Influence of uncorrelated overlayers on the magnetism in thin itinerant-electron films

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The influence of uncorrelated (nonmagnetic) overlayers on the magnetic properties of thin itinerant-electron films is investigated within the single-band Hubbard model. The Coulomb correlation between the electrons in the ferromagnetic layers is treated by using the spectral density approach (SDA). It is found that the presence of nonmagnetic layers has a strong effect on the magnetic properties of thin films. The Curie temperatures of very thin films are modified by the uncorrelated overlayers. The quasiparticle density of states is used to analyze the results. In addition, the coupling between the ferromagnetic layers and the nonmagnetic layers is discussed in detail. The coupling depends on the band occupation of the nonmagnetic layers, while it is almost independent of the number of the nonmagnetic layers. The induced polarization in the nonmagnetic layers shows a long-range decreasing oscillatory behavior and it depends on the coupling between ferromagnetic and nonmagnetic layers.

I. INTRODUCTION

In the past few years, there has been growing interest in the magnetic behavior of thin metallic films. This attention originates both from fundamental physics and from applications. The reduced symmetry and the lower coordination numbers at the surface offer the possibility of inducing new and exotic phenomena, such as perpendicular anisotropy in ultrathin films, interlayer coupling, and giant magnetoresistance (GMR) in ferromagnetic metal/nonmagnetic metal (FM/NM) multilayers. In experiment, it was shown that ultrathin transition metal films can display long range ferromagnetic order from a monolayer on. It is well known, that due to the Mermin-Wagner theorem, an effectively two-dimensional spin-isotropic system cannot display long-range magnetic order at any finite temperature. However, in real ultrathin films, there always exists an anisotropy which allows almost two-dimensional magnetism to occur.

In experiment, the magnetic thin films are normally grown on a nonmagnetic substrate. The effects of the presence of nonmagnetic overlayers on the magnetic properties of these thin films are widely studied both in experiment [1] and theory [2,3]. It has been shown that the interfaces between magnetic and nonmagnetic layers play an important role with respect to the magnetic properties of multilayers systems [4,5]. The composition of the interface between FM and NM has a strong effect on the magnetic properties of the FM films. The critical Co film thickness for the reorientation transition of the magnetization has been observed to shift from 3–4 ML up to 18 ML by the presence of carbon at the interface. In addition, very low coverage of nonmagnetic materials on top of a magnetic layers can have a strong effect on the direction of the magnetization [6,7]. For example, an almost 90° rotation from in-plane direction to out-of-plane direction of the magnetization is induced by 0.03 monolayer (ML) Cu on a 7 ML thick Co film on a stepped Cu(001) surface. The magnetic properties of ultrathin films do not change monotonically with the overlay thickness in some systems. The magnetic anisotropy of thin FM film is observed to rotate from in-plane direction to out-of-plane direction with very thin NM overlayers, while it will return to in-plane direction when the NM overlayers become thicker [8]. First principle calculations for a Co ML on Cu(111) show a switch from the in-plane anisotropy of the uncovered Co monolayer to perpendicular anisotropy only for a 1 ML thick Cu overlayer, while 2 ML Cu produce a slight in-plane anisotropy again [9].

The induced polarization in the NM layers has been investigated experimentally in various systems, such as Pt/Cu [10], Pd/NM [11], Pd/Fe [12], Pd/Co [13], and Cu/Co [14,15]. The direction of the induced polarization has been found to be different for different systems. In Pd/Fe films, the Pd near the interface is ferromagnetically coupled with the Fe film [16]. The induced moment of the Pd has been shown to enhance the Curie temperature $T_C$ of the film [17]. On the other hand, in Pt/Co systems with thicknesses up to 1.5 ML the Pt layer is negatively spin polarized (antiferromagnetic coupling) [18]. In Cu/Co systems the spin polarization of the Cu layers has been shown to oscillate as a function of the Cu thickness. This oscillation is regarded as the origin of the oscillation of the interlayer magnetic coupling in Cu/Co multilayers [19]. In theory, based on first principle calculations, the polarization has been found to be positive both in Pt/Fe and NM/TM (NM denotes noble metal such as Au, Ag and Cu, TM: Fe, Cr) systems. Systematic calculations show that Fe, Co and Ni overlayers on Pd favour a ferromagnetic configuration, whereas V, Cr and Mn overlayers lead to an antiferromagnetic superstructure [20].

Clearly, nonmagnetic overlayers play a very important role with respect to the magnetic properties of thin metallic films. Theoretically, the influence of nonmagnetic overlayers on transition metal films is mostly investigated within first principle calculations [21,22]. However, these calculations can give the zero temperature properties of the films only. Certain idealized model systems have proved to be a good starting point for investigating the magnetic behavior at finite temperatures. In order to investigate the temperature dependence of the magnetization, the Ising model was adopted in Ref. [23]. However, in transition metals, the magnetically active electrons are itinerant. It is by no means clear to what extent the results obtained by localized spin models are applicable to transition metal films.
In addition, the quantum interference of Bloch waves in the NM layers has been applied to study the interlayer magnetic coupling in the FM/NM multilayer.\textsuperscript{43} Within this theory, only the properties of the NM layers are considered, while the properties of the FM layers are neglected completely. In a theory of interlayer magnetic coupling in the FM/NM multilayers, Edwards \textit{et al}. obtained the difference of exchange coupling between two FM layers for difference band occupation in NM layers.\textsuperscript{43} Their results correspond to a Hartree-Fock treatment of a Hubbard-like one-band tight-binding model with on-site interaction $U = 0$ in the NM and with $U = \infty$ in the FM. However, they didn’t calculate the magnetization of the FM and NM, and the effect of the NM on the properties of the FM was neglected.

The aim of the present paper is to investigate the influence of NM overlayers on the magnetism of itinerant-electron thin films within the Hubbard model.\textsuperscript{44} The influence of the coupling between the FM and NM layers on both the magnetic properties of the FM layers and the induced magnetization in the NM layers will be investigated in detail.

The Hubbard model was originally introduced to explain band magnetism in transition metals and has become a standard model to study the essential physics of strongly correlated electron systems over years, such as spontaneous magnetism, metal-insulator transition and high-temperature superconductivity. It incorporates in the simplest way the interplay of the kinetic energy, the Coulomb interaction, the Pauli principle and the lattice geometry. In systems with reduced translational symmetry, the Hubbard model has been successfully applied to describe the temperature-driven reorientation transition of magnetization in itinerant-electron films,\textsuperscript{45} metal-insulator transition in thin films,\textsuperscript{46} the surface magnetism\textsuperscript{47} and low dimensional magnetism.\textsuperscript{48} The model, though in principle rather simple, nevertheless, provokes a non-trivial many-body problem, that could be solved up to now only for some special cases.\textsuperscript{49} In two and three dimensions, one still has to resort to approximate treatments. Due to the reduced translation symmetry in thin films even more complications are introduced. Recently a generalization of the spectral density approach (SDA)\textsuperscript{50} has been applied to study the magnetism of thin metallic films and surfaces.\textsuperscript{50} The SDA, which reproduces the exact results of Harris and Lange\textsuperscript{51} that concern the general shape of the spectral density in the strong-coupling limit ($U \gg W$, $U$: on-site Coulomb interaction, $W$: bandwidth of the Bloch density of states), leads to rather convincing results concerning the magnetic properties of the Hubbard model.\textsuperscript{50} By comparison with different approximation schemes for the Hubbard model as well as experimentally exact QMC calculations in the limit of infinite dimensions it has been shown that the correct inclusion of the exact results of Harris and Lange\textsuperscript{51} in the strong coupling regime is vital for a reasonable description of the magnetic behavior of the Hubbard model, especially at finite temperatures.

The structure of the paper is as follows. First, the Hamiltonian of our model is proposed. Then the SDA for the Hubbard film is described in a simple way. In section IV we show the results of the numerical evaluation of the model and discuss the magnetic behavior of the film system in terms of the layer and temperature dependent magnetizations and the quasiparticle density of states. Finally, a summary will be given.

II. HAMILTONIAN OF THE MODEL

In this paper, we will concentrate on the essence of the effect of NM overlayers on the magnetic properties of itinerant-electron thin films, as well as the influence of the FM layers on the NM layers. The structure discussed here is a NM/FM/NM sandwich structure. We study the symmetric situation where the numbers of the NM layers both above and below the FM layers are assumed to be equal.

The description of this film geometry requires some care. Each lattice vector of the film is decomposed into two parts:

$$ R_{i\alpha} = R_i + r_{\alpha} $$ (1)

$R_i$ denotes a lattice vector of the two-dimensional Bravais lattice of the surface layer with $N$ sites. To each lattice point $R_i$ a $d$-atom basis $r_{\alpha}$ ($\alpha = 1, 2, \cdots, d$) is associated, referring to the $d = 2d_{NM} + d_{FM}$ layers of the film. Here, $d_{NM}$ denotes the thickness of the NM layers and $d_{FM}$ the thickness of the FM layers. Within each layer we assume translational invariance. Then a Fourier transformation with respect to the underlying two-dimensional (surface) Bravais lattice can be applied.

The considered model Hamiltonian reads as follows:

$$ \mathcal{H} = \sum_{i,j,\alpha,\beta,\sigma} (T_{ij}^{\alpha\beta} - \mu)^{\alpha\beta} c_{i\alpha \sigma}^{\dagger} c_{j\beta \sigma} + \frac{U}{2} \sum_{i,\alpha,\sigma} V(\alpha) n_{i\alpha \sigma} n_{i\alpha - \sigma}, $$ (2)

where $c_{i\alpha \sigma}^{\dagger}$ ($c_{i\alpha \sigma}$) stands for the creation (annihilation) operator of an electron with spin $\sigma$ at the lattice site $R_{i\alpha}$, $n_{i\alpha \sigma} = c_{i\alpha \sigma}^{\dagger} c_{i\alpha \sigma}$ is the number operator, and $T_{ij}^{\alpha\beta}$ denotes the hopping-matrix element between the lattice sites $R_{i\alpha}$ and $R_{j\beta}$. The hopping-matrix element between nearest-neighbour sites is set to $-t_{FM}$ ($-t_{NM}$) in the FM (NM) layers and to $-t_{NF}$ between FM and NM layers. $U$ denotes the on-site Coulomb matrix element and $\mu$ is the chemical potential. The Coulomb interaction between the electrons is only considered in the FM layers. Therefore we choose for $V(\alpha)$:

$$ V(\alpha) = \begin{cases} 0, & \alpha \leq d_{NM} \text{ or } \alpha > d_{NM} + d_{FM}, \\ 1, & d_{NM} < \alpha \leq d_{NM} + d_{FM}. \end{cases} $$ (3)

In the following, all quantities related to the NM layers will be labelled by a subscript $NM$, those related to the FM layers by a subscript $FM$. 
III. SPECTRAL-DENSITY APPROACH TO THE HUBBARD FILM

Recently a generalization of SDA has been proposed to deal with the modifications due to reduced translational symmetry. In the following we give only a brief derivation of the SDA solution and refer the reader to previous papers for a detailed discussion.

The basic quantity to be calculated is the retarded single-electron Green function

\[ G_{ij\sigma}^{\alpha\beta}(E) = \langle \langle c_{i\alpha\sigma}^+ c_{j\beta\sigma}^\varepsilon \rangle \rangle_E. \] (4)

All relevant information about the system can be obtained from the Green function. For example, the spin- and layer-dependent quasiparticle density of states (QDOS) is determined by the diagonal part of \( G_{ij\sigma}^{\alpha\beta}(E) \):

\[ \rho_{\alpha\sigma}(E) = -\frac{1}{\pi} \text{Im} \int dE G_{ii\sigma}^{\alpha\alpha}(E - \mu). \] (5)

The band occupations \( n_{\alpha\sigma} \) are given by

\[ n_{\alpha\sigma} = \frac{1}{\pi} \text{Im} \int dE f_-(E) \rho_{\alpha\sigma}(E), \] (6)

where \( f_-(E) \) is the Fermi function. Ferromagnetism is indicated by a spin-asymmetry in the band occupations \( n_{\alpha\sigma} \) leading to non-zero layer magnetizations \( m_\alpha = n_{\alpha\uparrow} - n_{\alpha\downarrow} \). The band occupation in each layer is given by \( n_\sigma = n_{\sigma\uparrow} + n_{\sigma\downarrow} \).

The equation of motion for the single-electron Green function reads:

\[ \sum_{i,\gamma} [(E + \mu)\delta_{i\gamma}^{\alpha\gamma} - T_{ii\gamma}^{\alpha\gamma} - V(\gamma)\Sigma_{i\gamma\sigma}(E)]G_{ij\sigma}^{\gamma\beta}(E) = \hbar \delta_{ij}. \] (7)

Here we have introduced the electronic self-energy \( \Sigma_{i\gamma\sigma}(E) \) which incorporates all effects of electron correlations. The self-energy will automatically vanish within the NM layers due to \( V(\alpha) = 0 \). The local approximation for self-energy in the FM layers is adopted, which has been tested recently for the case of reduced translational symmetry. Because the translational invariance is assumed within each layer, we then have \( \Sigma_{i\gamma\sigma}(E) = \delta_{i\gamma}^{\alpha\beta} \Sigma_{i\sigma}(E) \).

The key point of the SDA is to find a reasonable ansatz for the self-energy in FM layers. Guided by the exactly soluble atomic limit of vanishing hopping \( (t_{FM} = 0) \) and by the findings of Harris and Lange, the strong-coupling limit \( (U/t_{FM} >> 1) \), a one-pole ansatz for the self-energy \( \Sigma_{i\sigma}(E) \) can be motivated:

\[ \Sigma_{i\sigma}(E) = g_{1\sigma}^{\alpha\alpha} \frac{E - g_{2\sigma}^{\alpha\alpha}}{E - g_{3\sigma}^{\alpha\alpha}} \] (8)

where the spin- and layer-dependent parameters \( g_{1\sigma}^{\alpha\alpha}, g_{2\sigma}^{\alpha\alpha} \) and \( g_{3\sigma}^{\alpha\alpha} \) are fixed by exploiting the equality between two alternative but exact representations for the moments of the layer-dependent QDOS:

\[ M_{ij\sigma}^{(m)\alpha\beta} = -\frac{1}{\pi} \text{Im} \int dE(E^m G_{ij\sigma}^{\alpha\beta}(E)) \]

\[ = \langle \langle \cdots \{c_{i\alpha\sigma}^+, \mathcal{H}, \cdots, \mathcal{H}, c_{j\alpha\sigma}\} \rangle \rangle_{m\text{-times}}. \] (9)

Here \( \langle \cdot \cdot \cdot \rangle \) denotes the grand-canonical average and \( \{ \cdots \} \) is the commutator (anticommutator). It has been shown\(^{[4]} \) that an inclusion of the first four moments of QDOS \( (m = 0-3) \) is vital for a proper description of ferromagnetism in the Hubbard model, especially for finite temperatures. Further, the first four moments represent a necessary condition to be consistent with the strong-coupling results of Harris and Lange. Taking into the first four moments to fix the three parameters \( g_{1\sigma}^{\alpha\alpha}, g_{2\sigma}^{\alpha\alpha} \) and \( g_{3\sigma}^{\alpha\alpha} \) in \( \Sigma_{i\sigma}(E) \), one obtains the following self-energy:

\[ \Sigma_{\sigma}(E) = U n_{\alpha\uparrow\sigma} \frac{E + \mu - B_{\alpha\uparrow\sigma}}{E - \mu - B_{\alpha\uparrow\sigma} - U(1 - n_{\alpha\uparrow\sigma})}. \] (10)

The self-energy depends on the spin-dependent occupation numbers \( n_{\alpha\sigma} \) and the so-called band-shift \( B_{\alpha\sigma} \) that consists of higher correlation functions:

\[ B_{\alpha\sigma} = T_{ii\sigma}^{\alpha\alpha} + \frac{1}{n_{\alpha\sigma}(1 - n_{\alpha\sigma})} \sum_{j,\beta \neq \alpha} T_{ij\sigma}^{\alpha\beta} \langle c_{i\alpha\sigma}^+ c_{j\beta\sigma}^\uparrow (2n_{i\alpha\sigma} - 1) \rangle. \] (11)

A spin-dependent shift of the band center of gravity \( n_{\alpha\downarrow\sigma} B_{\alpha\uparrow\sigma} ((1 - n_{\alpha\downarrow\sigma})B_{\alpha\downarrow\sigma}) \) may generate and stabilize ferromagnetic solutions. Although \( B_{\alpha\sigma} \) consists of higher correlation functions, it can be expressed exactly via \( \rho_{\alpha\sigma} \) and \( \Sigma_{\sigma}(E) \):\(^{[3,4]} \)

\[ B_{\alpha\sigma} = T_{ii\sigma}^{\alpha\alpha} + \frac{1}{n_{\alpha\sigma}(1 - n_{\alpha\sigma})} \frac{1}{\hbar} \int dE f_-(E) \times \left( \frac{\Sigma_{\sigma}(E - \mu) - 1}{\Sigma_{\sigma}(E - \mu) - T_{ii\sigma}^{\alpha\alpha}} \right) \rho_{\alpha\sigma}(E). \] (12)

Now a closed set of equations is established via Eqs.\(^{[4]} \), \(^{[6]} \), \(^{[7]} \) and \(^{[8]} \), which can be solved self-consistently.

IV. RESULTS AND DISCUSSION

In our calculations, a fcc(100) geometry is assumed for both the FM and the NM layers. We consider a uniform hopping \( t_{FM} = t_{NM} = t_{NF} = 0.25eV \) between nearest neighbour sites. The band occupation of the FM layers is set to \( n_{FM} = 1.4 \) for all calculations. The band occupation in the NM layers is denoted by \( n_{NM} \). By adjusting the on-site hopping integrals \( T_{ii\sigma}^{\alpha\alpha} \) we explicitly exclude charge transfer within the FM and the NM layers. Further, we keep the on-site Coulomb interaction in the FM layers fixed at \( U = 12eV \), which is three times the bandwidth of the three-dimensional fcc lattice and clearly refers to the strong-coupling regime. In the following we will refer to the considered structure as \( d_{NM}/d_{FM}/d_{NM} \).
datively. For (a)–(d), the number of NM layers is the interface FM layer, and parameters are: 

\[ \frac{T}{T_C} = 0.7 \ldots 0.9 \] has disappeared. The magnetization of the inner FM layers is only weakly affected by the presence of the NM layers (see Fig. 1d).

**FIG. 1.** The layer-dependent magnetization \( m_{\alpha} \) of the FM layers for a \( d_{NM}/d_{FM}/d_{NM} \) sandwich structure as a function of temperature for different numbers \( d_{FM} \) of FM layers. (a) \( d_{FM} = 1 \) and 2, (b), (c), (d) refer \( d_{FM} = 3, 4 \) and 5, respectively. For (a)–(d), the number of NM layers is \( d_{NM} = 4 \). (e) \( d_{FM} = 5 \) and \( d_{NM} = 0 \) (free standing FM film). \( \alpha = 1 \) denotes the interface FM layer, and \( \alpha = 2, 3 \) the inner FM layers. Other parameters are: \( n_{FM} = 1.4, n_{NM} = 0.8, T_C^B \) refers to the bulk Curie temperature.

In Fig. 1, the layer-dependent magnetizations are plotted as a function of temperature for different numbers of magnetic layers. The magnetizations are strongly layer-dependent. Without NM overlayers (Fig. 1c; 0/5/0 structure), the magnetization in each layer is fully polarized at very low temperatures. The magnetization curves of the inner layers show the usual Brillouin-type behavior. The surface magnetization, however, shows a very different behavior: It depends almost linearly on temperature in the temperature range \( T/T_C = 0.7 \ldots 0.9 \). Compared to the inner layers, the surface magnetization decreases significantly faster as a function of temperature and shows a tendency to a reduced Curie temperature. However, due to the coupling between the surface and the inner layers that is induced by the electron hopping, a unique Curie temperature for the whole film is obtained. When the NM overlayers are taken into account (see Fig. 1a, 1b, 1c, 1d; 4/d_{FM}/4 structure), the interface magnetization of the FM layers and its temperature behavior are strongly affected by the interaction between the FM and NM layers which is induced by the electron hopping at the interface. The interface is no longer fully polarized at low temperatures and decreases more rounded as a function of temperature than in the case without NM overlayers. The linear dependence of the interface magnetization in the range of \( T/T_C^B = 0.7 \ldots 0.9 \) has disappeared. The magnetization of the inner FM layers is only weakly affected by the presence of the NM layers (see Fig. 1d).

**FIG. 2.** The Curie temperature \( T_C \) as a function of the number \( d_{FM} \) of FM layers for different numbers \( d_{NM} \) of NM layers. \( d_{NM} = 0 \) refers to the free standing FM film. The parameters are: \( n_{FM} = 1.4, n_{NM} = 0.8 \).

From Fig. 1, one can also read off that the Curie temperature \( T_C \) increases gradually as a function of the number of the FM layers \( d_{FM} \) and reaches its bulk value for \( d_{FM} = 8 \ldots 10 \). The influence of the NM layers on the Curie temperature is analyzed in more detail in Fig. 2 where \( T_C(d_{FM}) \) is shown for different numbers of the NM layers. As can be seen in Fig. 2, the behavior of \( T_C \) as a function of \( d_{FM} \) is quite different for \( d_{NM} = 0 \) and \( d_{NM} \neq 0 \). In the case without NM overlayers \( (d_{NM} = 0) \) \( T_C \) increases very steeply as a function of \( d_{FM} \) and saturates already for \( d_{FM} = 3 \ldots 5 \). The influence of the NM layers is most important for very thin magnetic films \( d_{FM} < 6 \). For \( d_{FM} = 3, 4 \) the presence of only one NM overlayer leads to a reduction of the Curie temperature of about 5% compared to its free FM film value. It is interesting to note that there are only minor changes in \( T_C \) when the number of NM layers is further increased. Note that for \( d_{FM} \geq 3 \), the reduction of the \( T_C \) is strongest for just one NM layer. As \( d_{NM} \) is further increased, the reduction of the \( T_C \) becomes slightly decreasing again. \( T_C \) as a function of \( d_{NM} \) saturates already for \( d_{NM} = 3 \). This indicates that the influence of a very thin NM topping on the magnetic properties of the FM films is stronger than for thick NM overlayers. In experiment, it has also been observed that very thin NM layers have a stronger effect on the magnetic properties than thick overlayers. For example, the direction of the magnetization of a Co film shows a rotation from the in-plane direction to the out-of-plane direction induced only by very thin coverage of Cu, while for thick coverage of Cu, the direction of magnetization of the FM films will turn back to in-plane direction. First princi-
ple calculations for a Co ML on Cu(111) predict a switch from the in-plane anisotropy of the uncovered Co monolayer to perpendicular anisotropy only for 1 ML thick Cu overlayer, while 2 ML Cu produces a slight in-plane anisotropy again.\

In order to investigate the influence of the NM overlayers on the magnetism of the FM films in more detail, we have calculated the magnetization of the NM layer and the FM layers as a function of \( n \) layers as a function of \( n \). For very small \( n \) it decreases rapidly from the free FM film value \( T^0 \) (\( d_{NM} = 0 \)) to a minimum at \( n_{NM} = 0.35–0.4 \). Then it increases from the minimum to a maximum (at \( n_{NM} \approx 1.97 \)) which lies above \( T^0 \). Finally, it drops quickly to \( T^0 \) at \( n_{NM} = 2.0 \). The two limiting cases (\( T_C = 0 \) at \( n_{NM} = 0 \) and \( n_{NM} = 2.0 \)) are easy to understand. In these two situations, the NM bands are either empty or fully occupied and, therefore, have no influence on the properties of the FM film. To understand the behavior of \( T_C \) as a function of \( n_{NM} \), we have also calculated the magnetizations of the NM layer and the FM layers as a function of \( n_{NM} \) at low temperatures in Fig. 3b and Fig. 3c. The magnetization of the NM layer shows a similar dependence on \( n_{NM} \) as the Curie temperature (see Fig. 3b). Since the magnetization of the FM layers is always positive, the sign of magnetization of the NM layer represents the coupling between FM and NM at the interface. A positive sign corresponds to ferromagnetic coupling, a negative sign to antiferromagnetic coupling. The results indicate that \( T_C \) is strongly affected by the coupling of FM and NM. From Fig. 3c, one can see that the coupling of FM and NM has also a strong effect on the magnetizations in the FM layers, especially on the interface magnetization at low temperature.

![Curie temperature and magnetization](image_url)

**FIG. 3.** The Curie temperature \( T_C \) and magnetizations \( m_{NM} \) of a \( d_{NM}/d_{FM}/d_{NM} = 1/3/1 \) sandwich structure as functions of the band occupation \( n_{NM} \) of the NM layers. (a) \( T_C \), (b) the magnetization of the NM layer, and (c) the magnetizations of the FM layers. \( \alpha = 1 \) indicates the interface FM layer. The fully polarized magnetizations of the FM layers are 0.6. \( T^0 \) denotes the Curie temperature of the free FM film. Other parameters are: \( n_{FM} = 1.4 \). For (b) and (c) the temperature is \( T = 0.1T^0 \).

![Layer-dependent QDOS](image_url)

**FIG. 4.** Layer-dependent QDOS of a 1/3/1 sandwich structure for different \( n_{NM} \) at low temperature (\( T = 0.1T^0 \)). (a) \( n_{NM} = 0.4 \), (b) \( n_{NM} = 0.8 \), and (c) \( n_{NM} = 1.4 \).

Further insight about the coupling between the FM and the NM layers can be obtained from the layer-dependent QDOS. In Fig. 4 the QDOS of a 1/3/1 sandwich structure is shown for \( T = 0.1T^0 \) and three different values of the band occupation of the NM layers (\( n_{NM} = 0.4, 0.8, 1.4 \)). For \( n_{NM} = 0.8 \) the temperature dependence of the QDOS is plotted in Fig. 5 for \( T = 0.1, 0.9, 1.0T_C \). Two kinds of splittings are observed in the FM spectrum. The strong Coulomb interaction between the electrons leads to a splitting of the spectrum into a high and a low energy part ("Hubbard splitting"). These two quasiparticle subbands ("Hubbard bands") are separated by an energy amount of...
the order $U$. In the lower subband the electron mainly hops over empty lattice sites, whereas in the upper subband it hops over lattice sites that are already occupied by another electron with opposite spin. The weights of the subbands scale with the probability that a propagating electron meets the one or the other situation. The total weight of the QDOS of each layer is normalized to 1. In the strong coupling limit the weights of the lower and the upper subbands are given by $(1-n_{α-})$ and $n_{α-}$, respectively. Due to the vanishing Coulomb repulsion the Hubbard splitting disappears in the NM spectrum. For temperatures below $T_C$, an additional spin splitting ("exchange splitting") in majority- ($σ = \uparrow$) and minority- ($σ = \downarrow$) spin direction occurs in both the FM and the NM spectrum, leading to a non-zero magnetization $m_α = n_{α\uparrow} - n_{α\downarrow}$. Note that, in principle, the NM and the FM spectrum for each spin direction occupy exactly the same energy region, thus preventing the electrons to be trapped. However, the corresponding spectral weight may become very small as can be seen in Fig. 4 and Fig. 5.

First we want to discuss the $n_{NM}$-dependence of the QDOS at low temperatures. For the case of $d_{NM} = 0$, the majority QDOS lies completely below the chemical potential, and the system is fully polarized ($n_{α\uparrow} = 1$) at $T = 0$ (see also Fig. 1c). If the NM overlayer is taken into account (Fig. 4), the majority QDOS of both the interface and inner FM layers have tails above the chemical potential due to the hybridization between FM and NM layers. As a consequence the system is no longer fully polarized at low temperatures (see also Fig. 1a,1b,1c,1d). The weight of the tail determines the reduction of the magnetization compared to the fully polarized state. Since the weight of the tail becomes smaller as the band occupation of the NM layer increases from $n_{NM} = 0.4$ to $n_{NM} = 1.4$ the reduction of the magnetization in the interface gets weaker as well (see also Fig. 3c).

Let us now turn to the NM layer. As mentioned above, the QDOS of the NM layer has just one kind of splitting – the exchange splitting. The QDOS of the NM layer is quite different for majority- and minority-spin direction. Because there is no Coulomb interaction in the NM layers, the majority- and minority-QDOS do not affect each other. It is interesting to note, that above the chemical potential the majority NM-QDOS resembles the BDOS (Bloch density of states) of the square lattice which is equivalent to the free standing fcc(100) monolayer. This is because for energies above the chemical potential a ($σ = \uparrow$)-electron within the NM layer is effectively isolated since the spectral weight of the ($σ = \uparrow$)-FM-QDOS is very small in this energy region.

For $n_{NM} = 0.4$ (Fig. 4a), there is very low spectral weight in the majority NM-QDOS below the chemical potential. As a consequence the number of spin-up electrons is smaller than the number of spin-down electrons in the NM layer. The magnetization of the NM layer is negative, i.e., the NM and FM layers are antiferromagnetically coupled. With increasing $n_{NM}$ the center of gravity of the QDOS of the NM layer gets shifted to lower energies. When the peak of the majority NM-QDOS crosses the chemical potential, the number of the majority-spin electrons increases faster as a function of $n_{NM}$ than the number of minority-spin electrons. The magnetization of the NM layer increases and becomes positive (see Fig. 4b and 4c, also Fig. 3b). Of course, as $n_{NM}$ increases, the shape of the QDOS will also change. Until $n_{NM} = 1.97$, the magnetization of the NM layer will increase as a function of $n_{NM}$. Then it drops quickly, because both the majority- and minority-spin QDOS gets shifted below the chemical potential.

![FIG. 5. Temperature dependence of the layer-dependent QDOS for a 1/3/1 sandwich structure. (a) $T = 0.1T_C$, (b) $T = 0.9T_C$ and (c) $T = T_C$.](image)

The temperature dependence of the FM-QDOS (Fig. 5) is dominated by two correlation effects. As a function of increasing temperature the spin-splitting between the centers of gravity of the majority and minority quasiparticle subbands decreases. In addition there is a temperature-dependent transfer of spectral weight between the lower and the upper quasiparticle subband. The interplay of these two correlation effects leads to a rather rapid demagnetization of the system as a function of temperature and allows for Curie temperatures in a physically reasonable order of magnitude.

At $T = T_C$, the spin-splitting has disappeared completely, both in the FM and the NM spectrum (Fig. 5c).
Due to the coupling between FM and NM layers, the NM-QDOS becomes temperature dependent as well. While the band edges of the NM-QDOS stay fixed, there is a redistribution of spectral weight within the NM-QDOS as a function of temperature. We would like to point out that this temperature-dependence may even result in a temperature induced change from ferromagnetic to antiferromagnetic coupling between FM and NM layers. From Fig. 5b, one can read off that at \( T = 0.9T_C \) the number of spin-up electrons is smaller than the number of spin-down electrons. Due to the reduced spin-splitting in the FM spectrum, the main peak of the majority NM-QDOS gets shifted above the chemical potential. As a consequence, the total magnetization at the interface exhibits only a very small oscillation around a certain negative value as \( d_{NM} \geq 4 \) (see Fig. 6c). This indicates that the coupling between FM and NM layers is only affected by the properties of the FM and NM layers close to the interface, whereas it is independent of the thickness of the NM overlayers as \( d_{NM} \geq 4 \).

Due to the oscillatory behavior of the induced magnetization, we find the surface magnetization to be also oscillating as a function of the number of the NM layers (Fig. 6a). The induced magnetization at the interface exhibits only a very small oscillation around a certain negative value as \( d_{NM} \geq 4 \) (see Fig. 6c). This indicates that the coupling between FM and NM layers is only affected by the properties of the FM and NM layers close to the interface, whereas it is independent of the thickness of the NM overlayers as \( d_{NM} \geq 4 \).

Finally, we want to discuss the induced polarization in the NM layers which is shown in Fig. 6. The induced magnetization of the NM layers oscillates with the layer index for \( d_{NM} \geq 4 \). As a consequence, the total magnetization of the NM layers oscillates as a function of the thickness of the NM as well. An oscillatory behavior of total magnetization of the NM layers as a function of the thickness of the NM has also been obtained by Bruno within the theory of interlayer magnetic coupling. However, our starting point and our results are completely different. The quantum interference was introduced to understand the properties of the NM layers. The Bloch waves of the NM layers are regarded as to be confined within two FM perturbations (or one FM perturbation and one Vacuum). Due to the constructive and destructive reflection at this confinement, the densities of spin-up and/or spin-down electrons are found to be oscillating as a function of the thickness of the NM. While the long range magnetic order was excluded in his theory. Within this concept, one can find that the magnetization of the NM interface should oscillate around zero. On the contrary, in our calculation, the amplitude of the oscillation decreases from the interface to the surface (Fig. 6a) and the profile of the induced magnetization is almost independent of \( d_{NM} \) (Fig. 6a). The induced magnetization at the interface exhibits only a very small oscillation around a certain negative value as \( d_{NM} \geq 4 \).

### V. CONCLUSIONS

The effect of uncorrelated layers on the magnetic properties in thin Hubbard films is studied by the spectral density approach (SDA). The SDA, which reproduces the exact results of \( t/U \) -perturbation theory of Harris and Lange, in strong-coupling limit, leads to rather convincing results concerning the magnetic properties of the Hubbard model. By comparison with different approximation schemes for the Hubbard model as well as numerically exact QMC calculation in the limit of infinite dimensions it has been shown that the correct inclusion of the exact results of Harris and Lange in the strong coupling regime is vital for a reasonable description of the magnetic behavior of the Hubbard model, especially at finite temperatures. Within our theory, FM and NM layers are treated on the same footing. The effects of the coupling between FM and NM on the magnetic properties of the FM layers, as well as on the NM layers, have been studied in detail. The Curie temperature of thin FM films is modified by the presence of NM layers. For \( n_{FM} = 1.4 \) and \( n_{NM} = 0.8 \) the Curie temperature increases gradually as a function of the num-
number of FM layers and converges to the corresponding bulk value for $d_{FM} = 8 - 10$. The induced polarization in the NM layers displays a long-range decreasing oscillation with respect to the layer index of the NM layers. The induced magnetization of the interface NM layer hardly changes as a function of number of the NM layers when $d_{NM} \geq 4$. This means the coupling between the FM and NM layers is determined by the intrinsic properties of the FM and NM layers, such as the band occupation, the in-site Coulomb interaction and the hopping, and is independent of the numbers of the FM and NM layers. 

The magnetic properties of this thin film system have been microscopically understood by means of spin- layer- and temperature- dependent quasiparticle density of states (QDOS) for a 1/3/1 sandwich structure. There exist two correlation induced band splittings in the FM spectrum. Besides the Hubbard splitting there is an additional exchange splitting for temperatures below $T_C$. Due to the vanishing Coulomb repulsion the Hubbard splitting disappears in the NM spectrum. For the case of $d_{NM} = 0$, the majority FM-QDOS lies completely below the chemical potential, and the system is fully polarized ($n_{NM}^1 = 1$) at zero temperature. If the NM layers are taken into account, the majority QDOS of both the interface and inner FM layers have tails above the chemical potential due to the hybridization between the FM and NM layers. As a consequence the system is no longer fully polarized at low temperatures. There is a reduction of the FM magnetization compared to the fully polarized state. The reduction of the magnetization of the interface FM layer gets weaker as the band occupation of the NM layer is increased from $n_{NM} = 0.4$ to $n_{NM} = 1.4$. In addition for $n_{NM} = 0.4$, there is very low spectral weight in the majority NM-QDOS below the chemical potential. As a consequence the number of spin-up electrons is smaller than the number of spin-down electrons in the NM layer. The magnetization of the NM layer is negative, i.e., the NM and FM layers are antiferromagnetic coupled. As $n_{NM}$ increases, the magnetization of the NM layer increases and becomes positive. The change of the coupling between the FM and NM layers can also be induced by the temperature. This temperature induced change of the coupling is observed only for very thin NM layers.

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50 In order to see the oscillation clearly, we relabel the layer index, i.e., 1 refers to the interface, 2 next to the interface, etc.
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