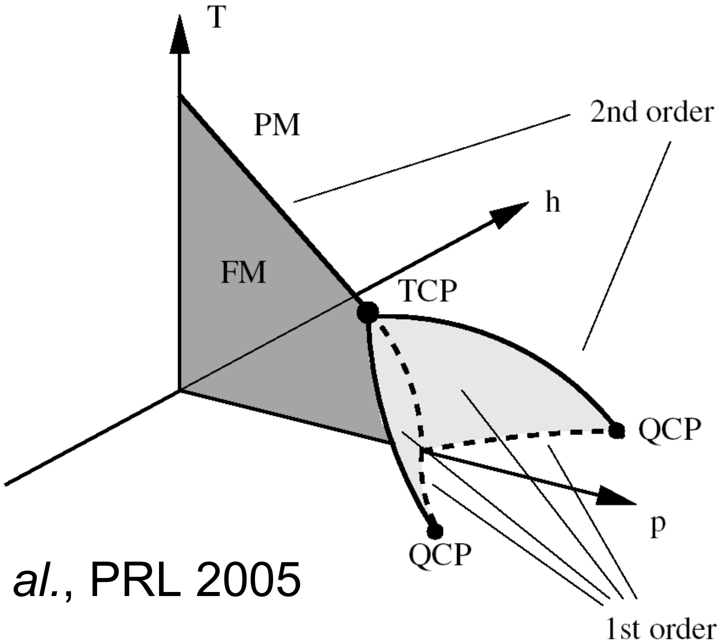
Inhomogeneous phase formation on the border of itinerant ferromagnetism



Belitz *et al.*, PRL 2005

Gareth Conduit[1], Andrew Green[2], Ben Simons[1]

1. University of Cambridge, 2. University of St Andrews

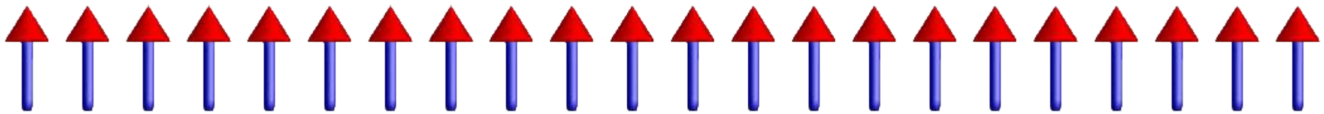
Itinerant ferromagnetism in an atomic Fermi gas: Influence of population imbalance
G.J. Conduit & B.D. Simons, Phys. Rev. A **79**, 053606 (2009)

Inhomogeneous phase formation on the border of itinerant ferromagnetism
G.J. Conduit, A.G. Green & B.D. Simons, arXiv:0906.1347

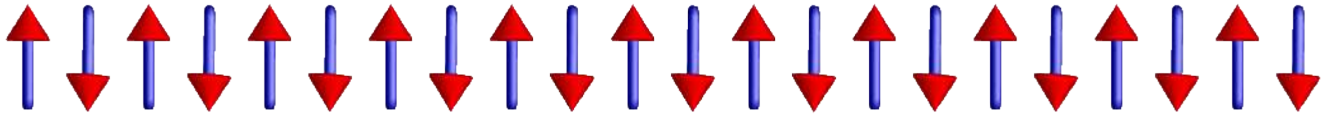
Two types of ferromagnetism

- *Localised ferromagnetism*: moments confined in real space

Ferromagnet

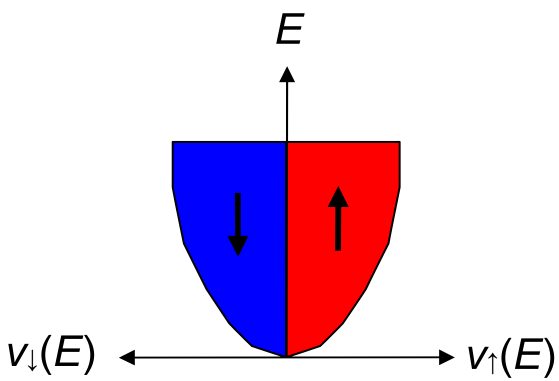


Antiferromagnet

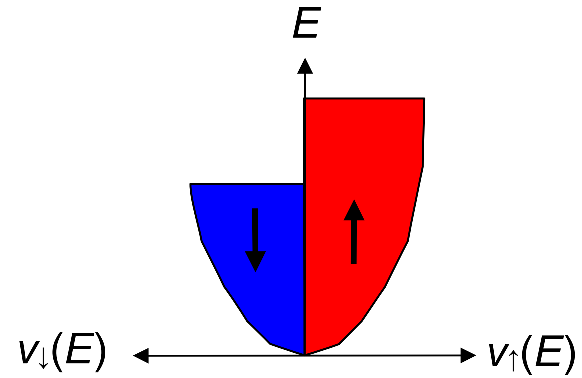


- *Itinerant ferromagnetism:* electrons in Bloch wave states

Not magnetised



Partially magnetised



Stoner model for itinerant ferromagnetism

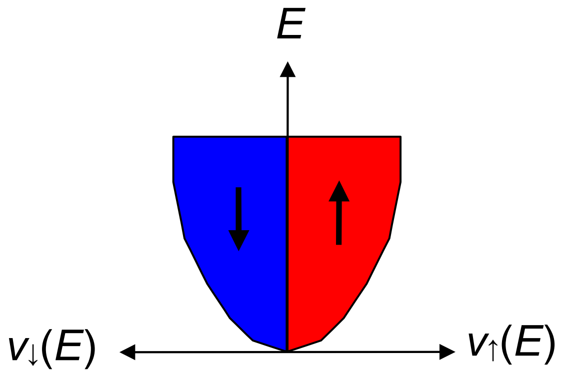
- Repulsive interaction energy $U = g n_\uparrow n_\downarrow$
- A ΔE shift in the Fermi surface causes:

  (1) Kinetic energy increase of $\frac{1}{2} v \Delta E^2$

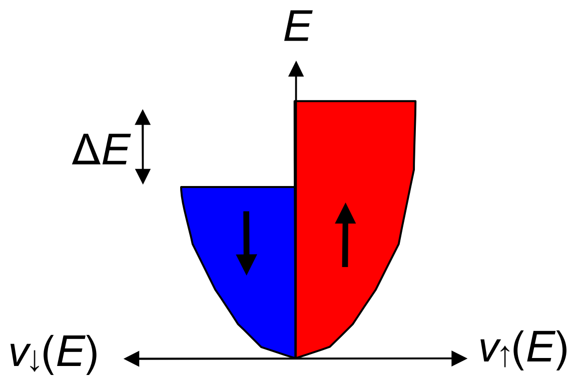
  (2) Reduction of repulsion of $-\frac{1}{2} g v^2 \Delta E^2$

- 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

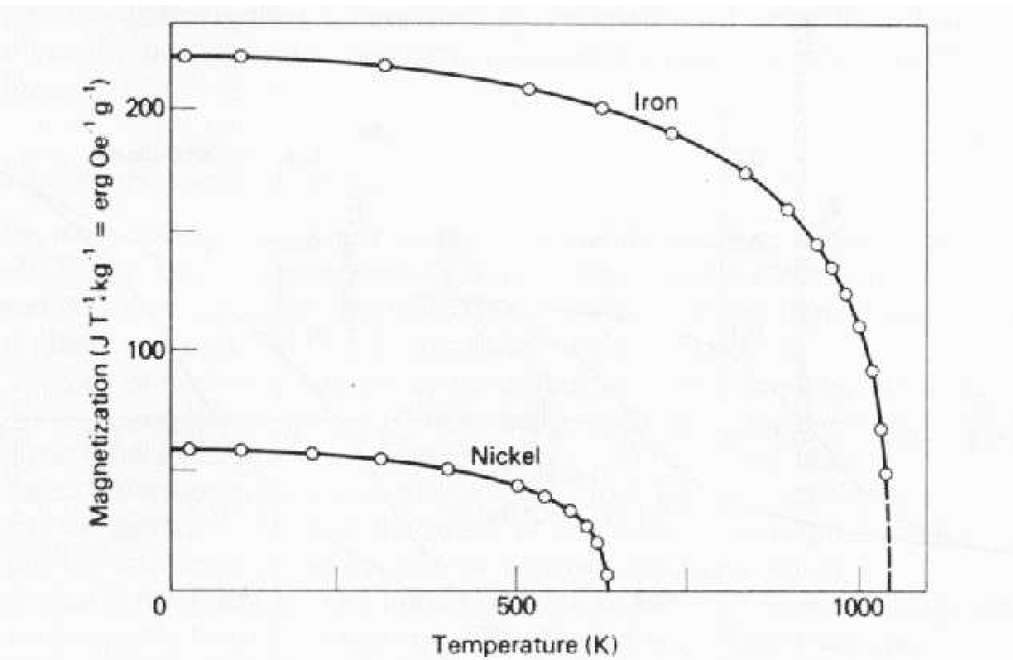


Figure 1.2 Spontaneous magnetization plotted against temperature for iron and nickel.

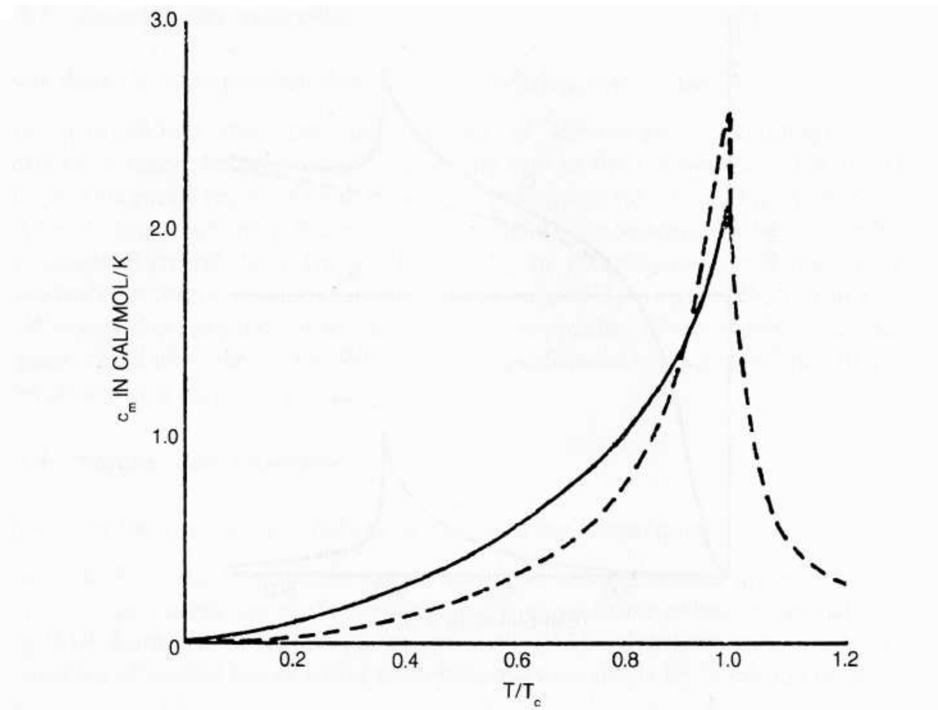
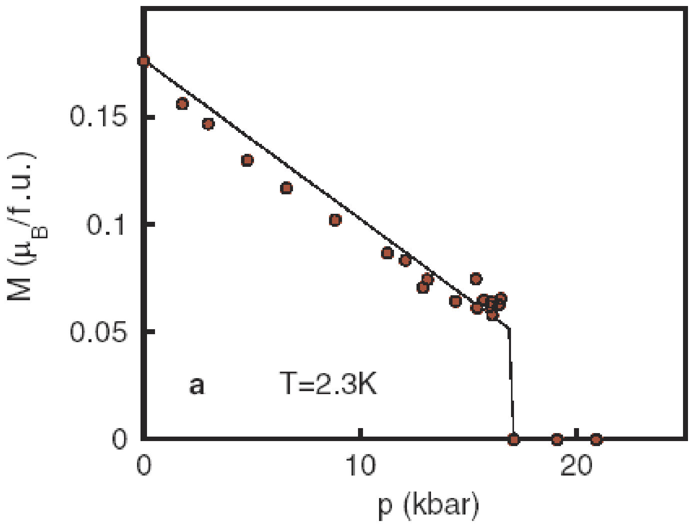


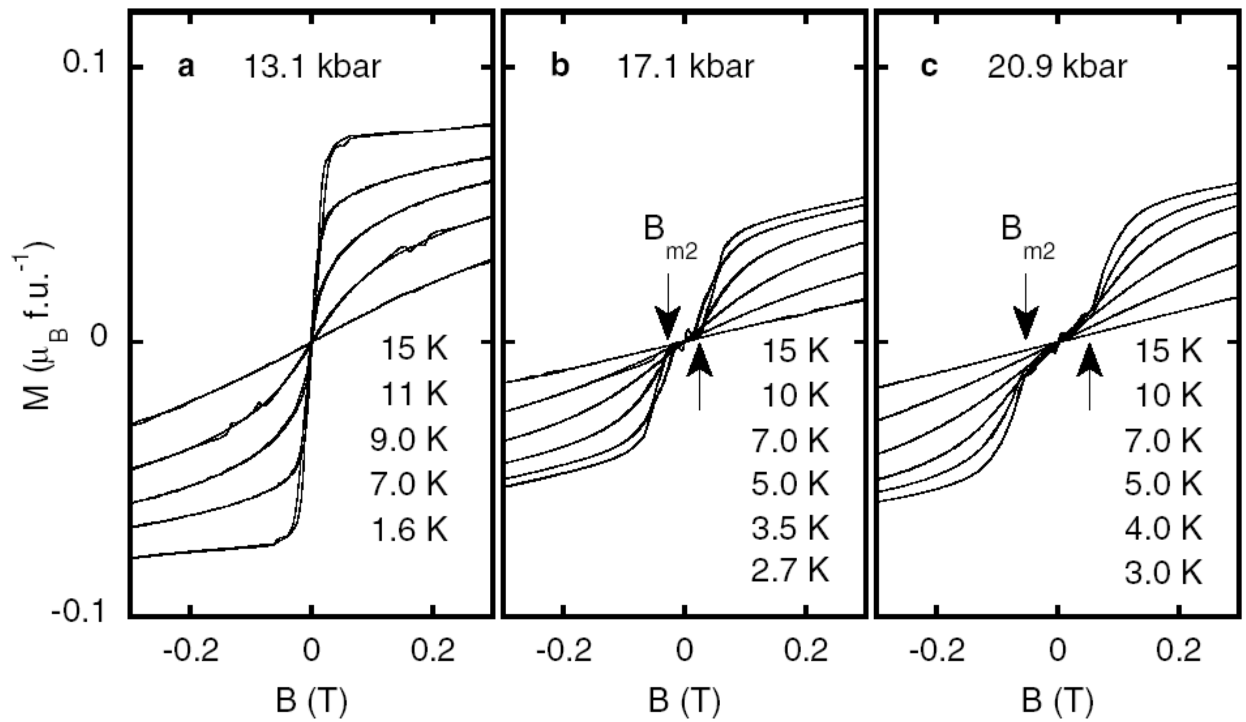
Fig. 9.20 Specific heat anomaly for nickel at its Curie point compared with the theoretical prediction.

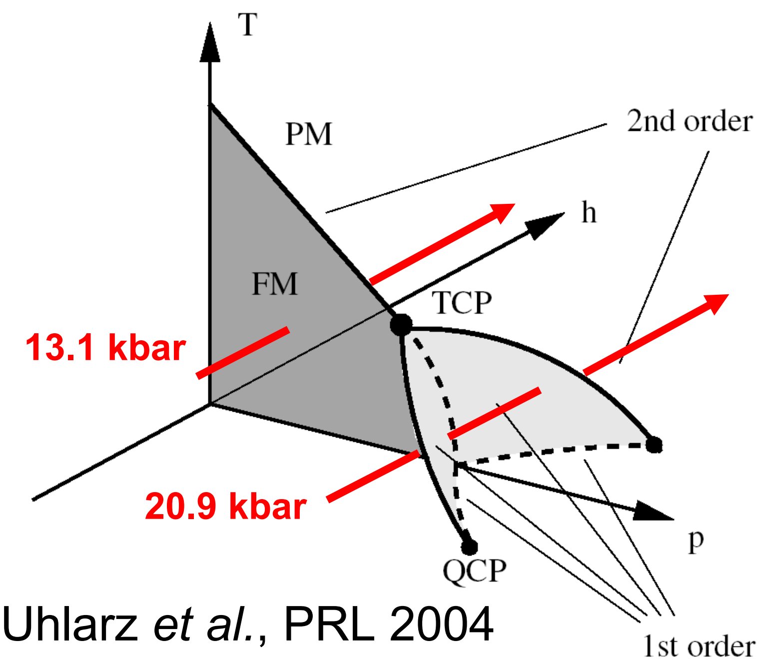
that is characterised by a divergence of length-scales (peaked heat capacity and susceptibility)

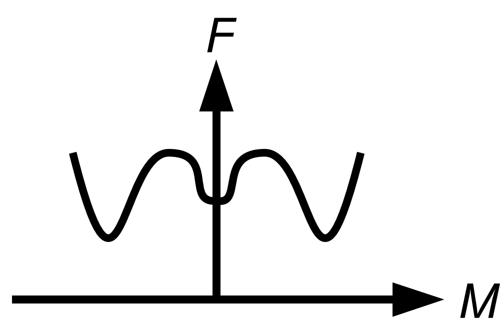
Breakdown of Stoner criterion — $ZrZn_2$

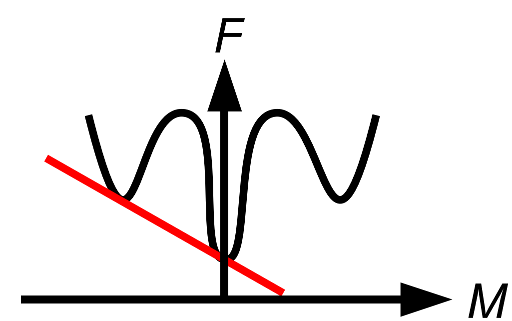
- At low temperature and high pressure $ZrZn_2$ has a first order transition







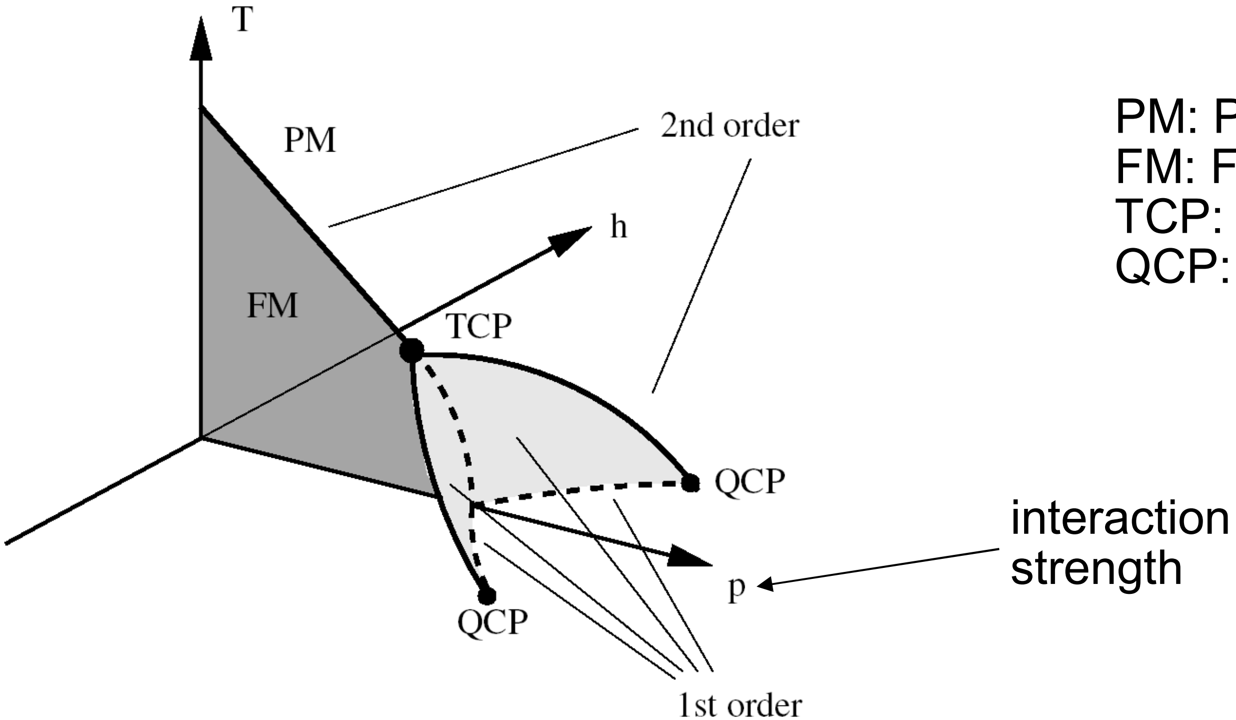




Uhlarz *et al.*, PRL 2004

Breakdown of Stoner criterion

- Generic phase diagram of the first order transition



PM: Partially magnetised
FM: Fully magnetised
TCP: Tricritical point
QCP: Quantum critical point

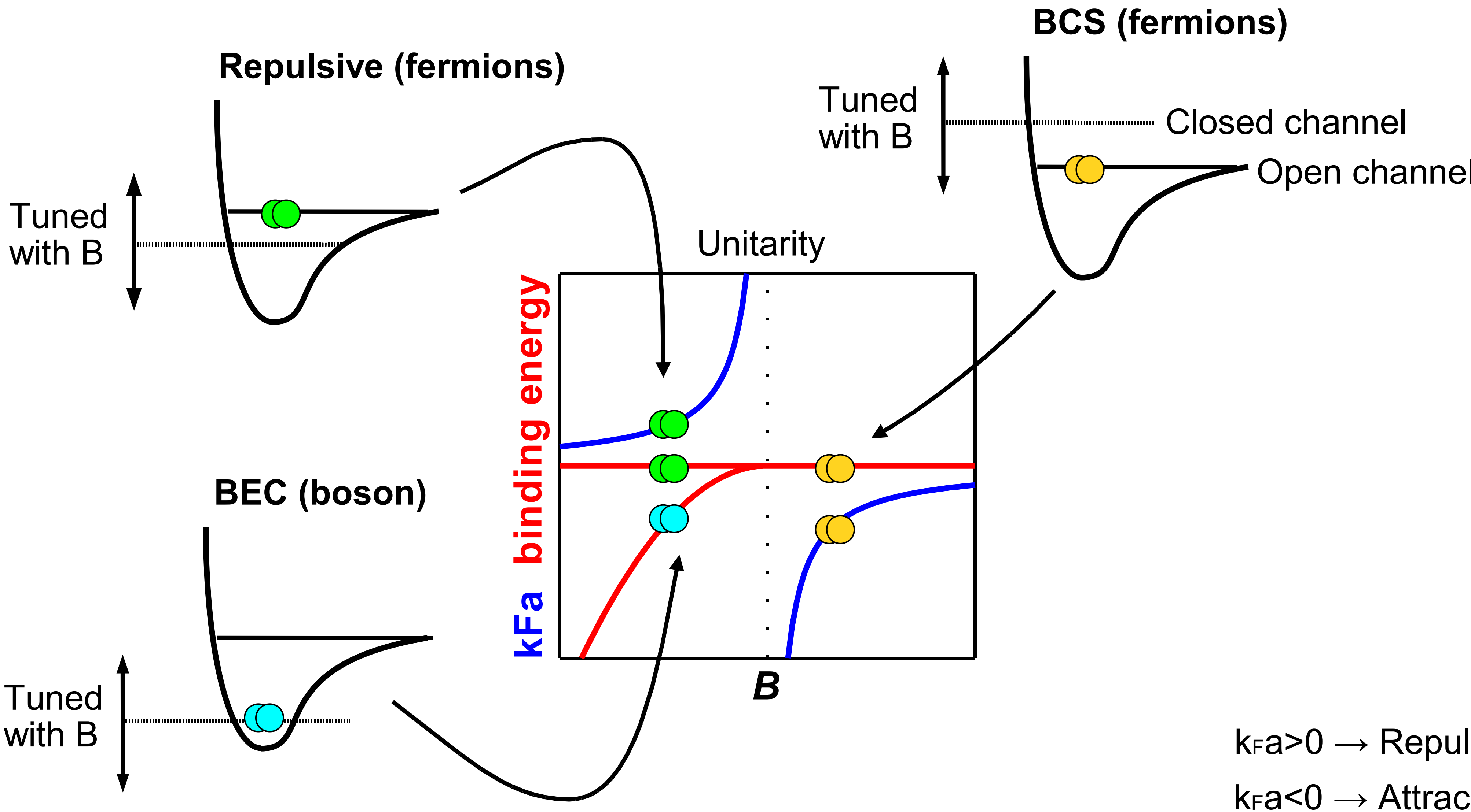
- Two explanations of first order behaviour:

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

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

Feshbach resonance

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



$k_F a > 0 \rightarrow$ Repulsive

$k_F a < 0 \rightarrow$ 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

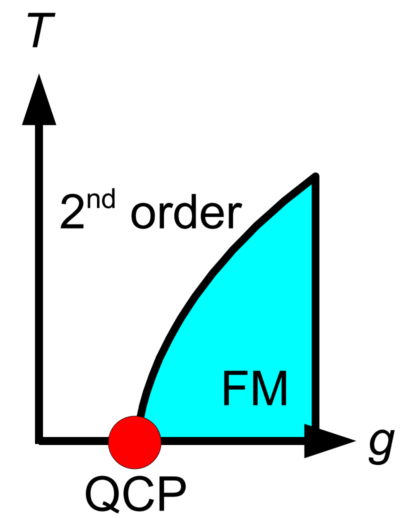
- Hertz-Millis (spin triplet channel) [Hertz PRB 1976 & Millis PRB 1993]

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

Extension to Hertz-Millis

- Coupling to auxiliary fields can drive a transition first order [Rice 1954, Garland & Renard 1966]

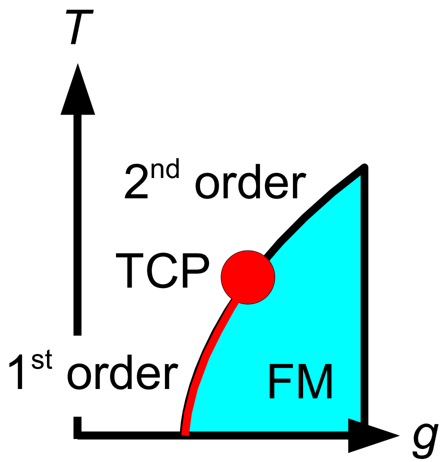
$$rm^2 + um^4 + a\phi^2 \pm 2am^2\phi$$
$$= rm^2 + (u-a)m^4 + a(\phi \pm m^2)^2$$
$$= rm^2 + (u-a)m^4$$



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

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

- 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

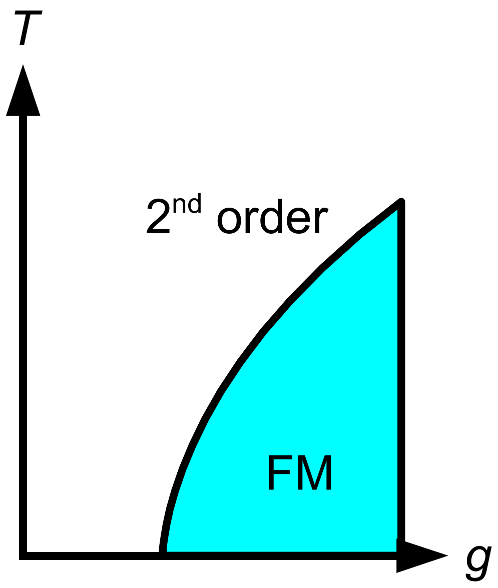
  5) Integrate out density and magnetisation fluctuations

Particle-hole perspective

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

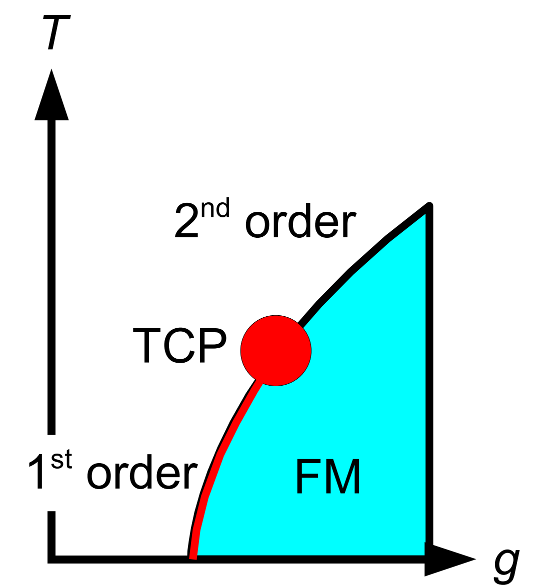
$$F = \sum_{\sigma,\boldsymbol{k}} \epsilon_{\boldsymbol{k}}^{\sigma} n(\epsilon_{\boldsymbol{k}}^{\sigma}) + gN^{\uparrow} N^{\downarrow} + \cdots$$

- 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



$$F=\sum_{\sigma,\boldsymbol{k}}\epsilon_{\boldsymbol{k}}^{\sigma}n(\epsilon_{\boldsymbol{k}}^{\sigma})+gN^{\uparrow}N^{\downarrow}$$
$$-\frac{2g^2}{V^3}\sum_{\boldsymbol{p}}\int\int\frac{\rho^{\uparrow}(\boldsymbol{p},\epsilon_{\uparrow})\rho^{\downarrow}(-\boldsymbol{p},\epsilon_{\downarrow})}{\epsilon_{\uparrow}+\epsilon_{\downarrow}}d\epsilon_{\uparrow}d\epsilon_{\downarrow}$$
$$+\frac{2g^2}{V^3}\sum_{\boldsymbol{k}_{1,2,3,4}}\frac{n(\epsilon_{\boldsymbol{k}_1}^{\uparrow})n(\epsilon_{\boldsymbol{k}_2}^{\downarrow})}{\epsilon_{\boldsymbol{k}_1}^{\uparrow}+\epsilon_{\boldsymbol{k}_2}^{\downarrow}-\epsilon_{\boldsymbol{k}_3}^{\uparrow}-\epsilon_{\boldsymbol{k}_4}^{\downarrow}}\delta(\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_3)$$

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

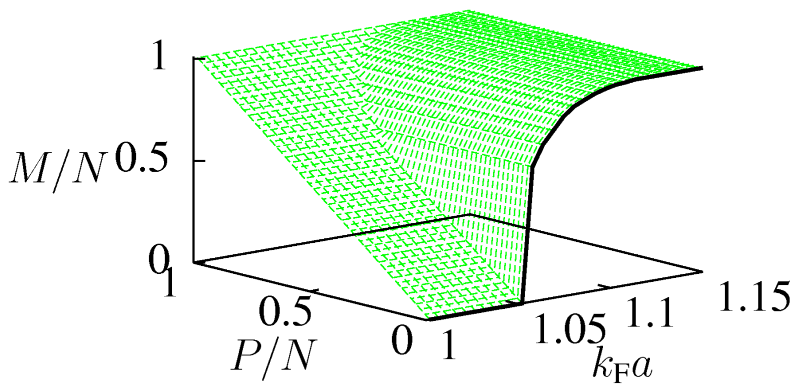
$$\rho^{\sigma}(\boldsymbol{p},\epsilon)=\sum_{\boldsymbol{k}}n(\epsilon_{\boldsymbol{k}+\boldsymbol{p}/2}^{\sigma})\left[1-n(\epsilon_{\boldsymbol{k}-\boldsymbol{p}/2}^{\sigma})\right]\delta\left(\epsilon-\epsilon_{\boldsymbol{k}+\boldsymbol{p}/2}^{\sigma}+\epsilon_{\boldsymbol{k}-\boldsymbol{p}/2}^{\sigma}\right)$$

- 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]

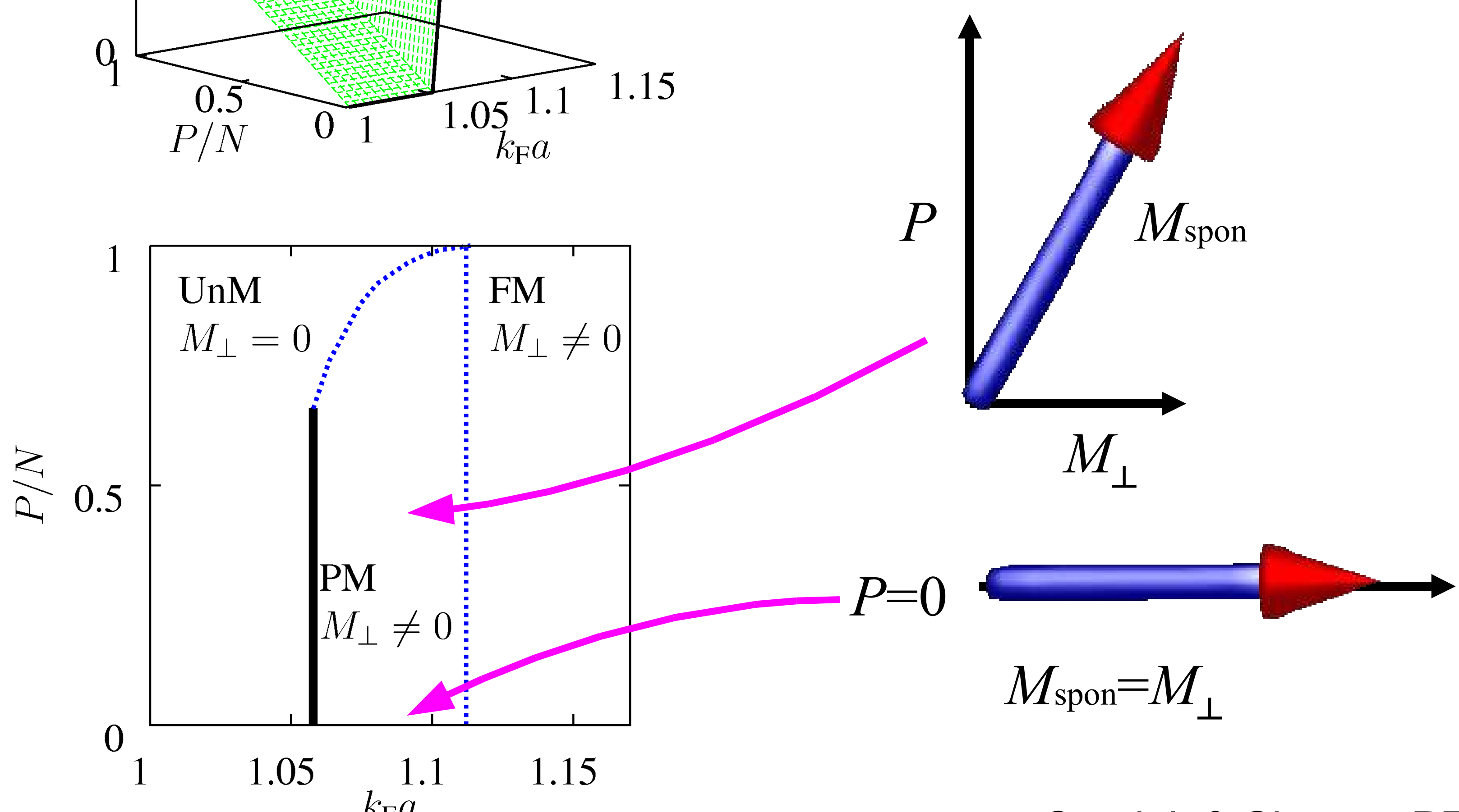
[1]Abrikosov 1958 & Duine & MacDonald 2005

Population imbalanced case

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



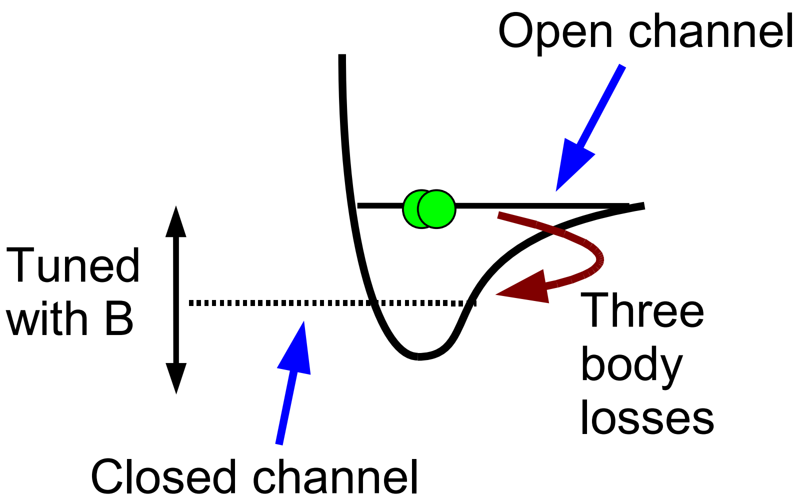
UnM: Unmagnetised
PM: Partially magnetised
FM: Fully magnetised

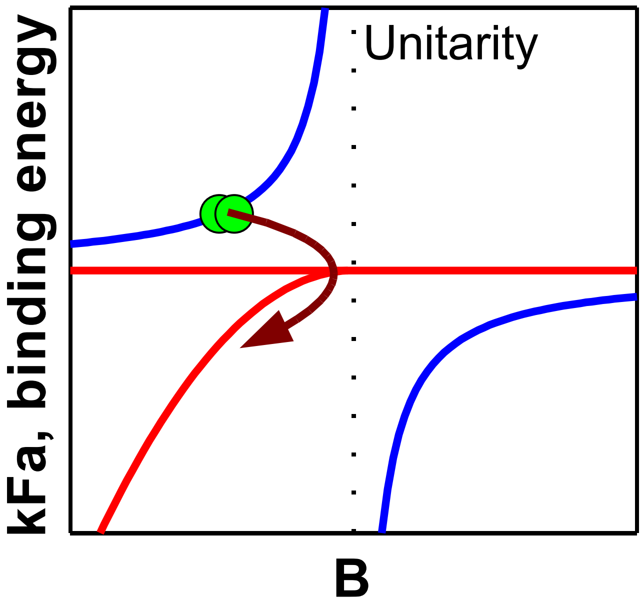


Conduit & Simons, PRB 2009

Experimental detection

- Three body losses inhibit stability of ferromagnetic state

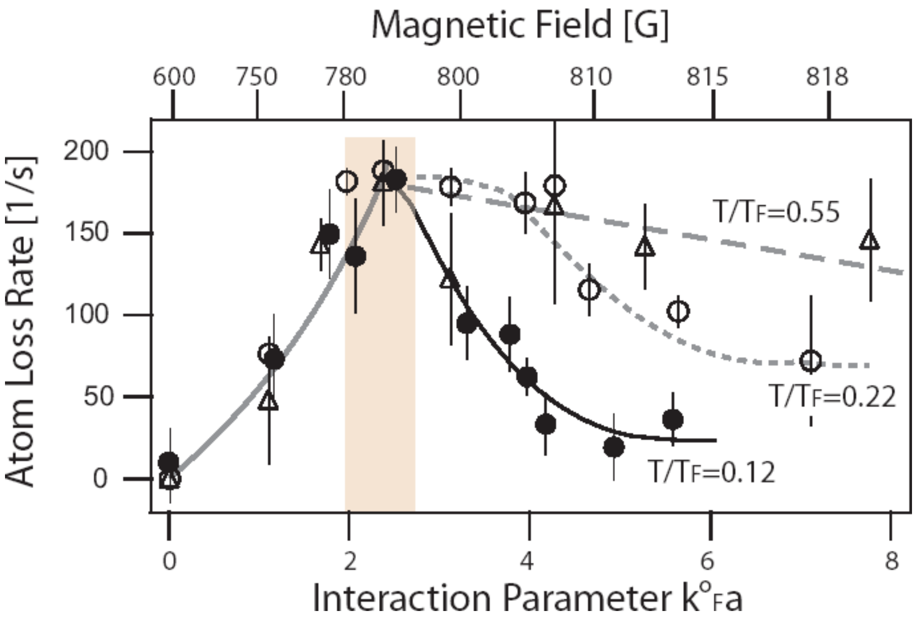




- Pauli exclusion prevents three-body losses in the ferromagnetic state
- Rather than disadvantage three-body losses can be a detection method of the absence of a ferromagnetic state, $a^6 n_\uparrow n_\downarrow$

Experimental study with cold atom gases

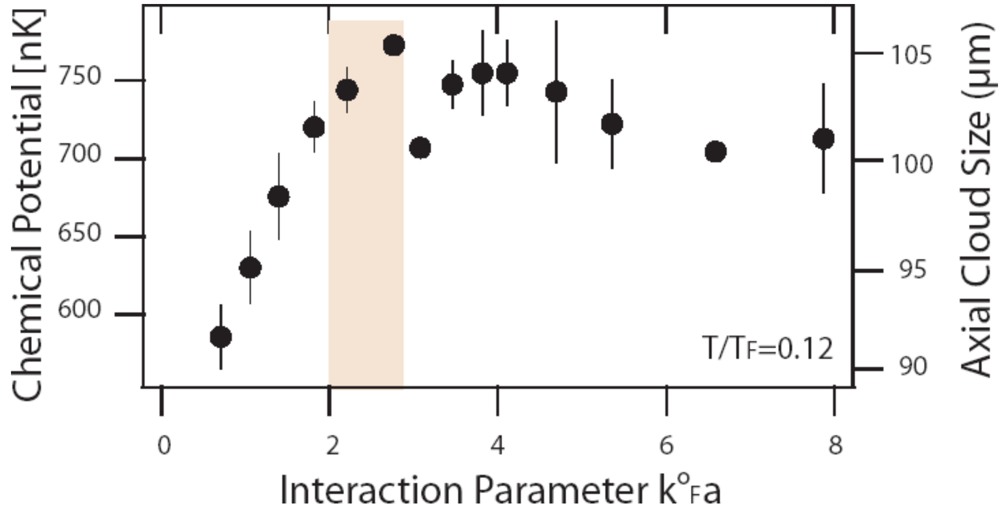
- G.-B. Jo and W. Ketterle have recently observed itinerant ferromagnetism in cold atom gases[1]
- Use ^{6}Li atoms and short 2.5ms ramp time
- Atom loss rate $a^6 n_\uparrow n_\downarrow$ is peaked at the transition



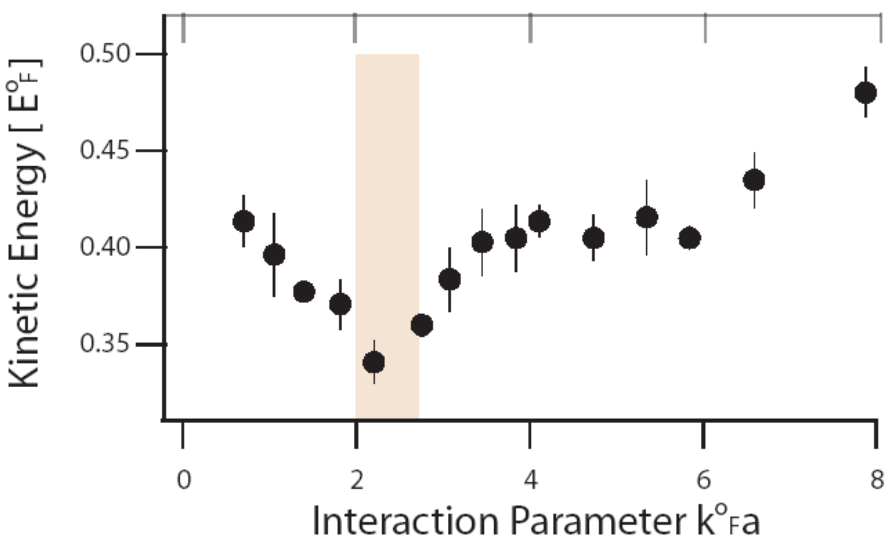
[1]Jo *et al.*, submitted 2009

Experimental study with cold atom gases

- Repulsive interactions increases the pressure, raising cloud size

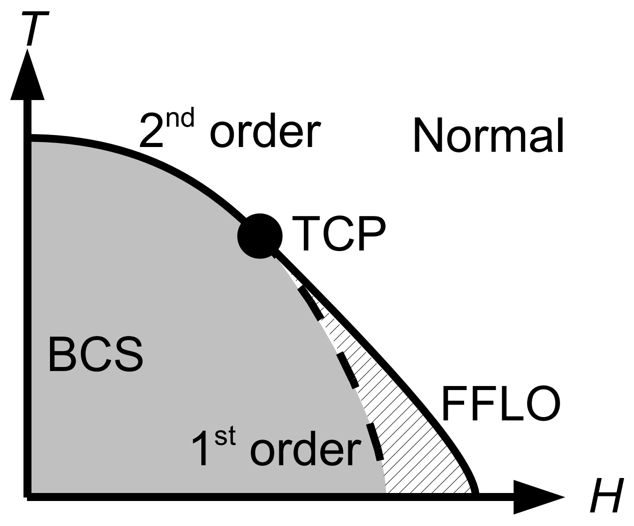


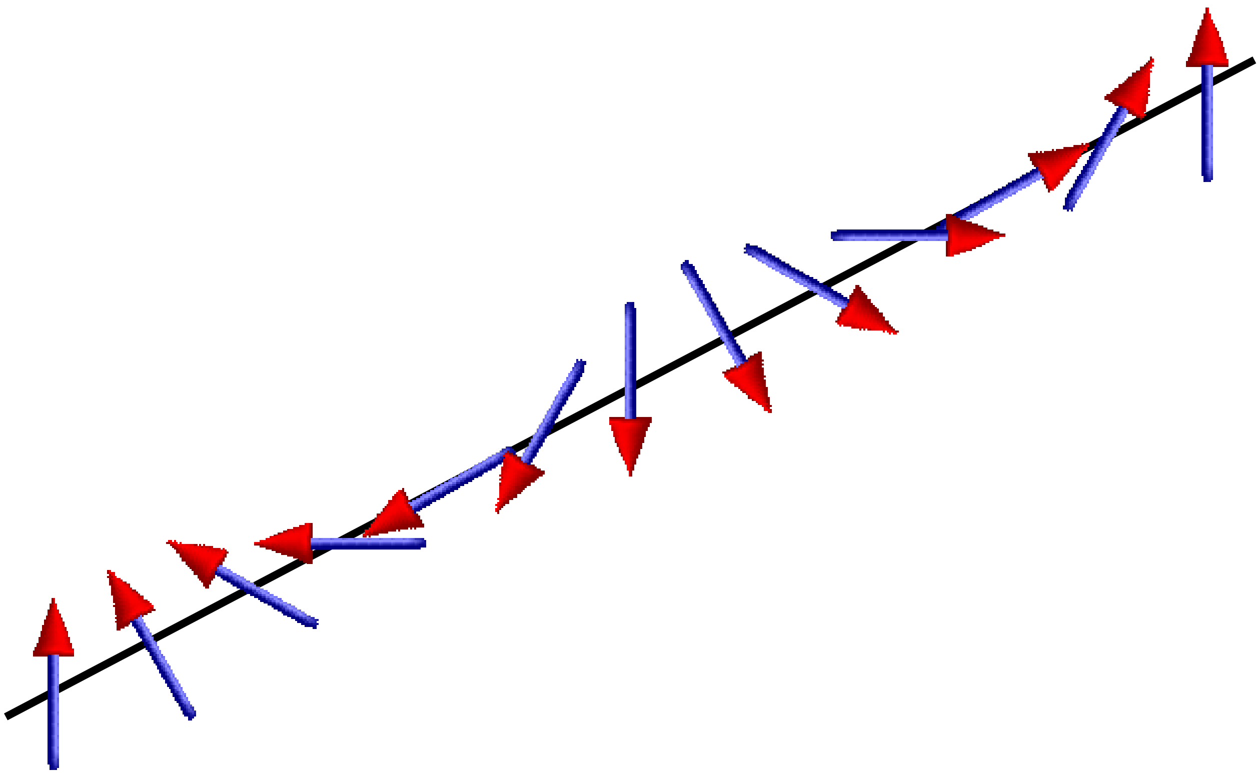
- But reducing the kinetic energy ~$n^{5/3}$ before the transition

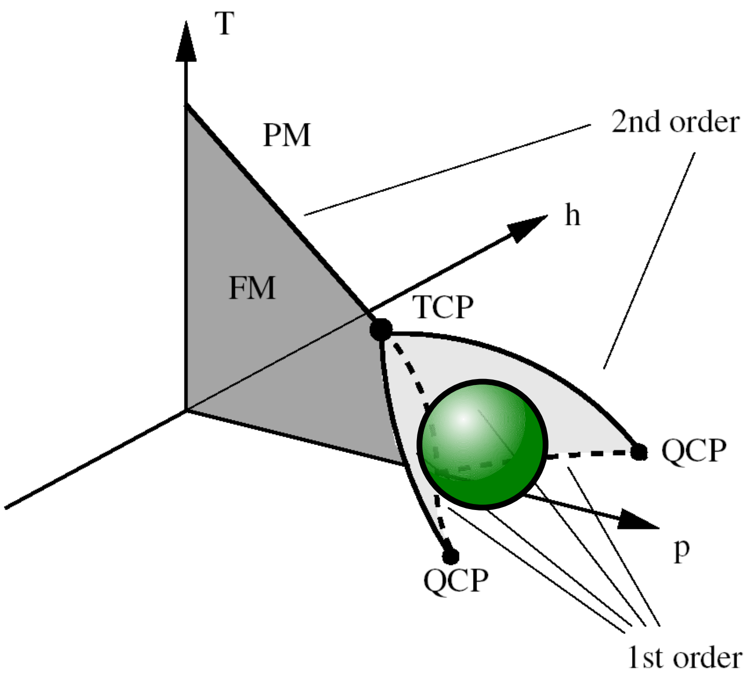


Summary of cold atoms work

- 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

Part I: Analyse uniform ferromagnetism for atomic gases

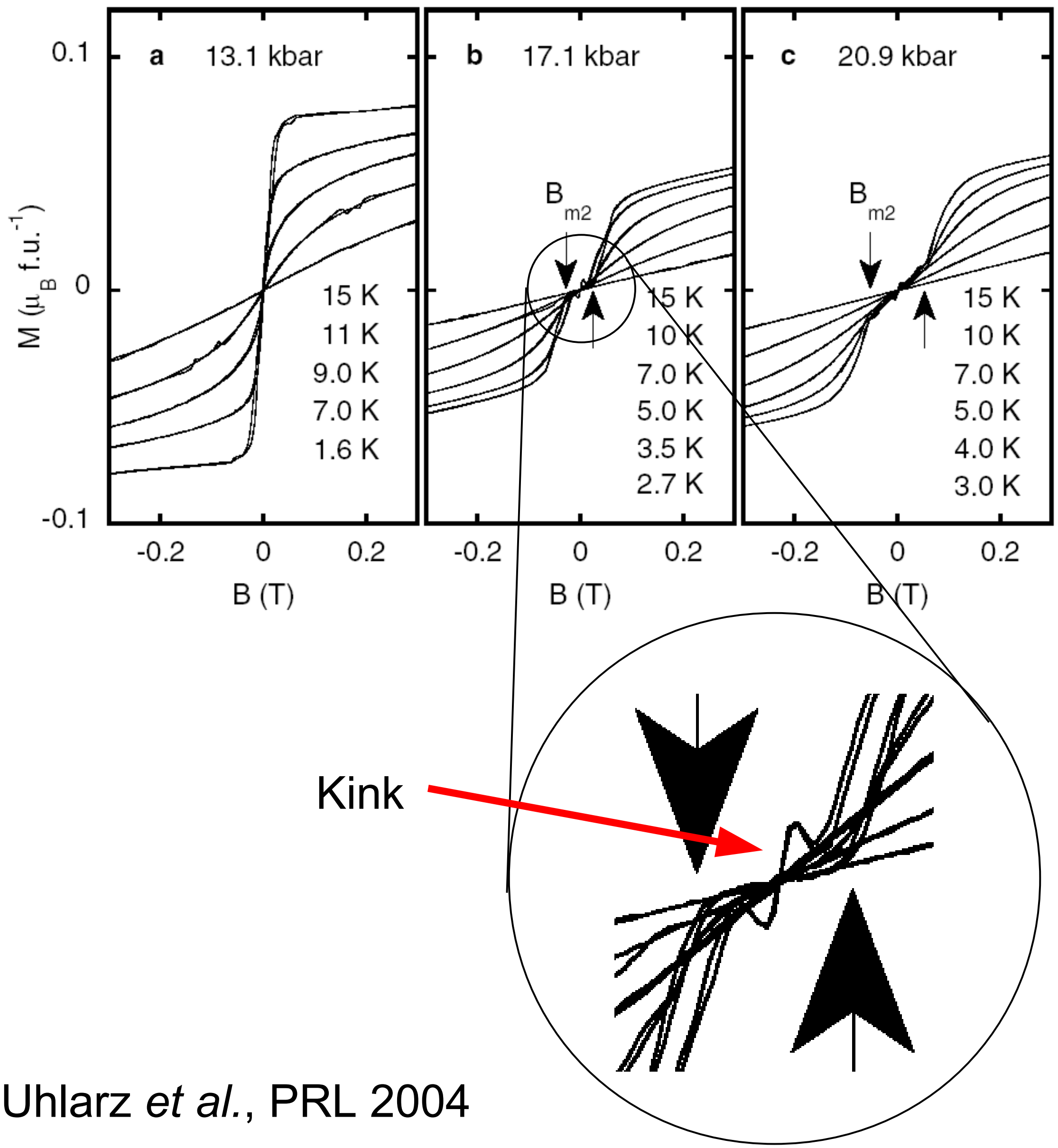
- Survey previous analytical work on itinerant ferromagnetism
- Demonstrate physical origin of first order transition
- Analyse population imbalance in cold atom gas
- Review ongoing cold atoms experiments

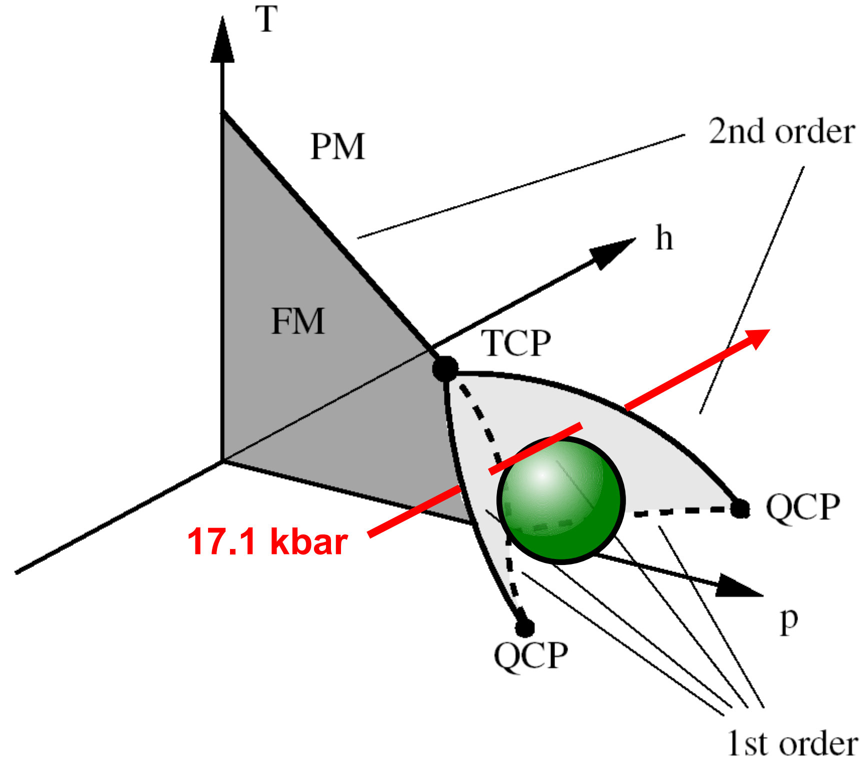
Part II: Search for inhomogeneous phase

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

$ZrZn_2$

- Kink in magnetisation indicative of novel phase behaviour





Uhlarz *et al.*, PRL 2004

Gauge transform analysis

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

$$F=\sum_{\sigma,\boldsymbol{k}} \epsilon^{\sigma}_{\boldsymbol{k},\boldsymbol{q}}\, n(\epsilon^{\sigma}_{\boldsymbol{k},\boldsymbol{q}}) + gN^{\uparrow}_{\boldsymbol{q}} N^{\downarrow}_{\boldsymbol{q}} - \frac{2\mathrm{g}^2}{V^3}\sum_{\boldsymbol{k}} \int\int \frac{\rho^{\uparrow}_{\boldsymbol{q}}(\boldsymbol{k},\epsilon_{\uparrow})\,\rho^{\downarrow}_{\boldsymbol{q}}(-\boldsymbol{k},\epsilon_{\downarrow})}{\epsilon_{\uparrow}+\epsilon_{\downarrow}}\, d\epsilon_{\uparrow}\, d\epsilon_{\downarrow}$$

$$+\frac{2\mathrm{g}^2}{V^3}\sum_{\boldsymbol{k}_{1,2,3,4}} \frac{n(\epsilon^{\uparrow}_{\boldsymbol{k}_1,\boldsymbol{q}})\, n_{\downarrow}(\epsilon^{\downarrow}_{\boldsymbol{k}_2,\boldsymbol{q}})}{\epsilon^{\uparrow}_{\boldsymbol{k}_1,\boldsymbol{q}}+\epsilon^{\downarrow}_{\boldsymbol{k}_2,\boldsymbol{q}}-\epsilon^{\uparrow}_{\boldsymbol{k}_3,\boldsymbol{q}}-\epsilon^{\downarrow}_{\boldsymbol{k}_4,\boldsymbol{q}}}\,\delta(\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_3)$$

- Modifies the electron dispersion

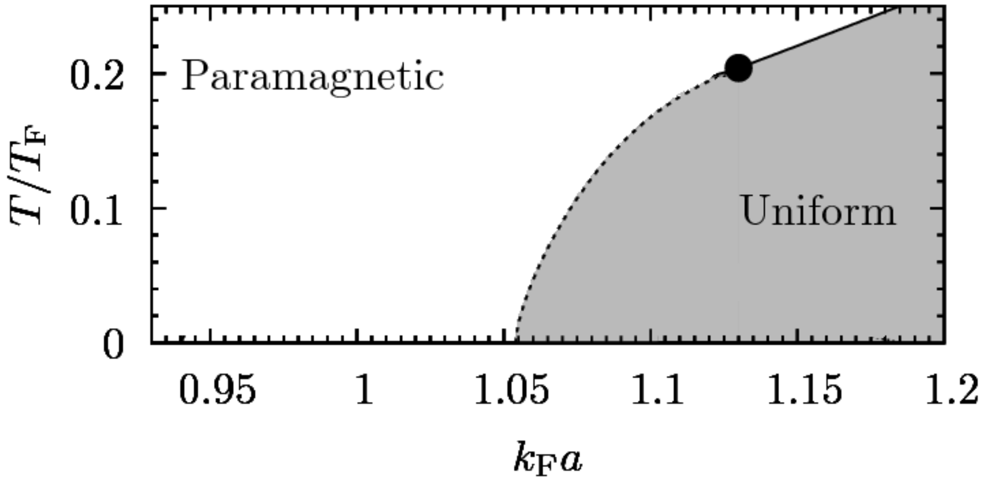
$$\epsilon^{\pm}_{\boldsymbol{p},\boldsymbol{q}}=\frac{\epsilon_{\boldsymbol{p}+\boldsymbol{q}/2}+\epsilon_{\boldsymbol{p}-\boldsymbol{q}/2}}{2}\pm\frac{\sqrt{(\epsilon_{\boldsymbol{p}+\boldsymbol{q}/2}-\epsilon_{\boldsymbol{p}-\boldsymbol{q}/2})^2+(2\,gm)^2}}{2}$$

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

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

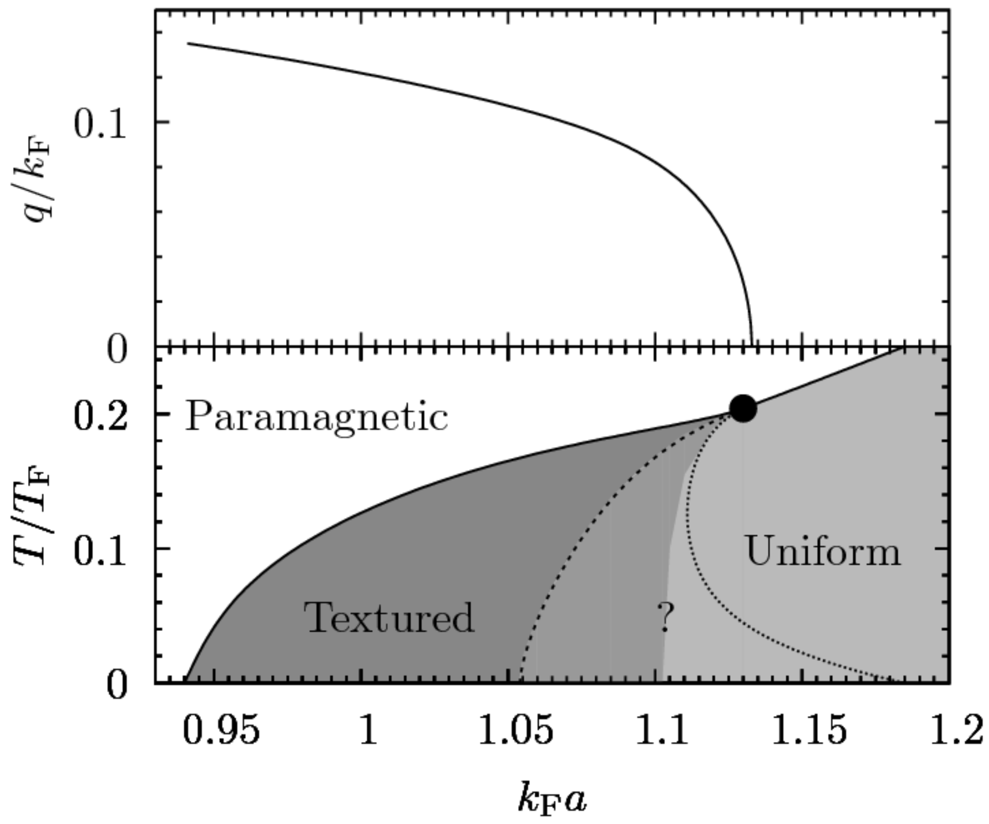
Results

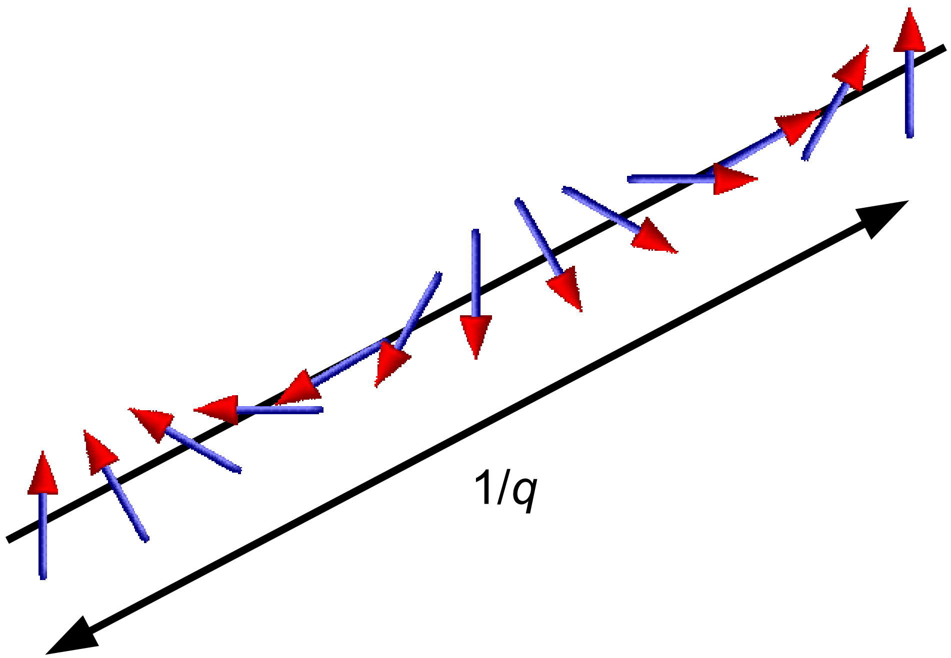
- Uniform ferromagnetic phase with tricritical point



Results

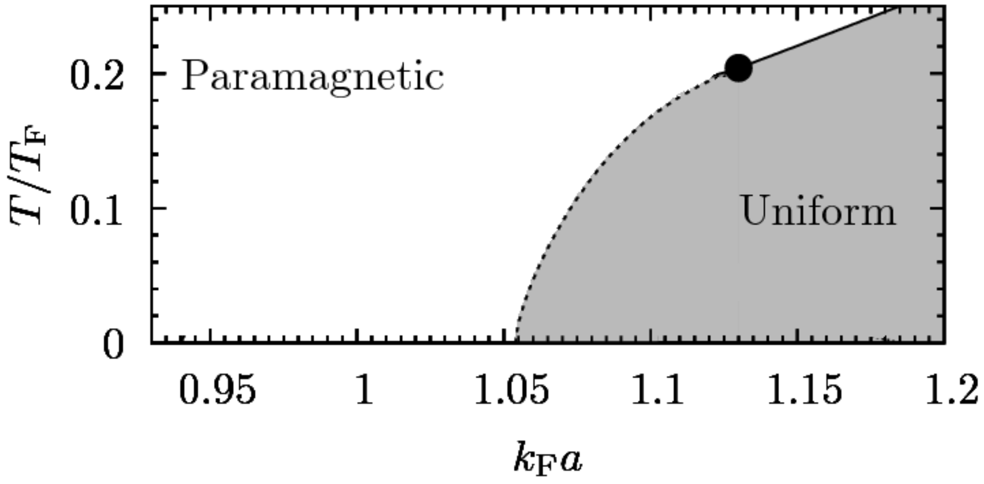
- Textured phase preempted transition with q=0.1k_F

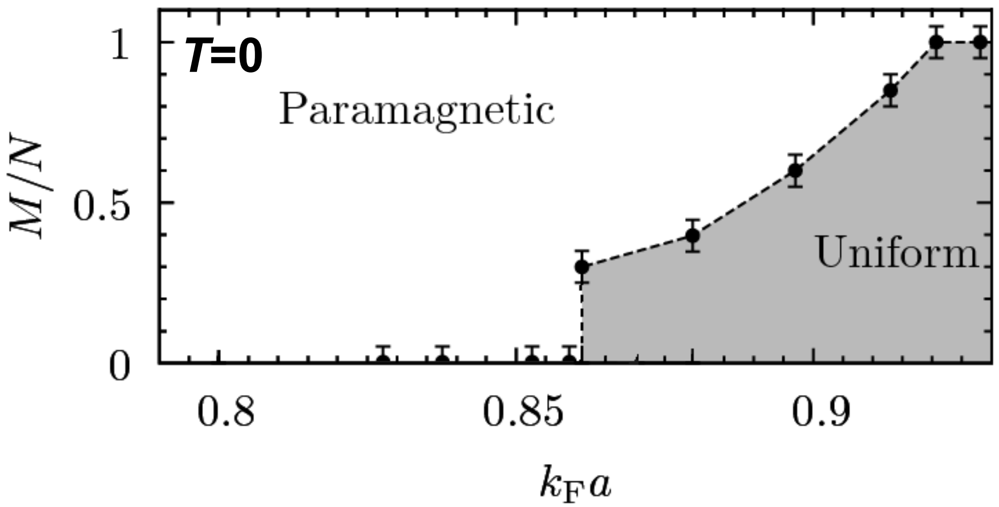




Quantum Monte Carlo: Uniform phase

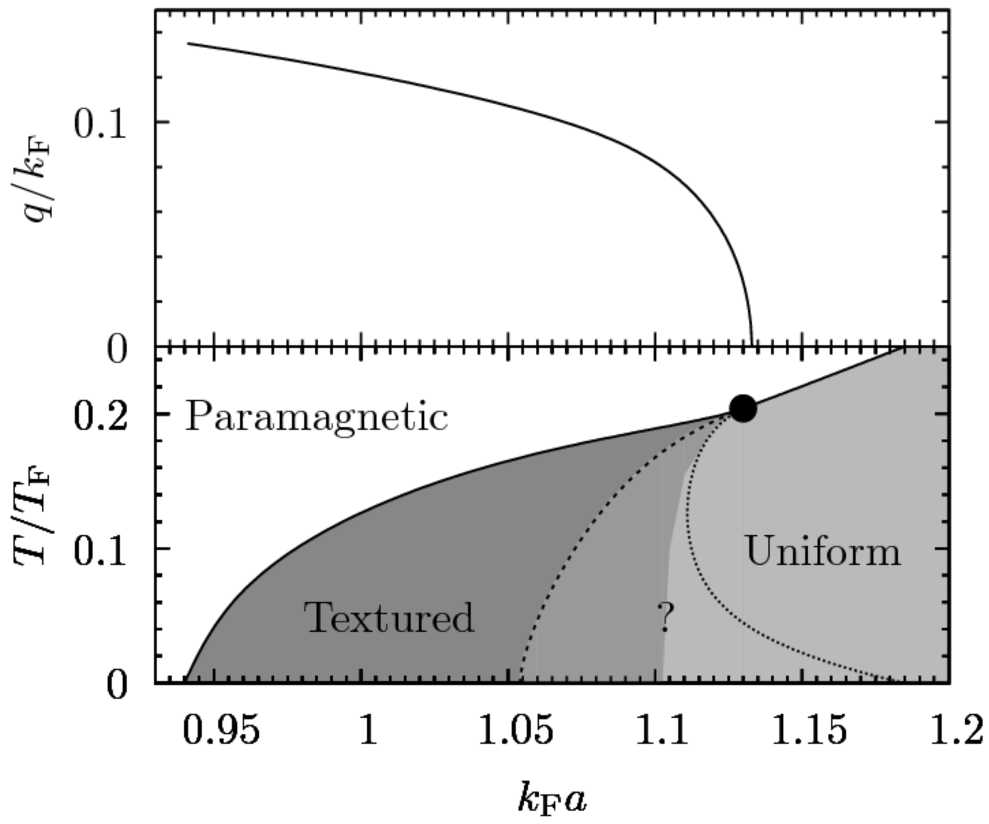
- First order transition into uniform phase

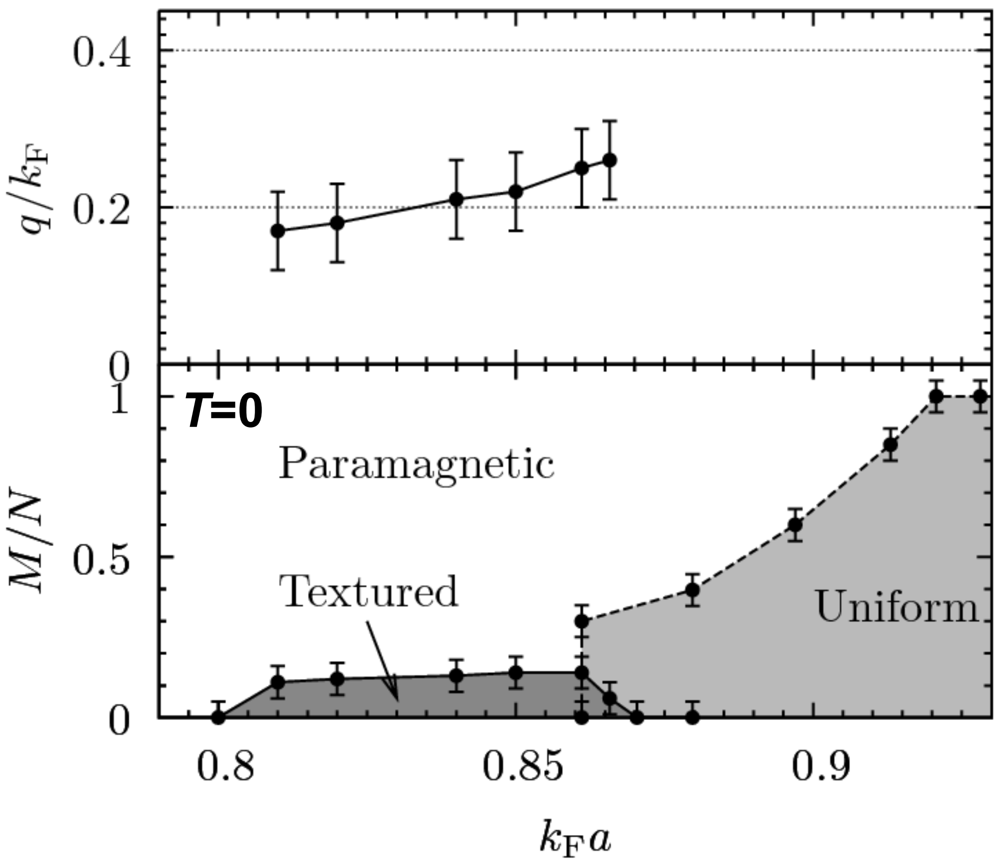




Quantum Monte Carlo: Textured phase

- Textured phase preempted transition with q=0.2k_F



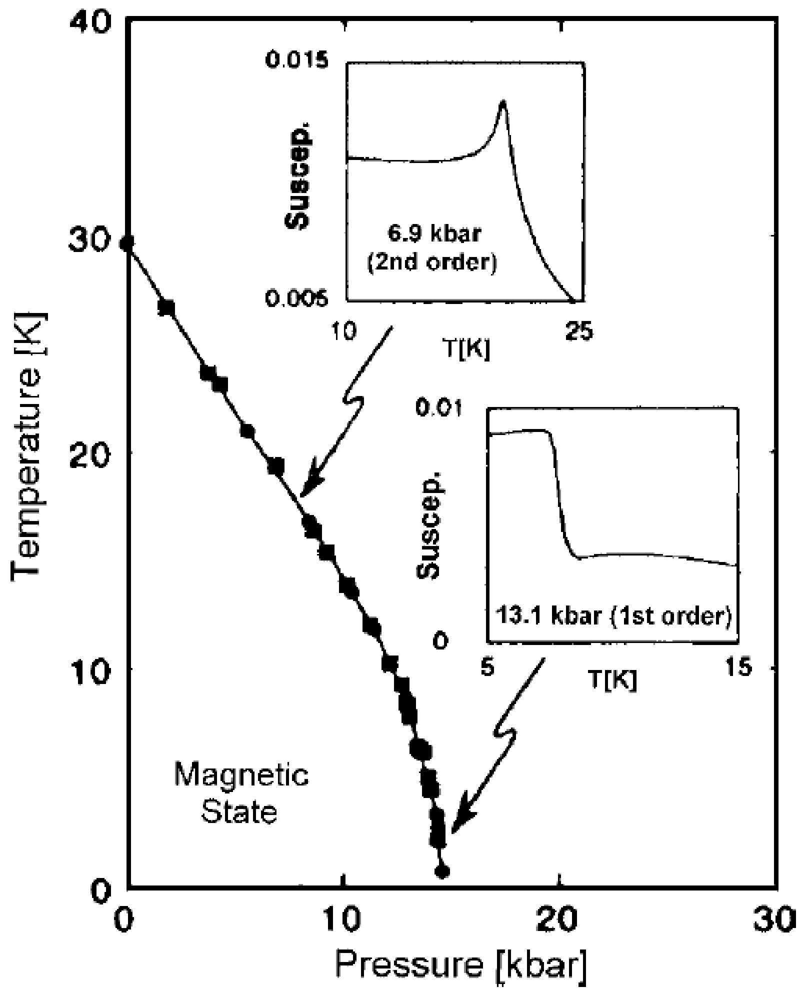


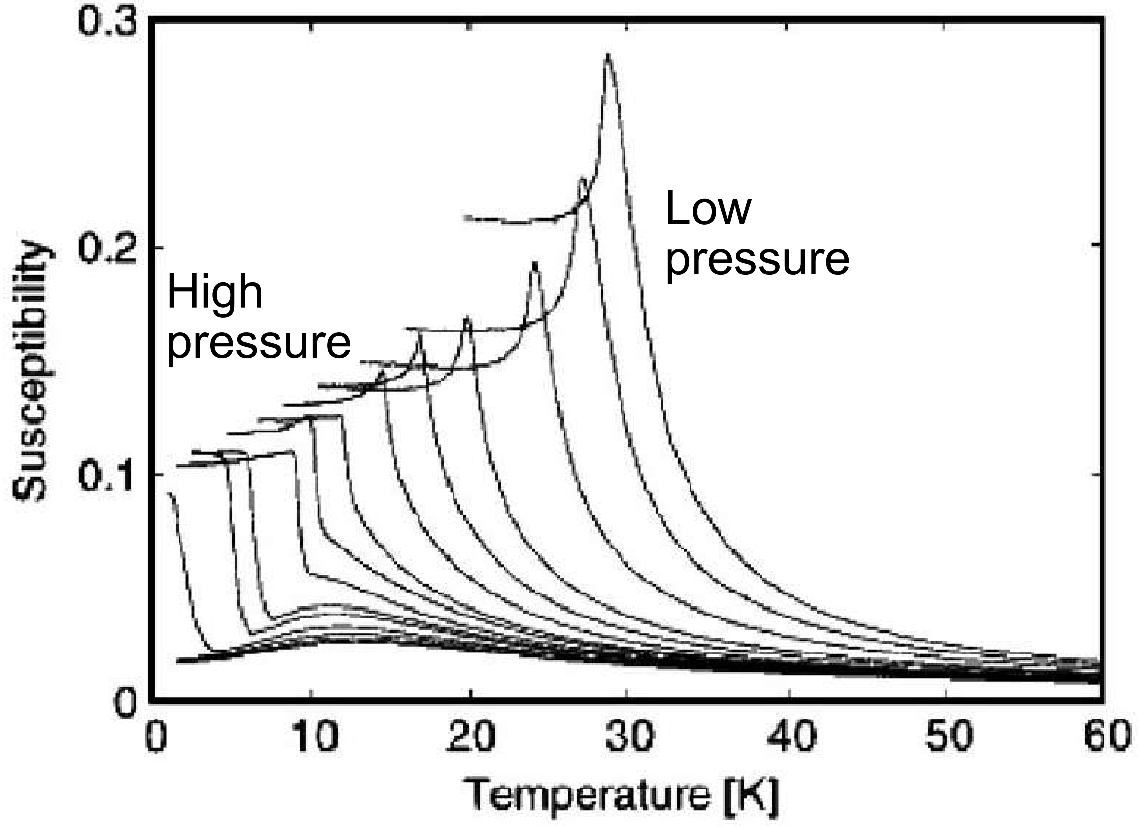
Summary

- Transfer from second to first order ferromagnetic transition at low temperature understood through soft transverse magnetic fluctuations
- Fluctuations responsible for development of nonanalytcities 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



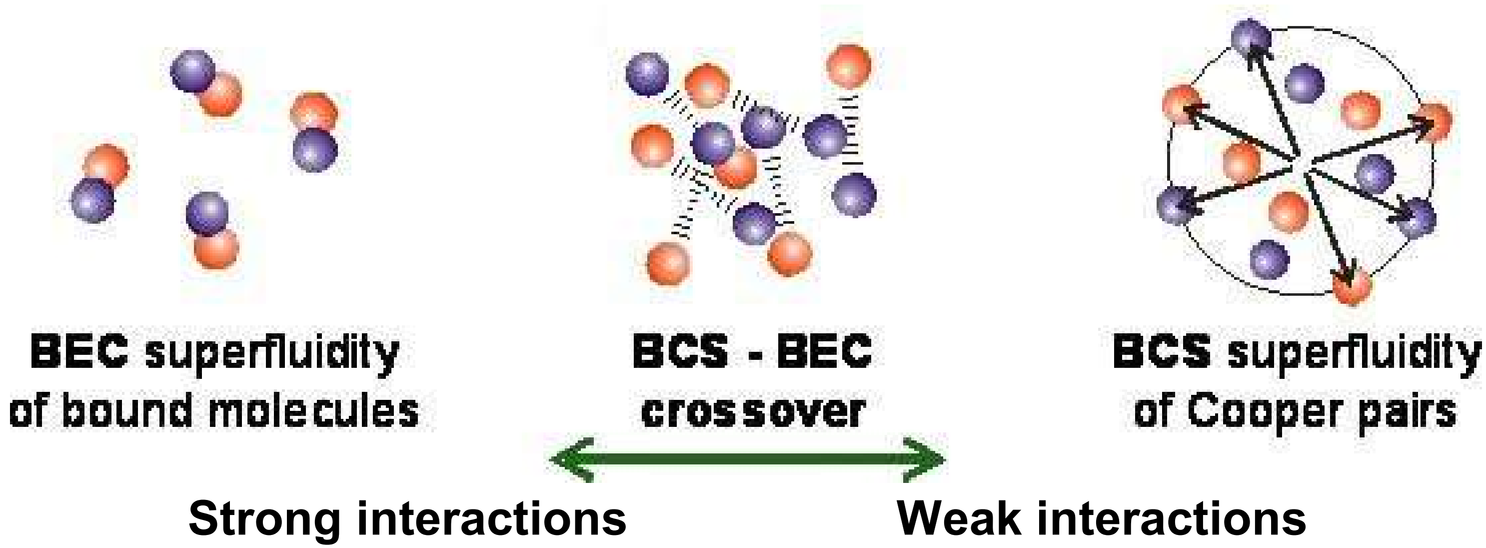


Pfleiderer *et al.*, PRB 1997

Pfleiderer *et al.*, PRB 1997
Vojta *et al.*, 1999 Ann. Phys. 1999

Cold atomic gases — interactions

- A gas of Fermionic atoms is laser and evaporatively cooled to ~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 allow us to investigate itinerant ferromagnetism

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

Cold atomic gases — spin

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

^{6}Li	$m_F=1/2$	maps to	spin 1/2
^{6}Li	$m_F=-1/2$	maps to	spin -1/2
^{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 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}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:

$\lvert\uparrow\uparrow\rangle$	S=1, S_z=1	State not possible as S_z has changed
$\lvert\downarrow\downarrow\rangle$	S=1, S_z=-1	State not possible as S_z has changed
$\left(\lvert\uparrow\downarrow\rangle+\lvert\downarrow\uparrow\rangle\right)/\sqrt{2}$	S=1, S_z=0	Magnetic moment in plane
$\left(\lvert\uparrow\downarrow\rangle-\lvert\downarrow\uparrow\rangle\right)/\sqrt{2}$	S=0, S_z=0	Non-magnetic state

- Ferromagnetism, if favourable, must form in plane

Integrating out electron fluctuations

- Partition function:

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

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

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

2) Integrate out electrons

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

Integrating out magnetisation fluctuations

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

3) Expand about uniform magnetisation *m*

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

4) Expand density and magnetisation fluctuations to second order

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

5) Integrate out density and magnetisation fluctuations

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

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

Result

- Final expression for the free energy

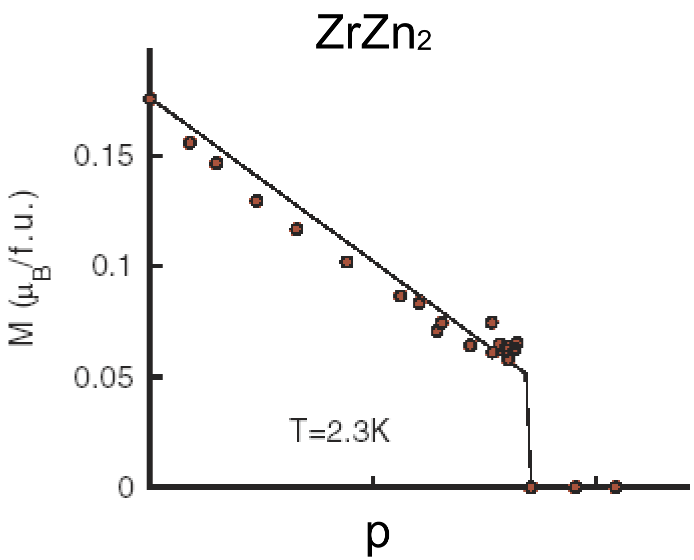
$$F = \sum_{\sigma,\boldsymbol{k}} \epsilon_{\boldsymbol{k}} n_\sigma(\epsilon_{\boldsymbol{k}}) + g N_\uparrow N_\downarrow$$

$$-\frac{2g^2}{V^3} \sum_{\boldsymbol{k}_{1,2,3,4}} \frac{n_\uparrow(\epsilon_{\boldsymbol{k}_1}) n_\downarrow(\epsilon_{\boldsymbol{k}_2}) [n_\uparrow(\epsilon_{\boldsymbol{k}_3}) + n_\downarrow(\epsilon_{\boldsymbol{k}_4})]}{\epsilon_{\boldsymbol{k}_1} + \epsilon_{\boldsymbol{k}_2} - \epsilon_{\boldsymbol{k}_3} - \epsilon_{\boldsymbol{k}_4}} \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 - \boldsymbol{k}_3 - \boldsymbol{k}_3)$$

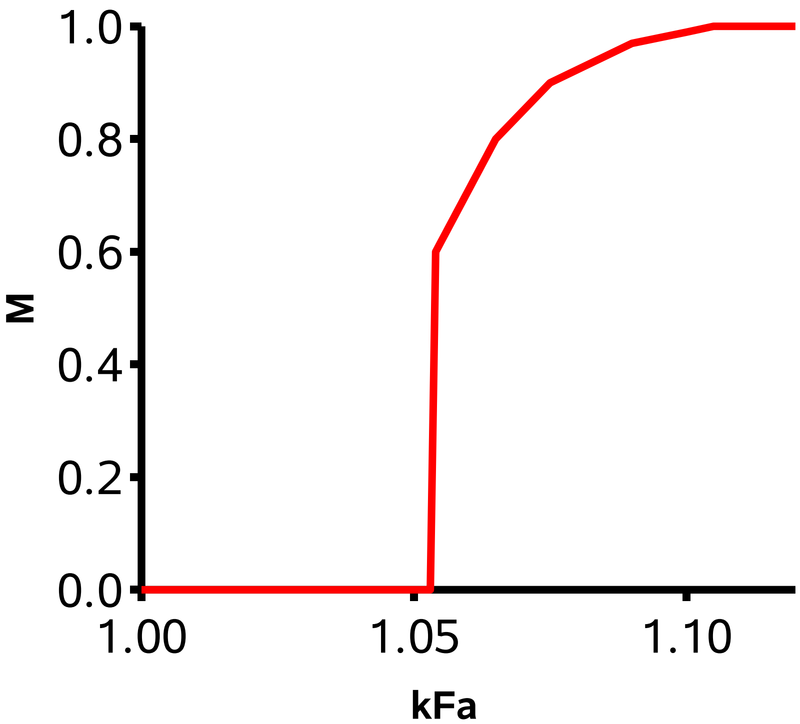
is identical to second order perturbation theory [Abrikosov 1958, Lee & Yang 1960, Mohling, 1961, Duine & MacDonald, 2005]

Ferromagnetic transition

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

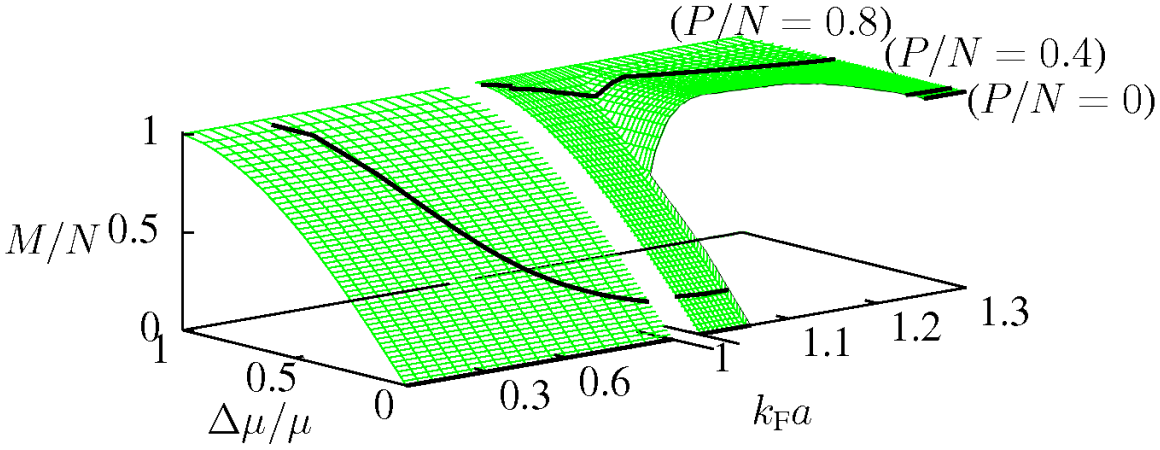


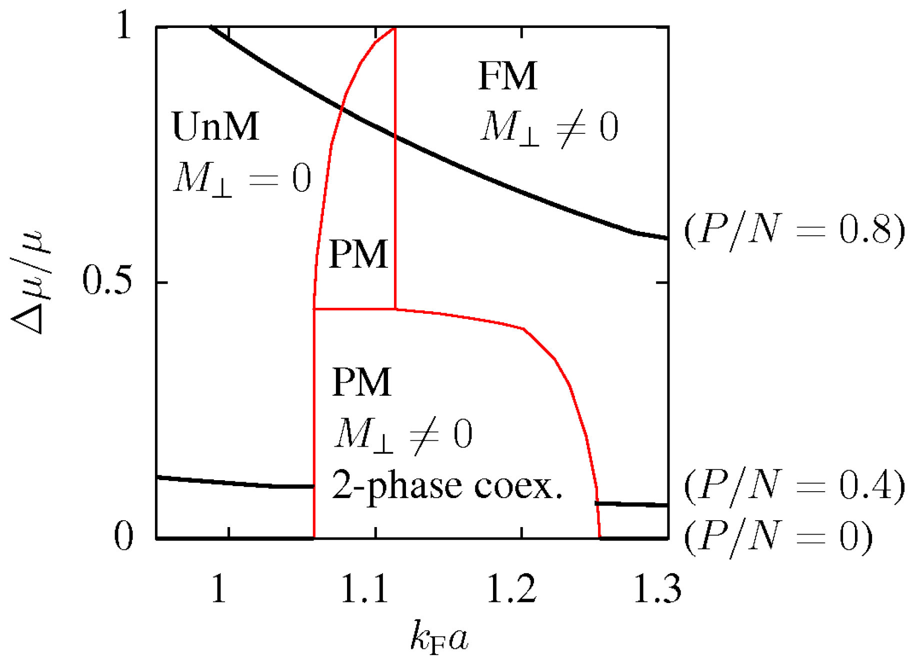
Uhlarz *et al.*, PRL 2004



Grand canonical ensemble

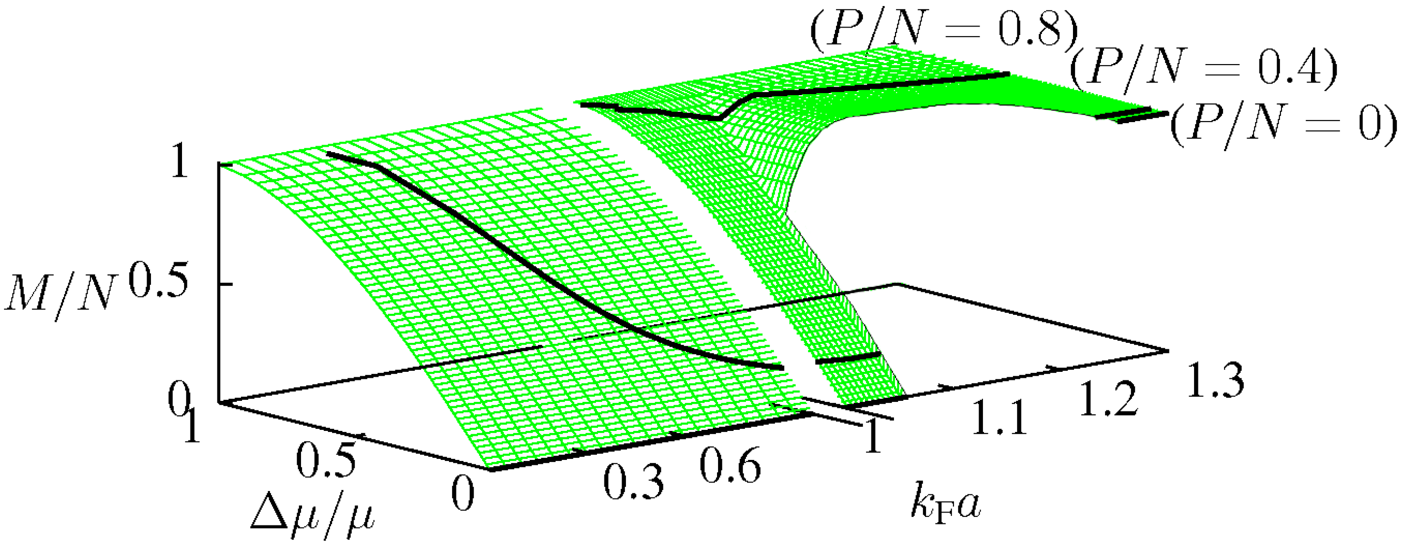
- In the grand canonical ensemble we obtain

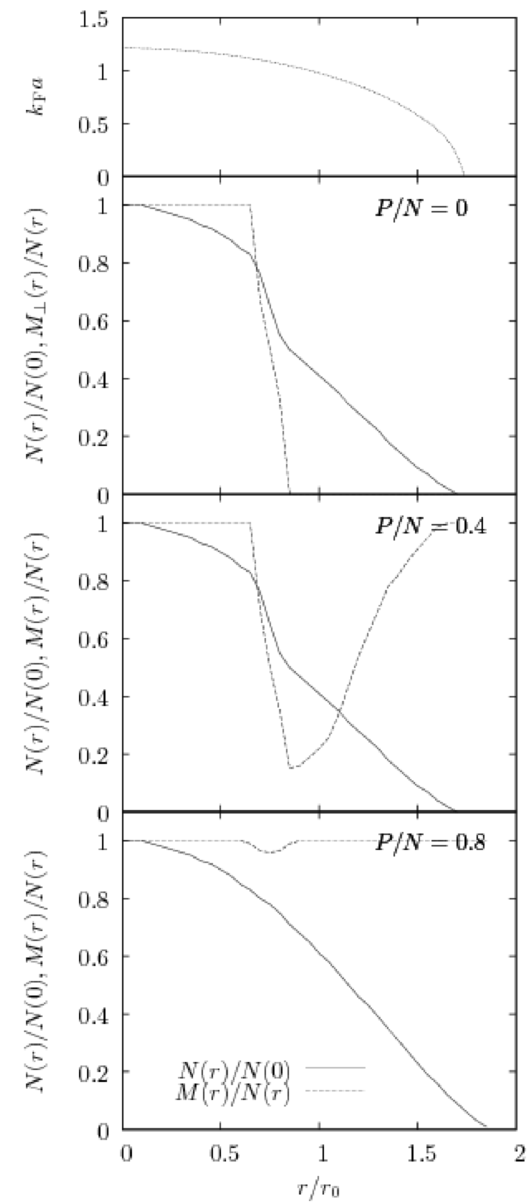




Trap behaviour

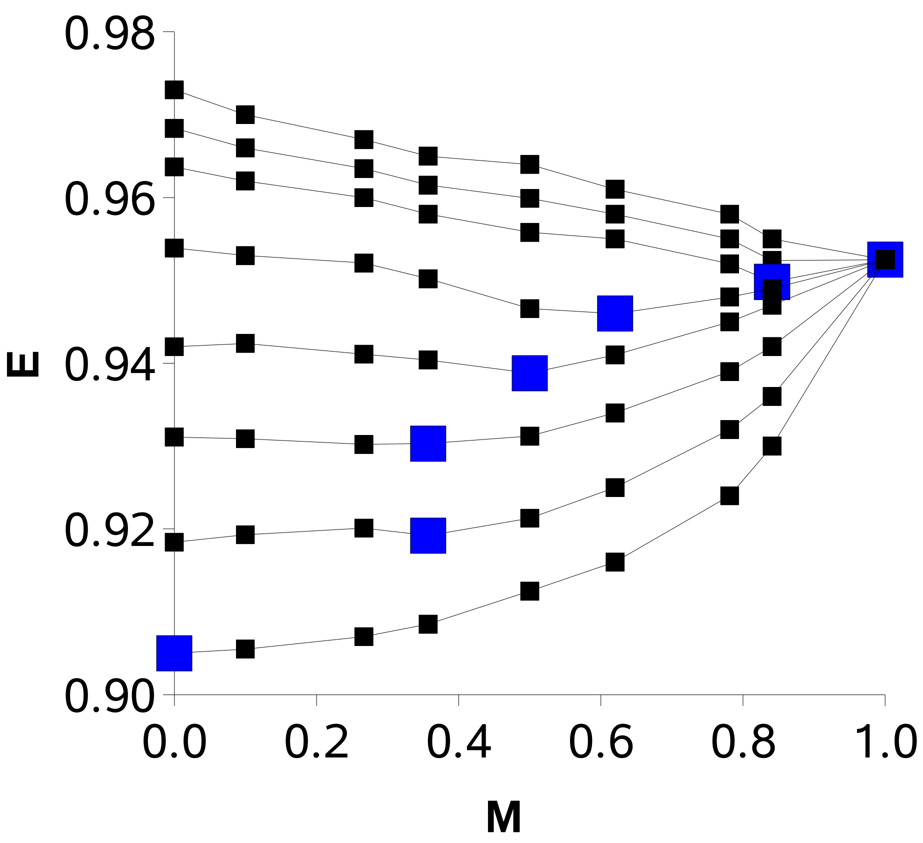
- Trap behaviour corresponds to three trajectories in the phase diagram

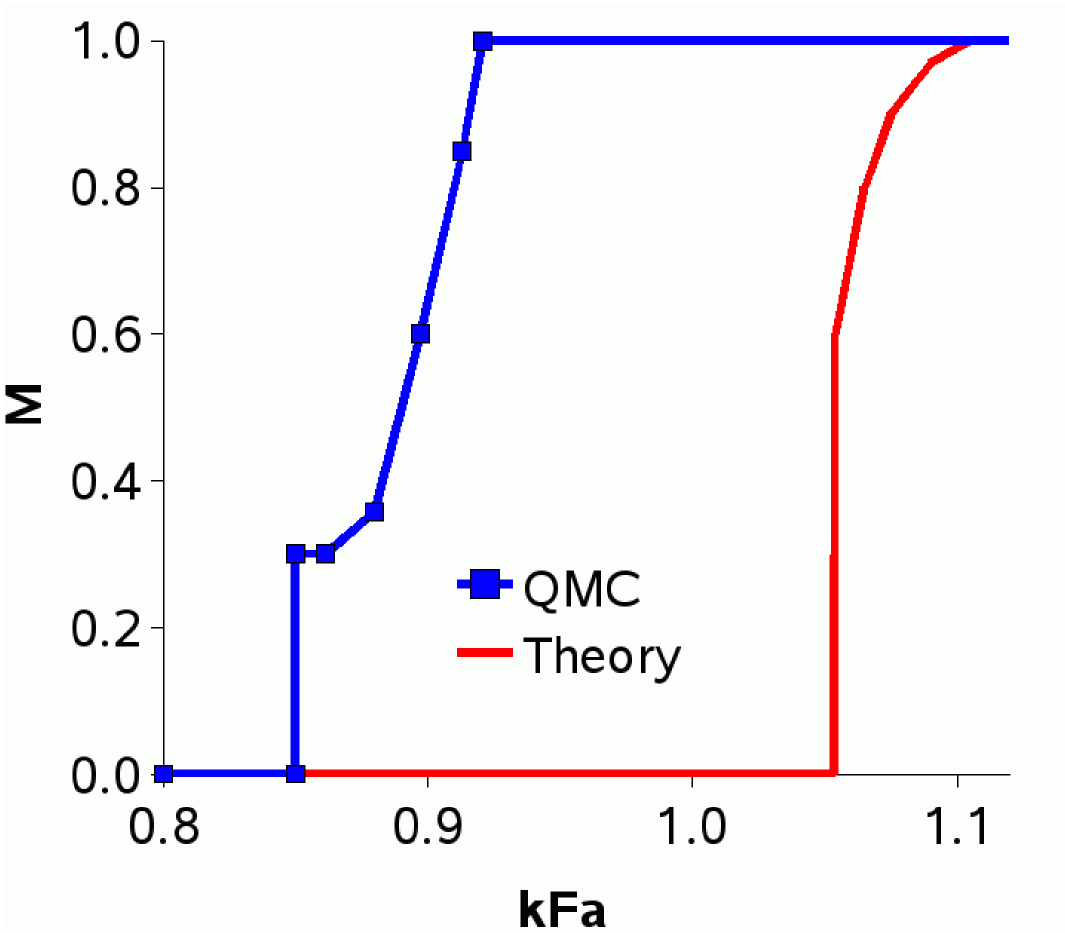




QMC calculations

- 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

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

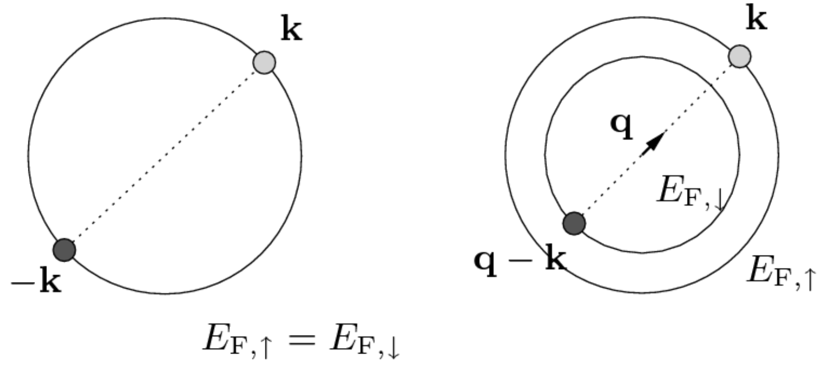
- The coupling of fields[1] can drive a transition first order

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

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

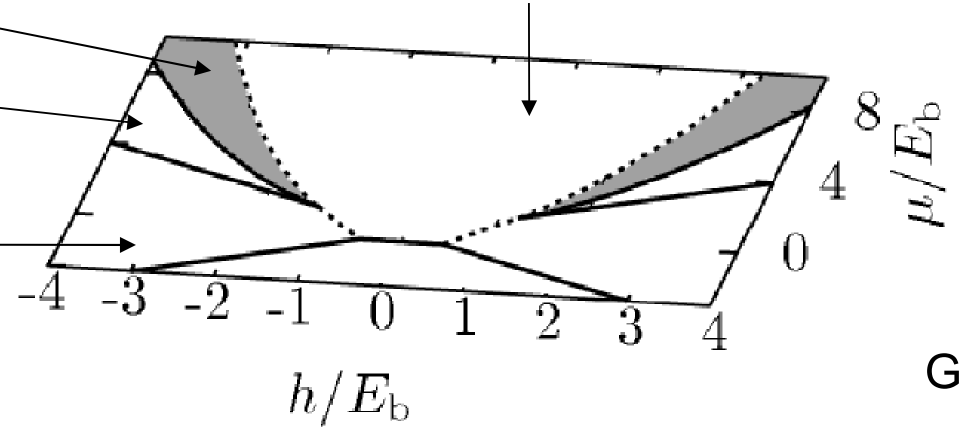
FFLO

- 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

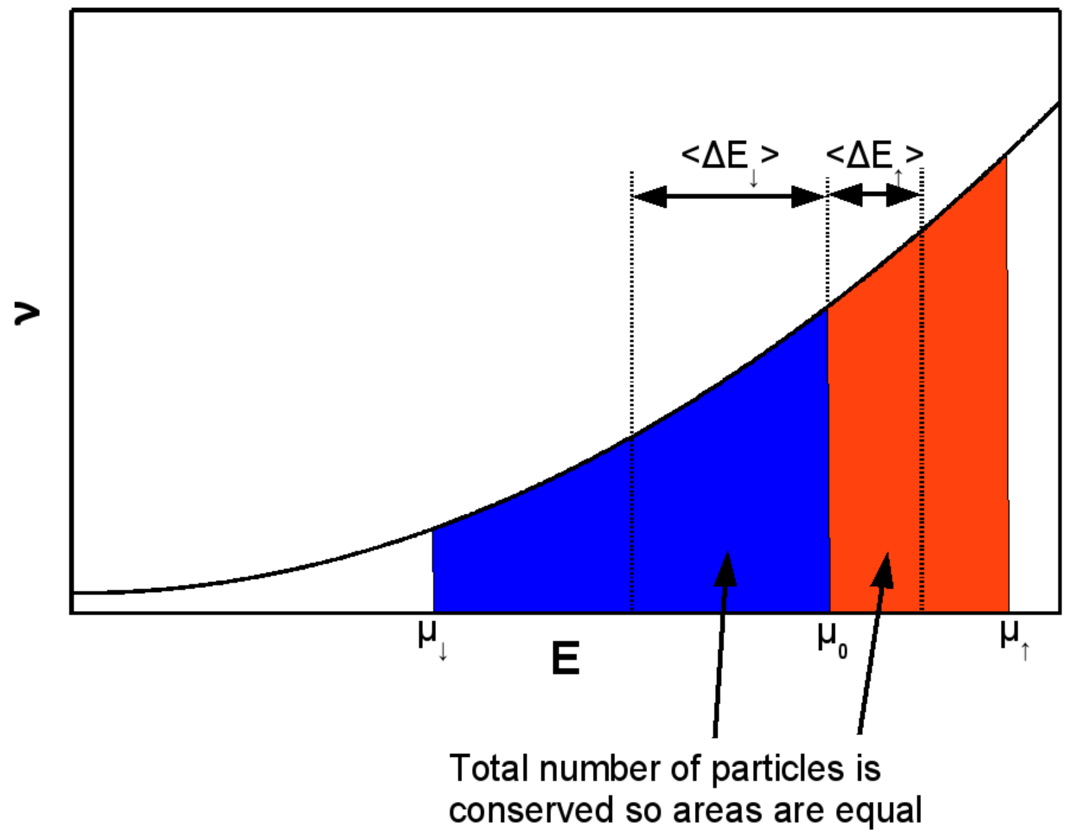


GJC *et al*. PRB 2008

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]

$$\nu\nu'' > 3(\nu')^2$$



Improved Wohlfarth Rhodes criterion

- Accounting for changes in the energy spectrum ε gives criterion

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

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

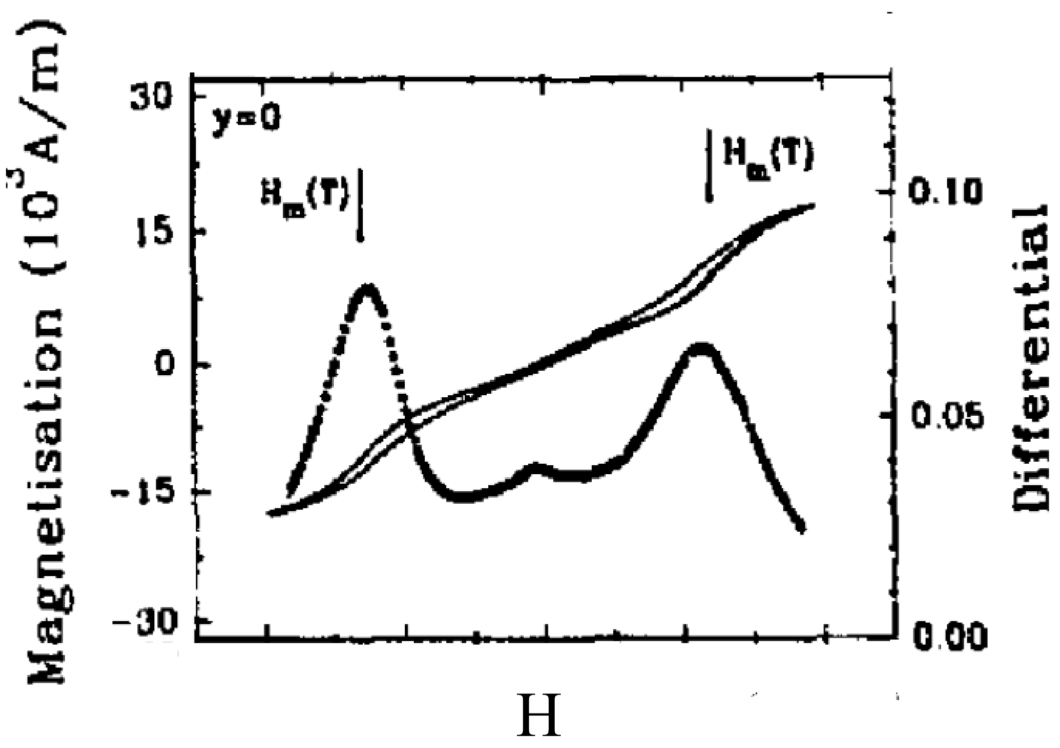
- The terms have magnitude

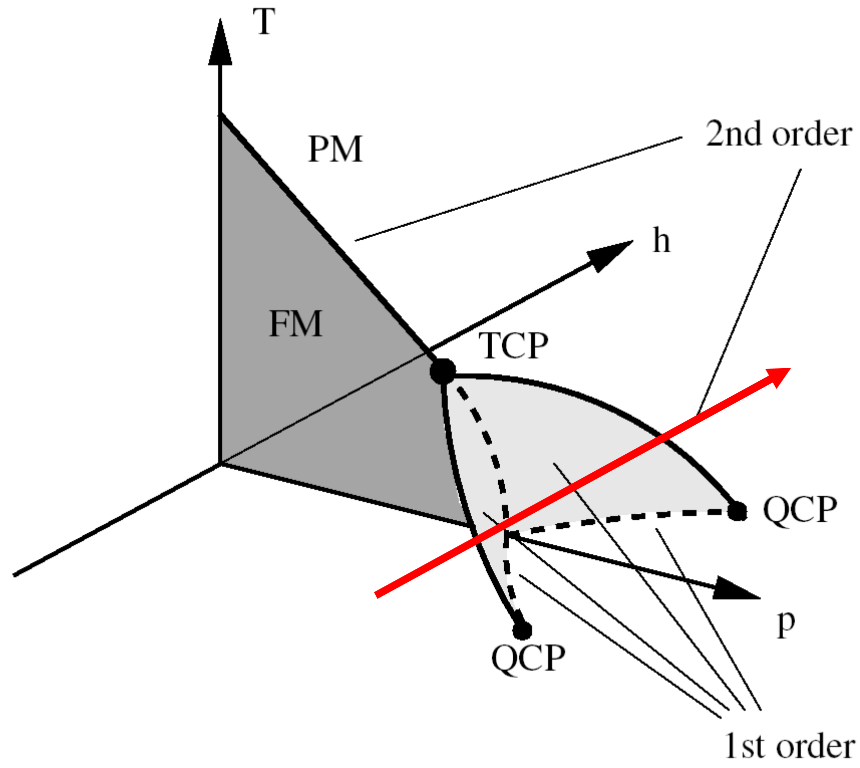
Term	Expansion
$\int_0^u \varepsilon^{(0,4)}(w,0)\mathrm{d}w$	$0.0k_\mathrm{F}a + 0.0086(k_\mathrm{F}a)^2$
$4\varepsilon^{(0,3)}(u,0)$	$0.0k_\mathrm{F}a - 0.04(k_\mathrm{F}a)^2$
$6\varepsilon^{(1,2)}(u,0)$	$0.024(k_\mathrm{F}a)^2$
$4\varepsilon^{(2,1)}(u,0)$	$0.0(k_\mathrm{F}a)^2$
$\varepsilon^{(3,0)}(u,0)$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

Transition due to changing energy spectrum at the Fermi surface (→ $4\varepsilon^{(0,3)}(u,0)$ row)

$NbFe_2$

- $NbFe_2$ displays antiferromagnetic order where it is expected to be ferromagnetic — could this be a textured ferromagnetic phase?

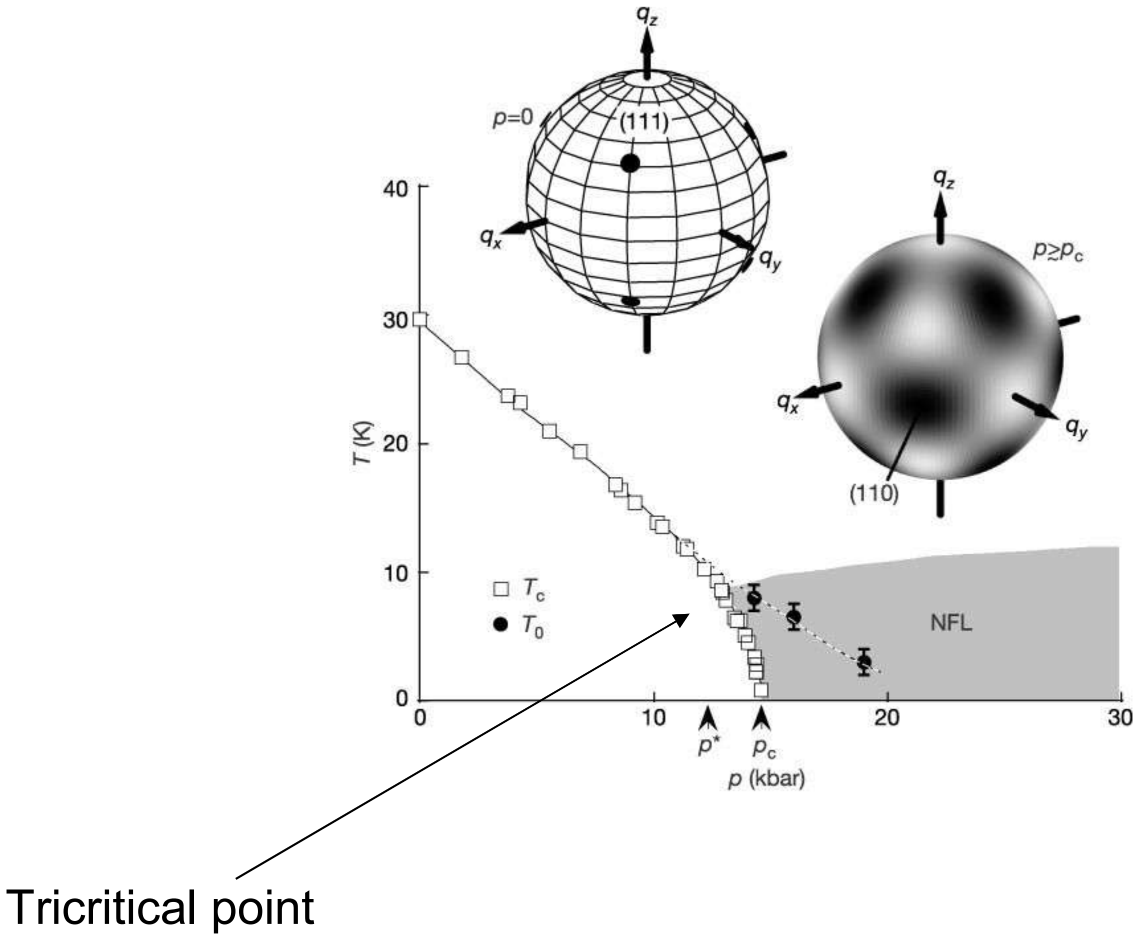




Crook & Cywinski, JMMM 1995

MnSi

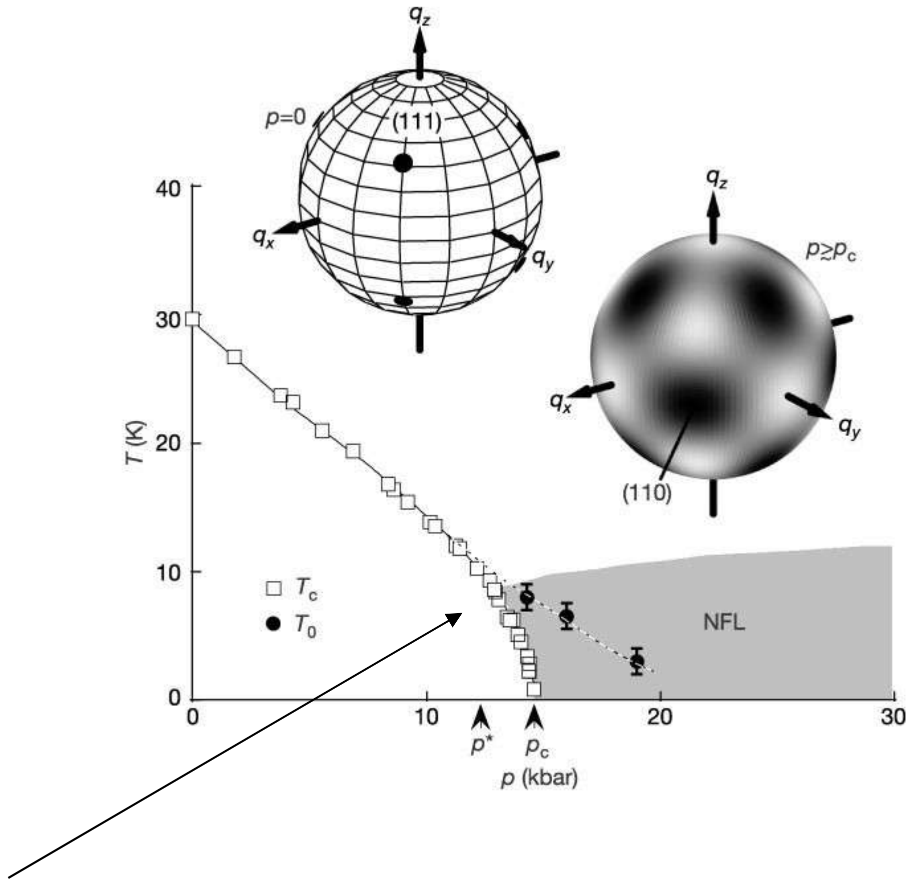
- MnSi displays non-Fermi liquid behaviour consistent with a spin state (though in a non-centrosymmetric crystal)



Pfleiderer *et al.*, Nature 2004

MnSi

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

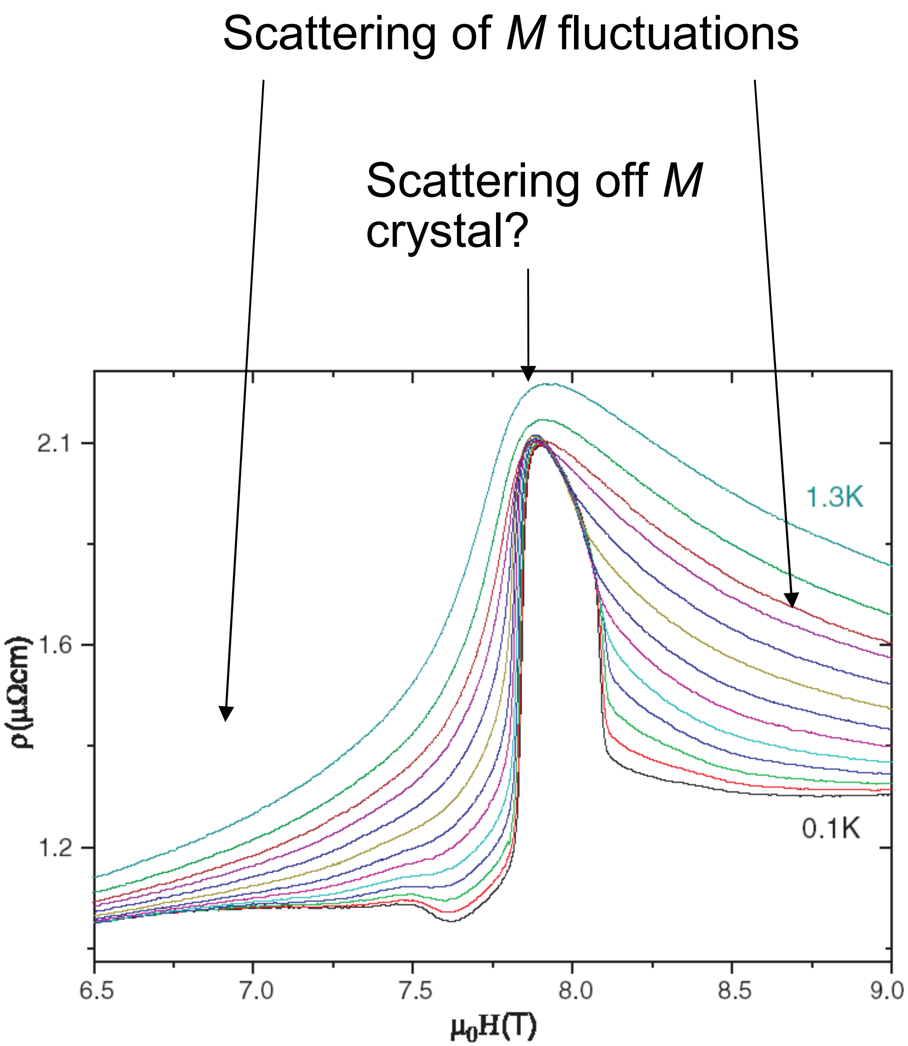


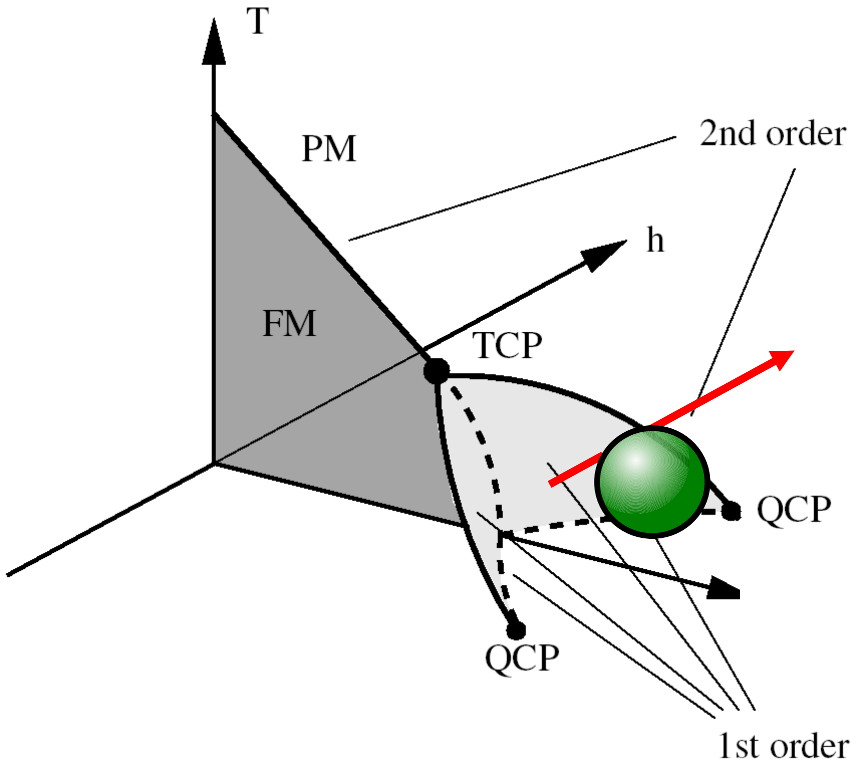
Tricritical point

Pfleiderer *et al.*, Nature 2004

$Sr_3Ru_2O_7$

- Resistance anomaly



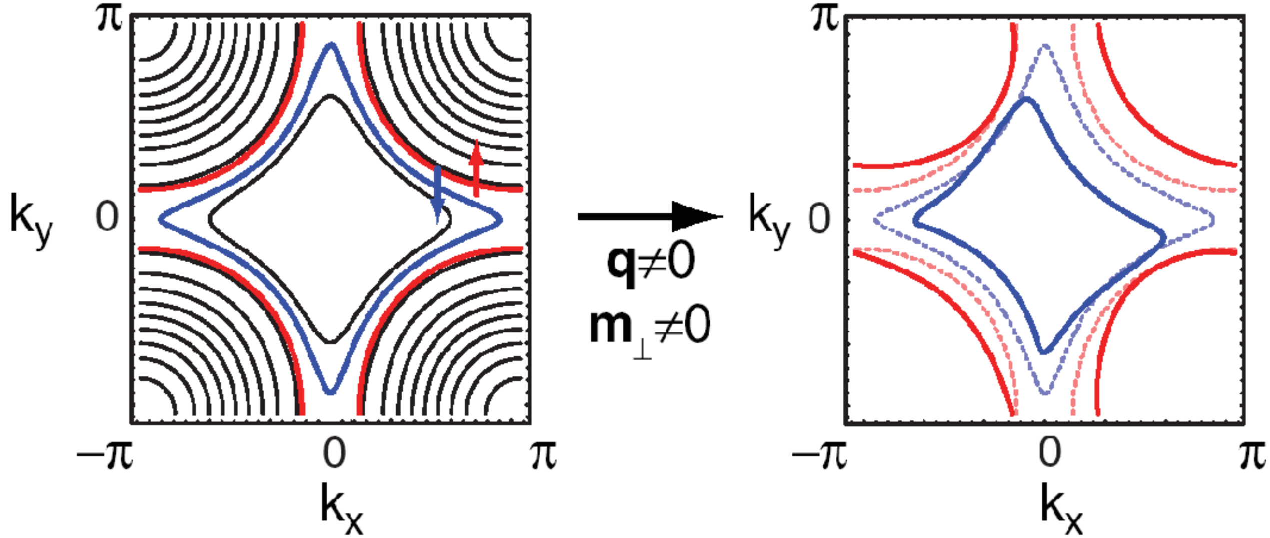


- Consistent with a new crystalline phase

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

$$\psi\to \mathrm{e}^{\frac{1}{2} i\,\boldsymbol{q}\cdot\boldsymbol{r}\,\sigma_z}\psi$$

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

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

- Diagonalisation gives the energies relative to a spiral

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

which replaces $\varepsilon_{\boldsymbol{p}}\pm gm$ in the uniform case

- Analysis then proceeds as before

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

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

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

- Single determinant not exact spin eigenstate in finite sized system

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

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