

Interfacing the susceptibility code with L-SIC

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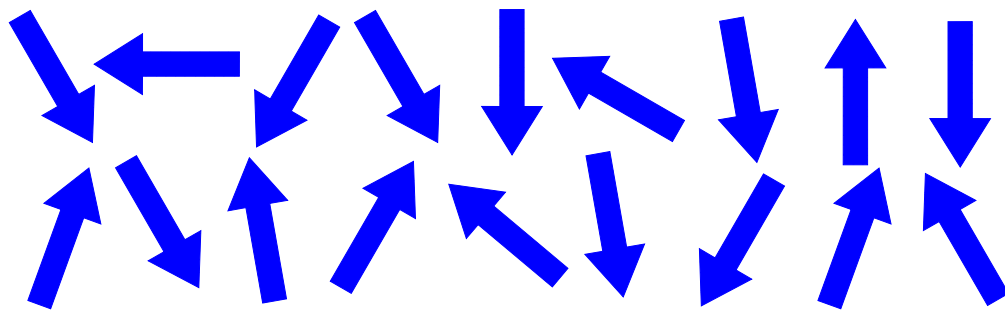
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Magnetism at finite temperature: Disordered Local Moments (DLM)

Time scale separation: For times, $\tau \gg \hbar/w$, (\hbar/w is electronic hopping time) but $\tau < \tau_{sf}$ (τ_{sf} is typical spin fluctuation time), the spin orientations of the electrons leaving an atomic site are sufficiently correlated with those arriving that the magnetisation integrated over a unit cell and averaged over τ is non-zero.



$$P(\{\hat{e}_i\}) = \frac{\exp[-\beta\Omega(\{\hat{e}_i\})]}{\prod_j \int d\hat{e}_j \exp[-\beta\Omega(\{\hat{e}_i\})]}$$

where $\Omega(\{\hat{e}_i\})$ is the 'generalised' electronic grand potential from SDFT and $\beta = (k_B T)^{-1}$. $\Omega(\{\hat{e}_i\})$ - classical 'spin' or 'local moment'

Choose 'reference' Hamiltonian $\Omega_0\{\hat{e}_i\}$ and use Feynman Inequality $F \leq F_0 + \langle \Omega - \Omega_0 \rangle^0$ with

$$F_0 = -(1/\beta) \ln \prod_i \int d\hat{e}_i \exp(-\beta\Omega_0)$$

and

$$\langle X \rangle^0 = \frac{\prod_i \int d\hat{e}_i X \exp(-\beta\Omega_0)}{\prod_i \int d\hat{e}_i \exp(-\beta\Omega_0)} = \prod_i \int d\mathbf{e}_i P_0\{\hat{e}_i\} X\{\hat{e}_i\}$$

With Ω_0 in the form

$$\Omega_0 = \sum_i \omega_i^{(1)}(\hat{e}_i) + \sum_{i,j,i \neq j} \omega_{ij}^{(2)}(\hat{e}_i, \hat{e}_j) + \dots$$

'First-Principles' Mean Field Theory (DLM picture) from $\omega_i^{(1)}$ only and averaging performed using techniques adapted from theory of the electronic structure of disordered alloys.

Paramagnetic DLM state *equivalent to Ising 'up-down' spin system.*

Onset of Magnetic Order and the paramagnetic susceptibility

Apply small, external spin-only magnetic field $\{\mathbf{h}_i\}$, varying from site to site and determine induced magnetisation. Local moments tend to align with field, hence $\delta P(\{\hat{e}_i\})$. Obtain paramagnetic spin susceptibility generalised to multi-sublattice systems with compositional disorder

$$\chi^{\alpha,n}(\mathbf{q}) = 1/3\beta\mu_n^\alpha c_n^\alpha + 1/3\beta \sum_l \sum_\epsilon c_l^\epsilon S_{n,l}^{(2),\alpha,\epsilon}(\mathbf{q}) \chi^{\epsilon,l}(\mathbf{q}),$$

Here n, l are sublattice indices and α, ϵ labels for the atoms occupying the sublattices. c_n^α defines the concentration of the α constituent on sublattice n and μ_n^α the magnitudes of the self-consistently determined local moments.

Type of magnetic order, transition temperatures

The key computational tasks for the susceptibility code are:

- the evaluation of Brillouin zone convolution integrals $\int \tau_{L_1, L_2}^{n, l}(\mathbf{k}, z) \tau_{L_3, L_4}^{l, n}(\mathbf{k} + \mathbf{q}) d\mathbf{k} - \tau_{L_1, L_2}^{nn} \tau_{L_3, L_4}^{nn} \delta_{n, l}$ (where L_1 etc. are angular momentum labels)
- the solution of the *Bethe-Salpeter equations* which arise from allowing the CPA effective medium to respond to the inhomogeneous magnetic field.

These tasks are carried out for energies z for path $z = \nu$ to $z = \nu + i\Delta$ where ν is the chemical potential and Δ a cutoff of order 1-2 Ryd.

The calculation of the susceptibility requires interpolation to a sum over Matsubara frequencies $z = \nu + ik_B T \pi(2m + 1)$.

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Including the L-SIC ...