Accounting for spin fluctuations beyond local spin density approximation in the density functional theory

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We present a method to correct the magnetic properties of itinerant systems in the local-spin-density approximation (LSDA), and we apply it to the ferromagnetic-paramagnetic transition under pressure in a typical itinerant system Ni_3Al. We obtain a scaling of the critical fluctuations as a function of pressure equivalent to the one obtained within Moryia's theory. Moreover, we show that in this material the role of the band structure is crucial in driving the transition. Finally, we calculate the magnetic moment as a function of pressure and find that it gives a scaling of the Curie temperature that is in good agreement with experiment. The method can be easily extended to the antiferromagnetic case and applied, for instance, to the Fe pnictides in order to correct the LSDA magnetic moment.

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Density functional theory (DFT), in its most common implementations [the local-(spin)-density-approximation (L(S)DA) with or without gradient corrections], is in principle the only way to access the ground states of real materials.[1] And indeed the agreement with experiment concerning the ground-state properties, such as crystal and electronic structures, is excellent, especially for itinerant systems wherein local correlations play a minor role. Nevertheless, a well known problem of the LSDA is the overestimation of the tendency to magnetism in itinerant magnets near the quantum critical point (QCP). This problem can be traced to the fact that the LSDA is essentially a mean-field theory, which does not take into account a detrimental effect of near-critical fluctuations on the long-range magnetism. Thus, while the itinerant nature of systems like FeAl,[2] Pd,[3] or the more recent and better known Fe pnictides[4–6] make the LSDA and generalized gradient approximation (GGA) reproduce very well the paramagnetic band structure, whenever a (magnetic) quantum critical point is approached the theory fails miserably. The importance of this problem is demonstrated by the number of papers dealing with the problem of correcting the magnetic moment of Fe pnicitides.[7–12] There, the usual argument is that correlations beyond the mean field suppress the (LSDA) local-ordered moment. It was shown that one can reduce the calculated magnetic moment by using the LDA + U method with a negative Hubbard parameter U,[8] but there is no physical justification for this procedure. Such many-body approaches as the dynamic mean-field theory (DMFT)[9–11] and Gutzwiller approximation[12] were also successfully used; since these methods introduce additional fluctuations into the system, they obviously work in the right direction. However, the concept of substituting long-range critical fluctuations by the on-site ones is rather questionable.[2] Furthermore, the effect of nonlocal fluctuations was recently found to be crucial, also in localized models, whenever the critical behavior is analyzed,[13] and in any event the computational load in these methods is incomparably heavier than in LDA calculations.

For these reasons we propose a different approach which corrects the LSDA within DFT and takes into account the itinerant nature of the system. Our method is easy to implement,[14] carries no additional computational cost, and has a transparent physical justification. The approach we describe in the following is based on the idea that an unknown more accurate DFT is very close to the conventional LSDA-GGA functional, but the energy gain due to spin polarization (the "Stoner interaction,"using the DFT parlance) is reduced by about as much as the Moriya self-consistent renormalization (SCR) theory,[15] successfully used before,[3,16,17] suggests. For this reason we call it reduced Stoner theory (RST). In fact, we show that there is a one to one and well defined connection between our method and the Moriya SCR theory in accounting for the effect of spin fluctuations in itinerant magnets. This allows us to make an *ab initio* prediction of the magnetic moment as a function of pressure for the archetypical Ni_3Al itinerant ferromagnet with the correct scaling of the Curie temperature which until now was impossible. For Ni_3Al, indeed, the effect of spin fluctuations on physical properties both in the magnetic state (magnetic moment and susceptibility) and in the paramagnetic one (dc resistivity) was demonstrated both theoretically[16,18] and experimentally.[19,20]

Applying the RST, we estimate the pressure dependence of the contribution due to spin fluctuations on the magnetic moment of Ni_3Al. Surprisingly, we find that this contribution is almost pressure independent. This means that spin fluctuations only act in shifting the Stoner condition. The rest is done by the band structure. As a consequence, we show that the way in which the spin fluctuations renormalize the effective Stoner interaction is encoded in the band structure itself. This is generally true, but in Ni_3Al it becomes particularly evident due to the perfect scaling of the density of states (DOS) with pressure.

Having established a link between the RST and the SCR theory indeed, we are able to give a reliable estimate of the Stoner parameter in itinerant magnets. Moreover, if one reverses the logic, a comparison between the experiment and the RST results gives an easy and reliable estimate of the spin fluctuations acting in the system. In the following we present the bare LSDA results for Ni_3Al under pressure, and

we interpret them within the so-called extended Stoner theory (EST).[21–23] We explain that the overestimation of both the magnetic moment at zero pressure and the critical pressure P_c comes essentially via the overestimation of the Stoner parameter in the LSDA. After that, we introduce the formalism for correcting the LSDA behavior, and we present the scaling equations used in the RST. In the last part of the paper, we apply these scaling equations to the ferromagnetic-paramagnetic transition of Ni_3Al under pressure.

First, we discuss the bare LDA (and LSDA) results for the magnetic transition in Ni_3Al under pressure. Ni_3Al crystallizes in the ideal cubic Cu_3Au $cP4$ structure. Neutron-scattering measurements indicate only a ferromagnetic instability, and no other instabilities play a role in the system.[24,25] We calculated the equilibrium lattice parameter $a = 3.4825$ Å in the LDA,[26] and we found it to be ≈2% smaller than the experimental one.[27] The calculated magnetic moment at $P = 0$ GPa is $m(0) = 0.68\ \mu_B$ in the LSDA ($0.73\ \mu_B$ in the GGA) in reasonable agreement with previous results.[16] After that, we calculated the magnetic moment as a function of pressure, and as shown in Fig. 1(a), we found that it decreases approximately linearly up to the critical pressure $P_c = 45$ GPa, much larger than the experimental one, which is $P_c^{\text{expt}} \approx 8$ GPa.[20] This behavior can be easily understood within the EST.[21–23] In fact, as shown in Fig. 1(b), the paramagnetic DOS $N(E)$ calculated in the LDA scales almost perfectly with the pressure P as

$$N(E,P) = \frac{N[Z(P)E,0]}{Z(P)} \tag{1}$$

in a wide energy range around the Fermi level, taken as the origin, where $Z(P) = 1 + 0.005P$ with P measured in GPa. This can be related to magnetization via the EST,[21–23] which combines the Stoner criterion with Andersen's force theorem

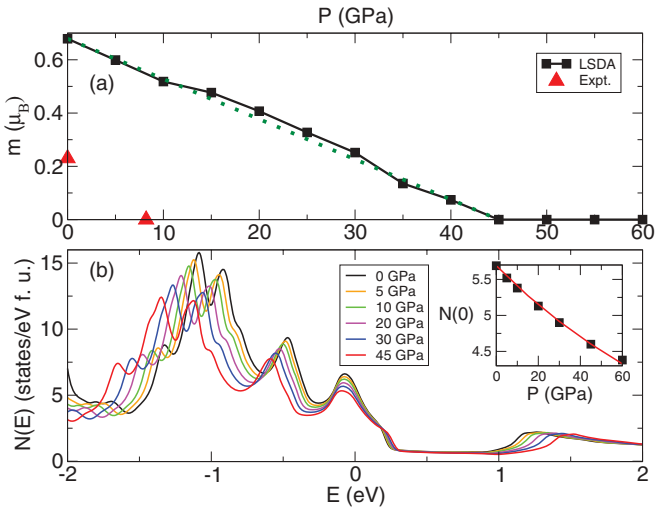

FIG. 1. (Color online) (a) Magnetic moment per unit cell of Ni_3Al calculated with the LSDA (black-dotted line). Both the magnetic moment at zero pressure $m(0)$ and the critical pressure P_c are overestimated with respect to the experimental ones (red triangles).[28] The green dots mark a linear interpolation of the data. (b) Paramagnetic density of states as a function of energy calculated for different pressures with the LDA. Inset: Density of states at the Fermi level calculated as a function of pressure (black squares). The data are fitted with Eq. (1) (red continuous line).

to show that in the lowest order in the magnetic moment m, the total LSDA energy is given in terms of the nonmagnetic DOS per spin:

$$E(m) = \frac{1}{2}\int_0^m \frac{m'dm'}{\tilde{N}(m')} - \frac{1}{4}Im^2, \tag{2}$$

where $\tilde{N}(m')$ is the extended DOS defined in Ref. 21 as the average DOS over an energy interval equal to the exchange splitting at a given m and I is the Stoner parameter. Stationary solutions appear where $\tilde{N}(m) = 1/I$ and $d\tilde{N}(m)/dm < 0$, forming a stable or a metastable (metamagnetic) ferromagnetic state with the magnetic moment m. If $N(E)$ scales according to Eq. (1), so also does $\tilde{N}(m)$. Comparing Eq. (2) with the fixed-spin-moment calculation, we found the Stoner parameter in the LSDA to be $I^{\text{LSDA}} \approx 0.41$ eV, independent of pressure (see the Appendix). In the GGA, the Stoner parameter is 17% larger: $I^{\text{GGA}} = 1.17I^{\text{LSDA}}$. In the following, we will consider only the LSDA results. Around the minimum of $E(m)$, $\tilde{N}(m)$ decreases monotonically. Thus, a reduction of I shifts the Stoner condition $[\tilde{N}(m) = 1/I]$ toward a smaller magnetic moment, bringing the LSDA results in agreement with the experiment. The aim of this paper is to find a way for reducing the LSDA Stoner parameter and getting, in this way, the correct magnetic moment in itinerant systems. In order to gain some understanding of how the standard LSDA needs to be corrected to account for spin fluctuations, let us recall the SCR theory for critical ferromagnets. It starts with the Ginzburg-Landau expansion,

$$E(M) = a_0 + a_2M^2/2 + a_4M^4/4 + a_6M^6/6 + \cdots, \tag{3}$$

where M is the magnetic moment and E is the LSDA energy. It is then assumed that M fluctuates around the average value $\bar{M}$ so that $M = \bar{M} + \delta M$. Assuming that δM follows a Gaussian distribution such that $\langle \delta M^2 \rangle = \xi^2$, we can rewrite Eq. (3) in terms of $\bar{M}$ as

$$E(\bar{M}) = \tilde{a}_0 + \tilde{a}_2\bar{M}^2/2 + \tilde{a}_4\bar{M}^4/4 + \tilde{a}_6\bar{M}^6/6 + \cdots, \tag{4}$$

where the explicit formula for the renormalized coefficients is given in Ref. 3 and the second-order coefficient $\tilde{a}_2 = a_2 + (5/3)a_4\xi^2 + (35/9)a_6\xi^4 + \cdots$. If we restrict our expansion to the second order, this SCR procedure is equivalent to renormalizing spin susceptibility.

The amplitude of the spin fluctuations ξ, in principle, can be obtained by the fluctuation-dissipation theorem (FDT):

$$\xi^2 = \frac{3\hbar}{\Omega}\int d\mathbf{q}\int \frac{d\omega}{\pi}\text{Im}\chi(\mathbf{q},\omega), \tag{5}$$

where Ω is the volume of the unit cell.[3,19] $\chi(\mathbf{q},\omega)$ in this formula is often expressed in terms of the noninteracting (Lindhard) susceptibility, which in turn is expanded to the lowest order in q and ω, $\chi_0(\mathbf{q},\omega) = \chi_0(\mathbf{0},0) - aq^2 + ib\omega/q$.[3] The coefficients a and b can be written down as functions of the Fermi velocity, averaged over the Fermi surface. However, in order to calculate ξ, using this expression one needs to apply a cutoff q_c, which is not a well defined quantity.

Let us now point out that the uniform spin susceptibility in the LSDA can be written in a particularly simple form, namely, $\chi^{-1} = \delta^2E/\delta M^2|_{M=0} = a_2 = \frac{1}{2}[\frac{1}{N_\sigma(E_F)} - I]$ (this can be considered as a rigorous definition of the LSDA Stoner

parameter I), where $N_\sigma(E_F)$ is the paramagnetic DOS per spin. Comparing this expression with the one for $\tilde{a}_2$, we see that the SCR procedure is equivalent to the renormalization of I according to

$$\tilde{I} = I - (10/3)a_4\xi^2, \tag{6}$$

which can also be written as $\tilde{I} = sI$, where $s < 1$ (see also Appendix).

This is a justification of the recipe of using I as an adjustable parameter,[29] often used in critical ferromagnets empirically. In this sense, $\tilde{I}$ can be perceived as derivable from an unknown, more accurate DFT in a specific material. One can also "reverse engineer" such an improved functional, using the standard von Bart-Hedin scaling,

$$E_{xc} = \int \varepsilon_{xc}(n,m)n(\mathbf{r})d\mathbf{r}, \tag{7}$$

$$\varepsilon_{xc}(n,\zeta) = \varepsilon^P_{xc}(n) + f(\zeta)\Delta\varepsilon_{xc}(n), \tag{8}$$

where $\zeta(\mathbf{r}) = m(\mathbf{r})/n(\mathbf{r})$, ε^P_{xc} and $\Delta\varepsilon_{xc}(n)$ do not depend on m, $f(\zeta)$ is a known function, $n = (n_\uparrow + n_\downarrow)$, and $m = (n_\uparrow - n_\downarrow)$. The response to magnetism is entirely defined by the $\Delta\varepsilon_{xc}(n)$ functional as the energy difference between the fully polarized and unpolarized electron gas:

$$\frac{\partial\varepsilon_{xc}}{\partial n} = \frac{\partial\varepsilon^P_{xc}}{\partial n} + f(\zeta)\frac{\partial\Delta\varepsilon_{xc}(n)}{\partial n} - f'(\zeta)\Delta\varepsilon_{xc}(n)\frac{\zeta}{n}, \tag{9}$$

$$\frac{\partial\varepsilon_{xc}}{\partial m} = f'(\zeta)\Delta\varepsilon_{xc}(n)\frac{1}{n}. \tag{10}$$

Note that the charge potential also acquires a term that disappears when $\zeta = 0$. In this sense, it is impossible in a physically meaningful way to reverse engineer f and $\Delta\varepsilon_{xc}$ in such a way that $\partial\varepsilon_{xc}/\partial m$ be scaled by a constant factor s, and $\partial\varepsilon_{xc}/\partial n$ would remain the same. Rather, a natural way to weaken the magnetism in this formalism is to scale $\Delta\varepsilon_{xc}(n)$ in Eq. (8). Then we will have the following set of scaled equations:

$$\varepsilon_{xc}(n,\zeta) = \varepsilon^P_{xc}(n) + sf(\zeta)\Delta\varepsilon_{xc}(n), \tag{11}$$

$$\frac{\partial\varepsilon_{xc}}{\partial n} = v^P_{xc} + s\left[f(\zeta)\Delta v_{xc}(n) - f'(\zeta)\Delta\varepsilon_{xc}(n)\frac{\zeta}{n}\right], \tag{12}$$

$$\frac{\partial\varepsilon_{xc}}{\partial m} = sf'(\zeta)\Delta\varepsilon_{xc}(n)\frac{1}{n}, \tag{13}$$

where the part in the square brackets is simply the additional charge potential that appears because of spin polarization. It is easy to verify that this functional produces an exchange-correlation potential scaled by s, and the charge potential is unchanged:

$$\begin{aligned}\tilde{V}_\uparrow(\mathbf{r}) - \tilde{V}_\downarrow(\mathbf{r}) &= s[V_\uparrow(\mathbf{r}) - V_\downarrow(\mathbf{r})],\\ \tilde{V}_\uparrow(\mathbf{r}) + \tilde{V}_\downarrow(\mathbf{r}) &= [V_\uparrow(\mathbf{r}) + V_\downarrow(\mathbf{r})].\end{aligned} \tag{14}$$

The Stoner kernel $\delta^2E_{xc}/\delta m(\mathbf{r})^2$ is also scaled by s as we wanted. Equation (14) can be easily implemented[14] and can be used to obtain correct magnetic moments, and the corresponding electronic structure in the materials near the ferro- *or* antiferromagnetic QCP. Moreover, given Eqs. (5) and (6), s gives also an indication of the strength of the spin fluctuations acting in the system. Below we use Eq. (14) for correcting the LSDA results obtained in the previous section in the case of Ni_3Al itinerant ferromagnets under pressure. As shown previously, Ni_3Al becomes paramagnetic under pressure,[20] and the LSDA overestimates not only the magnetic moment but also the critical pressure P_c. Empirically, by comparing the LSDA value of the magnetic moment with the experimental ones for $P = 0$ GPa and for $P = 6$ GPa, we found that in both cases the value of s needed to reconcile the LSDA result with experiment, using the scaling introduced in Eq. (14), is $s \approx 0.88$. This implies that ξ is almost pressure independent between 0 and 6 GPa. This value of s gives for $\tilde{I}$ the same value obtained by renormalizing I within the EST (see the Appendix). In general, one expects that spin fluctuations become stronger closer to the critical pressure so that their average amplitude ξ becomes larger and the scaling parameter $s = 1 - (10/3)a_4\xi^2/I$ in Eq. (6) smaller . On the other hand, ξ is defined by averaging over the entire Brillouin zone, and the fact that the susceptibility at one particular point $\mathbf{q} = \mathbf{0}$ diverges may or may not strongly affect ξ. In order to understand this result, we compared our calculations with Ref. 16 wherein ξ is calculated for $P = 0$ GPa in the approximations described above. By means of the scaling arguments described below, we found that the transition is driven entirely by the change in the DOS given by Eq. (1) while the renormalized Stoner parameter $\tilde{I}$ is, in the first approximation, pressure independent. Let us try to rationalize this fact, using the fluctuation-dissipation theorem [Eq. (5)].

Given Eq. (1) and since the Fermi velocity scales inversely with the DOS, $v(P) = v(0)Z(P)$ in the approximation described in the beginning, and used in Ref. 16, we found that ξ does actually scale with pressure as $\xi(P) \propto \sqrt{\frac{1}{\Omega(P)}}$, where $\Omega(P)$ is the unit-cell volume at pressure P.[30] We found indeed that it does not diverge or even grow substantially near the critical pressure [even though the model susceptibility at $q = 0$, $\omega = 0$ does diverge there as $\tilde{I}N(E_F) = 1$]. This result is particularly important because it tells us that the effect of spin fluctuations in Ni_3Al under pressure can be entirely accounted for by renormalizing the Stoner factor (the rest is a band-structure effect). Furthermore, the fact that the correlation length associated with the fluctuations (ξ) does not diverge approaching the transition is compatible with the fact that the system does not show other instabilities (like triplet superconductivity) at $P = P_c$. In fact if ξ would go to infinity, another (competing) instability could profit from this kind of long-range correlation in order to build up a competing order parameter. In fact, $\sqrt{\Omega(6\text{ GPa})/\Omega(0\text{ GPa})} = 0.98$, implying that ξ changes only by 2%. Applying the SCR theory starting from the fixed-spin-moment calculations and using ξ as a parameter (see the Appendix), we found that the best agreement with the experiment was achieved if ξ changes slightly more, by 5%, but simply using a pressure-independent ξ, corresponding to the scaling parameter $s = 0.88$ provides, apart from some underestimation of P_c, a very reasonable agreement with the experiment. This choice of s allows us also to make predictions about the magnetic moment between 0 and P_c as shown in Fig. 2.

There are no experimental measurements of magnetization as a function of pressure between 0 and 8 GPa in Ni_3Al, but the pressure dependence of the Curie temperature T_c was measured by Nicklovic *et al.*[20] They also analyzed the data

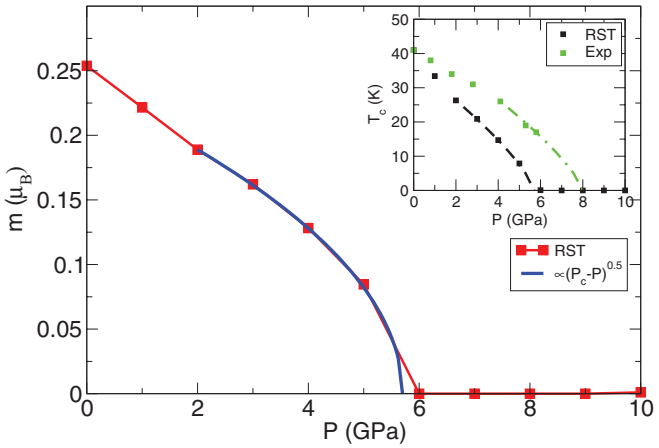

FIG. 2. (Color online) Predicted magnetic moment as a function of pressure calculated within the RST (red-dotted line). The critical behavior $m \propto (P_c - P)^{1/2}$ (blue line) is followed between 2 and 6 GPa. The Curie temperature $T_c \propto m^{3/2}$ is shown in the inset by black dots. Apart from the underestimation of the critical pressure, the agreement with the experimental data taken from Ref. 20 (green dots) is very good. In fact, both theoretically and experimentally, the extrapolation of the data at 5.7 GPa (black-dashed line) and 8 GPa (green-dashed line), respectively, give the same critical behavior $T_c \propto (P - P_c)^{3/4}$ as observed by Nicklovic *et al.* (Ref. 20).

using a Landau functional for the field

$$\mathbf{H} = a_2\mathbf{m} + a_4\mathbf{m}^3 - c\nabla^2\mathbf{m}. \tag{15}$$

By assuming $a_2 \propto (P - P_c)$, they found $T_c \propto (P - P_c)^{3/4}$ in good agreement with the experimental data. Within Moriya's theory,[18] $T_c \propto m^{3/2}$, where $m = |\mathbf{m}|$. Assuming $a_2 \propto (P - P_c)$ in Eq. (15) gives $m \propto (P - P_c)^{\beta}$ with $\beta = 1/2$ from which the result of Nicklovic *et al.* follows. In the following we show that the linearity of a_2 with respect to $(P - P_c)$ is a consequence of Eq. (1). For small values of the magnetic moment, in the fluctuation-corrected LSDA described above, $a_2 = \frac{1}{2N_\sigma(E_F)} - \frac{\tilde{I}}{2}$, $c = 0$, and $\tilde{I}$ is adjusted so as to have $N_\sigma(E_F)\tilde{I} = 1$ at $P = P_c$. Given Eq. (1), then $a_2 = \frac{Z(P)/Z(P_c)}{2N_\sigma(E_F),P_c} - \frac{\tilde{I}}{2} = \frac{\tilde{I}}{2Z(P_c)}[\alpha(P - P_c)] \propto (P - P_c)$, thus providing a microscopical justification for the model of Ref. 20. As shown in Fig. 1, in the LSDA (for large values of the magnetic moment), we found $\beta \approx 1$ while $\beta = 0.5$ is recovered for small values (see Fig. 2). This is due to the fact that at large magnetic moments, the coefficient a_2 must be corrected by adding high-order terms. Finally, using Moriya's relation for T_c, we find $T_c \propto (P - P_c)^{3/4}$ in full agreement with Nicklovic *et al.* The disagreement with experiment in the inset of Fig. 2 concerns only the underestimation of P_c caused by the approximation of s as a constant value and the underestimation of the equilibrium lattice parameter.[27]

To summarize, in this paper we have described a simplified method for accounting for near-critical spin fluctuations within the DFT. The method amounts to scaling the DFT exchange-correlation field by a phenomenological constant s and subsequent self-consistent solutions of the Kohn-Sham equations. This phenomenological constant can also be, in principle, calculated via the fluctuation-dissipation theorem[3] and in this sense is equivalent to the SCR theory by Moriya. Our method is complementary to the widely used similarly semiphenomenological LDA + U and plays for itinerant near-critical magnets the same role as LDA + U for systems near a Mott-Hubbard transition. We apply this method to the ferromagnetic QCP in Ni_3Al under pressure. We show that, due to a particular scaling property of the band structure, the parameter s is constant with pressure. In this way the method becomes completely *ab initio*. In fact, the ferromagnetic-paramagnetic transition in Ni_3Al is driven by the band-structure changes under pressure while the feedback to the critical fluctuations (parametrized by s) is small. Using this formalism, we make a prediction of the magnetic moment as a function of pressure, recovering the critical exponent for the magnetization $\beta = 1/2$ for small magnetic moments and explaining the observed dependence of the Curie temperature on pressure. The new method should be useful in cases when one needs to calculate electronic properties of materials wherein the LSDA overestimates the tendency to magnetism or when one wants to monitor theoretically the evolution of the electronic structure from nonmagnetic to magnetic and get an estimate of the spin-fluctuation amplitude.

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APPENDIX: CONNECTION BETWEEN RST AND SRC VIA EST

If we fit the fixed-spin-moment calculations with a Landau expansion up to the eighth order, we find the same result as in Ref. 16. However, as opposed to that work, we do not want to apply explicitly a fluctuation-induced renormalization but renormalize I directly, according to Eq. (14), that is, to scale down the *ab initio* Stoner parameter in order to obtain the correct magnetic moment for Ni_3Al. To make a direct connection

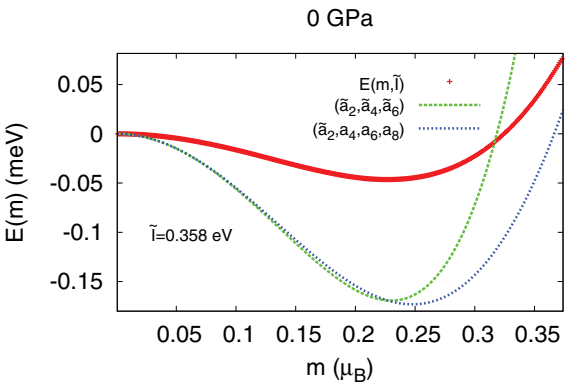

FIG. 3. (Color online) Energy E as a function of the magnetic moment m for $P = 0$ GPa. The red dots show the curve obtained by means of EST with a renormalized Stoner parameter $\tilde{I} = 0.358$. The green and the blue lines mark, respectively, the Landau functional in which all the coefficients are renormalized and the one in which only the first coefficient of the expansion is renormalized.

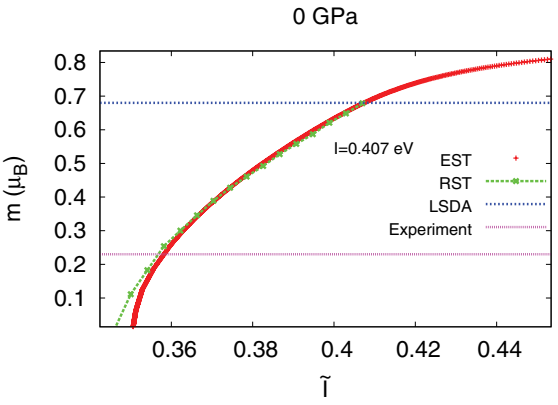

FIG. 4. (Color online) Magnetic moment m as a function of the reduced Stoner parameter $\tilde{I} = sI$ for Ni_3Al at 0 GPa in EST (red dots) and RST (green-dotted line). The bare value of the Stoner parameter $I = 0.407$ eV was chosen in order to have the same value of m for $s = 1$.

between the Landau approach and the RST approach, we can use the EST. Indeed, as discussed above, the RST method is equivalent to the SCR method if only the second-order coefficient a_2 (the inverse magnetic susceptibility) is renormalized. We can expand the EST total energy in Eq. (2) in m. Then renormalizing the Stoner parameter becomes exactly equivalent to renormalizing a_2. Figure 3 shows that, in fact, the a_2 renormalization only affects the equilibrium magnetic moment while the renormalization of the higher-order coefficients influences $E(m)$ at m larger than the experimental magnetic moment. Note that the red-dotted curve (EST) in Fig. 3 corresponds to rigid splitting of the unpolarized bands[21] while the coefficients of the Landau expansion were obtained by fitting fully self-consistent magnetic calculations.[16] Figure 4 shows the equilibrium magnetic moment m as a function of the reduced Stoner parameter $\tilde{I} = sI$, obtained both with the EST and by self-consistent calculations using the exchange scaling s of Eq. (14) at $P = 0$ GPa. The value of I is chosen, in the former case, in such a way that the LSDA and EST magnetic moments have the same value for $s = 1$. The agreement between the two curves is perfect, and the value of $\tilde{I}$ found in this way is in perfect agreement with the one extracted from the comparison of the EST with the renormalized Landau expansion in Fig. 3.

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[30]In Refs. 3 and 16, ξ is defined as

$$\xi^2(P) = \frac{b(P)v_F^2(P)N^2(E_F,P)}{8a^2(P)\Omega(P)}[Q^4\ln(1+Q^{-4}) + \ln(1+Q^4)],$$

where $a(P) = \frac{1}{12}\frac{d^2\langle N(E_F,P)v_x^2(P)\rangle}{dE_F^2}$ and $b(P) = \frac{1}{2}\langle N(E_F,P)v^{-1}(P)\rangle$. Since the Fermi velocity scales inversely with the DOS, $v(P) = v(0)Z(P)$, these parameters scale as $a(P) = a(0)Z(P)$ and $b(P) = b(0)/Z^2(P)$. The last parameter Q depends on the cutoff vector $Q = q_c\sqrt{a(P)/b(P)v_F(P)}$. A possible choice for q_c is $q_c = \sqrt{N(E_F)/a}$ because at that point the expansion of χ loses its physical meaning (χ_0 changes sign). Then $Q = \sqrt{N(E_F,P)/b(P)v_F(P)}$ does not depend on pressure. This implies that ξ does actually scale with pressure as $\xi(P) \propto \sqrt{\frac{1}{\Omega(P)}}$.

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