

# On the origin of surface states in a correlated local-moment film

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**Abstract.** The electronic quasiparticle structure of a ferromagnetic local moment film is investigated within the framework of the s-f model. For the special case of a single electron in an otherwise empty energy band being exchange coupled to a fully ordered localised spin system the problem can be solved exactly and, for the spin- $\downarrow$  electron, some marked correlation effects can be found. We extend our model to incorporate the influence of the surface on the electronic structure. Therefore we modify the hopping integrals in the vicinity of the surface. This leads to the existence of surface states, both for the spin- $\uparrow$  and the spin- $\downarrow$  spectral density of states. The interplay between the modification of the hopping integrals and the existence of surface states and correlation effects is discussed in detail.

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## 1 Introduction

In the recent past the s-f (or s-d) model has been the subject of intensive theoretical work [1–3]. The model describes the exchange coupling of itinerant band electrons to localised magnetic moments. The model is applicable to magnetic semiconductors like the europium chalcogenides [4] EuX (X = O, S, Se, Te) and the chromium chalcogenide spinels [5] MCr<sub>2</sub>Y<sub>4</sub> (M = Hg, Cd; Y = S, Se). It is also used to describe metallic local moment systems such as Gd, Tb, and Dy [6]. Many characteristics of these materials may be explained by a correlation between the localised “magnetic” states (4f, *e.g.*) and extended conduction band states (5d-6s, *e.g.*). In the s-f model this correlation is represented by an intraatomic exchange interaction.

At present magnetic phenomena at surfaces, interfaces, and in thin films attract broad attention both theoretically and experimentally due to the question of phase transitions in dimensionally reduced systems. In particular, the magnetism of thin Gd films has been the subject of intensive experimental effort. In contrast to 3d-metals, Gd surfaces seem to have a Curie temperature which is larger than the  $T_C$  value of the bulk material [7]. Similar surface enhanced magnetism has been observed in Tb [8]. Wu *et al.* [9] have modelled an antiferromagnetic coupling between the surface layer and the bulk. First experimental observations were made using spin-polarized low-energy electron diffraction (LEED) and photoemission spectroscopy (PES) [10]. Further spin-polarized photoemission studies [11–14] did not confirm the original observation and indicated a ferromagnetic coupling between surface and bulk. Farle *et al.* [15] measured the Curie-

temperature of layer-by-layer-grown Gd(0001) films as a function of film thickness. Donath *et al.* [16] using spin resolved inverse photoemission did not find any indication for exceptional surface magnetic properties such as an enhanced Curie-temperature or magnetic order at the surface which is different from bulk.

In particular, the behaviour of a Gd (0001) surface state has been discussed controversy. Federov *et al.* [17] and Weschke *et al.* [18] find a Stoner-like temperature dependence of the exchange splitting for the Gd (0001) surface. For the strained Gd(0001) Waldfried *et al.* [19] observe a wave vector dependent exchange splitting. They found the electronic structure at the surface to be different from that of bulk and a substantially increased Curie temperature at the surface. The FLAPW-calculations performed by Wu *et al.* [20] show a surface state near the  $\bar{\Gamma}$  point and an enhanced magnetic moment of the Gd (0001) surface.

It is not only the dimensionally reduced Gd which is of interest here, even bulk Gd is far from being completely understood. In an earlier study Nolting *et al.* [21] have observed that the a priori non-magnetic (5d, 6s)-conduction and valence bands exhibit a marked non uniform magnetic response which depends on the positions within the Brillouin zone and on the subband. This may be the reason for the fact that the experimental situation is controversial. Kim *et al.* [22] found a  $T$ -dependent spin splitting of occupied conduction electron states, which collapse in a Stoner-like fashion for  $T \rightarrow T_C$ . From photoemission experiments Li *et al.* [23,24] conclude that the exchange splitting must be wave-vector dependent, collapsing for some  $\mathbf{k}$  values, while for others no collapse occurs

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as a function of increasing temperature. This fairly complicated behaviour of the exchange splitting in the bulk material must be expected for Gd-films, too.

It is a challenge to perform an electronic structure calculation for a local-moment ferromagnet of reduced dimension in such a manner as to realistically incorporate correlation effects. In our previous paper [25] we proposed a simplified model which should be applicable to a local moment film of finite thickness. The special situation is considered of a single electron in an otherwise empty conduction band and coupled to the ferromagnetically saturated local spins of a simple cubic (s.c.) film. This model is applicable to a film of a ferromagnetic semiconductor such as EuO, EuS at  $T = 0$  K. This limiting case can be solved exactly for the bulk [26–28]. Its significance arises from the fact that all relevant correlation effects which are either found or expected to occur for finite band occupations and arbitrary temperatures [21, 29], do already appear in this simplified but tractable special model. In our previous paper [25] an exact solution of the model has been given for a film of finite thickness showing the interplay between structure and many-body effects. The film was formed by cutting a slab from the bulk material and leaving all bulk properties (such as intraatomic hopping) unmodified within the whole film. However, this assumption is somewhat unrealistic. Due to a wide range of physical effects near surfaces surface properties may be significantly different from bulk properties [7, 8, 10, 12, 30, 31].

In this work the variation of the hopping integrals is considered within the surface layer and between the surface layer and the layer nearest to the surface layer. We will demonstrate the modifying influence of the surface manifesting itself in the appearance of Tamm surface states [32]. We perform the model calculations to understand qualitatively the surface influence on a local moment film.

In the next section we briefly recall the model and its exact solution [25] and then show how the description can be extended to incorporate the variation of near surface hopping integrals. For a film of finite thickness the results of numerical calculations are presented in Section 3, followed by a summary and an outlook.

In this paper no concrete substance is focused on to as we perform the model calculations to qualitatively understand the surface influence of the surface on the electronic properties of the local moment film.

## 2 Theoretical model

We investigate a film with a simple cubic structure. The film is obtained by stacking  $n$  layers parallel to the (100)-plane of the s.c. crystal. Each lattice point of the film is indicated by a Greek letter  $\alpha, \beta, \gamma, \dots$  denoting the layer index and an index  $i, j, k, \dots$  numbering the sites within a given layer. Each layer possesses two-dimensional symmetry, *i.e.* the thermodynamic average of any site-dependent operator  $O_{i\alpha}$  depends only on the layer index  $\alpha$ .

We use the s-f (s-d) model as it is believed to yield a good description for local-moment semiconductors and metals [1–3]. The complete model-Hamiltonian

$$H = H_s + H_f + H_{sf} \quad (1)$$

consists of three parts. The first

$$H_s = \sum_{ij\alpha\beta} \left( T_{ij}^{\alpha\beta} - \mu \delta_{ij}^{\alpha\beta} \right) c_{i\alpha\sigma}^+ c_{j\beta\sigma} \quad (2)$$

describes the itinerant conduction electrons as s-electrons.  $c_{i\alpha\sigma}^+$  and  $c_{i\alpha\sigma}$  are, respectively, the creation and annihilation operators of an electron with the spin  $\sigma$  ( $\sigma = \uparrow, \downarrow$ ) at site  $\mathbf{R}_{i\alpha}$ .  $T_{ij}$  is the hopping integral.

Each lattice site  $\mathbf{R}_{i\alpha}$  is occupied by a localised magnetic moment, represented by a spin operator  $\mathbf{S}_{i\alpha}$ . The exchange coupling between these localised moments is expressed by the Heisenberg Hamiltonian:

$$H_f = \sum_{ij\alpha\beta} J_{ij}^{\alpha\beta} \mathbf{S}_{i\alpha} \mathbf{S}_{j\beta} \quad (3)$$

$J_{ij}^{\alpha\beta}$  are exchange integrals.

The interaction of electrons and localised spins occurs *via* an intraatomic exchange. It gives rise to the third term in equation (1):

$$H_{sf} = -J \sum_{i\alpha} \mathbf{S}_{i\alpha} \sigma_{i\alpha}. \quad (4)$$

$J$  is the s-f exchange coupling constant and  $\sigma_{i\alpha}$  is the Pauli spin operator of the conduction band electrons. Using the second-quantised form of  $\sigma_{i\alpha}$  and the abbreviations

$$\mathbf{S}_{j\alpha}^\sigma = \mathbf{S}_{j\alpha}^x + i z_\sigma \mathbf{S}_{j\alpha}^y; \quad z_\uparrow = +1, \quad z_\downarrow = -1, \quad (5)$$

$H_{sf}$  can be written as

$$H_{sf} = -\frac{1}{2} J \sum_{i\alpha\sigma} \left( z_\sigma \mathbf{S}_{i\alpha}^z n_{i\alpha\sigma} + \mathbf{S}_{i\alpha}^\sigma c_{i\alpha-\sigma}^+ c_{i\alpha\sigma} \right). \quad (6)$$

All physically relevant information of the system can be derived from the retarded single electron Green function:

$$\begin{aligned} G_{ij\sigma}^{\alpha\beta}(E) &= \left\langle \left\langle c_{i\alpha\sigma}; c_{j\beta\sigma}^+ \right\rangle \right\rangle_E \\ &= -i \int_0^\infty dt e^{-\frac{i}{\hbar} Et} \left\langle \left[ c_{i\alpha\sigma}(t), c_{j\beta\sigma}^+(0) \right]_+ \right\rangle. \quad (7) \end{aligned}$$

Here  $[\dots]_+$  is the anticommutator. The creation and annihilation operators are used in their (time dependent) Heisenberg representation. We perform a Fourier transformation within the layer

$$G_{\mathbf{k}\sigma}^{\alpha\beta}(E) = \frac{1}{N} \sum_{ij} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} G_{ij\sigma}^{\alpha\beta}. \quad (8)$$

Equation (8) conforms to the two-dimensional translation symmetry.  $N$  is the number of sites per layer,  $\mathbf{k}$  a wave-vector from the first two-dimensional Brillouin zone. Another relevant quantity is the spectral density, defined as the imaginary part of the Green function

$$S_{\mathbf{k}\sigma}^{\alpha\beta}(E) = -\frac{1}{\pi} \Im G_{\mathbf{k}\sigma}^{\alpha\beta}(E + i0^+). \quad (9)$$

$S_{\mathbf{k}\sigma}^{\alpha\beta}$  is directly connected to observable quantities within angle and spin resolved (inverse) photoemission experiments. The wave-vector summation of the spectral density equation (9) yields a layer-dependent (local) quasiparticle density of states,

$$\rho_{\alpha\sigma}(E) = \frac{1}{\hbar N} \sum_{\mathbf{k}} S_{\mathbf{k}\sigma}^{\alpha\alpha}(E) = \frac{1}{\hbar} S_{ii\sigma}^{\alpha\alpha}(E) \quad (10)$$

which will play an important role in following discussion.

The many-body problem posed by the Hamiltonian equation (1) is non trivial. Up to now no analytic solution is found even for the bulk. The model is widely used and has proved to be realistic for applications to semiconducting or metallic local moment ferro- and antiferromagnets [2–4, 21]. We investigate the special situation of a thin saturated ferromagnetically ordered film, *i.e.*  $\langle S_{i\alpha}^z \rangle = S$ , with a single electron in an otherwise empty conduction band at zero-temperature ( $n = 0, T = 0$ ) and interacting *via* the s-f exchange (6) with the localised spin system of the film.

The solution of the many-body problem is described very briefly. Details can be found in our previous paper [25]. The equation of motion of the single electron Green function (7) can be written

$$E G_{ij\sigma}^{\alpha\beta} = \hbar \delta_{ij}^{\alpha\beta} + \sum_{l\gamma} T_{il}^{\alpha\gamma} G_{lj\sigma}^{\gamma\beta} - \frac{J}{2} \left( z_{\sigma} \Gamma_{ij\sigma}^{\alpha\alpha\beta} + F_{ij\sigma}^{\alpha\alpha\beta} \right) \quad (11)$$

where we have introduced two “higher” Green functions

$$F_{ijk}^{\alpha\beta\gamma} = \left\langle \left\langle S_{i\alpha}^z c_{j\beta\sigma} ; c_{k\gamma\sigma}^+ \right\rangle \right\rangle_E \xrightarrow{n \rightarrow 0, T \rightarrow 0} \hbar S G_{jk\sigma}^{\beta\gamma}, \quad (12)$$

$$F_{ijk}^{\alpha\beta\gamma} = \left\langle \left\langle S_{i\alpha}^{-\sigma} c_{j\beta-\sigma} ; c_{k\gamma\sigma}^+ \right\rangle \right\rangle_E. \quad (13)$$

For the case of a completely saturated local moment system the function (12) can be expressed as a product of  $\hbar S$  and the single-electron Green function (7). This arises because in the Green functions (12, 13) the averaging has to be done using the magnon and electron vacuum ( $\sum_{\sigma} \langle n_{\alpha\sigma} \rangle \equiv 0$ ). Equation (13) can be interpreted as a function expressing “spin flips” at certain lattice sites. Applying a two-dimensional Fourier transformation to the equation of motion (11) yields

$$\begin{aligned} & (E + \frac{1}{2} J \hbar S) G_{\mathbf{k}\sigma}^{\alpha\beta} \\ &= \hbar \delta_{\alpha\beta} + \sum_{\gamma} T_{\mathbf{k}}^{\alpha\gamma} G_{\mathbf{k}\sigma}^{\gamma\beta} - \frac{J}{2\sqrt{N}} \sum_{\mathbf{q}} F_{\mathbf{k}\mathbf{q}\sigma}^{\alpha\alpha\beta} \end{aligned} \quad (14)$$

where  $\mathbf{k}$  and  $\mathbf{q}$  are wave vectors of the two dimensional Brillouin zone and

$$T_{\mathbf{k}}^{\alpha\beta} = \frac{1}{N} \sum_{ij} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} T_{ij}^{\alpha\beta} \quad (15)$$

is the energy in Bloch presentation.

In order to solve equation (14) we have to evaluate the “spin flip” function  $F_{\mathbf{k}\mathbf{q}\sigma}^{\alpha\gamma\beta}$ . If the spin  $\sigma$  of the single electron points into the same direction as the ferromagnetically saturated lattice ( $\sigma = \uparrow$ ) the electron cannot exchange its spin with the local moment system. This corresponds to the disappearance of the “spinflip” function (13),

$$F_{ii\uparrow}^{\alpha\alpha\beta} \xrightarrow{n \rightarrow 0, T \rightarrow 0} 0. \quad (16)$$

The case of a  $\sigma = \downarrow$  electron is more complex. There are many possibilities to exchange its spin with the local moment system. As a consequence the “spin flip” function (13) does not vanish as in the  $\uparrow$ -case. Nevertheless it turns out that the equation of motion for  $F_{ii\downarrow}^{\alpha\alpha\beta}$  decouples exactly. As a result the “spin-flip” function can be expressed in terms of the single electron Green function (for details see [25])

$$-\frac{J}{2\sqrt{N}} \sum_{\mathbf{q}} F_{\mathbf{k}\mathbf{q}\sigma}^{\alpha\alpha\beta} = C_{\alpha} G_{\mathbf{k}\downarrow}^{\alpha\beta} \quad (17)$$

where

$$C_{\alpha} = \frac{\frac{1}{2} J^2 \hbar^2 S B_{\alpha}}{1 - \frac{1}{2} J \hbar B_{\alpha}}, \quad (18)$$

$$B_{\alpha} = \frac{1}{N} \sum_{\mathbf{q}} \left( A_{\mathbf{q}\downarrow}^{-1} \right)^{\alpha\alpha}, \quad (19)$$

and

$$(A_{\mathbf{k}\sigma}(E))^{\alpha\beta} = -T_{\mathbf{k}}^{\alpha\beta} + \delta^{\alpha\beta} \left( E + \frac{1}{2} z_{\sigma} J \hbar S \right). \quad (20)$$

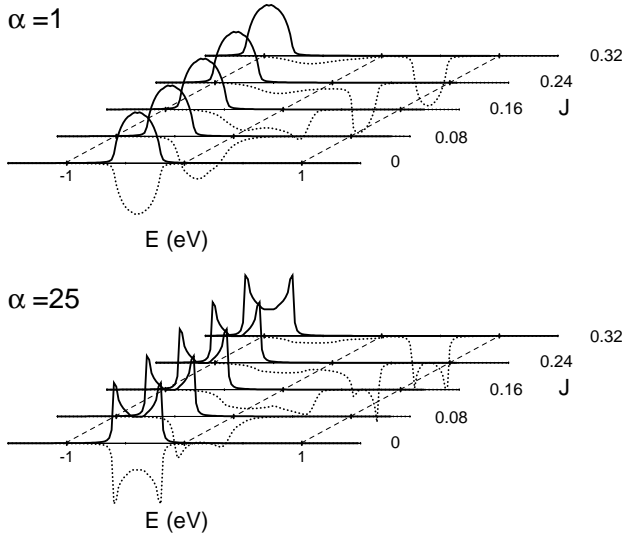
Combining equations (14, 16, 17) one obtains

$$\mathbf{G}_{\mathbf{k}\sigma} = \hbar \mathbf{D}_{\mathbf{k}\sigma}^{-1} \quad (21)$$

where

$$(\mathbf{D}_{\mathbf{k}\sigma})^{\alpha\beta} = (\mathbf{A}_{\mathbf{k}\sigma})^{\alpha\beta} - \delta_{\downarrow\sigma}^{\alpha\beta} C_{\alpha}. \quad (22)$$

To start our discussion we recall the basic features of the spectra of a single spin- $\sigma$  electron as presented in our previous paper [25]. Figure 1 shows the spectral densities of both spin- $\uparrow$  and spin- $\downarrow$  electron at  $\mathbf{k} = \bar{\Gamma}$  for the first and the centre layer of a 50-layer film with uniform hopping. For vanishing s-f interaction  $J$  there is no way to distinguish between a spin- $\uparrow$  and a spin- $\downarrow$  electron. The spectra therefore coincide. If the s-f interaction  $J$  is switched on the spectrum of the spin- $\uparrow$  electron is rigidly shifted by a constant energy of  $-\frac{1}{2} J S$ , since the electron has no chance to exchange its spin with the perfectly aligned



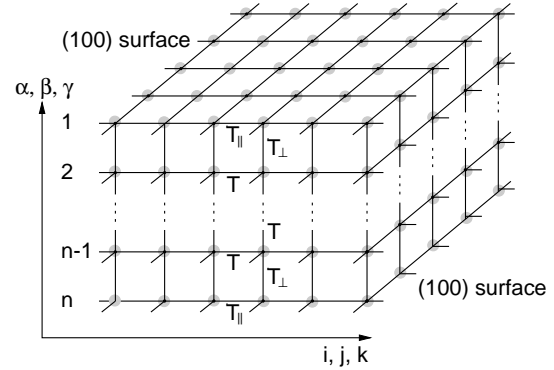
**Fig. 1.** Local spin- $\sigma$  spectral densities of the first and the 25th layer of a 50-layer s.c.-(100)-film with uniform hopping ( $\epsilon_{\parallel} = \epsilon_{\perp} = 1$ ) for different s-f exchange constants  $J = 0, 0.08, 0.16, 0.24, 0.32$ . The spectra for the spin- $\uparrow$  and the spin- $\downarrow$  electron are drawn as a solid line in positive direction and as a dotted line in negative direction, respectively.

local-moment system. However, this is possible for the spin- $\downarrow$  electron. For small exchange coupling  $J$  a slight deformation of the free spin- $\downarrow$  spectral density sets in. For intermediate and strong s-f-interaction the spectrum splits into two parts. The higher energetic part represents a polarisation of the immediate spin neighbourhood of the electron due to a repeated emission and reabsorption of magnons. The result is a polaron-like quasiparticle called the “magnetic polaron”. The low-energetic part of the spectrum is a scattering band which corresponds to the emission of a magnon by the spin- $\downarrow$  electron without reabsorption, but with a spin-flip of the electron. For details of the discussion see also [25].

In contrast to [25] we are here interested in surface states. We apply the above theory to a s. c. film consisting of  $n$  layers oriented parallel to the (100)-surface as drawn schematically in Figure 2. We restrict the electron hopping to nearest neighbours only *i.e.*

$$T_{ij}^{\alpha\beta} = \delta_{i,j\pm\Delta}^{\alpha\beta} T^{\alpha\alpha} + \delta_{ij}^{\alpha,\beta\pm 1} T^{\alpha\beta} \quad (23)$$

where  $\Delta = (0, 1), (0, \bar{1}), (1, 0), (\bar{1}, 0)$ .  $T^{\alpha\beta}$  is the hopping between the layers  $\alpha$  and  $\beta = \alpha \pm 1$  and  $T^{\alpha\alpha}$  within the layer  $\alpha$ . In order to study surface states we vary the hopping within the surface  $T_{\parallel} = \epsilon_{\parallel} T$  and between the surface and the layer nearest to the surface layer  $T_{\perp} = \epsilon_{\perp} T$  by



**Fig. 2.** Model structure of an 100-layer film with s. c. structure. Nearest neighbour hopping  $T_{\parallel}$ : within the surface layer;  $T_{\perp}$ : between the surface and the layer nearest to the surface layer;  $T$ : within and between inner layers.

introducing the parameters  $\epsilon_{\parallel}$  and  $\epsilon_{\perp}$

$$T^{\alpha\beta} = \begin{pmatrix} \epsilon_{\parallel} T & \epsilon_{\perp} T & 0 & \cdots & 0 \\ \epsilon_{\perp} T & T & T & & \vdots \\ 0 & T & \ddots & & \\ & & \ddots & T & 0 \\ \vdots & & & T & T & \epsilon_{\perp} T \\ 0 & \cdots & 0 & \epsilon_{\perp} T & \epsilon_{\parallel} T \end{pmatrix} \quad (24)$$

in contrast to a uniform hopping  $T$  in our previous paper [25]. Here  $\epsilon_{\parallel}$  and  $\epsilon_{\perp}$  are considered as model parameters. In the numerical calculations the bulk hopping is set to  $T = -0.1$  eV. The investigation of the influence of modified surface hopping is performed for the example of an infinite (100)-layer s.c. film. The elements of the Bloch matrix are defined in equation (15) where the summation includes nearest neighbours only. Thus the diagonal elements of the Bloch matrix are given by

$$T_{\mathbf{k}}^{11} = 2\epsilon_{\parallel} T(\cos(k_x a) + \cos(k_y a)), \quad (25)$$

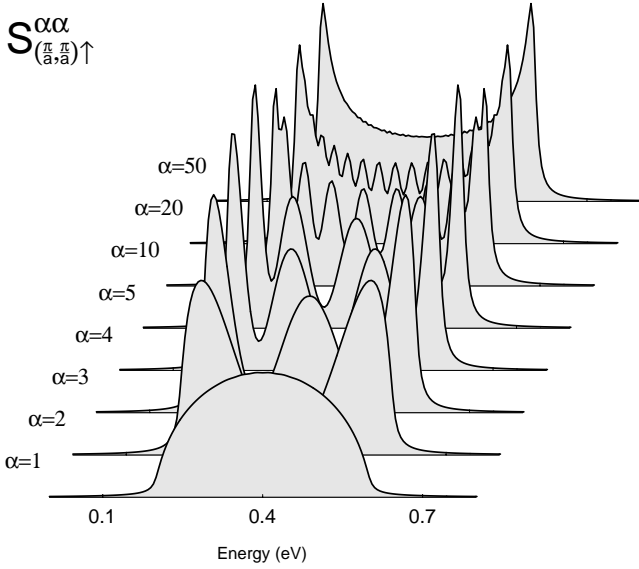
$$T_{\mathbf{k}}^{\alpha\alpha} = 2 T(\cos(k_x a) + \cos(k_y a)),$$

and the first upper and lower diagonal elements by

$$\begin{aligned} T_{\mathbf{k}}^{12} &= T_{\mathbf{k}}^{21} = \epsilon_{\perp} T, \\ T_{\mathbf{k}}^{\alpha,\alpha+1} &= T_{\mathbf{k}}^{\alpha+1,\alpha} = T. \end{aligned} \quad (26)$$

For either a semi-infinite system or a sufficiently thick film some essential analytical predictions can be made which are subject of a forthcoming paper [33]. For the  $\uparrow$ -electron the layer dependent retarded single electron Green function  $G_{\mathbf{k}\uparrow}^{\alpha\beta}(E)$  can be calculated analytically and both the existence and the behaviour of surface states can be studied.

Modifying the hopping within the first layer by more than 25% *i.e.* by a factor  $\epsilon_{\parallel} \leq \frac{3}{4}$  or  $\epsilon_{\parallel} \geq \frac{5}{4}$  and keeping all



**Fig. 3.** Local spin- $\sigma$  spectral densities ( $J = 0, \sigma = \uparrow, \downarrow$ ) of the layer ( $\alpha = 1, 2, 3, 4, 5, 10, 20, 50$ ) of a 100-layer film at  $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$  as a function of energy (eV). The hopping is uniform within the film:  $\epsilon_{\parallel} = \epsilon_{\perp} = 1$ .

the other hopping integrals unchanged results in a single surface state which splits off, at the lower or upper edge of the bulk band. This surface state first emerges for  $\mathbf{k} = \bar{\Gamma}$ ,  $\bar{M}$  from the bulk band and from there it spreads for larger modification to the rest of Brillouin zone.

If the hopping within the whole film remains constant but the hopping between the first and the second layer is changed by a factor  $\epsilon_{\perp} \geq \sqrt{2}$  then two surface states split off one on each side of the bulk band. The splitting is  $\mathbf{k}$  independent.

It proves that the maximum of the spectral weight of surface states is located either at the first or at the second layer. From there it drops exponentially as a function of the distance from the surface. The closer the surface state is located to bulk states the slower the descent.

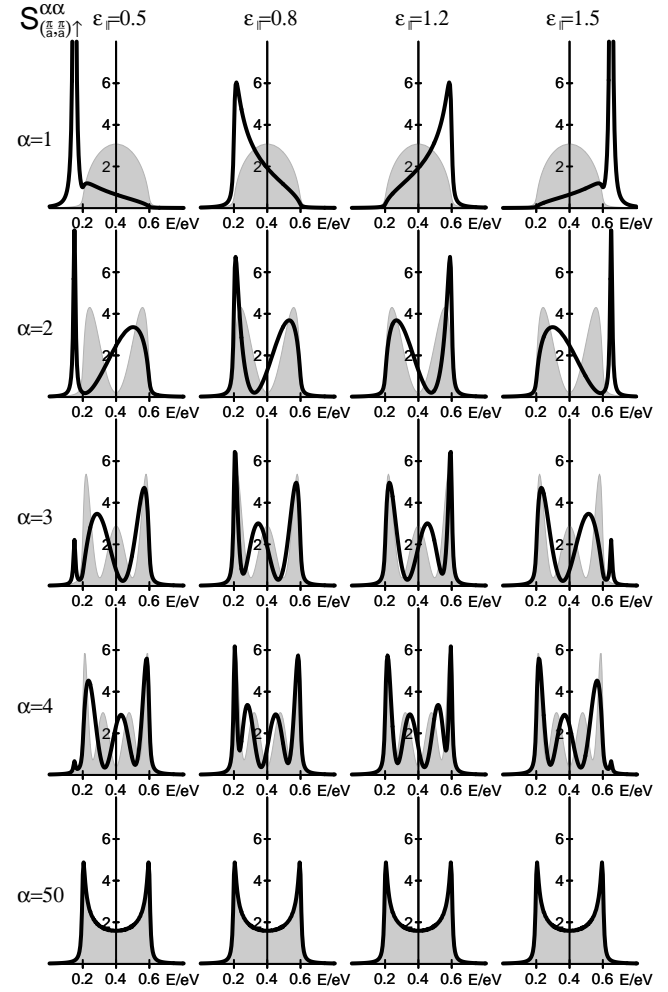
Generally the correlation is observed such that the more strongly modified the hopping ( $|\epsilon_{\parallel} - 1|, |\epsilon_{\perp} - 1|$ ) becomes the larger gets the spectral weight of surface states of the layers close to the surface.

### 3 Results

We discuss our results in terms of the spectral density  $S_{\mathbf{k}\sigma}^{\alpha\alpha}(E)$  as defined in equation (9), and the quasiparticle density of states  $\rho_{\alpha\sigma}(E)$ , equation (10).

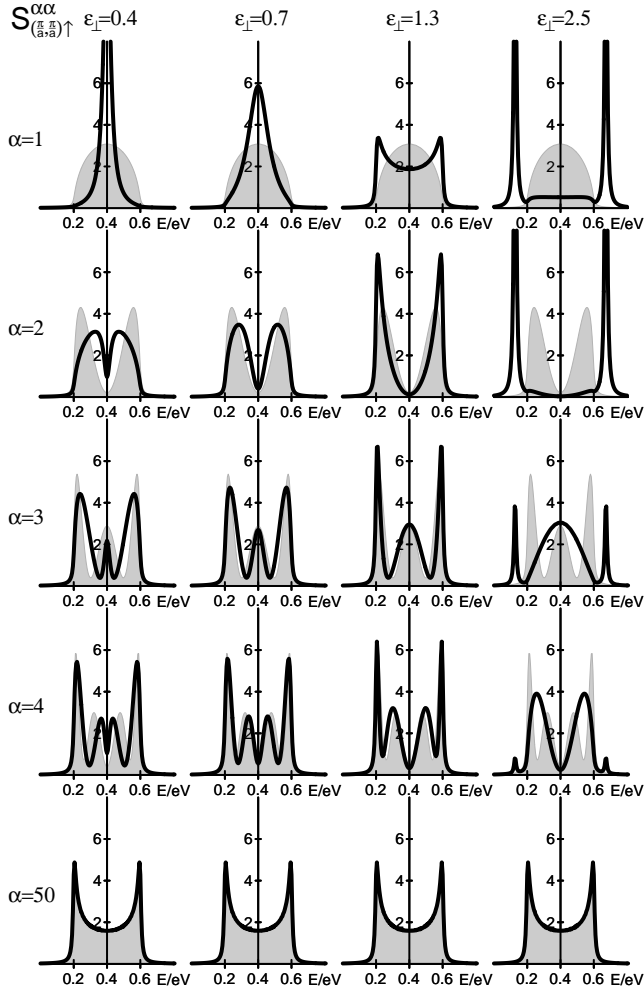
#### 3.1 Spin- $\uparrow$ -electron

For the  $\sigma = \uparrow$ -electron the s-f-exchange  $J$  results only in a rigid shift of the spectrum (20-22). Therefore we can choose  $J = 0$  to study the influence of modified hopping. Figure 3 shows the  $\sigma$ -spectral density  $S_{\mathbf{k}\sigma}^{\alpha\alpha}$  for the  $\alpha$ -th



**Fig. 4.** Local spin- $\uparrow$  spectral densities ( $J = 0, \sigma = \uparrow, \downarrow$ ) of the layer ( $\alpha = 1, 2, 3, 4, 50$ ) of a 100-layer film at  $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$  as a function of energy (eV) for modified hopping within the first layer by the factor  $\epsilon_{\parallel} = 0.5, 0.8, 1.2, 1.5$  and constant hopping between the first and the second layer ( $\epsilon_{\perp} = 1$ ) (black line). The grey background shows the spectral density for the case of uniform hopping.

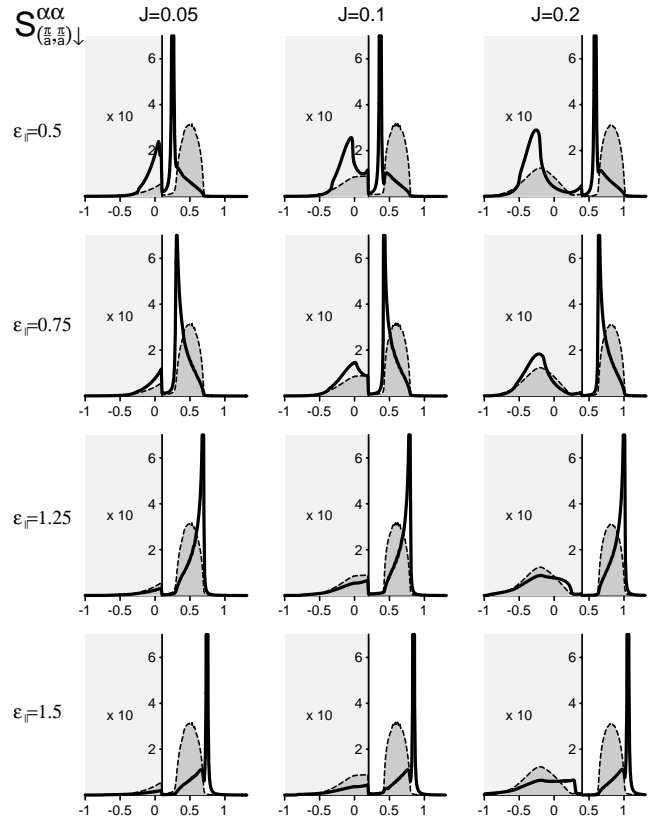
layer of a 100-layer film at  $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$  for uniform hopping ( $\epsilon_{\parallel} = \epsilon_{\perp} = 1$ ) and the s-f interaction  $J = 0$  switched-off. The spectral densities vary from layer to layer as a consequence of the broken symmetry at the surface. For each  $\mathbf{k}$  point the local spectral density of a given layer equals the density of states of an atom in a one-dimensional finite tight-binding linear chain. For the given situation at the  $\bar{M}$  point of the two dimensional Brillouin zone the centre of gravity for each layer is given by  $T^{\alpha\alpha}(\frac{\pi}{a}, \frac{\pi}{a}) = 0.4$  eV and the total bandwidth is  $-4T^{\alpha, \alpha+1} = 0.4$  eV. The lower and upper band edges are 0.2 eV and 0.6 eV respectively. For the innermost layers ( $\alpha = 50, 51$ ) the spectral density approaches the one dimensional tight-binding density of states whereas for the surface layers ( $\alpha = 1, 100$ ) it approaches the semi-elliptic one.



**Fig. 5.** Local spin- $\uparrow$  spectral densities ( $J = 0, \sigma = \uparrow, \downarrow$ ) of the layer ( $\alpha = 1, 2, 3, 4, 50$ ) of a 100-layer film at  $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$  as a function of energy (eV) for modified hopping between the first and second layer by the factors  $\epsilon_{\perp} = 0.4, 0.7, 1.3, 2.5$  and constant hopping within the first layer ( $\epsilon_{\parallel} = 1$ ) (black line). The grey background is the spectral density for the case of uniform hopping.

The variation of hopping is done by either varying  $\epsilon_{\parallel}$  or  $\epsilon_{\perp}$  while keeping the other fixed to determine the influence of both parameters.

Figure 4 exhibits the layer dependent local spin- $\uparrow$  spectral density for the same wave vector  $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$  as in Figure 3. The hopping is modified within the surface layer ( $\epsilon_{\parallel} \neq 1$ ) while  $\epsilon_{\perp} = 1$ . Deviations of intra layer hopping in the surface layer result in a transfer of spectral weight for  $\epsilon_{\parallel} < 1$  towards lower and for  $\epsilon_{\parallel} > 1$  towards higher energies, respectively. The transfer is most significant for the surface layers and decreases towards the bulk. For the inner (bulk like) layers the modification of hopping at the surface layers has no effect. If the difference between bulk and surface hopping is strong enough the transfer of spectral weight causes the splitting off of a surface  $\delta$ -like peak. This happens for  $\epsilon_{\parallel} < 0.75$  at the lower and for  $\epsilon_{\parallel} > 1.25$  at the upper band edge, respectively. The features ob-

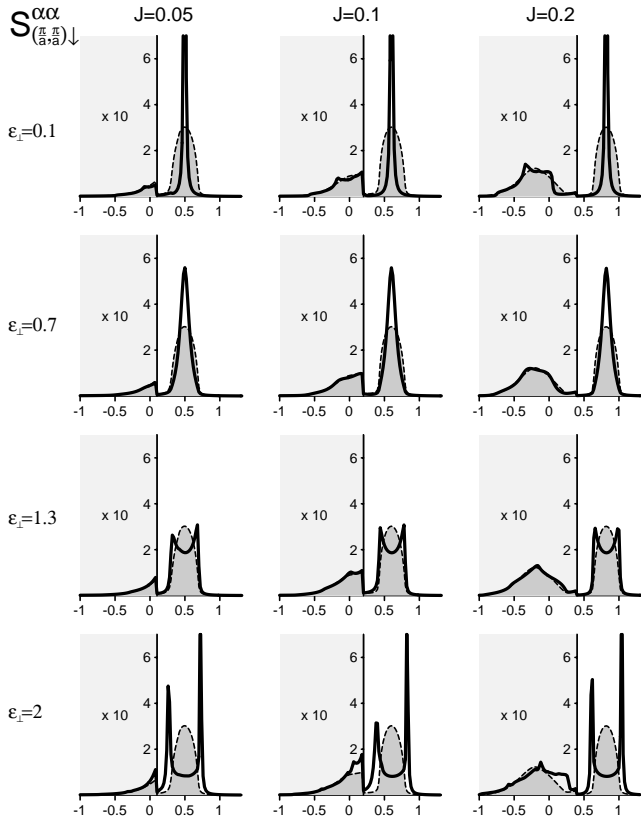


**Fig. 6.** Local spin- $\downarrow$  spectral density of the surface layer ( $\alpha = 1$ ) of a 100 layer film at  $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$  with modified hopping within the first layer ( $\epsilon_{\parallel} = 0.5, 0.75, 1.25$ ) while  $\epsilon_{\perp} = 1$  for different s-f exchange coupling constants  $J = 0.05, 0.1, 0.2$ . The dashed lines show the spectral density for the case of uniform hopping. The values on the low energy side of the spectra (light grey background) are multiplied by the factor 10.

served for reduction of hopping are symmetric to those observed for an increase of the hopping matrix element.

We obtain the curves shown in Figure 5 by varying the hopping between the surface layer and the layer nearest to the surface layer and leaving all other hopping integrals within a 100-layer film unchanged. If the hopping between the first and the second layer decreases ( $0 \leq \epsilon_{\perp} < 1$ ) spectral weight is symmetrically transferred from band edges towards the centre of the band for the spectral density. In the limiting case  $\epsilon_{\perp} \rightarrow 0$  the spectral density of the first layer is converted to a  $\delta$ -peak whereas the spectral density of the second layer  $\alpha = 2$  approaches the shape of the surface spectral density of a film with uniform hopping. The reason is that  $\epsilon_{\perp} = 0$  means a complete decoupling of the first layer from the rest of the film inasmuch the second layer plays the role of a surface.

If the hopping is augmented, as expressed by  $\epsilon_{\perp} > 1$ , the spectral weight is symmetrically distributed towards the edges of the bulk band. For a sufficiently large modification of the hopping we observe the simultaneous splitting off of two surface states, one at the lower and the other at the upper edge of the bulk band. These surface

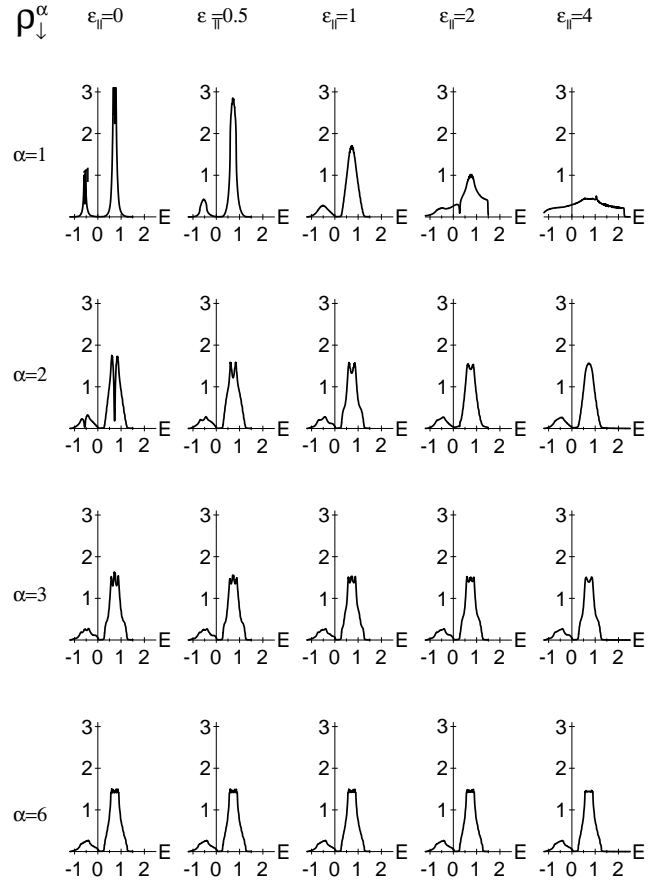


**Fig. 7.** Local spin- $\downarrow$  spectral density of the surface layer ( $\alpha = 1$ ) of a 100-layer film at  $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$  with modified hopping between the surface layer and the surface nearest layer ( $\epsilon_{\perp} = 0.25, 0.5, 2, 4$ ) and  $\epsilon_{\parallel} = 1$  for different s-f exchange coupling constants  $J = 0.05, 0.1, 0.2$ . The dashed lines show the spectral density for uniform hopping. The values on the low energy side of the spectra (light grey background) are multiplied by the factor 10.

states can be observed for the spectral densities ( $\epsilon_{\perp} = 2.5$ ) of the first four layers ( $\alpha = 1, 2, 3, 4$ ). The spectral weight of these states decreases exponentially with the distance from the surface layer. The energy position of the excitation is independent of the layer index  $\alpha$ . An analytical investigation of the limits in parameter space ( $\epsilon_{\perp}, \epsilon_{\parallel}$ ), separating regions with one two or without surface states, will be given in [33].

### 3.2 Spin- $\downarrow$ -electron

The local spin- $\downarrow$  spectral density of the surface layer of a 100-layer film at the  $\bar{M}$  point  $(\frac{\pi}{a}, \frac{\pi}{a})$  of the Brillouin zone in case of different s-f exchange coupling constants  $J$  can be seen in Figure 6. The hopping is modified within the topmost layer. In analogy to the case of the spin- $\uparrow$  electron there is a splitting off of a surface state at the polaron band of the spectrum. This effect is independent on the s-f interaction  $J$ . The scattering part located at lower energies is altered as a consequence of modification of the spin- $\uparrow$  spectrum by  $\epsilon_{\parallel}$ . This reflects the transfer of

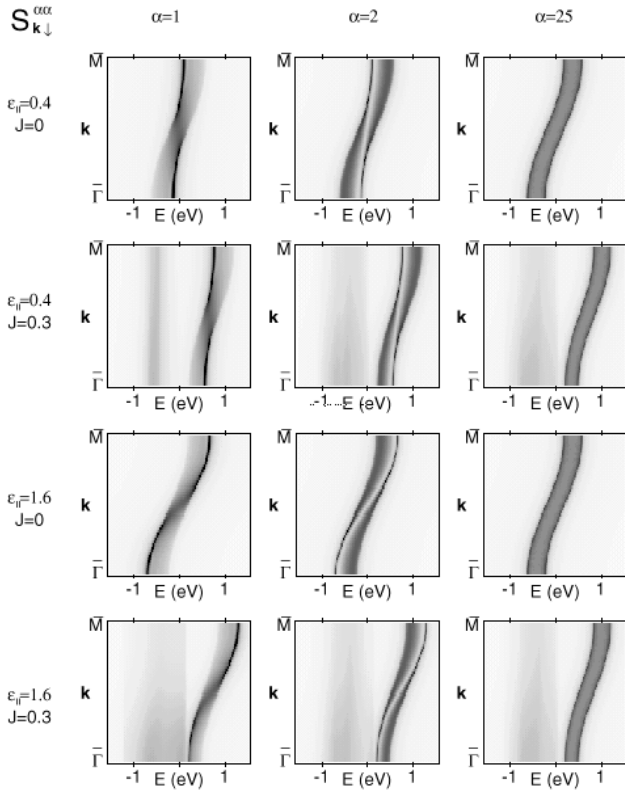


**Fig. 8.** Local spin- $\downarrow$  densities of states for  $J = 0.32$  of the layers ( $\alpha = 1, 2, 3, 6$ ) of a 12 layer film with modified hopping within the first layer and  $\epsilon_{\perp} = 1$ .

spectral weight in the spin- $\uparrow$  spectral density. However, a surface state does not show up at the scattering part of the spectral density.

The same holds for the spin- $\downarrow$  spectral density of states for the situation of modified hopping between first and the second layer of a 100-layer film as can be seen in Figure 7. Here also, the existence of surface states does only depend on the parameter  $\epsilon_{\perp}$  and is independent on the s-f exchange interaction  $J$ .

Figure 8 shows the local density of states (LDOS) of a 12-layer film. The hopping within the surface layer is modified while all the other hopping integrals are left unchanged. For the surface layer ( $\alpha = 1$ ) we observe a drastic dependence of the LDOS on the hopping  $\epsilon_{\parallel}$ . A reduction of the hopping within the first layer results in a narrowing of the scattering and the polaron part of the LDOS of the first layer. An increase of the hopping causes a broadening of both scattering and polaron parts. For a substantial modification of the hopping  $\epsilon_{\parallel} > 2$  both parts merge and the LDOS of the second layer approaches the LDOS of the surface layer in the case of uniform hopping. One possible explanation is that if the hopping within the surface layer becomes infinite ( $\epsilon_{\parallel} \rightarrow \infty$ ) and the hopping between the surface layer and the surface nearest layer remains finite



**Fig. 9.** Density plots of the local spin- $\downarrow$  spectral density of the  $\alpha = 1, 2, 25$  layer of a 50 layer film as a function of energy and  $\mathbf{k} \in (\bar{\Gamma}, \bar{M})$  for two s-f exchange coupling constants  $J = 0, 0.3$  and modified hopping within the first layer ( $\epsilon_{\parallel} = 0.4, 1.6$ ). The hopping between all layers remains constant.

the electron can only move within the surface layer and will not jump to the second layer. The consequence is an “effective” decoupling of the surface layer from the rest of the film as in the case of ( $\epsilon_{\perp} = 0, \epsilon_{\parallel} = 1$ ) discussed in Subsection 3.1. The analytical solution [33] for  $\sigma = \uparrow$  shows that in the limit  $\epsilon_{\parallel} \rightarrow \infty$  and  $\epsilon_{\perp} = \text{const.}$  the Green function of the second layer becomes equal to the Green function of the surface layer in case of uniform hopping.

Figure 9 offers a series of density plots of the local spectral density of the first, second, and central layer of a 50 layer film as a function of energy and wave vector  $\mathbf{k}$  for different values of the s-f exchange ( $J = 0, 0.3$ ) and modified hopping within the first layer. In the spectra of the first and second layer we observe the splitting off of a surface state from the bulk band ( $\alpha = 25$ ) near the  $\bar{\Gamma}$  and near the  $\bar{M}$  point of Brillouin zone. For  $\epsilon_{\parallel} = 0.4 < 1$  the splitting off takes place on the inner side of dispersion curve causing a narrowing of polaron band of the LDOS for  $\epsilon_{\parallel} = 1.6 > 1$  on the outer side resulting in a broadening of it. As a consequence of the broadened or narrowed  $\sigma = \uparrow$  LDOS (see Fig. 9) for  $\epsilon_{\parallel} = 1.6$  the scattering part is broadened but for  $\epsilon_{\parallel} = 0.4$  it is narrowed.

## 4 Summary

We have investigated the electronic quasiparticle spectrum of a ferromagnetic local-moment film of finite thickness. A single band electron is coupled by an intraatomic s-f interaction to the magnetic local-moment system. For a ferromagnetically saturated localised spin system,  $T = 0$  K, an exact solution of the problem was given in our previous work [25].

In contrast to this, in this work the investigation has been focused on the influence of modified hopping integrals near the surface of the film. In tight binding approximation for the hopping integrals, either the hopping within the topmost layer or the hopping between the first and the second layer has been modified.

Generally the modification of the hopping causes a transfer of spectral weight within the spectra.

For sufficiently modified hopping within the surface layer ( $|\epsilon_{\parallel} - 1| > \frac{1}{4}$ ), both for increased and decreased hopping and for both spin directions  $\sigma$  of the single electron a surface state splits off from the bulk band ( $\sigma = \uparrow$ ) or the polaron band ( $\sigma = \downarrow$ ), respectively. The existence of surface states for a given  $\epsilon_{\parallel}$  depends on the wave vector  $\mathbf{k}$  of the two dimensional Brillouin zone and starts at the  $\bar{\Gamma}$  and  $\bar{M}$  point.

If the hopping between the surface layer and the surface nearest layer  $\epsilon_{\perp}$  is adequately increased two surface states show up, one at the lower edge and one at the upper edge of the bulk spectrum.

The spectral weight of the surface states exponentially decays from the surface into the bulk. The surface effects induced by modified hopping visible in the spin- $\uparrow$  spectrum are rendered by correlation in the spin- $\downarrow$  spectrum.

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