Description of magnetically ordered stratified state in the periodic Anderson model

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The mechanism for magnetic ordering near the surface of a $3d$ metal is analyzed in the periodic Anderson model. A simple criterion for the occurrence of antiferromagnetic order in a bulk sample is given. A numerical solution of the self-consistent equations (in the approximation of a very simple Fermi-liquid closure) shows that there may be either a surface magnetism or "dead layers" at the surface of a metal, depending on the parameter values. A criterion for choosing between the two situations is given. When the jump parameter is relatively large, an antiferromagnetic order with hyperstructures of a fold type may occur. The onset of magnetic order in thin films is analyzed (assuming a constant Fermi energy).

1. INTRODUCTION

Advances in experimental capabilities have recently attracted much more research interest to situations in which a surface and surface layers play a decisive role in determining the properties of a sample. Of particular interest here are thin films and other stratified systems. Two approaches are ordinarily taken in the theoretical work on the electron structures of metal surfaces and other stratified systems. The first approach is based on a density-functional method and requires lengthy numerical calculations.[1–3] The second approach presupposes the use of model Hamiltonians,[4–6] in the construction of which one focuses on only some small fraction of the interactions which play the most important role in the description of phenomena of the given class. The calculations are greatly simplified in this second approach, and the qualitative picture of the phenomenon is still conveyed correctly.

Foremost among the models which successfully describe the magnetic properties of $3d$ transition metals and their compounds are the Hubbard model and the periodic Anderson model. The Hubbard Hamiltonian incorporates only direct transitions between d states in the absence of an s-type conduction band, so the width of the d level tends toward zero with decreasing value of the jump parameter.[7] The periodic Anderson model is based on the idea of hybridizing pure s- and d-type bands, so the renormalized parameters which are found for the quasilocalized d electrons contain contributions determined by the interaction with s electrons. In particular, an intrinsic width of the d level, which does not depend on the jump parameter, appears. The Anderson model thus presupposes that the coupling of the d and s electrons at a site is comparatively strong, while the coupling between d electrons in different sites due to the d–s–d interaction is relatively weak. A situation of this sort arises with decreasing distance between impurities in the ordinary Anderson model.[8] One should first construct resonant d states having a finite width (as in Anderson's model of an isolated impurity) and the consider the interaction between different atoms. A characteristic parameter useful for assessing the plausibility of a model is the ratio V/Γ, of the jump integral V to the width of the d level, Γ. A relation $V/\Gamma \lesssim 1$ is assumed. More precisely, this theory has a solid basis under the conditions $|E_0 - \varepsilon_F|/\Gamma \gg V/\Gamma$ and $U/\Gamma \gg V/\Gamma$, where U is the Coulomb repulsion of the d electrons which are localized at a site, E_0 is the energy of the unperturbed d level, and ε_F is the Fermi energy. This circumstance constitutes an important distinction between the periodic Anderson model and the Hubbard model, which was used in Ref. 6, where it was pointed out that the surface influences the magnetic properties of the layers near the surface by virtue of the decrease in the number of geometric neighbors. Borman *et al.* made some definite assumptions, which limit the application of that study to weakly magnetized samples. In real $3d$ metals, the parameters of the Anderson model are given in order of magnitude by U, $|E_0 - \varepsilon_F| \sim 6$–$10$ eV, V, and $\Gamma \sim 1$ eV (Refs. 9 and 10). It is thus natural to assume $U > V$ and $|E_0 - \varepsilon_F| > V$, as we do in the present paper, in contrast with the approach taken by Borman *et al.*[6] who studied the behavior of systems which are approximately paramagnetic, with small values of U.

In the present paper we study the magnetic properties of surfaces and films in the stratified approximation on the basis of the periodic Anderson model. As in Ref. 6, we use the linear approximation in the exact self-consistent equations. We derive a condition for an instability of the paramagnetic state with respect to ferromagnetic and antiferromagnetic ordering. In the linear regime we study the transition from the surface to the interior of a sample for an arbitrary type of magnetic order. We use the initial nonlinear equations to carry out an exact numerical calculation. The results of this calculation show that near a surface the magnetic moment may either decrease (to the point of the formation of "dead layers") or increase (a surface magnetism). We derive a first simple semiempirical condition for the occurrence of one situation or another. We compare the results of the numerical solution with the results found in the linear approximation. We show that the linear approximation corresponds to the numerical solution at small values of V in the interior of the sample. At large values of $V (V/\Gamma \sim 1.5)$, the equations have many solutions, mostly antiferromagnetic, including some with magnetic hyperstructures of a fold type (a breakdown of antiferromagnetic order in a single layer).

2. EQUATIONS FOR THE GREEN'S FUNCTIONS; THE LINEAR APPROXIMATION

In the transition metals of the iron group, the energy spectrum can be approximated well by a model of two bands corresponding to $3d$ and $4s$ atomic electrons. In describing

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stratified structures in 3d metals, we thus start from the equations for the matrix elements of the Green's function of the periodic Anderson model[11]:

$$\sum_{i_1}[\omega\delta_{ii_1}-E_{ii_1}(\omega)]g_{i_1i'}(\omega)-\sum_{\mathbf{k}}V_{i\mathbf{k}}(\omega)g_{\mathbf{k}i'}(\omega)=\delta_{ii'},$$

$$[\omega-E_{\mathbf{k}}(\omega)]g_{\mathbf{k}i}(\omega)-\sum_{i_1}V_{\mathbf{k}i_1}(\omega)g_{i_1i}(\omega)=0,$$

where the index i specifies the site in the crystal lattice, and **k** is the quasimomentum of the electron in the s band. The diagonal elements E_{ii} are interpreted as the energies of d electrons which are localized at site i; the nondiagonal elements, $E_{ii'}$ describe jumps of d electrons from one lattice site to another. The quantities $V_{i\mathbf{k}}$ and $V_{\mathbf{k}i}$ are treated as seed-band hybridization potentials. All the quantities which appear in the equations are diagonal in the spin indices; to streamline the notation, we will omit these indices. For the matrix elements $g_{ii'}$ we find the closed equation

$$[\omega-E_i(\omega)]g_{ii'}(\omega)-\sum_{i_1}V_{ii_1}(\omega)g_{i_1i'}(\omega)=\delta_{ii'}. \qquad (1)$$

The energy of a d electron, E_i, and the transition integrals V_{ii_1} contain contributions from an s–d interaction:

$$E_i(\omega)=E_{ii}(\omega)+\sum_{\mathbf{k}}\frac{V_{i\mathbf{k}}(\omega)V_{\mathbf{k}i}(\omega)}{\omega-E_{\mathbf{k}}},$$

$$V_{ii'}(\omega)=E_{ii'}(\omega)+\sum_{\mathbf{k}}\frac{V_{i\mathbf{k}}(\omega)V_{\mathbf{k}i'}(\omega)}{\omega-E_{\mathbf{k}}(\omega)}.$$

The energy levels E_i have an intrinsic width Γ, which is determined by s–d hybridization effects:

$$\Gamma(\omega)=\operatorname{Im}E_i(\omega)=\pi\sum_{\mathbf{k}}|V_{\mathbf{k}i}(\omega)|^2\delta(\omega-E_{\mathbf{k}}(\omega)).$$

An iterative solution of system of equations (1) leads to the following expression for the function g_{ii}:

$$g_{ii}(\omega)=[\omega-E_i(\omega)-\sigma_i(\omega)]^{-1},$$

$$\sigma_i(\omega)=\sum_{i_1\neq i}\frac{V_{ii_1}(\omega)V_{i_1i}(\omega)}{\omega-E_{i_1}(\omega)}$$

$$+\sum_{\substack{i_1\neq i\\ i_2\neq i,i_1}}\frac{V_{ii_1}(\omega)V_{i_1i_2}(\omega)V_{i_2i}(\omega)}{[(\omega-E_{i_1}(\omega)][\omega-E_{i_2}(\omega)]}+\dots .$$

For a metal with a bcc lattice, and with a d–d interaction within a single coordination sphere, the series for the mass operator σ_i is cut off at the first term. For homogeneously ordered ferromagnetic and antiferromagnetic samples we find

$$\sigma_\Phi{}^\alpha(\omega)=8V^2/(\omega-E^\alpha), \qquad \sigma_A{}^\alpha(\omega)=8V^2/(\omega-E^{-\alpha}).$$

Here V is the integral representing jumps between nearest neighbors, which is assumed to be independent of the spin α and the frequency ω. Similar expressions for σ can be written for other types of lattices, e.g., an fcc lattice, but they are considerably more complicated even when the interaction of d electrons within the first coordination sphere is taken into account.

The energy of a d electron with a spin projection α must be determined self-consistently in the spirit of the Fermi-liquid theory,[11,12] along with the occupation numbers of the electron states, n^α. In a case in which the kernel of the Fermi-liquid approximation is approximated by a single constant U, the self-consistency condition becomes

$$E^\alpha=E_0+Un^{-\alpha}.$$

The parameter U is phenomenological and is not associated with the restrictions imposed by the Hartree-Fock approximation.[13] This approximation is the simplest one; it does not describe effects such as the Kondo effect.[14] Finding a description of such effects in a stratified sample is an independent and significant problem.

The density of d states with a definite spin projection is expressed in terms of the imaginary part of the Green's function. It is the sum of two Lorentzian functions centered at $E^\alpha \pm 2^{3/2}V$. In the case of a ferromagnetic order, the two lines have the same amplitude. States with different spin projections are displaced an amount UM with respect to each other, where M is the magnitude of the magnetic moment. For an antiferromagnetic material, the positions of the Lorentzian lines corresponding to different values of α are the same, but their amplitudes are different (Fig. 1).

We now consider the simplest inhomogeneous state: a stratified state in which the magnetic moments of the atoms are identical in the same layer and change from one layer to another. An inhomogeneity of this type arises, for example, because of an absolutely smooth boundary of a sample. In this case the energy of a d electron in layer i differs from the energies in the preceding and succeeding layers, so that mass operator σ_i changes:

$$\sigma_i{}^\alpha=4V^2/(\omega-E^\alpha_{i-1})+4V^2/(\omega-E^\alpha_{i+1}).$$

Assuming that the deviations from homogeneity (parametric, ferromagnetic, or antiferromagnetic) are slight, we restrict the analysis to the approximation linear in Δn in the equations for the occupation numbers. Denoting by Δ_i the

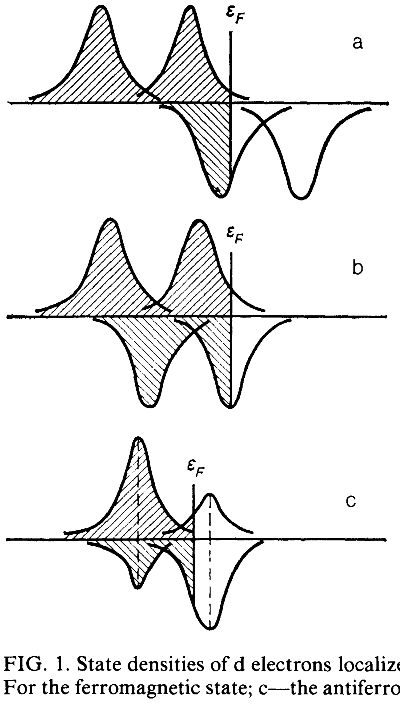

FIG. 1. State densities of d electrons localized at a site of interest. a,b—For the ferromagnetic state; c—the antiferromagnetic state.

energy shift for a *d* electron with respect to the energy in a homogeneously ordered sample, we find the following system of equations for the linear approximation:

$$\Delta_i^{-\alpha}=A^{\alpha}_{\Phi,\mathrm{A}}\Delta_i^{\alpha}+B^{\alpha}_{\Phi,\mathrm{A}}(\Delta_{i-1}^{\pm\alpha}+\Delta_{i+1}^{\pm\alpha}). \qquad (2)$$

The upper sign in this expression corresponds to a ferromagnetic ground state, and the lower sign to an antiferromagnetic ground state. The coefficients *A* and *B* are given by

$$A_\Phi{}^\alpha=-\frac{U}{8\pi}\left[\frac{1}{2^{1/2}V}\operatorname{arcctg}\frac{(E^\alpha-\varepsilon_F)^2-8V^2+\Gamma^2}{2^{5/2}V\Gamma}\right.$$
$$\left.+\frac{2\Gamma}{(E^\alpha+2^{3/2}V-\varepsilon_F)^2+\Gamma^2}+\frac{2\Gamma}{(E^\alpha-2^{3/2}V-\varepsilon_F)^2+\Gamma^2}\right], \qquad (3)$$

$$B_\Phi{}^\alpha=\frac{U}{8\pi}\left[\frac{1}{2^{3/2}V}\operatorname{arcctg}\frac{(E^\alpha-\varepsilon_F)^2-8V^2+\Gamma^2}{2^{5/2}V\Gamma}-\right.$$
$$\left.-\frac{\Gamma}{(E^\alpha+2^{3/2}V-\varepsilon_F)^2+\Gamma^2}-\frac{\Gamma}{(E^\alpha-2^{3/2}V-\varepsilon_F)^2+\Gamma^2}\right]$$

in the case of ferromagnetism and

$$A_\mathrm{A}{}^\alpha=-\frac{8V^2U}{\pi W^2}\left[\frac{2}{W}\operatorname{arcctg}\frac{(E^\alpha-\varepsilon_F)(E^{-\alpha}-\varepsilon_F)-8V^2+\Gamma^2}{\Gamma W}\right.$$
$$\left.+\frac{8\Gamma}{(E^\alpha+E^{-\alpha}+W-2\varepsilon_F)^2+4\Gamma^2}+\frac{8\Gamma}{(E^\alpha+E^{-\alpha}-W-2\varepsilon_F)^2+4\Gamma^2}\right],$$
$$B_\mathrm{A}{}^\alpha=\frac{U}{2\pi}\left[\frac{16V^2}{W^3}\operatorname{arcctg}\frac{(E^\alpha-\varepsilon_F)(E^{-\alpha}-\varepsilon_F)-8V^2+\Gamma^2}{\Gamma W}\right. \qquad (4)$$
$$-\left(1+\frac{E^\alpha-E^{-\alpha}}{W}\right)^2\frac{\Gamma}{(E^\alpha+E^{-\alpha}+W-2\varepsilon_F)^2+4\Gamma^2}$$
$$\left.-\left(1-\frac{E^\alpha-E^{-\alpha}}{W}\right)^2\frac{\Gamma}{(E^\alpha+E^{-\alpha}-W-2\varepsilon_F)^2+4\Gamma^2}\right],$$

where $W=[(E^\alpha-E^{-\alpha})^2+32V^2]^{1/2}$, for an antiferromagnetic state.

Equation (2) has a simple physical meaning: A perturbation of the occupation numbers of the electron states of a selected atom results from both a change in the state of the electrons which are localized at the same atom and which have the opposite spin [the first term on the right side of Eq. (2)] and the electrons which are localized at neighboring atoms (the second term). In the linear approximation, the state density is again written as the sum of two Lorentzian functions, although the positions of the centers of these functions and their amplitudes are not the same as the corresponding quantities in the homogeneous case.

We seek a solution of Eq. (2) in the form

$$\Delta_j{}^\alpha=C_\alpha q^j.$$

For the quantities *q* we then find

$$q^2-zq+1=0,$$

where

$$z=-\frac{1}{2}\left(\frac{A_\Phi{}^\alpha}{B_\Phi{}^\alpha}+\frac{A_\Phi{}^{-\alpha}}{B_\Phi{}^{-\alpha}}\right)$$
$$\pm\left[\frac{1}{4}\left(\frac{A_\Phi{}^\alpha}{B_\Phi{}^\alpha}-\frac{A_\Phi{}^{-\alpha}}{B_\Phi{}^{-\alpha}}\right)^2+\frac{1}{B_\Phi{}^\alpha B_\Phi{}^{-\alpha}}\right]^{1/2}$$

in the ferromagnetic case and

$$z=\frac{1}{2}\left(\frac{1}{B_\mathrm{A}{}^\alpha}+\frac{1}{B_\mathrm{A}{}^{-\alpha}}\right)\pm\left[\frac{1}{4}\left(\frac{1}{B_\mathrm{A}{}^\alpha}-\frac{1}{B_\mathrm{A}{}^{-\alpha}}\right)^2+\frac{A_\mathrm{A}{}^\alpha A_\mathrm{A}{}^{-\alpha}}{B_\mathrm{A}{}^\alpha B_\mathrm{A}{}^{-\alpha}}\right]^{1/2}$$

in the antiferromagnetic case.

For real values of z such that $|z|>2$, there exist two real roots q which correspond to an exponential growth and an exponential decay of the magnetic moment with distance into the sample (with increasing j). The increasing solution must be discarded if there is only a single surface. For values $|z|<2$ there are two complex roots, which correspond to an oscillatory profile of the magnetic moment in the layer with distance to the surface of the sample. In this case we can speak of the formation of a long-range order in the layered structure. Complex values of z describe oscillations of the magnetic moment which decay with distance into the sample.

If the homogeneous state is paramagnetic, the quantities $A^{\alpha}_{\Phi}, A^{\alpha}_{A}$, and $B^{\alpha}_{\Phi}, B^{\alpha}_{A}$ are identical and do not depend on the spin projection α. The value $q=1$ corresponds to an instability of the paramagnetic state with respect to ferromagnetic ordering. In this case we have

$$A+2B=-1. \qquad (5)$$

Substituting expressions (3) into (5), we find the usual Stoner condition,

$$U\rho(\varepsilon_F)=1,$$

where $\rho(\varepsilon_F)$ is the state density at the Fermi level. An instability with respect to a transition to an antiferromagnetic state arises at $q=-1$. In this case we have

$$A-2B=-1.$$

Using the explicit expressions [(3) and (4)] for A and B, we find

$$U\Delta N/2^{3/2}V=1, \qquad (6)$$

where ΔN is the difference between the occupation numbers of the sublevels into which the *d* level splits because of the *d*–*d* interaction. The denominator in (6) contains the energy separation of the two split sublevels.

The conditions which have been found for a ferromagnetic ordering, (5), and for an antiferromagnetic ordering, (6), become clear when we examine the energy spectrum of the *d* electrons. In the case of a paramagnet-ferromagnet transition, two mechanisms acting to perturb the amplitude of the Lorentzian profiles of the state density of the *d* electrons localized at a site of interest cancel out. These mechanisms are that caused by the effect of *d* electrons localized at the same site and that caused by the effect of *d* electrons localized at neighboring atoms. With increasing interaction U, a state in which the state-density curves corresponding to opposite values of the spin projection are shifted with respect to one another becomes preferred from the energy standpoint. At the transition from the paramagnetic order to an antiferromagnetic order, on the other hand, the shifts in the positions of the state-density peaks cancel out, while the energy benefit is achieved thanks to a transition of electrons from one sublevel of the *d* level to the other.

The linear approximation makes possible a correct description of the behavior of the magnetic moment in the case in which the system is not far from any homogeneous state

TABLE I. The magnetic moment M_0 and the number of d electrons, N_0, in a homogeneous sample and deviations from the homogeneous state in the surface layer and in the following layers $[x=(E_0-\varepsilon_F)/\Gamma, y=U/\Gamma]$.

V/Γ	M_0, μ_B	N_0	ΔM_1, μ_B	ΔM_2, $10^{-1}\mu_B$	ΔN_1	$\Delta N_2 \cdot 10^2$
$x=-10,\ y=10$						
0,5	1,50	7.60	−0.45	−0,19	0.30	0.15
0.6	1.65	7,47	−0.33	−0.12	0.26	−0,17
0.7	1,74	7.38	−0,23	−0.16	0.22	0,13
0.8	1,78	7,31	−0.14	−0.24	0,19	0,63
0,9	1,79	7.25	−0,06	−0.33	0.17	1,21
1,0	1.78	7,19	0.03	−0.46	0.15	1,88
1,1	1.74	7.12	0,13	−0.62	0,15	2,71
1,2	1.67	7.04	0.25	−0.86	0,15	3,74
1,3	1,57	6.95	0.41	−0,12	0,17	5,08
1,4	1.39	6.81	0,66	−0.20	0,21	6,60
1,5	1.08	6,61	1,07	−0,45	0,27	5.72
1.6	0.34	6.28	1,78	−0.64	0,47	4.87
1.7	0	6,12	2,06	−0.38	0.56	7.27
$x=-10,\ y=12$						
0,3	3.65	5,91	0.11	0,01	−0.10	−0,07
0,5	3.17	6,30	0.38	0,08	−0.30	−0.50
0.7	2.58	6.70	0.57	0	−0.39	0.81
0.9	2.18	6.81	0.59	−0.30	−0.26	3.92
1.0	2.00	6.80	0,68	−0.54	−0,19	5,78
1,1	1.78	6,71	0.88	−1,00	−0.14	8,30

(paramagnetic, ferromagnetic, or antiferromagnetic). However, this approximation is not sufficient for describing the surface layers, where the perturbation of the magnetic moments may be pronounced. A calculation of the magnetic moments of the surface requires an exact solution of the self-consistent equations.

3. RESULTS OF AN EXACT CALCULATION FOR A NONUNIFORMLY MAGNETIZED METAL

To solve the problem of the distribution of magnetic moments in a stratified magnetic material, we need to determine the occupation numbers n_i^α of the electron states in each layer. For interior layers, the values of n_i^α can be found from the system of equations

$$n_i^\alpha = \frac{1}{\pi}\sum_{j=1}^{3} C_j^{(i)} \operatorname{arcctg} x_j^{(i)}. \qquad (7)$$

Here the $x_j^{(i)}$ are determined by the roots of the denominator of the Green's function g_{ii}, which in our case is a polynomial of third degree in ω, and the $C_j^{(i)}$ are the coefficients in the decomposition of the Green's functions into simple fractions. The equations for the surface layer is similar to (7), but since the atoms of this layer contain only four neighbors in the first coordination sphere the quantities $x_j^{(i)}$ are found from a quadratic equation.

In the numerical calculation of the magnetic moments in thin metal films and near the surface of a metal, the following algorithm was used. The first step is to find the occupation numbers of the electron states corresponding to the uniformly ordered sample. These occupation numbers are used as an initial approximation for the subsequent calculations. The values of the magnetic moment and of the number of electrons in the next approximation are then determined in succession, beginning with the surface layer. To find the occupation numbers in layer i, we need to specify the energies in layers $i-1$ and $i+1$. For E_{i-1} we use the value found immediately before this value, and for E_{i+1} we use the value of the preceding approximation. This procedure is repeated until the magnetic moment and the number of electrons in each layer stop varying. A method of this sort for finding self-consistent solutions does not guarantee the uniqueness of the solution, so different magnetic structures may be found for given parameter values, depending on the initial homogeneous state.

Table I shows values of the magnetic moment and of the number of d electrons $[M=5(n^+-n^-),\ N=5(n^+ + n^-)]$ in the interior of the sample, along with the ratios of the magnetic moments and the numbers of electrons at the surface layer and in the next layer in the case of a ferromagnetic order, for various values of V/Γ. The other parameter values were taken to be $x=(E_0-\varepsilon_F)/\Gamma=-10$, $y=U/\Gamma=10$; 12. The magnetic moment of the surface layer may be substantially greater than the value in the interior of the sample (the near-surface mechanism[6,15]), but it may also be smaller ("dead layers" at the surface of a metal[16]), according to the calculations. The decrease and increase in the magnetic moment at the surface are determined by the position of the Fermi level with respect to the state-density curve. We suggest the following simple criterion: If the Fermi level lies between the centers of gravity of the d levels with opposite spin projections (Fig. 1a), the magnetic moment of the surface atoms increases. The point is that the surface atoms have fewer neighbors than the interior atoms, so there is an effective decrease in the hopping parameter V. Consequently, the distance between the sublevels of the d level of the electrons with each of the spin projections decreases. The number of electrons with the predominant spin direction becomes even greater, while the number with the opposite spin decreases. If the centers of the d levels lie below ε_F (Fig. 1b), the number of electrons will increase in both sublevels with decreasing V. However, because of the difference in the densities of the states with the different spin projections at the Fermi level, the resultant moment decreases. This semiempirical criterion is confirmed by an analysis of all the data obtained, in particular, the data shown in Table I. In real samples, the parameter V may also change as a result of a

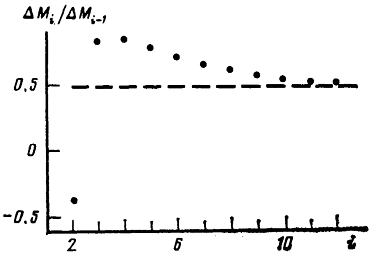

FIG. 2. Formation of the magnetic moment near the surface. Transition to the linear regime (i is the layer number).

reconstruction of the lattice or under the influence of adsorbed atoms. In this case the criterion must be reformulated. The perturbation of the magnetic moment even in the second layer is considerably smaller than that in the first, so the effect of the surface usually extends to only a few atomic layers. Despite the rapid decay of the quantity $\Delta M_i = M_i - M_0$, one can verify that in several cases the linear approximation correctly conveys the picture of the perturbation of the magnetic moments. With $x = -10$, $y = 10$, and $V/\Gamma = 1.3$, for example, we find, in the linear approximation of damped oscillations,

$$\Delta M_k = (0.2)^k \sin(\varphi_0 + \pi k/2).$$

It is this behavior, with a change in the sign of the perturbation after every other layer, that is found in the exact solution.

There are parameter values for which the effect of the surface is felt down to 10 or 20 atomic layers. Figure 2 shows the quantity $q_i = \Delta M_i/\Delta M_{i-1}$ as a function of the layer index i for one such case ($x = -10$, $y = 10$, and $V/\Gamma = 1.6$). The dashed line shows the linear approximation. Corresponding results could be found for an antiferromagnetic ground state.

With increasing V/Γ, the effect of neighboring atoms on the magnetic moment of an atom of interest increases. It turns out that the deviations from the homogeneous state are not small, so the linear approximation does not describe the magnetic order. The nonuniform magnetic structures which arise in this case have a typical size ranging from a few atomic distances to some tens of atomic distances. In several cases the magnetic moment of an atom in layer i is not determined unambiguously by the preceding layers, and several magnetic structures can exist simultaneously in a sample. One of these structures—a fold superposed on antiferromagnetic order—is shown in Fig. 3.

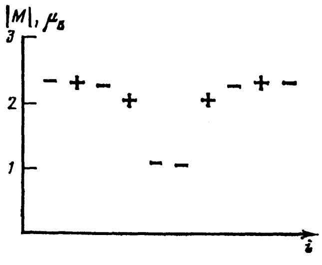

FIG. 3. Fold superposed on antiferromagnetic order for the case $x = -10$, $y = 12$, and $V/\Gamma = 1.2$. The plus and minus signs correspond to different directions of the spin projection.

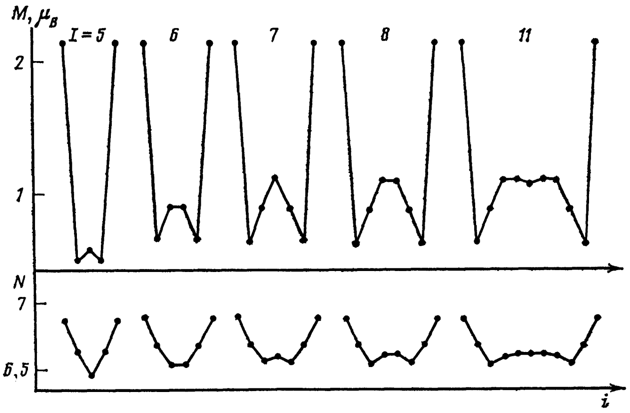

FIG. 4. Distributions of the magnetic moments and of the number of d electrons in films of various thicknesses. Here I is the number of layers in the film; $x = -10$, $y = 10$, $V/\Gamma = 1$.

The effect of the surface on the magnetic properties turns out to be particularly strong in thin metal films consisting of a few atomic layers. In this case, the magnetic moments are acted upon by both surfaces simultaneously, and they differ greatly from the corresponding values in a bulk sample. Figure 4 shows the distributions of the magnetic moments and the number of electrons for films of various thicknesses. We see that the behavior of the magnetic moments near the surface of a thin film is quite different from that in the case of a semi-infinite metal. A change in the occupation numbers in the electron states may lead to a shift of the position of the Fermi level from that in a bulk sample and to a change in the very nature of the magnetic order. In this case the Fermi level is assumed to be fixed.

It is interesting to compare the results calculated for real materials on the basis of the theory derived here with the data found by other approaches, in particular, the density-functional method. The density-functional method was used in Ref. 1 to study the distribution of magnetic moments in an iron film consisting of seven atomic layers. The data from that calculation are shown in Table II along with results found in the present theory on the basis of the periodic Anderson model. The parameters describing the d electrons in iron correspond to those used in Ref. 9. The behavior of the surface layer is the same in the two approaches. There is a substantial increase in the magnetic moment. This result agrees well with experimental results on the photoelectric effect of polarized electrons.[17,18] The second layer has a magnetic moment M_2 smaller than that of the first or third. In Ref. 1, however, the value of M_2 was larger than the moment in the interior of the sample, while in our case it turns out to be smaller. On the whole, there is a fairly good agreement between the two calculations.

TABLE II. Results calculated for the magnetic moments in an α-Fe film consisting of seven layers ($x = -11$, $y = 13$, $V/\Gamma = 0.9$).

i	M_i, μ_B [1]	M_i, μ_B (present theory)
1	2.98	2.84
2	2,35	2.30
3	2.39	2.32
4	2,25	2.32

We have not taken up the temperature dependence of the properties of stratified systems. Such an analysis would present some further difficulties since it would be necessary to deal with the temperature-induced shift of the Fermi level. The position of the Fermi level is determined by the requirement that the total number of electrons remain constant. It can be dealt with accurately only for a metal with a relatively small number of s electrons.

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[1] E. Wimmer, H. Krakauer, A. J. Freeman, Adv. Electron. and Electron. Phys. **65**, 357 (1985).

[2] N. Lang, *Theory of an Inhomogeneous Electron Gas* [Russ. transl., Mir. Moscow, 1987].

[3] O. Jepsen, J. Madsen, and O. K. Anderson, Phys. Rev. **B18**, 605 (1978).

[4] G. Allen, Phys. Rev. **B19**, 474 (1979).

[5] G. Allen, Surf. Sci. **1**, 121 (1981).

[6] V. D. Borman, L. A. Maksimov, and A. P. Popov, Zh. Eksp. Teor. Fiz. **90**, 697 (1986) [Sov. Phys. JETP **63**, 407 (1986)].

[7] E. V. Kuz'min, *Fizika magnitouporyadochennykh beshchestv. (Physics of Magnetically Ordered Substances),* Nauka, Novosibirsk, 1976, p. 6.

[8] P. W. Anderson, Phys. Rev. **124**, 41 (1961).

[9] V. L. Sedov, Zh. Eksp. Teor. Fiz. **74**, 2066 (1978) [Sov. Phys. JETP **47**, 1074 (1978)].

[10] J. B. Boyce and C. P. Slichter, Phys. Rev. **B13**, 379 (1976).

[11] V. N. Gittsovich, A. S. Kondrat'ev, and V. M. Uzdin, Fiz. Met. Metalloved. **55**, 649 (1983).

[12] V. P. Silin, *Fizika mnogochastichnykh sistem. (Physics of Multiparticle Systems),* Naukova dumka, Kiev, 1984, p. 37.

[13] P. W. Anderson, Usp. Fiz. Nauk **127**, 19 (1979).

[14] C. Lacroix, J. Phys. **F11**, 2389 (1981).

[15] M. I. Kaganov, Zh. Eksp. Teor. Fiz. **62**, 1196 (1972) [Sov. Phys. JETP **35**, 631 (1972)].

[16] R. M. White and T. H. Geballe, *Long-Range Order in Solids, Solid State Physics Supplement No. 15,* Academic, Orlando (1984).

[17] A. M. Turner, Yu. Jeng Chang, and J. L. Erskine, Phys. Rev. Lett. **48**, 348 (1982).

[18] A. M. Turner and J. L. Erskine, Phys. Rev. **B28**, 5628 (1983).

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