Spin-wave relaxation in diluted magnetic semiconductors within the self-consistent Green’s function approach

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The authors employ a self-consistent Green’s function approach to investigate the spin-wave relaxation $\Gamma(p)$ in diluted magnetic semiconductors. They find that the trend of the spin-wave relaxation strongly depends on the ratio of the itinerant and impurity spin densities. For density ratios in the Ruderman-Kittel-Kasuya-Yosida phase, $\Gamma(p)$ decreases even though thermal fluctuations increase. On the other hand, in the strong coupling phase, an interesting peak structure appears. They discuss the implications of their numerical results for experiments. © 2006 American Institute of Physics. [DOI: 10.1063/1.2335666]

Carrier-mediated ferromagnetism, found in diluted magnetic semiconductors (DMSs) such as III–V semiconductors doped with transition metals, opens up the possibility of electric manipulations of magnetic and optical properties because of the exchange coupling between the localized moments of the transition metal and the itinerant spins in the semiconducting bands. In recent years, experimental progress has stimulated intense theoretical investigations of DMSs, which mainly focus on estimates of the critical temperature. Although some experimental data are available, little theoretical attention has been paid to spin dynamics, which is crucially important in understanding the spin coherence.

To analyze how spin waves relax in DMS, both the itinerant and impurity spins need to be treated on an equal footing. In this letter, we employ the self-consistent Green’s function approach, which retains both spatial and thermal averages. To complete the self-consistency, it is necessary to introduce another Green’s function which describes the correlations between the itinerant and impurity spins, $i\hat{D}(r_1, r_2; t) = \langle [\hat{S}^+ (r_1, t) \hat{S}^- (r_2, 0)] \rangle$, where $T$ is the time ordering operator and the double bracket implies both quantum and thermal averages. To simplify the calculations, we assume that the disorders is not strong, i.e., not close to the percolation threshold, and the virtual crystal approximation is valid. Therefore, after a coarse-graining procedure, the translational invariance is approximately restored and the Green’s functions only depend on the relative distance. This approximation is justified by $=150$ meV nm$^3$ and the impurity spin density $n_i = 1$ nm$^{-3}$ but vary the ratio of itinerant to impurity spin densities $n_p/n_i$ in the following.

We now introduce the self-consistent Green’s function approach. Note that, instead of treating spin waves as bosons, the Green’s function approach respects the spin kinematics which is crucially important when thermal fluctuations are not small. The thermal Green’s function, describing the (impurity) spin-wave propagation, is defined as $i\hat{D}(r_1, r_2; t) = \langle [\hat{S}^+ (r_1, t) \hat{S}^- (r_2, 0)] \rangle$, where $T$ is the time ordering operator and the double bracket implies both quantum and thermal averages. To complete the self-consistency, it is necessary to introduce another Green’s function which describes the correlations between the itinerant and impurity spins, $i\hat{D}(r_1, r_2; t) = \langle [\hat{S}^+ (r_1, t) \hat{S}^- (r_2, 0)] \rangle$. To simplify the calculations, we assume that the disorder is not strong, i.e., not close to the percolation threshold, and the virtual crystal approximation is valid. Therefore, after a coarse-graining procedure, the translational invariance is approximately restored and the Green’s functions only depend on the relative distance. This approximation is justified by

![Graph](image)

FIG. 1. (Color online) Spin spectral function $A(p; \Omega)/(2(\Omega^2))$ at temperatures $T = 2$ and $28$ K with density ratio $n_p/n_i = 0.3$. Against common intuition, the half-width shrinks as the temperature increases.
The spin-wave propagator is solved, \( F(\mathbf{k}, \mathbf{k} + p; \Omega) \), which found that magnetization curves with different disorder configurations are almost identical.

The dynamical equations for the Green’s functions can be derived by the standard approach and higher-order Green’s functions may be decoupled within the random phase approximation. Making use of the translational invariance and the decoupling scheme, the dynamical equation for \( D(r; t) \) in the Fourier space is

\[
\Omega D(p, \Omega) = 2\langle S^2 \rangle - J(\sigma^2)D(p, \Omega) + J\langle S^2 \rangle \int \frac{d^3k}{(2\pi)^3} F(k, k + p; \Omega),
\]

where \( F(\mathbf{k}, \mathbf{k} + p; \Omega) \) is the Fourier transformed Green’s function \( F(r, r'; t) \). Similarly, the other dynamical equation is

\[
\langle \Sigma(p, \Omega) \rangle = \frac{2\langle S^2 \rangle}{\Omega - \Sigma(p, \Omega) + i\gamma},
\]

where the prefactor \( 2\langle S^2 \rangle \) comes from the exact treatment of spin-wave kinematics. The self-energy \( \Sigma(p, \Omega) \) arises from interactions between the itinerant and the impurity spins and contains two terms,

\[
\Sigma(p, \Omega) = -J(\sigma^2) + \Delta \int \frac{d^3k}{(2\pi)^3} G(k, k + p; \Omega).
\]

If only the first term is retained, it coincides with the Weiss mean-field approximation. However, since the first term is always real, dropping the second term would remove all information about the Landau damping of the spin waves, described by the imaginary part of the self-energy \( \Sigma_I(p, \Omega) \), inside the Stoner continuum.

Once the spin-wave dispersion is obtained from \( \omega_p = \Sigma_I(p, \omega_p) = 0 \), the polarization of the impurity spins can be computed by Callen’s formula

\[
\langle S^2 \rangle = \langle n_{sw} \rangle + \frac{(2S + 1)(\langle n_{sw} \rangle)^{2S+1}}{(1 + \langle n_{sw} \rangle)^{2S+1} - \langle n_{sw} \rangle^{2S+1}},
\]

where the average number of spin waves is \( \langle n_{sw} \rangle \) and \( (\langle n_{sw} \rangle) = (1/n_p) \int d^3k/(2\pi)^3 [e^{\beta\omega_q} - 1]^{-1} \). The difference between the independent spin-wave theory and the self-consistent Green’s function method lies in the third term, which correctly accounts for the spin kinematics. The magnetization curves for different density ratios \( n_i/n_f \) are shown in Fig. 2. While this is not the main focus of our results, we emphasize the sensitivity in the shape of the magnetization curve to the density ratio. From previous studies in the diffusive regime, there are three phases for the Zener model—mean-field, RKKY, and strong coupling. For \( n_i/n_f = 0.3 \), it lies in the strong coupling phase and the magnetization curve decreases linearly with a very small gradient and, only in the narrow regime near the critical temperature, the magnetization diverges to zero and the phase transition occurs. Similar magnetization curves, quite different from what we expect for a Heisenberg-like model, have been observed in some experiments.19 Finally, we choose \( n_i/n_f = 0.01 \) (also in the strong coupling phase) to demonstrate that the magnetization curve can turn concave, though this is not necessarily related to percolation near the metal-insulator transition.

The unique feature of the Green’s function approach is that we can also study the temperature evolution of the spin spectral function, \( A(p, \omega) = -(1/\pi)\text{Im } D(p, \Omega) \), as shown in Fig. 1. From Eq. (4), the imaginary part of the spin-wave propagator takes the Lorentzian form

\[
A(p, \omega) = 2\langle S^2 \rangle \frac{Z}{\pi} \frac{\Gamma(p)}{(\Omega - \omega_p)^2 + \Gamma(p)^2},
\]

where \( Z = 1 \) is the spectral weight for the gapless spin wave. After the Taylor expansion of \( \Sigma_I(p, \Omega) \) in the vicinity of the spin-wave dispersion \( \Omega = \omega_p \), the relaxation rate of the spin waves \( \Gamma(p) = \Sigma_I(\omega_p) \). The numerical results for the spin-wave relaxation rate versus temperature with \( n_i/n_f = 0.3, 0.1 \) are shown in Fig. 3. One may expect that increasing thermal fluctuations lead to an increasing relaxation rate, but our numerical results show a decrease in the relaxation rate in the high-density regime.

![FIG. 2. (Color online) Magnetization curves of impurity and itinerant spins at different density ratios \( n_i/n_f = 0.01, 0.1, 0.3 \).](image1)

![FIG. 3. (Color online) Spin-wave relaxation rate \( \Gamma(p) \) at different momenta and density ratios \( n_i/n_f = 0.3, 0.1 \). The solid (broken) lines correspond to the left (right) axis.](image2)
merical results disagree. In the RKKY phase with \( n_h/n_I = 0.3 \), the spin relaxation rate \( \Gamma(p) \) decreases as the tempera-
ture increases. This reduction can be understood as the weak-
ening of the effective coupling strength between the itinerant and impurity spins in proportion to the spin polarization.
However, since the decoupling scheme in the self-consistent
approach only includes decaying channels in the diagonal
parts (as in all random phase approximations), the computa-
tion of \( \Gamma(p) \) breaks down in the vicinity of the critical
temperature where off-diagonal channels dominate. Therefore,
one should not take the vanishing \( \Gamma(p) \) at the Curie tempera-
ture seriously. However, in the low temperature regime, the
diagonal channels do dominate and our numerical result of
decreasing \( \Gamma(p) \) with increasing temperature is a real effect.

In the strong coupling phase with \( n_h/n_I = 0.1 \), the trend of
the spin relaxation is completely different. The spin relax-
ation \( \Gamma(p) \) is small and does not change much at low tem-
peratures, then a peak structure appears just before hitting the
critical temperature. This nonmonotonic trend can be explained
by the energy shift of the Stoner continuum. In the strong
coupling phase, the Stoner continuum is separated from the gapless
spin waves at low temperatures by a finite gap. The gap suppresses
\( \Gamma(p) \) and makes it insensitive to temperature changes. The gap
disappears at the temperature where the polarization of the itinerant spins \( \langle \sigma^z \rangle \) is no longer
totally polarized. Due to the intersection of the spin-wave dis-

cersion and the Stoner continuum, enhanced spin relaxation
is expected. An analysis of our numerical results reveals that
the partial polarization of \( \langle \sigma^z \rangle \) and the peak in \( \Gamma(p) \) occur at the
same temperature.

One may notice the close relationship between the mag-
netization curve and the spin relaxation rate and their sensi-
tive dependence on the density ratio \( n_h/n_I \). This is reminis-
cent of the interesting differences between as-grown samples and
annealed ones.\(^1\) The annealing process removes intersti-
tial impurities and reduces the disorder strength. However, if
the as-grown sample is already in the diffusive regime, the
annealed one can also be described by the virtual crystal
approximation. We believe that the major difference arises
from the increase in carrier density and thus the density ratio
\( n_h/n_I \). The annealing process increases \( n_h/n_I \) from the strong
coupling to the RKKY phase which changes the shape of the
magnetization curve. Therefore, it would be exciting to study the
spin dynamics for both as-grown and annealed samples and
compare the experimental outcomes with our numerical
predictions. Note that we did not include the realistic six-
band Luttinger model here. In principle, our approach can be
generalized to include more bands by introducing more
Green’s functions but the self-consistent equations will be
rather complicated, not fatal though. However, it is important
to emphasize that the ratio \( n_h/n_I \) to enter the RKKY regime
is expected to be larger, as compared to the estimate from the
two-band model.

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