On the magnetic stability at the surface in strongly correlated electron systems

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The stability of ferromagnetism at the surface at finite temperatures is investigated within the strongly correlated Hubbard model on a semi-infinite lattice. Due to the reduced surface coordination number the effective Coulomb correlation is enhanced at the surface compared to the bulk. Therefore, within the well-known Stoner-picture of band ferromagnetism one would expect the magnetic stability at the surface to be enhanced as well. However, by taking electron correlations into account well beyond the Hartree-Fock (Stoner) level we find the opposite behavior: As a function of temperature the magnetization of the surface layer decreases faster than in the bulk. By varying the hopping integral within the surface layer this behavior becomes even more pronounced. A reduced hopping integral at the surface tends to destabilize surface ferromagnetism whereas the magnetic stability gets enhanced by an increased hopping integral. This behavior represents a pure correlation effect and can be understood in terms of general arguments which are based on exact results in the limit of strong Coulomb interaction.

I. INTRODUCTION

There is currently active interest in the influence of reduced translational symmetry on the magnetic properties at surfaces, in ultra-thin films and in multi-layer structures. One class of materials that is intensively studied are the magnetic transition metals, within which the magnetically active electrons are itinerant. Theoretically it is possible to calculate the ground state properties like the magnetic moments at and near surfaces and in thin films in great detail by use of \textit{ab initio} methods. However, these approaches are strictly based on a Stoner-type picture of ferromagnetism and treat electron correlation effects that are responsible for the spontaneous magnetic order on a low level only. Further, an extension to finite temperatures states a difficult problem.

To study the temperature behavior of spontaneous ferromagnetism rather idealized model systems have proven to be a good starting point. What concerns the magnetic properties of systems with reduced translational symmetry, the temperature behavior has been, up to now, almost exclusively studied within localized spin models (Ising model, Heisenberg model). In these systems the magnetic stability at the surface is found to be reduced compared to the bulk. The reduced magnetic stability results simply from the reduced exchange coupling at the surface due to the lower coordination number. However, it is not clear at all to what extent this argument applies also for the magnetic transition metals Fe, Co, Ni, which are prototypical materials of the so-called band magnetism of itinerant electrons. As it is well known, within a tight-binding scheme for the description of the bandstructure the reduced coordination number at the surface leads to a reduced effective bandwidth in the surface layer. As a consequence the effective correlation at the surface will be enhanced. Thus, on the basis of the well-known Stoner-picture of band magnetism one may intuitively expect the magnetic stability at the surface to be enhanced compared to the bulk.

In this paper we investigate the magnetic stability at the surface in strongly correlated electron systems within the Hubbard model on a semi-infinite lattice. Based on the limit of strong Coulomb interaction we give general arguments concerning the magnetic stability at the surface. In addition we will show results of numerical evaluations within the spectral density approach to the semi-infinite Hubbard model. The spectral density approach is based on exact results about the general shape of the spectral density in the limit of strong Coulomb interaction. To emphasize the importance of correlation effects we will show, in addition, results obtained within the Hartree-Fock approximation (Stoner-model).

II. THEORY

To describe the geometry of the semi-infinite lattice each lattice vector is decomposed into two parts \( \mathbf{R}_i = \mathbf{R}_0 + \mathbf{r}_i \). Throughout the paper \( \mathbf{R}_0 \) (Latin index) denotes a lattice vector parallel to the film surface whereas \( \mathbf{r}_i \) (Greek index) refers to the distance from the surface \((\alpha = 1: \) surface layer). Each lattice plane parallel to the surface contains \( N \) lattice sites. Within the layers we assume translational invariance.

Using this notation the Hubbard model for the semi-infinite lattice reads:

\[
\mathcal{H} = \sum_{i, j, \alpha, \beta, \sigma} (T_{ij}^{\alpha\beta} - \mu \delta_{ij}^{\alpha\beta}) c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + \frac{U}{2} \sum_{i, \alpha, \sigma} n_{i\alpha\sigma} n_{i\alpha\sigma}.
\] (1)

Here \( c_{i\alpha\sigma} (c_{i\alpha\sigma}^\dagger) \) stands for the annihilation (creation) operator of an electron with spin \( \sigma \) at the lattice site \( \mathbf{R}_i \), \( n_{i\alpha\sigma} = c_{i\alpha\sigma}^\dagger c_{i\alpha\sigma} \) is the number operator. \( U \) denotes the on-site Coulomb matrix element and \( \mu \) the chemical potential. \( T_{ij}^{\alpha\beta} \) is the hopping integral between the lattice sites \( \mathbf{R}_i \) and \( \mathbf{R}_j \).

Let us first discuss the kinetic part of the system \((U = 0)\) that is treated within the tight-binding approxi-
ation. A two-dimensional Fourier transformation yields the corresponding dispersions

\[ T^{\alpha \beta}_{\mathbf{k}} = \frac{1}{N} \sum_{ij} T^{\alpha \beta}_{ij} e^{-i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \]  
(2)

\[ = T^{\alpha \beta}_{00} \delta^{\alpha \beta} + T^{\alpha \beta}_{ij} (\mathbf{k}), \]  
(3)

that can be easily calculated. Here and in the following \( \mathbf{k} \) denotes a wave-vector from the underlying two-dimensional (surface) Brillouin zone. \( t \) is the hopping integral between nearest neighbor atoms. The on-site hopping integral \( T^{\alpha \beta}_{00} \) gives the center of gravity of the dispersion of the \( \alpha \)-th layer. The dispersions \( T^{\alpha \beta}_{ij} \) determine the Bloch density of states (BDOS) \( \rho_0(E) \). The bandwidth of the BDOS is denoted by \( W \). A moment analysis of the BDOS \( \Delta^{(n)}_\alpha \) shows the variance at the surface \( \Delta^{(2)}_\alpha (\alpha = 1) \) to be considerably reduced compared to the variance of the inner layers \( \Delta^{(2)}_\alpha (\alpha = 2, \ldots, \infty) \). Mathematically, the square root of the variance \( \sqrt{\Delta^{(2)}_\alpha} \) gives a measure of the effective bandwidth of the BDOS. In addition, for an asymmetric BDOS also the skewness \( \Delta^{(3)}_\alpha \) is reduced at the surface compared to the bulk. For fcc-type semi-infinite lattices with surface orientations (100) and (111) that are considered in the numerical calculation (see below) we find:

\[ \frac{\Delta^{(2)}_\alpha}{\Delta^{(2)}_\alpha}(100) = 0.667, \quad \frac{\Delta^{(2)}_\alpha}{\Delta^{(2)}_\alpha}(111) = 0.750, \]
\[ \frac{\Delta^{(3)}_\alpha}{\Delta^{(3)}_\alpha}(100) = 0.5, \quad \frac{\Delta^{(3)}_\alpha}{\Delta^{(3)}_\alpha}(111) = 0.625. \]

The basic quantity from which all relevant information on the system can be obtained is the retarded single-electron Green function

\[ G^{\alpha \beta}_{ij\sigma}(E) = \langle \langle c_{i \alpha \sigma} c_{j \beta \sigma}^\dagger \rangle \rangle E. \]  
(5)

After a two-dimensional Fourier transformation one obtains from \( G^{\alpha \beta}_{ij\sigma}(E) \) the spectral density \( \Sigma^{\alpha \beta}_{ij\sigma}(E) = -\frac{1}{\pi} \text{Im} G^{\alpha \beta}_{ij\sigma}(E) \), which represents the bare line-shape of a (direct, inverse) photoemission experiment. The diagonal elements of the Green function determine the spin- and layer-dependent quasiparticle density of states (QDOS): \( \rho_{\alpha \sigma}(E) = -\frac{1}{\pi} \text{Im} G^{\alpha \alpha}_{ii\sigma}(E - \mu) \). Via an energy integration one immediately gets from \( \rho_{\alpha \sigma}(E) \) the band occupations

\[ n_{\alpha \sigma} \equiv \langle n_{i \alpha \sigma} \rangle = \int_{-\infty}^{\infty} dE f_-(E) \rho_{\alpha \sigma}(E). \]  
(6)

\( \langle \ldots \rangle \) denotes the grand-canonical average and \( f_-(E) \) is the Fermi function. Ferromagnetism is indicated by a spin-asymmetry in the band occupations \( n_{\alpha \sigma} \) leading to non-zero magnetizations \( m_\alpha = n_{\alpha \uparrow} - n_{\alpha \downarrow} \). The mean band occupation \( n \) and the mean magnetization \( m \) are given by \( n = \frac{1}{2} \sum_{\alpha \sigma} n_{\alpha \sigma} \) and \( m = \frac{1}{2} \sum_{\alpha} m_\alpha \), which are, of course, identical to the respective bulk values \( (\alpha \rightarrow \infty) \).

For the generalization of the SDA to systems with reduced translational symmetry we adopt the local approximation for the self-energy \( \Sigma_{ij\sigma}(E) = \delta_{ij} \delta^{\alpha \beta} \Sigma_{\alpha \sigma}(E) \) which has been tested recently for a semi-infinite lattice. The decisive step is to find a reasonable ansatz for the self-energy \( \Sigma_{\alpha \sigma}(E) \). Guided by the exactly solvable atomic limit of vanishing hopping \( U = 0, W = 0 \) and by the findings of Harris and Lange in the strong-coupling limit \( (U/W \gg 1) \), a one-pole ansatz for the self-energy \( \Sigma_{\alpha \sigma}(E) \) can be motivated

\[ \Sigma_{\alpha \sigma}(E) = g_0^\alpha E - g_0^\sigma \frac{E - \delta_{\alpha \sigma}}{E - \delta_{\alpha \sigma}}, \]  
(7)

The spin- and layer-dependent parameters \( g_0^\alpha, g_0^\sigma \) and \( \delta_{\alpha \sigma} \) are chosen by exploiting the equality between two alternative but exact representations for the moments of the Green function.
The deviation from the bulk magnetization is almost completely restricted to the topmost layer. Note, that the influence of the surface is stronger for the more open (100) structure. Due to the coupling between the layers that is induced by the electron hopping a unique Curie temperature is found for the whole system. We have to conclude from Fig. 1 that within the strongly correlated Hubbard model the magnetic order is less stable at the surface than in the bulk, although the effective correlation is enhanced at the surface. This observation clearly contradicts the expectation on the basis of the well-known Stoner-picture of band ferromagnetism. Indeed, repeating the same calculations within the HFA we find the magnetic order to be more stable at the surface compared to the bulk. For very strong Coulomb interaction the layer magnetizations within the HFA become almost independent of the layer index.

The reduced magnetic stability at the surface in strongly correlated electron systems can be understood in terms of general arguments by use of the moment analysis of the BDOS of the semi-infinite lattice (see Eq. (8)). The arguments are based on the magnetic behavior of bulk systems with full translational symmetry, which have been studied in very detail. Both the reduced variance ($\Delta_s^2 < \Delta_b^2$) as well as the reduced skewness ($\Delta_s^3 < \Delta_b^3$) at the surface lead to the same trend:

\[
-\frac{1}{\pi} \text{Im} \int_{-\infty}^{\infty} dE E^m G_{ij\sigma}^\beta(E) = \left\langle \left\{ \left[ [\ldots c_{i\alpha\sigma}, \mathcal{H}]_{\ldots\ldots\ldots}, c_{j\beta\sigma}^\dagger \right] \right\}_m \right\rangle \tag{8}
\]

Here $[\ldots\ldots\ldots]_m$ denotes the commutator (anticommutator). Eq. (8) imposes rigorous sum rules on the Green function which have been recognized to state important guidelines when constructing approximate solutions for the Hubbard model. By comparing various approximation schemes it has been shown that the inclusion of the first four sum rules is vital for a reasonable description of spontaneous ferromagnetism in the Hubbard model, especially at finite temperatures. Taking the first four sum rules ($m = 0, \ldots, 3$) into account to determine the free parameters of the SDA aspect for the self-energy yields a closed set of equations that has to be solved self-consistently. Note, that the self-energy incorporates the so-called bandshift $B_{\alpha-\sigma}$ which is layer dependent and consists of higher correlation functions $B_{\alpha-\sigma}$ and is uniformly magnetized ($n_{\alpha-\sigma}(1-n_{\alpha-\sigma})B_{\alpha-\sigma} \sim E_{\text{kin},-\sigma}, U \gg W$).

A spin-asymmetry of the bandshift, which can occur within the self-consistent calculation in certain parameter regions, may generate or stabilize ferromagnetic solutions in the strongly correlated Hubbard model. For strong Coulomb interaction the bandshift is found to be proportional to the kinetic energy of the system ($n_{\alpha-\sigma}(1-n_{\alpha-\sigma})B_{\alpha-\sigma} \sim E_{\text{kin},-\sigma}, U \gg W$).

III. RESULTS AND DISCUSSION

The numerical evaluations have been done for a semi-infinite fcc lattice. To study the influence of the reduced coordination number we have considered two different surface orientations (100) and (111). The mean band occupation is kept fixed at $n = 1.4$ and the Coulomb interaction is chosen to be $U = 3W$ which clearly refers to the strong coupling region. In order to avoid a mixture of charge transfer and electron correlation effects we have included charge transfer between the layers by requiring $n_\alpha = n, \forall \alpha$. This is achieved by adjusting the layer-dependent on-site hopping integral $T_{\alpha\alpha}$.

Fig. 1 shows the spontaneous magnetization of the semi-infinite fcc lattice as a function of increasing temperature. At low temperatures the system shows full polarization ($m = 2 - n$) and is uniformly magnetized ($m_\alpha = m, \forall \alpha$) since we have explicitly excluded charge transfer between the layers. As the temperature increases the magnetization of the surface layer $m_1$ decreases faster than the bulk magnetization $m_b$. This behavior holds for both considered surface orientations, (100) and (111). The deviation from the bulk magnetization is almost

\[
\left(1 + \frac{\alpha}{2}\right)
\]

FIG. 1. Magnetization $m_\alpha$ for a semi-infinite fcc lattice as a function of the reduced temperature $T/T_C$. $\alpha = 1$ corresponds to the surface layer. (a) (100) surface; (b) (111) surface. Further parameters: $U/W = 3; n = 1.4$

(i) Within various approximation schemes, as well as DMFT-QMC calculations, it has been established, that a large skewness of the BDOS tends to stabi-
lize spontaneous ferromagnetism in the Hubbard model. Since the skewness of the surface layer BDOS is reduced compared to the inner layers this explains the trend to a reduced magnetic stability at the surface.

(ii) In order to understand the influence of the reduced variance of the BDOS at the surface on the magnetic stability we have plotted in Fig. 2 the Curie temperature $T_C$ for an fcc bulk system in two different ways. Fig. 2(a) shows $k_B T_C/W$ as a function of the effective correlation $U/W$. This corresponds to the situation where the bandwidth $W$ of the uncorrelated Bloch band is kept fixed while the Coulomb interaction $U$ is varied. Within the SDA the Curie temperature steeply increases as soon as $U/W$ exceeds a critical lower bound. But already for $U/W \approx 1 - 2$ the Curie temperature starts to saturate and approaches a finite value as $U \to \infty$. This behavior can be understood by inspecting the quasiparticle spectrum. In the strongly correlated Hubbard model the quasiparticle spectrum splits into a high and a low energy subband ("Hubbard-bands"; for a detailed discussion see, e.g., Refs. 24,25). Both subbands are separated by an energy amount of approximately $U$. In the ferromagnetic phase there is an additional spin splitting within each subband between the majority and the minority spin direction. According to the results of Harris and Lange24 the spin splitting is \( \Delta_2 \) determined by the spin-asymmetry in the kinetic energy \( E_{\text{kin}} = E_{\text{kin},\uparrow} + E_{\text{kin},\downarrow} \) of the system. This can be seen, e.g., for the spin-splitting \( \Delta_2 \) between the centers of gravity \( \langle T_2 \rangle \) of the upper Hubbard-bands within which the chemical potential \( \mu \) is located for the more than half-filled case \( n > 1 \). Here one finds

\[
\Delta_2 = T_2 \uparrow - T_2 \downarrow \approx W \frac{E_{\text{kin},\uparrow}}{n_\uparrow} - \frac{E_{\text{kin},\downarrow}}{n_\downarrow}.
\]

The kinetic energy, however, becomes independent of \( U \) in the limit of strong Coulomb interaction and the bandwidth \( W \) remains the only relevant energy scale with respect to the magnetic properties of the system. Therefore, the spin splitting (9) as well as the Curie temperature saturate as a function of increasing \( U \) (Fig. 2(a)). The same behavior has been observed within several strong coupling approaches to the Hubbard model24 as well as DMFT-QMC calculations.26 Within the HFA the spectrum shows a completely different behavior. Here, the Hubbard splitting is absent and the spin splitting is given by $U\mu$. Both, the spin splitting and the Curie temperature increase linearly with $U$ in the strong coupling limit as can be seen in Fig. 2(a). In Fig. 2(b) we have plotted $k_B T_C/U$ as a function of the effective correlation $U/W$. This means that the Bloch bandwidth $W$ is varied while the Coulomb interaction $U$ is kept fixed. Note, that this corresponds to the situation in semi-infinite lattices as well as in thin films where $U$ is uniform for all layers, the effective bandwidth ($\sim \sqrt{\Delta_2^2}$) of the BDOS being, however, different at the surface and in the bulk. As we have discussed above, in the strong coupling regime the energy scale being important for the magnetic properties is given by $W$. Therefore, for fixed $U$ the Curie temperature within the SDA decreases proportional to $1/W$ as $U/W \to \infty$ (see Fig. 2(b)). In the limit $W = 0$ we find a vanishing Curie temperature, which reproduces the exact result in the so-called "atomic limit" of vanishing hopping. Again, the Hartree-Fock solution fails to describe the strong coupling behavior correctly, giving a finite Curie temperature even for $W = 0$. Since the energy scale determining the magnetic properties is given by $U$ within the HFA the Curie temperature saturates at a finite value as $W \to 0$ in Fig. 2(b). By applying the results of Fig. 2(b) to the semi-infinite system it is clear that in the limit of strong Coulomb interaction the reduced effective bandwidth in the surface layer ($\sqrt{\Delta_2^2} < \sqrt{\Delta_2^2}$) enhances the effective correlation but reduces the magnetic stability at the surface. In addition, Fig. 2(b) explains the qualitatively different behavior concerning the magnetic stability at the surface within the HFA and the SDA.

![Fig. 2. Curie temperature $T_C$ as a function of the effective correlation $U/W$ for an fcc lattice (bulk calculation). (a) constant bandwidth $W$ of the BDOS, (b) constant Coulomb interaction $U$. $k_B$ is the Boltzmann constant. Further parameters: $n = 1.4$](image-url)
the exact results of the $W/U$ perturbation theory of Harris and Langreth. It is clear that argument (ii) holds only for strong Coulomb interaction. In the case of moderate coupling strengths the effective correlation $U/W$ has to exceed a lower critical bound for spontaneous ferromagnetism to occur.

\[
T_C(U, rW) = rT_C\left(\frac{U}{r}, W\right), \quad r > 0
\]  
\[
T_C(U, rW) = T_C(U, W) \left[ 1 + \frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right) (1 - r) \right]
\]

For $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right) > 1$ a reduction of the bandwidth $W$ by a factor $r$ will increase the Curie temperature, for $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right) < 1$ the Curie temperature will be reduced. In Fig. 3 numerical results for $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$ are plotted as a function of $U/W$ for both the SDA and the HFA. $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$, that is defined in the ferromagnetic phase only, diverges as $U/W$ approaches the lower critical correlation. Thus, for moderate coupling strength we find $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right) > 1$ within the HFA and the SDA. However, within the SDA $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$ becomes smaller than 1 very rapidly with increasing $U/W$ and vanishes as $U/W \to \infty$. Thus, by inspecting $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$ we can distinguish between two different regimes: For moderate correlation we expect the magnetic stability at the surface to be enhanced, whereas it will be reduced for strong Coulomb interaction. Again, a similar behavior is to be expected within other strong coupling approaches to the Hubbard model as well.

FIG. 3. $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$ (see Eq. (11)) calculated within the HFA and the SDA as a function of the effective correlation $U/W$ for an fcc lattice (bulk calculation). Further parameter: $n = 1.4$.

Let us discuss the boundary between these two regimes (moderate coupling $\leftrightarrow$ strong coupling behavior) in more detail. Due to the scaling property of the Hubbard model (moderate coupling strength) the exact results of the perturbation theory of Harris and Langreth [10] can be utilized. The bulk calculation within the SDA as a function of the effective correlation $U/W$ up to the first order yields:

\[
T_C(U, rW) = rT_C\left(\frac{U}{r}, W\right), \quad r > 0
\]  
\[
T_C(U, rW) = T_C(U, W) \left[ 1 + \frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right) (1 - r) \right]
\]  

For $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right) > 1$ a reduction of the bandwidth $W$ by a factor $r$ will increase the Curie temperature, for $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right) < 1$ the Curie temperature will be reduced. In Fig. 3 numerical results for $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$ are plotted as a function of $U/W$ for both the SDA and the HFA. $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$, that is defined in the ferromagnetic phase only, diverges as $U/W$ approaches the lower critical correlation. Thus, for moderate coupling strength we find $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right) > 1$ within the HFA and the SDA. However, within the SDA $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$ becomes smaller than 1 very rapidly with increasing $U/W$ and vanishes as $U/W \to \infty$. Thus, by inspecting $\frac{U}{T_C} \left( \frac{\partial T_C}{\partial U} \right)$ we can distinguish between two different regimes: For moderate correlation we expect the magnetic stability at the surface to be enhanced, whereas it will be reduced for strong Coulomb interaction. Again, a similar behavior is to be expected within other strong coupling approaches to the Hubbard model as well.

FIG. 4. Bulk magnetization $m_b$ and surface layer magnetization $m_s$ as a function of the reduced temperature $T/T_C$ for a semi-infinite fcc lattice with a (111) surface. The hopping integral within the first layer has been varied according to $T_k^{11} = T_01 + \epsilon t_{11}(k)$, $\epsilon > 0$. (a) $\epsilon = 1.0, 0.9, 0.8, 0.7$. (b) $\epsilon = 1.0, 1.1, 1.2, 1.3$. The thick lines correspond to the uniform situation $\epsilon = 1.0$. Further parameters: $U/W = 3$; $n = 1.4$

To further investigate the magnetic stability at the surface we have modified the hopping integral within the surface layer of the semi-infinite fcc(111) lattice according to $T_k^{11} = T_01 + \epsilon t_{11}(k)$, $\epsilon > 0$. In Fig. 2(b) we find the corresponding layer magnetizations as a function of the reduced temperature $T/T_C^{bulk}$. We have considered deviations from the unperturbed hopping $\epsilon = 1.0$ within 30% only. A reduced hopping integral in the surface layer $\epsilon < 1$ (Fig. 2(a)) results in a reduced magnetic stability at the surface. As in the uniform situation ($\epsilon = 1$, see also Fig. 2) we find a unique Curie temperature $T_C = T_C^{bulk}$ for all $\epsilon < 1$ due to the coupling between the surface layer and the bulk. As the hopping at the surface is enhanced compared to the bulk ($\epsilon > 1$, Fig. 2(b)), the magnetic stability at the surface increases. Note that already a 30% enhancement of the surface hopping integral ($\epsilon = 1.3$) leads to an enhanced surface Curie temperature $T_C^{surf}$ which lies clearly above $T_C^{bulk}$. For $T_C^{bulk} < T < T_C^{surf}$ the polarization of the surface layer induces a finite polarization in the adjacent layers. However, the induced
magnetization decreases very fast with increasing distance from the surface. In this sense we find two separate Curie temperatures in the system. The bulk Curie temperature is, of course, not affected by the enhanced surface Curie temperature. Qualitatively, the influence of the modified hopping at the surface on the magnetic stability can be understood by argument (ii) that was introduced above. A reduced (enhanced) hopping integral at the surface leads to a reduction (enhancement) of the effective bandwidth of the surface layer BDOS and, therefore, to a reduced (enhanced) magnetic stability. Again, the opposite behavior is found within the HFA.

IV. CONCLUSION

In conclusion we have investigated the magnetic stability at the surface in strongly correlated electron systems within the semi-infinite Hubbard model. For strong Coulomb correlation we find the magnetic stability at the surface to be reduced compared to the bulk. This behavior represents a pure correlation effect that cannot be explained within the well-known Stoner-picture of band-magnetism which is justified for weak Coulomb interaction only. However, based on exact results concerning the general shape of the spectral density in the strong coupling limit the reduced magnetic stability at the surface can be understood by a moment analysis of the BDOS. It has been shown that both the reduced variance (effective bandwidth) as well as the reduced skewness of the surface layer BDOS tend to reduce the magnetic stability at the surface.

By modifying the nearest neighbor hopping integral within the surface layer we have investigated the magnetic stability at the surface in more detail. Again, the same trend is observed. A reduced (enhanced) hopping integral at the surface leads to a reduced (enhanced) magnetic stability at the surface. For an fcc(111) geometry already a 30% enhancement of the surface hopping integral results in a surface Curie temperature which lies well above the bulk Curie temperature.

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