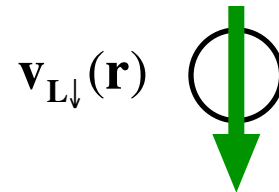
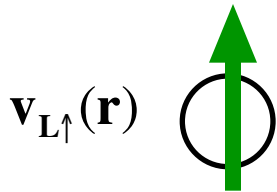


Interfacing L-SIC with Susceptibility Code

1] Potential Generation

- Use L-SIC code to generate potentials for a disordered system, where atoms have equal probabilities for up and down orientations of their local moments.



2] Evaluation of t-matrices

- $v_{L\uparrow(\downarrow)}$ are used to evaluate scattering matrices $t_{L\uparrow(\downarrow)}$,

$$\bar{t}_{L\uparrow(\downarrow)} = t_{L\uparrow(\downarrow)}^{\text{LSD}} (1 - \delta_{L\bar{L}}) + t_{L\uparrow(\downarrow)}^{\text{SIC-LSD}} \delta_{L\bar{L}}.$$

[See M. Lueders *et al*, cond-mat/0406515.]

- Typical energy grid used for a susceptibility calculation is $E = E_F + i(0.005)10^{0.2m}$, where $m=0,1,2,\dots$
- DLM code interpolates onto *Matsubara frequencies*.

3] t-matrices passed into susceptibility code

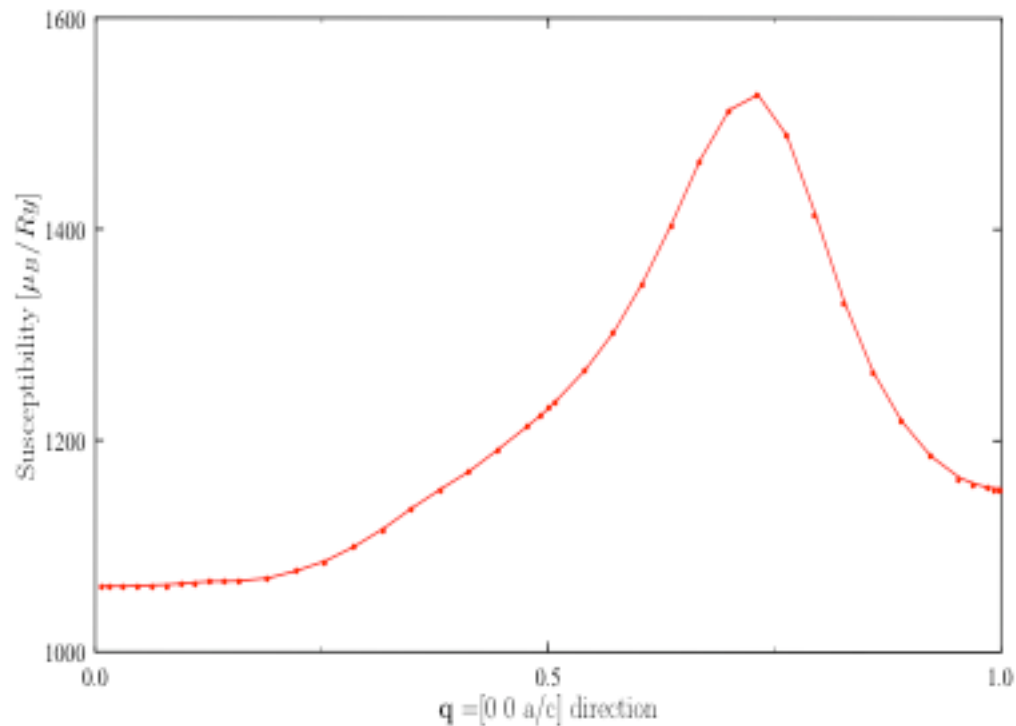
- Susceptibility code evaluates the wavevector dependent direct-correlation function $S^{(2)}(\mathbf{q})$
-From which the susceptibility is calculated according to

$$\chi(\mathbf{q}) = \frac{1/3\beta\mu}{1 - 1/3\beta S^{(2)}(\mathbf{q})}.$$

hcp-Gadolinium

- Experimentally observed to be ferromagnetic, with a Curie temperature of 293K.
- The highly localised nature of the 4f electrons make it a good test case for the applicability of density functional theory methods to rare earth systems.
- In previous investigations [see for example M. Heinemann & W.M. Temmerman, Phys. Rev. B, **49**, 4348 (1994)] use of the LDA within the LMTO-ASA predicts that an *antiferromagnetic* groundstate is energetically favourable.
- DLM susceptibility calculations also reveal an antiferromagnetic ordering tendency...

Wavevector Dependent Paramagnetic Susceptibility (LDA calculation)

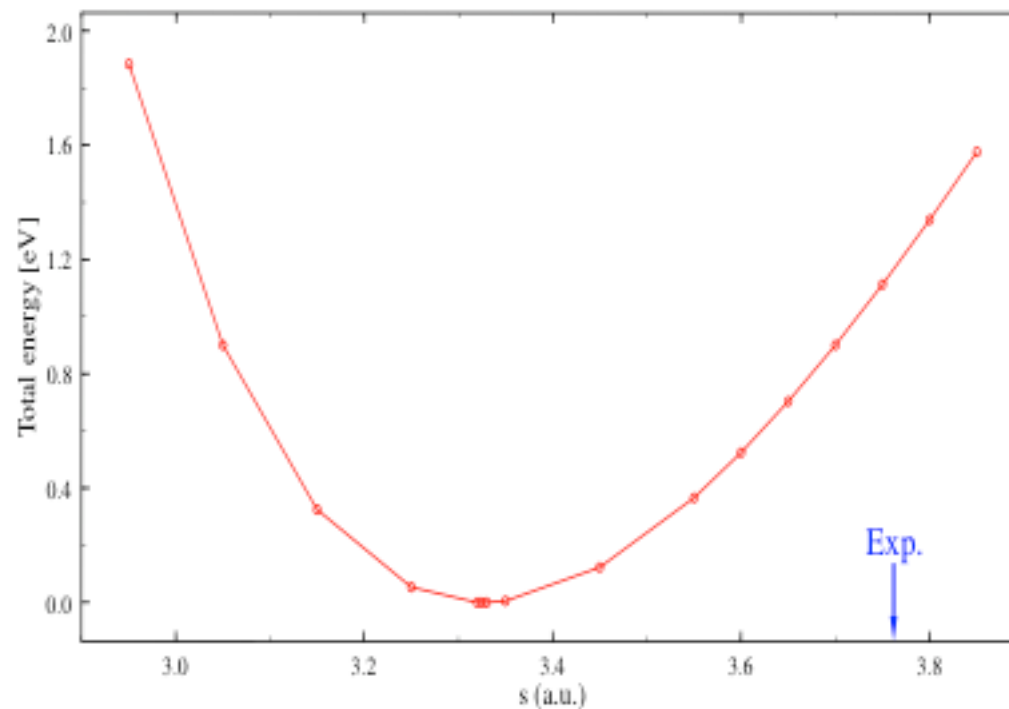


- Applying a GGA correction [A. C. Jenkins *et al*, J.Phys. :Condens. Matter, **12**, 10441 (2000)] or treating the 4f electrons as localised core electrons [I. Turek *et al*, J.Phys. :Condens. Matter, **15**, 2771 (2003)] leads to the correct prediction of a ferromagnetic groundstate.
- We have performed a DLM calculation with all the majority 4f states *SIC-corrected*.

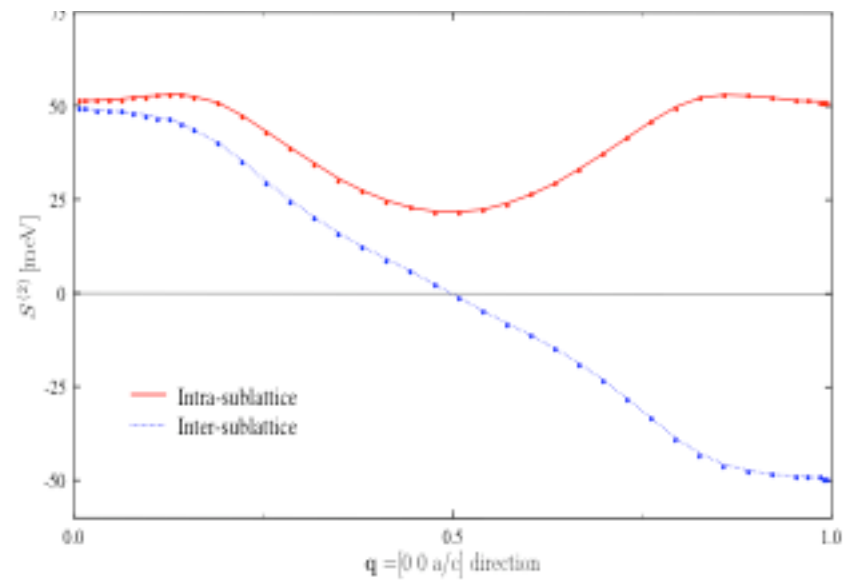
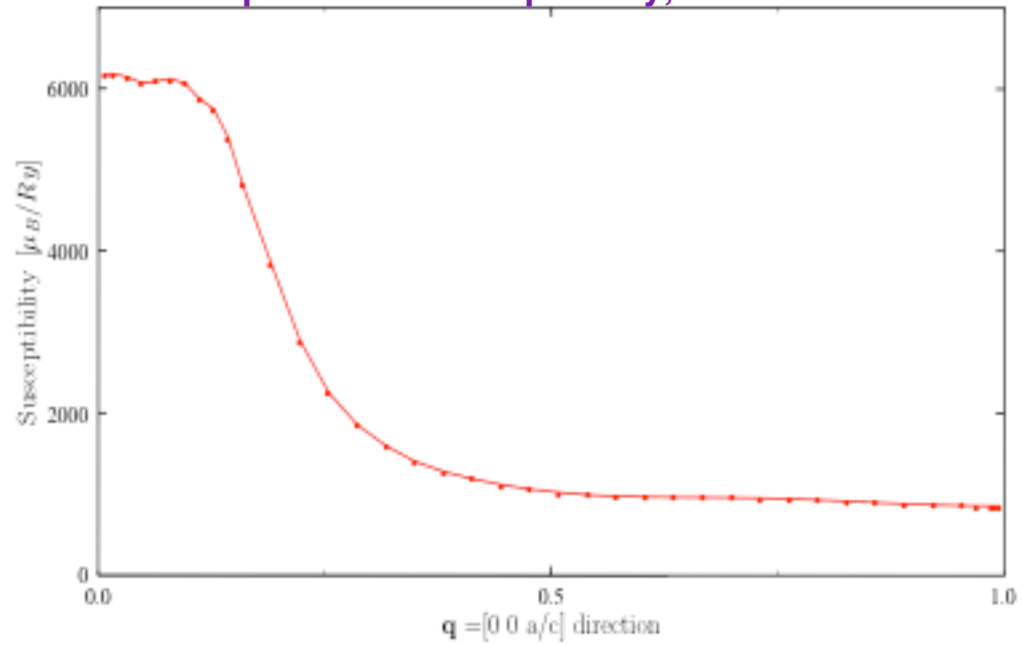
Lattice Parameters

- Fixed c/a ratio at experimental value (1.597)
- Minimised total energy w.r.t Wigner-Seitz (WS) radius, s.

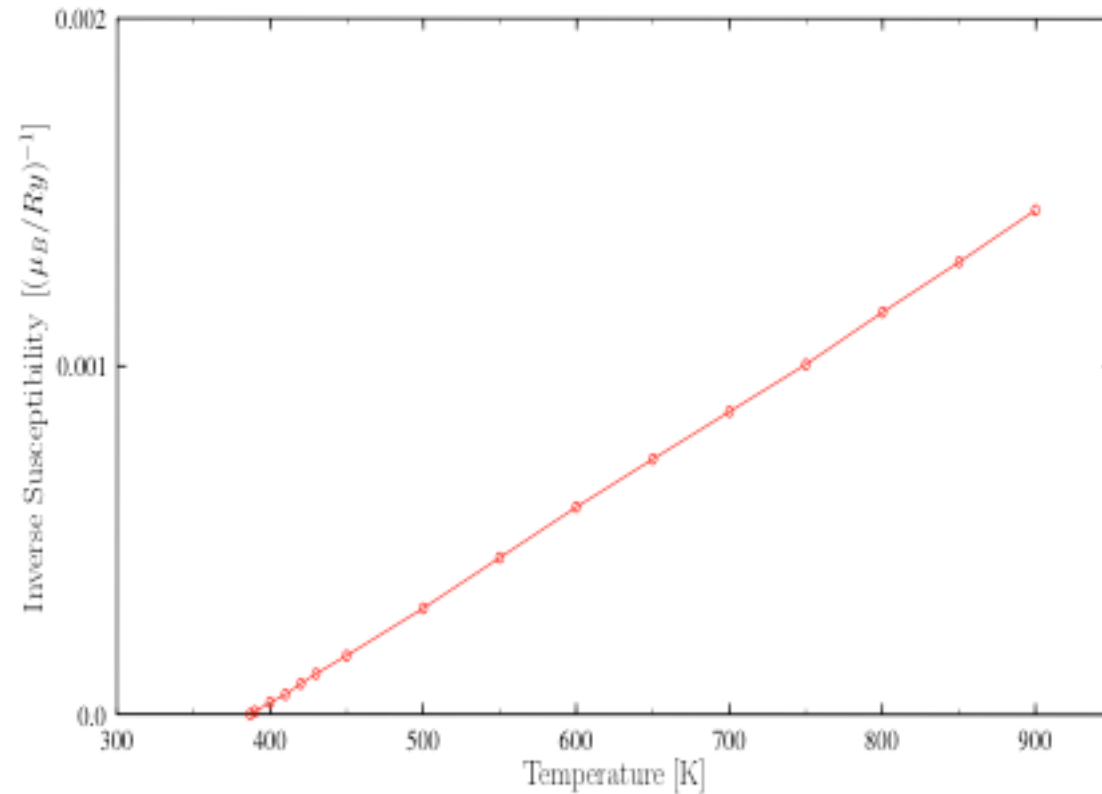
Total energy as a function of WS radius, s.



Wavevector Dependent Susceptibility, evaluated at $T=1.15T_c$



Curie-Weiss Behaviour

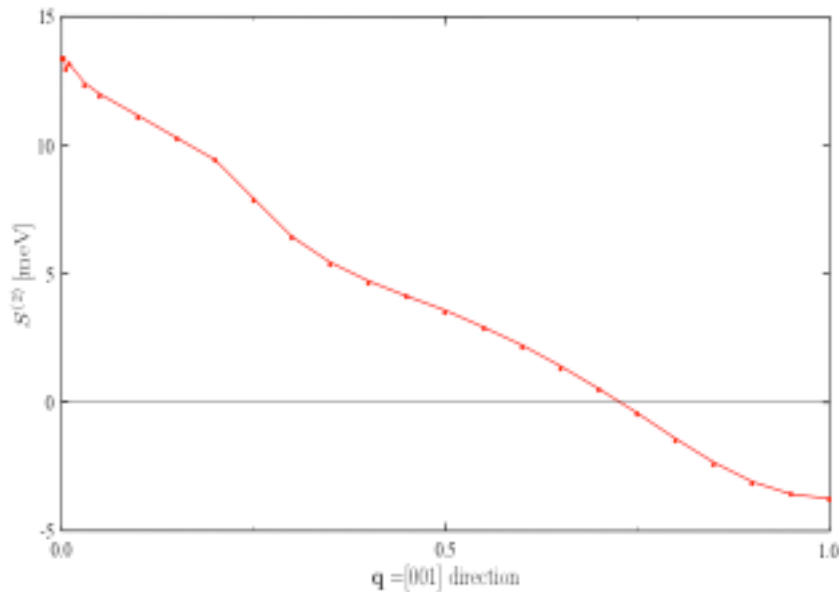


- Magnetic Ordering temperature $\approx 390\text{K}$.
- 33% higher than experimental value.
- An overestimate of this size is what would be expected from a mean-field theory.

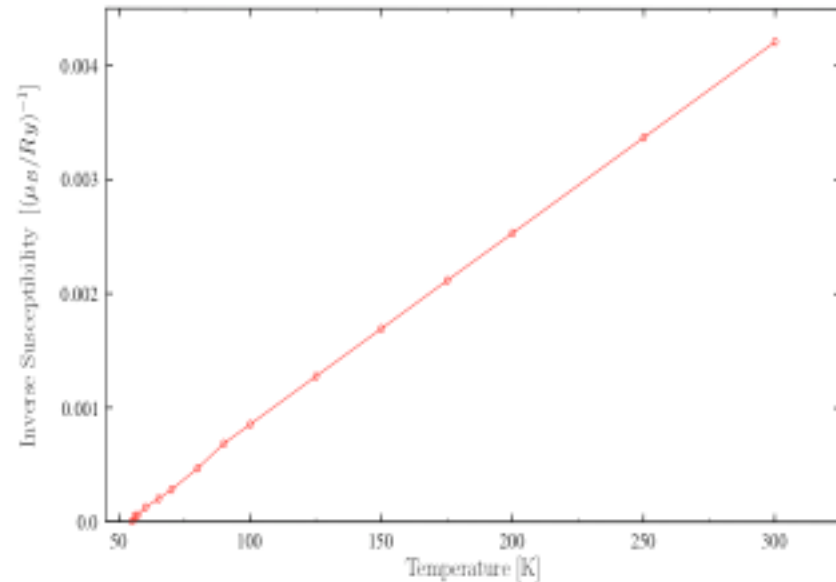
Cerium

- At the temperatures in which the γ -phase of Ce is experimentally accessible it is in a paramagnetic state.
- Our calculations indicate a ferromagnetic ordering tendency.
- If it were possible to stabilise the γ phase at low temperatures, we predict it would adopt a ferromagnetic structure at a temperature of 55K.

Ferromagnetic Correlations.....



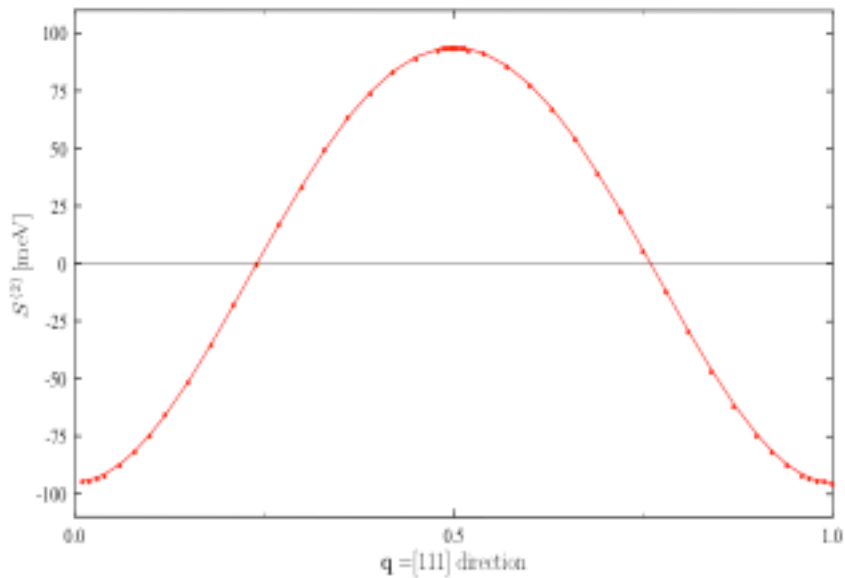
Magnetic Ordering Temperature.....



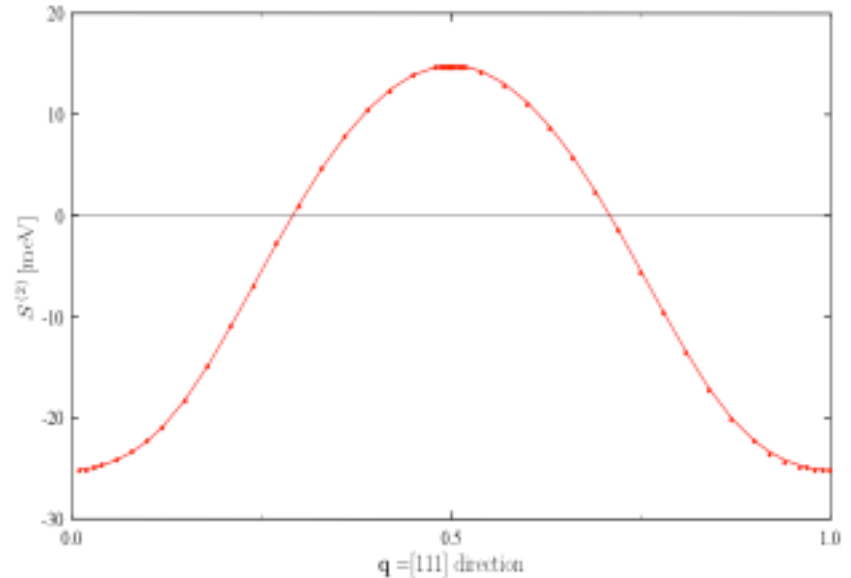
Transition Metal Oxides: NiO & MnO

- Experimentally observed to exhibit type-II antiferromagnetic ordering, with moments oppositely aligned in adjacent (111) planes.
- Preliminary results, from calculations in which the transition metal 3d states are SIC-corrected, predict the correct magnetic ordering.

NiO



MnO



Magnetic Ordering Temperatures

	Theory	Experiment
NiO	363K	523K
MnO	57K	118K

- Systematic underestimation of the transition temperature.
- The effect of including *empty spheres* needs to be investigated.

Future Projects

- Extend the Gadolinium work to GdY alloys.
- Look at whole Transition Metal Oxide Series.
- Investigate *layered* systems.