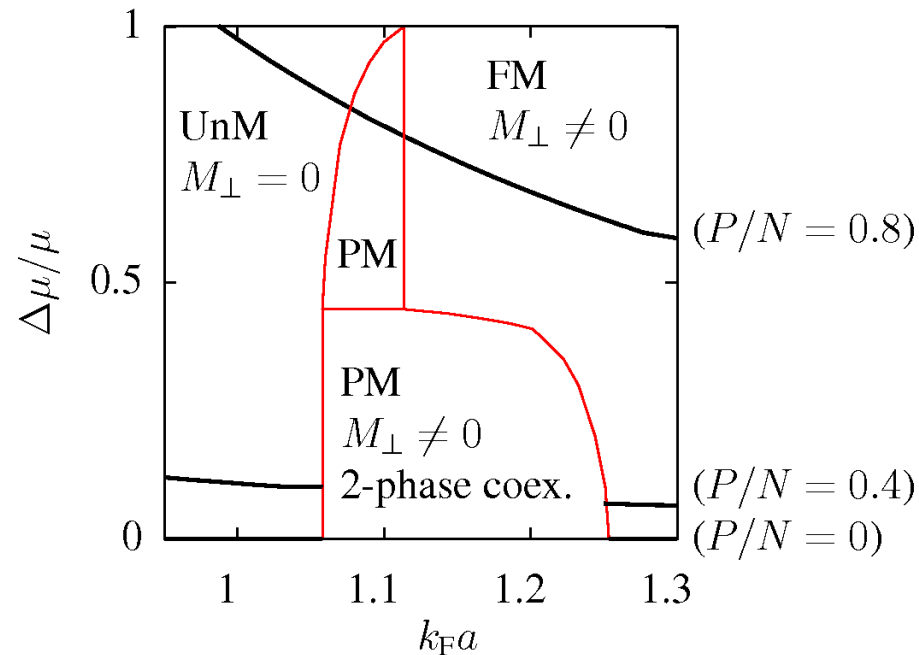
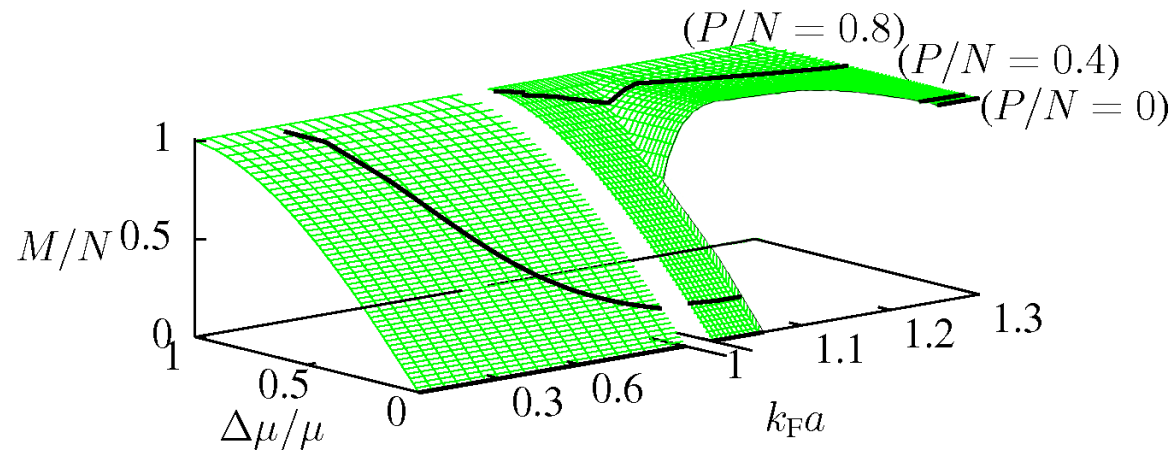


Summary

- Considering soft particle-hole modes, density & magnetic fluctuations revealed a first order transition
- Probed population imbalance in atomic gases
- Quantum fluctuation driven textured ferromagnetic phase reconstruction
- Confirmed phases with *ab initio* QMC calculations
- Further questions: interplay of lattice & quantum fluctuations and possible nematic or other phases
- Acknowledge EPSRC funding

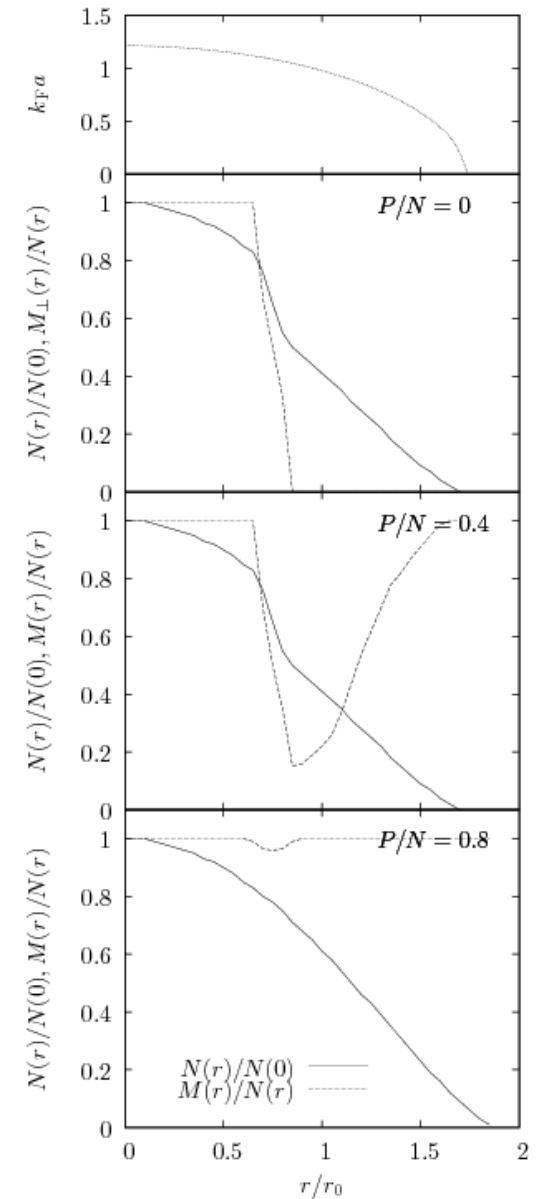
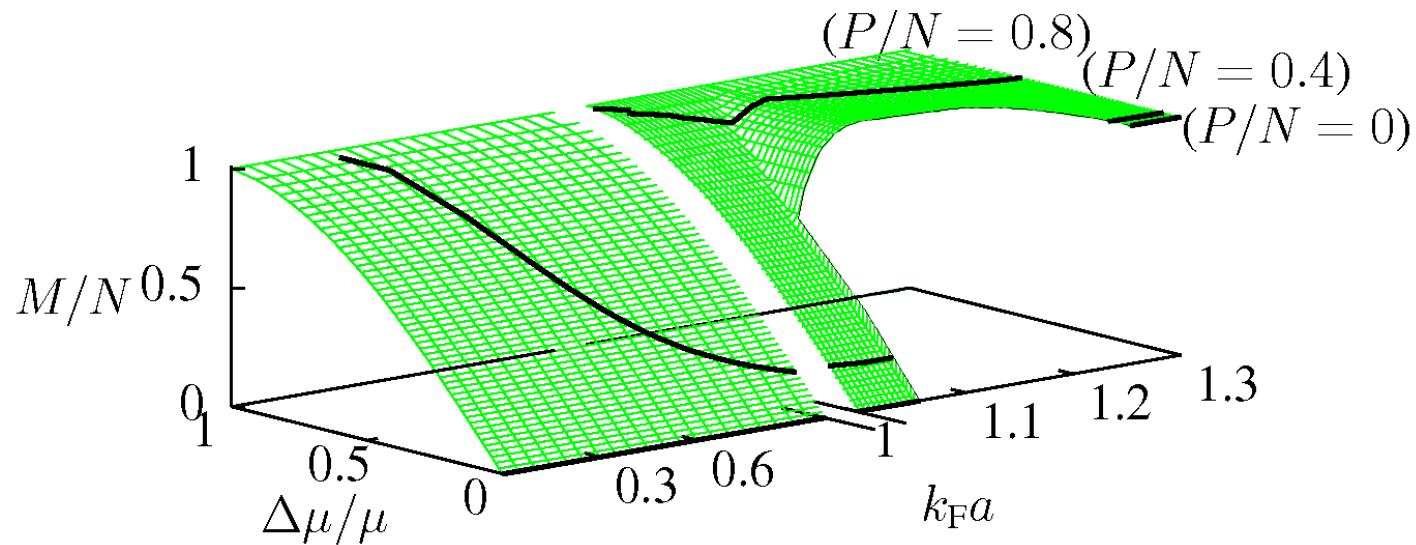
Grand canonical ensemble

- In the grand canonical ensemble we obtain



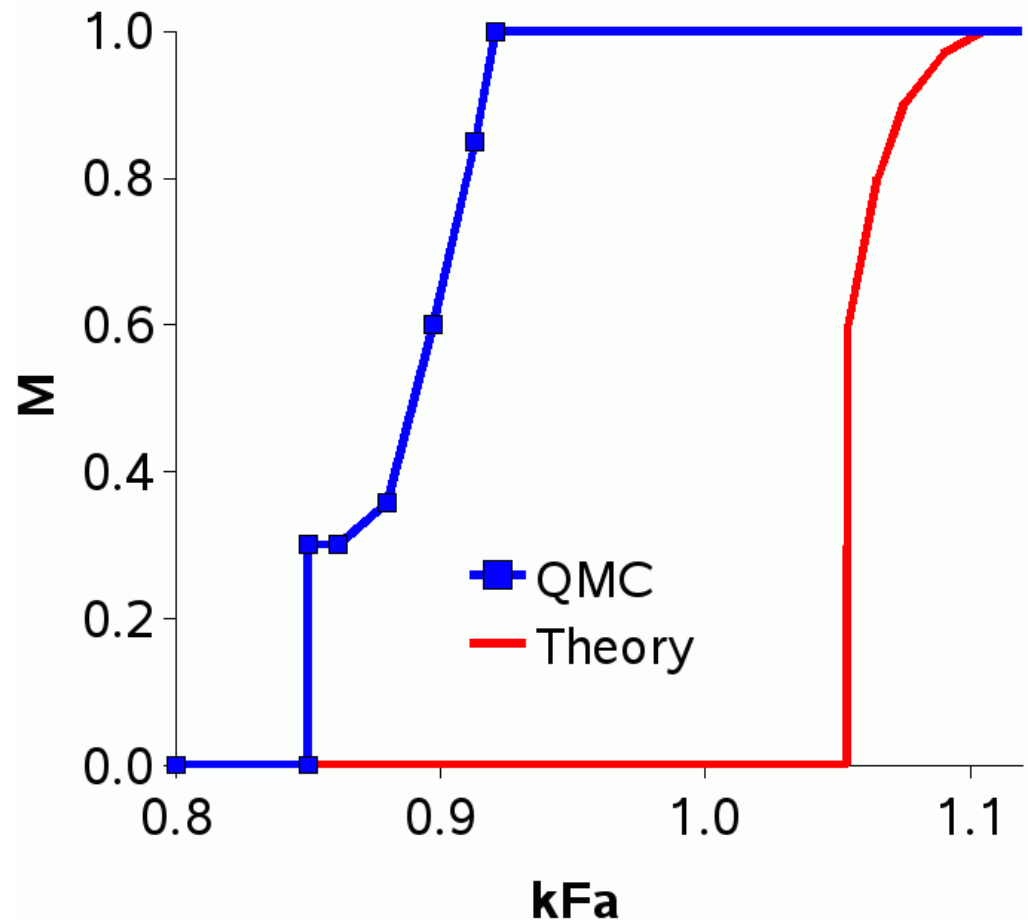
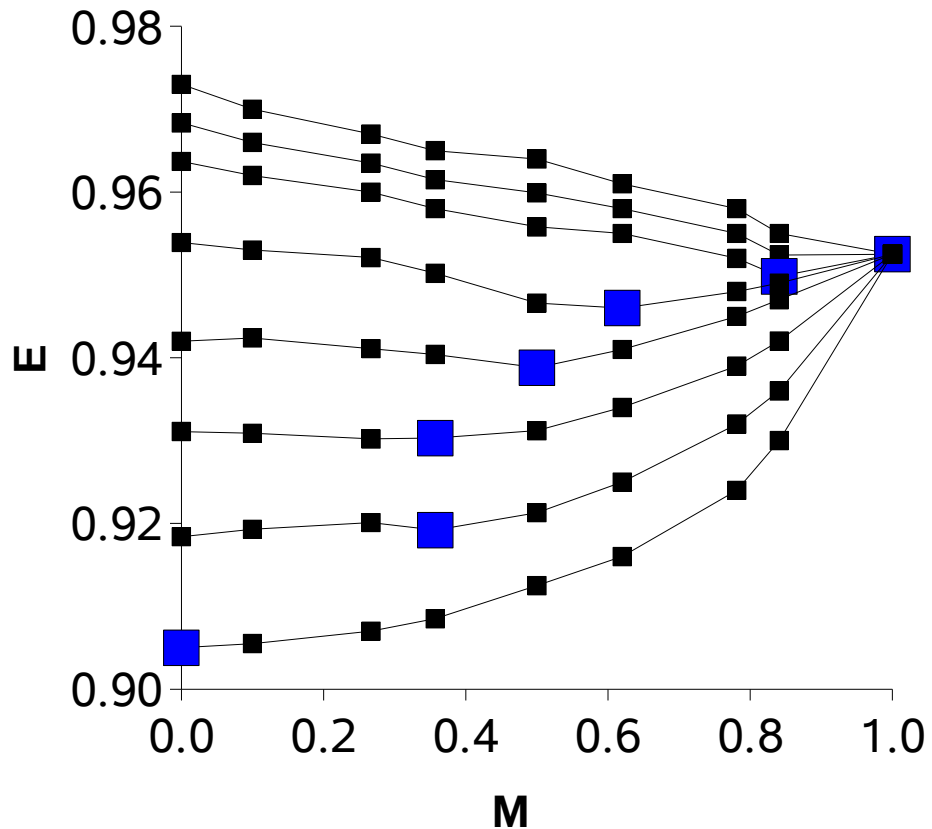
Trap behaviour

- 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



Consequences of fluctuations

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

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

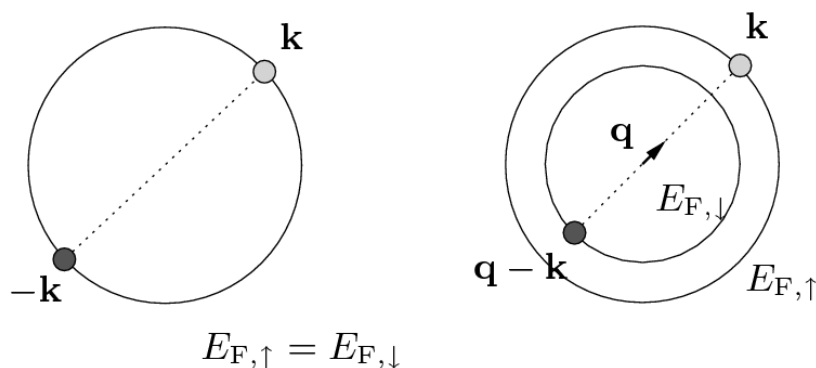
- The coupling of fields¹ can drive a transition first order

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

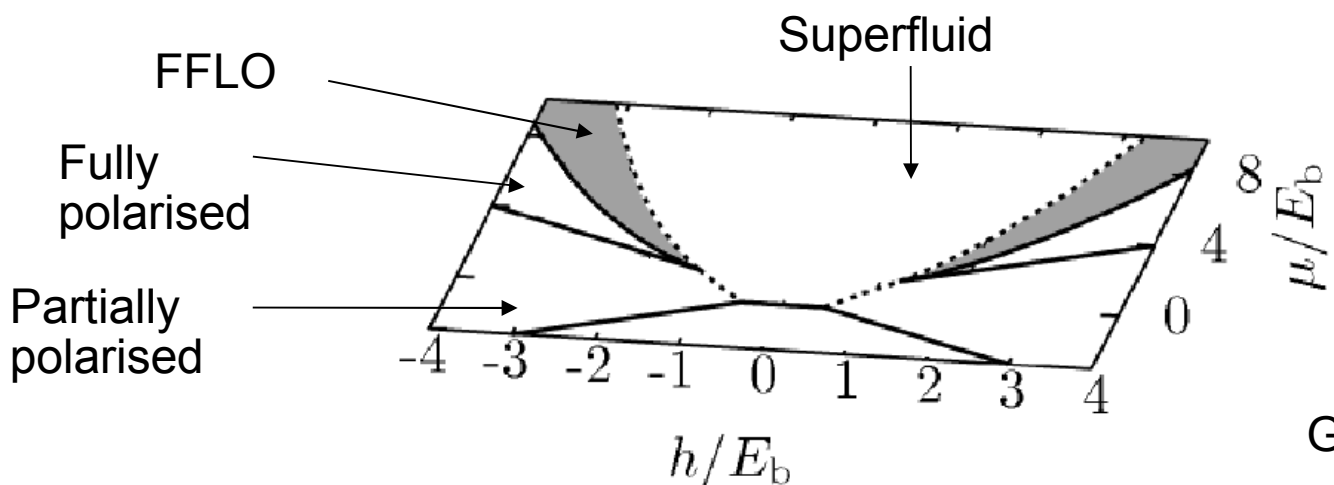
¹Rice 1954, Garland & Renard 1966, Larkin & Pikin 1969

FFLO

- The Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) phase has a modulated superconducting gap



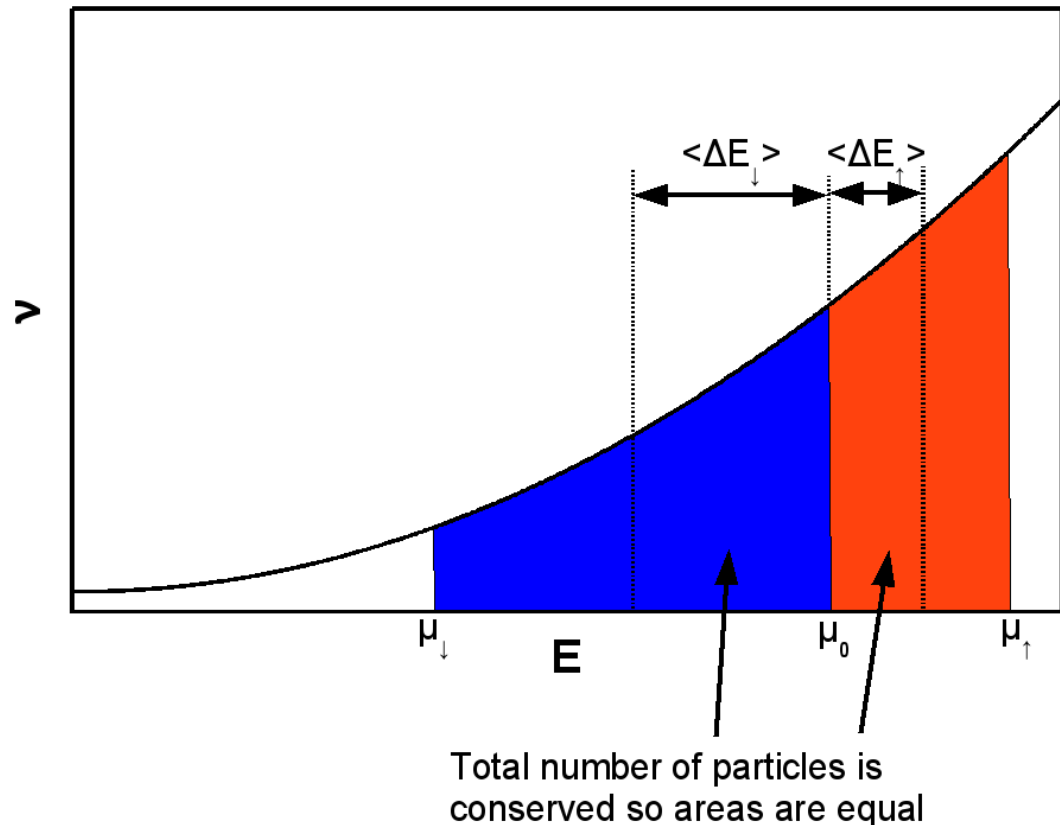
- A Cooper pair has zero momentum, with unequal Fermi surfaces the Cooper pair carries momentum, causing a modulated superconducting gap parameter Δ
- The FFLO phase preempts the normal phase-superfluid transition



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, Pfeleiderer *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 ε gives criterion

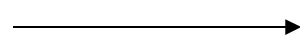
$$\int_0^u \varepsilon^{(0,4)}(w, 0)dw + 4\varepsilon^{(0,3)}(u, 0) + 6\varepsilon^{(1,2)}(u, 0) + 4\varepsilon^{(2,1)}(u, 0) + \varepsilon^{(3,0)}(u, 0) < 0$$

Overall change in energy spectrum during the transition

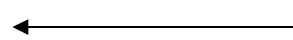
How energy spectrum changes during transition at the Fermi surface

Wohlfarth Rhodes criterion

Differential of energy spectrum curve



$\varepsilon^{(a,b)}$

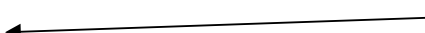


Differentiate energy spectrum wrt changing Fermi surface

- The terms have magnitude

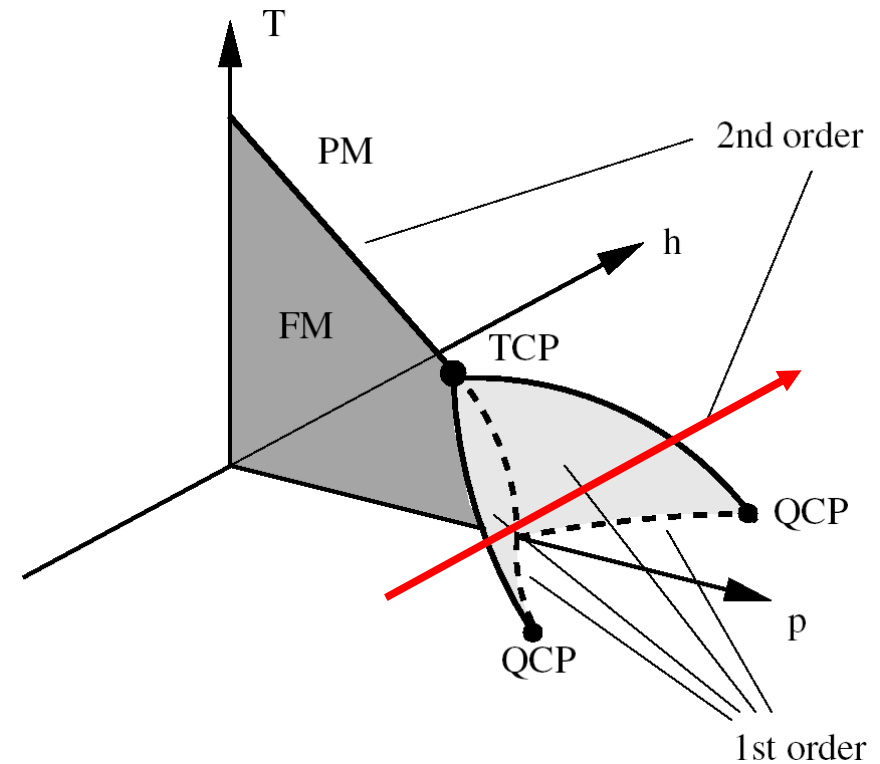
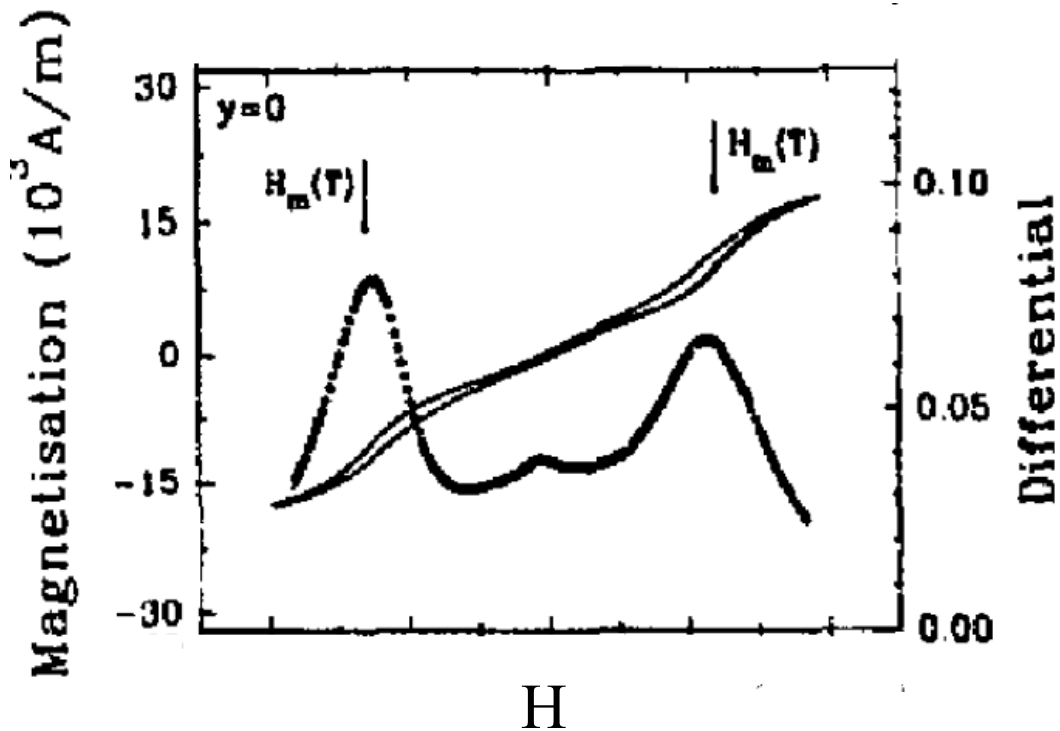
Term	Expansion
$\int_0^u \varepsilon^{(0,4)}(w, 0)dw$	$0.0k_F a + 0.0086(k_F a)^2$
$4\varepsilon^{(0,3)}(u, 0)$	$0.0k_F a - 0.04(k_F a)^2$
$6\varepsilon^{(1,2)}(u, 0)$	$0.024(k_F a)^2$
$4\varepsilon^{(2,1)}(u, 0)$	$0.0(k_F a)^2$
$\varepsilon^{(3,0)}(u, 0)$	$2^{-3/2}/27 - 0.0055(k_F a)^2$

Transition due to changing energy spectrum at the Fermi surface



NbFe₂

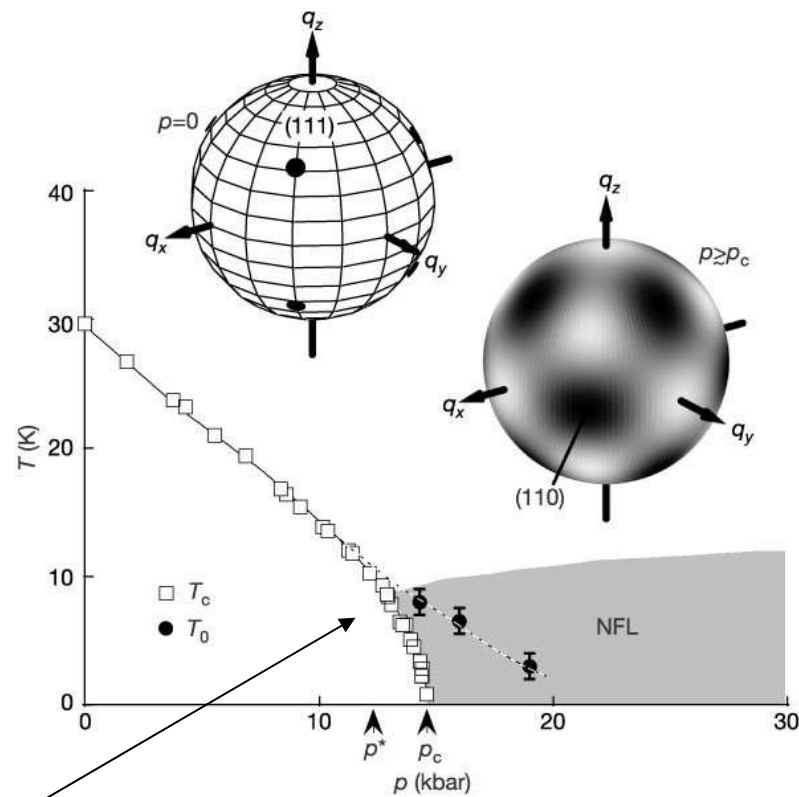
- NbFe₂ displays antiferromagnetic order where it is expected to be ferromagnetic — could this be a textured ferromagnetic phase?



Crook & Cywinski, JMMM 1995

MnSi

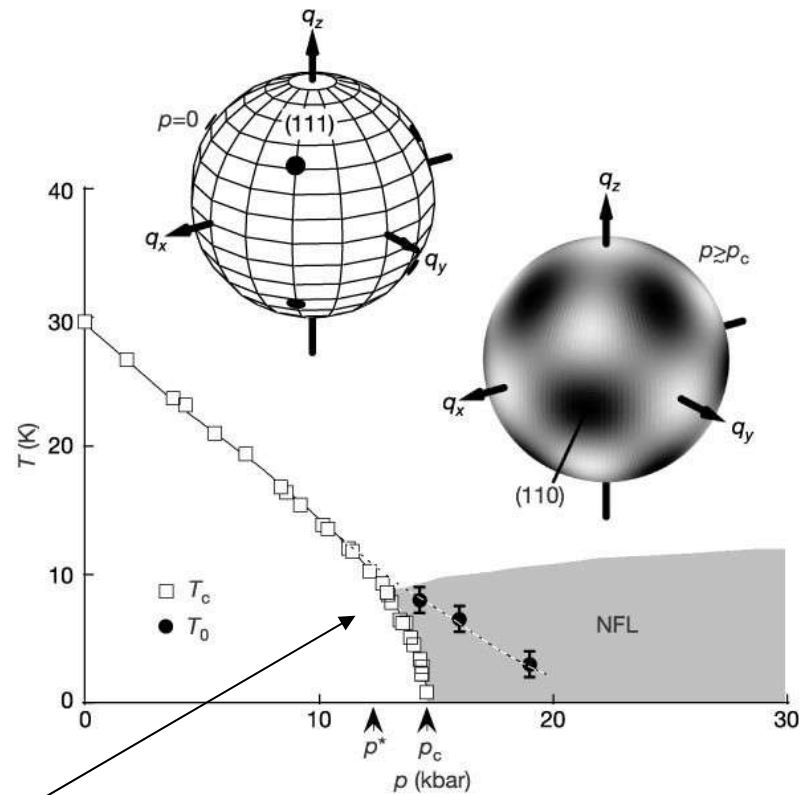
- MnSi displays non-Fermi liquid behaviour consistent with a spin state (though in a non-centrosymmetric crystal)



Tricritical point

MnSi

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



Tricritical point