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SPIN SUSCEPTIBILITY IN A NARROW DEGENERATE BAND (*)

F. BROUERS
Laboratoire de Physique des Solides (**) , Université Paris-Sud, 91405 Orsay, France

and

F. DUCASTELLE
Office National d’Etudes et de Recherches Aérospatiales, 92320 Châtillon, France

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Résumé. — On a montré récemment que la susceptibilité statique de spin dans le modèle de
Hubbard calculé en CPA reste finie dans le cas d’une bande non dégénérée quel que soit le nombre
de porteurs, excepté peut-être dans le cas d’une bande à moitié remplie.

Nous montrons que cette propriété est plus générale et serait toujours valable si le modèle de
Hubbard pouvait être résolu exactement dans le cadre de l’approximation de l’analogie d’alliage.
On considère ensuite un modèle avec dégénérescence orbitale et l’on montre que dans ce cas, on
peut obtenir une instabilité de la susceptibilité. On relle cette instabilité à la règle de Hund.

Abstract. — It has been shown that the static spin susceptibility of the Hubbard model of correla-
tions for a narrow band calculated in the CPA remains finite for any simple-band model and the
carrier number, except possibly in the case of a precisely half filled band. We show that this statement
is more general and should be true if the Hubbard model could be solved exactly within the alloy
analogy approximation. We then consider a model with orbital degeneracy and show that in this
case there can be an instability in the susceptibility and we correlate this instability with Hund’s
rule.

1. Introduction. — Efforts have been recently
devoted to incorporate many body effects in the
theory of disordered systems particularly in the
type of alloys (Hasegawa and Kanamori [1],
Levin et al. [2], Brouers et al. [3, 4], Lederer et al. [5],
Abito and Schweitzer [6], Elk [7], Yonezawa [8]).
Electron-electron interactions are to be considered
if one wants to calculate self-consistently the charge
transfers in alloys and the variation of the alloy
constituents potentials with concentration (Gautier
et al. [9], Brouers et al. [10], Van der Rest et al. [11])
and are essential in determining the magnetic pro-
erties of the alloy. The model usually employed
to investigate the itinerant electron magnetism in
narrow band binary alloys is represented by the
Hubbard Hamiltonian

\[ H = \sum_{i,\sigma} E_i n_{i\sigma} + \sum_{i,j,\sigma,\sigma'} W_{ij} C_{i\sigma}^+ C_{j\sigma'} + \sum_{i,\sigma} U_i n_{i\sigma} n_{i-\sigma} \]

(1)

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exhibit any ferromagnetic instability for any single-band model and carriers number except possibly in the case of a precisely half-filled band. The CPA treatment of the Hubbard Hamiltonian neglects the dynamical character of the problem. As they are thought to be unfavorable for ferromagnetism their inclusion would make the possibility of a ferromagnetic instability even less likely. Fukuyama and Ehrenreich have therefore concluded that one could suggest that there exists no such instability in the Hubbard model without orbital degeneracy.

The present paper deals with this problem and indicates how the spin susceptibility of a doubly degenerate tight binding band exhibits a ferromagnetic instability if one treats the degenerate Hubbard Hamiltonian in the framework of the alloy analogy approximation.

In section 2, we show that Fukuyama and Ehrenreich [13] conclusions can be obtained in a more straightforward manner by relating the spin susceptibility to the partial Green’s functions. Using this procedure, one can show that the statement can be made more general since we prove that the exact solution of the alloy analogy approximation of the Hubbard model would yield a susceptibility which would never exhibit any instability if the Fermi level lies in a region of non-zero density of states. In section 3, we take advantage of our more general expression relating the spin susceptibility to the partial densities of states to calculate the susceptibility of a doubly degenerate tight binding band in the CPA and obtain for that quantity an expression which in some cases can be divergent if the Fermi level lies in a nonzero density of states. Finally, a numerical example illustrates this possibility.

2. The spin susceptibility in the alloy analogy. — 2.1 ALLOY ANALOGY. — As was first pointed out by Hubbard (1964) for the ordered case, the motion of electrons with spin \( s = + \sigma \) can be described approximately by the following alloy Hamiltonian

\[
H_s = W_s + H_s^{\sigma - \sigma} = \sum_{ij} W_{ij} C_{i\sigma} C_{j\sigma} + \sum_i \varepsilon_{i\sigma} C_{i\sigma}^+ C_{i\sigma}
\]

where \( \varepsilon_{i\sigma} \) is equal to \( \varepsilon^0 \equiv 0 \) or \( \varepsilon^0 \equiv U \), depending on whether an electron with spin \( -\sigma \) is at site \( i \) or not. At a fixed instant in time the electrons with opposite spins are regarded as occupying given positions on randomly distributed lattice sites. One neglects the dynamical effects of opposite spin electrons and one replaces the time average which arises because of the continuous rearrangement of spin by a configuration average as in the alloy problem. Hamiltonian eq. (2) can therefore be viewed as describing two independent binary alloys : \( A_{-n_{-\sigma}} B_{n_{-\sigma}} \). Here \( n_{+\sigma} \) is the average number of electrons per site with spin \( +\sigma \) :
where \( \mu_B \) is the Bohr magneton and \( g_\sigma(E_F) \) the density of states at Fermi level of \( \sigma \) spin electrons:
\[
g_\sigma(E_F) = -\frac{1}{\pi N} \operatorname{Im} \operatorname{Tr} \langle G_\sigma(E_F + i\epsilon) \rangle. \quad (12)
\]

The susceptibility diverges if \( \delta n_\sigma / \delta n_{-\sigma} \) is equal to \(-1\). Fukuyama and Ehrenreich have shown that if that quantity is calculated for a one orbital tight binding band using CPA within the alloy analogy approximation, this condition is never fulfilled. The susceptibility is always positive and finite; therefore, the system can never be ferromagnetic.

In order to obtain this result in a more direct and more natural way, it is convenient to derive a compact expression for \( n_\sigma \) and then take its derivative with respect to the concentration \( n_{-\sigma} \). The formula for \( n_\sigma \) we shall use in the following subsection has been established by one of us in the context of a discussion of the general properties of CPA and extensions (Ducastelle [15]). We refer to that forthcoming paper for a detailed discussion of its application in the theory of alloys.

2.3 An expression for \( n_{-\sigma} \). Its application to the spin susceptibility. — If \( \langle G_\sigma(E) \rangle \) is the exact alloy average Green’s function, one can write
\[
\langle \operatorname{Tr} \frac{dG}{dE} G^{-1} \rangle = -\operatorname{Tr} \langle G \rangle = \frac{d}{dE} \langle \operatorname{Tr} \log G \rangle
\]
and therefore substituting in eq. (4)
\[
n_{+,\sigma} = \frac{1}{\pi N} \operatorname{Im} \operatorname{Tr} \langle \log G_\sigma(E_F) \rangle. \quad (14)
\]

In the CPA, one can write
\[
\frac{d}{dE} \langle \operatorname{Tr} \log G \rangle = -\operatorname{Tr} \langle G \rangle \left( 1 - \frac{d\Sigma}{dE} \right) \quad (15)
\]
where \( \Sigma \) is the single-site CPA self-energy (Velicky et al. [16]) and
\[
X \equiv \operatorname{Tr} \int_{-\infty}^{E_F} \langle G(E) \rangle dE = -\operatorname{Tr} \log \langle G(E_F) \rangle + \int_{-\infty}^{E_F} F \frac{d\Sigma}{dE} dE \quad (16)
\]
where \( F = \langle G_{00} \rangle \) is the CPA average site-diagonal Green’s function. If we make use of the relation
\[
\frac{d}{dE} \langle \log [1 - (\epsilon - \Sigma) F] \rangle = -\langle t \rangle \frac{dF}{dE} + F \frac{d\Sigma}{dE} (1 + F) = F \frac{d\Sigma}{dE} \quad (17)
\]
where
\[
\langle t \rangle_{\text{CPA}} = \left\langle \frac{\epsilon - \Sigma}{1 - (\epsilon - \Sigma) F} \right\rangle = 0 \quad (18)
\]
one obtains the final result:
\[
n_{+,\sigma}^{\text{CPA}} = -\frac{1}{\pi N} \operatorname{Im} X_{+,\sigma}^{\text{CPA}} \quad (19)
\]
and
\[
X_{+,\sigma}^{\text{CPA}} = -\operatorname{Tr} \log \langle G_\sigma(E_F) \rangle + N \langle \log [1 - (\epsilon - \Sigma) F_\sigma(E_F)] \rangle \quad (20)
\]
which is to be compared with the exact result eq. (14).

There is no ambiguity in the determination of the log in the complex plane since one can write:
\[
\langle \log [1 - (\epsilon - \Sigma) F] \rangle = -\left\langle \frac{F}{1 - (\epsilon - \Sigma) F} \right\rangle + \log F. \quad (21)
\]

The imaginary part of \( F \) and of the conditional average Green’s function \( F [1 - (\epsilon - \Sigma) F]^{-1} \) are always negative (Ducastelle [16]) and the argument of the log are always comprised between 0 and \( -\pi \).

The generalization of eq. (20) to molecular CPA (Tsukada [18], Ducastelle [17, 19] is straightforward and discussed in Appendix A).

In order to obtain the spin susceptibility we need the derivative of \( X_{-,\sigma} \) with respect to concentration \( n_{-\sigma} \). Quite generally and supposing that the average could be calculated exactly, the derivative of any operator \( \hat{O} \) of an alloy \( A_1 - c B_c \) with respect to \( c \) concentration is given by
\[
\frac{d\langle \hat{O} \rangle}{dc} = \sum_\sigma \langle \hat{O}_{a-B} \rangle - \langle \hat{O}_{a-A} \rangle \quad (22)
\]
where \( \langle \hat{O}_{a-B(A)} \rangle \) is the conditional average when site \( n \) is occupied by an atom B. One has therefore:
\[
-\frac{dX}{dc} = \sum_\sigma \operatorname{Tr} \left\langle \log \frac{G_{a-B}}{G_{a-A}} \right\rangle. \quad (23)
\]

The two partial Green’s functions are related by:
\[
G_{a-B} = G_{a-A} + G_{a-B}(\epsilon_B - \epsilon_A) |n \rangle \langle n | G_{a-B} \quad (24)
\]
which allows us to write:
\[
-\frac{dX}{dc} = \sum_\sigma \operatorname{Tr} \left\langle \log (1 + \delta |n \rangle \langle n | G_{a-B}) \right\rangle. \quad (25)
\]

Or since
\[
\operatorname{Tr} \langle \log (1 + \delta |n \rangle \langle n | G_{a-B}) \rangle = \operatorname{Tr} \langle \log (1 + \delta \langle n | G_{a-B} | n \rangle) \rangle \quad (26)
\]
\[
-\frac{dX}{dc} = N \log (1 + \delta \langle n | G_{a-B} | n \rangle). \quad (27)
\]
For the Hubbard model, $\varepsilon_A = 0$, $\varepsilon_B = U$ and $c = n_{-\sigma}$, we have therefore
\[
\frac{dn_{\sigma}}{dn_{-\sigma}} = -\frac{1}{\pi N} \text{Im} \frac{dX_{\sigma}}{dn_{-\sigma}} = \frac{1}{\pi} \text{Im} \langle \log (1 + U \langle n \mid G_{n,n}^{\sigma} \mid n \rangle) \rangle \tag{28}
\]
where $G_{n,n}^{\sigma} = \langle \sigma \rangle$ is the partial Green's function of a $\sigma$ electron on site $n$ occupied by an electron of spin $-\sigma$.

As the imaginary part of this quantity is always negative inside the band, it is straightforward to show that if the density of states is non zero one always has
\[
-1 < \frac{dn_{\sigma}}{dn_{-\sigma}} < 0 \tag{29}
\]
and therefore
\[
\chi = \frac{2 \mu_B^2 g_{\sigma}(E_F)}{1 + \frac{dn_{\sigma}}{dn_{-\sigma}}} \tag{30}
\]
is never divergent inside the band. The statement is more general than the one given by Fukuyama and Ehrenreich since we did not use any specific approximation for the average Green's function.

One can show and this is an interesting result of the present paper that CPA yields a final expression for $dn_{\sigma}/dn_{-\sigma}$ which is quite similar to eq. (28) if the average is the alloys CPA eq. (20). The derivation with respect to $c$ gives
\[
\frac{dX}{dc} = - \text{Tr} \langle G \rangle \frac{d\Sigma}{dc} + N \langle t \rangle \frac{dF}{dc} - \frac{N}{2} \frac{d}{dc} \langle \log [1 - (\varepsilon - \Sigma) F] \rangle \tag{31}
\]
and since $\langle t \rangle_{\text{CPA}} = 0$ (eq. (18)) one has
\[
\frac{dn}{dc} = -\frac{1}{\pi N} \text{Im} \frac{dX}{dc} = \frac{1}{\pi} \text{Im} \frac{\partial}{dc} \langle \log [1 - (\varepsilon - \Sigma) F] \rangle \tag{32}
\]
and finally introducing the site diagonal CPA partial Green's function
\[
F = \frac{1}{1 - (\varepsilon_{A(B)} - \Sigma)} F = F_{A(B)} \tag{33}
\]
\[
\frac{dn}{dc} = \frac{1}{\pi} \text{Im} \log (1 + \delta F_{\alpha}) = -\frac{1}{\pi} \text{Im} \log (1 - \delta F_{\alpha}) \tag{34}
\]
In the Hubbard Hamiltonian alloy analogy approximation, we can write eq. (34) as
\[
\frac{dn_{\sigma}}{dn_{-\sigma}} = \frac{1}{\pi} \text{Im} \log (1 + UF_{n,n}^{\sigma} \langle \sigma \rangle) \tag{35}
\]
For the same reasons as in the exact expression (28), one has $-1 < dn_{\sigma}/dn_{-\sigma} < 0$ and the static susceptibility does not diverge. In appendix A, we show how these expressions can be generalized to the molecular CPA. In appendix B, we prove that CPA eq. (35) approximate expression of the more general eq. (28) is equivalent to the Fukuyama and Ehrenreich result.

In the next section, we generalize the alloy analogy approximation to a two orbital Hubbard Hamiltonian and derive a static expression of the susceptibility generalizing the procedure we have discussed in this section.

3. Orbital degeneracy. — 3.1 SPIN SUSCEPTIBILITY.

Starting from the general expression given by Hubbard [14] (1964), one can write the electron-electron interaction contribution to the two-orbital system $H_{v'v} = \frac{1}{2} \sum_{i,s} v_{i,s} n_{i,s} - U_{i,s} n_{i,s} n_{i,-s} + \sum_{i,s} (U_{i,s} - J) n_{i,s} n_{i,-s}$
\[
- J \sum_{i,s} (C_{i,s}^{+} C_{i,-s} C_{i,s}^{+} C_{i,-s}) + C.C. \tag{36}
\]
v and $v'$ are one of the two orbitals $\alpha, \beta$, $U_{\alpha\alpha}$ and $U_{\beta\beta}$ are the two intraband Coulomb interaction, $U_{\alpha\beta}$ is the interband Coulomb interaction and $J$, the exchange interaction. One can find a detailed discussion of the properties of this Hamiltonian in the paper of Cyrot and Lyon-Caen [20]. Using the canonical transformation method the authors have discussed the possibility of the occurrence of an orbital order. One of the conclusion of the authors is that ferromagnetism is only possible if the exchange energy $J$ is non zero. A generalization of the alloy analogy approximation to the two orbital Hamiltonian is only possible if the two last terms are neglected. In this paper, we do not intend to discuss the validity of such an approximation. Our aim is to show that if one neglects them and moreover suppose that $U_{\alpha\alpha} = U_{\beta\beta} = U_{\alpha\beta} = U$, the spin susceptibility can exhibit a ferromagnetic instability and this is in contrast to what is obtained in a one orbital model.

If we keep the two first terms of eq. (36), one can write an alloy analogy approximation of the two orbital Hamiltonian : as a set of four effective Hamiltonians.
\[
H_{v\alpha} = W_{v\alpha} + \sum_{i,s} v_{i,s}^\alpha n_{i,s}^\alpha v = \alpha, \beta \quad s = \pm \sigma \tag{37}
\]
with for example
\[
\varepsilon_{v\alpha} = U(n_{\alpha} - n_{\beta - \alpha}) + (U - J) n_{\beta - \alpha} \tag{38}
\]
for example
\[
n_{v\alpha} = \langle n_{i,s}^\alpha \rangle
\]
is the site average number of \( \nu \) orbital electron with spin \( s \). In writing eq. (37), we assume that one can write \( W = W_0 + W_p \) so that there is no hopping between the two orbitals and that the two orbitals have the same shape.

One needs to calculate the four quantities

\[
\nu_{\alpha} = -\frac{1}{N} \int_{-\infty}^{\infty} G_{\nu \alpha} \, dE \tag{39}
\]
each of which depends on the three others playing the role of concentrations. We consider the paramagnetic case where

\[\nu_{\alpha} = \nu_{\alpha - \sigma} = \nu_{\beta} = \nu_{\beta - \sigma}.\]

The spin susceptibility reads

\[\chi = 2 \mu B \frac{d\nu_\alpha}{dE} \text{ with } \nu_\alpha = \nu_{\alpha - \sigma} + \nu_{\beta} \tag{40}\]

and

\[
\frac{d\nu_{\alpha}}{dE} = \frac{\partial\nu_{\alpha}}{\partial E} + \frac{\partial\nu_{\alpha}}{\partial E_{\sigma - \sigma}} \frac{d\nu_{\sigma - \sigma}}{dE} + \frac{\partial\nu_{\beta}}{\partial E_{\sigma - \sigma}} \frac{d\nu_{\sigma - \sigma}}{dE} + \frac{\partial\nu_{\beta}}{\partial E_{\beta - \sigma}} \frac{d\nu_{\beta - \sigma}}{dE} + \frac{\partial\nu_{\beta}}{\partial E_{\beta - \sigma}} \frac{d\nu_{\beta - \sigma}}{dE}. \tag{41}\]

As the two concentrations \( \nu_{\alpha - \sigma} \) and \( \nu_{\beta - \sigma} \) correspond to the same potential \( U \), we have

\[
\frac{\partial\nu_{\alpha}}{\partial E_{\alpha - \sigma}} = \frac{\partial\nu_{\alpha}}{\partial E_{\beta - \sigma}} = a \tag{42}\]

and

\[
\frac{\partial\nu_{\beta}}{\partial E_{\beta - \sigma}} = b. \tag{43}\]

One has therefore

\[
\frac{d\nu_{\alpha}}{dE} = \frac{\partial\nu_{\alpha}}{\partial E} + a \frac{d\nu_{\sigma - \sigma}}{dE} + b \frac{d\nu_{\beta - \sigma}}{dE} \tag{44}\]

and similarly

\[
\frac{d\nu_{\beta}}{dE} = \frac{\partial\nu_{\beta}}{\partial E} + a \frac{d\nu_{\sigma - \sigma}}{dE} + b \frac{d\nu_{\beta - \sigma}}{dE} \tag{45}\]

and this yields for the susceptibility (40)

\[\chi = 2 \mu B \frac{\partial\nu_{\alpha}}{\partial E} \left[ 1 + 2a - b \right]^{-1}. \tag{46}\]

3.2 Enhancement factor. — We know calculate the enhancement factor \( [1 + 2a - b]^{-1} \) by generalizing the discussion of section 2.3.

Let us consider the Hamiltonian \( H_{\text{net}} \), the alloy analogy approximation consists in averaging over the eight possible spins configurations of table I.

The exact formula (20) can be generalized. One finds

\[
\frac{d\overline{\mathcal{O}}}{d\nu_{\nu}} = \sum_i (\overline{\mathcal{O}}_{\nu_{\nu}} - \overline{\mathcal{O}}_{\nu_{\nu} \text{empty}}) \tag{47}
\]

where \( \overline{\mathcal{O}}_{\nu_{\nu} \text{empty}} \) designates the conditional average, the site \( i \) being occupied by an electron of spin \( s \) on \( \nu \) orbital and the generalization of eq. (28) reads :

\[
\frac{\partial\nu_{\nu}}{\partial E_{\nu'}} = \frac{\partial\nu_{\nu}}{\partial E_{\nu'}}. \tag{48}
\]

In particular

\[
a = \frac{\partial\nu_{\nu}}{\partial E_{\nu}} = \frac{1}{\pi} \text{ Im } \langle 1 + U_{\nu'\nu} \langle i | G_{\nu'\nu} (\text{occ}) | i \rangle \rangle \tag{49}
\]

and

\[
b = \frac{\partial\nu_{\nu}}{\partial E_{\nu}} = \frac{1}{\pi} \text{ Im } \langle 1 + (U_{\nu'\nu} - J) \langle i | G_{\nu'\nu} (\text{occ}) | i \rangle \rangle. \tag{50}
\]

Because of the analytical properties of the Green's functions, one has

\[-1 < a < 0 \quad \text{and} \quad -1 < b < 0 \tag{51}\]

since \( U > 0 \) and \( U - J > 0 \). This leads to the condition for the denominator of the susceptibility eq. (45)

\[(a - b) < 1 + 2a - b < (a - b) + 1. \tag{52}\]

We shall see next section that in some cases \((a - b)\) can be negative yielding an instability of the susceptibility.

4. Numerical illustration. — Using the alloy analogy approximation (eq. (37), (38)) of the two orbital Hubbard Hamiltonian (eq. (36)), we have calculated the density of states and the partial Green's functions.
of the eight-component alloy the potentials and the concentration of which are given in table I. We have used the coherent potential approximation using the self-consistent iterative formula (Brouers et al. [21])

\[
\Sigma(z) = \sigma(z) + \left[ \langle i | \overline{G}(\sigma) | i \rangle \right]^{-1} - \left( \sum_{\lambda=1}^{8} P(\lambda) \langle i | \overline{G}^{(\lambda)}(\sigma) | i \rangle \right)^{-1}, \tag{53}
\]

The summation is taken over the eight alloy-components, the \( P(\lambda) \) are the corresponding concentrations and the \( \overline{G}^{(\lambda)} \), the partial Green's functions. The quantities \( a \) and \( b \) (eq. (49) and (50)) and the denominator of the spin susceptibility \( \chi \) (eq. (45)) are then determined. If \( n_{\alpha \sigma} = n_{\sigma \alpha} = n \) one can, as a result of some cancellations, derive:

\[
1 + 2 a - b = 1 + 2(1 - n)^2 \arctg \frac{U \text{Im} \overline{G}^{(3)}_{\sigma}}{1 + U \text{Re} \overline{G}^{(3)}_{\sigma}} + 2(1 - n) n \arctg \frac{2 U \text{Im} \overline{G}^{(7)}_{\sigma}}{1 + 2 U \text{Re} \overline{G}^{(7)}_{\sigma}} + n^2 \arctg \frac{(3 U - J) \text{Im} \overline{G}^{(8)}_{\sigma}}{1 + (3 U - J) \text{Re} \overline{G}^{(8)}_{\sigma}} - (1 - n)^2 \arctg \frac{(U - J) \text{Im} \overline{G}^{(2)}_{\sigma}}{1 - (U - J) \text{Im} \overline{G}^{(2)}_{\sigma}}. \tag{54}
\]

We take for the non-interacting electron density of states, corresponding to \( H_{\text{vs}} = W_{\text{vs}} \) in eq. (37), the semi-elliptic band

\[
g^{0}(\varepsilon) = \begin{cases} 
\frac{2}{\pi} (1 - \varepsilon^2)^{1/2} & \text{for } |\varepsilon| \leq 1 \\
0 & \text{for } |\varepsilon| \geq 1.
\end{cases} \tag{55}
\]

The energies are expressed in units of one-half bandwidth. When \( J = 0 \), \( a = b \) and from eq. (51) the denominator is always positive. The ferromagnetic instability of the susceptibility does not appear for all values of \( J \) and \( U \). For the semi-elliptic density eq. (55) there is no instability for \( J/U < 0.3 \) and \( U < 1.5 \) moreover we have noticed that this instability depends strongly on the form of the chosen density of states. If one starts from a density of states with a peak at the top of the band as the one used by Van der Rest et al. (1975), the instability can appear for \( U = 1 \). Therefore, our numerical results are to be considered merely as a numerical example showing the possibility of ferromagnetic instability when the exchange interaction \( J \neq 0 \). We have taken \( U = 2 \), \( J/U = 0.4 \) and \( n_{\alpha} = n_{\sigma} = \frac{1}{4} \). Figure 1 shows the density of states for this case. The range of the density of states for which the denominator is negative has been shaded. As the Fermi level is located in that region, the paramagnetic state is unstable for that system. We have also considered the case \( n = \frac{1}{2} \) for the same value of \( U \) and \( J \) but in that case the Fermi level which lies in a gap of density of states is outside the instability region. Here (Fig. 1) in the vicinity of the Fermi level, the contribution to the denominator comes entirely from the configurations (2) and (3) of table I. The corresponding angles in eq. (53) are comprised between \( -\pi/2 \) and \( \pi \) and the divergence therefore appears in a region where the states come essentially from the partial density of states \( g^{(1)}_{\text{vs}} \). This condition is fulfilled only if \( U \) and \( J \) are larger than some critical values. In our example, the correspondence between the instability of the susceptibility and the tendency of the spin of the two orbitals to be aligned is in agreement with Hund's rule.

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Appendix A. — Eq. (20) can be generalized to molecular CPA (Tsukada [18], Ducastelle [17], [19]). The number of atoms \( N \) is equal to \( q_{e} N_{e} \), \( q_{e} \) being the number of atoms in a cluster and \( N_{e} \) the number of clusters

\[
X = - \text{Tr} \log \langle G \rangle + \sum_{\text{clusters}} N_{e} \text{Tr} \log [1 - (\varepsilon_{c} - \Sigma_{c}) \overline{G}_{cc}] \tag{A1}
\]

where the trace in the second term of the r.h.s. is taken over the cluster states. Following a discussion analogous to that of section 2.3, one obtains:

\[
\frac{1}{N} \frac{dn}{dc} = - \frac{1}{\pi} \frac{\partial}{\partial \varepsilon} \text{Tr} \log [1 - (\varepsilon_{c} - \Sigma_{c}) \overline{G}_{cc}] \tag{A2}
\]

\[
= \frac{1}{\pi} \sum_{\text{clusters}} \langle \log [1 + \delta \overline{G}_{pp}] \rangle \tag{A3}
\]
where

$$\bar{\psi}^+_{i-B} = \langle i \mid \bar{\psi}_{i-B} \mid 1 - (\epsilon_i - \Sigma_i) \bar{\psi}_{i-B} \rangle e^{-i}$$

and $\epsilon_i = \epsilon_B$.

**Appendix B.** In this appendix, we show how one can obtain Fukuyama and Ehrenreich result for the single-band spin susceptibility. Starting from eq. (32), one has for an alloy within CPA

$$\frac{\partial}{\partial c} \log \left[ 1 - (\epsilon - \Sigma) F \right] = \log \frac{1 - (\epsilon_B - \Sigma) F}{1 - (\epsilon_A - \Sigma) F}$$

(A5)

$$= \log \frac{t_B}{t_A} + \frac{v_B}{v_A} \text{ with } v = \epsilon - \Sigma$$

(A6)

and $t = v[1 - vF]^{-1}$ and since

$$ct_B + (1 - c)t_A = 0, \quad \text{Im} \log \frac{t_A}{t_B} e^{-i} = 0$$

we have seen in section 2.2 that the denominator $1 + (dn_a/dn_{-a})$ is always $> 0$. More generally, we ask the question whether the paramagnetic solution is the only possible uniform solution.

We have

$$n_{n_{-a}} = -\frac{1}{\pi N} \text{Im} \text{Tr} \int_{-\infty}^{\infty} \langle G_{n_{-a}} \rangle \, dE$$

(A11)

$$n_{n_{-a}} + n_{-a} = n = \text{Const.}$$

$G_{n}$ is a function of $-n_{-a}$. Therefore we can write the set of equations

$$n_{n_{-a}} = \varphi(E_F, n_{-a})$$

(A12)

$$n_{-a} = \varphi(E_F, n_{n_{-a}})$$

(A13)

$$n_{n_{-a}} + n_{-a} = n$$

(A14)

Let us suppose that the system of two eq. (A13) and (A14) has been solved. We know $E_F$ and $n_{-a}$ in terms of $n_{n_{-a}}$ and thus the function

$$n_{n_{-a}} = \psi(n_{n_{-a}})$$

(A15)

Let us calculate

$$\frac{d\psi}{dn_{n_{-a}}} = \frac{\partial \varphi}{\partial E_F} \frac{dE_F}{dn_{n_{-a}}} + \frac{\partial \varphi}{\partial n_{-a}} \frac{dn_{-a}}{dn_{n_{-a}}}$$

(A16)

From (A14) and (A13) we have

$$\frac{dn_{-a}}{dn_{n_{-a}}} = -1 = \frac{\partial \varphi}{\partial E_F} \frac{dE_F}{dn_{n_{-a}}} + \frac{\partial \varphi}{\partial n_{-a}}$$

(A17)

which gives

$$\frac{dE_F}{dn_{n_{-a}}} = -\frac{1 + (\partial \varphi_{-a}/\partial n_{-a})}{(\partial \varphi_{-a}/\partial E_F)}.$$  

(A18)

If we now substitute these results in (A16) we obtain

$$\frac{d\psi}{dn_{n_{-a}}} = -\frac{\partial \varphi_{-a}}{\partial E_F} \frac{dE_F}{dn_{n_{-a}}} \left( 1 + \frac{\partial \varphi_{-a}}{\partial n_{-a}} \right) - \frac{\partial \varphi_{-a}}{\partial n_{-a}}.$$  

(A19)

The quantities

$$\frac{\partial \varphi_{-a}}{\partial E_F} = g_{-a}(E_F) \text{ and } \frac{\partial \varphi_{-a}}{\partial n_{-a}} = g_{-a}(E_F)$$

are positive quantities.

We have moreover shown in section 2.3 that

$$0 < 1 + \frac{\partial \varphi_{-a}}{\partial n_{-a}} < 1.$$  

(A20)

The same conditions hold for $\partial \varphi_{-a}/\partial n_{-a}$. Collecting these results, one can see that

$$\frac{d\psi}{dn_{n_{-a}}} < 1.$$  

Consequently, the function $n_{n_{-a}} - \psi(n_{n_{-a}})$ has a positive and continuous derivative (provided $g_{-a}(E_F)$ is non zero) and is equal to zero only once when $n_{n_{-a}} = n_{-a}$. 

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In appendix C, we show that there is one and only one solution, i.e. $n_{n_{-a}} = n_{-a}$.

**Appendix C.** In section 2.2, we have shown that the single-band spin susceptibility in the alloy analogy approximation of the Hubbard Hamiltonian is given by:

$$\chi = 2 \mu_B \frac{dn_{n_{-a}}}{d \Sigma} = \frac{2 \mu_B g(E_F)}{1 + \frac{dn_{n_{-a}}}{dn_{-a}} \bigg|_{E_F = \text{const}}}$$

(A10)
References