Frustration and long-range behavior of the exchange interactions in AuFe spin-glass alloys

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We calculate the effective exchange pair interactions between Fe atoms in fcc Au-rich AuFe spin-glass alloys from first principles. The character of magnetic frustrations as well as the asymptotic behavior of the exchange interactions are strongly concentration dependent: the AuFe magnetic system becomes less frustrated as the Fe concentration increases since the antiferromagnetic interactions are stronger reduced than the ferromagnetic ones. It is also found that, as compared to the standard Rudermann-Kittel-Kasuya-Yosida (RKKY) theory, the distance dependence of the exchange interactions strongly varies with the Fe concentration. For example, for 5% of Fe we already find a pronounced exponential damping of the exchange interactions due to disorder, which in turn is in striking contrast to the well-known power-law decay predicted by ordinary RKKY.

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I. INTRODUCTION

After more than three decades of intense research, the basic phenomena related to the spin-glass behavior of magnetic matter have been well established experimentally,[1] resulting in well-defined empirical definitions for spin glasses. These are, e.g., absence of long-range magnetic order and macroscopically long relaxation times below the freezing temperature, the existence of a cusp in the temperature dependence of the susceptibility, etc. A commonly accepted microscopic definition of the spin-glass phenomenon is, however, absent at present despite the fact that the spin-glass problem was formally solved mathematically by Parisi and co-workers in terms of a bond disorder model. In this model magnetic moments on a regular lattice interact via randomly distributed exchange forces and simplified assumptions of the long-range and distance-independent exchange coupling are employed (see Binder and Young[2]). It is still unclear how bond disorder models such as the short-range Edwards-Anderson[3] model or the long-range Kirkpartrick-Sherrington[4] and Gabay-Toulouse[5] models can be related to real spin-glass materials such as, e.g., CuMn or AuFe alloys. In these alloys the magnetic atoms are randomly distributed on the lattice (quenched site disorder) and the exchange interactions depend strongly on the distance between the magnetic sites and much less on the local environment of a given site occupied by a magnetic atom. There are other models which are based on a more realistic picture of site disorder and fixed exchange interactions, which have been in the focus of spin-glass research[2] because they allow one to be more material specific. For example, one can choose a Ruderman-Kittel-Kasuya-Yosida (RKKY) form of the exchange interaction with parameters representing spin glasses such as CuMn and perform Monte Carlo simulations of the corresponding random Heisenberg model.[6] There are quite a few so-called "realistic"[2] approaches to the spin-glass problem which have already been reviewed several times.[1,2,7,8] They all agree on one point, namely, that the essential ingredients of a spin glass are the site (chemical) randomness and the frustration of the magnetic interactions on the underlying lattice.[1] The frustration in metallic spin glasses is the result of either the nearest-neighbor antiferromagnetic (AF) interaction on the geometrically frustrated lattice and/or competitions between distant AF and ferromagnetic interactions. Here we discuss only the frustration of the exchange interactions, which we explicitly understand as the competition between distant ferromagnetic and antiferromagnetic interactions. However, other sources of magnetic frustration connected with inhomogeneities in AuFe alloys cannot be ruled out completely and may eventually be important. While the overall necessity of the long-range interactions for the system to be a spin glass is still under debate, the features of the long-distance behavior of magnetic interactions seems to be relevant for many spin-glass theories.

In the case of metallic spin glasses it is believed that the required competition between antiferromagnetic and ferromagnetic coupling is caused by strong and long-range oscillatory RKKY interactions and as such is commonly used during spin-glass simulations, because of its simple analytical form, particularly in the case of spherical Fermi surfaces.[1] There have been various attempts to estimate the exchange interactions in metallic spin-glass alloys by fitting the experimental results for the magnetic susceptibility to the results of the cluster Heisenberg-type models corresponding to low concentrations of magnetic atoms ($\leqslant 5\%$). The results of such studies[9] suggested that there are significant deviations from RKKY behavior with respect to the first few neighboring sites even for low concentrations of magnetic atoms.[1] On the other hand, *ab initio* calculations of the exchange interactions for the first nine nearest neighbors in the $Cu_{85}Mn_{15}$ spin glass alloy[10] showed that these exchange interactions can be fitted to a RKKY form using an additional exponential damping factor. This conclusion agrees with a general behavior of exchange interactions in random systems.[11]

While detailed knowledge of exchange interactions is relevant for numerical simulations in real spin-glass alloys, questions of general interest concerning the character of magnetic interactions in metallic spin-glass materials have to

be answered, namely, (i) is the asymptotic behavior of the exchange interactions of RKKY character or not, (ii) how is the overall character of interactions changed if one moves from the spin-glass regime towards alloys with higher concentrations of magnetic atoms in which ordered magnetic structures may be stabilized at low temperatures and (iii) what is the cause of the frustration as the alloy composition is varied. These questions become important in the case of alloys with dominating ferromagnetic interactions such as, e.g., AuFe alloys.

In this paper we try to answer some of the above raised questions by performing a systematic first-principles study of pair exchange interactions in AuFe alloys for concentrations in the range of $0-30\,\%$ of Fe. We shall employ the well-known approach[12] which allows one to estimate exchange interactions reliably and efficiently from first principles and which was also adapted to random alloys[13] thus extending the two-impurity result of Blackman and Elliott[14] to the case of concentrated metallic alloys. We have recently implemented this approach in the framework of the tight-binding (TB) linear muffin-tin orbital (LMTO) method[15] and applied successfully to the case of transition metal ferromagnets,[16] $4f$-metal ferromagnets Gd,[17] and bcc Eu (Ref. 18) as well as to diluted magnetic semiconductors.[19,20] Recently, exchange interactions in amorphous Co and Fe were determined using the supercell approach in Ref. 21 while the evaluation of on-site exchange coupling parameters for ternary Invar alloys was reported in Ref. 22.

In the present paper Au-rich AuFe alloys are investigated because of the richness of the phase diagram and the fact that the magnetic frustration in these alloys does not follow merely from the geometrical arguments, as may be the case in AuMn alloys where the nearest-neighbor interaction is antiferromagnetic. In particular, we shall concentrate on those general aspects of the spin-glass problem which are related to magnetic interactions, such as their frustration and their spatial extent.

II. METHOD OF CALCULATION

We have determined the electronic structure of AuFe alloys by employing the first-principles all-electron scalar-relativistic TB-LMTO method in the atomic-sphere approximation by making use of the coherent potential approximation (CPA),[23] which neglects local environment effects but correctly reproduces the concentration trends. The neglect of short-range order effects can be justified from ^{197}Au Mössbauer experiments[24] which suggest that over a wide concentration range the Fe atoms in AuFe alloys are homogeneously distributed. It should be noted that in principle an *ab initio* treatment of short-range effects in AuFe is also possible (see Ref. 25). The charge self-consistency is treated in the framework of the local spin-density approximation using a Vosko-Wilk-Nusair parametrization for the exchange-correlation potential.[26] Details of the method can be found in Ref. 23.

For each Fe concentration we have determined the theoretical equilibrium volume and calculated the corresponding pair exchange interactions. The calculated Fe moments are of the order of $3\mu_B$ and independent of the alloy composition. For example, the magnetic moments for a single (isolated) impurity and for $Au_{0.75}Fe_{0.25}$ are $3.05\mu_B$ and $2.95\mu_B$. The evaluation of exchange interactions as developed in Ref. 12 requires that the magnetic moments are not changed when rotated in spin space. To verify the validity of this assumption, we have also performed calculations in the antiferromagnetic, disordered local moment (DLM) state. The DLM picture is the simplest way of treating the noncollinearity of the magnetic moments by assuming that all moment directions are equally probable and thus result in a zero net magnetization. Under such an assumption the problem can be mapped onto a ternary alloy $Au_{1-x}Fe^{+}_{x/2}Fe^{-}_{x/2}$ with the Fe atoms being collinearly aligned, but with random spin-up (Fe^{+}) and spin-down (Fe^{-}) orientations. This situation can be treated straightforwardly within the framework of the CPA.[23] The corresponding Fe moment for $Au_{0.75}Fe_{0.25}$ in the DLM state is essentially the same as in the ferromagnetic state, namely, $2.97\mu_B$. On the other hand, the magnetic moments induced by Fe atoms on Au sites are negligible (less than $0.01\mu_B$).

We have also verified the robustness of the present results for magnetic moments with respect to charge fluctuations on Fe and Au sites.[27,28] These charge fluctuations can be included approximately into the present formalism by assuming that extra charges at a given random site (Fe or Au) are screened within the first nearest-neighbor shell of atoms. In terms of this approximations an additional term to the potential (local Madelung term[27,28]) has to be taken into account with a corresponding correction appearing in the expression for the total energy. It was found that the effect of charge fluctuations on the pair exchange interactions is rather small causing changes of the order 1–2 %.

The resulting total energies are mapped onto an effective classical Heisenberg Hamiltonian[12,16]

$$H = -\sum_{i \neq j} J_{ij} \mathbf{e}_i \cdot \mathbf{e}_j \,, \tag{1}$$

where $\mathbf{e}_i$ and $\mathbf{e}_j$ are unit vectors at sites i and j, and J_{ij} represents the effective pair exchange interactions between magnetic atoms. The values of spin moments are included in the definition of the J_{ij}'s: positive/negative values correspond to the ferromagnetic/antiferromagnetic coupling. The Heisenberg parameters J_{ij} are obtained using the magnetic force theorem[12,29] by (i) directly evaluating the change of energy associated with a small rotation of the spin-polarization axes in atomic cells i and j and (ii) by using the vertex-cancellation theorem (VCT).[30] We refer to Refs. 13,20 for more details concerning the formalism.

The exchange interactions of the Fe spins in Au-rich AuFe alloys are mediated via a random medium which has to properly describe relevant alloy properties, namely, the concentration dependence and the carrier lifetime due to randomness. All these properties critically influence the alloy Fermi surface. The CPA describes such an effective medium surprisingly well. Local environment effects can, of course, influence the values of exchange interactions, in particular for very specific configurations. A recent study,[31] however, indicated that the CPA is a very reasonable estimate of configu-

rationally averaged interactions which as such are sampled directly or indirectly in experiment. Finally, we wish to mention that electron correlations beyond the local spin-density approximation can also influence exchange interactions in spin-glass alloys such as AuFe and CuMn. Although in principle an approach as proposed in Ref. 32 is feasible, it is beyond the scope of the present paper.

It should be noted that the exchange interactions J_{ij} can be evaluated reliably for distant pairs of magnetic atoms[16–18,20] over the whole concentration range. The asymptotic behavior of the exchange interactions is determined by the system Fermi surface and thus can also be studied analytically. The concept of a Fermi surface in general is, however, ill defined in disordered alloys and can only be used safely in the low-concentration limit. For concentrated alloys this concept is not suitable at all: it can at best provide qualitative arguments. This is the main reason why we present an asymptotic study of distant exchange interactions based on the direct numerical evaluation. It should be noted that an accurate evaluation of these interactions requires careful energy and Brillouin zone integrations; we used several million k points in the Brillouin zone.

III. SPIN-GLASS STATES AND EXCHANGE INTERACTIONS IN AuFe ALLOYS

AuFe and CuMn alloys are perhaps the most studied "canonical"[1] spin glasses. Extensive experimental studies of AuFe alloys lead to a well established magnetic phase diagram as well as to a multitude of empirical data of magnetic properties (see, e.g., Refs. 1 and 33–35, and references therein). At low Fe concentrations ($x \lesssim 0.16$) fcc$-Au_{1-x}Fe_x$ alloys exhibit a paramagnetic to spin-glass transition at a freezing temperatures below 40 K. AuFe alloys are ferromagnetic for concentrations $x > 0.24$. In the intermediate concentration regime ($0.16 < x < 0.24$) an additional transition occurs from the ferromagnetic state below the critical temperature to a low-temperature reentrant spin-glass (RSG) phase. The RSG transition has attracted considerable experimental and theoretical interest during the last three decades. The possibility of a RSG transition was predicted by the random bond model of Gabay and Toulouse[5] for a certain choice of parameters for the Gaussian distributions of bond probabilities. In site-disorder models the existence of such a transition is not yet well understood. An alternative explanation of the RSG transition is based on the picture of the Fe-rich clusters present in AuFe (Refs. 36 and 37) which, however, was questioned by later experimental investigations.[35,38]

In Fig. 1 we present the calculated exchange interactions and their dependence on the Fe concentration for the first ten nearest-neighbor (NN) shells, where 0% of Fe corresponds to the interaction between two isolated Fe impurities in the Au fcc host. The dominant first nearest-neighbor interaction [Fig. 1(a)] is strongly ferromagnetic and $\approx 5-10$ times larger in absolute value than the next few NN interactions [Fig. 1(b)]. From the first six shells only the first NN and the third NN interactions are ferromagnetic for $x < 0.15$ while the remaining interactions are antiferromagnetic. Obviously in

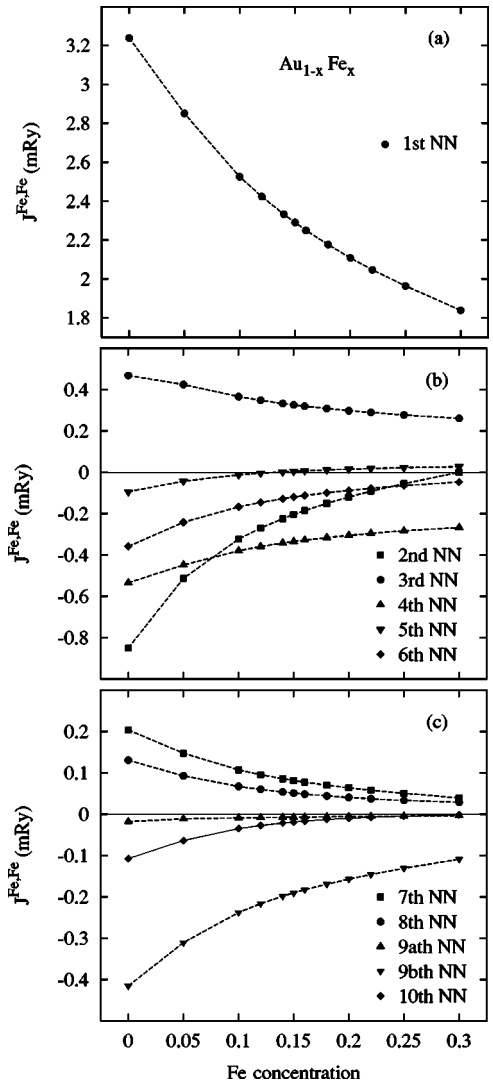

FIG. 1. Dependence of pair exchange interactions in the ferromagnetic $Au_{1-x}Fe_x$ on the concentration x: (a) $J_1^{Fe,Fe}$, (b) $J_n^{Fe,Fe}$, $n=2$–6, and (c) $J_n^{Fe,Fe}$, $n=7$–10. There are two different exchange interactions corresponding to different sites $(1/2,1/2,2)$ and $(0,3/2,3/2)$ with the same intersite distance ($n=9a$ and $n=9b$).

AuFe alloys a strong frustration due to the competition between the distant ferromagnetic and antiferromagnetic interactions occurs. In order to characterize the amount of the frustration in the system, we consider partial sums I_0^n of exchange interactions defined as follows:

$$I_0^{(n)} = \sum_{i=n}^{\infty} N_n J_n^{\mathrm{Fe,Fe}} \approx \sum_{i=n}^{M} N_n J_n^{\mathrm{Fe,Fe}} . \qquad (2)$$

In Eq. (2) N_n is the number of sites in the nth shell, and $J_n^{Fe,Fe}$ are the calculated exchange interactions between the central magnetic atom and an arbitrary magnetic atom in the nth shell. We have verified that above infinite sum is well approximated by about two hundreds of shells ($M=231$ in the present case). It should be noted that this number provides a well converged result for $n \lesssim 100$. Clearly, the quantity $xI_0^{(n)}$, where x is the concentration of Fe atoms in AuFe, has the

meaning of an effective exchange interaction between a given magnetic atom and all other sites occupied by magnetic atoms beyond the $(n-1)$th shell. In this way the quantity $xI_0^{(1)}$ is just the effective coupling constant which appears in a conventional mean-field theory. For all considered concentrations $I_0^{(1)}$, $I_0^{(2)}$, $I_0^{(3)}>0$, while $I_0^{(4)}<0$. This means that the average interaction of a given magnetic atom with all magnetic atoms beyond the third NN shell is effectively antiferromagnetic and this is, in our opinion, one reason for the magnetic frustration in AuFe alloys. It should be noted that this behavior can also be found in other ferromagnetic systems, which at present does not allow to judge with any degree of certainty whether or not these features are a prerequisite for a spin-glass formation. However, the study of $I_0^{(n)}$ can thus be considered as an alternative way of looking at frustration. The results presented in Fig. 1 show two basic features of the concentration dependence of the exchange interactions. First, all interactions decrease with increasing Fe concentration. The only exception is the fifth NN interaction which changes sign from negative to positive at about 15% of Fe. It should be noted that this is just the concentration at which, at higher temperatures, the ferromagnetic phase starts to develop from the RSG phase. Second, there is a significant difference in the decrease of the ferromagnetic and antiferromagnetic interactions with respect to the concentration of Fe atoms. All ferromagnetic interactions (first, third, seventh, and eighth NN) in Fig. 1 decrease slowly with increasing Fe concentration. On the contrary, some of the antiferromagnetic interactions, including the strong second NN interaction, are reduced by more than an order of magnitude for the concentration indicating the onset of ferromagnetism $(x>0.24)$. A similar picture pertains for more distant interactions. Furthermore quite a few of the antiferromagnetic interactions change sign at certain Fe concentrations which is not the case for ferromagnetic interactions. This means, that the total amount of the antiferromagnetic interactions decreases relatively to the total amount of the ferromagnetic interactions as AuFe becomes ferromagnetic. Viewed alternatively, the positive effective exchange interactions $I_0^{(n)}$ decrease with increasing Fe concentrations much slower than the negative ones. It can therefore be concluded that the frustration in AuFe alloys *gradually vanishes* with increasing Fe content and simultaneously the ferromagnetic order starts to develop. In other words, the frustration in the spin-glass concentration range is one order of magnitude larger than in the ferromagnetic range. The qualitative differences between exchange interactions for alloys with different compositions can be seen in more detail in Fig. 2, where we show the calculated exchange interactions for three different AuFe alloys: a spin-glass alloy with low Fe concentration (5% Fe), an alloy close to the border between the spin glass and the RSG regimes (15% Fe), and for a ferromagnetic alloy (30% Fe). It can clearly be seen that (i) the different variation of exchange interactions with the distance, which will be discussed in detail in the next section and (ii) the vanishing of the frustration with increasing Fe content. It should be noted that the explanation of the magnetic phase diagram in AuFe alloys, i.e., the development of the spin-glass phase at low concentrations, cannot be fully understood in the framework of percolation theory because the balance between the ferromagnetic and antiferromagnetic interactions has to be taken into account properly.

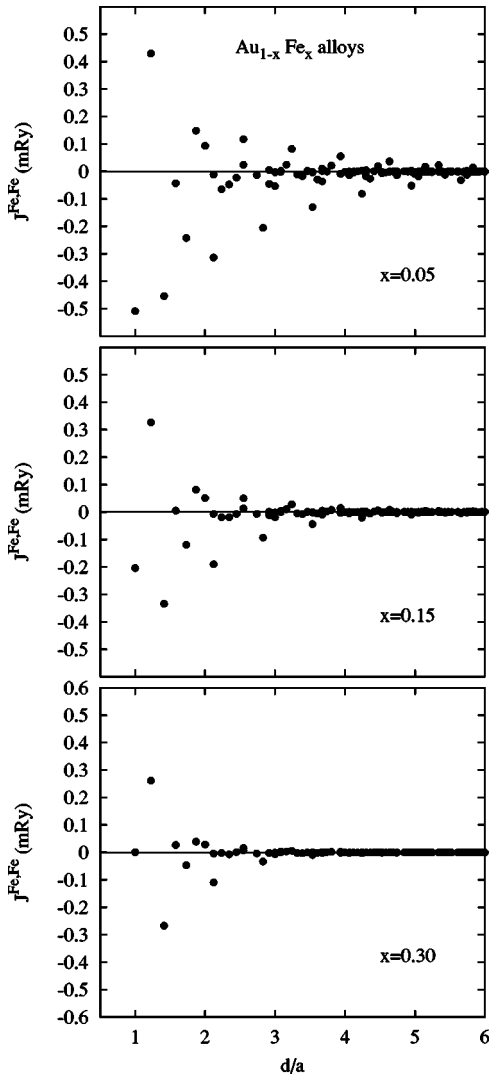

FIG. 2. Dependence of pair exchange interactions on the distance between two Fe atoms (in units of the lattice constant) in the ferromagnetic $Au_{1-x}Fe_x$ for $x=0.05$, $x=0.15$, and $x=0.30$.

IV. ASYMPTOTIC LONG-RANGE BEHAVIOR OF EXCHANGE INTERACTIONS

In this section we want to discuss the long-range behavior of the exchange interactions in more detail and, in particular, try to give an answer to the question of whether or not RKKY interactions are relevant for the description of the asymptotic behavior of the exchange interactions in metallic spin glasses. In Fig. 3 we show the calculated J_{ij} along the nearest-neighbor [110] direction, which gives the dominating contribution to exchange interactions. To view the asymptotic behavior at far distances, the exchange interactions in Fig. 3(a) are multiplied by a RKKY-like factor $(d/a)^3$ (d is the distance between the pair of Fe atoms and a is the lattice constant). In the limit of very low concentra-

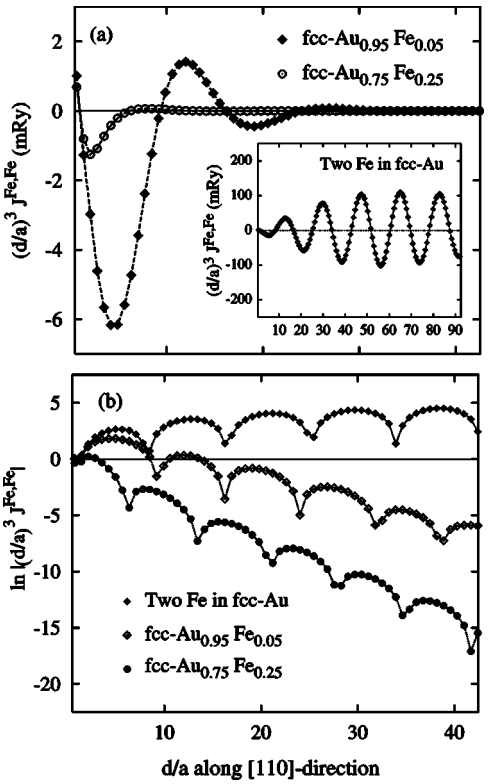

FIG. 3. Dependence of pair exchange interactions on the distance d between two Fe atoms along the nearest-neighbor direction [110] in the ferromagnetic $Au_{1-x}Fe_x$ for three different concentrations x: (a) $(d/a)^3 J^{Fe,Fe}(d)$ and (b) $\ln|(d/a)^3 J^{Fe,Fe}(d)|$.

tions, represented here by two isolated Fe impurities embedded in a Au host (see inset), we indeed recover the asymptotic RKKY behavior for large distances. However, it takes a few oscillations (the preasymptotic regime) before the asymptotic value of the oscillation amplitudes is recovered. This preasymptotic regime occurs due to the strong direct exchange interactions over short distances. Oscillations of exchange interactions as a function of the distance between Fe atoms are strongly damped with increasing Fe content. The character of the damping is changed qualitatively: instead of a power-law form familiar from the RKKY picture we observe an exponential decay. This point is clearly illustrated in Fig. 3(b) where we show the quantity $\ln|(d/a)^3 J^{Fe,Fe}(d)|$ as a function of the distance d. The undamped RKKY oscillations (two-impurity limit) are in sharp contrast to the exponential damping in AuFe alloys which increases with increasing Fe concentration. Because AuFe alloys exhibit spin-glass behavior up to 15% of Fe and the RSG phase exists up to 25% of Fe, it seems that the long-range character of the RKKY interaction assumed in model theories *is not a prerequisite* for the spin-glass behavior. The physical reason of the exponential damping of the exchange interactions in disordered alloys can be easily understood qualitatively within the framework of the theory of disordered alloys. For large distances, which are only relevant when we discuss asymptotic behavior, the magnetic interaction is mediated by the conduction electrons (RKKY-like mechanism) since the other mechanisms related to direct exchange or superexchange are relatively short ranged (here one can also ignore the weak dipole-dipole interaction). For ordered systems, in general, this RKKY-type interaction shows a power law decay of the interaction amplitude as a function of distance. In chemically disordered systems the conduction electrons, which mediate the magnetic interaction, are subject to the scattering by the random potentials. It is well known from basic alloy theory that this random scattering leads to a finite lifetime and thus to an exponential damping of the one-electron states. The fact that the amplitude of the exchange interaction between the Fe moments decreases as the Fe concentration is increased can be understood from the changes of the local Fe density of states. We note that this decreasing interaction amplitude is not due to disorder effects such as the exponential damping described above but is related to the electronic structure changes coming from the shift of the Fermi level due to the fact that Fe has less conduction electrons than Au. It is known from electron scattering models such as the Korringa-Kohn-Rostoker (KKR) formalism that the strength of the interaction between two magnetic impurities in metals depends on the position of the Fermi level with respect to the resonance of the impurity local DOS. More precisely the amplitude of the interaction contains a factor $\sin(\eta_l)$, where η_l is the ordinary phase shift at the Fermi energy as defined in the KKR method. This factor is maximal for the Fermi level being at the impurity band resonance and becomes weaker if E_f moves out of it. In Fig. 4 we show the calculated local Fe density of states at three different Fe concentrations in Au. It can clearly be seen that E_f moves out of the resonance (maximum of the DOS) in the minority spin band as the Fe concentration increases and therefore the amplitude of the exchange interaction becomes weaker. This observation is also correlated to the observed decrease of the magnitude of the Fe moments in the Au host for less diluted alloys. Finally we would like to point out that Au-Fe alloys are not a special case concerning the overall behavior[39] of the exchange interactions in diluted magnetic alloys, and that the results of this paper can be easily understood in the framework of basic alloy theory. However, it is vital to point out that very often important details of the exchange interaction behavior become ignored in spin-glass modeling based on oversimplified models of exchange interactions.

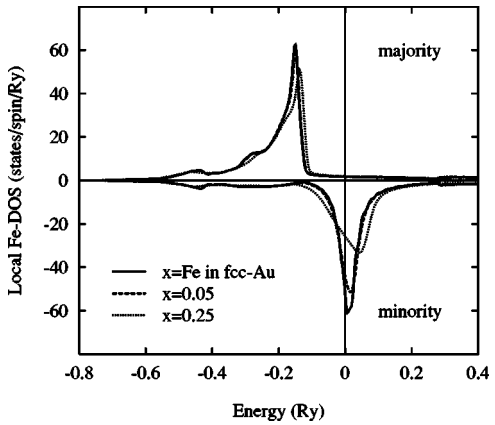

FIG. 4. Local Fe densitiy of states for three concentrations of Fe in $Au_{1-x}Fe_x$.

V. CONCLUSIONS

We find that the frustration of the pair-exchange interactions, defined as the competition between antiferromagnetic and ferromagnetic interactions, vanishes gradually as the Fe concentration increases. The formation of the spin-glass state is not caused solely by percolation effects, but to a large extent is also determined by changes in the electronic structure which change the distribution of the antiferromagnetic and ferromagnetic exchange interactions. Our results suggest that the long-range behavior of magnetic interactions in AuFe spin-glass alloys is much shorter ranged than to be expected from ordinary RKKY interactions. As compared to the case of the very dilute limit, where the asymptotic RKKY behavior was verified numerically (the oscillations are damped by a factor d^{-3}, where d is the distance between magnetic sites), for 5% of Fe impurities there is already a pronounced exponential damping of the calculated exchange interactions, which, however, is a general feature of disordered magnetic alloys. Because the damping increases further with increasing Fe concentrations, the short-range theories[2] seem to be more appropriate for a study of the spin-glass behavior in the AuFe metallic system.

The results of present calculations may be useful for numerical studies of the spin-glass behavior in AuFe alloys by using, e.g., Monte Carlo simulations.[6] A full set of calculated exchange constants is available on request.[40]

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