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# Periodic Anderson model for the description of noncollinear magnetic structure in low-dimensional 3d-systems

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**Abstract**

Distribution of magnetic moments in the low-dimensional metallic structures has been studied theoretically on the basis of periodic Anderson model. Calculation of noncollinear magnetic order was performed in the Hartree–Fock approximation using tight binding real space recursion method. Iteration process includes self-consistent determination of population numbers for the electrons with different directions of the magnetic moments at given atom relatively to the fixed axis. Energies of all states corresponding to the different directions of magnetic moments at the atom under consideration have been calculated, and the state with minimal energy being accepted for the next step.

Analytical transformations based on the generalised "zeros and poles method" were performed for the Green function that allows to avoid some time-consuming numerical procedures. It gives the possibility to develop efficient algorithm for the calculation of noncollinear magnetic structure of complex space nonhomogeneous systems.

Calculations performed for the parameters corresponding to Fe and Cr show the qualitatively different dependencies of the magnetic moment magnitude and the energies of d-electrons on the angles, which define the direction of magnetic moments.


*Keywords:* Model Hamiltonians; Noncollinear magnetism; 3d-metals

Magnetic structure of low-dimensional metallic systems (LDMS) has been recently studied quite intensively. It is connected with a number of new physical phenomena discovered in these structures as well as with development of new technologies which allow to create systems with well-controlled parameters. For most of the new phenomena the magnetic structure on atomic scale plays a crucial role. Imperfections such as surface roughness and interdiffusion lead to the breakdown of space homogeneity. It makes the theoretical description of real systems under experimental investigation extremely complex and time-consuming problem. So far ab initio calculations of such complex systems are out of the possibilities of modern computers. That is why the approach of tight binding model Hamiltonians such as Hubbard-like model (HM) and periodic Anderson model (PAM) is used for this purpose.

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HM has been applied to describe the distribution of magnetic moments on the stepped Cr surface. The results allow a rationalisation of the apparently contradictory observations obtained by spin-resolved and angle-and-energy resolved photoemission [1]. In [2] for a Fe (Cr) monolayer deposited on a vicinal Cr (Fe) substrate different self-consistent solutions were obtained. This is important for the description of experimental results of samples prepared under similar but not identical conditions.

PAM has been used to calculate the magnetic properties of Cr atoms impurity in the Fe matrix [3] and Fe clusters embedded near Cr surface, Fe/Cr interface [4], and pinhole defects in Fe/Cr superlattices [5]. Special algorithm was suggested for the modelling of rough surfaces and interfaces with consequent self-consistent calculation of obtained nonideal structure [6].

However, all these theories were developed only for the description of collinear magnetism. Whereas the distribution of magnetic moments with directions in LDMS is very important to understand the physical nature of phenomena in these systems. For example, the mechanisms of noncollinear exchange coupling and giant magnetoresistance in the Fe/Cr and Fe/Si multilayers are unknown, despite the essential efforts undertaken in this direction. So, the development of theoretical scheme for the description of complex nonhomogeneous systems taking into account the noncollinear magnetic structure is of great significance.

Variants of such a theory based on Hubbard Hamiltonian in mean-field approximation were developed in [7] for description of magnetism in transition metals at finite temperature and in [8] for investigation of helical spin density wave state in fcc iron. Modification of the theory was used to study the dependence of exchange coupling in Fe/Cr superlattices as a function of the relative orientation of the magnetic moments at the centre of two adjacent Fe layers [9] and for description of magnetic structure of Mn monolayer on Fe substrate [10].

In this work on the basis of PAM we develop the approach for the self-consistent calculation of noncollinear distribution of the magnetic moments in complex space nonhomogeneous systems. PAM assumes the existence of two bands, one of which corresponds to the quasilocalised d-band and another one to the itinerant s-electrons [3–6,11,12]. The s–d coupling on the site is presupposed to be more stronger than d–s–d interaction of d-electron on different sites. In this case, at first, one should construct resonant d-states and only after that to introduce the electron hopping between different states. d-electron energies have a finite width which is determined by s–d interaction

$$\Gamma_i = \mathrm{Im} \sum_{sk} \frac{V_{i,sk} V_{sk,i}}{\omega - \varepsilon_{sk}},$$

where $V_{i,sk}$ is the s–d hybridisation, $\varepsilon_{sk}$ the energy of itinerant s-electrons and $i$ is the coordinate of the site for localised d-electron.

For the description of noncollinear magnetism the Hamiltonian of PAM can be rewritten either in terms of spin quantisation along a global $z$-axis which is the same for all atoms or using a local spin-quantisation axis along local magnetic moment at site. We will use here the first possibility. In this case after Hartree–Fock approximation in the PAM Hamiltonian one can obtain together with intersite hopping without change of spin-projection $V$ the hopping on site with spin inversion $V^{\uparrow\downarrow}$.

It is schematically depicted in Fig. 1, where every site is shown as two circles corresponding to the up and down spin projection, the solid lines show the usual intersite hopping, the hopping on the site is shown by dash-lines. Parameters $V_{ll}^{\uparrow\downarrow}$ and $V_{ll}^{\downarrow\uparrow}$ depend on the magnitude of magnetic moment on given site as well as on its direction

$$V_{ll}^{\uparrow\downarrow} = (V_{ll}^{\downarrow\uparrow})^* = -\mathrm{e}^{-\mathrm{i}\varphi_l} \sin\theta_l \frac{U_l M_l}{2}.$$

Here $U_l$ and $M_l$ are Coulomb integral and magnetic moment on $l$-site correspondingly; $\theta_l$ and $\varphi_l$ are polar angles which define the magnetic moments direction.

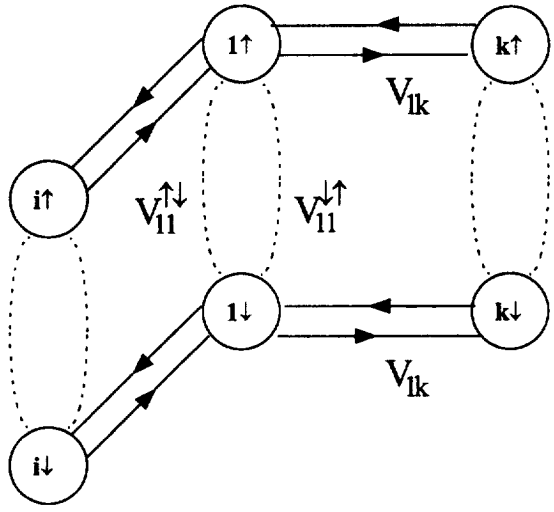


Fig. 1. Schematic representation of hopping in PAM. Solid lines correspond to the intersite hopping without change of spin projection, dash-lines correspond to the hopping on site with the change of spin projection.

Using the recursive method in real space, when the d–d interaction is taken into account inside of first coordination sphere of given atom, one can obtain expression for the d-electron Green function

$$g_{ll}^{\uparrow\uparrow} = \frac{1}{\omega - E_l^{\uparrow} - \sigma_{ll}^{\uparrow\uparrow}},$$

where $E_l^{\uparrow}$ is the energy of d-electron with up spin projection on $z$-axis, mass operator $\sigma_{ll}^{\uparrow\uparrow}$ is defined as

$$\sigma_{ll}^{\uparrow\uparrow} = Z_l^{-1}\left\{\frac{U_l^2 M_l^2}{4}\sin^2\theta_l \prod_{i=1}^{8} D_i + \sum_{j=1}^{8}\left(\frac{U_l U_j M_l M_j}{2}\sin\theta_l \sin\theta_j \cos(\varphi_l - \varphi_j) - a_1^{\downarrow} a_j^{\downarrow} - V^2\right) V^2 \prod_{i\neq j}^{8} D_i \right.$$
$$\left. -V^2 \sum_{j=1}^{8}\sum_{i<j}^{8}\left(a_i^{\downarrow} a_j^{\uparrow} + a_j^{\downarrow} a_i^{\uparrow} - \frac{U_i U_j}{2} M_i M_j \sin\theta_i \sin\theta_j \cos(\varphi_i - \varphi_j)\right) \prod_{i'\neq i,j}^{8} D_{i'}\right\},$$

and following notifications were introduced:

$$Z_l = \left(a_l^{\downarrow} - \sum_{j=1}^{8}\frac{a_j^{\uparrow} V^2}{D_j}\right)\prod_{i=1}^{8} D_i, \quad D_i = a_i^{\uparrow} a_i^{\downarrow} - \frac{U_i^2 M_i^2}{4}\sin^2\theta_i, \quad a_i^{\uparrow} = \omega - E_i^{\uparrow}.$$

For the numerical calculations we used the modification of "zeros and poles"method, which allows to determine very effectively the poles of mass operator and Green function and to avoid time-consuming numerical integration of density of d-electron states in the process of self-consistency.

Fig. 2 illustrates the graphical solution of equation $Z_l = 0$ for the determination of mass operator poles. It is easy to see that all poles $x_i$ are separated from each other, so that $x_i \in (\omega_{i-1}, \omega_i)$, where the $\omega_i$ are the roots in ascending order of equation $D_j = 0$ for different $j$. All $x_i$ can be obtained by means of bisection of the interval $(\omega_{i-1}, \omega_i)$ and choosing the interval where the function $Z_l(\omega)$ has different signs at the ends of interval. After calculation of mass operator poles one can rewrite mass operator as a sum of simple fraction so that the denominator of Green

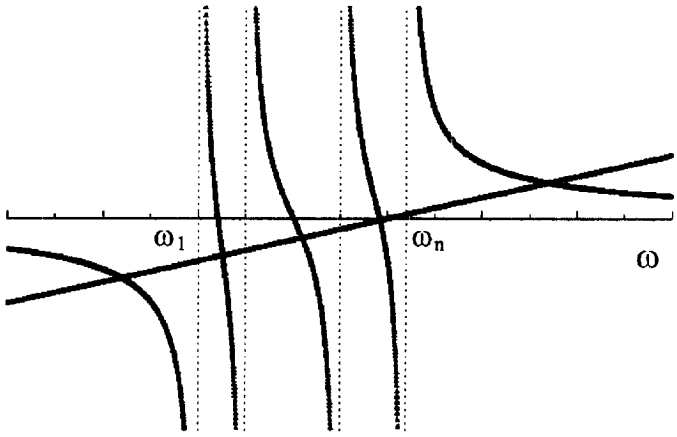


Fig. 2. Graphical solution of the equation $Z_l = 0$. Dash-lines show zeros of $D_i$ for different $i$.

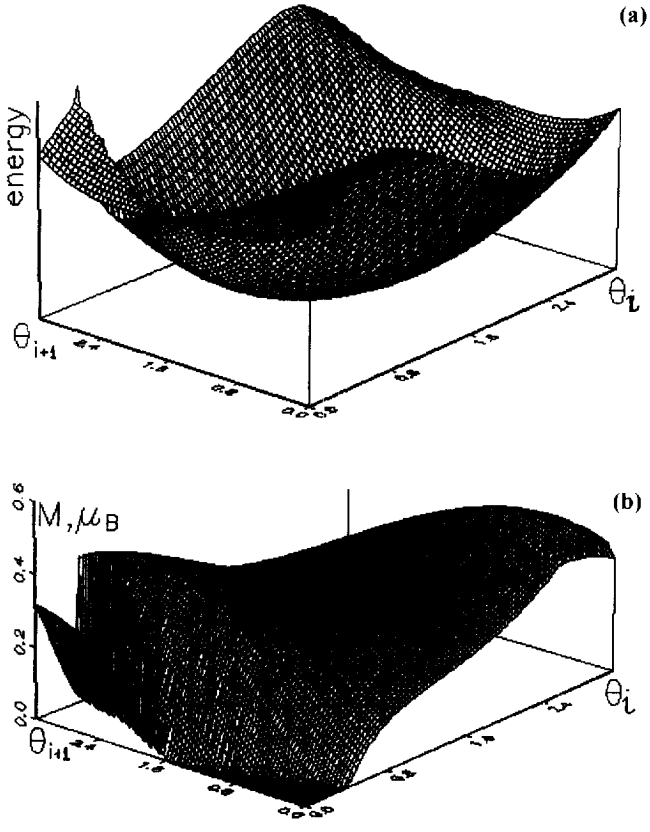


Fig. 3. Energy of d-electrons on $i$-site (a) and its magnetic moment $M$ (b) as a function of angles $\theta_i$ and $\theta_{i+1}$ between axis of quantisation and magnetic moments on $i$ and $i+1$-layer, $\theta_{i-1} = \pi/2$, $\varphi = 0$ for all atoms. All other parameters correspond to the antiferromagnetic Cr in collinear case.

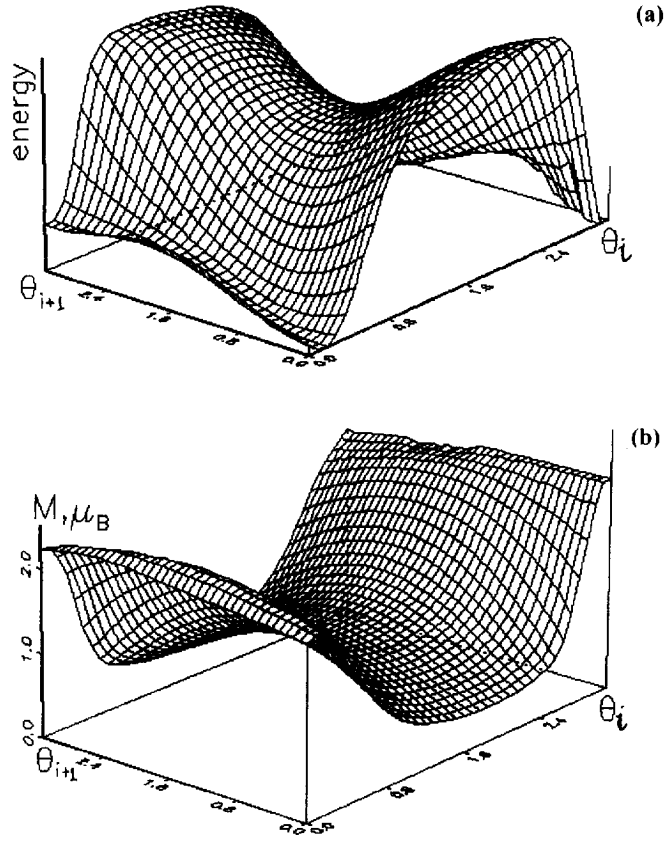


Fig. 4. The same as in Fig. 3 with parameters correspond to ferromagnetic Fe in collinear case.

function will have the same structure as $Z_l$. Green function roots $y_i(l)$ can be obtained after that by the same way. So the d-electron Green function takes the form

$$g_{ll}^{\uparrow\uparrow} = \sum_i \frac{C_i(l)}{\omega - y_i(l)},$$

and the population number can be found analytically without numerical calculations and it is essentially reduced the time of calculations.

Magnetic moment $M_l$ and occupation number $N_l$ on each site have been determined self-consistently for the different angles $\theta_l$ and $\varphi_l$, and the state with minimal energy is saved for the next iteration. The magnitude of the moments and their direction for other atoms are kept constant during the self-consistency on a given site.

The dependence of the energy and of the magnetic moments on the polar angles $\theta_l$ between quantisation axis and direction of magnetic moment depends essentially on the parameters of the model. As an example, we calculated the magnetic moments of atom in the layer $i$ as a function of $\theta_i$ and $\theta_{i+1}$ when for the previous layer $i-1$ the value $\theta_{i-1} = \pi/2$ is taken. In Fig. 3 all $\varphi$ were taken zero and all other parameters correspond to the antiferromagnetic chromium in collinear case. Fig. 4 displays the results where the same calculations were performed for the ferromagnetic iron. The shape of the surfaces in Figs. 3 and 4 differs essentially. First of all there is a minimum of energy in Fig. 3 for $\theta_i$ and $\theta_{i+1}$ not equal to 0 or $\pi$. In Fig. 4 on the contrary the dependence of energy on angles looks like saddle. So, minimal energy will be for $\theta_i = 0$ or $\theta_i = \pi$. It means that for Cr the formation of noncollinear structure can be

much more probable than for Fe. Dependence of magnetic moment on the $\theta_i$ and $\theta_{i+1}$ appears to be complex for Cr, so that first phase transition [13] can take place with change of the direction of spin of the nearest neighbours. Note that such behaviour can take place near domain walls in the bulk material. Self-consistent calculations of space nonhomogeneous structures like steps on the surface and pinholes in the superlattices show that such defects of the structure lead to the noncollinear ordering of magnetic moments.

In summary we have developed the theory within the framework of PAM for calculation of noncollinear magnetism in LDMS. Calculation performed shows the different sensitivity of Fe and Cr relatively to perturbation of collinear structure and displays the role of space defects in formation of noncollinear magnetism.

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