The magnetic RKKY-interaction in the superconducting phase of thulium borocarbide

by Jens Jensen, Ørsted Laboratory

Collaborators:

Risø:

Niels Hessel Andersen

Katrine Nørgaard
Morten Ring Eskildsen
Stine Nyborg Klausen
Kim Lefmann

Ørsted Laboratory:

Per Hedegård
Thorsten Hansen

Ames Laboratory:

Paul C. Canfield

Posters:

Katrine Nørgaard: "Exotic interplay between magnetism and superconductivity in $TmNi_2B_2C$" (FF38P).

Thorsten Hansen: "Ferromagnetic vortex cores in $TmNi_2B_2C$" (FF40p).

Outline of the talk

- Introduction
- The RKKY-interaction
- The RKKY-interaction in a BCS-superconductor
- The upper critical field in $TmNi_2B_2C$ (paramagnetic phase)
- The c-axis phase diagram of $TmNi_2B_2C$
- Neutron experiment on $TmNi_2B_2C$
  - field along the a-axis -
- The a-axis phase diagram of $TmNi_2B_2C$
- The spin-density wave induced via the RKKY-interaction
- The total free energy as a function of the magnetic ordering wave vector
- Conclusion

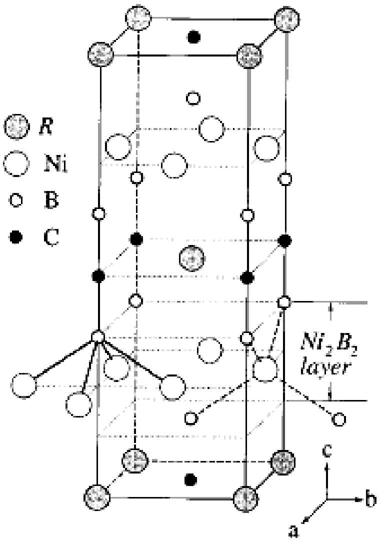
Introduction

The coexistence of superconductivity and antiferromagnetic ordering in the **rare-earth nickel borocarbides** ($R\,Ni_2B_2C$) discovered 1994.

More well-defined systems than the Chevrel-phase ($R\,Mo_6S_8$) and rhodium borides ($R\,Rh_4B_4$) studied 20 years ago.

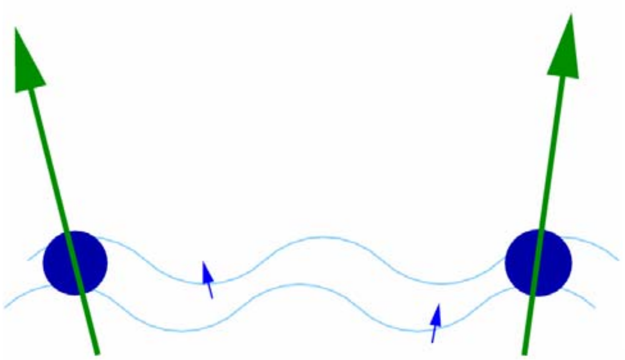
Crystal structure of
$R\,Ni_2B_2C$

body-centered-tetragonal
(I4/mmm)

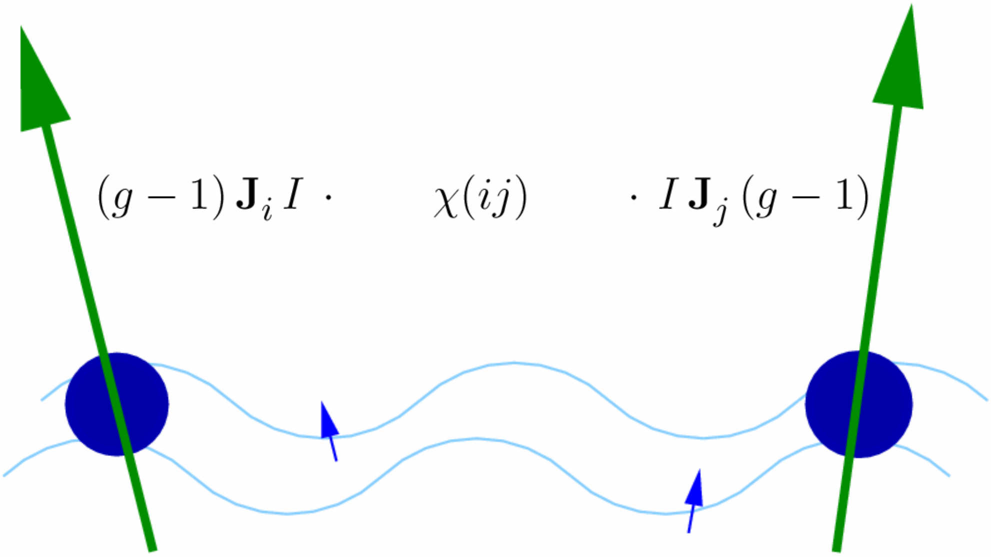


Magnetic moments:
Localized 4f-electrons on the rare-earth ions
interacting via the metallic electrons:

The RKKY:



The RKKY interaction



$$(g-1)\,\mathbf{J}_i\,I\;\cdot\qquad\chi(ij)\qquad\cdot\;I\,\mathbf{J}_j\,(g-1)$$

$$\mathcal{H}_{\mathrm{H}} = -\tfrac{1}{2}\sum_{i,j}\mathcal{J}(ij)\mathbf{J}_i\cdot\mathbf{J}_j$$

$$\mathcal{J}(\mathbf{q}) = \sum_{\boldsymbol{\tau}}|j(\mathbf{q}+\boldsymbol{\tau})|^2\chi(\mathbf{q}+\boldsymbol{\tau}) - \frac{1}{N}\sum_{\mathbf{q}'}\sum_{\boldsymbol{\tau}}|j(\mathbf{q}'+\boldsymbol{\tau})|^2\chi(\mathbf{q}'+\boldsymbol{\tau})$$

$j(\mathbf{q}) = (g-1)I(\mathbf{q})$, $\boldsymbol{\tau}$ is a reciprocal lattice vector.

In the normal phase the susceptibility of the conduction electrons is

$$\chi(\mathbf{q}) = \frac{1}{2N}\sum_{\mathbf{k}}\frac{f(\epsilon_{\mathbf{k}})-f(\epsilon_{\mathbf{k}-\mathbf{q}})}{\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}}} \qquad ; \qquad \chi(\mathbf{0}) = \tfrac{1}{2}\mathcal{N}(0)$$

The RKKY interaction in a BCS-superconductor

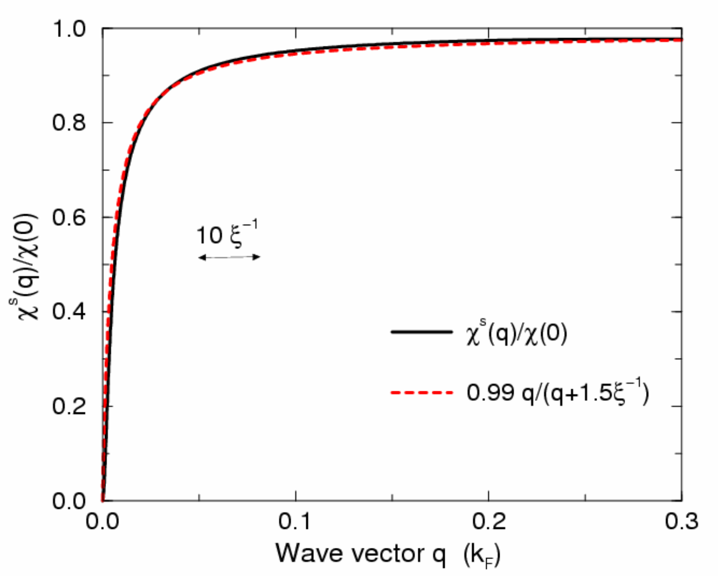
Introducing the relative electron energies $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$ and the quasiparticle energies $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$, then the susceptibility in the super-conducting phase is

$$\chi^s(\mathbf{q}) = \frac{1}{2N}\sum_{\mathbf{k}} \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k-q}})}{E_{\mathbf{k-q}} - E_{\mathbf{k}}} + \frac{1}{2N}\sum_{\mathbf{k}} \left[\frac{1-2f(E_{\mathbf{k-q}})}{2E_{\mathbf{k-q}}} - \frac{1-2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}}\right] \frac{\xi_{\mathbf{k-q}}\xi_{\mathbf{k}} + \Delta^2 - E_{\mathbf{k-q}}E_{\mathbf{k}}}{E_{\mathbf{k-q}}^2 - E_{\mathbf{k}}^2}$$

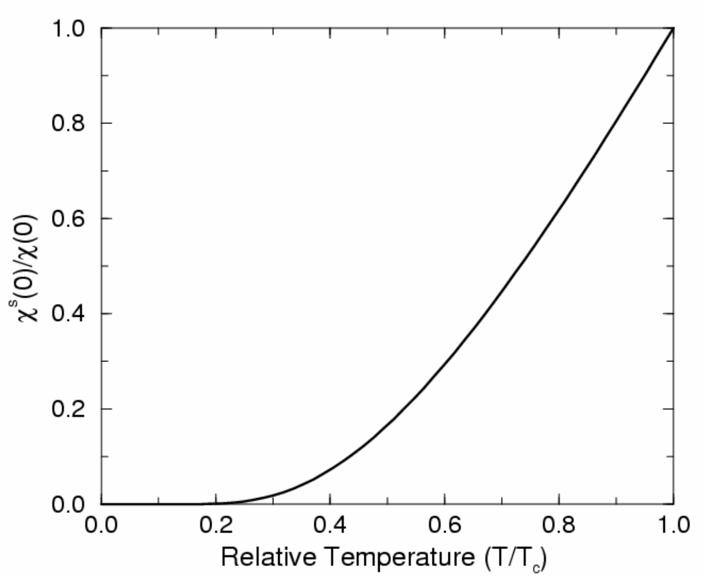
The q-dependence at T = 0 (spherical Fermi surface).

$\xi = \frac{\hbar v_F}{\pi\Delta}$ is the correlation length of the superconductor.

(Anderson-Suhl,1959)



The temperature dependence at q = 0.



The upper critical field in $TmNi_2B_2C$ (paramagnetic phase)

$TmNi_2B_2C$ is superconducting below T_c = 11 K of type II with

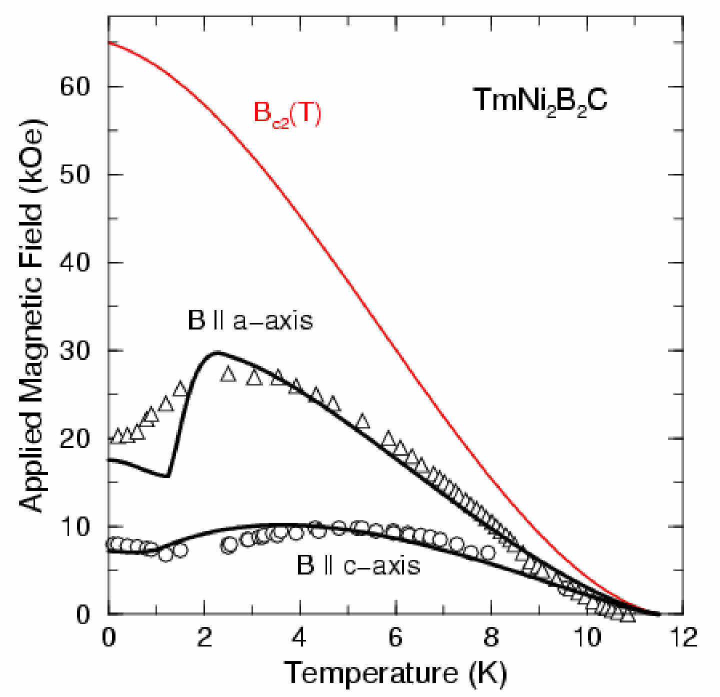
$$\kappa = \lambda/\xi \approx 7; \quad \xi(0) \simeq 70 \text{ Å}; \quad \lambda(0) \simeq 500 \text{ Å}; \quad \Delta(0) \simeq 1.7 \text{ meV}$$

and the free energy is (Abrikosov):

$$F_s(T, B_i) - F_n = -\frac{(B_{c2}(T) - B_i)^2}{1.16 \cdot 8\pi(2\kappa^2 - 1)}$$

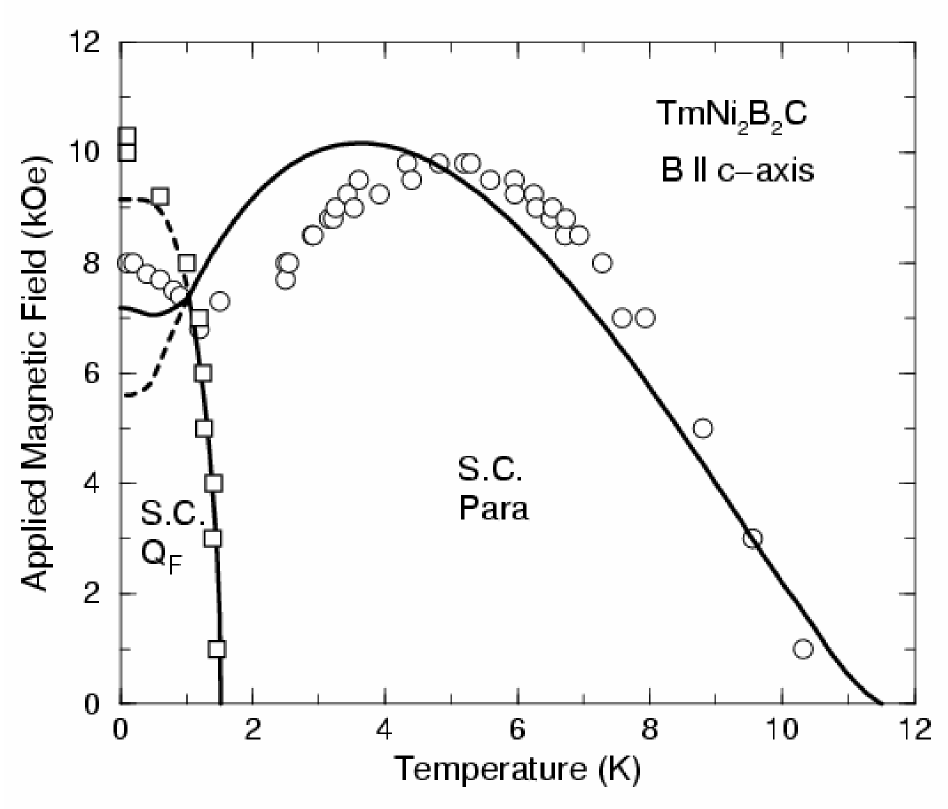
The magnetic properties of the Tm-ions are well characterized (strongly anisotropic with an easy c-axis). The magnetic free energy changes abruptly at the upper critical field:

$$\langle \mathcal{H}_H \rangle = \begin{cases} -\frac{1}{2} N \mathcal{J}_s(\mathbf{0}) \langle J_z \rangle^2; \text{ (S.C.)} \\ -\frac{1}{2} N \mathcal{J}(\mathbf{0}) \langle J_z \rangle^2; \text{ (normal)} \end{cases} \qquad \mathcal{J}_s(\mathbf{0}) = \mathcal{J}(\mathbf{0}) \frac{(1-\alpha)\chi(0) + \alpha \chi_T^s(0)}{\chi(0)}$$



T_c is about 16 K in the two non-magnetic Lu and Y borocarbides, and B_{c2}(Lu) = 76 kOe and B_{c2}(Y) = 110 kOe at T = 0.

The c-axis phase diagram of $TmNi_2B_2C$



- $TmNi_2B_2C$ orders antiferromagnetically with the moments along the c-axis at T_N = 1.5 K (zero field).

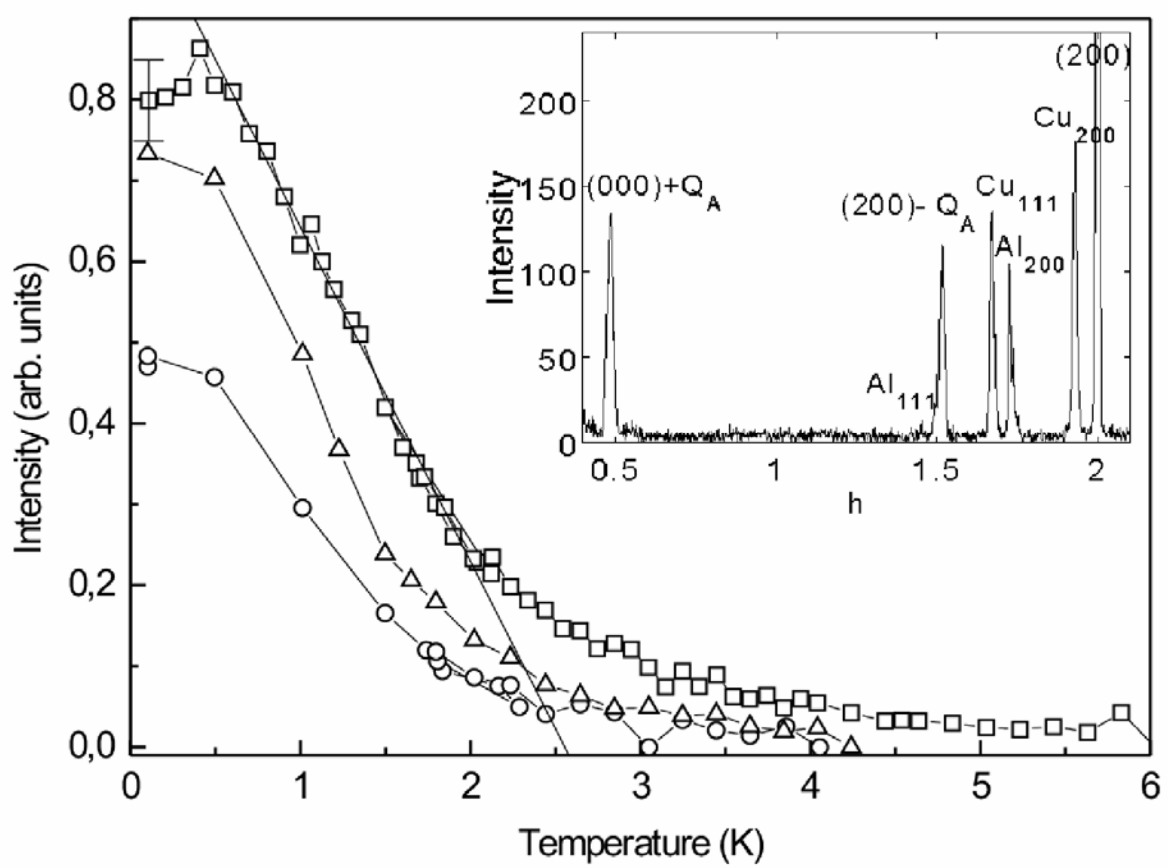
- The ordering wave vector along [110] is small, $Q_F = 0.13\, a^* \cong 16\, \xi^{-1}$.

- This value agrees with the estimated shift of a maximum in $\mathcal{J}(\mathbf{q})$ from $\mathbf{q} = \mathbf{0}$ in the normal phase to a non-zero value, due to the Anderson-Suhl mechanism in the superconducting phase.

$$T_N(H{=}0) \;\Rightarrow\; \mathcal{J}_s(\mathbf{Q_F}) \approx \mathcal{J}(\mathbf{Q_F}) \approx \mathcal{J}(\mathbf{0}) = 8.6\ \mu\text{eV}.$$

$$T_N(H) - T_N(H{=}0) \text{ is determined by } \mathcal{J}_s(\mathbf{Q_F}) - \mathcal{J}_s(\mathbf{0}) \;\Rightarrow \alpha \approx 1.$$

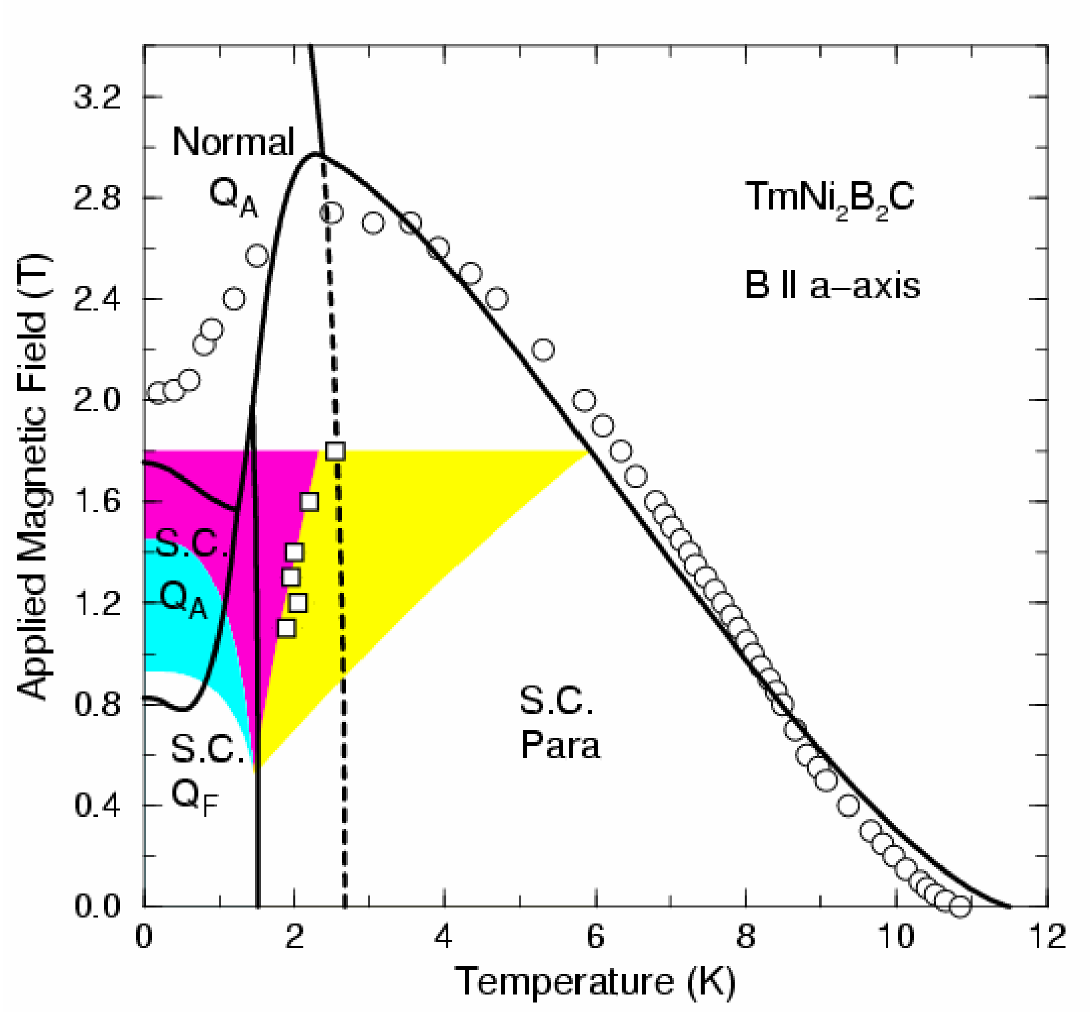
Neutron experiment on $TmNi_2B_2C$
- field along the a-axis -



Neutron scattering intensities at $\mathbf{Q_A}$ = (0.482,0,0)
o : 1.2 T ; Δ : 1.4 T ; □ : 1.8 T
Insert: Neutron scan along [h 0 0] (at 100 mK and 1.8 T).

The a-axis field changes the magnetic ordering, not to a c-axis ferromagnet, but to a new antiferromagnetically structure with the wave vector Q_A = 0.48 $a*$ along [100] instead of [110].

The a-axis phase diagram of $TmNi_2B_2C$



□: The experimental value of $T_N(H)$.

🟦 Coexistence of the Q_F and the Q_A scattering peaks.

🟪 The experimental Q_A phase.

🟨 The long tail region with low-intensity scattering at Q_A.

The spin-density wave induced via the RKKY interaction

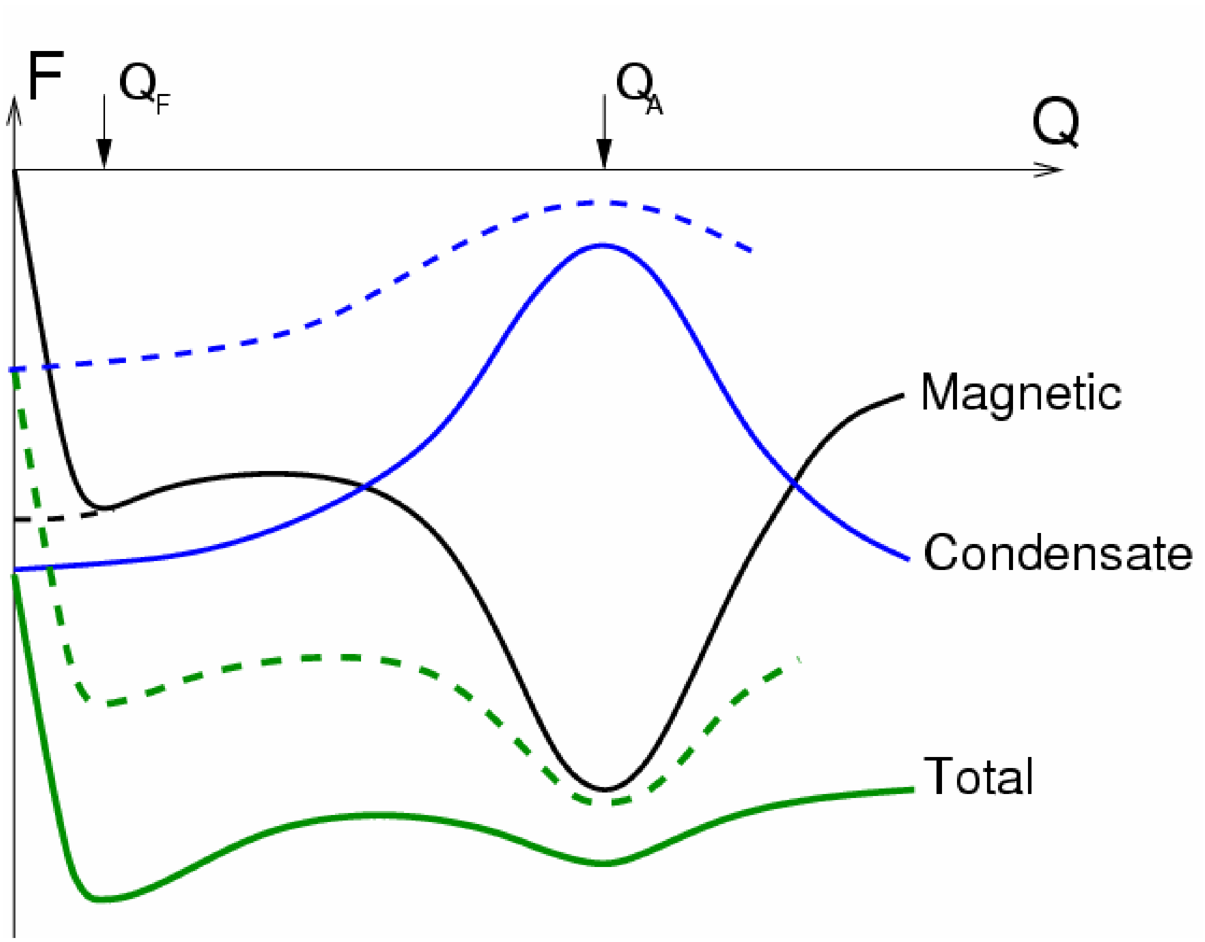
- The antiferromagnetically ordering at $\mathbf{Q}$ of the local 4f-moments acts as an effective magnetic field on the spins of the conduction electrons $\Rightarrow$a spin-density wave at $\mathbf{Q}$ and gaps in the energy bands of the conduction electrons at $\pm\mathbf{Q}/2$.

- The spin degrees of freedom of the conduction electrons, and thus the possibility for creating Cooper-pairs, is reduced proportionally to the magnetic order parameter (the amplitude of the modulated moments).

$$\frac{T_c}{T_c^0} = \frac{B_{c2}}{B_{c2}^0} = \exp\left[\frac{\delta}{1-\delta}\ln\left(\frac{\Delta(0)}{\omega_D}\right)\right] \simeq \exp\left[-\frac{2\delta}{1-\delta}\right]$$
$$\delta = d_A\left\langle J_z(\mathbf{Q})\right\rangle$$

- Nesting effects on the Fermi surface: Band structure calculations indicate that states separated by wave vectors close to $\mathbf{Q_A}$ contribute much to $\mathcal{N}$(0), i.e. d_A is large when $\mathbf{Q} \approx \mathbf{Q_A}$ but may be neglected when $\mathbf{Q} \approx \mathbf{Q_F}$ (the effect vanishes at $\mathbf{Q} = \mathbf{0}$).

The total free energy as a function of the magnetic ordering wave vector



Conclusion

- The Anderson-Suhl reduction of $\mathcal{J}(\mathbf{0})$ in $TmNi_2B_2C$ explains the strong anisotropy of the upper critical field and its small value in comparison with the non-magnetic rare-earth borocarbides.

- Nesting effects on the Fermi surface close to $\mathbf{Q}_A$ implies that $\mathcal{J}(\mathbf{Q}_A)$ is large. However, a magnetic ordering at this wave vector is suppressed because the energy of the superconducting condensate is strongly reduced by the induced spin density wave at $\mathbf{Q}_A$ (by the same reason).

- The new neutron scattering experiments show an increase of the stability of the $\mathbf{Q}_A$-phase in the normal metal when the a-axis field is increased above the upper critical field.

- Antiferromagnetically ordered moments on the Ni-sites?
- Creation of quasi-localized moments on the Ni-sites due to the applied field?
- ??