

# Non colinear magnetism

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## 1 Notations and theoretical considerations

\* We will denote the spinor by  $\Psi^{\alpha\beta}$ ,  $\alpha, \beta$  being the two spin indexes.

\* The magnetic properties are well represented by introducing the spin density matrix:  $\rho^{\alpha,\beta}(r) = \sum_n f_n \langle r | \Psi_n^\alpha \rangle \langle \Psi_n^\beta | r \rangle$  where the sum runs over all states and  $f_n$  is the occupation of state  $n$ .

\* With  $\rho^{\alpha,\beta}(r)$ , we can express the scalar density by  $\rho(r) = \sum_{\alpha,\alpha} \rho^{\alpha,\alpha}(r)$  and the magnetisation density  $\vec{m}(r)$  (in units of  $\hbar/2$ ) whose components are  $m_i(r) = \sum_{\alpha,\beta} \rho^{\alpha,\beta}(r) \sigma_i^{\alpha,\beta}$ , where the  $\sigma_i$  are the Pauli matrices.

\* In general,  $E_{xc}$  is a functional of  $\rho^{\alpha,\beta}(r)$ , or equivalently of  $\vec{m}(r)$  and  $\rho(r)$ . It is therefore denoted as  $E_{xc}(n(r), \vec{m}(r))$

\* The expression of  $V_{xc}$  taking into account the above expression of  $E_{xc}$  is:

$$V_{xc}^{\alpha,\beta}(r) = \frac{\delta E_{xc}}{\delta \rho(r)} \delta_{\alpha,\beta} + \sum_{i=1}^3 \frac{\delta E_{xc}}{\delta m_i(r)} \sigma_i^{\alpha,\beta}$$

\* In the LDA approximation, due to its rotational invariance,  $E_{xc}$  is indeed a functional of  $n(r)$  and  $|m(r)|$  only. In the GGA approximation, we *assume* that it is a functional of  $n(r)$  and  $|m(r)|$  and their gradients. (This is not the most general functional of  $\vec{m}(r)$  dependent upon first order derivatives, and rotationally invariant.) We therefore use exactly the same functional as in the spin polarized situation, using the local direction of  $\vec{m}(r)$  as polarization direction. We have  $\frac{\delta E_{xc}}{\delta m_i(r)} = \frac{\delta E_{xc}}{\delta |m_i(r)|} \widehat{m}(r)$ , where  $\widehat{m}(r) = \frac{m(r)}{|m(r)|}$ . Now, in the LDA-GGA formulations,  $n \uparrow + n \downarrow = n$  and  $|n \uparrow - n \downarrow| = |m|$  and therefore, if we set  $n \uparrow = (n + m)/2$  and  $n \downarrow = (n - m)/2$ , we have:

$$\frac{\delta E_{xc}}{\delta \rho(r)} = \frac{1}{2} \left( \frac{\delta E_{xc}}{\delta n \uparrow(r)} + \frac{\delta E_{xc}}{\delta n \downarrow(r)} \right)$$

and

$$\frac{\delta E_{xc}}{\delta |m(r)|} = \frac{1}{2} \left( \frac{\delta E_{xc}}{\delta n \uparrow (r)} - \frac{\delta E_{xc}}{\delta n \downarrow (r)} \right)$$

This makes the connection with the more usual spin polarized case.

\* Expression of  $V_{xc}$  in LDA-GGA

$$V_{xc}(r) = \frac{\delta E_{xc}}{\delta \rho(r)} \delta_{\alpha,\beta} + \frac{\delta E_{xc}}{\delta |m(r)|} \hat{m}(r) \cdot \sigma$$

\* Implementation

\* Computation of  $\rho^{\alpha,\beta}(r) = \sum_n f_n \langle r | \Psi^\alpha \rangle \langle \Psi^\beta | r \rangle$  One would like to use the routine `mkrho.f` which does precisely this. But this routine transforms only real quantities, whereas  $\rho^{\alpha,\beta}(r)$  is hermitian and can have complex elements. The “trick” is to use only the real quantities:

$$\begin{aligned} \rho^{1,1}(r) &= \sum_n f_n \langle r | \Psi^1 \rangle \langle \Psi^1 | r \rangle \\ \rho^{2,2}(r) &= \sum_n f_n \langle r | \Psi^2 \rangle \langle \Psi^2 | r \rangle \\ \rho(r) + m_x(r) &= \sum_n f_n (\Psi^1 + \Psi^2)_n^* (\Psi^1 + \Psi^2)_n \\ \rho(r) + m_y(r) &= \sum_n f_n (\Psi^1 - i\Psi^2)_n^* (\Psi^1 - i\Psi^2)_n \end{aligned}$$

and compute  $(\rho(r), \vec{m}(r))$  with the help of the additionnal:

$$\begin{aligned} \rho(r) &= \rho^{1,1}(r) + \rho^{2,2}(r) \\ m_z(r) &= \rho^{1,1}(r) - \rho^{2,2}(r) \end{aligned}$$

Note that only the forurier transform are performed in `mkrho.f` the final transformation to  $(\rho(r), \vec{m}(r))$  is performed in `symrhg.f`.

\* The computation of  $V_{xc}$  is performed in `rhoexc.f`. The only transformation to this routine, is to compute  $|\vec{m}(r)|$  as input of the usual (i.e spin polarized) `rhoexc.f` and yield back the four component  $V_{xc}$ , from the expression of  $\frac{\delta E_{xc}}{\delta |m(r)|}$ .

\* For more information, see: Hobbs et al., PRB, 62, 11556 ; Perdew et al. PRB, 46, 6671 (for the xc functional)