Incommensurate and Commensurate Antiferromagnetic Spin Fluctuations in Cr and Cr Alloys from *Ab Initio* Dynamical Spin Susceptibility Calculations

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A scheme for making *ab initio* calculations of the dynamic paramagnetic spin susceptibilities of solids at finite temperatures is described. It is based on time-dependent density functional theory and employs an electronic multiple scattering formalism. Incommensurate and commensurate antiferromagnetic spin fluctuations in paramagnetic Cr and compositionally disordered $Cr_{95}V_5$ and $Cr_{95}Re_5$ alloys are studied together with the connection with the nesting of their Fermi surfaces. We find that the spin fluctuations can be described rather simply in terms of an overdamped oscillator model. Good agreement with inelastic neutron scattering data is obtained. [S0031-9007(99)08949-8]

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Chromium is the archetypal itinerant antiferromagnet (AF) whose famous incommensurate spin density wave (SDW) ground state is determined by the nesting wave vectors $\mathbf{q}_{\mathrm{nest}}$ identified in the Fermi surface [1]. Chromium alloys also have varied AF properties [1] and their paramagnetic states have recently attracted attention owing, in part, to analogies drawn with the high temperature superconducting cuprates especially $(La_cSr_{1-c})_2CuO_4$. The incommensurate SDW fluctuations in these materials [2] are rather similar to those seen in the paramagnetic phase of Cr close to T_N. Moreover "parent" materials La_2CuO_4, in the one instance, and $Cr_{95}Mn_5$ or $Cr_{95}Re_5$, in the other, are simple commensurate AF materials which on lowering the electron concentration by suitable doping develop incommensurate spin fluctuations which may be promoted by imperfectly nested Fermi surfaces.

Here we examine the nature of damped diffusive spin fluctuations in chromium above the Néel temperature T_N which are precursory to the SDW ground state. We also study dilute chromium alloys, $Cr_{95}Re_5$ and $Cr_{95}V_5$, and obtain good agreement with experimental data. For example, recent inelastic neutron scattering experiments [1,3] have measured incommensurate AF "paramagnons," persisting up to high frequencies in the latter system. We explore the temperature dependence, the variation with dopant concentration, and the evolution of the spin fluctuations in these systems from incommensurability to commensurability with increasing frequency and provide the first *ab initio* description of these effects. To this end we describe a new scheme for calculating the wave vector and frequency dependent dynamic spin susceptibility of metals which is based on the time-dependent density functional theory (TDDFT) of Gross *et al.* [4] and as such is an all-electron theory. For the first time the temperature dependent dynamic spin susceptibility of metals and alloys is calculated from this basis. There have been several simple parametrized models to describe the magnetic properties of Cr and its alloys [5]. All of these have concentrated on the approximately nested electron "jack" and slightly larger octahedral hole pieces of the Fermi surface [1] and, at best, have included only the effects of all the remaining electrons via an electron reservoir. We find similarities between our results and results from such models but show that a complete picture is obtained only when an electronic band-filling effect which favors a simple AF ordering at low temperature is also considered. We also find that the spin fluctuations are given an accurate description as overdamped diffusive simple harmonic oscillator modes which are at the heart of theories of the effects of spin fluctuations upon the properties of itinerant electron systems [6].

Over the past few years great progress has been made in establishing TDDFT [4]. Analogs of the Hohenberg-Kohn [7] theorem of the static density functional formalism have been proved and rigorous properties found. Here we consider a paramagnetic metal subjected to a small, time-dependent external magnetic field, $\mathbf{b}(\mathbf{r}, t)$ which induces a magnetization $\mathbf{m}(\mathbf{r}, t)$ and uses TDDFT to derive an expression for the dynamic paramagnetic spin susceptibility $\chi(\mathbf{q}, w)$ via a variational linear response approach [8]. Accurate calculations of dynamic susceptibilities from this basis are scarce (e.g., [9]) because they are difficult and computationally demanding. Here we mitigate these problems by accessing $\chi(\mathbf{q}, w)$ via the corresponding *temperature* susceptibility $\bar{\chi}(\mathbf{q}, w_n)$ where w_n denotes a bosonic Matsubara frequency [10]. We outline this approach below.

The equilibrium state of a paramagnetic metal, described by standard DFT, has density $\rho_0(\mathbf{r})$ and its magnetic response function $\chi(\mathbf{r}t; \mathbf{r}'t') = \{\delta m[b](\mathbf{r}, t)/\delta b(\mathbf{r}', t')\}|_{b=0,\rho_0}$ is given by the following Dyson-type

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equation:

$$\chi(\mathbf{r}t;\mathbf{r}'t') = \chi_s(\mathbf{r}t;\mathbf{r}'t') + \int d\mathbf{r}_1 \int dt_1 \int d\mathbf{r}_2 \int dt_2 \times \chi_s(\mathbf{r}t;\mathbf{r}_1t_1)K_{xc}(\mathbf{r}_1t_1;\mathbf{r}_2t_2)\chi(\mathbf{r}_2t_2,\mathbf{r}'t'). \quad (1)$$

χ_s is the magnetic response function of the Kohn-Sham noninteracting system with the same unperturbed density ρ_0 as the full interacting electron system, and $K_{xc}(\mathbf{r}t;\mathbf{r}'t') = [\delta b_{xc}(\mathbf{r},t)/\delta m(\mathbf{r}',t')]|_{b=0,\rho_0}$ is the functional derivative of the effective exchange-correlation magnetic field with respect to the induced magnetization. As emphasized in Ref. [4] Eq. (1) represents an exact representation of the linear magnetic response. The corresponding development for systems at finite temperature in thermal equilibrium has also been described [8]. In practice approximations to K_{xc} must be made and this work employs the adiabatic local density approximation (ALDA) [4] so that $K_{xc}^{\mathrm{ALDA}}(\mathbf{r}t;\mathbf{r}'t') = \{db_{xc}^{\mathrm{LDA}}[\rho(\mathbf{r},t),m(\mathbf{r},t)]/dm(\mathbf{r},t)\}|_{\rho_0,m=0}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') = I_{xc}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\times\delta(t-t')$. On taking the Fourier transform with respect to time we obtain the dynamic spin susceptibility $\chi(\mathbf{r},\mathbf{r}';w)$.

For computational expediency we consider the corresponding *temperature* susceptibility [10] $\bar{\chi}(\mathbf{r},\mathbf{r}';w_n)$ which occurs in the Fourier representation of the temperature function $\bar{\chi}(\mathbf{r}\tau;\mathbf{r}'\tau')$ that depends on imaginary time variables τ,τ' and w_n as the bosonic Matsubara frequencies $w_n = 2n\pi k_BT$. Now $\bar{\chi}(\mathbf{r},\mathbf{r}';w_n) \equiv \chi(\mathbf{r},\mathbf{r}';iw_n)$ and an analytical continuation to the upper side of the real w axis produces the dynamic susceptibility $\chi(\mathbf{r},\mathbf{r}';w)$. Using crystal symmetry and carrying out a lattice Fourier transform we obtain the following Dyson equation for the temperature susceptibility:

$$\bar{\chi}(\mathbf{x},\mathbf{x}',\mathbf{q},w_n) = \bar{\chi}_s(\mathbf{x},\mathbf{x}',\mathbf{q},w_n) + \int d\mathbf{x}_1\bar{\chi}_s(\mathbf{x},\mathbf{x}_1,\mathbf{q},w_n)I_{xc}(\mathbf{x}_1) \times \bar{\chi}(\mathbf{x}_1,\mathbf{x}',\mathbf{q},w_n), \quad (2)$$

with $\mathbf{x}$,$\mathbf{x}'$ and $\mathbf{x}_1$ measured relative to crystal lattice unit cells of volume V_{WS}.

In terms of the DFT Kohn-Sham Green function of the static unperturbed system,

$$\bar{\chi}_s(\mathbf{x},\mathbf{x}',\mathbf{q},w_n) = -\frac{1}{\beta N}\,\mathrm{Tr}\sum_{\mathbf{R}}\sum_m G(\mathbf{x},\mathbf{x}',\mathbf{R},\mu+i\nu_m) \times G[\mathbf{x}',\mathbf{x},-\mathbf{R},\mu+i(\nu_m+w_n)]e^{i\mathbf{q}\cdot\mathbf{R}}, \quad (3)$$

where $\mathbf{R}$ is a lattice vector between the cells from which $\mathbf{x}$ and $\mathbf{x}'$ are measured, μ is the chemical potential, and ν_m is a fermionic Matsubara frequency $(2n+1)\pi k_BT$. The Green function can be obtained within the framework of multiple scattering (Korringa-Kohn-Rostoker, KKR) theory [11]. This makes this formalism applicable to disordered alloys as well as ordered compounds and elemental metals, the disorder being treated by the coherent potential approximation (CPA) [12]. Then the partially averaged Green function, $\langle G(\mathbf{r},\mathbf{r}',z)\rangle_{\mathbf{r}\alpha,\mathbf{r}'\beta}$, where $\mathbf{r},\mathbf{r}'$ lie within unit cells occupied by α and β atoms, respectively, can be evaluated in terms of deviations from the Green function of an electron propagating through a lattice of identical potentials determined by the CPA ansatz [13].

To solve Eq. (2), we use the direct method of matrix inversion and local field effects are fully incorporated. $\bar{\chi}(\mathbf{q},\mathbf{q};w_n) = (1/V_{WS})\int d\mathbf{x}\int d\mathbf{x}'\,e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}\bar{\chi}(\mathbf{x},\mathbf{x}',\mathbf{q},w_n)$ can then be constructed. The most computationally demanding parts of the calculation are the convolution integrals over the Brillouin zone which result from the expression for $\bar{\chi}_s$; see Eq. (3). Since all electronic structure quantities are evaluated at complex energies, these convolution integrals have no sharp structure and can be evaluated straightforwardly by an application of adaptive quadrature [14].

As discussed in Ref. [10], for example, we can define the retarded response function $\chi(\mathbf{q},\mathbf{q},z)$ of a complex variable z. Since it can be shown [10] formally that $\lim_{z\to\infty}\chi(z) \sim 1/z^2$ and we can obtain $\chi(iw_n)$ from the above analysis it is possible to continue analytically to values of z just above the real axis, i.e., $z = w + i\eta$. In order to achieve this we fit our data to a rational function $\bar{\chi}(\mathbf{q},\mathbf{q},w_n) = \chi(\mathbf{q})[1 + \sum_{k=1}^{M-2}U_k(\mathbf{q})w_n^k]/[1 + \sum_{k=1}^{M}D_k(\mathbf{q})w_n^k]$ with the choice of coefficients U_k, D_k ensuring that the sum rule involving the static susceptibility $\chi(\mathbf{q})$ is satisfied, i.e., $\chi(\mathbf{q}) = (2/\pi)\int_0^\infty dw\,\mathrm{Im}\,\chi(\mathbf{q},\mathbf{q},w)/w$. We find that very good fits are obtained with small M.

For chromium and its alloys, we find that $M = 2$ is sufficient to provide excellent fits to the calculations of $\bar{\chi}$ over a wide range of w_n's, so that $\chi^{-1}(\mathbf{q},\mathbf{q},w) = \chi^{-1}(\mathbf{q})[1 - i(w/\Gamma(\mathbf{q})) - (w/\Omega(\mathbf{q}))^2]$ (standard error $<3\%$ of mean). For the systems studied here we find $\Omega(\mathbf{q})/\Gamma(\mathbf{q}) < 0.15 \ll 1$ and so the *spin dynamics can be described in terms of a heavily overdamped oscillator model*. Evidently $t_{SF}(\mathbf{q}) = \hbar/\Gamma(\mathbf{q})$ represents a relaxation time for a damped diffusive spin fluctuation with wave vector $\mathbf{q}$. Moreover, the imaginary part of the dynamical susceptibility which, when multiplied by $[1 - \exp(-\beta w)]^{-1}$, is proportional to the scattering cross sections measured in inelastic neutron scattering experiments, is written $\mathrm{Im}\,\chi(\mathbf{q},\mathbf{q},w) = \chi(\mathbf{q})w\Gamma^{-1}(\mathbf{q})/\{[1 - (w/\Omega(\mathbf{q}))^2]^2 + (w/\Gamma(\mathbf{q}))^2\}$. We note that theories for the spin fluctuation effects upon itinerant electron properties, including quantum critical phenomena, also invoke such a model [6]. The small $\mathbf{Q}$, $= (\mathbf{q} - \mathbf{q}_0)$, dependence of $\chi^{-1}(\mathbf{q}_0 + \mathbf{Q})$ and $\Gamma(\mathbf{q}_0 + \mathbf{Q})$ is of particular importance. [$\mathbf{q}_0$ is where $\chi^{-1}(\mathbf{q})$ is smallest.]

Finite-temperature calculations were carried out for the static susceptibilities of the three systems, using the experimental bcc lattice spacing of Cr, 2.88 Å, and von Barth–Hedin local exchange and correlation [15]. We find that (i) Cr orders into an incommensurate AF state below 280 K specified by $\mathbf{q}_0 = \{0,0,0.93\}$, where experiment yields $T_N = 311$ K and $\mathbf{q}_0 = \{0,0,0.95\}$ [1]; (ii) $Cr_{95}V_5$ does not develop magnetic order at any

temperature, as found in experiment [1,3]; and (iii) $Cr_{95}Re_5$ orders into a weakly incommensurate AF state below $T = 410$ K ($\mathbf{q}_0 = \{0, 0, 0.96\}$), whereas experimentally it forms a commensurate AF state below T_N of 570 K [1].

Our calculations for $\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$ are shown in Figs. 1(a) and 1(b) for $Cr_{95}V_5$ and $Cr_{95}Re_5$, respectively. Our calculation of $\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$ for paramagnetic Cr at $T = 300$ K is broadly similar to that for paramagnetic Cr at $T = 0$ K by Savrasov [9] so a figure is not presented. It shows incommensurate spin fluctuations for small frequencies which are signified by peaks in $\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$ at $\mathbf{q}_0$ which is equal to the Fermi surface nesting vector $\mathbf{q}_{\mathrm{nest}}$. For increasing w the peaks move to $\mathbf{q} = \{0, 0, 1\}$; i.e., the spin fluctuations become commensurate. The spin fluctuations at 300 K shown in Fig. 1(a) for $Cr_{95}V_5$, on the other hand, remain incommensurate up to much higher frequencies maintaining intensity comparable to that at the peak at low w. This qualitative difference between the two systems has not been described before

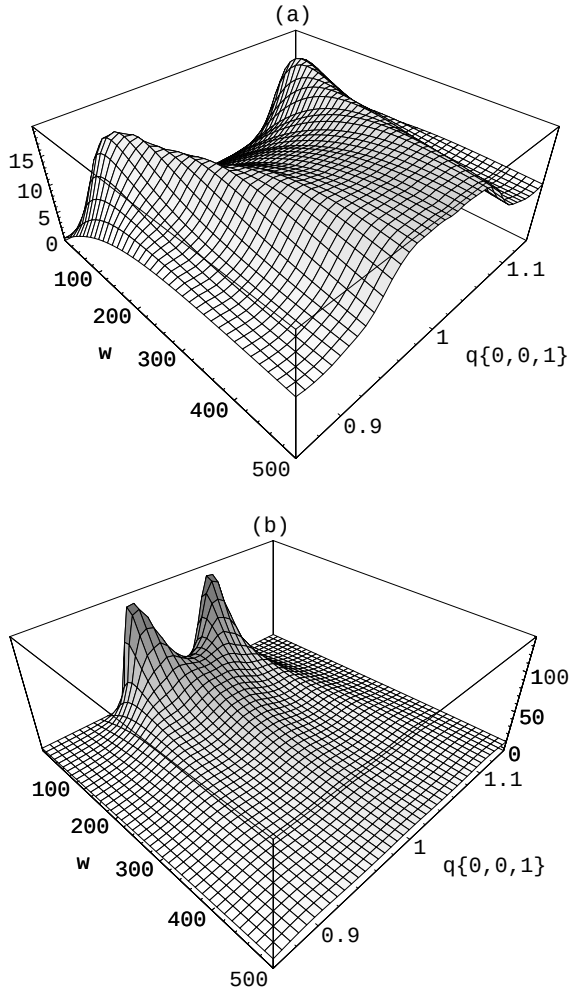

FIG. 1. $\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$ of (a) $Cr_{95}V_5$ at $T = 300$ K and (b) $Cr_{95}Re_5$ at $T = 1.09T_N$ (450 K) in units of $\mu_B^2\,\mathrm{eV}^{-1}$ for wave vectors $\mathbf{q}$ along the $\{0, 0, 1\}$ direction where $\mathbf{q}$ is in units of π/a (a is the lattice spacing). The frequency axis w is marked in meV.

by a first-principles theory although found experimentally [1,3]. For lower temperatures we find that $\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$ of $Cr_{95}V_5$ becomes a sharper function of w and we can also infer that $[1 - \exp(-\beta w)]^{-1}\,\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$ should vanish for small w when $T \to 0$ K. These aspects have also been noted from experimental measurements [1].

It is striking that the alloy's Fermi surface is well defined [12] despite impurity scattering although it is more poorly nested (the difference between the sizes of the electron and hole octahedra is larger) than that of Cr owing to its fewer electrons. Once again the peaks in $\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$ occur at the nesting vectors $\mathbf{q}_{\mathrm{nest}} = \{0, 0, 0.9\}$. The spin fluctuations in the paramagnetic phase of $Cr_{95}Re_5$ are shown in Fig. 1(b). Here adding electrons by doping with Re has improved the Fermi surface nesting so that $\mathbf{q}_{\mathrm{nest}} = \{0, 0, 0.96\}$ and $\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$ has a weight spread from $\mathbf{q}_{\mathrm{nest}}$ to $\{0, 0, 1\}$. The dominant spin fluctuations now rapidly become commensurate with increasing w. We obtain a rather similar picture from the calculations for Cr by artificially raising the chemical potential by a small amount. Interestingly when we account for thermally induced electron-phonon scattering [5] by adding a small shift ($\approx$20 meV) to the Matsubara frequencies ν_m in Eq. (3), we find a tendency for the dominant spin fluctuations to become commensurate at lower w in both Cr and $Cr_{95}Re_5$.

Some of these features also emerge qualitatively from the simple parametrized models based on that part of the band structure near μ which leads to the nested electron and hole octahedra at the Fermi surface [5]. Our "first-principles" calculations, being based on an all-electron theory, however, need some additional interpretation. As analyzed by recent total energy calculations [16], bcc Cr with the experimentally measured lattice spacing tends to form a commensurate AF phase at low temperatures which is modulated by a spin density wave of appropriate wavelength. The overall AF instability of the paramagnetic phase is promoted by the approximate half filling of the narrow $3d$ bands [17] which is further modified by a weak perturbation coming from the Fermi surface nesting. As dopants such as V and Re are added not only is the Fermi surface nesting altered but also the d bands become either farther from or closer to being half filled.

The calculations can be summarized in terms of the damped oscillator model. $\chi^{-1}(\mathbf{q}_0 + \mathbf{Q}) \simeq \chi^{-1}(\mathbf{q}_0) + cQ^2$ for small $\mathbf{Q}$ for Cr and $Cr_{95}V_5$ whereas for $Cr_{95}Re_5$, $\chi^{-1}(\mathbf{q})$ is nearly constant for a range of $\mathbf{q}$ between $\mathbf{q}_{\mathrm{nest}}$ and $\{0, 0, 1\}$. We find the product $\gamma(\mathbf{q})$ of $\chi(\mathbf{q})$ with damping factor $\Gamma(\mathbf{q})$ to be only very weakly temperature dependent in these three systems and $\simeq\gamma(\mathbf{q}_0)$, a constant, for small $\mathbf{Q}$, yielding a dynamical critical exponent [6] of 2 typically assumed for antiferromagnetic itinerant electron systems. The nature of the spin fluctuations can be succinctly described via the variance $\langle m^2(\mathbf{q})\rangle$. From the fluctuation dissipation theorem, $\langle m^2(\mathbf{q})\rangle = (1/\pi)\int_{-\infty}^{\infty} \times dw\,[1 - \exp(-\beta w)]^{-1}\,\mathrm{Im}\,\chi(\mathbf{q}, \mathbf{q}, w)$. Figure 2 shows $\langle m^2(\mathbf{q})\rangle$ at several temperatures for Cr where we have

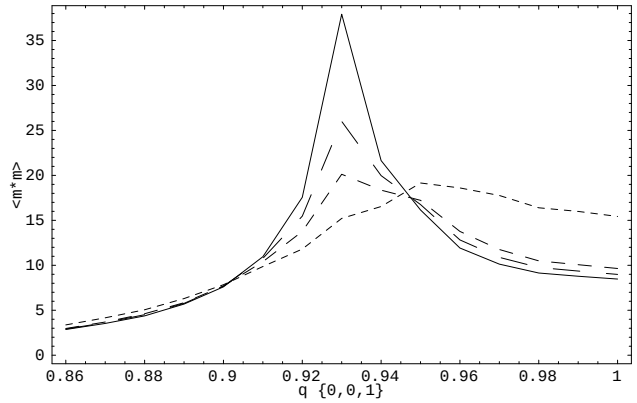

FIG. 2. The variance of the spin fluctuations in Cr $\langle m^2(\mathbf{q})\rangle$ in μ_B^2 for wave vectors $\mathbf{q}$ along the $\{0,0,1\}$ direction at 350 K (solid line), 400 K (long dashed line), 450 K (medium dashed line), and 700 K (short dashed line).

used a frequency cutoff of 500 meV and so have not included the faster of the quantum fluctuations. Near T_N the magnetic fluctuations have their greatest weight around the $\mathbf{q}_{\text{nest}}$. At higher T the peak diminishes and weight grows at $\mathbf{q}$'s nearer $\{0,0,1\}$ reflecting the shift in the peak in $\text{Im}\,\chi(\mathbf{q},\mathbf{q},w)$ from $\mathbf{q}_{\text{nest}}$ to commensurate $\mathbf{q}$'s with increase in frequency w. Similar plots to Fig. 2 for $Cr_{95}V_5$ and $Cr_{95}Re_5$ show, respectively, a smaller and greater tendency for the weight in $\langle m^2(\mathbf{q})\rangle$ to transfer in this way. If the frequency cutoff is reduced, $\langle m^2(\mathbf{q})\rangle$ near $\{0,0,1\}$ is sharply diminished so that the Brillouin zone integral of $\langle m^2(\mathbf{q})\rangle$, $\langle m^2\rangle$ decreases with increasing temperature as inferred from neutron scattering data [1].

We have not included the effects of spin fluctuation interactions, i.e., mode-mode coupling [18] into our calculations and have determined T_N and the static susceptibility by what is essentially an *ab initio* Stoner theory. In weak itinerant ferromagnets, for example, mode-mode coupling causes a dramatic suppression of the Curie temperatures from those estimated from a Stoner theory. For the Cr systems studied here, the fair agreement with experiment which we obtain for T_N and the relatively large value of the damping factor $\Gamma(\mathbf{q})$ with respect to that in weakly itinerant ferromagnets is suggesting that such spin fluctuation effects are small. Spin fluctuation calculations have, however, been carried out by Hasegawa and others for simple parametrized models of Cr neglecting Stoner particle-hole excitations and Fermi surface nesting [19]. Using a functional integral technique he made a high temperature (static) approximation so that all the thermally induced fluctuations were treated classically and found T_N for commensurate AF order to be 370 K and $\sqrt{\langle m^2\rangle}$ to increase linearly with temperature above T_N. A quantitative calculation, however, in which the Stoner particle-hole excitations and spin fluctuations are treated within the same framework is needed to determine unequivocally whether or not a Stoner-like picture is adequate for these systems.

In summary, we have presented a first-principles framework for the calculation of dynamic paramagnetic spin susceptibilities of metals and their alloys at finite temperatures. At this point we add that the approach can also be applied to the study of magnetic excitations in magnetically ordered materials. The first applications on the AF spin fluctuations in Cr and $Cr_{95}Re_5$ above T_N and in paramagnetic $Cr_{95}V_5$ have found good agreement with available experimental data.

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