Magnetic exchange in α–iron from the ab initio calculations in the paramagnetic phase

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Applying the local density approximation (LDA) and dynamical mean field theory (DMFT) to paramagnetic α-iron, we revisit a problem of theoretical description of its magnetic properties. The analysis of local magnetic susceptibility shows that at sufficiently low temperatures \( T < 1500K \), both, \( e_g \) and \( t_{2g} \) states equally contribute to the formation of the effective magnetic moment with spin \( S = 1 \). By considering the non-uniform magnetic susceptibility we find that the non-quasiparticle form of \( e_g \) states is crucial for obtaining ferromagnetic instability in α-iron. The main contribution to the exchange interaction, renormalized by the effects of electron interaction, comes from the hybridization between \( t_{2g} \) and \( e_g \) states. We furthermore suggest the effective spin-fermion model for α-iron, which allows us to estimate the exchange interaction from paramagnetic phase, which is in agreement with previous calculations in the ordered state within the LDA approaches.

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Elemental iron in its low-temperature body-centered cubic (bcc) phase, which is stable below approximately 1200 K, provides unique example of itinerant magnetic \( d \)-electron systems, where formation of well-defined local magnetic moments can be expected. Indeed, the Rhodes-Wolfarth ratio \( p_C/p_S \) for this substance is very close to one, which is characteristic feature of systems, containing (almost) localized \( d \)-electrons (\( p_C \) corresponds to the magnetic moment, extracted from the Curie–Weiss law for magnetic susceptibility in the paramagnetic phase \( \chi = \gamma_B^2 p_C(p_C + 1) / T \), and \( p_S \) is the saturation moment, \( g \) is a Lande factor, \( T \) denotes temperature). At the same time, the moment \( p_C = 1.1 \) has a small fractional part, which is natural for the itinerant material.

This poses natural questions: which electrons mainly contribute to the local-moment spin degrees of freedom of α-iron? What is the appropriate physical model, that describes spin degrees of this substance? Attempting to answer the former question, Goodenough suggested, that the \( e_g \) electrons are localized, while \( t_{2g} \) electrons are itinerant. This suggestion was later on refined in Ref. 2, pointing to a possibility, that only some fraction of \( e_g \) electrons, contributing to formation of the peak of the density of states near the Fermi level, named by the authors as giant van Hove singularity, is localized. (The intimate relation between peaks of density of states and electron localization was also previously pointed out in Ref. 3.) On contrary, there were statements made that 95% of electrons are localized in iron. On the model side, the thermodynamic properties of α-iron were described within the effective spin \( S = 1 \) Heisenberg model, assuming therefore that the main part of magnetic moment is localized, in agreement with the above-mentioned Rhodes-Wolfarth arguments. Use of the effective Heisenberg model was justified from the ab-initio analysis of spin spiral energies yielding reasonable values of the exchange integrals.

These considerations however did not take into account strong electronic correlations in α–iron, which important role was emphasized first in Ref. 7. Previous calculations within the local density approximation (LDA), combined with the dynamical mean-field theory (DMFT) revealed the presence of non-quasiparticle states formed by \( e_g \) electrons. To answer the question of the effect of different orbital states on magnetic properties, in the present paper we investigate the non-local magnetic susceptibility using the electronic spectrum, obtained within the state–of–art dynamical mean–field theory (DMFT) calculation, combined with the ab-initio local density approximation (LDA), in the paramagnetic phase. Simultaneously, we compare the results of these calculations to the low–temperature local magnetic properties. We argue, that for magnetic properties, \( t_{2g} \) electrons are almost equally contribute to the effective local magnetic moment, as the \( e_g \) electrons, and play crucial role in the mechanism of magnetic exchange in iron. In particular, the most important contribution to the exchange integrals comes from the hybridization of \( t_{2g} \) and \( e_g \) states, which yields nearest-neighbour magnetic exchange interaction, which agrees well with the experimental data.

For the ab initio calculations we consider the bcc lattice with the parameter \( a = 2.8664 \) Å, corresponding to room temperature. Band–structure calculations have been carried out in LDA approximation within tight–binding–linear muffin–tin orbital–atomic spheres approximation framework; the von Barth-Hedin local exchange-correlation potential was used. Primitive reciprocal translation vectors were discretized into 12 points along each direction which leads to 72 k–points in irreducible part of the Brillouin zone. For DMFT calculations, we use the Hamiltonian of Hubbard type with the kinetic term containing all s–p–d states, being extracted from the LDA solution, and the interaction part with density-density contributions for d electrons only. The Coulomb interaction parameter value \( U = 2.3 \) eV and the Hund’s parameter \( I = 0.9 \) eV used in our work are the same as in earlier LDA+DMFT calculations. To treat
a problem of formation of local moments we consider paramagnetic phase. The effective impurity model for DMFT was solved by continuous-time quantum-Monte–Carlo (QMC) method. This allows us to reach the room temperature, which is inaccessible for the calculations within the previously used Hirsch–Fye Monte-Carlo approach.\textsuperscript{7,8,11}

We consider first the results for the orbital–resolved temperature–dependent local static spin susceptibility
$$\chi_{\text{loc,}mn} = 4\mu_B^2 \int_0^\beta \langle s_{\text{loc,}m}^z (\tau) s_{\text{loc,}n}^z (0) \rangle \, d\tau,$$
where $s_{\text{loc,}m}^z$ is the $z$–projection of the spin of $d$–electrons, belonging to the orbitals $m = 2g$, $e_g$ at a given lattice site $i$, see Fig. 1 (for completeness, we also show the total susceptibility $\chi_{\text{loc}} = \sum_{mn} \chi_{\text{loc,}mn}$). The temperature dependence of the static inverse local susceptibility is linear (as was also observed in previous studies\textsuperscript{7,8,11}), however being resolved with respect to orbital contributions (see Fig. 1) it appears to manifest very different nature of $e_g$ and $t_{2g}$ moments. The inverse $e_g$ orbital contribution behaves approximately linearly with $T$ in a broad temperature range. At the same time, $\chi_{\text{loc,t}_{2g}-t_{2g}}$ demonstrates a crossover at $T^* \sim 1500$ K between two linear dependences with the low–temperature part having higher slope (i. e. smaller effective moment). The scale $T^*$ corresponds to the characteristic scale of peculiarities of the bare density of states of $t_{2g}$ states, see Ref. 8.

To get further insight into the local magnetic properties of $\alpha$–iron, we consider the temperature dependence of the effective magnetic moment $\mu_{m,\text{eff}} = 3/(d\chi_{\text{loc,}mmn}/dT)$ and the instantaneous average $\langle \langle s_{\text{loc,}m}^z \rangle \rangle^2$, corresponding to different orbital states, see Fig. 2. We find, that for $e_g$ electrons both moments saturate at temperatures $T < 1500$ K and remain approximately constant up to sufficiently low temperatures. Yet, the value of the square of the moment $\mu_{e_g,\text{eff}}^2/(3\mu_B^2) = 1.2$, extracted from the Curie-Weiss law for local susceptibility, and the instantaneous average $4\langle \langle s_{\text{loc,}e_g}^z \rangle \rangle^2 = 1.8$ appear to be respectively almost twice and 1.4 times smaller, than the corresponding filling $n_{e_g} \simeq 2.6$. This points that while the major part of $e_g$ electrons determine the instantaneous average $\langle \langle s_{\text{loc,}e_g}^z \rangle \rangle^2$, only approximately half of them contribute to the sufficiently long-living (on the scale of $1/T$) local moments, while other part of the $e_g$ electrons can be considered as itinerant for description of magnetic properties. At the same time, for $t_{2g}$ electronic states the abovementioned crossover between the high-temperature value $\mu_{t_{2g},\text{eff}}^2/(3\mu_B^2) = 1.95$ and the low temperature value $\mu_{t_{2g},\text{eff}}^2/(3\mu_B^2) \simeq 0.82$ is present, which, comparing to $n_{t_{2g}} \simeq 4.4$, shows that only approximately $20\%$ of $t_{2g}$ electrons participate in the effective local moment formation at low temperatures. Nevertheless, the corresponding low-temperature effective moments $\mu_{e_g,\text{eff}}^2$ and $\mu_{t_{2g},\text{eff}}^2$ are comparable (each of them is approximately $3\mu_B^2$, corresponding to the effective spin $s \simeq 1/2$), showing important role of $t_{2g}$ electrons in the formation of the total spin $S = 1$ state. Although according to the self-energy calculations\textsuperscript{22} $t_{2g}$ electrons are not localized themselves,

![FIG. 1: (Color online) Temperature dependence of inverse local magnetic susceptibility, and the corresponding $e_g$ and $t_{2g}$ orbital contributions. Dashed lines show linear behavior in different temperature intervals.](image1)

![FIG. 2: (Color online) The temperature dependence of the effective magnetic moment and instantaneous average $\langle \langle s^z \rangle \rangle^2$ and $\mu_{\text{eff}}^2$ in $\alpha$–iron, extracted from the temperature dependence of local susceptibility, together with the contribution of the $e_g$ and $t_{2g}$ orbitals.](image2)
-\left(2\mu_B^2/\beta\right) \sum_{\mathbf{k}, \mathbf{m}} \text{Tr} \left[ \mathbf{g}_{\mathbf{k}, \mathbf{m}}(i\nu_l) \mathbf{g}_{\mathbf{k}+\mathbf{q}, \mathbf{m}}(i\nu_l) \right],

which is obtained using paramagnetic LDA and LDA+DMFT electronic spectrum \( \mathbf{g}_{\mathbf{k}, \mathbf{m}}(i\nu_l) \) is the corresponding electronic Green function for the transition from the orbital state \( \mathbf{m} \) to \( \mathbf{n} \), \( \nu_l \) is a fermionic Matsubara frequency; for more details on the calculation procedure see Ref. [11]. The results for LDA and LDA+DMFT approaches at \( T = 290 \) K are presented in the Fig. 3 (we find that the LDA+DMFT results are almost temperature-independent at low \( T \)). For the susceptibility, calculated using purely LDA spectrum (i.e. with the assumption that all electrons are itinerant), the maximum of the susceptibility \( \chi^{irr} \) is located at the point \( \mathbf{q} = \mathbf{q}_p = (\pi, \pi, \pi)/a \), which contradicts the existence of the ferromagnetic instability in \( a \)-iron at low \( T \), requiring maximum of \( \chi^{irr} \) at \( \mathbf{q} = 0 \). One can observe, that the main contribution to this “incorrect” behavior originates from the \( e_g \) electron part, \( \chi^{irr, e_g-\text{eg}} \). Both \( \chi^{irr, e_g-\text{eg}} \) and \( \chi^{irr, e_g-\text{t}_{2g}} \) contributions are however strongly influenced by the account of the local self-energy corrections to the Green’s function in DMFT approach. The self-energy corrections to \( \chi^{irr, e_g-\text{eg}} \) (which correspond physically to account of partial localization of \( d \)-electrons) shift the maximum of the non-uniform susceptibility to \( \Gamma \) point (\( \mathbf{q} = 0 \)). Note that within LDA+DMFT, intra-orbital contributions to the susceptibility \( \chi^{irr, e_g-\text{eg}} \) and \( \chi^{irr, t_{2g}-\text{t}_{2g}} \) are only weakly momentum-dependent; they also behave similarly, varying “counter-phase”. According to the general ideas of spin-fluctuation theory\[20\], this weak momentum dependence can be ascribed to the formation of the effective moments from \( e_g \) and \( t_{2g} \) states. In agreement with the above discussed consideration, the \( \chi^{irr, e_g-\text{eg}} \) contribution has even weaker dispersion than the \( \chi^{irr, t_{2g}-\text{t}_{2g}} \) part. At the same time, strongly dispersive \( \chi^{irr} \) contribution, which is assumed to correspond to the (remaining) itinerant degrees of freedom, provides the maximum of the resulting \( \chi^{irr} \) at \( \mathbf{q} = 0 \) and appears to be the main source of the stability of the ferromagnetic ordering in iron within LDA+DMFT approximation.

To see the quantitative implications of the described physical picture, we consider the effective spin-fermion model

\[
S = \frac{1}{2} \sum_{\mathbf{k}, \nu, \omega} \chi_S^{-1}(\mathbf{k}, \nu, \omega) \hat{S}_\mathbf{k}(\nu) \hat{S}_{-\mathbf{k}}(-\nu) e^{i\mathbf{q}(\mathbf{R}_{\mathbf{k}} - \mathbf{R}_{-\mathbf{k}})} \quad (1)
\]

\[
+ 2I \sum_{\mathbf{k}, \nu, \omega} \hat{S}_\mathbf{k}(\nu) \hat{S}_{-\mathbf{k}}(-\nu) \sum_{\nu', \sigma} c_\mathbf{k}^\dagger(\nu) \left[i \nu_\sigma \delta_{\nu, \nu'} + H_{\nu'} + \Sigma_{\nu'}(\nu_\sigma)\right] c_{-\mathbf{k}}(\nu),
\]

\((\omega_\nu) \) is a bosonic Matsubara frequency, \( l, l' \) combines site and orbital indices\), describing interaction of itinerant electrons with (almost) local spin fluctuations (in contrast to critical spin fluctuation in cuprates\[13,14\], see also Ref.\[22\]. We assume here that the Coulomb and Hund’s interaction acting within \( e_g \) and \( t_{2g} \) orbitals results in a formation of some common local moment (field \( S \)), while the remaining itinerant degrees of freedom are described by the field \( s_l = s_l^{e_g} + s_l^{t_{2g}} \), formed from the Grassmann variables \( c_{\nu' \sigma} \); \( H_{\nu'} \) and \( \Sigma_{\nu'} \) are the Hamiltonian and local self-energy corrections to the LDA spectrum (the latter is assumed to be local and therefore diagonal with respect to orbital indices). Note that both (localized and itinerant) electronic subsystems present two \textit{modus} of the same \( d \)-electronic states. The interaction between these two subsystems is driven by Hund’s constant coupling \( I \).

To determine bare propagator of magnetic degrees of freedom \( \chi_S(\mathbf{q}, \nu, \omega) \), we require that the dressed propagator of \( \mathbf{S} \) field is equal to the susceptibility of itinerant subsystem. Using the random-phase-type approximation, which reduces the three-frequency dependence of irreducible susceptibility and vertex to the respective single-frequency orbital “averaged” quantities, \( \chi^{irr} = \sum_{mn} \chi^{irr, mn} \) and \( \Gamma \), we obtain

\[
\chi_S^{-1}(\mathbf{q}, \nu, \omega) = 4\mu_B^2 \left(\chi^{irr}\right)^{-1} - 2\Gamma + (I/\mu_B)^2 \chi^{irr} \quad (2)
\]

where the last term is added to cancel the corresponding bosonic self-energy correction from itinerant degrees of freedom to avoid double-counting, cf. Ref.\[26\]. From the results of Fig. 3 it follows that \( \chi^{irr} = \chi^{irr} + \delta \chi^{irr} \) with momentum-independent \( \chi^{irr} \) and \( \delta \chi^{irr} \ll \chi^{irr} \); without loss of generality, we can assume \( \sum_{\mathbf{q}} \delta \chi^{irr} = 0 \), such that \( \delta \chi^{irr} = \sum_{\mathbf{q}} \delta \chi^{irr} \). Expanding Eq. (2) to first order in \( \delta \chi^{irr} \), we obtain

\[
\chi_S^{-1}(\mathbf{q}, \nu, \omega) = 4\mu_B^2 \left(\chi^{irr}\right)^{-1} - 2\Gamma + (I/\mu_B)^2 \chi^{irr} + [(I/\mu_B)^2 - 4\mu_B^2 \left(\chi^{irr}\right)^{-2}] \delta \chi^{irr} \quad (3)
\]
Since $\chi^{\text{irr}} \simeq 2\mu_B^2/eV$ and $I \simeq 1eV$ the momentum dependence is almost cancelled, and we obtain the local bare propagator of spin degrees of freedom,

$$\chi_S^{-1}(q, i\omega_n) \simeq \chi_S^{\text{loc}}^{-1}(i\omega_n) = 4\mu_B^2 \chi_S^{\text{loc}}(i\omega_n) + (I/\mu_B)^2 \chi^{\text{irr}}$$

with $\chi_S^{\text{loc}}(i\omega_n) = (\tau^{\text{irr}})^{-1} - 2I/(4\mu_B^2)$. In practice, the frequency dependence $\chi^{\text{loc}}(i\omega_n) = \mu_B^2/(3(T + \theta)(1 + |\omega_n|/\delta))$ can be obtained from the dynamic local spin correlation functions, which is characterized by the temperature-independent moment $\mu_B$, its damping $\delta \propto T$, and the corresponding Weiss temperature $\theta$ (see Refs. [11]).

Considering the renormalization of the propagator $\chi_S$ by the corresponding boson self-energy corrections, we obtain for the non-uniform susceptibility similarly to the single-band case,

$$\chi^{-1}(q, i\omega_n) = \chi^{\text{loc}}^{-1}(i\omega_n) - J_q/(4\mu_B^2),$$

where the exchange interaction

$$J_q = (I/\mu_B)^2(\chi^{\text{irr}} - \chi^{\text{irr}}) = J_q^{(1)} + J_q^{(2)},$$

fulfills $\sum_q J_q = 0$ (no spin self-interaction). Here $J_q^{(1)} = (I/\mu_B)^2 \sum_m [\chi^{\text{irr},mm} - \sum_p \chi^{\text{irr},pm}]$ is the intra-orbital part, while $J_q^{(2)} = 2(I/\mu_B)^2 \chi^{\text{irr},t_{2g}e_g}$ results from the hybridization of states of different symmetry (we use also here that by symmetry $\sum_p \chi^{\text{irr},t_{2g}e_g} = 0$). The contribution $J_q^{(1)}$ is approximately twice smaller than $J_q^{(2)}$, and therefore the main contribution to the magnetic exchange comes from the hybridization of $t_{2g}$ and $e_g$ states. The whole momentum dependence of $J_q^{(2)}$ can be well captured by the nearest-neighbor approximation for effective exchange integrals only, $J_q^{(2)} = J_0 \cos(qz/2) \cos(qx/2) \cos(qy/2)$, while $J_q^{(1)}$ has more complicated momentum dependence.

Restricting ourselves by considering the contribution $J_q = J_q^{(2)}$, (we assume that the contribution $J_q^{(1)}$ is further suppressed by the non-local and vertex corrections), from Fig. 4 we find at $T = 290$ K the value $J_q = 0.20$ eV. This value, as well as the momentum dependence of $J_q^{(2)}$ agrees well with the result of S.V. Okatov et al. The obtained results provide an estimate for the Curie temperature (we assume $T_C \gg \theta$), which can be obtained from the divergence of $\chi^{-1}(q, 0)$:

$$T_C = \frac{\mu_B^2 c_{\text{eff}} J_0}{4\mu_B^2 3} \approx 0.17 \text{ eV}$$

and appears comparable with the result of full DMFT calculation, and therefore shows that the above model is adequate for describing magnetic properties of the full 5-band Hubbard model. (Note that the overestimation of $T_C$ in DMFT approach in comparison with the experimental data is due to density-density approximation for the Coulomb interaction$^{17}$ and (to minor extent) due to presence of non-local fluctuations, not accounted by DMFT).

Neglecting longitudinal fluctuations of field $S$ we can map the model [1] to an effective $S = 1$ Heisenberg model $\mathcal{H}_H = (1/2)\sum_{ij} J_{ij} S_i S_j$ to estimate the spin–wave spectrum:

$$\omega_q = S(J_0 - J_q) = S(I/\mu_B)^2(\chi^{\text{irr},t_{2g}e_g} - \chi^{\text{irr},t_{2g}e_g})$$

We obtain the corresponding spin stiffness $D = \lim_{q \rightarrow 0}(\omega_q/q^2) = 290 \text{ meV} \cdot \text{Å}^2$ in a good agreement with the experimental data $D = 280 \text{ meV} \cdot \text{Å}^2$ (Ref. [19]).

In conclusion, we have considered the problem of the description of effective local moments in $\alpha$-iron based on the electronic spectrum in paramagnetic phase within LDA+DMFT approximation. We find that local moments are formed by both $e_g$- and $t_{2g}$-orbital states, each of them contributing a half of the total moment $S = 1$.

The effective spin–fermion model is proposed for $\alpha$-iron on the basis of the performed analysis. This model considers two modus operandi of $d$-electron states, forming local moment and itinerant states, interacting with each other. The magnetic exchange between the local-moment states is provided by the effective RKKY-type mechanism. The obtained exchange integrals are well captured by the LDA+DMFT approach. The main origin of the intersite interaction of these moments is attributed to the $e_g$-$t_{2g}$ hybridization, which yields magnetic exchange, dominating on the nearest-neighbour cites. Contrary to the previous studies$^{16,18}$, we do not however assume some magnetic ordering for the electronic system.

We also emphasize that non–local self–energy corrections, as well as vertex corrections, missed in our investigation, can make the described physical picture more precise. In particular, non-local effects allow for the non–zero non-diagonal $e_g$-$t_{2g}$ self-energy matrix elements and therefore possibly renormalize the strength of exchange interaction, as well as the self-energy of $t_{2g}$ electronic states. Therefore further investigation using powerful theoretical techniques of dynamic vertex approximation$^{20}$, dual fermion$^{21}$, or other non-local approaches are required.

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