

MSM 2009

**NON-COLLINEAR MAGNETISM IN
DISORDERED ALLOYS**

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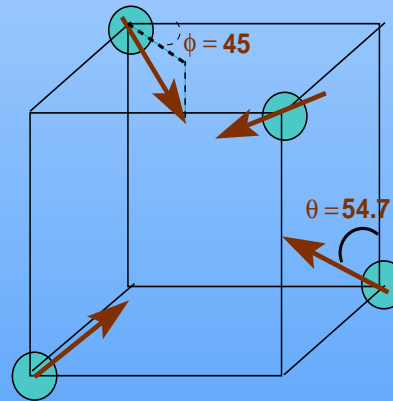
Anders Bergman, Biplab Sanyal

Uppsala University, Uppsala

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It may sometimes happen that the local axis of quantization of spins (the direction along which magnetic moment points) is different from a global axis. This local axes may be different in different atomic sites $\{\hat{e}_R\}$. This can happen in bulk, stepped and rough surfaces and interfaces, in spin-glasses.

For example :



The 3Q non-collinear magnetic structure in disordered FeMn has the lowest energy.

With average moment $1.7\mu_B$. Akimasa Sukuma, *J. Phys. Soc. (Japan)*, 3072 (2000)

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Generalizations required to describe non-collinear magnetism in alloys :

- **Density Functional Approximation \Rightarrow Density Matrix Functionals (Kübler)**
- **Lack of lattice translational symmetry \Rightarrow (Heine) “throw out k-space” \Rightarrow Matrix Recursion Method (Haydock/Godin)**
- **Disorder \Rightarrow Augmented Space Method (Mookerjee/Kaplan,Johnson,Leath)- Beyond standard mean-field CPA**
- **Basis of representation \Rightarrow TB-LMTO - gives a sparse representation of the Hamiltonian - essential for Recursion**

Disorder

- If disorder were homogeneous, i.e. perfectly random, then the single site mean-field theory : the coherent potential approximation (CPA) is good enough.
- We want to describe situations where we may have **inhomogeneous disorder** : **short-range ordering or clustering**, or where because of large difference in atomic sizes of constituents we have **random local lattice distortions** : which lead to **“off-diagonal disorder”** in the Hamiltonian.
- In all such situations the neighbourhood plays an important role and single-site mean-field approximations are incapable of describing them.
- Can we devise a way of describing effects of **“configuration fluctuations”** about the mean-field ?

Disorder

A. Mookerjee, “Electronic structure of clusters, surfaces and alloys” (Taylor-Francis, 2003) ed. A. Mookerjee and D.D. Sarma.

Hamiltonian has parameters which are disordered

$$H = H(\{p_i\})$$

Taking a leaf from measurement theory :

- Associate with each random parameter p_i an operator P_i
- The eigenvalues of P_i are the values taken by p_i .
- The spectral density of P_i is the probability density of the parameter.
- P_i is an operator in the configuration space of p_i .

Example :

$$Pr(p) = x \delta(p) + y \delta(p - 1)$$

$$P = \begin{pmatrix} x & \sqrt{xy} \\ \sqrt{xy} & y \end{pmatrix}$$

Disorder

A. Mookerjee, *J Phys C6 L205 (1973)*

- In configuration space construct a 'reference state' $|0\rangle = \sum_p \sqrt{Pr(p)}|p\rangle$.
- Augmented space Theorem \Rightarrow

$$\ll f(p) \gg = \langle 0 | \tilde{\mathbf{f}}(P) | 0 \rangle$$

- The average of the Green function :

$$\ll G[H(\{p_i\}) \gg = \langle 0 | \tilde{\mathbf{G}}[\tilde{\mathbf{H}}[\{P_i\}]] | 0 \rangle$$

- The result is formally exact. Approximations can now be introduced in a controlled way.

Disorder

- We can now set up a multiple scattering picture where the scattering is by configuration fluctuations about the 'mean' configuration.
- If we neglect all configurations where there are correlated fluctuations at more than one site, we get the CPA.
- Other earlier approximations like **TCA** (Kaplan-Gray) and **ICPA** (Leath-Cohen) are all based on this Augmented space theorem.
 - Kaplan, Leath and Gray, PR B21 4230 (1984) ;
 - Ghosh, Leath and Cohen, PR B66 214206 (2002)
- We shall couple this formalism with Recursion and introduce formal approximations there.

Recursion

R. Haydock and T. Godin, Comp. Phys. Commun. 64, 123 (1991)

Our approach would be to express $\ll G(z) \gg$ as a continued fraction through the Recursion method (Haydock-Heine).

- **Recursion is a real-space method. It visualizes the solid as a gigantic molecule. It requires no lattice translation symmetry.** Surfaces, interfaces, disordered crystals, amorphous networks all can come under its orbit.
- The continued fraction for an (semi) infinite system also stretches infinitely far down.
- **The only approximation is ‘termination’.** Excellent terminators are available which can be self-consistently obtained from the initial coefficients and their asymptotic behaviour.
- **Estimates of errors in such ‘termination’ are available** and therefore the approximations are controlled.

R. Haydock, Lecture Notes in Physics, vol 35 (Academic Press)

Non-Collinear Magnetism

- Wave functions become **bi-spinors** : $\Phi(r, E) = \begin{pmatrix} \phi_1(r, E) \\ \phi_2(r, E) \end{pmatrix}$
- Density Functionals \Rightarrow **Density matrix functionals** :

$$E[\rho] \Rightarrow E[\rho_{\alpha\alpha'}] \quad \rho_{\alpha\alpha'}(r) = \sum_{\lambda \in \text{occ}} \phi_{\alpha}^*(r, E_{\lambda}) \phi_{\alpha'}(r, E_{\lambda})$$

- **Modified Kohn-Sham equation** :

$$\sum_{\alpha'} [-\nabla^2 \delta_{\alpha\alpha'} + V_{\alpha\alpha'}(r)] \phi_{\alpha'} = E \phi_{\alpha}(r)$$

- **Effective matrix potential** :

$$V_{\alpha\alpha'}(r) = [V_{\text{ion}} + V_{\text{H}} + V_{\text{xc}}^{(1)} + V_{\text{SR}}] \delta_{\alpha\alpha'} + [\vec{B}(r) + v(r)\vec{L}] \cdot \vec{S}_{\alpha\alpha'}$$

$$\vec{B}(r) = \sum_R V_{\text{xc}}^{(2)}(r-R) \hat{e}_R$$

This $\vec{B}(r)$ is a ‘local internal field’ which gives rise to exchange splitting when magnetism occurs.

Non-Collinear Magnetism

- **If magnetism is collinear and all \hat{e}_R point is the global z direction, $\vec{B}(r) = B(r)\hat{z}$**

- **and**

$$V_{xc}^{(1)} = V_{xc}^{\uparrow} + V_{xc}^{\downarrow} \quad V_{xc}^{(2)} = V_{xc}^{\uparrow} - V_{xc}^{\downarrow}$$

The matrix potential diagonalizes and the up and down Kohn-Sham equations become separable.

- **When magnetism is non-collinear the Hamiltonian takes the form :**

$$\mathbf{H} = H^{(0)}\mathbf{I} + \left[\vec{B} + v\vec{L} \right] \cdot \vec{S}$$

- **In the TB-LMTO representation the Hamiltonian is characterised by potential parameters $C_{RL\alpha}, \Delta_{RL\alpha}$ which may be random and a structure matrix $S_{RL,R'L'}$ which is short-ranged making the Hamiltonian sparse and may also be **random**.**

Non-Collinear Magnetism

- The random potential parameters are replaced by their corresponding operators and the augmented Hamiltonian is built up as :

$$\tilde{\mathbf{H}} = \tilde{\mathbf{H}}^{(0)} \mathbf{I} + \left[\tilde{\mathbf{B}} + \tilde{\mathbf{v}} \tilde{\mathbf{L}} \right] \cdot \tilde{\mathbf{S}}$$

- The averaged magnetic moment is given by :

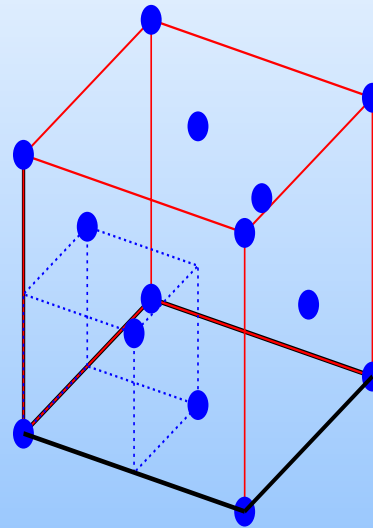
$$\langle\langle \vec{m}_R \rangle\rangle = \sum_L \int_{-\infty}^{E_F} dE \langle\langle \vec{m}_{RL}(E) \rangle\rangle$$

with

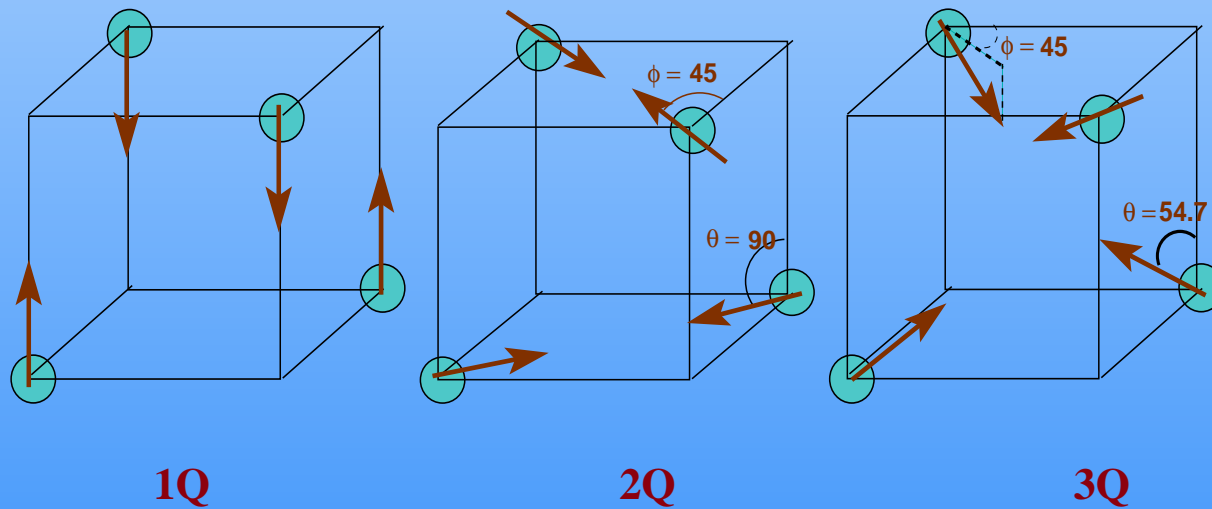
$$\langle\langle \vec{m}_{RL}(E) \rangle\rangle = -\frac{1}{\pi} \Im m \operatorname{Tr} \left\{ \tilde{\mathbf{S}} \langle 0RL | \tilde{\mathbf{G}}(E + i0) | 0RL \rangle \right\}$$

- The three terms in the above expressions are obtained by three recursions first diagonalizing S_x, S_y, S_z using SU(2) rotation matrices.

MnPt disordered alloy

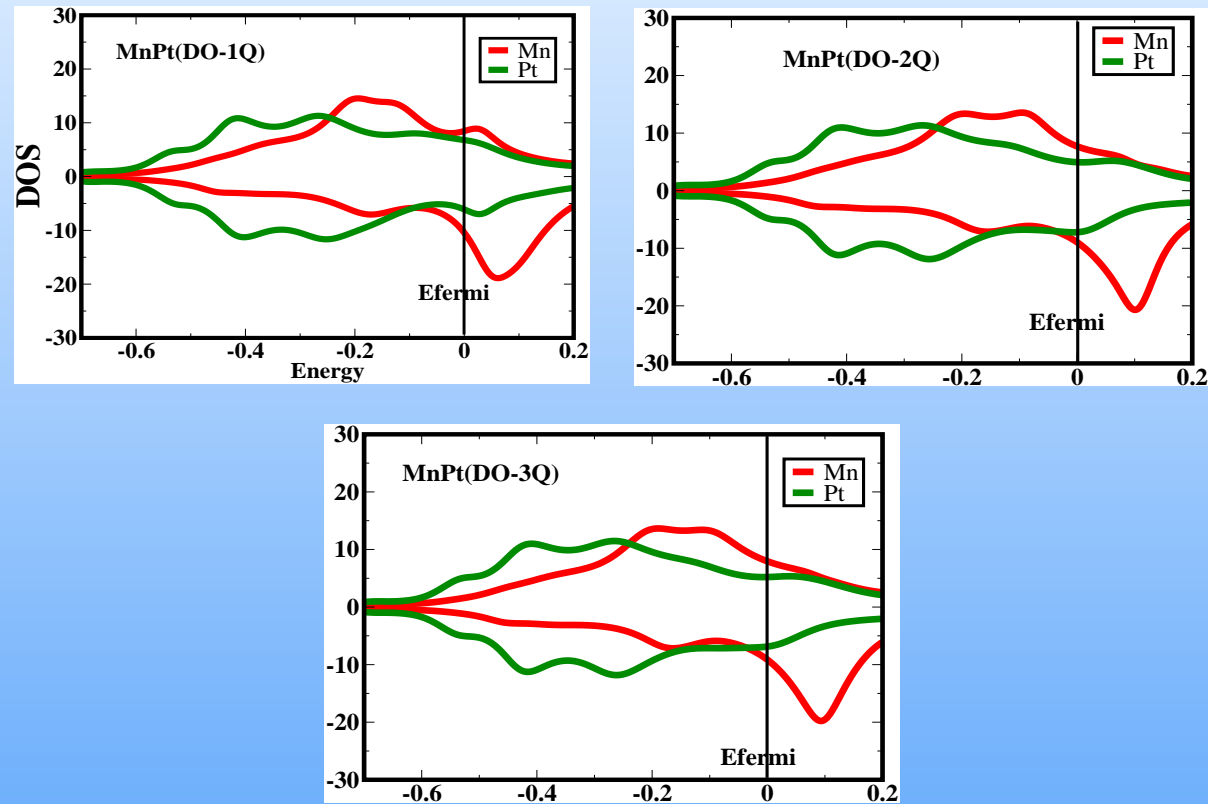


A fcc cubic unit and the magnetic unit cell.



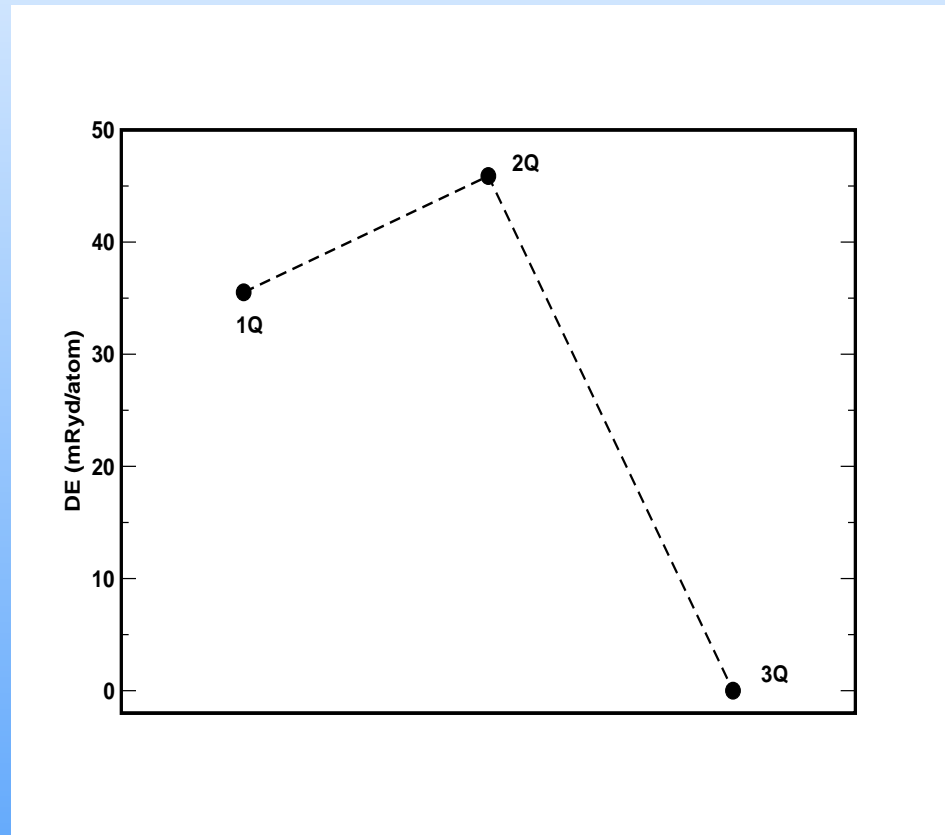
Collinear and non-collinear magnetic arrangements.

MnPt disordered alloy



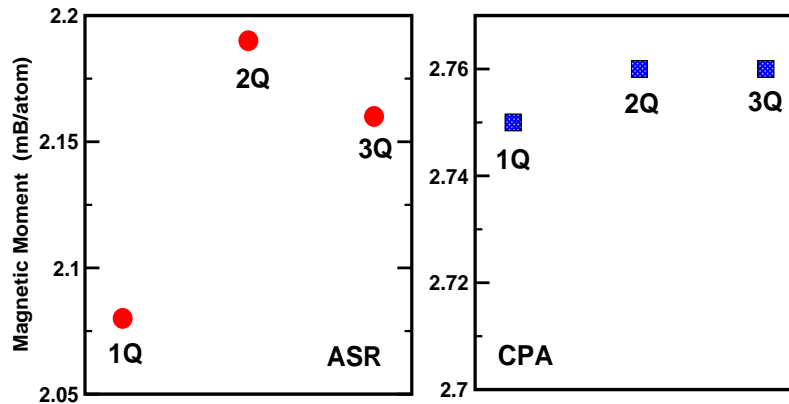
Density of states for the three arrangements.

MnPt disordered alloy



3Q has the lowest energy. Energy difference of 1Q,2Q with 3Q are shown.

MnPt disordered alloy



Local magnetic moments for the three arrangements in ASR and CPA.