Accounting for spin fluctuations beyond LSDA in the density functional theory

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(Dated: May 1, 2014)

We present a method to correct the magnetic properties of itinerant systems in local spin density approximation (LSDA) and we apply it to the ferromagnetic-paramagnetic transition under pressure in a typical itinerant system, Ni$_3$Al. We obtain a scaling of the critical fluctuations as a function of pressure equivalent to the one obtained within Moriya’s theory. Moreover we show that in this material the role of the bandstructure 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 the 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.

PACS numbers: 71.15.Mb, 71.20.Be, 75.40.-s, 75.50.Cc

Density functional theory (DFT), in its most common implementations (local spin density approximation, LSDA, with or without gradient corrections, GGA), is in principle the only way to access the ground state of real materials. And indeed the agreement with experiment concerning the ground state properties, such as crystal and electronic structures, is excellent, especially for itinerant systems, where local correlations play a minor role. Nevertheless, a well known problem of LSDA is the overestimation of the tendency to magnetism in itinerant magnets near the quantum critical point (QCP). This problem can be traced down to the fact that 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, FeP or the more recent and better known Fe-pnictides make LDA and GGA reproduce very well the paramagnetic bandstructure, whenever a (magnetic) quantum critical point (QCP) is approached the theory fails miserably. The importance of this problem is demonstrated by the amount of papers dealing with the problem of correcting the magnetic moment of Fe-pnictides. There, the usual argument is that correlations beyond 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 U$, but there is no physical justification for this procedure. Such many-body approaches as Dynamic Mean Field Theory (DMFT) and Gutzwiller 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. Furthermore the effect of non-local fluctuations was recently found to be crucial, also in localized models, whenever the critical behavior is analyzed, and in any event computational load in these methods is incomparably heavier than in LDA calculations.

For these reasons we propose a different approach which corrects LSDA within DFT and takes into account the itinerant nature of the system. Our method is easy to implement and carries no additional computational cost, and has a transparent physical justification. The approach we describe in the following is based on the idea that unknown more accurate DFT is very close to the conventional LSDA-GGA functional, but the energy gain due to spin polarization (“Stoner interaction”, using the DFT parlance) is reduced by about as much as the Moriya selfconsistent renormalization (SCR) theory, successfully used before, 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$_3$Al itinerant ferromagnet, with the correct scaling of the Curie temperature, which until now was impossible. For Ni$_3$Al 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 and experimentally and experimentally.

Applying the RST we estimate the pressure dependence of the contribution due to spin fluctuations on the magnetic moment of Ni$_3$Al. 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 bandstructure. As a consequence we show that the way in which the spin fluctuations renormalize the effective Stoner interaction is encoded in the bandstructure itself. This is generally true but in Ni$_3$Al 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.
calculated the equilibrium lattice parameter in GGA) in reasonable agreement with previous results.

After that we calculated the magnetic moment as a function of pressure (black squares). The data are fitted with eq. 1 (red continuous line).

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$_3$Al under pressure and we interpret them within the so-called extended Stoner Theory (EST). We explain that the overestimation of both the magnetic moment at zero pressure, and the critical pressure $P_c$ come essentially by the overestimation of the Stoner parameter in 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$_3$Al under pressure.

First we discuss the bare LDA (and LSDA) results for the magnetic transition in Ni$_3$Al under pressure. Ni$_3$Al crystallizes in the ideal cubic Cu$_3$Au $cP4$ structure. We calculated the equilibrium lattice parameter $a = 3.4825$ Å in LDA and we found it to be $\approx 2\%$ smaller than the experimental one. The calculated magnetic moment at $P = 0$ GPa is $m(0) = 0.68 \mu_B$ in LSDA ($0.73 \mu_B$ in GGA) in reasonable agreement with previous results.

After that we calculated the magnetic moment as a function of pressure and, as shown in the top of Fig. 1, we found that it decreases approximately linearly up to the critical pressure $P_c = 45$ GPa, much larger than the experimental one, which is $P_c^{\text{exp}} \approx 8$ GPa. This behavior can be easily understood within the EST. In fact, as shown in Fig. 1 (bottom), the paramagnetic DOS $N(E)$ calculated in LDA scales almost perfectly with the pressure $P$ as:

$$N(E, P) = \frac{N(E \ast Z(P), 0)}{Z(P)},$$

in a wide energy range around the Fermi level taken as the origin, where $Z(P) = 1 + 0.005 \ast P$ with $P$ measured in GPa. This can be related to magnetization via the EST, which combines the Stoner criterion with the Andersen’s force theorem to show that in the lowest order in the magnetic moment $m$ the total LSDA energy is given in terms of the non magnetic DOS per spin:

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

where $N(m')$ 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 $N(m) = 1/I$, and $dN(m)/dm < 0$, forming a stable or a metastable (paramagnetic) ferromagnetic state with the magnetic moment $m$. If $N(E)$ scales according to eq. 1 so does also $\tilde{N}(m)$. Comparing eq. 2 with the fixed spin moment calculation we found the Stoner parameter in LSDA to be $I_{LSDA} \approx 0.41$ eV independent on pressure (see appendix A). In GGA the Stoner parameter is 17% larger, $I_{GGA} = 1.17I_{LSDA}$. 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,

$$E(M) = a_0 + a_2 M^2/2 + a_4 M^4/4 + a_6 M^6/6 + \cdots ,$$

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 $\delta M$ follows a Gaussian distribution such that $\langle \delta M^2 \rangle = \xi^2$, we can rewrite eq. 3 in terms of $\bar{M}$ as

$$E(M) = a_0 + \bar{a}_2 M^2/2 + \bar{a}_4 M^4/4 + \bar{a}_6 M^6/6 + \cdots ,$$

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

The amplitude of the spin fluctuations, $\xi$, in principle, can be obtained by the fluctuation-dissipation theorem.
\[ \xi^2 = \frac{4\hbar}{\Omega} \int dq \int \frac{d\omega}{2\pi^2} I m \chi(q, \omega) \]  

where \( \Omega \) is the volume of the unit cell, \( \chi(q, \omega) \) 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 \( \omega \), \( \chi_0(q, \omega) = \chi_0(0, 0) - aq^2 + ibq/\omega \). 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 \( \xi \) 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 \( \chi^{-1} = \delta^2 E/\delta M^2 \mid_{\mathbf{M}=0} \) \( a_2 = \frac{1}{2} \left[ \frac{1}{N_s(E_F)} - I \right] \) (this can be considered as a rigorous definition of the LSDA Stoner parameter \( I \), where \( N_s(E_F) \) is the paramagnetic DOS per spin. Comparing this expression with the one for \( a_2 \) we see that the SCR procedure is equivalent to renormalization of \( I \) according to

\[ \tilde{I} = I - (10/3)a_4\xi^2, \]  

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

This is a justification of the recipe of using \( I \) as an adjustable parameter, often used in critical ferromagnets empirically. In this sense, \( I \) 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,

\[ E_{xc} = \int \varepsilon_{xc}(n, m)n(r)dr \]  

\[ \varepsilon_{xc}(n, \zeta) = \varepsilon_{xc}^p(n) + f(\zeta)\Delta \varepsilon_{xc}(n), \]  

where \( \zeta(r) = m(r)/n(r) \), \( \varepsilon_{xc}^p \) and \( \Delta \varepsilon_{xc}(n) \) do not depend on \( m \) and \( f(\zeta) \) is a known function, and \( n = (n_\uparrow + n_\downarrow) \), \( m = (n_\uparrow - n_\downarrow) \). 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:

\[ \frac{\partial \varepsilon_{xc}}{\partial m} = \frac{\partial \varepsilon_{xc}^p}{\partial m} + f(\zeta)\frac{\partial \Delta \varepsilon_{xc}(n)}{\partial m} - f'(\zeta)\Delta \varepsilon_{xc}(n)\frac{\zeta}{n} \]  

\[ \frac{\partial \varepsilon_{xc}}{\partial n} = f'(\zeta)\Delta \varepsilon_{xc}(n)\frac{1}{n} \]  

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:

\[ \varepsilon_{xc}(n, \zeta) = \varepsilon_{xc}^p(n) + s f(\zeta)\Delta \varepsilon_{xc}(n) \]  

\[ \frac{\partial \varepsilon_{xc}}{\partial n} = v_{xc}^p + s [f(\zeta)\Delta \varepsilon_{xc}(n) - f'(\zeta)\Delta \varepsilon_{xc}(n)\frac{\zeta}{n}] \]  

\[ \frac{\partial \varepsilon_{xc}}{\partial m} = s f'(\zeta)\Delta \varepsilon_{xc}(n)\frac{1}{n} \]  

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 unstached:

\[ V_{\uparrow}(\mathbf{r}) - V_{\downarrow}(\mathbf{r}) = s[V_{\uparrow}(\mathbf{r}) - V_{\downarrow}(\mathbf{r})] \]  

\[ V_{\uparrow}(\mathbf{r}) + V_{\downarrow}(\mathbf{r}) = [V_{\uparrow}(\mathbf{r}) + V_{\downarrow}(\mathbf{r})] \]  

and the Stoner kernel \( \delta^2 E_{xc}/\delta m(r)^2 \) also scaled by \( s \), as we wanted. Eq. 13 can be easily implemented, and can be used to obtain correct magnetic moments and the corresponding electronic structure in the materials near ferro or antiferromagnetic QCP. Moreover, given eq. 6 and 9, \( s \) gives also an indication of the strength of spin fluctuations acting in the system. Below we use eq. 13 for correcting the LSDA results obtained in the previous section in the case of Ni3Al itinerant ferromagnet under pressure. As shown previously, Ni3Al becomes paramagnetic under pressure, and LSDA overestimates not only the magnetic moment, but also the critical pressure. Empirically, by comparing the LSDA value of the magnetic moment with the experimental one 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. 13 is \( s \approx 0.88 \). This implies that \( \xi \) 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 appendix A). In general, one expects that spin fluctuations become stronger closer to the critical pressure, so that their average amplitude \( \xi \) becomes larger, and the scaling parameter \( s = 1 - (10/3)a_4\xi^2/I \) in eq. 6 smaller. On the other hand, \( \xi \) is defined by averaging over the entire Brillouin zone, and the fact that susceptibility at one particular point \( q = 0 \) diverges may or may not strongly affect \( \xi \). In order to understand this result, we compared our calculations with Ref. 16, where \( \xi \) is calculated for \( P = 0 \) GPa in the approximations described above. By means of scaling arguments described below, we found that the transition is driven entirely by the change in DOS given by eq. 11 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. 11 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 Refs. 16, we found that \( \xi \) does actually scale with pressure as \( \xi(P) \propto 1/\Omega(P) \), where \( \Omega(P) \) is the unit cell volume at
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, \( \tilde{\chi}_\infty \) = 1). This result is particularly important because it tells us that the effect of spin fluctuations in Ni₃Al under pressure can be entirely accounted for by renormalizing the Stoner factor (the rest is a bandstructure effect). Furthermore, the fact that the correlation length associated with the fluctuations (\( \xi \)) 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 \( \xi \) would go to infinity, another (competing) instability could profit of this kind of long range correlation in order to build up a competing order parameter. In fact, \( \sqrt{\Omega(6 \text{ GPa})/\Omega(0 \text{ GPa})} = 0.98 \), which implies that \( \xi \) changes only by 2%. Applying the SCR theory starting from the fixed spin moment calculations and using \( \xi \) as a parameter (see appendix A), we found that the best agreement with the experiment was achieved if \( \xi \) changes slightly more, by 5%, but simply using a pressure-independent \( \xi \), 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 Ni₃Al, but the pressure dependence of the Curie temperature \( T_c \) was measured by Nicklovic et al. They also analyzed the data using a Landau functional for the field

\[
H = a_2 m + a_4 m^3 - c \nabla^2 m.
\]  

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, \( T_c \propto m^{3/2} \) where \( m = |m| \). Assuming \( a_2 \propto (P - P_c) \) in eq. \( 1 \) gives \( m \propto (P - P_c)^{3/2} \) 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, \( a_2 = \frac{2N_s(E_F)}{Z} - \frac{i}{2}, \) \( c = 0 \), and \( \tilde{I} \) is adjusted so as to have \( N_s(E_F)\tilde{I} = 1 \) at \( P = P_c \). Given eq. \( 1 \) then

\[
a_2 = \frac{2\tilde{I}(P)/2\tilde{I}(P_c)}{2N_s(E_F)/Z} - \frac{i}{2} = \frac{i}{2\tilde{I}(P_c)}[\alpha(P - P_c)] \propto (P - P_c),
\]

thus providing a microscopical justification for the model of Ref. 21. As shown in Fig. 1 in 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 moment 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 Fig. 2 (inset) 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. 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 solution of the Kohn-Sham equations. This phenomenological constant can also be, in principle, calculated via the fluctuation dissipation theorem and, in this sense is equivalent to the SCR theory by Moriya. Our method is complementary to the widely used similarly semi-phenomenological 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 Ni₃Al under pressure. We show that, due to a particular scaling property of the bandstructure, the parameter \( s \) is constant with pressure. In this way the method becomes completely ab initio. In fact, the ferromagnetic-paramagnetic transition in Ni₃Al is driven by the band structure changes under pressure, while the feedback to the critical fluctuations (parameterized by \( s \)) is small. Using this formalism, we make a prediction of the magnetic moment as a function of pressure, which recovers the critical exponent for the magnetization \( s = 1 \) for small magnetic moments and explains 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 where LSDA overestimates the tendency to magnetism, or when one wants to monitor theoretically the evolution of the electronic structure from non magnetic to magnetic and get an estimate of the spin fluctu-
ation amplitude.

This research was supported by the Deutsche Forschungsgemeinschaft under Priority Program 1458, grant number Boe/3536-1. We are grateful to Alaska Subedi, Tobias Schickling and Mark Hoeppner for a careful reading of our manuscript.

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25 Our LDA and LSDA calculations were done using the general potential linearized augmented-plane-wave (LAPW) method as implemented in the Wien2k package.\textsuperscript{22,28} Up to 1330 k points were used in the self-consistent calculations with an LAPW basis defined by the cutoff $R_{\text{S}}K_{\text{max}} = 9$ both in the magnetic and in the non magnetic calculations. A larger number of 4960 k points were used for calculating the non magnetic DOS. We fitted the total energy as a function of the unit cell volume with the equation of state that we used is the one by Murnaghan.\textsuperscript{22} $E = E_0 + |B| V^0 / |B|^r - 1) / 14703.6$ where $V/V_0$ is the volume compression, $P = B/B^{r^r} - 1$ with $V_0 = 284.5961$ Bohr$^3$, $B = 237.0284$ GPa, $B^r = 3.8413$, $E_0 = -9594.376522$ Ry. $B$ and $B^r$ are the Bulk modulus and derivative. The lattice parameters both in the magnetic and in the non magnetic case were found to be the same.
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31 In Refs.\textsuperscript{16} $\xi$ is defined as $\xi^2 (P) = \frac{\partial (P \nu_0 (P))^2 (P)^2 (E_F, P) [Q^4 \log (1 + Q^{-4}) + \log (1 + Q^4)]}{8 a^2 (P) \Omega(P)}$ where: $a(P) = \frac{\partial (N(E_F, P))}{\partial Q}$ $b(P) = \frac{\partial (N(E_F, P))}{\partial Q}$ 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, $Q = q \sqrt{a(P) / b(P) v(P)}$. A possible choice for $q_c$ is $q_c = \sqrt{N(E_F)/a}$, because at that point the expansion of $\chi$ loses its physical meaning ($\chi_0$ changes sign). Then $Q = \sqrt{N(E_F, P) / b(P) v(0)}$ does not depend on pressure. This implies that $\xi$ does actually scale with pressure as $\xi (P) \propto \frac{1}{\sqrt{P}}$.

Appendix A: Connection between RST and SRC via EST

If we fit the fixed spin moment calculations with a Landau expansion up to the 8-th order we find the same result as in Ref.\textsuperscript{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.\textsuperscript{14} that is, to scale down \textit{ab-initio} the Stoner parameter in order to achieve the correct magnetic moment for Ni$_3$Al. To make a direct connection 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 $\alpha_2$ (the inverse magnetic susceptibility) is renormalized. We can expand the EST total energy in eq.\textsuperscript{2} in $m$, and then renormalizing the Stoner parameter becomes exactly equivalent to a renormalization of $\alpha_2$. Fig.\textsuperscript{9} shows that, in fact, only the $\alpha_2$ renormalization affects the equilibrium magnetic moment, while the renormalization of the higher order coefficients influences $E(m)$ at
FIG. 3: 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 where all the coefficients are renormalized and the one where only the first coefficient of the expansion is renormalized.
FIG. 4: Magnetic moment $m$ as a function of the reduced Stoner parameter $\tilde{I} = s^* I$ for Ni$_3$Al 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 $s = 1$. 

$\mu_B$