Title

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Surface Properties of A Heavy-Fermion System: An Exact Many-Body Solution to A Periodic-Cluster Hubbard Model

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ABSTRACT

An exact solution of an eight-site crystal model with periodic boundary conditions, a {001} thin-film with face-centered-cubic crystal structure, is presented for the case of a heavy-fermion system. The object is to study modifications of the many-body electronic structure in the presence of surfaces. The model consists of: (a) a single, fully symmetric orbital per site, with nearest-neighbor and second nearest-neighbor hopping; (b) an *infinite* Coulomb repulsion between electrons on the same site; (c) antiferromagnetic superexchange interactions; and (d) a nearly half-filled band (7/8 electron per site). Two structures are investigated: a two-layer, and a four-layer *fcc* slabs. The nature of the change from bulk to surface is studied by introducing a variable coupling between periodically extended slabs. The many-body spectrum, the one-electron occupancy and the change in properties from bulk to surface are obtained and discussed.

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I. INTRODUCTION

Heavy-fermion materials, with their large heat capacities and other unusual properties at low temperatures, exhibit interesting behavior related to electron many-body interactions in highly correlated narrow-band systems.[1–6] These materials provide a good subject for investigating changes in many-body interactions in various environments.

Techniques used in solving strongly interacting systems, such as heavy-fermion systems have included variational, perturbative, diagrammatic and Monte Carlo approaches[7–12]. Recently, the method of reducing the computational overhead by use of group-theoretical techniques, allowing exact solution of moderate-size clusters, has been shown to be powerful[13].

The small-cluster approach has been successfully applied to various problems where local many-body effects are important: a four-atom cluster Hubbard model[14], photoemission behavior[15] in Nickel, intermediate-valence behavior[16,17] in Cerium, magnetic behavior in Iron, Cobalt, and the Iron-Cobalt alloy[18,19], alloying in the Cooper-Silver-Gold system[20], as well as thermodynamic properties[21] and valence-bond formation[22]. The work has shown that single-site and short-range correlations are well

taken into account in this approach. Although incapable of exhibiting phase transitions, the approach has also shown indications of possible mechanisms involved in long-range correlations.

In a previous paper[23] (referred to as RF hereafter), the small-cluster method has been used to explore the Fermi surface, spin-wave and transport properties of an eight-site, seven electron *fcc* cluster, which proved to be a heavy-fermion system. Superconducting and magnetic fluctuations have also been studied in this approach[24]. Insight into the problem of heavy-fermion, and high-temperature superconductivities has been obtained.

Highly correlated rare-earth metals and compounds are known to have electronic properties which differ drastically at the surface from those in the bulk[25–28]. It is the purpose of the present contribution to modify the approach of RF so as to study the surface electronic structure of the same heavy-fermion model, and examine the transition in those properties from bulk to surface.

Section II reviews the Hamiltonians used to study the thin-film structures of the heavy-fermion model of RF, and the scheme used to link the surface and the original bulk structures. Section III describes the method of calculation. Section IV presents and discusses the results. Conclusions are given in section V.

II. THE HAMILTONIAN

The Hamiltonian for the bulk of the heavy-fermion systems considered here is given in RF. There are essentially, following Hubbard[29], three terms, i.e. nearest-neighbor-site hopping, second nearest-neighbor-site hopping, and an on-site Coulomb repulsion. The limit of large on-site Coulomb repulsion, $U \rightarrow \infty$, reduces the Hamiltonian[30–32] to the form:

$$H = H_{1nn} + H_{2nn} + H_{AF} \quad . \tag{2.1}$$

The first term is the nearest-neighbor hopping, with transfer integral t. The second term is the second-neighbor hopping, with transfer integral T. The third term, a correction of the order t^2/U, represents the antiferromagnetic nearest-neighbor Heisenberg interaction. In this contribution, two thin-film structures for the heavy-fermion system of RF are investigated. The first is a two-layer slab (see Figure 1). The cluster under consideration here is comprised of eight atoms. If repeated via periodic boundary conditions through the two-dimensional plane, a two-layer slab cut from the original bulk *fcc* lattice in the [001] direction is obtained. Each atom in this structure has only eight nearest neighbors instead of twelve, i.e. four in the same layer and four in the adjacent layer. For the same reason, each atom has only four second neighbors rather than the six of the bulk structure. The eight sites in the cluster are labeled i=0,1,...,7, with sites 0, 3, 4, and 7 in one layer, and the remaining ones in the other. The three terms of the Hamiltonian can be written as:

$$H_{1nn} = -t \sum_{\substack{(i,j)=1nn;\sigma \\ interlayer}} c_{i\sigma}^{\dagger} c_{j\sigma} - 2t \sum_{\substack{(i,j)=1nn;\sigma \\ intralayer}} c_{i\sigma}^{\dagger} c_{j\sigma} \tag{2.2}$$

$$H_{2nn} = -4T \sum_{(i,j)=2nn;\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \tag{2.3}$$

$$H_{AF} = J \sum_{\substack{(i,j)=1nn \\ interlayer}} \vec{S}_i \cdot \vec{S}_j + 2J \sum_{\substack{(i,j)=1nn \\ intralayer}} \vec{S}_i \cdot \vec{S}_j \tag{2.4}$$

The notation is standard, similar to that of RF. It should be noted that the sums on the

sites are restricted to the eight-atom cluster, and the eight nearest neighbors of each site are, in the periodic cluster, two each of two of the sites in the same layer and one each of all four sites in the other layer (e.g. the eight nearest neighbors of site 0 are two each of sites 3 and 7, and one each of sites 1, 2, 5, and 6). Therefore the terms in equation (2.2) have coefficients t and $2t$ respectively. The site labeled $(i \pm 4)$ is always the second neighbor of site i.

The second thin-film structure is a four-layer slab (see Figure 2). Here there are two surface layers (where the sites have the nearest-neighbor structure described above), and two interior layers with full twelve nearest neighbors and five second neighbors. There are two sites in each layer of the eight-atom cluster. (For instance the eight nearest neighbors of site 0 are four sites 3, two sites 5 and two sites 6; the five second neighbors are four sites 0 -- i.e. itself -- and one site 4. Similarly the twelve nearest neighbors of site 4 are four sites 7, two sites 1, two sites 2, two sites 5, and two sites 6; the five second neighbors are four sites 4 and one site 0.) Therefore the three terms of the Hamiltonian for this structure can be written as

$$H_{1nn} = -2t \sum_{\substack{(i,j)=1nn;\sigma \\ interlayer}} c_{i\sigma}^{\dagger} c_{j\sigma} - 4t \sum_{\substack{(i,j)=1nn;\sigma \\ intralayer}} c_{i\sigma}^{\dagger} c_{j\sigma} \tag{2.5}$$

$$H_{2nn} = -T \sum_{i=0...7;\sigma} c_{i\sigma}^{\dagger} c_{(i\pm4)\sigma} - 4T' \sum_{i=0...7;\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} \tag{2.6}$$

$$H_{AF} = 2J \sum_{\substack{(i,j)=1nn \\ interlayer}} \vec{S}_i \cdot \vec{S}_j + 4J \sum_{\substack{(i,j)=1nn \\ intralayer}} \vec{S}_i \cdot \vec{S}_j \tag{2.7}$$

At this point, an interesting question arises: is there a smooth transition from bulk to surface structure? To address this question, three coupling terms, corresponding to the three terms in the Hamiltonian, are introduced between adjacent slabs, provided they are periodically arranged along the [001] direction. The hopping and antiferromagnetic Heisenberg parameters between different slabs are denoted by αt, αT, and αJ respectively. For $\alpha = 0$, the thin-film structure is achieved. In the $\alpha = 1$ limit, the original bulk *fcc* lattice is recovered. By setting $0 < \alpha < 1$, a continuous set of intermediate cases can be obtained.

III. METHOD OF CALCULATION

The Hamiltonian presented above, for the eight-atom cluster, exhibits many symmetries and constraints which can be exploited to reduce greatly the computational demands of the problem.

With sixteen orbitals, the number of many-body states for N electrons is $[16!/(16-N)!N!]$, which in the case of seven electrons (nearly-half filled band) amounts to 11440. An infinite on-site repulsion reduces the number of states to $[2^N 8!/(8-N)!N!]$, which is 1024 for seven electrons, a sizable reduction. Furthermore, these 1024 states separate, according to spin, into 64 octets, 288 sextets, 448 quartets and 224 doublets. There is also a space-group decomposition. In the following, the space-group properties of the two thin-film structures are discussed separately.

A. Two-layer thin-film structure

The space group for the two-layer, eight-atom cluster (Figure 1) is a nonsymmorphic one, of order 32. In addition to the identity there are three translations along the plane of the layers, the $x-y$ plane, which provide 4 operations. There are two four-fold and one two-fold rotations around the z axis (C_{4z}, C_{4z}^2, C_{4z}^{-1}, where z axis is chosen to be the [001] direction, i.e. the normal to the surface, and the origin is on site

0). With the four intralayer translations these give 3×4 = 12 additional operations. There are also sixteen two-fold screw axes parallel to the x-y plane (their rotation part is formed by one of the four point operations $C_{2x}, C_{2y}, C_{2d}, C_{2d'}$). This nonsymmorphic space group possesses 11 irreducible representations with the following degeneracies: γ_1 (d = 1), γ_2 (d = 1), γ_3 (d = 1), γ_4 (d = 1), γ_5 (d = 2), m_1 (d = 1), m_2 (d = 1), m_3 (d = 1), m_4 (d = 1), m_5 (d = 2), and y_1 (d = 4). These γ, m, and y representations, labeled by the translation-group k-vectors, correspond to the following points of the two-dimensional square Brillouin zone (which extends over the region $-2\pi/a < \pm k_x \pm k_y \leq 2\pi/a$):

$$[0, 0]: \quad \gamma \ , \tag{3.1}$$

$$[2\pi/a, 0]: \quad m \ , \tag{3.2}$$

$$[\pi/a, \pi/a] \text{ and } [\pi/a, -\pi/a]: \quad y \ , \tag{3.3}$$

where a is the cubic lattice constant of the *fcc* structure. These four points constitute the finite sampling of reciprocal space inherent in the periodic-cluster approach[13]. The character table of the group[33] is given in Table I.

The two-layer structure discussed here can be obtained directly from the original bulk structure (see RF), by symmetry reduction. There are compatibility relations between the irreducible representations of the group of the eight-atom cluster *fcc* bulk structure and those of the two-layer structure (see Table II). With all the symmetries taken into account the largest block to diagonalize is 14×14, a considerable reduction over 11440×11440, or 1024×1024, or even 448×448. The various block sizes are shown in Table III.

In the finite, four-point sampling of the eight-atom periodic cluster, there are two one-electron energy levels at γ ($\gamma_{i\sigma}$; i =1, 2), two at m ($m_{i\sigma}$; i =1, 2), and four levels at y ($y_{i\sigma}$; i =1, 2, 3, 4). One can make the transformation between (Wannier) one-electron localized states $c_{i\sigma}$, and Bloch states (referred to collectively as $a_{i\sigma}$) by:

$$\vec{a} = 8^{-1/2}\ \vec{\vec{M}} \cdot \vec{c} \tag{3.4}$$

where the eight-component column vectors $\vec{a}$ and $\vec{c}$ are connected by the 8×8 Wannier-Bloch matrix, $\vec{\vec{M}}$:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \end{bmatrix} \tag{3.5}$$

These one-electron orbitals γ, m and y, have symmetries ${}^2\gamma_1$, ${}^2\gamma_2$, ${}^2m_5$, and ${}^2y_1$, respectively, and one-electron energies:

$$\varepsilon_{\gamma_1} = -8t - 4T \quad , \tag{3.6}$$

$$\varepsilon_{\gamma_2} = 0t - 4T \quad , \tag{3.7}$$

$$\varepsilon_{y_1} = 0t + 4T \quad , \tag{3.8}$$

and

$$\varepsilon_{m_5} = 4t - 4T \quad . \tag{3.9}$$

The bandwidth is $(4t - 4T) - (-8t - 4T) = 12t$, i.e. 75% of that of the bulk structure ($16t$). This reduction results from the surface effect: atoms at the surface layer have fewer neighbors. It is worth noting that there is a one-electron level crossover. Comparison with the one-electron bulk structure (see RF and Table II) shows that a level split off the three-fold bulk x_1 manifold, of γ_2 symmetry, drops below the four-fold degenerate bulk level l_1, middle-of-the-band states, now converted into the y_1 four-fold set.

It is now possible to write down the non-interacting 7-electron energies. They are shown in Table IV.

B. Four-layer thin-film structure

The symmetry of the four-layer thin-film structure (see Figure 2) is lower than that of the two-layer one. The space group in this case is also nonsymmorphic, but of order 16. The only translation in the cluster (in addition to the identity) is $\tau = [a/2, a/2, 0]$, which connects the two atom in the same layer in the cluster (say, site 0 and 3). Again, here a is the cubic lattice constant in the *fcc* structure. The eight point-group operations are: the identity E, five two-fold rotations C_{4z}^2, C_{2x}, C_{2y}, C_{2d}, and $C_{2d'}$, and two four-fold rotations C_{4z}, and C_{4z}^{-1}. Four of the operations appear, in the space group, only together with the translations $\theta \equiv [a/2, 0, 0]$ and $\theta + \tau$: $\{C_{4z} \mid \theta\}$, $\{C_{4z}^{-1} \mid \theta\}$, $\{C_{2d} \mid \theta\}$, $\{C_{2d'} \mid \theta\}$, and similarly for $\theta + \tau$. The elements involving C_{2d} and $C_{2d'}$ are intrinsic two-fold screw axes. This nonsymmorphic space group has 10 irreducible representations corresponding to only two points in the two-dimensional Brillouin zone (which extends over the region $-2\pi/a < \pm k_x \pm k_y \leq 2\pi/a$):

$$[0, 0]: \quad \gamma \ , \tag{3.10}$$

$$[2\pi/a, 0] \quad \text{and} \quad [0, 2\pi/a]: \quad h \ . \tag{3.11}$$

The representations are: γ_1 (d = 1), γ_2 (d = 1), γ_3 (d = 1), γ_4 (d = 1), γ_5 (d = 2), h_1 (d = 1), h_2 (d = 1), h_3 (d = 1), h_4 (d = 1), and h_5 (d = 2). The character table of the group[33] is shown in Table V. In this case there are no simple compatibility relations between the symmetries of the present system and those of the original bulk *fcc* structure of RF. The reason is that if this periodic arrangement of the four-layer structure is repeated periodically along the z-axis, the *fcc* structure is obtained, but the periodic cluster is different from that in RF. In fact, it corresponds to an eight-point sampling of the Brillouin zone that, instead of sampling (as in RF) one Γ, three X, and four L points, it samples at

$$\Gamma = [0, 0, 0] \ , \tag{3.12}$$

$$X = [2\pi/a, 0, 0], \quad [0, 2\pi/a, 0], \quad \text{and} \quad [0, 0, 2\pi/a] \ , \tag{3.13}$$

$$Z = [0, 0, \pi/a] \quad \text{and} \quad [0, 0, -\pi/a] \ , \tag{3.14}$$

$$W = [2\pi/a, 0, \pi/a] \quad \text{and} \quad [2\pi/a, 0, -\pi/a] \ . \tag{3.15}$$

This bulk sampling has only tetragonal symmetry; it destroys the cubic symmetry of the original *fcc* structure[34]. In the four-layer thin-film structure, four of the eight bulk points (Γ, $X_z = [0, 0, 2\pi/a]$, and the two Z points) are projected onto the γ point of the surface Brillouin zone. The other four points of the bulk structure (two X and the two W points) are projected onto the h point of the surface zone.

With all the symmetries taken into account, the largest block to diagonalize is 28×28, still a sizable reduction over those obtained before the application of group-theoretical techniques. The block sizes for all representations and spins are presented in Table VI.

In this finite, two-point sampling of the eight-atom cluster, there are four one-electron energy levels at each of the γ and h point ($\gamma_{i\sigma}$ and $h_{i\sigma}$; i=1, 2, 3, 4). Similar to the two-layer thin-film case, the 8×8 Wannier-Bloch matrix $\vec{M}$, which connects the (Wannier) one-electron localized states and Bloch states in this case can be obtained:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \end{bmatrix} \tag{3.16}$$

The one-electron orbitals γ and h, have symmetries γ_1, γ_4, and h_5 respectively, and one-electron energies:

$$\varepsilon_{\gamma_1\pm} = -6t - 4T \pm [4t^2 + (4t + T)^2]^{1/2} \ , \tag{3.17}$$

$$\varepsilon_{\gamma_4\pm} = -2t - 4T \pm [4t^2 + (4t - T)^2]^{1/2} \ , \tag{3.18}$$

$$\varepsilon_{h_5\alpha} = 4t - 5T \ , \tag{3.19}$$

$$\varepsilon_{h_5\beta} = 4t - 3T \quad , \tag{3.20}$$

respectively. The one-electron energies are very different from those of the two-layer thin-film structure discussed above or the original bulk *fcc* structure in RF. The bandwidth in this case is

$$(4t - 3T) - \{-6t - 4T \pm [4t^2 + (4t + T)^2]^{1/2}\} = 10t + T + [4t^2 + (4t + T)^2]^{1/2}.$$

This is about 90% of the bandwidth of the bulk *fcc* structure, an amount 15% larger than that in the two-layer thin-film case. This additional part comes from the contribution of the two interior layers which have two more (full twelve all together) nearest neighbors and one more (five in total) second neighbors.

Because there are six one-electron levels in the present case, the whole spectrum of non-interacting 7-electron energies is a very long list (there are 282 different energy levels for 11440 states). Only the energies of the ground state (GS) and the lowest excited state (LES) for $t < 0$ and $t > 0$ cases, with the corresponding degeneracy, are written down here:

$$\varepsilon_{GS}\ (t < 0) = 28t - 29T \quad , \quad d=4, \tag{3.21}$$

$$\varepsilon_{LES}\ (t < 0) = 28t - 27T \quad , \quad d=4, \tag{3.22}$$

$$\varepsilon_{GS}\ (t > 0) = -30t - 28T - [4t^2 + (4t - T)^2]^{1/2} \quad , \quad d=2, \tag{3.23}$$

$$\varepsilon_{LES}\ (t > 0) = -24t - 29T - 2\,[4t^2 + (4t - T)^2]^{1/2} \quad , \quad d=4. \tag{3.24}$$

IV. RESULTS AND DISCUSSION

A. Many-body spectrum of the thin-film structures

There are two entirely different physical situations, i.e. ferromagnetic and heavy-fermion, corresponding to $t < 0$ and $t > 0$ respectively, for the bulk *fcc* structure with nearly-half-filled bands (7/8 electron per site) and infinite Coulomb repulsion U (see RF). The purpose of the present contribution is to investigate how the results change in the presence of surfaces. In the following, we will focus our attention on the heavy-fermion ($t > 0$) case. Corresponding results for the ferromagnetic ($t < 0$) case are presented in the appendix.

In the bulk structure of RF, ninety-six of the total possible 1024, a huge pile-up of many-body states, are present in the ground-state manifold of energy (for $J = 0$) $E=-6t+6T$, with various symmetries. It is thus a true "heavy fermion" system. The many-body energies of the bulk heavy-fermion ground-state manifold ($\alpha = 1$) are given in Table VII, together with the results of the lowest sixteen levels of the two-layer thin-film structure ($\alpha = 0$). The results for the lowest twelve levels of the four-layer thin-film structure ($\alpha = 0$) and the corresponding bulk levels ($\alpha = 1$) are shown in Table VIII. In the presence of surfaces the many-body electronic structure is drastically changed. In the case of the two-layer thin-film structure, the ground state (except for spin degeneracy) is non-degenerate and of energy $E=-5t+4T+(1/4)J$, with symmetry ${}^6\gamma_4$. It is quite surprising that the ground state has spin 5/2, corresponding to a partially saturated ferromagnetic state, rather than spin 1/2, as appeared in the bulk structure. For the four-layer thin-film structure, the ground state is also non-degenerate, with symmetry ${}^2\gamma_4$. Although it is still a spin minimally aligned state as in the bulk case, a clear trend toward a more ferromagnetic state can be seen from the many-body spectrum: a spin 3/2 state, with symmetry ${}^4\gamma_3$, drops in energy toward the ground state ${}^2\gamma_4$. More discussion on this point is presented below.

By setting J and/or T equal to zero, the degeneracy of the many-body spectrum of both thin-film structures remains essentially the same, with only energy shifts and some slight energy-level rearrangement. This fact indicates that one-electron effect is the dominant factor in thin-film structure of these heavy-fermion systems: the accidental degeneracies of the bulk case are removed by the presence of the surfaces. In other words, the surfaces of this heavy-fermion system are no longer "heavy-fermionic".

The highly degenerate ground-state manifold of the bulk structure is absent in the many-body spectra of both thin-film structures. The separation between the low-lying states are much larger than the corresponding values of the bulk structure and, more importantly, they are dominated by the nearest-neighbor hopping interaction as mentioned above. This indicates that the formation of the heavy-fermion state is the result of a delicate balance of both many-body effect and one-electron band-structure effect, with appropriate crystal symmetry. For the thin-film structures, symmetry reduction alters the condition for this balance; consequently it destroys the pile-up of many-body states at the lowest energies and leads to the non-degenerate (non-heavy-fermion) surface-structure ground state.

B. One-electron occupancy

It is instructive to have a look at one-electron occupancy in the thin-film structures. First, it is interesting to see how the Fermi surface behavior changes. The notion of Fermi surface of these highly correlated systems has been discussed in RF in the context of an eight-atom cluster providing finite reciprocal-space sampling of the Brillouin zone. It is important to keep in mind that the information is only obtained on a small, discrete set of one-electron energy states, rather than the conventional one-electron continuum. The occupancy of one-electron states is obtained by finding the expectation values:

$$\langle a_{i\sigma}^{\dagger} a_{i\sigma} \rangle = \sum_{j,k=0}^{7} M_{ij} M_{ik} \langle c_{j\sigma}^{\dagger} c_{k\sigma} \rangle \quad , \tag{4.1}$$

where the matrix elements M_{ij} are given by (3.5) and (3.16) for the two-layer and four-layer thin-film structures respectively.

Results for two-layer structure are shown in Table IX for $U = \infty$, $t > 0$ and $U = \infty$, $t < 0$ (see Appendix) cases, along with the isolated atom and non-interacting cases. It can be seen that the Fermi surface behavior of this thin-film heavy-fermion system is very similar to the result of the bulk fcc structure, although its ground state has been drastically changed. It has a monotonically decreasing electron distribution close to the isolated-atom picture, rather than the sharp drop-off of the non-interacting picture. However, a quantitative change occurs here. The total amount of probability drop-off from the bottom (γ_1) to the top (m_5) of the one-electron band is 3/16, somewhat smaller than the amount of the corresponding drop-off, 1/4, in the bulk case.

The situation for the four-layer thin-film structure is slightly different. The results are presented in Table X. Note that the one-electron levels are arranged (in order of increasing energy) as following: γ_{1-} , γ_{4-} , γ_{1+} , γ_{4+} , $h_{5\beta}$, and $h_{5\alpha}$. The change of the probability with increasing energy is non-monotonic, a somewhat surprising many-body effect. There is a small increase (0.04) from γ_{4+} to $h_{5\alpha}$. The total amount of probability decrease from γ_{1-} to γ_{4+} is 0.18, approximately the same as in the two-layer structure. These results show that the one-electron occupancies of this strongly interacting system is weakly structure dependent.

Another item of interest is the one-hole occupancy probability on the localized orbitals of different sites. There is one hole per cluster in the present model. In the bulk and in the two-layer structures, all the sites are equivalent. Therefore, the occupancy probability should be the same, (1/8) on every site. However, in the case of four-layer structure, the sites in the surface layers have fewer nearest neighbors than

those in the interior layers. It is thus expected that the one-hole occupancy probability will be higher on the sites in the interior layers, because of an almost full band and larger spectral bandwidth (number of neighbors) there. This is confirmed by calculations, as shown in Table XI.

C. Bulk-to-surface transition

Since the properties of the thin-film structures of the heavy-fermion system considered here are quite different from those of the bulk structure, it is of interest to know how is the many-body electronic spectrum modified as the system changes from bulk to thin-film structure. It has been pointed out in Section II that this can be achieved by introducing variable coupling terms, with parameters αt, αT and αJ, (α is the bulk-to-surface coupling ratio in the [001] direction) between the periodically extended slabs. In the limit of $\alpha = 1$, the original bulk *fcc* lattice is recovered; thin-film structure is obtained for $\alpha = 0$. The many-body spectrum for the bulk-to-surface transition, i.e. for $0 \leq \alpha \leq 1$, has been obtained. To compare the results with those obtained for the bulk structure in RF, the two-layer slab structure which, as mentioned in sections II and III, is directly related to the original bulk *fcc* structure, is considered first. It is worth noting the splitting of the ground-state manifold (ninety-six states all together for $\alpha = 1$ in the absence of antiferromagnetic-superexchange interaction) as $\alpha < 1$. The separation between the states in this manifold increases with decreasing α. When α reaches zero, i.e. the system possesses the thin-film structure, the energy separation between the ground state ${}^6\gamma_4$ and the first excited state ${}^4\gamma_3$ is fairly large (of order $0.08t$). This clearly indicates that one of the consequences of the surface is to destroy the huge accumulation of many-body states in the ground-state manifold of the bulk heavy-fermion system.

The second interesting point is the crossover behavior, shown in Figure 3. The ground state of the system is ${}^2\gamma_4$ for $0.92 \leq \alpha < 1.0$. This state is split off the heavy-

fermion ground-state manifold of the original bulk structure (i.e. the $\alpha = 1$ limit). For $0.83 \leq \alpha \leq 0.92$, the state of symmetry ${}^4\gamma_3$ drops below ${}^2\gamma_4$ and becomes the ground state of the system. Finally, when $\alpha \leq 0.83$, the ${}^6\gamma_4$ ground state of the thin-film structure (i.e. $\alpha = 0$), has the lowest energy. This cross-over shows another surface-effect induced behavior, i.e. a transition from antiferromagnet (spin minimally aligned) to partially saturated ferromagnet.

In the case of the four-layer thin-film structure, the ground state is a spin minimally aligned one with symmetry ${}^2\gamma_4$ for the whole region $0 \leq \alpha \leq 1$. Nevertheless, a clear trend toward ferromagnetism can be seen. Two partially saturated ferromagnetic states, with symmetries ${}^4\gamma_3$ and ${}^4h_5$ which are third and eleventh excited state in the $\alpha = 1$ (bulk) limit respectively, drop in energy when α decreases from one. They become more stable than a spin minimally aligned state with symmetry ${}^2h_5$, (the second excited state in the bulk limit) at $\alpha = 0.21$ and $\alpha = 0.09$, and become the second and the third excited states of the system, respectively.

V. CONCLUSION

A model for a {001} thin film of an *fcc* structure heavy-fermion system, in the infinite-U limit and for an occupation of seven-eighth of an electron per site was examined in the periodic small-cluster approach. Two thin-film structures, i.e. a two-layer and a four-layer slabs, were investigated. The most important result is that one-electron effects tend to dominate the electronic behavior in the presence of surfaces. The many-body spectrum is essentially determined by the nearest-neighbor one-electron hopping interaction, which in this case overwhelms all other electronic and magnetic effects.

The nature of the ground state is drastically changed from that in the bulk. The ground state for the two-layer thin-film structure, which is directly related to the original bulk structure, is a non-degenerate partially saturated ferromagnetic state with

symmetry ${}^6\gamma_4$. Furthermore, it is well separated from all excited states. This means that the surface electronic structure is no longer heavy-fermionic. This is in contrast to the bulk system, where there is a huge accumulation of many-body states in the ground-state manifold, only partially split by the antiferromagnetic-superexchange interaction. The heavy-fermion state therefore is very sensitive to local atomic environment. For the four-layer thin-film structure, which arises from a different, asymmetric finite sampling in the Brillouin zone, the ground state is also non-degenerate, but with symmetry ${}^2\gamma_4$, i.e. a spin minimally aligned state. However, a clear trend towards ferromagnetism can be seen from the low-energy excitations in the many-body spectrum.

Although the ground state is drastically altered, the discontinuity of one-electron occupancy probabilities is still small, as in the case of the bulk heavy-fermion state. The details of the one-electron occupancy behavior seem to be weakly structure (bulk or thin-film) and symmetry (tetragonal or cubic) dependent. It is also found that, in the case of the four-layer thin-film structure, the hole has a larger probability of being in the interior layers, where the projected bandwidth is larger, rather than in the surface layers.

The bulk-to-surface transition was examined by introducing a variable coupling term between periodically repeated slabs. Results show that the ground-state manifold of the bulk heavy-fermion system splits as the system changes from bulk to thin-film structure, with a concomitant transition from antiferromagnetic (spin minimally aligned) state to partially saturated ferromagnet.

APPENDIX: The ferromagnetic state

The properties of the present system are very sensitive to the one-electron hopping parameter t. In the case of $t > 0$, the electronic structure of the bulk corresponds to a heavy-fermion system; for $t < 0$, it becomes a fully saturated ferromagnet (see RF). The nature of the change from bulk to surface structure of the heavy-fermion system has been discussed in the main text. In this appendix, the situation for the ferromagnetic case, $t < 0$, is presented.

The ground states of the two thin-film structures for $t < 0$ case are both non-degenerate with energies

$$E_{2\ layer} = -8|t| + 4T + 3J \quad , \tag{A.1}$$

$$E_{4\ layer} = -6|t| + (15/4)J - [[2t - (1/4)J]^2 + (4t + 5T)^2]^{1/2} \tag{A.2}$$

respectively, and both with spin 7/2, i.e. spin maximally aligned. They are thus fully saturated ferromagnets. One-electron band-structure effects overwhelm the antiferromagnetic-superexchange mechanism and always produce ferromagnetic ordering. This is similar to the result in the bulk case. A simple Hartree-Fock state, with all electrons with parallel spins, would yield the correct ground state for the thin-film structure under these conditions. Thus the ferromagnetic state is stable under the change from bulk to thin-film structure, independently of the symmetry reduction.

By setting J and/or T equal to zero, the degeneracy of the many-body spectra of both thin-film structures remains essentially unchanged, with some energy shifts and slight energy-level rearrangements. This fact indicates that one-electron effects are also dominant, similarly to the heavy-fermion case discussed in the main text.

The one-electron occupancy is calculated by use of equations (4.1), (3.5) and (3.16). Results for the two-layer and four-layer thin-film structures are presented in Table IX and Table X respectively. For the two-layer thin-film structure, it shows an occupation of one half for the lower-energy orbitals and zero for the higher ones. This is the well known Stoner state, with spin-up and spin-down electron distributions split by the interaction: an ordinary Fermi distribution and Fermi surface for the "majority" spins, and "minority" spin states completely empty. The situation for the four-layer thin-film structure is different. Note that the one-electron energy levels in the ferromagnet ($t<0$) case are arranged (in order of increasing energy) as: $h_{5\beta}$, $h_{5\alpha}$, γ_{4-} , γ_{1-} , γ_{4+} , and γ_{1+}. The "minority" spin levels are still empty. The ferromagnetic interactions preserves the symmetry of the many-body state, but hybridizes one-electron orbitals of the *same* symmetry. As a consequence, even though a full γ_1 orbital is unoccupied, this orbital is *not* the original non-interacting γ_{1+}. The hole is instead comprised of the bulk γ_{1+} (96%) and the γ_{1-} (4%) orbitals, as shown by occupancy. These results further confirm the conclusions obtained for the heavy-fermion system, i.e. the one-electron-occupancy behavior of this strongly interacting system is weakly structure (bulk or thin-film) and symmetry (cubic or tetragonal) dependent. Unlike the heavy-fermion system, the fully saturated ferromagnetic state is quite stable under the change from bulk to thin-film structure. The results of the many-body spectrum calculation show that the fully saturated ferromagnetic state with symmetry ${}^8\gamma_1$ is the ground state throughout the range $0 \leq \alpha \leq 1$.

One-hole occupancy probability on the localized orbitals of different sites (i.e. in surface or interior layers) is calculated for the four-layer thin-film structure. The result is shown in Table IX. It can be seen that, in contrast to the heavy-fermion case, the hole tends to stay in the outermost (surface) layers.

In summary, the results show that the properties of the ferromagnet are qualitatively the same under the change from bulk to thin-film structure. Some details, e.g.

the many-body eigenvalues and one-electron occupancy probabilities, are slightly modified by the presence of the surface.

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34 Notice that there are six Z points and six W points in the Brillouin zone of the *fcc* structure. The sampling described in (3.12)-(3.15) selects only one third of them, which results in a reduction from cubic to tetragonal symmetry.

TABLE I.

The character table of the eight-atom-cluster nonsymmorphic space group for the two-layer thin-film structure of Figure 1.

	1	1	2	2	2	4	4	4	4	4	4
	E	E	E	C_{4z}^2	C_{4z}^2	$C_{4z};C_{4z}^{-1}$	$C_{4z};C_{4z}^{-1}$	$C_{2x};C_{2y}$	$C_{2x};C_{2y}$	$C_{2d};C_{2d'}$	$C_{2d};C_{2d'}$
	0	4	3,7	0,4	3,7	0,4;3,7	3,7;0,4	1,5;2,6	2,6;1,5	1,5;2,6	2,6;1,5
γ_1	1	1	1	1	1	1	1	1	1	1	1
γ_2	1	1	1	1	1	1	1	-1	-1	-1	-1
γ_3	1	1	1	1	1	-1	-1	1	1	-1	-1
γ_4	1	1	1	1	1	-1	-1	-1	-1	1	1
γ_5	2	2	2	-2	-2	0	0	0	0-	0	0
m_1	1	1	-1	-1	1	i	-i	1	-1	i	-i
m_2	1	1	-1	-1	1	-i	i	1	-1	-i	i
m_3	1	1	-1	-1	1	-i	i	-1	1	i	-i
m_4	1	1	-1	-1	1	i	-i	-1	1	-i	i
m_5	2	2	-2	2	-2	0	0	0	0	0	0
y_1	4	-4	0	0	0	0	0	0	0	0	0

TABLE II.

Compatibility relations between the representations of the group for the bulk structure and those for the group of the two-layer thin-film structure. The original representations are given in Reference 23.

Original representations of the bulk structure	Reduce to the following representations of the two-layer structure
Γ_1	γ_1
Γ_2	γ_3
Γ_{12}	$\gamma_1 \oplus \gamma_3$
$\Gamma_{15'}$	$\gamma_2 \oplus \gamma_5$
$\Gamma_{25'}$	$\gamma_4 \oplus \gamma_5$
X_1	$\gamma_2 \oplus m_5$
X_2	$\gamma_4 \oplus m_5$
X_3	$\gamma_3 \oplus m_1 \oplus m_2$
X_4	$\gamma_1 \oplus m_1 \oplus m_2$
X_5	$\gamma_5 \oplus m_3 \oplus m_4 \oplus m_5$
L_1	y_1
L_2	y_1
L_3	$y_1 \oplus y_1$

TABLE III.

Sizes of blocks of the various representations for the two-layer thin-film-structure space group.

	γ_1	γ_2	γ_3	γ_4	γ_5	m_1	m_2	m_3	m_4	m_5	y_1
S = 7/2	1	1	0	0	0	0	0	0	0	1	1
S = 5/2	2	2	2	2	2	1	1	1	1	4	6
S = 3/2	4	4	4	4	6	3	3	3	3	8	14
S = 1/2	4	4	4	4	6	3	3	3	3	8	14

TABLE IV.
Many-body energies for 7 electrons in the non-interacting, $U = J = 0$, limit for the two-layer thin-film structure.

Occupation $\gamma\gamma' ym$	Energy		Degeneracy	Notes
2230	$-16t$	$-4T$	56	ground state, ($t > 0$)
2140	$-16t$	$+4T$	140	lowest one-electron excitations, ($t > 0$)
2050	$-16t$	$+12T$	56	
2221	$-12t$	$-12T$	48	
2131	$-12t$	$-4T$	448	
2041	$-12t$	$+4T$	280	
2212	$-8t$	$-20T$	48	
2122	$-8t$	$-12T$	336	
2032	$-8t$	$-4T$	336	
1240	$-8t$	$+4T$	140	
1150	$-8t$	$+12T$	224	
1060	$-8t$	$+20T$	56	
2203	$-4t$	$-28T$	4	
2113	$-4t$	$-20T$	64	
2023	$-4t$	$-12T$	112	
1231	$-4t$	$-4T$	448	highest one-electron excitations, ($t > 0$)
1141	$-4t$	$+4T$	1120	
1051	$-4t$	$+12T$	448	
2104		$-28T$	2	
2014		$-20T$	8	
1222		$-12T$	336	
1132		$-4T$	1344	
1042		$+4T$	840	
0250		$+12T$	56	
0160		$+20T$	56	
0070		$+28T$	8	
1213	$4t$	$-20T$	64	
1123	$4t$	$-12T$	448	
1033	$4t$	$-4T$	448	highest one-electron excitations, ($t < 0$)
0241	$4t$	$+4T$	280	
0151	$4t$	$+12T$	448	
0061	$4t$	$+20T$	112	
1204	$8t$	$-28T$	2	
1114	$8t$	$-20T$	32	
1024	$8t$	$-12T$	56	
0232	$8t$	$-4T$	336	
0142	$8t$	$+4T$	840	
0052	$8t$	$+12T$	336	
0223	$12t$	$-12T$	112	
0133	$12t$	$-4T$	448	
0043	$12t$	$+4T$	280	
0214	$16t$	$-20T$	8	
0124	$16t$	$-12T$	56	lowest one-electron excitations, ($t < 0$)
0034	$16t$	$-4T$	56	ground state, ($t < 0$)
	total		11440	

TABLE V.

The character table of the eight-atom-cluster nonsymmorphic space group for the four-layer thin-film structure of Figure 2.

There is only one translation τ in the cluster.

	1	1	2	1	1	2	2	2	2	2
	E	C_{4z}^2	$C_{2x}\ C_{2y}$	E	C_{4z}^2	$C_{2x}\ C_{2y}$	$C_{4z}\ C_{4z}^{-1}$	$C_{2d}\ C_{2d'}$	$C_{4z}\ C_{4z}^{-1}$	$C_{2d}\ C_{2d'}$
				τ	τ	τ			τ	τ
γ_1	1	1	1	1	1	1	1	1	1	1
γ_2	1	1	1	1	1	1	-1	-1	-1	-1
γ_3	1	1	-1	1	1	-1	-1	1	-1	1
γ_4	1	1	-1	1	1	-1	1	-1	1	-1
γ_5	2	-2	0	2	-2	0	0	0	0	0
h_1	1	1	1	-1	-1	-1	i	i	-i	-i
h_2	1	1	1	-1	-1	-1	-i	-i	i	i
h_3	1	1	-1	-1	-1	1	-i	i	i	-i
h_4	1	1	-1	-1	-1	1	i	-i	-i	i
h_5	2	-2	0	-2	2	0	0	0	0	0

TABLE VI.

Sizes of blocks of the various representations for the four-layer thin-film-structure space group.

	γ_1	γ_2	γ_3	γ_4	γ_5	h_1	h_2	h_3	h_4	h_5
$S = 7/2$	2	0	0	2	0	0	0	0	0	2
$S = 5/2$	8	4	4	8	0	0	0	0	0	12
$S = 3/2$	16	12	12	16	0	0	0	0	0	28
$S = 1/2$	16	12	12	16	0	0	0	0	0	28

TABLE VII.

Many-body energies of the bulk ($\alpha = 1$) heavy-fermion ground-state manifold and the lowest sixteen states of the two-layer thin-film structure ($\alpha = 0$).

Energies are in units of t. Other parameters are $T = 0.1t$ and $J = 0.01t$.

$\alpha = 1$		$\alpha = 0$	
Energy	Symmetry	Energy	Symmetry
-5.430	${}^2\gamma_2$	-5.000	${}^6\gamma_4$
-5.430	${}^2\gamma_3$	-4.899	${}^4\gamma_3$
-5.430	${}^2\gamma_4$	-4.772	${}^2\gamma_4$
-5.430	${}^2m_5$	-4.732	${}^4m_5$
-5.430	${}^2m_5$	-4.649	${}^2y_1$
-5.420	${}^2y_1$	-4.583	${}^2m_5$
-5.420	${}^2y_1$	-4.545	${}^4y_1$
-5.415	${}^4\gamma_1$	-4.507	${}^4m_5$
-5.415	${}^4\gamma_2$	-4.372	${}^2\gamma_3$
-5.415	${}^4\gamma_3$	-4.350	${}^6m_5$
-5.415	${}^4\gamma_4$	-4.317	${}^4m_5$
-5.415	${}^4m_5$	-4.236	${}^6y_1$
-5.415	${}^4m_5$	-4.000	${}^2\gamma_2$
-5.405	${}^4y_1$	-4.000	${}^4\gamma_4$
-5.390	${}^6\gamma_4$	-4.000	${}^8m_5$
-5.390	${}^6m_5$	-4.000	${}^2y_1$

TABLE VIII.

Many-body energies of the lowest twelve states of the four-layer thin-film structure ($\alpha = 0$) and the corresponding bulk structure ($\alpha = 1$).

Energies are in units of t. Other parameters are $T = 0.1t$ and $J = 0.01t$.

$\alpha = 1$		$\alpha = 0$	
Energy	Symmetry	Energy	Symmetry
-7.765	${}^2\gamma_4$	-7.065	${}^2\gamma_4$
-7.763	${}^2h_5$	-7.003	${}^2h_5$
-7.627	${}^2h_5$	-6.858	${}^4\gamma_3$
-7.217	${}^4\gamma_2$	-6.823	${}^4h_5$
-7.217	${}^4\gamma_3$	-6.800	${}^2\gamma_2$
-7.157	${}^4\gamma_4$	-6.768	${}^2h_5$
-7.157	${}^4\gamma_1$	-6.646	${}^2\gamma_3$
-7.143	${}^4\gamma_3$	-6.627	${}^4\gamma_2$
-7.127	${}^4\gamma_3$	-6.599	${}^2\gamma_2$
-7.040	${}^2\gamma_2$	-6.583	${}^4\gamma_3$
-7.040	${}^2\gamma_3$	-6.581	${}^2\gamma_3$
-7.039	${}^4h_5$	-6.498	${}^4\gamma_2$

TABLE IX.

Orbital occupation probabilities of the two-layer thin-film structure.

State	γ_1	γ_2	y_1	m_5
isolated-atom ($t = T = 0$)	7/16	7/16	7/16	7/16
heavy-fermion ($U = \infty$; $t > 0$; $T = 0.1t$, $J = 0.01t$)	9/16	1/2	27/64	3/8
ferromagnet ($U = \infty$; $t < 0$, $T = 0.1t$, $J = 0.01t$)	0	1/2	1/2	1/2
non-interacting ($U = 0$; $t > 0$)	1	1	3/8	0
non-interacting ($U = 0$; $t < 0$)	0	0	3/8	1

TABLE X.

Orbital occupation probabilities of the four-layer thin-film structure.

State	γ_{1-}	γ_{4-}	γ_{1+}	γ_{4+}	$h_{5\beta}$	$h_{5\alpha}$
isolated-atom ($t = T = 0$)	7/16	7/16	7/16	7/16	7/16	7/16
heavy-fermion ($U = \infty$; $t > 0, T = 0.1t, J = 0.01t$)	0.54	0.54	0.54	0.36	0.37	0.39
ferromagnet ($U = \infty$; $t < 0, T = 0.1t, J = 0.01t$)	0.48	1/2	0.02	1/2	1/2	1/2
non-interacting ($U = 0$; $t > 0$)	1	1	1	1/2	0	0
non-interacting ($U = 0$; $t < 0$)	0	0	0	0	1	3/4

TABLE XI.

One-particle occupation probabilities of atomic orbitals in the four-layer thin-film structure.

	Electron		Hole	
	Surface Site	Interior Site	Surface Site	Interior Site
heavy-fermion ($U = \infty$; $t > 0$, $T = 0.1t$, $J = 0.01t$)	0.903	0.847	0.097	0.153
ferromagnet ($U = \infty$; $t < 0$, $T = 0.1t$, $J = 0.01t$)	0.824	0.926	0.176	0.074

FIGURE CAPTIONS

[1] The eight-atom cluster in the two-layer slab structure. With periodic boundary conditions this cluster, which forms an infinite two-layer slab, is equivalent to sampling the Brillouin zone at the points γ, m, and y (see the text for details). For each site, there are eight nearest neighbors and four second neighbors.

[2] The eight-atom cluster in the four-layer slab structure. With periodic boundary conditions this cluster, which forms an infinite four-layer slab, is equivalent to sampling the Brillouin zone at the points γ and h (see the text for details). In this structure, there are two surface layers where each site has eight nearest neighbors and five second neighbors, and two interior layers where each site has the full twelve nearest neighbors and five second neighbors.

[3] The crossover behavior of the ground states as a function of bulk-to-surface coupling ratio α, for $T=0.1t$ and $J=0.01t$. Note that these three states are degenerate at $\alpha = 1$ (bulk) limit when J equals zero, but are split apart at the $\alpha = 0$ (thin-film) limit even when both J and T equal zero.

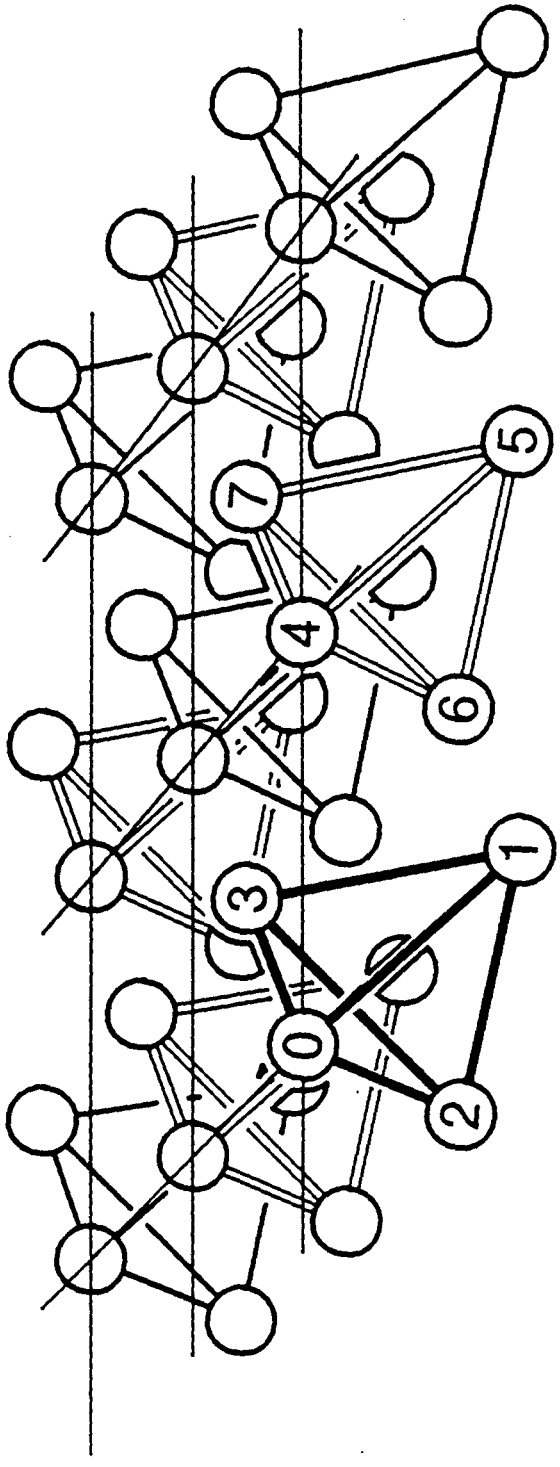

Figure 1

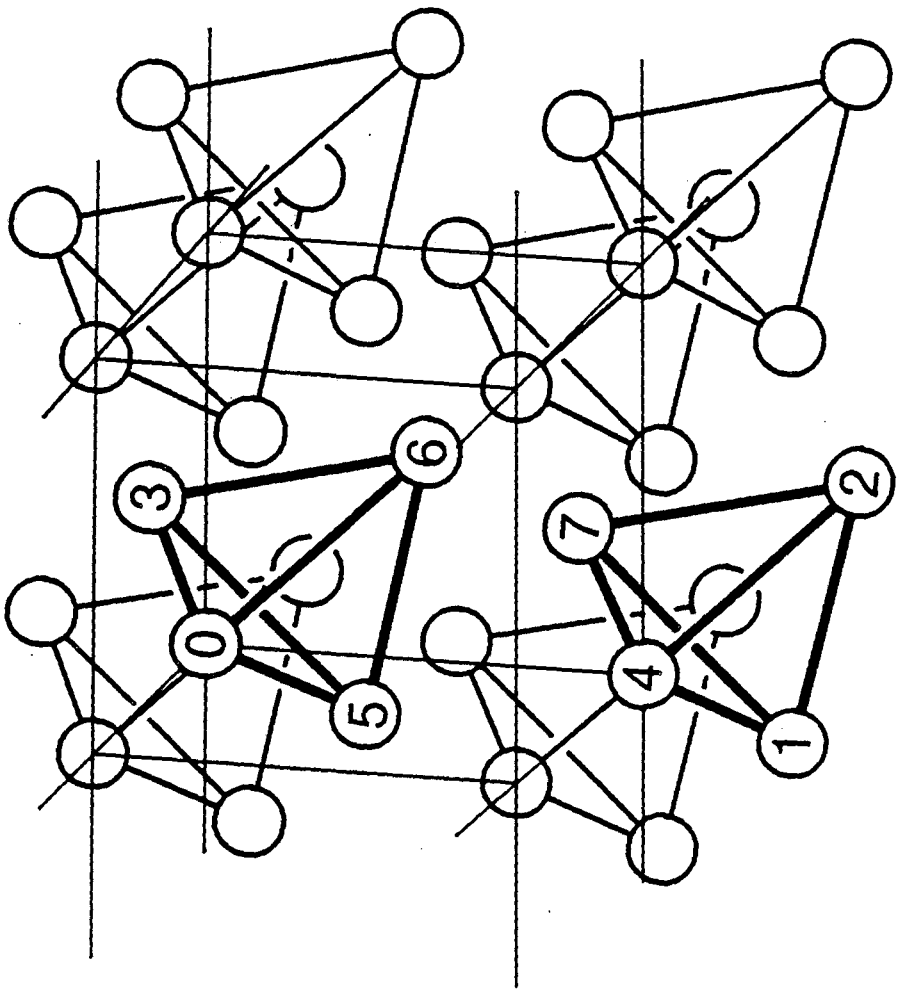

Figure 2

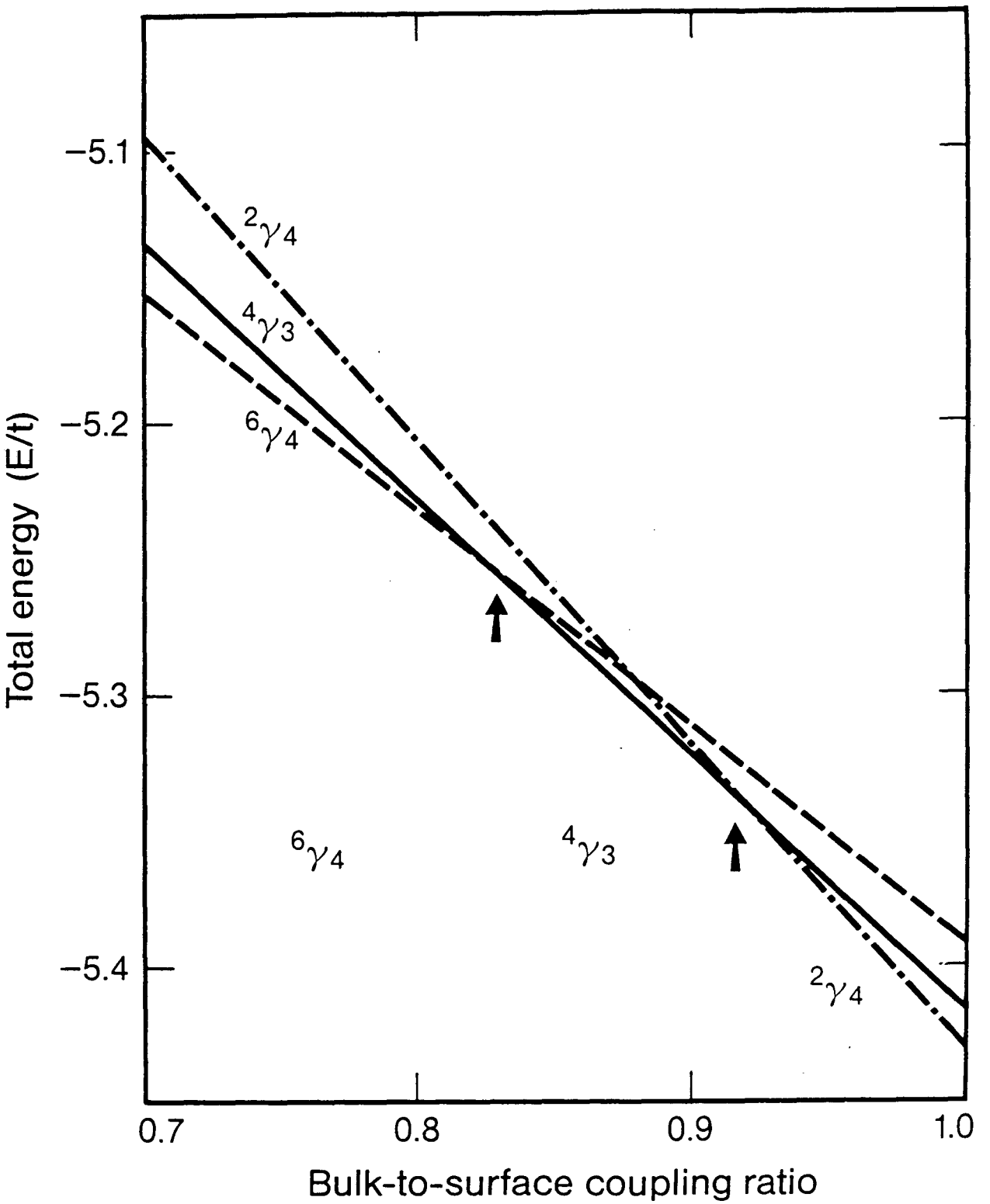
−5.1
−5.2
−5.3
−5.4
Total energy (E/t)
$^2\gamma_4$
$^4\gamma_3$
$^6\gamma_4$
$^6\gamma_4$
$^4\gamma_3$
$^2\gamma_4$
0.7
0.8
0.9
1.0
Bulk-to-surface coupling ratio

Figure 3

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