Phonon-assisted magnetopolaron effect in diluted magnetic semiconductors

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A phonon-assisted magnetopolaron effect in diluted magnetic semiconductors is theoretically investigated. It is shown that the binding energy of magnetic polarons can be substantially enhanced if coupling between the magnetic and phonon subsystems is taken into account. In the particular case of ''soft'' lattice dynamics, the stability range of the hole-induced magnetic polaron can be extended to temperatures of a few tens of kelvin and magnetic fields of several tesla. [S0163-1829(99)06104-4]

I. INTRODUCTION

The concept of magnetic polarons (MP's) (or, more precisely, paramagnetic polarons) was introduced in the 1970s[1,2] and became especially interesting for its role in the understanding of diluted magnetic semiconductors (DMS's).[3–6] The exchange interaction between the spin of a free charge carrier and the spins of magnetic ions substantially modifies the energy bands in a magnetic field, giving rise to new spin-dependent phenomena observable at low temperatures. This interaction leads to a noticeable alignment of localized magnetic moments even in the absence of an external magnetic field. Such a local polarization results in the splitting of spin states both for electrons and for holes. The charge carrier, in turn, holds the polarization cloud which causes the appearance of a self-consistent MP state.

It is worthwhile mentioning that considerable recent attention has also been focused on MP physics in studies of high-temperature superconductivity. An analysis conducted in the framework of the t-J model[7] revealed the possibility of a hole-hole superconductive pairing, with a single hole being a magnetic polaron of small radius (see Ref. 8).

Although there is abundant evidence for bound magnetic polaron existence,[9,10] the severely restrictive conditions required for free magnetic polaron (FMP) stability have made this sort of polaron very difficult to observe experimentally. According to Kasuya *et al.*,[1] a polaron becomes stable when its free energy approaches zero, a condition that cannot be satisfied at temperatures above about 1 K for the electron due to its small mass and the comparatively small exchange constant value for all known DMS's. Stability conditions are more favorable for the FMP associated with a hole, but are still strongly dependent on the content of the magnetic component, the temperature, and the details of the band structure. Calculations of the stability of the hole-type FMP in $Zn_{1-x}Mn_xSe$ have shown that the hole-type FMP is stable only for temperatures below some characteristic value T_d, which for $x=0.05$ is in the range of 0.2–1 K.[11] The value of T_d for the electron-type FMP is expected to be about one or two orders of magnitude smaller.

Several experiments, on the other hand, show evidence of MP existence at temperatures higher than 1 K.[12–16] Golnik *et al.*[12] explain a peak in luminescence from $Cd_{1-x}Mn_xTe$, which is visible for $x\approx 0.05$ and dominates the exciton-related luminescence spectrum for $x\geqslant 0.1$, as originating from a magnetically localized exciton formation. In experiments on spin-flip Raman scattering and luminescence, Warnock *et al.*[13] observe peculiarities in the spin relaxation of the Stokes-shifted radiation as well as a shift with narrowing of the exciton luminescence towards that of a free exciton when the CdMnSe(Te) crystals were measured in a magnetic field.

Unusual luminescence data were also reported recently for $Hg_{1-x}Mn_xTe$ single crystals $(0.09\leqslant x\leqslant 0.20)$.[14–16] Simple theoretical estimates indicate that exciton states within the mobility gap exist approximately 1 meV below the bottom of conduction band. Luminescence from these levels is difficult to detect experimentally at zero magnetic field due to the presence of a band tail. Occasionally, however, a weak luminescent signal transforms into a strong and surprisingly narrow peak, increasing in intensity as the magnetic field is increased. It appears possible to treat this behavior as if it were due to the formation of a gap in the electron density of states, with the exciton states being within the gap at some intermediate value of the magnetic field. According to the theory developed by Karpov and Tsidil'kovskii[17] for diluted magnetic semiconductors, a gap in the density of states in a band tail originates from the magnetopolaron effect. The magnetic field shifts the effective gap to lower energies. Additionally, the magnetic field controls the position of the exciton energy level through the modification of the exciton localization length. As the magnetic field is varied, the repositioning of the energy levels

can lead to a shift of the exciton level into the gap, resulting in the appearance of an excitonic state and, hence, of a luminescence signal. Thus, the key point here is the existence of the MP, which allows the existence of the gap in the electron density of states. The commonly used models for the magnetopolaron restrict the MP state to temperatures below about 1–2 K, whereas MP-associated effects have been observed at 5–10 K.

In this paper the problem of the MP-phonon interaction is solved analytically within the ''exchange box'' model. Our study shows that taking the magnetic polaron-phonon interaction into account can explain the enhancement of the characteristic temperature of MP formation and, therefore, provides a formal theoretical basis for our earlier experimental results.[14–16]

II. MODEL AND DISCUSSION

The qualitative and quantitative description of autolocalization of the electron state due to the exchange interaction with the magnetic subsystem has been presented by several authors.[4–6] If the magnetic system is in the paramagnetic phase, magnetization fluctuations result in a stable discrete electron level, provided that the free energy is diminished. Ordinarily, the electron-localized ion exchange interaction is considered as[18]

$$H_{exc}=-2\sum_{j=1}^{N_m} A_j \vec{S}_e\cdot\vec{S}_m^j, \tag{1}$$

where $A_j=JV_c|\psi(R_j)|^2$, J is the exchange parameter, V_c is the volume of the unit cell, $\psi(R)$ is the spatial part of the electron wave function, and the index j runs over all localized spin moments (LSM's). The direct spin-spin exchange interaction between magnetic ions is taken into account phenomenologically by introducing an effective temperature of the Curie-Weiss parameter type and the effective concentration, which excludes the part of the ions forming antiferromagnetic clusters. It is also possible to take into account the influence of an external magnetic field by adding the Zeeman contributions for electron and localized magnetic spins to Eq. (1) ($\hbar=1$):

$$H_{exc}=-2\sum_{j=1}^{N_m} A_j\vec{S}_e\cdot\vec{S}_m^j+\omega_0\left(S_{e_z}+\sum_{j=1}^{N_m} S_{m_z}^j\right), \tag{2}$$

where

$$\omega_0=g_m\mu_B H\left(1+\left[\frac{g_e}{g_m}-1\right]\frac{S_{e_z}}{S_{e_z}+\sum_{j=1}^{N_m} S_{m_z}^j}\right)\simeq g_m\mu_B H, \tag{3}$$

g factors are assumed to be isotropic for simplicity, μ_B is the Bohr magneton, and the z axis is aligned with the magnetic field H.[19] In Eq. (1) or (2), the electron wave function $\psi(R)$ is usually found through a self-consistent variational procedure. As a rule, the hydrogenlike trial function

$$\psi(R)=\frac{1}{\sqrt{\pi a^3}}\exp(-R/a) \tag{4}$$

is chosen, where the unique variational parameter a converts to the effective-mass Bohr radius a_B^* in the limiting case of small exchange contribution.

As the analysis[3,18] shows, once the central limit theorem is applicable to the problem, the specific form of the $A_j(R)$ dependence is only indirectly responsible for the spin fluctuation distribution, which remains Gaussian in form. Since in our case the inequality $n_m a^3\gg 1$ (where n_m is the concentration of magnetic ions) takes place, there is a sufficient number of localized uncorrelated magnetic spins to make the central limit theorem applicable.

Thus, in this case it is possible to confine consideration to the ''exchange box'' model Hamiltonian[4] of the form

$$H_{exc}=-2\overline{A}\sum_{j=1}^{\overline{N}} \vec{S}_e\cdot\vec{S}_m^j, \tag{5}$$

where a step function is substituted in Eq. (1) instead of $\psi(R)$. Here

$$\overline{A}=\frac{Jx}{\overline{N}},\quad \overline{N}=n_m\overline{V},\quad \overline{V}=\gamma a^3,$$

x is the molar fraction of magnetic ions, and γ is a numerical factor, which determines the dispersion of the spin fluctuations in the system. $\overline{N}$ is the number of particles enclosed by the box with volume $\overline{V}$.

In other words, we replace the nonuniform rapidly decaying interaction over all space, by a uniform interaction over a finite space. The specific form of the $\psi(R_j)$ dependence only affects the numerical coefficient γ.[4]

The Hamiltonian of Eq. (1) commutes with the operator of total spin of the LSM system. Once the finite number $\overline{N}$ has been determined, the eigenvalue spectrum of H_{exc} may be characterized by, among other quantum numbers, the total spin $F=|\vec{S}_e+\vec{S}_\Sigma|$ and μ, the projection of $\vec{F}$ on the direction of the magnetic field H (if $H\neq 0$). Alternatively, we may specify the system's state by $f=F-S_\Sigma$ and μ, where different values of f correspond to states where the electron spin is aligned with the total spin of the localized magnetic system $\vec{S}_\Sigma$ or opposed to it.

A standard technique for the determination of $\overline{N}$ was developed in Ref. 4, where $\overline{V}$ is assumed to be the volume of the region where the spectrum of spin fluctuations corresponding to the Hamiltonian of Eq. (5) agrees with the original spectrum that corresponds to Eq. (1), with $\psi(R)$ being determined by Eq. (4). The fitting constant has been evaluated to be about $\gamma\approx 26$.

Now let us consider the spectrum of Eq. (1). The nonuniformity of the exchange interaction is bound to some lattice distortion because the localized magnetic ions surrounding an electron tend to rearrange themselves so as to minimize their energy.

To include the contribution of spin-phonon coupling to the ''exchange box'' Hamiltonian of Eq. (5), we analyze the exchange coefficient $A_j \propto |\psi(R_j)|^2$ in Eq. (1). The displacement of an ion from its equilibrium position at a lattice site j results in the change of the electron wave function $\psi(R_j)$ induced by the deformation generator[20,21]

$$V=\exp\left[\sum_j v_j \frac{\partial}{\partial u_j}\right].$$

The displacement v_j may be in general expressed as a Fourier series of the form

$$v_j=\sum_k c_k e^{-ikR_j^0},$$

where c_k is the displacement amplitude of a mode with the momentum k and[22]

$$\frac{\partial}{\partial u_j}=\sum_{\alpha,k}\left[\frac{M_i\Omega_{\alpha,k}}{2N_i}\right]^{1/2} e(\alpha,k)[a_{\alpha,k}e^{ikR_j^0}-a^{\dagger}_{\alpha,-k}e^{-ikR_j^0}].$$

Here R_j^0 is the ion equilibrium position, $e(\alpha,k)$ is the polarization vector, and $a^{\dagger}_{\alpha,k}$ and $a_{\alpha,k}$ are the creation and annihilation operators of a phonon with the momentum k, polarization direction α, and frequency $\Omega_{\alpha,k}$. Thus we get

$$V=\exp\left(\sum_{\alpha,k}\left[\frac{M_iN_i\Omega_{\alpha,k}}{2}\right]^{1/2} e(\alpha,k)[c_k a_{\alpha,k}-c_{-k}a^{\dagger}_{\alpha,-k}]\right),$$

where M_i and N_i are the ionic mass and the number of ions, respectively. To first order in the displacement we obtain

$$|\psi(R_j)|^2 \simeq |\psi(R_j^0)|^2+\sum_{\alpha,k}\left[\frac{M_iN_i\Omega_{\alpha,k}}{2}\right]^{1/2} \times e(\alpha,k)[c_k+c_k^*][a_{\alpha,k}+a^{\dagger}_{\alpha,-k}]|\psi(R_j^0)|^2. \tag{6}$$

Thus, we arrive at the model Hamiltonian

$$H_t=-2\overline{A}\vec{S}_e\cdot\vec{S}_\Sigma+\omega_0(S_{e_z}+S_{\Sigma_z})-\sqrt{2\overline{A}}(\vec{S}_e\cdot\vec{S}_\Sigma) \times\sum_{\alpha,k} g_{ph}(\alpha,k)(a_{\alpha,k}+a^{\dagger}_{\alpha,-k})+\sum_{\alpha,k}\Omega_{\alpha,k}a^{\dagger}_{\alpha,k}a_{\alpha,k}, \tag{7}$$

where the last term represents the pure phonon contribution and $g_{ph}(\alpha,k)$ is the spin-phonon coupling function:

$$g_{ph}(\alpha,k)\simeq[M_iN_i\Omega_{\alpha,k}]^{1/2}e(\alpha,k)[c_k+c_k^*].$$

It seems reasonable to suppose a further stabilization of the system due to the spin-phonon interaction. Physically, the tendency of magnetic ions to be pulled into the region ''polarized'' by the carrier spin leads to a local distortion of the magnetic subsystem, which in turn results in the strengthening of carrier localization.

One can partially diagonalize the Hamiltonian of Eq. (7) $\tilde{H}_t=U^{-1}H_tU$ with the matrix

$$U=\exp\left[-\sqrt{2\overline{A}}(\vec{S}_e\cdot\vec{S}_\Sigma)\sum_{\alpha,k} g_{ph}(\alpha,k)(a_{\alpha,k}-a^{\dagger}_{\alpha,-k})\right]. \tag{8}$$

As a result we get

$$\tilde{H}_t=-2\overline{A}\vec{S}_e\cdot\vec{S}_\Sigma+\omega_0(S_{e_z}+S_{\Sigma_z})-2\overline{A^2}\chi S_e^2S_\Sigma^2 +\sum_{\alpha,k}\Omega_{\alpha,k}a^{\dagger}_{\alpha,k}a_{\alpha,k}, \tag{9}$$

where

$$\chi=\sum_{\alpha,k}\frac{g_{ph}(\alpha,k)g_{ph}(\alpha,-k)}{\Omega_{\alpha,k}}. \tag{10}$$

The appropriate eigenstates are characterized by three numbers S_Σ, μ, f and correspond to the energy:

$$\varepsilon_{S_\Sigma,\mu,f}=-2\overline{A}f\left(S_\Sigma+\frac{1}{2}\right)+\frac{\overline{A}}{2}+\omega_0\mu-\frac{3}{2}\overline{A^2}\chi S_\Sigma(S_\Sigma+1) +\sum_{\alpha,k}\Omega_k(n_k+1/2). \tag{11}$$

It is necessary to calculate the partition function $Z(k_B=1)$:

$$Z=\sum_{f=-1/2}^{1/2}\sum_{S_\Sigma=\sigma}^{\overline{N}S_M}\sum_{\mu=-S_\Sigma-f}^{S_\Sigma+f} U_\mu^{S_\Sigma}\exp[-\beta\varepsilon_{S_\Sigma,\mu,f}], \tag{12}$$

where $\sigma=0$ or 1/2 depending on whether $2\overline{N}S_M$ is even or odd, and $\beta=1/T$. The calculation shows that the weight $U_\mu^{S_\Sigma}$ of the state specified by the total spin S_Σ and its projection μ can be expressed as the weight difference for states specified by the total spin projection[4]

$$U_\mu^{S_\Sigma}=U_{S_\Sigma-1}-U_{S_\Sigma}=U_{S_\Sigma}-U_{S_\Sigma+1}, \tag{13}$$

which does not depend on μ.

Thus, the summation of Z over μ reduces to the much simpler form

$$Z_0=\sum_{-\overline{N}S_M}^{\overline{N}S_M}U_\mu\exp[-\beta\omega_0\mu] =\sum_{\sigma}^{\overline{N}S_M}(2-\delta_{\mu,0})U_\mu\cosh[-\beta\omega_0\mu],$$

which is well known to be

$$Z_0=\left\{\frac{\sinh[\beta\omega_0(S_M+1/2)]}{\sinh[\beta\omega_0/2]}\right\}^{\overline{N}}. \tag{14}$$

Finally we deduce

$$Z=Z_{ph}\frac{e^{\beta\lambda(\overline{S}_\Sigma-1/2)}}{2\sinh[\beta\omega_0/2]}(e^{-\beta\overline{A}}[K_1^--K_1^+] +e^{\beta\omega_0}K_2^+-e^{-\beta\omega_0}K_2^-), \tag{15}$$

where Z_{ph} is the pure phonon contribution.

Here we introduced

$$K_{1,2}^{\pm}=K(x_{1,2}\pm\beta\omega_0),$$

$$K(x)=\left\{\frac{\sinh[x(S_M+1/2)]}{\sinh[x/2]}\right\}^{\overline{N}},\quad x_{1,2}=\beta\left(\overline{A}\mp\frac{\lambda}{2\overline{S_\Sigma}}\right),$$

and

$$\lambda=\frac{3}{2}\overline{A^2}\chi(\overline{S_\Sigma}+1),\quad \overline{S_\Sigma}=\frac{1}{\beta}\frac{1}{\tilde{Z}}\frac{\partial\tilde{Z}}{\partial\lambda},$$

with $\tilde{Z}=Z/Z_\infty$ being the normalized partition function, which is further described in the discussion below.

The correct procedure requires that we retain only those contributions to Z that correspond to the localized magnetic polaron state formation. When $\overline{N}\to\infty$, the region of localization grows ($a\to\infty$) and the electron becomes free. This means that Z in Eq. (15) should be normalized to

$$Z_\infty=K(\beta\omega_0)\frac{\sinh[\beta(\omega_0+y)]-\sinh[\beta y]}{\sinh[\beta\omega_0/2]},\qquad(16)$$

where

$$y=Jxb_{S_M}(\beta\omega_0),$$

where $b_{S_M}(\beta\omega_0)$ is the Brillouin function. In the absence of a magnetic field $\omega_0=0$ and Eq. (16) reduces to

$$Z_\infty^0=2(2S_M+1)^{\overline{N}}.$$

Finally, $\overline{S_\Sigma}$ is determined self-consistently as

$$\frac{2}{\overline{N}}\overline{S_\Sigma^2}=\frac{e^{-\beta\overline{A}}[K_1^+b_1^+-K_1^-b_1^-]+e^{\beta\omega_0}K_2^+b_2^+-e^{-\beta\omega_0}K_2^-b_2^-}{e^{-\beta\overline{A}}[K_1^--K_1^+]+e^{\beta\omega_0}K_2^+-e^{-\beta\omega_0}K_2^-}$$

$$-b_{S_M}(\beta\omega_0)\frac{\cosh[\beta(\omega_0+y)]+\cosh[\beta y]}{\sinh[\beta(\omega_0+y)]-\sinh[\beta y]},\qquad(17)$$

where $b_{1,2}^{\pm}=b_{S_M}(x_{1,2}\pm\beta\omega_0)$. When $\overline{N}$ tends to infinity, $\overline{S_\Sigma}$ tends to zero.

The magnetic part of free energy can be determined as

$$F_m=-T[\ln Z-\ln Z_{ph}-\ln Z_\infty].\qquad(18)$$

Apart from F_m one should add to the total free energy the kinetic contribution originating from the uncertainty principle

$$F_k\simeq\frac{1}{2m^*a^2},\qquad(19)$$

where m^* is the effective electron mass. The equation for the equilibrium value of the localization length $\tilde{a}$ is

$$\frac{\partial F_m}{\partial a}+\frac{\partial F_k}{\partial a}=0.\qquad(20)$$

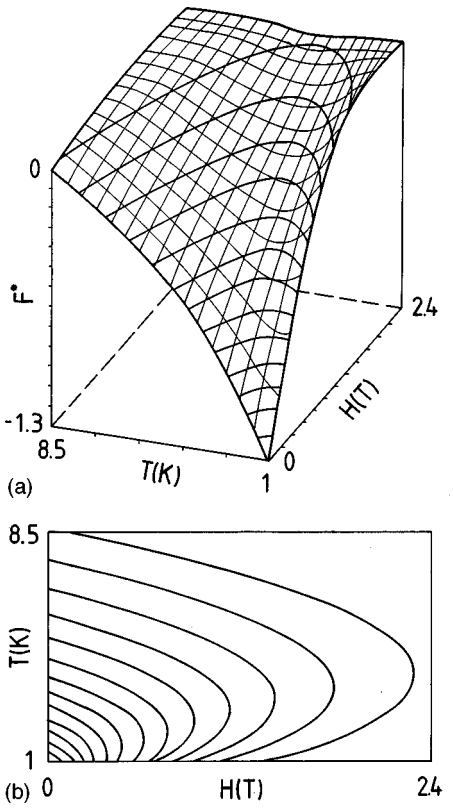

FIG. 1. Free energy versus temperature and magnetic field in the absence of a spin-lattice interaction, $\chi=0$, for the common set of parameters: $J=-0.8$ eV, $m_h^*\simeq0.1m_e$, $x=0.1$, $S_h=3/2$, $S_M=5/2$ (Mn^{2+}). (a) $F^*(T,H)$ plot; F^* is taken in units $|Jx|$. (b) Isoenergy cross sections of the $F^*(T,H)$ dependence.

When the value of the total free energy $F_t=F_m+F_k$ corresponding to the root $\tilde{a}$ of Eq. (20) is negative, there appears a localized magnetic polaron state.

From an experimental point of view it is more interesting to discuss the hole magnetic polaron instead of the electron one because the former appears at helium temperatures, whereas the latter exists only at milli-kelvin temperatures. To do this we need to substitute m_h^* for m^* in Eq. (19) and also $\vec{S}_h$ for $\vec{S}_e$ in Eq. (9) which in particular causes the parameter λ in Eq. (15) to increase.

First we analyze the case of no spin-lattice interaction. To discuss the possibility of MP existence we consider the free energy behavior, namely, the $F_t(a)$ or $F_t(\overline{N})$ dependence. Qualitative patterns for the principal regimes show a two-minimum curve. The MP formation occurs when the local minimum of the $F_t(a)$ curve at $a\neq0$ becomes absolute and, hence, the proper free energy value $F^*=F_t(\tilde{a})$ becomes negative.

Using this criterion it is possible to examine the behavior of F^* for different values of T and H (Fig. 1). The nontrivial feature here is that the temperature increase originally favors the polaron formation at higher magnetic field values. The reason for this lies in the fact that the intensive magnetic field freezes the ion's spins, preventing their rearrangement which is necessary for hole spin localization. The temperature growth acts in the opposite way and so facilitates the spin realignment.

Now we consider the case of a nonzero spin-lattice inter-

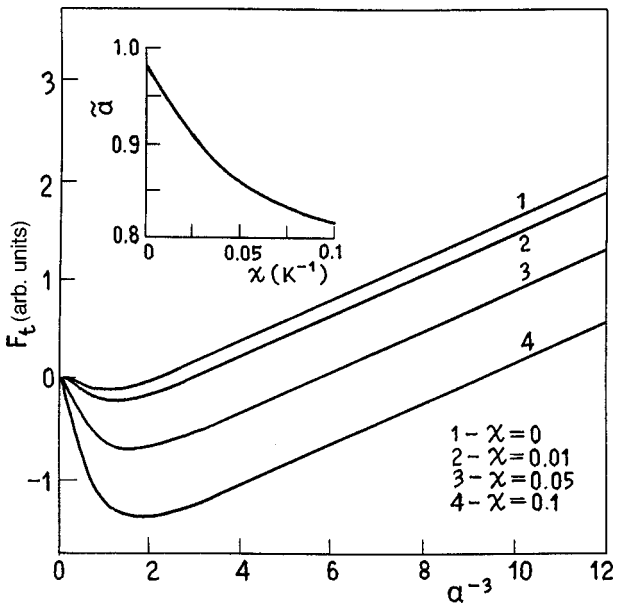

FIG. 2. Free energy dependence F_t versus a^{-3} for different spin-lattice coupling χ. Dimensionless parameter a is presented in units of $(|J|x/k_BTn_m\gamma)^{1/3}$. $T=2$ K. All parameters are the same as in Fig. 1. Inset: dependence of the MP radius on parameter χ.

action and, hence, allow the ions to shift from their equilibrium lattice positions. This shift results in a potential well which further localizes the hole. Figure 2 depicts the $F_t(a^{-3})$ dependence for different strengths of spin-lattice coupling in the particular case of magnetic field $H=1$ T and temperature $T=2$ K. The MP radius $\tilde{a}$ diminishes with increasing χ value as shown in the inset of Fig. 2. We can also introduce the characteristic temperature of the MP state formation T_d which corresponds to the condition $F_t(\tilde{a})=0$. The dependence of T_d on the spin-lattice coupling parameter χ is presented in Fig. 3 for different values of the magnetic field. The growth of the absolute value of χ results in an increased T_d.

To evaluate χ we consider Eq. (10). Inasmuch as the mean internal energy is represented as[23]

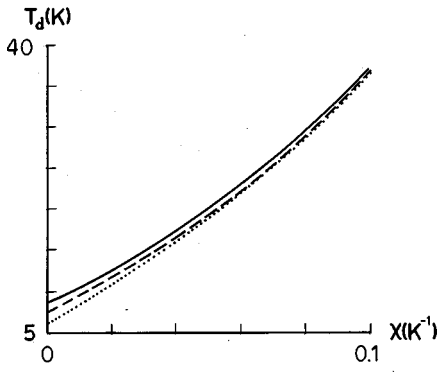

FIG. 3. The dependence of the characteristic temperature for MP formation T_d on the spin-lattice coupling strength for different intensities of applied magnetic field. The set of material parameters is the same as in Fig. 1. $H=0$ (solid line), $H=1$ T (dashed line), $H=2$ T (dotted line).

$$\overline{\varepsilon}=\sum_{\alpha,k} N_i M_i \Omega_{\alpha,k}^2 |U_{\alpha,k}|^2=\sum_{\alpha,k} (\overline{N}_k+1/2)\Omega_{\alpha,k}, \quad (21)$$

where

$$\overline{N}_k=[\exp(\Omega_k/T)-1]^{-1}$$

and $|U_{\alpha,k}|^2$ is the square of displacement amplitude, we get

$$\chi\simeq\sum_{\alpha,k}\frac{1}{\Omega_{\alpha,k}}(1/2+[\exp\Omega_{\alpha,k}/T-1]^{-1})$$

or

$$\chi\simeq 3\overline{N}\int\frac{d\Omega}{\Omega}D(\Omega)(1/2+[\exp\Omega/T-1]^{-1}), \quad (22)$$

where $D(\Omega)$ is the density of phonon states. In the framework of the Debye model Eq. (22) simply reduces to

$$\chi\simeq\frac{9}{4}\frac{\overline{N}T^2}{\Theta^3}\int_0^{\Theta/T}(1/2+[\exp z-1]^{-1})z\,dz, \quad (23)$$

where Θ is the characteristic Debye temperature for the magnetic sublattice.

At low temperatures $T\ll\Theta$, Eq. (23) reduces to

$$\chi\simeq\frac{9}{16}\frac{\overline{N}}{\Theta}. \quad (24)$$

For ordinary crystalline lattices Θ is of the order of 200 K and consequently (see Fig. 3) the gain in T_d for polaron formation is essential, even in the case of a small polarons[17] ($\overline{N}\simeq 30$). But if one of the phonon modes gets soft, its contribution to the χ value becomes dominant, which leads to the further growth of χ and T_d.

From the point of view of possible lattice softening, mercury-containing DMS's of the type $Hg_{1-x-y}Cd_xMn_yTe$ or $Hg_{1-x}Mn_xTe$ seem to be the most promising model materials. The mercury ion is able to exhibit the valence number of both 1 and 2 in different mercury-based compounds. There is a hybridization of the ground electronic d^2p^{n-1} and d^1p^n states in real systems, with fluctuations being also able to change the configuration weights in a mixed state. As a result, the materials of this group are rather flexible and exhibit the ability to easily vary their structure under pressure. For example, HgTe undergoes a structural transition at pressures of only 16 kbar.[24] Evidence of an anomalously large mean-square displacement of a heavy Hg ion has also been found.[25] From the viewpoint of these peculiarities, crystals of the HgTe family closely resemble the superionic crystals of the AgI family. Both the HgTe-type and AgI-type crystals exhibit a strong hybridization between the p (Te, I) and d (Hg, Ag) electronic states at the top of the valence band. This feature has been shown to be a crucial prerequisite to lattice instability with a local double-well (DW) formation.[21,26] It should be mentioned that the hypothesis for off-center displacement of Hg has recently been put forward phenomenologically in order to explain the anomalous features of the TO lattice spectrum in HgTe.[27] Following this hypothesis we have also developed a theory which predicts the nonsymmetric DW appearance for Hg ions.[28] As a result, the lattice

dynamics softens and the close proximity of electron and phonon excitation energies should be taken into account. One can expect a violation of the adiabatic condition in this material with a substantial enhancement of the spin-lattice interaction parameter χ. We assumed such an enhancement to be responsible for a development of the strong excitonic resonance observed in Ref. 15, where a hybridized ''exciton-hole MP'' model was suggested to explain the experimental data on the magnetoluminescence of $Hg_{1-x}Mn_xTe$ single crystals.

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[19] The approximation made in Eq. (3) has its origin in the relation [see Eq. (14) and notation below]

$$\left| S_{e_z} + \sum_{j=1}^{N_m} S^j_{m_z} \right| \sim \frac{1}{\beta} \frac{1}{Z_0} \frac{\partial Z_0}{\partial \omega_0} = \overline{N} b_{S_M}(\beta\omega_0), \quad \overline{N} \gg 1.$$

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