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ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

STABILIZATION OF FERROMAGNETIS IN NARROW-BAND SOLIDS BY s-d - HYBRIDIZATION

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STABILIZATION OF FERROMAGNETISM IN NARROW-BAND SOLIDS BY s-d - HYBRIDIZATION

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Эльк К. E4-5842

Стабилизация ферромагнетизма в модели Хаббарда в результате $s-d$ -гибридизации

Рассмотрена простая модель влияния s-полосы на d-электроны в переходных металлах. На основе этой модели исследуется существование ферромагнитного основного состояния.

Препринт Объединенного института ядерных исследований.
Дубна, 1971

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Stabilization of Ferromagnetism in Narrow-Band Solids by $s-d$ Hybridization

A simple model is considered, describing the influence of the s band on the d electrons in transition metals. Possibilities for a ferromagnetic ground state are obtained.

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For the description of the small d-bands in transition metals and their compounds the Hubbard model [1]

$$H = \sum_{ij\sigma} \Delta_{ij} d^{+}_{i\sigma} d_{j\sigma} + U \sum_{i} n_{i-\sigma} n_{i\sigma}, \quad n_{i\sigma} = d^{+}_{i\sigma} d_{i\sigma} \tag{1}$$

is applied with good results in many cases. In (1) are used creation operators $d^{+}_{i\sigma}$ for electrons with spin σ in a Wannier state of the i-th atom, Δ_{ij} is the kinetic energy and U the repulsive interaction between electrons on the same atom. We choose $\Delta_{ii} = 0$. With the simple decoupling procedure [1]

$$\Delta_{ij} n_{i-\sigma} d_{j\sigma} \approx \langle n_{i-\sigma} \rangle \Delta_{ij} d_{j\sigma} \qquad \text{for} \quad i \neq j \tag{2}$$

we get an one-particle Green's function, possessing singularities at

$$\omega = \Delta(\vec{k})(1 - \langle n_{i-\sigma} \rangle), \quad \Delta(\vec{k}) = \sum \Delta \quad e^{-i\vec{k}\vec{R}_{i}} \tag{3}$$

in the strong correlated limit ($U \to \infty$). Here the presence of the $-\sigma$ spins effectively narrows the σ spin band, but does not change the center of gravity of the band. Therefore in this approximation the Hamiltonian (1) gives only a paramagnetic state at $T = 0$ [2,3], but many of these narrow-band solids really have a ferro - or antiferromagnetic ground state. Therefore several authors tried other approximations to get ferromagnetic states /2,4/. Especially the decoupling procedure of Roth /4/ yields a band shift, depending on $<n_{l-\sigma}>$, which can result in ferromagnetism in special cases.

Whereas Roth /4/ obtains the band shift only by a special approximation, which is not at all exact /5/ , the $s-d$ hybridization gives a real shift. Therefore we consider the influence of the empty s-band, neglected usually. The Hamiltonian is

$$\tilde{H} = H + \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \frac{1}{\sqrt{N}} \sum_{lk\sigma} (a_k e^{-ikR_l} c^+_{k\sigma} d_{l\sigma} + h.c.), \qquad (4)$$

with H from (1) and the creation operator $c^+_{k\sigma}$ for electrons with spin σ and energy ϵ_k in the s-band. Analogous two-band models are also considered in other papers /2,6/, but either both bands are assumed to be small and energetically clear distinct /2/ or the hopping term Δ_{ll} , important for d-bands, is neglected /6/. The Hamiltonian (4) is also considered by Kishore and Joshi /7/, using mainly the Hartree-Fock approximation. A Hamiltonian of the form (4) with a wide s-band may be important for several compounds of transition metals, in which a clear dictinction between s- and d-band is impossible. $\tilde{H}$ can be solved with the approximation

$$[\tilde{H}, n_{l-\sigma} d_{l\sigma}] \approx -U n_{l-\sigma} d_{l\sigma} - <n_{l-\sigma}> \sum_{l} \Delta_{ll} d_{l\sigma} - <n_{l-\sigma}> \sum_{k} e^{ikR_l} a^*_k c_{k\sigma}, \qquad (5)$$

analogously to (2). Then a set of 4 Green's functions follows, resulting in a Green's function of the d-electrons

$$G^{-1}_{\sigma}(k, \omega) = F_{\sigma}(\omega) - \Delta(k) - |a_k|^2 / (\omega - \epsilon_k). \qquad (6)$$

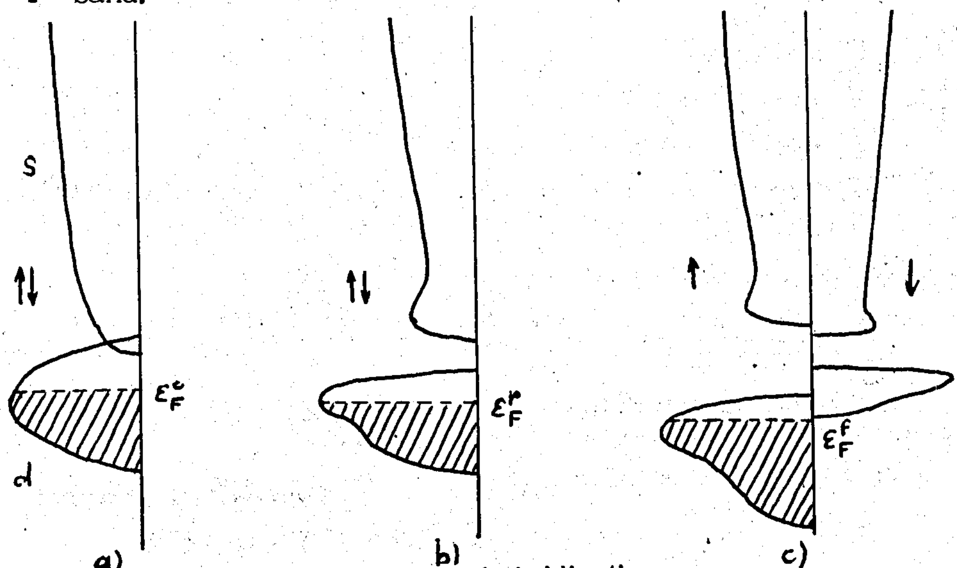
Comparing with the simple Hubbard model /1/ here only the additional term $|a_k|^2/(\omega-\epsilon_k)$ appears. $F_\sigma(\omega)$ is the well-known function

$$F_\sigma^{-1}(\omega) = \frac{1-n_{-\sigma}}{\omega} + \frac{n_{-\sigma}}{\omega - U}, \qquad n_\sigma = \langle n_{l\sigma} \rangle . \tag{7}$$

In the strong correlated limit the singularities of $G_\sigma(k,\omega)$ lie at

$$\omega = \Delta(k)(1-n_{-\sigma}) + \frac{|a_k|^2(1-n_{-\sigma})}{(\omega-\epsilon_k)}, \tag{8}$$

Additionally to (3) we get from (8) not only a narrowing of the d-band, but also a shift down and a change of the form of the d-band, depending on the position of the empty s-band and on the hybridization a_k. This change of the form gives an effective support of the d-band shift and is especially important by an overlapping of s- and d-band These effects are illustrated in the figure for the case of a small overlapping and an empty s-band.



The effect of the $s-d$ hybridization.
a) Band positions without hybridization; b) Bandsplitting , paramagnetic case; c) Shift by different occupation of up- and down-spin band.

By the complex effect of narrowing, shift and change of form it is possible to get a ferromagnetic ground-state, if the density of particles $n = n_\uparrow + n_\downarrow$ overcomes a critical value $n \geq n_1$, analogously to Roth /4/. The band shift has the most drastical effect at $n = 1$, but, generally, saturated ferromagnetism appears at $n_2 \leq n < 1$. However, n_1 and n_2 are strongly dependent on the form and position of the s-band and on the hybridization a_k, so that only crude estimations are possible.

At all events we get the fact, that the empty s-band in consequence of the "repulsion" of the d-band may result in ferromagnetic solutions in narrow band solids. On the other hand neglecting of the s-band can give incorrect solutions.

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