Spin susceptibility of the doubly degenerate Hubbard model

J. van der Rest
Institut de Physique, B5, Université de Liège, B-4000 Sart Tilman, Belgium

F. Brouers
Institut für Theoretische Physik, Freie Universität Berlin Arnimalee 3, Berlin 33, Germany

(Received 4 March 1981)

It has been shown that the static spin susceptibility of the Hubbard model for a narrow band calculated in the alloy-analogy approximation remains finite for any single-band model and carrier number, except possibly in the case of half-filled bands. In the same way one does not find any instability if one looks for a possible divergence of the susceptibility for a wave vector corresponding to an antiferromagnetic ordering in a half-filled or nearly-half-filled band. In this paper we consider a model with orbital degeneracy. We calculate the spin susceptibility in the alloy-analogy approximation using self-consistent expressions for the configuration probabilities. We investigate how these quantities vary with the model parameters. In this case also we do not find any ferromagnetic instability. The discrepancy with previous results is discussed.

I. INTRODUCTION

The possibility of ferromagnetic and antiferromagnetic solutions and their stability with respect to the paramagnetic solutions of the Hubbard model used in the discussion of the magnetic and conductivity properties of narrow-band materials has been investigated by many authors.

It is now well established that the Hubbard III approximation[1] does not provide a stable ferromagnetic solution. As was shown by Velicky *et al.*,[2] the Hubbard III solution which includes only the scattering corrections is identical to the coherent-potential approximation (CPA)[3] of the theory of alloys.

Fukujama and Ehrenreich[4] have shown that the static spin susceptibility of the Hubbard model calculated in the CPA remains finite for any single-band model and carrier number except possibly in the case of precisely half-filled split band. Brouers and Ducastelle[5] have shown that this statement is more general and should be true if the Hubbard model could be solved exactly within the alloy-analogy approximation. This statement is therefore true for any extension of the CPA. In a subsequent paper Brouers *et al.*[6] have calculated the response to a periodic external magnetic field of the magnetically disordered phase of the Hubbard model in the alloy-analogy approximation. They looked for a possible divergence of the susceptibility for a wave vector corresponding to an antiferromagnetic ordering. They did not find any instability for a half-filled or nearly-half-filled band.

The case of the doubly degenerate Hubbard model was also considered by Brouers and Ducastelle[5] and the conclusion of that paper was that there can be an instability related to the Hund's rule and that ferromagnetism is possible in that model. That paper was criticized by Lacroix-Lyon-Caen and Cyrot[7] (LLCC) on the ground that the occupation probabilities had not been calculated self-consistently. These two authors considered the solution of the strong-coupling limit and using energy arguments concluded that for a band filling per spin and per orbital ($\bar{n}$) between 0.25 and 0.75 a ferromagnetic instability occurs.

The purpose of the present paper is to reconsider the results of Brouers and Ducastelle[5] taking account of the remarks of LLCC[7] and to calculate the spin susceptibility for any value of the Coulomb and exchange interaction and of the band filling. The conclusion of the present work is that if the configuration probabilities are calculated self-consistently there is no ferromagnetic instability in the doubly degenerate Hubbard model treated within the CPA. The instability found in the previous work[5] was not due to the neglect of the correlations in the probabilities but to an error in the computing program which has been now corrected.

The magnetic state found by LLCC[7] is based on an energy calculation. Their expression gives a lower energy for the ferromagnetic phase in the strong-coupling limit for a band filling between 0.25 and 0.75. We must, however, point out that the criterion for magnetic instability derived from the divergence of the magnetic susceptibility is unambiguous in the framework of the CPA. On the contrary, the definition of the total energy is not unique in the CPA, since CPA is not derived from a variational principle. The definition of the total energy used by LLCC, based on the Hartree-Fock expression of the total energy, is therefore questionable. We have, however, noticed that we find a high enhancement of the mag-

netic susceptibility—but no divergence—in the region where they find a lower energy for the ferromagnetic state.

We are also interested in this article in the configuration probabilities as such. These probabilities had not been self-consistently calculated previously, and we find it worthwhile therefore to study rather thoroughly their dependence upon the parameters of the model.

The outline of the paper is as follows: in a first part (Sec. II) we present the model and study some exact limiting cases; in a second part (Sec. III) we study in detail the configuration probabilities as a function of the band filling ($\bar{n}$) and of the strength of the e-e interactions (U); in a last part (Sec. IV) we study the magnetic susceptibility of the system and we show that it never diverges.

II. The model: exact limiting cases

In the alloy-analogy approximation of the two-orbital Hubbard Hamiltonian, the motion of the electrons with spin $\sigma(=\uparrow,\downarrow)$ on the $m(=1,2)$ orbitals is described by the following Hamiltonian[5]

$$H_m^\sigma = \sum_\alpha \epsilon_{\lambda m}^\sigma |\alpha m\rangle\langle m\alpha| + \sum_\alpha \sum_\beta{}' h |\alpha m\rangle\langle m\beta| \ , \tag{1}$$

where α is the site index, λ describes the electrons configuration on the α site, $\epsilon_{\lambda m}^\sigma$ is the energy level when an electron with spin σ is on the $|\alpha m\rangle$ orbital, and where $\sum_\beta'$ is a sum over the first neighbors of α.

The eight possible values for $\epsilon_{\lambda 1}^\uparrow$ are given in Table I with their corresponding probabilities $P_{\lambda 1}^\uparrow$; similar tables exist for the $1\downarrow$, $2\uparrow$, and $2\downarrow$ electrons. The two orbitals being equivalent, the values of $\epsilon_{\lambda m}^\sigma$ and $P_{\lambda m}^\sigma$ are in fact independent of m; in the paramagnetic state, they are furthermore independent of σ. From now on, we will therefore drop the m and σ indices whenever the context allows it without loss of clarity.

Hamiltonian (1) describes a pure metal but the energy levels are nevertheless varying from site to site; it has therefore to be studied as a disordered system. CPA[3] has therefore been used to study it, but the probabilities P_λ were not computed self-consistently by Brouers and Ducastelle,[5] who replaced the average of the products as given by Table I by the product of the averages. LLCC[7] showed how to go beyond this approximation. The probabilities of the various energy states or configuration probabilities are given explicitly in Appendix A in terms of the correlation functions $\langle n_{m\sigma} n_{m'\sigma'}\rangle$ and $\langle n_{m\sigma} n_{m'\sigma'} n_{m''\sigma''}\rangle$. Once the P_λ are known, the magnetic susceptibility of the system (χ) can be calculated as explained by Brouers and Ducastelle.[5] We give, nevertheless, in Appendix B the explicit formulas for χ firstly because there is a mistake in the last formula of Ref. 5—which gave rise to the mistake in their computer program—and secondly because we consider that the intraorbital Coulomb interaction U differs from the interorbital one U'.

The probabilities and the occupation numbers are easily calculated for the two limiting cases of negligible e-e interactions and of infinitely large e-e interac-

TABLE I. Energy levels $\epsilon_{\lambda 1}^\uparrow$ and configuration probabilities $P_{\lambda 1}^\uparrow$ for a $1\uparrow$ electron. U, U', and J are, respectively, the e-e intraorbital Coulomb interaction, the interorbital Coulomb interaction, and the exchange interaction, and $n_{m\sigma}$ is the number of electrons with spin σ on the m orbital. The probabilities must be computed self-consistently as explained is Appendix A, the brackets indicating that the average of the products has to be taken. Similar tables exist for the $1\downarrow$, $2\uparrow$, and $2\downarrow$ electrons.

Configuration (λ)	Orbitals occupation $1\uparrow$	$1\downarrow$	$2\uparrow$	$2\downarrow$	Energy levels ($\epsilon_{\lambda 1}^\uparrow$)	Probabilities ($P_{\lambda 1}^\uparrow$)
1	x	· · ·	· · ·	· · ·	0	$\langle(1-n_{1\downarrow})(1-n_{2\uparrow})(1-n_{2\downarrow})\rangle$
2	x	· · ·	x	· · ·	$U'-J$	$\langle(1-n_{1\downarrow})n_{2\uparrow}(1-n_{2\downarrow})\rangle$
3	x	· · ·	· · ·	x	U'	$\langle(1-n_{1\downarrow})(1-n_{2\uparrow})n_{2\downarrow}\rangle$
4	x	x	· · ·	· · ·	U	$\langle n_{1\downarrow}(1-n_{2\uparrow})(1-n_{2\downarrow})\rangle$
5	x	· · ·	x	x	$2U'-J$	$\langle(1-n_{1\downarrow})n_{2\uparrow}n_{2\downarrow}\rangle$
6	x	x	x	· · ·	$U+U'-J$	$\langle n_{1\downarrow}n_{2\uparrow}(1-n_{2\downarrow})\rangle$
7	x	x	· · ·	x	$U+U'$	$\langle n_{1\downarrow}(1-n_{2\uparrow})n_{2\downarrow}\rangle$
8	x	x	x	x	$U+2U'-J$	$\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle$

TABLE II. Configuration probabilities P_λ in the $U=0$ and ∞ limits. The probabilities for $\bar{n}>0.5$ are easily obtained from the symmetry relation $P_\lambda(\bar{n})=P_{9-\lambda}(1-\bar{n})$. The $U=\infty$ limit is taken under the conditions $0<J<U'\leq U$.

	$0\leq\bar{n}\leq 0.25$		$\bar{n}=0.25$		$0.25\leq\bar{n}\leq 0.5$		$\bar{n}=0.5$	
λ	$U=0$	$U=\infty$	$U=0$	$U=\infty$	$U=0$	$U=\infty$	$U=0$	$U=\infty$
1	$(1-\bar{n})^3$	$1-3\bar{n}$	0.422	0.25	$(1-\bar{n})^3$	$0.5-\bar{n}$	0.125	0
2	$(1-\bar{n})^2\bar{n}$	$\bar{n}$	0.141	0.25	$(1-\bar{n})^2\bar{n}$	$\bar{n}$	0.125	0.5
3,4	$(1-\bar{n})^2\bar{n}$	$\bar{n}$	0.141	0.25	$(1-\bar{n})^2\bar{n}$	$0.5-\bar{n}$	0.125	0
5,6	$(1-\bar{n})\bar{n}^2$	0	0.047	0	$(1-\bar{n})\bar{n}^2$	0	0.125	0
7	$(1-\bar{n})\bar{n}^2$	0	0.047	0	$(1-\bar{n})\bar{n}^2$	$2\bar{n}-0.5$	0.125	0.5
8	$\bar{n}^3$	0	0.016	0	$\bar{n}^3$	0	0.125	0

tions (Tables II and III). These limits are interesting because they have been extensively used previously and also because one point of this article is to show that the transition between these two limits is not always monotonous. Let us simply point out here that these two limits coincide for nearly empty bands and that they differ most for half-filled bands.

For intermediate values of U, U', and J, the probabilities and occupation numbers depend upon the empty band density of states. We take here the same density of states as Ref. 5, namely,

$$g^0(\epsilon)=\begin{cases}\frac{2}{\pi}(1-\epsilon^2)^{1/2}, & |\epsilon|\leq 1\\ 0, & |\epsilon|>1\end{cases}, \tag{2}$$

and we have checked that our conclusions are independent of this choice. The bandwidth for noninteracting electrons (W) equals 2 according to Eq. (2) which determines, therefore, the range of realistic values of U because W and U are known to be of the same order of magnitude for transition metals.

We have assumed in this article that $U'/U=0.8$ and $J/U=0.2$ in order to simplify the discussion; these values have been chosen because they are of the right order of magnitude and because they avoid any degeneracy of the energy levels. Nothing special happens if these ratios are changed as long as the energy levels stay in the same order as in Table I; for example, if one assumes that $J=(U-U')/2=0.1U$, one would simply decrease $\epsilon_3-\epsilon_2$ and $\epsilon_7-\epsilon_6$ and one would merely have to go to higher values of U for $0.25<\bar{n}<0.75$ before reaching the $U=\infty$ limit for P_2, P_3, P_6, and P_7. On the contrary, assuming $J=0$ implies $\epsilon_2=\epsilon_3$ and $\epsilon_6=\epsilon_7$ and therefore $P_2=P_3$ and $P_6=P_7$ which would change drastically the particular results presented here for $0.25<\bar{n}<0.75$; this is nevertheless expected because magnetism is known to arise from a nonzero exchange interaction and one therefore expects large values for dP_λ/dJ near $J=0$.

TABLE III. Occupation numbers n_λ in the $U=0$ and ∞ limits; they give the number of $1\uparrow$ electrons for each configuration. The question marks indicate that the corresponding states have a vanishingly small probability (see Table II) and fall in a gap of the density of states; the Fermi level can therefore be placed at will below or above these states.

	$0\leq\bar{n}\leq 0.25$		$\bar{n}=0.25$		$0.25\leq\bar{n}\leq 0.5$		$\bar{n}=0.5$	
λ	$U=0$	$U=\infty$	$U=0$	$U=\infty$	$U=0$	$U=\infty$	$U=0$	$U=\infty$
1	$\bar{n}$	$\frac{\bar{n}}{1-3\bar{n}}$	0.25	1	$\bar{n}$	1	0.5	1
2	$\bar{n}$	0	0.25	0	$\bar{n}$	$\frac{2\bar{n}-0.5}{\bar{n}}$	0.5	1
3,4	$\bar{n}$	0	0.25	0	$\bar{n}$	0	0.5	?
5,6	$\bar{n}$	0	0.25	0	$\bar{n}$	0	0.5	?
7	$\bar{n}$	0	0.25	0	$\bar{n}$	0	0.5	0
8	$\bar{n}$	0	0.25	0	$\bar{n}$	0	0.5	0

III. e-e CORRELATIONS: SELF-CONSISTENT RESULTS FOR THE PROBABILITIES

We discuss rather thoroughly in this section the probabilities P_λ because it is the first time that they have been self-consistently calculated from the e-e correlations $\langle n_{m\sigma} n_{m'\sigma'} \rangle$ for any value of the e-e interactions; this section gives, therefore, new information even without reference to the stability of the paramagnetic phase.

We will first stress the dependence of the probabilities upon the average number of electrons per orbital and per spin ($\bar{n}$) and secondly show their dependence upon the strength of the e-e interactions (U). We present then on Fig. 1 the probabilities P_1 to P_4 as a function of $\bar{n}$ and for various values of U. The values of P_5 to P_8 can be deduced immediately from the symmetry of the Hamiltonian

$$P_\lambda(\bar{n}) = P_{9-\lambda}(1-\bar{n}), \quad 5 \leq \lambda \leq 8 \ . \tag{3}$$

Let us review the main conclusions which can be deduced from it. One notices firstly [Fig. 1(a)] that P_1 is a monotonously decreasing function of $\bar{n}$ for all values of U. This is quite easy to understand: the larger the number of electrons in the system, the smaller the probability to encounter an empty state. Secondly, one sees that P_2 [Fig. 1(b)] is an increasing function of $\bar{n}$ up to 0.35 for $U=0$ and up to $\bar{n}=0.5$ for $U=\infty$ and is a decreasing function of $\bar{n}$ for larger values of $\bar{n}$; the fact that the value of $\bar{n}$ for which P_2 is maximum increases with U simply means that the larger the e-e interactions, the larger the number of

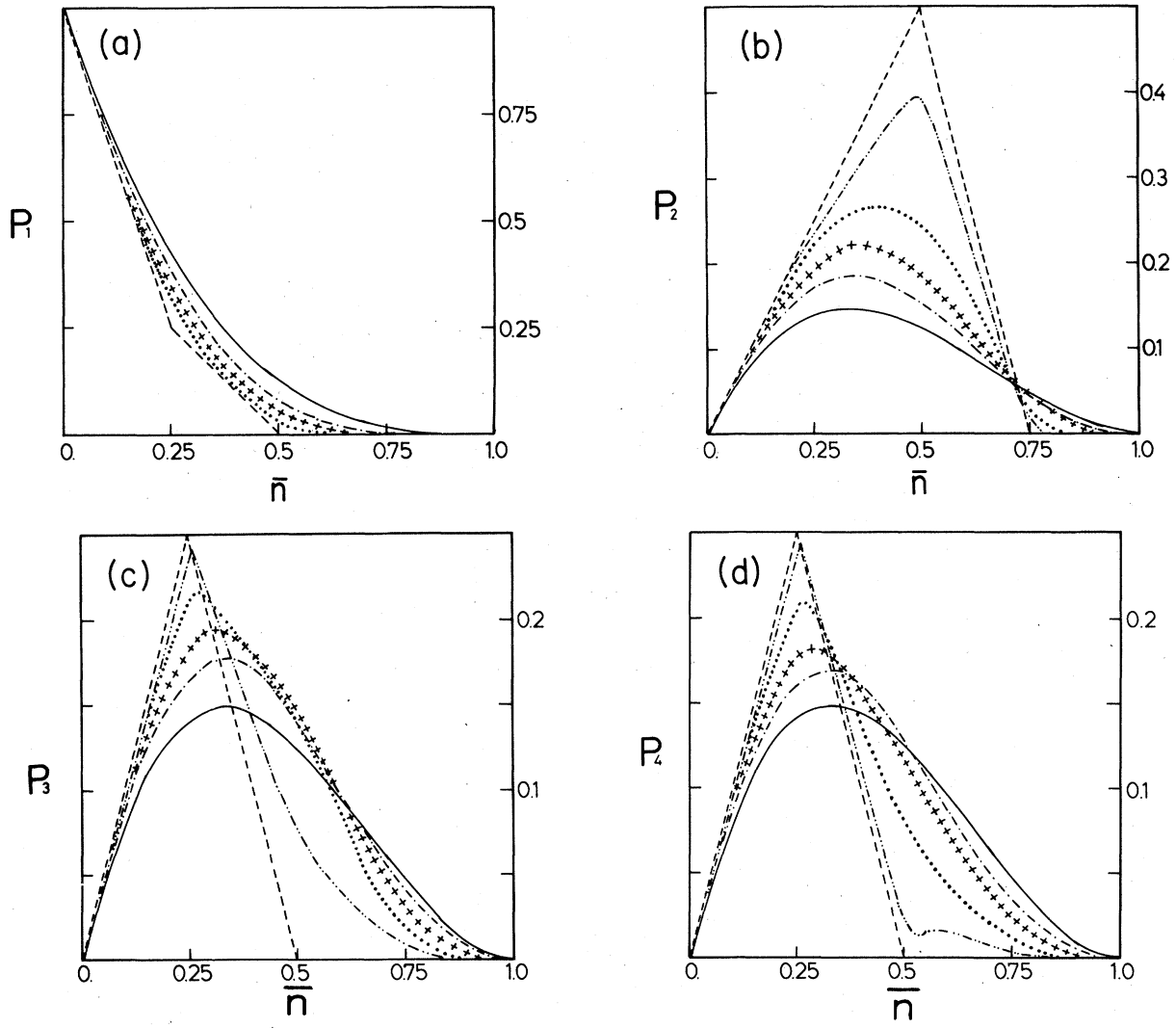

FIG. 1. (a)–(d) Configuration probabilities P_1 to P_4 as a function of $\bar{n}$ and for various values of U: —— $U=0$; —·—· $U=0.25$; ++++ $U=0.5$; ···· $U=1$; —·—· $U=2$; – – – $U=\infty$.

electrons the system can take in before starting to create the states of higher energy ($i=3$ to 8). Thirdly, P_3 and P_4 [Figs. 1(c) and 1(d)] are identical to each other both in the $U=0$ and in the $U=\infty$ limits, but they behave differently for intermediate values of U; they would obviously become identical for all values of U if one sets $U'=U$. They provide, therefore, a good test for the influence of the value of the ratio U'/U on the results and one can see that this influence is relatively small for realistic values of the ratio. Fourthly, one notices for all the probabilities that the difference between the $U=0$ and ∞ limits is maximum for $\bar{n}$ of the order of 0.5. This is in agreement with the well-known fact that the correlations are maximum for a half-filled band and become negligible for nearly empty (or full) bands. Fifthly, let us point out that P_1 is not very sensitive to the value of U while P_2, P_3, and P_4 change tremendously with U for most values of $\bar{n}$.

In order to analyze in more detail this dependence upon U, we have plotted on Fig. 2 the same probabilities P_1 to P_4 as a function of U and for various values of $\bar{n}$.

One notices firstly [Fig. 2(a)] that P_1 is a decreasing function of U for all values of $\bar{n}$. This is easy to understand, because the e-e interactions tend to spread the electrons on all the sites of the crystal by avoiding multiple occupancy on a given site; the probability to encounter an empty site is therefore lowered by the e-e interactions. The situation is less simple for the other probabilities and the situation is summarized in Table II. It appears from it that all

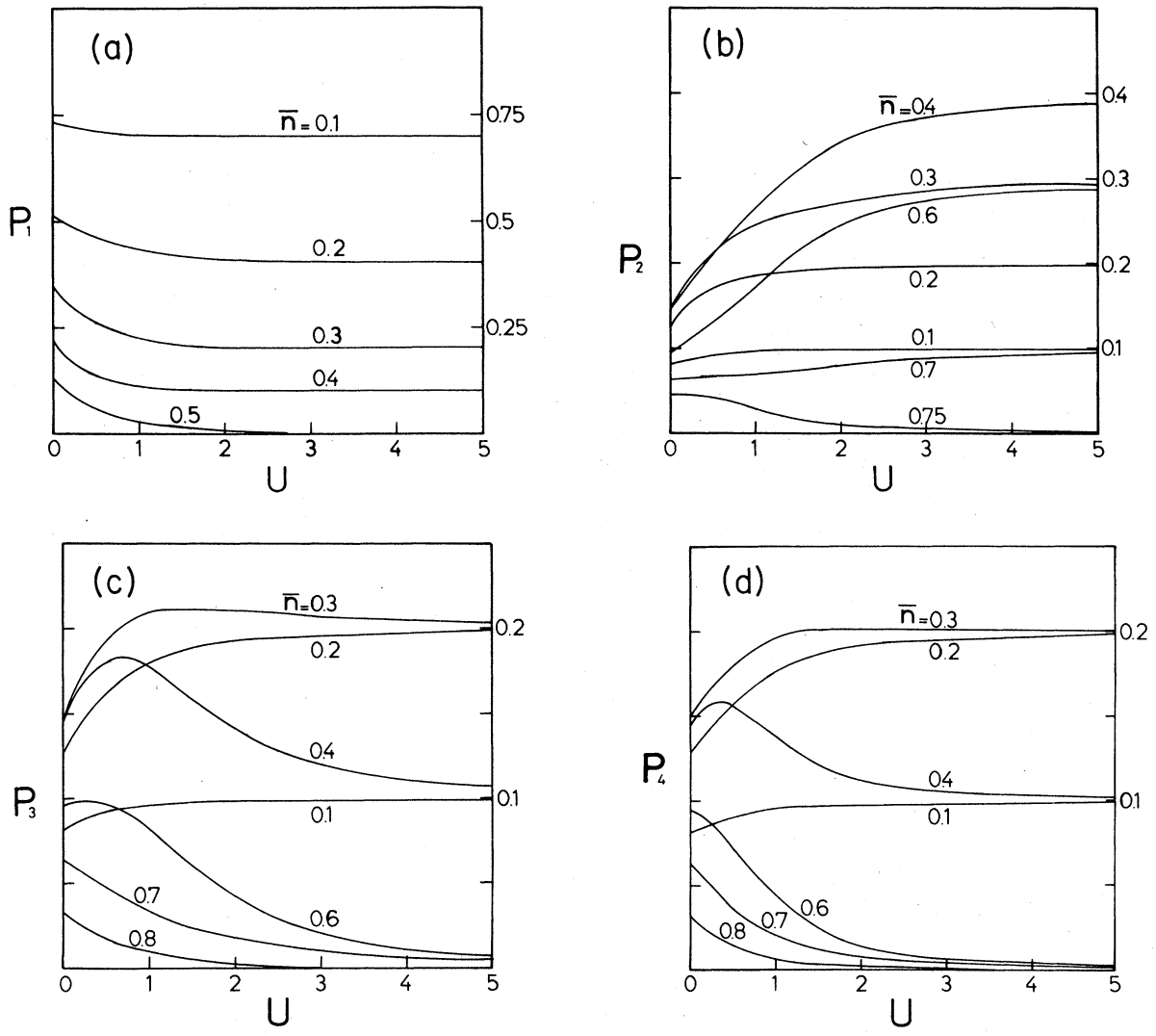

FIG. 2. (a)–(d) Configuration probabilities P_1 to P_4 as a function of U and for various values of $\bar{n}$; the values of $\bar{n}$ are indicated on the figure.

the probabilities have a monotonous dependence upon U only for $0 \leq \bar{n} \leq 0.25$ (and, by symmetry, also for $0.75 \leq \bar{n} \leq 1$). This can be understood as follows: as long as there is less than one electron per atom, the e-e interactions will tend to put at most one electron per site; the probabilities of multiple occupation (P_λ, $\lambda \geq 5$) decrease therefore with U; P_1 decreasing also as explained above, the other probabilities ($\lambda = 2$ to 4) must increase because the sum of all probabilities is a constant. This means that the probability that an electron arriving on a given site encounters another electron on the same site is an increasing function of U, for $0 \leq \bar{n} \leq 0.25$; this might look strange, but in fact even if the number of states corresponding to that situation increases with increasing U, it must be noticed that most of these states are empty and that the number of these occupied states decreases with increasing U.

For $0.25 \leq \bar{n} \leq 0.75$, at least one of the probabilities has a nonmonotonous dependence upon U and the situation can no longer be analyzed by simple qualitative arguments. Let us finally pay special attention in Fig. 2 to the region $0.5 \leq U \leq 2$, i.e., the region for realistic values for transition metals—to see how the probabilities behave in this region with respect to the limiting cases $U = 0$ and ∞.

A quick look shows us immediately the impossibility of interpolating between the $U = 0$ and ∞ limits: for $U = 0.5$, the probabilities can be either very close to the $U = 0$ limit (see P_2 for $\bar{n} = 0.75$ or P_3 for $\bar{n} = 0.6$), or very close to the $U = \infty$ limit (see P_3 for $\bar{n} = 0.3$), or somewhere in between these two limits (see P_2 for $\bar{n} = 0.3$, 0.4, and 0.6), or even not in-between these two limits (see P_3 and P_4 for $\bar{n} = 0.4$). And for $U = 2$, though the probabilities are generally very close to their $U = \infty$ limit, they are sometimes not even half-way between the $U = 0$ and the $U = \infty$ limits (see P_3 for $\bar{n} = 0.4$). One can therefore conclude that for U larger than the bandwidth, the $U = \infty$ limit is a fair approximation but that for realistic values of U (of the order of a half bandwidth) neither the $U = 0$ limit nor the $U = \infty$ limit or an average between these two limits seem fair approximations.

The influence of the e-e interactions on the e-e correlations can also be visualized on Fig. 3 which shows, for fixed values of $\bar{n}$, the evolution of the probabilities as a function of U. One sees very clearly that the correlations are negligible for nearly empty bands and that they become more and more important when the number of electrons increases; as expected, they are maximum for a half-filled band. For $0 \leq \bar{n} \leq 0.25$ there is indeed no major deformation of the curve when one goes from $U = 0$ to ∞; on the contrary for $0.3 \leq \bar{n} \leq 0.5$ two states (states 2 and 7) which are not more probable than the others in the $U = 0$ limit become much more likely than the others in the $U = \infty$ limit. The change is maximum for $\bar{n} = 0.5$ where in the $U = 0$ limit all states arise with equal probability, while in the $U = \infty$ limit only two states exist with nonzero probability. Another striking result is that the e-e interactions diminish in general the probability of occurrence of the states which have either the highest or the lowest probabilities of occurrence without e-e interactions. The e-e interactions tend then to favor the states which have an average probability of occurrence in the absence of e-e interactions. These two effects can reverse the order of the probabilities as occurs for example for P_1 and P_2 on Figs. 3(d) and 3(e): for small U one has $P_1 > P_2$ while $P_2 > P_1$ for a large enough value of U.

IV. MAGNETIC SUSCEPTIBILITY

According to Eq. (B8), the paramagnetic phase becomes unstable whenever the Fermi level (ϵ_F) lies in a region where $D = 1 + a_1 + a_2 - b < 0$. We show in this section that it never happens.

There is nevertheless an important difference between these results and the single-band results: the equivalent of D for a single band is positive for all energies where the density of states is nonzero.[4,5] Ferromagnetism is therefore never possible in such systems. On the contrary, our results show that if D is always positive at the Fermi level for a model with two-fold orbital degeneracy, there are nevertheless regions of nonzero density of states where D is negative.

To make this point clear, we consider, therefore, the whole curve $D(\epsilon)$ and not only its value at the Fermi level $D(\epsilon_F)$ and we look for the values of ϵ where $D(\epsilon) = 0$. Now, in the regions of nonzero density of states the integrated density of states $n(\epsilon) = \int_{-\infty}^{\epsilon} g(\epsilon')\, d\epsilon'$ is a monotonously increasing function of the energy ϵ which means that the energy itself is a well-defined function of the integrated density of states: $\epsilon = \epsilon(n)$. We can therefore consider D as a function of the integrated density of states $D(n)$ and look for the condition $D(\bar{n} \equiv n(\epsilon_F)) < 0$. For a given value of U, the equation $D(n) = 0$ therefore defines a curve in the $(\bar{n}, n)$ plane whose intersection with the $\bar{n} = n$ line gives the domain of $\bar{n}$ where $D(\bar{n}) < 0$; we show here that this domain contains at most the point $\bar{n} = 0.5$ for large enough values of U.

The advantage of this presentation of the results is that the results for all values of U and all values of $\bar{n}$ can be given with a single figure, namely, Fig. 4. Point (0.5, 0.5) being a center of symmetry, we present only the region $0 \leq \bar{n} \leq 0.5$. One sees that the domain enclosed in the $D(n) = 0$ curve vanishes for small values of U and that its extension is nearly independent of U for large enough values of U. For small values of U, the instability appears first around the point (0,1) and develops then along the line

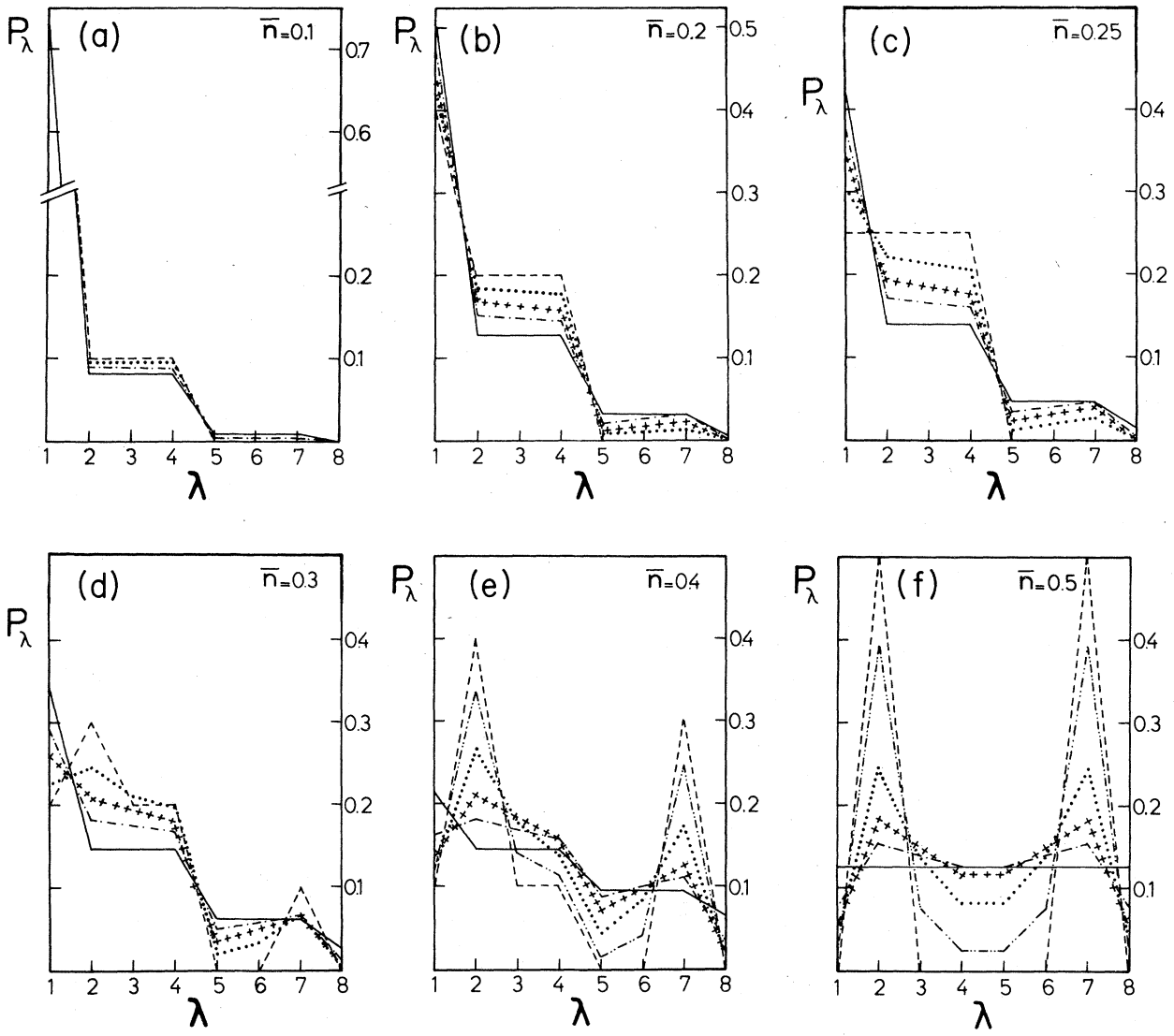

FIG. 3. (a)–(f) Configuration probabilities P_λ as a function of λ and for various values of U; the lines are labeled as on Fig. 1.

$n = 1 - 2\bar{n}$; another instability appears around the point (0.5, 0.5) and develops along the line $n = 1.5 - 2\bar{n}$. The two domains merge together for U around 2.5 along the line $n = 0.5$.

It is well known[4,5] that, for a half-filled band with ϵ_F in a gap of the density of states, the results depend upon the way the limit is taken. One expects therefore, the point (0.5, 0.5) to be on the border between stability and instability of the magnetic phase; this is indeed the case as can be seen on Fig. 4.

On the other hand, when $\bar{n} = 0$ we have $P_1 = 1$ and $P_\lambda = 0$ ($\lambda \neq 1$) (see Table II); this implies $a_1 = a_2 = b = 0$ (see Appendix B) and $D = 1$. There is, therefore, no solution for $D(n) = 0$ corresponding to $\bar{n} = 0$. This is indeed the case.

There is another special point in Fig. 4, namely, the point (0.35, 0.8); we could find no reason why all the curves pass by this point for large enough values of U. We have drawn the same figure for several values of the ratios U'/U and J/U and the position of that point did not change at all.

It can be seen from Fig. 4 that for large values of U there are two regions for $\bar{n}$: (1) when $0 \leq \bar{n} \leq 0.25$, the system is far from instability but it gets closer to instability when $\bar{n}$ increases, and (2) when $0.25 \leq \bar{n} \leq 0.5$, the system is close to instability but it stays at a constant distance from the instability region; it only gets nearer to instability when $\bar{n}$ is very close to 0.5.

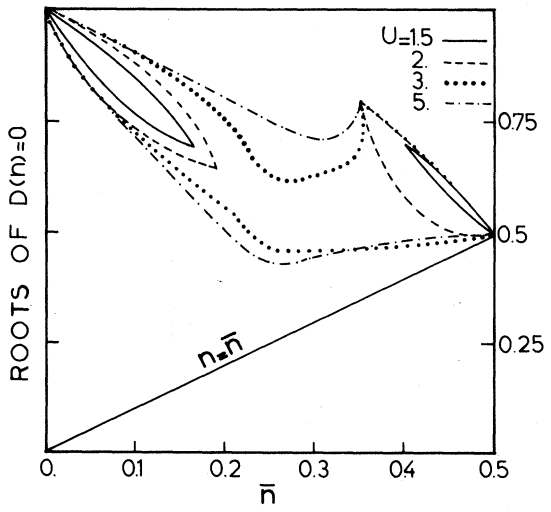

FIG. 4. Roots of $D(n)=0$ as a function of $\bar{n}$ and for various values of U. The straight line corresponds to $n=\bar{n}$. The figure shows that $D(n(\epsilon_F))>0$ for all values of U.

These results are in agreement with the qualitative results of LLCC[7] who found no instability for $0 \leq \bar{n} \leq 0.25$ and an instability for $0.25 \leq \bar{n} \leq 0.5$ for large enough values of U; as explained in the Introduction, their total energy calculations are only approximate and one cannot expect more than a qualitative agreement between their results and ours.

V. CONCLUSIONS

We have shown in this paper that there is no magnetic instability in the alloy analogy of the doubly degenerate Hubbard model when the configuration probabilities are self-consistently calculated with the occupation numbers and the correlation functions. We conclude, therefore, that the paramagnetic phase is stable for all strengths of the e-e interactions and for all values of the band filling. The reason of the discrepancy with LLCC[7] results has been discussed in the Introduction.

While it had been proved for a single-band model that the expression for the susceptibility remains finite within the whole band and not only at the Fermi level, the corresponding expression for a doubly degenerate model diverges sometimes within the band but never at the Fermi level. It would be interesting therefore to see if the corresponding expression will diverge at the Fermi level for higher degeneracies.

We have also discussed the configuration probabilities and we found that they do not vary monotonously between the $U=0$ and ∞ limits. It is therefore impossible to give a general interpolation formula between these limits.

APPENDIX A

We show in this Appendix how to calculate the configuration probabilities P_λ in terms of the occupation numbers n_λ. From Table I one gets immediately

$$P_1=\langle(1-n_{1\downarrow})(1-n_{2\uparrow})(1-n_{2\downarrow})\rangle=1-\langle n_{1\downarrow}\rangle-\langle n_{2\uparrow}\rangle-\langle n_{2\downarrow}\rangle+\langle n_{1\downarrow}n_{2\uparrow}\rangle+\langle n_{1\downarrow}n_{2\downarrow}\rangle+\langle n_{2\uparrow}n_{2\downarrow}\rangle-\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle \ ,$$

$$P_2=\langle(1-n_{1\downarrow})n_{2\uparrow}(1-n_{2\downarrow})\rangle=\langle n_{2\uparrow}\rangle-\langle n_{1\downarrow}n_{2\uparrow}\rangle-\langle n_{2\uparrow}n_{2\downarrow}\rangle+\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle \ ,$$

$$P_3=\langle n_{2\downarrow}\rangle-\langle n_{1\downarrow}n_{2\downarrow}\rangle-\langle n_{2\uparrow}n_{2\downarrow}\rangle+\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle \ ,$$

$$P_4=\langle n_{1\downarrow}\rangle-\langle n_{1\downarrow}n_{2\uparrow}\rangle-\langle n_{1\downarrow}n_{2\downarrow}\rangle+\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle \ ,$$

$$P_5=\langle n_{2\uparrow}n_{2\downarrow}\rangle-\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle \ ,$$

$$P_6=\langle n_{1\downarrow}n_{2\uparrow}\rangle-\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle \ ,$$

$$P_7=\langle n_{1\downarrow}n_{2\downarrow}\rangle-\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle \ ,$$

$$P_8=\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle \ .$$

The two orbitals being identical, we have for the paramagnetic state the following equalities

$$\langle n_{1\downarrow}\rangle=\langle n_{2\uparrow}\rangle=\langle n_{2\downarrow}\rangle=\bar{n} \ ,$$

$$\langle n_{1\downarrow}n_{2\uparrow}\rangle=\langle n_{1\uparrow}n_{2\downarrow}\rangle \ ,$$

$$\langle n_{1\downarrow}n_{2\downarrow}\rangle=\langle n_{1\uparrow}n_{2\uparrow}\rangle \ ,$$

$$\langle n_{2\uparrow}n_{2\downarrow}\rangle=\langle n_{1\uparrow}n_{1\downarrow}\rangle \ ,$$

where the last three equalities allow the use of Table I for the calculation of all the two electron correlation functions. One has

$$\langle n_{1\uparrow}n_{2\downarrow}\rangle=P_3n_3+P_5n_5+P_7n_7+P_8n_8 \ ,$$

$$\langle n_{1\uparrow}n_{2\uparrow}\rangle=P_2n_2+P_5n_5+P_6n_6+P_8n_8 \ ,$$

$$\langle n_{1\uparrow}n_{1\downarrow}\rangle=P_4n_4+P_6n_6+P_7n_7+P_8n_8 \ .$$

As usual, the three electron correlations are not as easy to write down as the two electron correlations; one has from Table I

$$\langle n_{1\uparrow}n_{2\uparrow}n_{2\downarrow}\rangle = P_5 n_5 + P_8 n_8 \ ,$$

$$\langle n_{1\uparrow}n_{1\downarrow}n_{2\uparrow}\rangle = P_6 n_6 + P_8 n_8 \ ,$$

$$\langle n_{1\uparrow}n_{1\downarrow}n_{2\downarrow}\rangle = P_7 n_7 + P_8 n_8 \ ,$$

and the left-hand sides should be equal by symmetry while the right-hand sides are different except in the $U=0$ limit. We therefore made the standard assumption, namely,

$$\langle n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle = \tfrac{1}{3}\langle n_{1\uparrow}n_{2\uparrow}n_{2\downarrow} + n_{1\uparrow}n_{1\downarrow}n_{2\uparrow} + n_{1\uparrow}n_{1\downarrow}n_{2\downarrow}\rangle \ .$$

APPENDIX B

We calculate in this Appendix the magnetic susceptibility of the system. The reasoning follows the same lines as Ref. 5 but it is slightly more general and it corrects the mistakes of that work.

$$\chi = 2\mu_B \frac{dn_\sigma}{d\mathcal{H}} \ , \tag{B1}$$

with

$$n_\sigma = n_{1\sigma} + n_{2\sigma} \ ,$$

and where $\mathcal{H}$ is an external magnetic field. We have then

$$\frac{dn_{1\sigma}}{d\mathcal{H}} = \frac{\partial n_{1\sigma}}{\partial \mathcal{H}} + \frac{\partial n_{1\sigma}}{\partial n_{1-\sigma}}\frac{dn_{1-\sigma}}{d\mathcal{H}} + \frac{\partial n_{1\sigma}}{\partial n_{2\sigma}}\frac{dn_{2\sigma}}{d\mathcal{H}} + \frac{\partial n_{1\sigma}}{\partial n_{2-\sigma}}\frac{dn_{2-\sigma}}{d\mathcal{H}} \ . \tag{B2}$$

Defining

$$\frac{\partial n_{1\sigma}}{\partial n_{1-\sigma}} = a_1 \ , \tag{B3}$$

$$\frac{\partial n_{1\sigma}}{\partial n_{2-\sigma}} = a_2 \ , \tag{B4}$$

$$\frac{\partial n_{1\sigma}}{\partial n_{2\sigma}} = b \ , \tag{B5}$$

we get

$$\frac{dn_{1\sigma}}{d\mathcal{H}} = \frac{\partial n_{1\sigma}}{\partial \mathcal{H}} + a_1\frac{dn_{1-\sigma}}{d\mathcal{H}} + a_2\frac{dn_{2-\sigma}}{d\mathcal{H}} + b\frac{dn_{2\sigma}}{d\mathcal{H}} \ , \tag{B6}$$

and similarly

$$\frac{dn_{2\sigma}}{d\mathcal{H}} = \frac{\partial n_{2\sigma}}{\partial \mathcal{H}} + a_1\frac{dn_{2-\sigma}}{d\mathcal{H}} + a_2\frac{dn_{1-\sigma}}{d\mathcal{H}} + b\frac{dn_{1\sigma}}{d\mathcal{H}} \ . \tag{B7}$$

Replacing Eqs. (B6) and (B7) into Eq. (B1), one obtains

$$\chi = 2\mu_B \frac{\partial n_\sigma}{\partial \mathcal{H}}(1 + a_1 + a_2 - b)^{-1} \ . \tag{B8}$$

Following the arguments of BD,[5] one gets

$$a_1 = \frac{\partial n_{1\uparrow}}{\partial n_{1\downarrow}} = \frac{1}{\pi}\,\mathrm{Im}[P_4 \ln(1+UG_4) + P_6\ln(1+UG_6) + P_7\ln(1+UG_7) + P_8\ln(1+UG_8)] \ , \tag{B9}$$

$$a_2 = \frac{\partial n_{1\uparrow}}{\partial n_{2\downarrow}} = \frac{1}{\pi}\,\mathrm{Im}[P_3 \ln(1+U'G_3) + P_5\ln(1+U'G_5) + P_7\ln(1+U'G_7) + P_8\ln(1+U'G_8)] \ , \tag{B10}$$

$$b = \frac{\partial n_{1\uparrow}}{\partial n_{2\uparrow}} = \frac{1}{\pi}\,\mathrm{Im}[P_2 \ln(1+(U'-J)G_2) + P_5\ln(1+(U'-J)G_5) + P_6\ln(1+(U'-J)G_6) + P_8\ln(1+(U'-J)G_8)] \ , \tag{B11}$$

where G_λ is the Green's function for the λ configuration and is given by

$$G_\lambda = \frac{\bar{G}}{1-(\epsilon_\lambda - \Sigma)\bar{G}} \ , \tag{B12}$$

where $\bar{G}$ is the Green's function of the effective medium for which the potential on all the sites equals Σ (see Ref. 3 for more details on CPA). It is in the computation of a_1, a_2, and b that a mistake was made in Ref. 5.

[1]J. Hubbard, Proc. R. Soc. London Ser. A 281, 401 (1964).
[2]B. Velicky, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. 175, 747 (1968).
[3]P. Soven, Phys. Rev. 156, 809 (1967); R. Elliott, J. Krumhansl, and P. Leath, Rev. Mod. Phys. 46, 465 (1974).
[4]H. Fukuyama and H. Ehrenreich, Phys. Rev. B 7, 3266 (1973).
[5]F. Brouers and F. Ducastelle, J. Phys. (Paris) 36, 851 (1975).
[6]F. Brouers, F. Ducastelle, and J. Giner, J. Phys. (Paris) 37, 1427 (1976).
[7]C. Lacroix-Lyon-Caen and M. Cyrot, Solid State Commun. 21, 837 (1977).