Influence of elastic and magnetic fields on the phonon scattering and thermal conductivity of acceptor defects in cubic semiconductors

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Magnetic and elastic fields have a strong influence on the phonon-scattering properties of acceptor states, which is experimentally well known from thermal conductivity measurements at low temperatures. Our theoretical approach starts with a former theory of the degenerate electronic defect states which are of the Γ_8 type. It uses high-order Green-function techniques together with unitary transformations. For the calculation of the thermal conductivity we take Callaway's formula together with a one-mode relaxation rate of the phonons. We discuss the dependence of the calculated scattering rates on physical parameters of the system. Under the influence of static fields the dynamical behavior of the electron-phonon coupling can be disturbed (e.g., resonance structures in the thermal conductivity curve can be destroyed). The changes due to those external perturbations are studied and it is shown that our theory qualitatively explains the experimental thermal conductivity results.

I. INTRODUCTION

In recent years the study of defects in solids by measurements with phonon techniques gained much interest. Because of their high resolution these methods are better suited for studying the dynamical behavior of the electron-phonon interaction than optical methods. New kinds of resonance structures were found, e.g., in p-doped semiconductors.[1–6] These additional phonon-scattering mechanisms were seen in thermal conductivity measurements as well as in experiments with monochromatic phonon techniques.[7] They are typically of nonadiabatic origin, i.e., they are due to the coupled dynamics of the interacting subsystems (electrons and phonons), which have to be solved. In previous papers[8,9] the connection between these resonances and the Jahn-Teller effect was demonstrated. Therefore these resonances are a dominating feature if degenerate electronic levels which can be split dynamically are present in the system. Therefore we call these resonances "dynamic resonances."

By applying external elastic or magnetic fields the original degeneracy can be destroyed by splitting the electronic levels in a static sense. This has been used in several experiments[3,4] to influence these resonances. Together with the static splitting in the electronic system direct phonon transitions may occur. By varying the field strength one has a tool to switch between both types of resonanes (the static and the dynamic ones).

The existing theories of phonon scattering at such statically split electronic states use a perturbational approach[10,11] and are not able to describe the dynamical resonances in the vanishing field limit. A first approach to a more general theory was given in a recent paper for donor states in semiconductors where the ground state is split even in the absence of fields.[12]

II. DEFECT HAMILTONIAN WITH FIELDS

In the following we consider acceptor systems (such as Mn in GaAs, In in Si, etc.) with Γ_8 ground states. The derivation of the defect Hamiltonian without fields was given in a previous paper of the authors[9] and therefore omitted here. We give the result which reads

$$H_{e\text{-ph}}=\sum_{q,\lambda}\left[D_\epsilon \sum_{i=1}^{2}\rho_i r_i^{q\lambda}+D_\tau\rho_3\sum_{j=1}^{3}\sigma_j s_j^{q\lambda}\right](b_{q\lambda}+b_{q\lambda}^{\dagger}) , \tag{1}$$

where D_ϵ and D_τ are the two independent deformation potential constants. $\{\rho_i\}$ and $\{\sigma_j\}$ are two commuting sets of spin operators. Together with the functions $r_i^{q\lambda}$ and $s_j^{q\lambda}$ they are shown in Appendix A.

These functions project the different phonon branches which are labeled by λ onto the normal modes of the cubic cell around the defect. Group-theoretical arguments show that only e and t phonons can interact with the defect. For simplicity we will use the abbreviation

$$\Lambda^{q\lambda}=\sum_{i=1}^{2}D_\epsilon\rho_i r_i^{q\lambda}+\sum_{j=1}^{3}D_\tau\rho_3\sigma_j s_j^{q\lambda} . \tag{2}$$

If we include elastic fields we arrive at a Hamiltonian of the following form:

$$H=\sum_{q,\lambda}\omega_{q\lambda}b_{q\lambda}^{\dagger}b_{q\lambda}+\sum_{q,\lambda}\Lambda^{q\lambda}(b_{q\lambda}+b_{q\lambda}^{\dagger})+\sum_{j=1}^{5}\xi_j\tau_j , \tag{3}$$

where the ξ_j's are abbreviations for the spin operators ρ_i,σ_j and $\rho_i\sigma_j$. They are defined in Appendix B. The τ_i are the elastic tensions instead of the deformations. Like the phonons two e- and three t-type deformations may couple to the defect. These fields split the original Γ_8

ground state into two Kramers doublets with energy difference:[13,14]

$$\Delta\epsilon = \left[\sum_{i=1}^{5} (2\tau_i)^2 \right]^{1/2} . \tag{4}$$

The interaction of the Γ_8 state with magnetic fields removes all degeneracies. The coupling terms are easily derived by the use of group theory: A magnetic field transforms like Γ_4. The coupling is with bilinear electronic operators and therefore the decomposition of the Kronecker product[15] of Γ_8 is needed:

$$\Gamma_8 \times \Gamma_8 = \Gamma_1 + \Gamma_2 + \Gamma_3 + 2\Gamma_4 + 2\Gamma_5 . \tag{5}$$

Γ_4 is contained twice in this product. The operators given in Eq. (1) belong to different irreducible representations of the cubic group. The details are given in Appendix A. The result for the Hamiltonian then reads:

$$H_{\text{field}} = g_1''(\hat{O}^1_{\Gamma_4,1}B_x + \hat{O}^1_{\Gamma_4,2}B_y + \hat{O}^1_{\Gamma_4,3}B_z) + g_2''(\hat{O}^2_{\Gamma_4,1}B_x + \hat{O}^2_{\Gamma_4,2}B_y + \hat{O}^2_{\Gamma_4,3}B_z) . \tag{6}$$

For our purposes, in this paper only magnetic fields in the z direction are considered. In this case the Hamiltonian for elastic and magnetic fields has the following form:

$$H_{\text{field}} = \tau_k \xi_k + H_1 \xi_9 + H_2 \xi_{15} \tag{7}$$

with

$$H_1 = g_2'' B_z, \quad H_2 = g_1'' B_z .$$

This operator is not yet diagonal in the electronic subspace. The operators of a fourfold state form a SU(4)- Lie algebra which is given in Appendix B. This Lie algebra has rank 3 (Ref. 16), every diagonal electronic operator therefore may be written as a combination of up to 3 simultaneously diagonal operators of the algebra which in our case are

$$\Delta\epsilon_1 \rho_3 + \Delta\epsilon_2 \sigma_3 + \Delta\epsilon_3 \rho_3 \sigma_3 . \tag{8}$$

Figure 1 shows the level scheme in the general case. For further use we take only one single τ_k nonvanishing. In this case the energy splittings of the system are easily calculated:

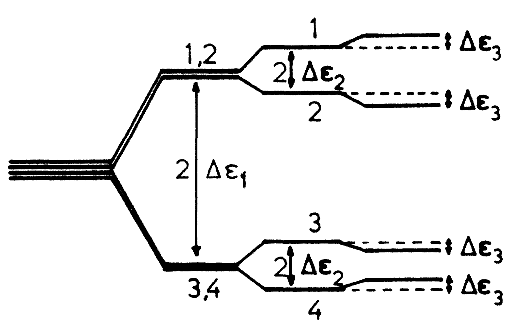

FIG. 1. Energy levels of the electronic Γ_8 state split by external fields.

(a) For $k=1$,

$$\Delta\epsilon_1 = \tau_1, \quad \Delta\epsilon_2 = H_1, \quad \Delta\epsilon_3 = H_2 . \tag{9a}$$

(b) For $k=2,5$,

$$\Delta\epsilon_1 = (H_1^2 + \tau_k^2)^{1/2}, \quad \Delta\epsilon_2 = H_2, \quad \Delta\epsilon_3 = 0 . \tag{9b}$$

(c) For $k=3,4$,

$$\Delta\epsilon_1 = (H_2^2 + \tau_k^2)^{1/2}, \quad \Delta\epsilon_2 = H_1, \quad \Delta\epsilon_3 = 0 . \tag{9c}$$

In cases (b) and (c) only four different energy differences appear. To simplify the formulas in the text and the numerical calculation we will therefore neglect case (a).

Because of the two independent Γ_4 representations contained in the Γ_8 Kronecker space the shape of the magnetic coupling terms is not unique. The usual way[10] to derive this interaction is by the use of angular momentum operators. Here we give the connection between the different g factors used in the literature:

$$g_1'' = 0.5 g_1 + 5 g_2 , \tag{10a}$$

$$g_2'' = 5.66 g_2 . \tag{10b}$$

To clarify the following expressions and calculations we introduce the parameter

$$D = \begin{cases} \dfrac{|H_1|}{(H_1^2 + \tau_k^2)^{1/2}} & \text{in case (b)} \\ \dfrac{|H_2|}{(H_2^2 + \tau_k^2)^{1/2}} & \text{in case (c)} \end{cases}$$

and

$$E = (1 - D^2)^{1/2} . \tag{11}$$

$D=0$ marks the case of the pure elastic field, whereas $D=1$ gives the pure magnetic one. In the discussion of transitions the introduction of energy differences is useful:

$$\hat{\epsilon}_0 = 0, \quad \hat{\epsilon}_1 = 2|\Delta\epsilon_2|, \quad \hat{\epsilon}_2 = 2|\,|\Delta\epsilon_1| - |\Delta\epsilon_2|\,| , \quad \hat{\epsilon}_3 = 2|\Delta\epsilon_1|, \quad \hat{\epsilon}_4 = 2(|\Delta\epsilon_1| + |\Delta\epsilon_2|) . \tag{12}$$

Instead of Eq. (7) we use the short form

$$H_{\text{field}} = \sum_m K_m \xi_m , \tag{13}$$

where the summation is restricted to the values k (index of applied elastic field, from 1 to 5, 9, and 15).

III. EQUATION OF MOTION HIERARCHY

In a Green-function-based approach the relaxation rate of a physical system is related to the imaginary part of the T matrix which can be expressed by a thermodynamical Green function.[17,18,8] This reads

$$G = G_0 - G_0 T G_0 . \tag{14}$$

The index 0 denotes the unperturbed system where no relaxation occurs. The calculations of the relaxation rate

$\tau_{q\lambda}^{-1}$ therefore implies a determination of the Green function of the perturbed system G.

For the relaxation of a phonon the phonon Green function is needed which has the form $\langle\langle \xi_i;\xi_i \rangle\rangle$. We use the equation-of-motion method for the evaluation of this Green function. The first step reads

$$\omega\langle\langle \xi_i;\xi_i \rangle\rangle = \sum_{q,\lambda} \langle\langle Q[\xi_i,\Lambda];\xi_i \rangle\rangle + \sum_m \tau_m \langle\langle [\xi_i,\xi_m];\xi_i \rangle\rangle \; . \tag{15}$$

For the next Green function $\langle\langle QE;\xi_i \rangle\rangle$ the following expression results:

$$\begin{aligned}(\omega^2-\omega_{q\lambda}^2)\langle\langle QE,\xi_i \rangle\rangle + \sum_{l,m} K_l K_m \langle\langle Q[[E,\xi_l],\xi_m];\xi_i \rangle\rangle \\ = \frac{\omega}{2\pi}\langle Q[E,\xi_i]\rangle_T + \frac{\omega_{q\lambda}}{2\pi}\langle P[E,\xi_i]\rangle_T + \omega\sum_{q',\lambda'}\langle\langle QQ'[E,\Lambda'];\xi_i \rangle\rangle + \omega\sum_l K_l \langle\langle Q[E,\xi_l];\xi_i \rangle\rangle \\ + \omega_{q\lambda}\sum_{q',\lambda'}\langle\langle PQ'[E,\Lambda'];\xi_i \rangle\rangle + 2\omega_{q\lambda}\langle\langle \Lambda E,\xi_i \rangle\rangle + \sum_l K_l \left[\omega\langle\langle Q[E,\xi_l];\xi_i \rangle\rangle - \frac{1}{2\pi}\langle Q[[E,\xi_l],\xi_i]\rangle_T \right. \\ \left. - \sum_{q',\lambda'}\langle\langle QQ'[[E,\xi_l],\Lambda'];\xi_i \rangle\rangle \right] \; . \end{aligned} \tag{16}$$

In this context E denotes an arbitrary electronic operator of the Lie algebra SU(4). In general $[[E,\xi],\xi]$ will not reduce to E. Therefore Eq. (16) leads to a system of linear equations. The solution can most easily be accomplished by a unitary transformation technique with

$$\hat{\xi}_i = U_{ij}\xi_j, \quad i,j=1,2,\ldots,15 \tag{17}$$

and the demand

$$[[\hat{\xi}_m,\hat{\xi}_n],\hat{\xi}_l] = A_{nl}^{(m)}\hat{\xi}_m, \quad n,l=k,9,15 \; . \tag{18}$$

This matrix is easily found because the double commutator in Eq. (18) decomposes in small units which are analytically diagonalized. For one case we give the matrix U in Appendix D. In transformed space Eq. (16) closes to yield E. With the abbreviation

$$\left[\frac{1}{\Delta(\omega,\omega_{q\lambda})}\right]_{EE'} = \sum_{\hat{E}} U_{E\hat{E}}^T \frac{1}{\hat{\Delta}_{\hat{E}}(\omega,\omega_{q\lambda})} U_{\hat{E}E'} \; , \tag{19}$$

this equation reads

$$\begin{aligned}\langle\langle QE;\xi_i \rangle\rangle = \sum_{E'} \left[\frac{1}{\Delta(\omega,\omega_{q\lambda})}\right]_{EE'} \left[\frac{\omega}{2\pi}\langle Q[E',\xi_i]\rangle_T + \frac{\omega_{q\lambda}}{2\pi}\langle P[E',\xi_i]\rangle_T - \frac{1}{2\pi}\sum_l K_l\langle Q[[E',\xi_l],\xi_i]\rangle_T \right. \\ + \omega\sum_{q',\lambda'}\langle\langle QQ'[E',\Lambda'];\xi_i \rangle\rangle - \sum_l K_l \sum_{q',\lambda'}\langle\langle QQ'[[E',\xi_l],\Lambda'];\xi_i \rangle\rangle + 2\omega_{q\lambda}\langle\langle \Lambda E';\xi_i \rangle\rangle \\ \left. + \omega_{q\lambda}\sum_{q',\lambda'}\langle\langle PQ'[E',\Lambda'];\xi_i \rangle\rangle + 2\omega\sum_l K_l\langle\langle Q[E',\xi_l];\xi_i \rangle\rangle \right] \; . \end{aligned} \tag{20}$$

With the additional definitions

$$\left[\frac{1}{K(\omega,\omega_{q\lambda})}\right]_{EE'} = \sum_{\hat{E}} U_{E\hat{E}}^T \frac{1}{\hat{K}_{\hat{E}}(\omega,\omega_{q\lambda})} U_{EE'} \; , \tag{21}$$

$$\left[\frac{1}{M(\omega,\omega_{q\lambda})}\right]_{EE'} = \sum_{E''} \frac{1}{[K(\omega,\omega_{q\lambda})]_{EE''}} \sum_l \hat{K}_l \left[\frac{1}{\Delta(\omega,\omega_{q\lambda})}\right] \; , \tag{22}$$

this is transformed to

$$\langle\langle QE;\xi_i\rangle\rangle=\sum_{E'}\left[\frac{1}{K(\omega,\omega_{q\lambda})}\right]_{EE'}\left[\frac{\omega}{2\pi}\langle Q[E',\xi_i]\rangle_T+\frac{\omega_{q\lambda}}{2\pi}\langle P[E',\xi_i]\rangle_T-\frac{1}{2\pi}\sum_l K_l\langle Q[[E',\xi_l],\xi_i]\rangle_T\right.$$
$$+\omega_{q\lambda}\sum_{q',\lambda'}\langle\langle PQ'[E',\Lambda'];\xi_i\rangle\rangle+2\omega_{q\lambda}\langle\langle \Lambda E';\xi_i\rangle\rangle+\omega\sum_{q',\lambda'}\langle\langle QQ'[E',\Lambda'];\xi_i\rangle\rangle$$
$$\left.-\sum_l K_l\sum_{q',\lambda'}\langle\langle QQ'[[E',\xi_l],\Lambda'];\xi_i\rangle\rangle\right]$$
$$+2\omega\sum_{E''}\left[\frac{1}{M(\omega,\omega_{q\lambda})}\right]_{EE''}\left[\frac{\omega}{2\pi}\langle Q[E'',\xi_i]\rangle_T+\frac{\omega_{q\lambda}}{2\pi}\langle P[E'',\xi_i]\rangle_T-\frac{1}{2\pi}\sum_m K_m\langle Q[[E'',\xi_m],\xi_i]\rangle_T\right.$$
$$+\omega\sum_{q',\lambda'}\langle\langle QQ'[E'',\Lambda'];\xi_i\rangle\rangle-\sum_m K_m\sum_{q',\lambda'}\langle\langle QQ'[[E'',\xi_m],\Lambda'];\xi_i\rangle\rangle$$
$$\left.+\omega_{q\lambda}\sum_{q',\lambda'}\langle\langle PQ'[E'',\Lambda'];\xi_i\rangle\rangle\right]. \quad (23)$$

From Eq. (14) the relaxation rate is given in terms of the electronic Green functions:

$$\tau_{q\lambda}^{-1}=4\pi nV\,\mathrm{Im}\langle\langle \Lambda^{q\lambda};\Lambda^{q\lambda}\rangle\rangle\ , \quad (24)$$

where n is the defect concentration and V the volume of the crystal. Therefore, only the "diagonal" Green functions are needed for the calculation. With the introduction of a projector $\hat{P}$ in the electronic space and the complementary projector $\hat{Q}$ one obtains

$$\left[\omega^2-\sum_{l,m}K_lK_m\hat{P}([[\xi_i,\xi_l],\xi_m]\to\xi_i)\right]\langle\langle\xi_i;\xi_i\rangle\rangle$$
$$=\frac{1}{2\pi}\sum_l K_l\langle[[\xi_i,\xi_l],\xi_i]\rangle_T+\omega\sum_{q,\lambda}\langle\langle Q[\xi_i,\Lambda];\xi_i\rangle\rangle+\sum_l K_l\sum_{q,\lambda}\langle\langle Q[[\xi_i,\xi_l],\Lambda];\xi_i\rangle\rangle$$
$$+\sum_{l,m}K_lK_m\hat{Q}([[\xi_i,\xi_l],\xi_m]\to\xi_i)\langle\langle[[\xi_i,\xi_l],\xi_m];\xi_i\rangle\rangle\ . \quad (25)$$

From the Green functions on the right-hand side of Eq. (16) only $\langle\langle PQ'[E,\Lambda'];\xi_i\rangle\rangle$ has phonon terms which do not commute with the unperturbed Hamiltonian. Therefore this function is expanded and yields

$$\omega\langle\langle PQ'E;\xi_i\rangle\rangle=\frac{1}{2\pi}\langle PQ'[E,\xi_i]\rangle_T+\omega_{q\lambda}\langle\langle QQ'E;\xi_i\rangle\rangle$$
$$+\omega_{q'\lambda'}\langle\langle PP'E;\xi_i\rangle\rangle+2\langle\langle Q'\Lambda E;\xi_i\rangle\rangle$$
$$+\sum_m K_m\langle\langle PQ'[E,\xi_m];\xi_i\rangle\rangle$$
$$+\sum_{q'',\lambda''}\langle\langle PQ'Q''[E,\Lambda''];\xi_i\rangle\rangle\ . \quad (26)$$

Inserting Eq. (26) in Eq. (16) gives the final equation for the relaxation rate calculation which reads in a formal way

$$\left[\omega^2-\sum_{l,m}K_lK_m\hat{P}([[\xi_i,\xi_l],\xi_m]\to\xi_i)\right]\langle\langle\xi_i;\xi_i\rangle\rangle$$
$$=\frac{1}{2\pi}E(\omega)+G(\omega)\ , \quad (27)$$

where $E(\omega)$ denotes the expectation values and $G(\omega)$ the higher Green functions. To reach a closure of the hierarchy Eq. (27) the following approximations are used

(a) RPA factorization of all quadratic phonon terms ($A\cong P,Q$):

$$\langle\langle AA'\xi_i;\xi_j\rangle\rangle\approx\langle AA'\rangle_T\langle\langle\xi_i;\xi_j\rangle\rangle\ .$$

(b) Neglect of all terms higher than quadratic in the static splittings K_l.

(c) Further development of nonclosing functions $\langle\langle\xi_k;\xi_i\rangle\rangle$ with respect to b.

(d) Simplification of electronic operator products by the limitation to one-electron-parts, i.e.,

$$\xi_i\xi_j\cong\tfrac{1}{2}[\xi_i,\xi_j]\ .$$

(e) Closure of all remaining terms with odd numbers of phonon operators with restriction to b with an expectation value:

$$\omega\langle\langle A\xi_i;\xi_j\rangle\rangle\approx\frac{1}{2\pi}\langle A[\xi_i,\xi_j]\rangle_T\ .$$

For the control of the approximations several sum rules[19] and especially the required positive definiteness of the result (24) are checked.

IV. CALCULATION OF EXPECTATION VALUES

The application of the equation-of-motion technique together with the described RPA approximation leads to several thermal expectation values which have to be calculated in the base of the perturbed Hamiltonian. To ensure high accuracy we use a unitary transformation approach.[20] The expectation value is written as

$$\langle \xi_i \rangle_H = \langle \tilde{\xi}_i \rangle_{\tilde{H}} = \langle e^{-S} \xi_i e^{S} \rangle_{\tilde{H}} \approx \langle \xi_i \rangle_{\tilde{H}} + \langle [\xi_i, S] \rangle_{\tilde{H}} + \cdots , \tag{28}$$

where S denotes a Hermitian matrix which may be determined by the U matrix equation. With the abbreviations

$$W_i^{q\lambda} = \frac{\omega_{q\lambda}}{\omega_{q\lambda}^2 - \hat{\epsilon}_i^2}, \quad D_i^{q\lambda} = \frac{\hat{\epsilon}_i}{\omega_{q\lambda}^2 - \hat{\epsilon}_i^2}, \quad i = 0, \ldots, 4 \tag{29}$$

the S matrix can be brought to the following form:

$$S = \sum_{q,\lambda} \sum_{i=1}^{5} \eta_j^{q\lambda} \sum_{j=1}^{15} (R_{ij}^P P^{q\lambda} + i R_{ij}^Q Q^{q\lambda}) \xi_j . \tag{30}$$

The coefficients R^P and R^Q are given in Appendix D. In the transformed space according to Eq. (30) the following electronic operators give nonvanishing expectation values:

$$\begin{aligned}
\langle \tilde{\xi}_1 \rangle_T &= D \langle \xi_5 \rangle_T = D(1 - e^{-\beta\hat{\epsilon}_1} - e^{-\beta\hat{\epsilon}_3} + e^{-\beta\hat{\epsilon}_4})/Z^c , \\
\langle \tilde{\xi}_2 \rangle_T &= -E \langle \xi_6 \rangle_T = E(e^{-\beta\hat{\epsilon}_3} + e^{-\beta\hat{\epsilon}_4} - e^{-\beta\hat{\epsilon}_1} - 1)/Z^c , \\
\langle \tilde{\xi}_9 \rangle_T &= -D \langle \xi_6 \rangle_T = D(e^{-\beta\hat{\epsilon}_3} + e^{-\beta\hat{\epsilon}_4} - e^{-\beta\hat{\epsilon}_1} - 1)/Z^c ,
\end{aligned} \tag{31}$$

$$\begin{aligned}
\langle \tilde{\xi}_{12} \rangle_T &= E \langle \xi_5 \rangle_T = E(1 - e^{-\beta\hat{\epsilon}_1} - e^{-\beta\hat{\epsilon}_3} + e^{-\beta\hat{\epsilon}_4})/Z^c , \\
\langle \tilde{\xi}_{15} \rangle_T &= -\langle \xi_{15} \rangle_T = (e^{-\beta\hat{\epsilon}_1} - e^{-\beta\hat{\epsilon}_3} + e^{-\beta\hat{\epsilon}_4} - 1)/Z^c ,
\end{aligned}$$

with $Z^c = 1 + e^{-\beta\hat{\epsilon}_1} + e^{-\beta\hat{\epsilon}_3} + e^{-\beta\hat{\epsilon}_4}$, where Z^c denotes the canonical *Zustandsumme*. The other expectation values read

$$\begin{aligned}
\langle QQ' \rangle_T = {} & \delta_{qq'} \delta_{\lambda\lambda'} \coth\left[\frac{\beta\omega_{q\lambda}}{2}\right] + 4 \sum_{j,k,l,m} C_{jklm}^{\langle QQ' \rangle} W_j^{q\lambda} W_j^{q'\lambda'} \eta_k^{q\lambda} \eta_l^{q'\lambda'} \langle \tilde{\xi}_m \rangle_T \\
& - 2 \sum_{j,k,l,m} F_{jklm}^{\langle QQ' \rangle} \langle \tilde{\xi}_m \rangle_T \left[\coth\left[\frac{\beta\omega_{q\lambda}}{2}\right] W_j^{q'\lambda'} D_j^{q\lambda} \eta_k^{q'\lambda'} \eta_l^{q\lambda} + \coth\left[\frac{\beta\omega_{q'\lambda'}}{2}\right] W_j^{q\lambda} D_j^{q'\lambda'} \eta_k^{q\lambda} \eta_l^{q'\lambda'} \right] ,
\end{aligned} \tag{32a}$$

$$\begin{aligned}
\langle PP' \rangle_T = {} & -\delta_{qq'} \delta_{\lambda\lambda'} \coth\left[\frac{\beta\omega_{q\lambda}}{2}\right] - 4 \sum_{j,k,l,m} C_{jklm}^{\langle PP' \rangle} D_j^{q\lambda} D_j^{q'\lambda'} \eta_k^{q\lambda} \eta_l^{q'\lambda'} \langle \tilde{\xi}_m \rangle_T \\
& + 2 \sum_{j,k,l,m} F_{jklm}^{\langle PP' \rangle} \langle \tilde{\xi}_m \rangle_T \left[\coth\left[\frac{\beta\omega_{q\lambda}}{2}\right] W_j^{q'\lambda'} D_j^{q\lambda} \eta_k^{q'\lambda'} \eta_l^{q\lambda} + \coth\left[\frac{\beta\omega_{q'\lambda'}}{2}\right] W_j^{q\lambda} D_j^{q'\lambda'} \eta_k^{q\lambda} \eta_l^{q'\lambda'} \right] ,
\end{aligned} \tag{32b}$$

$$\langle PQ' \rangle_T = \langle PQ' \rangle_T^{H_0} = \delta_{qq'} \delta_{\lambda\lambda'} , \tag{32c}$$

$$\langle Q\xi_t \rangle_T = -2 \sum_{j,l,m} C_{jlmt}^{\langle Q\xi \rangle} W_j^{q\lambda} \eta_l^{q\lambda} \langle \tilde{\xi}_m \rangle_T + 2\coth\left[\frac{\beta\omega_{q\lambda}}{2}\right] \sum_{j,l,m} F_{jlmt}^{\langle Q\xi \rangle} D_j^{q\lambda} \eta_l^{q\lambda} \langle \tilde{\xi}_m \rangle_T , \tag{32d}$$

$$\langle P\xi_t \rangle_T = 2i \sum_{j,l,m} C_{jlmt}^{\langle P\xi \rangle} D_j^{q\lambda} \eta_l^{q\lambda} \langle \tilde{\xi}_m \rangle_T - 2i\coth\left[\frac{\beta\omega_{q\lambda}}{2}\right] \sum_{j,l,m} F_{jlmt}^{\langle P\xi \rangle} W_j^{q\lambda} \eta_l^{q\lambda} \langle \tilde{\xi}_m \rangle_T , \tag{32e}$$

where the respective summation range is evident from the definition. The various types of $\underline{F}$ and $\underline{C}$ matrices were determined by a numerical procedure.

V. DISCUSSIONS OF RELAXATION RATES

From Eq. (24) the expression for the phonon relaxation rate can be brought to the following form:

$$\langle \tau_\lambda^{-1}(\omega) \rangle = n \frac{\hbar\omega f_\lambda^2(\omega) \bar{c}^3}{2\rho c_A^5} \sum_j A_j^\lambda \mathrm{Im} \langle\langle \xi_j ; \xi_j \rangle\rangle , \tag{33}$$

where the A's result from the angular integration within a isotropic Debye model. They are given in Appendix E. $\rho = M/V$ is the mass density, c_λ ($\lambda = l,t$) the longitudinal and transverse sound velocity, respectively, and $\bar{c}^3 = 1/(\sum_\lambda 1/c_\lambda^3)$. By standard methods all q summations are converted to integrals with nontrivial imaginary parts which describe the irreversible behavior of the system. The temperature dependence of some of these integrals is caused by the expectation values. The integrals are given in Appendix F.

The formal structure of the result for the relaxation rate is the same for the applied magnetic and elastic field.[21] The difference appears only in the summation of the splittings and the actual values of the coefficients. The result can be brought to the following form:

$$\langle\langle \xi_j ; \xi_j \rangle\rangle = \frac{Z(\omega)}{N(\omega)} , \tag{34}$$

where $N(\omega)$ and $Z(\omega)$ are given as

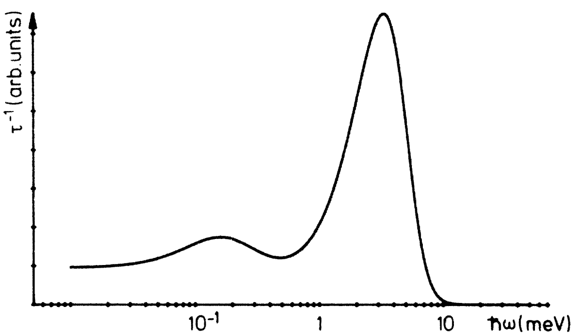

FIG. 2. Phonon relaxation rate of GaAs (Mn) with small magnetic field (1 T).

$$N(\omega)=\sum_{i=1}^{14} n_i(\omega),\quad Z(\omega)=\frac{1}{2\pi}\sum_{j=1}^{7} Z_j(\omega)\ .$$

The explicit form of the terms $n_i(\omega)$ and $z_j(\omega)$ is given in Appendix G.

It is easily seen that the dynamical terms (A_j^λ) contribute as well as the static splittings (κ_1). For small electron-phonon couplings A_j^λ the perturbational result[10] is obtained. In this limiting case the terms n_2 to n_{14} in the denominator can be neglected as well as z_6 and z_7 in the numerator. In contrast to perturbation theory our method gives a closed form for all scattering terms without distinction between direct and Raman processes.

The numerical evaluation for different cases is shown in Figs. 2–4. Independent of the kind of applied field the direct resonance is sharp only if the static splitting is larger than the Jahn-Teller resonance. Smaller static fields appear only through a broad absorption structure. This result fits very well in the intuitive picture of the dynamical scattering mechanism.

The small fields do not destroy the dynamics of the Jahn-Teller effect, therefore the static splitting is modulated by the momentary dynamical splittings and therefore smeared out.

Figure 5 shows very well the disturbance of the JT resonance by the application of a magnetic field. In the upper right the magnetic field applied to GaAs (Mn) in the z direction is weak and therefore the JT resonance, shown as a small peak is not disturbed. With higher magnetic field this resonance structure gets weaker and weaker, i.e., it is smeared out by the static splittings induced by the external field. Figure 6 shows the completely different

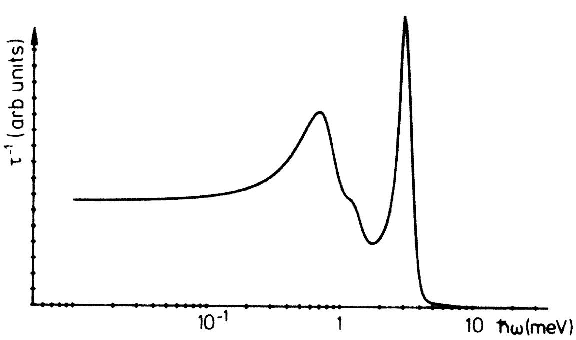

FIG. 3. Phonon relaxation rate of GaAs (Mn) with magnetic field strength of 10 T.

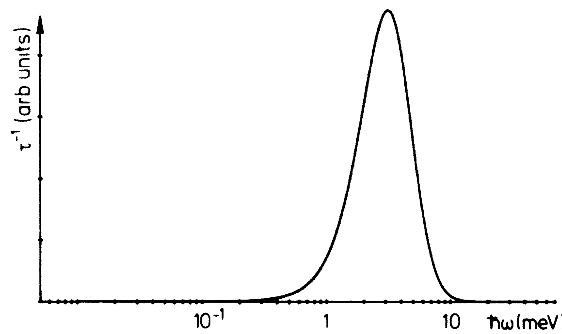

FIG. 4. Phonon relaxation rate of GaAs (Mn) with applied magnetic field of 500 T.

temperature behavior for the static and the dynamical resonance. In this case a static splitting of $\Delta\epsilon=4$ meV is applied to GaAs (Mn) by an elastic field. At low temperatures the static splitting is easily seen because it is at higher energies than the dynamical splittings and therefore it is not smeared out. For higher temperatures the occupation numbers of both static levels get the same and therefore this resonance is saturated. The dynamical resonance, which at low temperatures is completely dominated by the static one, survives at higher temperatures nearly unchanged because there are no static levels which can be equally populated. Therefore only this resonance is seen at higher temperatures.

The range of validity of the theory given here is limited by two parameters which are used for an expansion. The coefficients A_j^λ (respectively, D_ϵ, D_τ) and the static splittings κ_1. Both are required to be small. Additionally, we included the electronic splitting term in the unperturbed H_0. For very small fields this is not adapted to the physical situation in which the fields act as a perturbation for the stronger electron-phonon coupling.

VI. CALCULATION OF THERMAL CONDUCTIVITY

With the relaxation rate Eq. (34) the thermal conductivity can be calculated using Callaway's formula[22] ($x=\hbar\omega/kT$):

$$K(T)=\frac{k_B^4T^3}{6\pi^2}\sum_\lambda\frac{1}{c_\lambda}\int_0^{\theta_D/k_B}dx\frac{x^4e^x}{(e^x-1)^2}\tau_\lambda(x)\ ,\qquad(35)$$

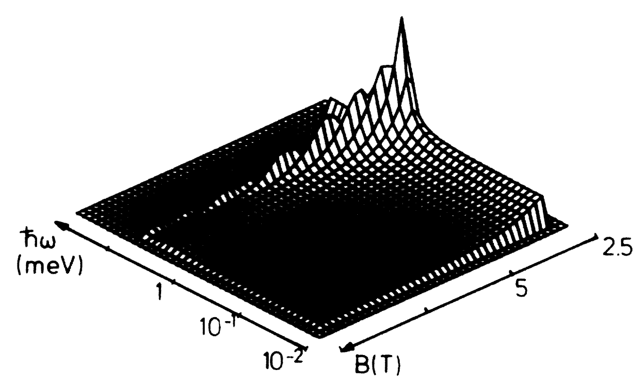

FIG. 5. Phonon relaxation rate plotted against magnetic field strength and phonon energy. The energy scale is logarithmic, the magnetic field scale is linear.

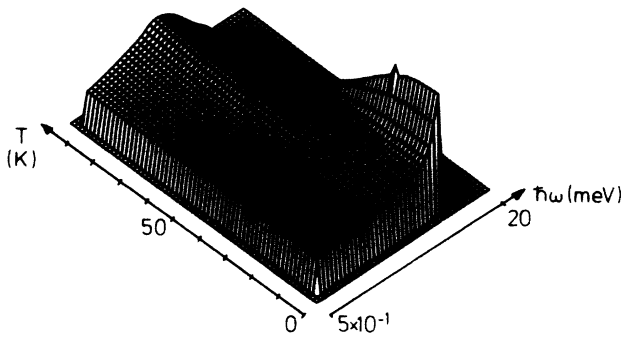

FIG. 6. Temperature dependence of the relaxation rate for an applied elastic field with $\Delta\epsilon=4$ meV. The energy scale is logarithmic, the temperature scale is linear.

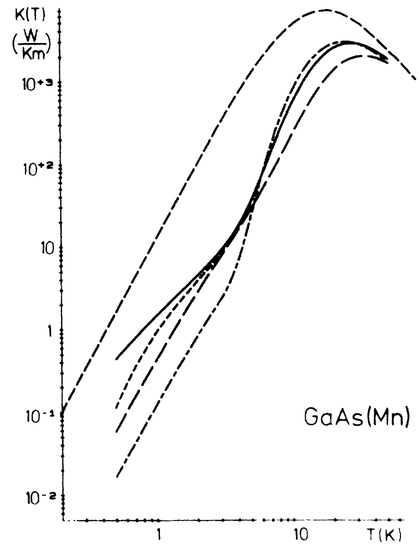

FIG. 8. Calculated thermal conductivity of GaAs (Mn) for different elastic field strengths: without field (solid line); $\Delta\epsilon=50$ μ eV (dashed line); $\Delta\epsilon=1.5$ meV (long-dashed—short-dashed line); $\Delta\epsilon=3$ meV (broken line). The upper curve corresponds to the undoped crystal.

where $\tau_\lambda(\omega)$ gives the total relaxation time of phonons of branch λ. For independent scattering processes the inverse relaxation rates have to be summed up:

$$\tau^{-1}=\sum_i \tau_i^{-1} . \tag{36}$$

For the evaluation of the thermal conductivity we added boundary scattering (τ_B), Rayleigh scattering (τ_R), and Umklapp scattering (τ_U) to the calculated relaxation rate Eq. (34) (Refs. 22—26). The parameters of the acceptor systems are given in Ref. 9. It should be stressed that our theory contains no adjustable parameters and the values used are determined by independent experiments.

The thermal conductivity for different cases and concentrations is given in Figs. 7 and 8. Figure 7 shows the influence of elastic fields on the thermal conductivity of Si(In). The solid lines gives the degenerate case (without applied field). A small elastic field reduces the thermal conductivity at low temperatures in analogy to experiments with a distribution of internal fields. A further increase of the field reduces the thermal conductivity in the whole range of temperatures and destroys completely the resonancelike structure. Figure 8 shows the influence of elastic fields on the thermal conductivity of GaAs (Mn). Fields much smaller than the resonance energy do not affect the dynamical resonance structure but reduce the

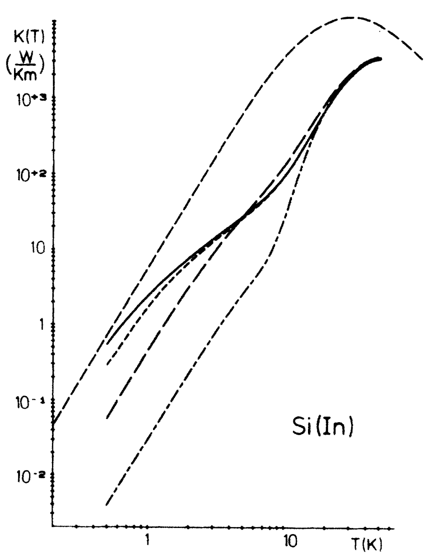

FIG. 7. Calculated thermal conductivity of Si (In) with different elastic fields: without field (solid line); $\Delta\epsilon=50$ μeV (dashed line); $\Delta\epsilon=3$ meV (long-dashed—short-dashed line); $\Delta\epsilon=10$ meV (broken line). The upper curve corresponds to the undoped crystal.

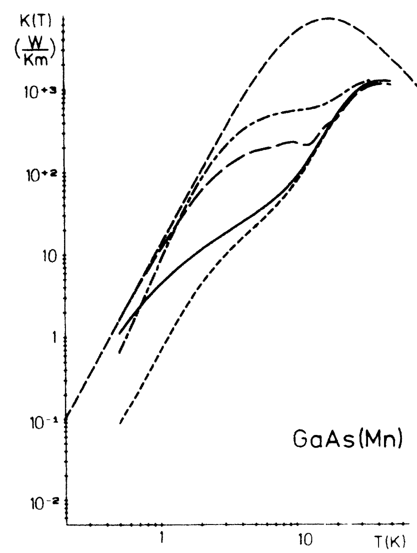

FIG. 9. Influence of a magnetic field on the thermal conductivity of GaAs (Mn): without field (solid line); 1 T (long-dashed—short-dashed line); 5 T (broken line); 20 T (dashed line). The upper curve corresponds to the undoped crystal.

thermal conductivity at lower temperatures. For very high fields the resonance structure gets weaker and finally disappears.

For magnetic field splittings the situation is analogous as is shown in Fig. 9 for the case of GaAs (Mn). In contrast to the case with elastic fields a minimum in thermal conductivity is built up at medium magnetic field strengths. Such a minimum was experimentally detected.[3] In contrast to former approaches for the degenerate case[9] the theory presented here cannot reproduce the thermal conductivity minimum of the field-free case in GaAs (Mn). This is due to the much simpler approximation scheme in the case here which was necessary for the inclusion of the field terms. Nevertheless, our theory shows qualitatively the influence of fields on thermal conductivity of these defect systems.

VII. CONCLUSIONS

Based on former work on the degenerate Γ_8 state[9,27] we investigated the dynamics of the field-split electronic Γ_8 state at acceptor defects in cubic semiconductors. We developed a Green-function method to evaluate the phonon-scattering rate due to the electron-phonon interaction.

By changing the field-induced splitting one can switch between the degenerate case (dynamical limit) and the nondegenerate one-level case (static limit) without JT interaction. Therefore these systems are very well suited to study the electron-phonon dynamics in detail.

From our Green-function result of the relaxation rate we calculated the thermal conductivity. The theoretical results agree qualitatively with several measurements on these systems. For a more quantitative approach in the case of the acceptor systems considered here the higher-order terms have to be evaluated, which seems to be not feasible with the numerical methods available to the authors. Nevertheless, the behavior of the electron-phonon system studied here is of theoretical interest and may be a dominant feature in other systems with a weak dynamical JT effect within a defect level.

ACKNOWLEDGMENTS

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APPENDIX A

The definitions of the spin operators ρ_i and σ_j and of the coupling functions $r_i^{q\lambda}$ and $s_i^{q\lambda}$ are given below. The spin operators ρ_i and σ_j can be represented as 4×4 matrices:[28]

$$\rho_1=\begin{bmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{bmatrix},\quad \rho_2=\begin{bmatrix}0&0&-i&0\\0&0&0&-i\\i&0&0&0\\0&i&0&0\end{bmatrix},\quad \rho_3=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix},$$

$$\sigma_1=\begin{bmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix},\quad \sigma_2=\begin{bmatrix}0&-i&0&0\\i&0&0&0\\0&0&0&-i\\0&0&i&0\end{bmatrix},\quad \sigma_3=\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&-1\end{bmatrix}.$$

They satisfy the relations $\rho_i^2=\sigma_j^2=1$, $[\rho_i,\sigma_j]=0$, and the usual spin commutation relations $[\rho_1,\rho_2]=2i\rho_3$; $[\sigma_1,\sigma_2]=2i\sigma_3$, and cyclic.

From these definitions the representations of the products $\rho_i\sigma_j$ can easily be found. The commutation relations are given in Appendix B. The two sets of electronic operators which transform according to the two Γ_4 representations and which couple to the magnetic field have the form:[29]

$$\hat{O}^{1}_{\Gamma_4,1}=\sigma_1;\quad \hat{O}^{1}_{\Gamma_4,2}=\sigma_2;\quad \hat{O}^{1}_{\Gamma_4,3}=\sigma_3$$

and

$$\hat{O}^{2}_{\Gamma_4,1}=-\tfrac{1}{2}\rho_1\sigma_1+\frac{\sqrt{3}}{2}\rho_2\sigma_1\ ,$$

$$\hat{O}^{2}_{\Gamma_4,2}=-\tfrac{1}{2}\rho_1\sigma_2-\frac{\sqrt{3}}{2}\rho_2\sigma_2\ ,$$

$$\hat{O}^{2}_{\Gamma_4,3}=\rho_1\sigma_3\ .$$

The coupling functions are defined by

$$r_1^{q\lambda}=\alpha(q)f(q)\frac{1}{3}(2\hat{q}_z n_{\lambda z}-\hat{q}_x n_{\lambda x}-\hat{q}_y n_{\lambda y})\ ,$$

$$r_2^{q\lambda}=\alpha(q)f(q)\frac{1}{\sqrt{3}}(\hat{q}_x n_{\lambda x}-\hat{q}_y n_{\lambda y})\ ,$$

TABLE I. Definitions of the operators ξ_i $(i=1,2,\ldots,15)$ and commutation relations for SU(4) in the product-spin representation. The results have to be multiplied by $2i$.

	ρ_1	ρ_2	$\rho_3\sigma_1$	$\rho_3\sigma_2$	$\rho_3\sigma_3$	ρ_3	$\rho_1\sigma_1$	$\rho_1\sigma_2$	$\rho_1\sigma_3$	$\rho_2\sigma_1$	$\rho_2\sigma_2$	$\rho_2\sigma_3$	σ_1	σ_2	σ_3
$\rho_1\cong\xi_1$	0	ρ_3	$-\rho_2\sigma_1$	$-\rho_2\sigma_2$	$-\rho_2\sigma_3$	$-\rho_2$	0	0	0	$\rho_3\sigma_1$	$\rho_3\sigma_2$	$\rho_3\sigma_3$	0	0	0
$\rho_2\cong\xi_2$	$-\rho_3$	0	$\rho_1\sigma_1$	$\rho_1\sigma_2$	$\rho_1\sigma_3$	ρ_1	$-\rho_3\sigma_1$	$-\rho_3\sigma_2$	$-\rho_3\sigma_3$	0	0	0	0	0	0
$\rho_3\sigma_1\cong\xi_3$	$\rho_2\sigma_1$	$-\rho_1\sigma_1$	0	σ_3	$-\sigma_2$	0	ρ_2	0	0	$-\rho_1$	0	0	0	$\rho_3\sigma_3$	$-\rho_3\sigma_2$
$\rho_3\sigma_2\cong\xi_4$	$\rho_2\sigma_2$	$-\rho_1\sigma_2$	$-\sigma_3$	0	σ_1	0	0	ρ_2	0	0	$-\rho_1$	0	$-\rho_3\sigma_3$	0	$\rho_3\sigma_1$
$\rho_3\sigma_3\cong\xi_5$	$\rho_2\sigma_3$	$-\rho_1\sigma_3$	σ_2	$-\sigma_1$	0	0	0	0	ρ_2	0	0	$-\rho_1$	$\rho_3\sigma_2$	$-\rho_3\sigma_1$	0
$\rho_3\cong\xi_6$	ρ_2	$-\rho_1$	0	0	0	0	$\rho_2\sigma_1$	$\rho_2\sigma_2$	$\rho_2\sigma_3$	$-\rho_1\sigma_1$	$-\rho_1\sigma_2$	$-\rho_1\sigma_3$	0	0	0
$\rho_1\sigma_1\cong\xi_7$	0	$\rho_3\sigma_1$	$-\rho_2$	0	0	$-\rho_2\sigma_1$	0	σ_3	$-\sigma_2$	ρ_3	0	0	0	$\rho_1\sigma_3$	$-\rho_1\sigma_2$
$\rho_1\sigma_2\cong\xi_8$	0	$\rho_3\sigma_2$	0	$-\rho_2$	0	$-\rho_2\sigma_2$	$-\sigma_3$	0	σ_1	0	ρ_3	0	$-\rho_1\sigma_3$	0	$\rho_1\sigma_1$
$\rho_1\sigma_3\cong\xi_9$	0	$\rho_3\sigma_3$	0	0	$-\rho_2$	$-\rho_2\sigma_3$	σ_2	$-\sigma_1$	0	0	0	ρ_3	$\rho_1\sigma_2$	$-\rho_1\sigma_1$	0
$\rho_2\sigma_1\cong\xi_{10}$	$-\rho_3\sigma_1$	0	ρ_1	0	0	$\rho_1\sigma_1$	$-\rho_3$	0	0	0	σ_3	$-\sigma_2$	0	$\rho_2\sigma_3$	$-\rho_2\sigma_2$
$\rho_2\sigma_2\cong\xi_{11}$	$-\rho_3\sigma_2$	0	0	ρ_1	0	$\rho_1\sigma_2$	0	$-\rho_3$	0	$-\sigma_3$	0	σ_1	$-\rho_2\sigma_3$	0	$\rho_2\sigma_1$
$\rho_2\sigma_3\cong\xi_{12}$	$-\rho_3\sigma_3$	0	0	0	ρ_1	$\rho_1\sigma_3$	0	0	$-\rho_3$	σ_2	$-\sigma_1$	0	$\rho_2\sigma_2$	$-\rho_2\sigma_1$	0
$\sigma_1\cong\xi_{13}$	0	0	0	$\rho_3\sigma_3$	$-\rho_3\sigma_2$	0	0	$\rho_1\sigma_3$	$-\rho_1\sigma_2$	0	$\rho_2\sigma_3$	$-\rho_2\sigma_2$	0	σ_3	$-\sigma_2$
$\sigma_2\cong\xi_{14}$	0	0	$-\rho_3\sigma_3$	0	$\rho_3\sigma_1$	0	$-\rho_1\sigma_3$	0	$\rho_1\sigma_1$	$-\rho_2\sigma_3$	0	$\rho_2\sigma_1$	$-\sigma_3$	0	σ_1
$\sigma_3\cong\xi_{15}$	0	0	$\rho_3\sigma_2$	$-\rho_3\sigma_1$	0	0	$\rho_1\sigma_2$	$-\rho_1\sigma_1$	0	$\rho_2\sigma_2$	$-\rho_2\sigma_1$	0	σ_2	$-\sigma_1$	0

$$s_1^{q\lambda}=\alpha(q)f(q)\frac{1}{\sqrt{3}}(\hat{q}_z n_{\lambda y}+\hat{q}_y n_{\lambda z}) ,$$

$$s_2^{q\lambda}=\alpha(q)f(q)\frac{1}{\sqrt{3}}(\hat{q}_z n_{\lambda x}+\hat{q}_x n_{\lambda z}) ,$$

$$s_3^{q\lambda}=\alpha(q)f(q)\frac{1}{\sqrt{3}}(\hat{q}_x n_{\lambda y}+\hat{q}_y n_{\lambda x}) ,$$

with $\hat{q}_i:=q_i/|\mathbf{q}|$ and $\alpha(q)=(\hbar\omega_{q\lambda}/2Mc_\lambda^2)^{1/2}$. $\mathbf{n}_\lambda(=n_{\lambda x},n_{\lambda y},n_{\lambda z})$ is the polarization vector. $f(q)$ is a cutoff function. In the most simple case it is given as

$$f(q)=[1+\tfrac{1}{4}(a^*)^2q^2]^{-2} ,$$

where a^* is the Bohr radius of the defect, describing the extension of the defect wave function.[21]

APPENDIX B

Table I represents the operators for a fourfold state.

APPENDIX C

The transformation of the electronic operator set for $k=2$ is shown as

$$\hat{\xi}_1=-D\xi_1-E\xi_{12} ,$$
$$\hat{\xi}_2=(1/\sqrt{2})(E\xi_2+D\xi_9+\xi_{15}) ,$$
$$\hat{\xi}_3=-D\xi_3-E\xi_{14} ,$$
$$\hat{\xi}_4=-D\xi_4+E\xi_{13} ,$$
$$\hat{\xi}_5=\xi_5 ,$$
$$\hat{\xi}_6=\xi_6 ,$$
$$\hat{\xi}_7=(1/\sqrt{2})(E\xi_4-\xi_7+D\xi_{13}) ,$$
$$\hat{\xi}_8=(1/\sqrt{2})(-E\xi_3-\xi_8+D\xi_{14}) ,$$
$$\hat{\xi}_9=-D\xi_2+E\xi_9 ,$$
$$\hat{\xi}_{10}=\xi_{10} ,$$
$$\hat{\xi}_{11}=\xi_{11} ,$$
$$\hat{\xi}_{12}=-E\xi_1+D\xi_{12} ,$$
$$\hat{\xi}_{13}=(1/\sqrt{2})(-E\xi_4-\xi_7-D\xi_{13}) ,$$
$$\hat{\xi}_{14}=(1/\sqrt{2})(E\xi_3-\xi_8-D\xi_{14}) ,$$
$$\hat{\xi}_{15}=(1/\sqrt{2})(E\xi_2+D\xi_9-\xi_{15}) .$$

APPENDIX D

The coefficients R^P and R^Q of the S matrix are given below. If we restrict ourselves to the case of an elastic field $\tau=\tau_2$ and an arbitrary magnetic field we have

TABLE II. Definition of the functions A_j^λ as the result of an angle-dependent integration over the phonon coordinates.

$\downarrow j\ \vec{\lambda}$	1	2	3
1	$\frac{16}{45}\pi D_\epsilon^2$	$\frac{8}{15}\pi D_\epsilon^2$	0
2	$\frac{16}{45}\pi D_\epsilon^2$	$\frac{4}{45}\pi D_\epsilon^2$	$\frac{4}{9}\pi D_\epsilon^2$
3	$\frac{16}{45}\pi D_\tau^2$	$\frac{16}{45}\pi D_\tau^2$	$\frac{2}{9}\pi D_\tau^2$
4	$\frac{16}{45}\pi D_\tau^2$	$\frac{16}{45}\pi D_\tau^2$	$\frac{2}{9}\pi D_\tau^2$
5	$\frac{16}{45}\pi D_\tau^2$	$\frac{4}{45}\pi D_\tau^2$	$\frac{4}{9}\pi D_\tau^2$

$$R^P_{1\,1}=E^2W_3^{q\lambda}+D^2W_0^{q\lambda},\quad R^Q_{5\,2}=DD_3^{q\lambda}\ ,$$
$$R^P_{2\,2}=E^2W_0^{q\lambda}+D^2W_3^{q\lambda},\quad R^Q_{4\,3}=0.5E^2(D_4^{q\lambda}-D_2^{q\lambda})+D^2D_1^{q\lambda}\ ,$$
$$R^P_{3\,3}=0.5E^2(W_2^{q\lambda}+W_4^{q\lambda})+D^2W_1^{q\lambda},\quad R^Q_{3\,4}=0.5E^2(D_2^{q\lambda}-D_4^{q\lambda})-D^2D_1^{q\lambda}\ ,$$
$$R^P_{4\,4}=0.5E^2(W_2^{q\lambda}+W_4^{q\lambda})+D^2W_1^{q\lambda},\quad R^Q_{2\,5}=-DD_3^{q\lambda}\ ,$$
$$R^P_{5\,5}=W_3^{q\lambda},\quad R^Q_{1\,6}=ED_3^{q\lambda}\ ,$$
$$R^P_{4\,7}=0.5E(W_4^{q\lambda}-W_2^{q\lambda}),\quad R^Q_{3\,7}=-0.5E(D_2^{q\lambda}+D_4^{q\lambda})\ ,$$
$$R^P_{3\,8}=0.5E(W_2^{q\lambda}-W_4^{q\lambda}),\quad R^Q_{4\,8}=-0.5E(D_2^{q\lambda}+D_4^{q\lambda})\ ,$$
$$R^P_{2\,9}=E\,D(W_0^{q\lambda}-W_3^{q\lambda}),\quad R^Q_{5\,9}=-ED_3^{q\lambda}\ ,$$
$$R^P_{1\,12}=E\,D(W_0^{q\lambda}-W_3^{q\lambda}),\quad R^Q_{3\,13}=-E\,D(0.5(D_4^{q\lambda}-D_2^{q\lambda})-D_1^{q\lambda})\ ,$$
$$R^P_{4\,13}=E\,D(0.5(W_2^{q\lambda}+W_4^{q\lambda})-W_1^{q\lambda}),\quad R^Q_{4\,14}=E\,D(0.5(D_4^{q\lambda}-D_2^{q\lambda})+D_1^{q\lambda})\ ,$$
$$R^P_{3\,14}=-E\,D(0.5(W_2^{q\lambda}+W_4^{q\lambda})-W_1^{q\lambda})\ .$$

All the other coefficients vanish. The expressions can be simplified to those of an elastic field alone by

$$E=1,\ D=0,\quad W_1^{q\lambda}=W_0^{q\lambda},\quad W_2^{q\lambda}=W_3^{q\lambda}=W_4^{q\lambda}=W^{q\lambda}\ .$$

APPENDIX E

Table II represents the angular integration within an isotropic Debye model.

APPENDIX F

The definitions of integrals needed for the Green-function equations are given below. We use the following abbreviations for the integrals, where s,g,d may have the values 0 to 4:

$$R_s^\lambda(n):=\int_0^{\omega_D}d\omega_{q\lambda}\frac{\omega_{q\lambda}^n}{\omega_{q\lambda}^2-\hat{\epsilon}_s^2}f_\lambda^2(\omega_{q\lambda})\ ,$$

$$\tilde{R}_s^\lambda(n):=\int_0^{\omega_D}d\omega_{q\lambda}\frac{\omega_{q\lambda}^n\coth\left[\dfrac{\beta\omega_{q\lambda}}{2}\right]}{\omega_{q\lambda}^2-\hat{\epsilon}_s^2}f_\lambda^2(\omega_{q\lambda})\ ,$$

$$S_{gd}^\lambda(\omega,n):=\int_0^{\omega_D}d\omega_{q\lambda}\frac{\omega^2-\omega_{q\lambda}^2+\hat{\epsilon}_d^2}{[(\omega-\hat{\epsilon}_d)^2-\omega_{q\lambda}^2][(\omega+\hat{\epsilon}_d)^2-\omega_{q\lambda}^2]}\frac{\omega_{q\lambda}^n}{\omega_{q\lambda}^2-\hat{\epsilon}_g^2}f_\lambda^2(\omega_{q\lambda})\ ,$$

$$\tilde{S}_{gd}^\lambda(\omega,n):=\int_0^{\omega_D}d\omega_{q\lambda}\frac{\omega^2-\omega_{q\lambda}^2+\hat{\epsilon}_d^2}{[(\omega-\hat{\epsilon}_d)^2-\omega_{q\lambda}^2][(\omega+\hat{\epsilon}_d)^2-\omega_{q\lambda}^2]}\frac{\omega_{q\lambda}^n\coth\left[\dfrac{\beta\omega_{q\lambda}}{2}\right]}{\omega_{q\lambda}^2-\hat{\epsilon}_q^2}f_\lambda^2(\omega_{q\lambda})\ ,$$

$$V_{gd}^\lambda(\omega,n):=\int_0^{\omega_D}d\omega_{q\lambda}\frac{1}{[(\omega-\hat{\epsilon}_d)^2-\omega_{q\lambda}^2][(\omega+\hat{\epsilon}_d)^2-\omega_{q\lambda}^2]}\frac{\omega_{q\lambda}^n}{\omega_{q\lambda}^2-\hat{\epsilon}_g^2}f_\lambda^2(\omega_{q\lambda})\ ,$$

$$\widetilde{V}^{\lambda}_{gd}(\omega,n):=\int_0^{\omega_D} d\omega_{q\lambda}\frac{1}{[(\omega-\hat{\epsilon}_d)^2-\omega_{q\lambda}^2][(\omega+\hat{\epsilon}_d)^2-\omega_{q\lambda}^2]}\frac{\omega_{q\lambda}^n\coth\left[\frac{\beta\omega_{q\lambda}}{2}\right]}{\omega_{q\lambda}^2-\hat{\epsilon}_g^2}f_\lambda^2(\omega_{q\lambda}) .$$

Restricting ourselves to the simple Lorentzian form of the cutoff function, i.e.,

$$f_\lambda(\omega_{q\lambda})=\left[1+\left[\frac{a^*}{2c_\lambda}\right]^2\omega_{q\lambda}^2\right]^{-2}$$

the temperature-independent integrals result in rational functions. So they may be easily solved.[30] The calculation of the temperature-dependent integrals cannot be done analytically. A numerial integration is impossible due to CPU-time considerations. We therefore developed the coth-part:[31]

$$\coth x=\frac{1}{x}+\sum_{k=1}^{\infty}\frac{2^{2k}B_{2k}}{(2k)!}x^{2k-1},\quad B_n\text{: Bernoulli's numbers} .$$

This series converges for $|x|<\pi$. Even for $k\leq 5$ good results are received in accordance with numerical calculations. Together with this series no new type of integral is needed, therefore this method was chosen despite other methods with better convergence conditions.[31] All the integrals are of Cauchy-principal-value type. The imaginary parts of the integrals can be calculated analytically.

APPENDIX G

A listing of the terms appearing in expression (35) is given below. In the following, summation convention is used:

$$n_1(\omega)=\omega^4-\omega^2N^{(1)}_{jlm}K_lK_m ,$$

$$n_2(\omega)=\omega^4\sum_{q,\lambda}\gamma_\lambda[N^{(2)}_{ja}\widetilde{S}^{\lambda}(\omega,5)+N^{(3)}_{jalm}\widetilde{V}^{\lambda}(\omega,5)K_lK_m]A_a^\lambda ,$$

$$n_3(\omega)=\omega^4\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(4)}_{jab}S^{\lambda}(\omega,4)+N^{(5)}_{jablm}V^{\lambda}(\omega,4)K_lK_m]A_a^\lambda A_b^{\lambda'}R^{\lambda'}(4) ,$$

$$n_4(\omega)=\omega^4\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(6)}_{jabkn}\widetilde{S}^{\lambda}(\omega,3)+N^{(7)}_{jabknlm}\widetilde{V}^{\lambda}(\omega,3)K_lK_m]R^{\lambda'}(4)A_a^\lambda A_b^{\lambda'}K_n\langle\xi_k\rangle_T ,$$

$$n_5(\omega)=\omega^4\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(8)}_{jabkn}S^{\lambda}(\omega,4)+N^{(8)}_{jabknlm}V^{\lambda}(\omega,4)K_lK_m]\widetilde{R}^{\lambda'}(3)A_a^\lambda A_b^{\lambda'}K_n\langle\xi_k\rangle_T ,$$

$$n_6(\omega)=\omega^2\sum_{q,\lambda}\gamma_\lambda[N^{(10)}_{ja}S^{\lambda}(\omega,6)+N^{(11)}_{jalm}V^{\lambda}(\omega,6)K_lK_m]A_a^\lambda ,$$

$$n_7(\omega)=\omega^2\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(12)}_{jabnp}S^{\lambda}(\omega,4)+N^{(13)}_{jabnplm}V^{\lambda}(\omega,4)K_lK_m]A_a^\lambda A_b^{\lambda'}R^{\lambda'}(4)K_nK_p ,$$

$$n_8(\omega)=\omega^2\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(14)}_{jabnp}\widetilde{S}^{\lambda}(\omega,5)+N^{(15)}_{jabnplm}\widetilde{V}^{\lambda}(\omega,5)K_lK_m]A_a^\lambda A_b^{\lambda'}R^{\lambda'}(4)K_n\langle\xi_p\rangle_T ,$$

$$n_8(\omega)=\omega^2\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(14)}_{jabnp}\widetilde{S}^{\lambda}(\omega,5)+N^{(15)}_{jabnplm}\widetilde{V}^{\lambda}(\omega,5)K_{lm}K_m]A_a^\lambda A_b^{\lambda'}R^{\lambda'}(4)K_n\langle\xi_p\rangle_T ,$$

$$n_9(\omega)=\omega^2\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(16)}_{jabnp}S^{\lambda}(\omega,6)+N^{(17)}_{jabnplm}V^{\lambda}(\omega,6)K_lK_m]A_a^\lambda A_b^{\lambda'}\widetilde{R}^{\lambda'}(3)K_n\langle\xi_p\rangle_T ,$$

$$n_{10}(\omega)=\omega^2\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(18)}_{jabnp}S^{\lambda}(\omega,4)+N^{(19)}_{jabnplm}V^{\lambda}(\omega,4)K_lK_m]A_a^\lambda A_b^{\lambda'}\widetilde{R}^{\lambda'}(5)K_n\langle\xi_p\rangle_T ,$$

$$n_{11}(\omega)=\omega^2\sum_{q,\lambda}\gamma_\lambda[N^{(20)}_{jalm}\widetilde{S}^{\lambda}(\omega,3)+\omega^2N^{(21)}_{jalm}\widetilde{V}^{\lambda}(\omega,3)]K_lK_mA_a^\lambda ,$$

$$n_{12}(\omega)=\omega^2\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(22)}_{jablm}S^{\lambda}(\omega,4)+\omega^2N^{(23)}_{jablm}V^{\lambda}(\omega,4)]K_lK_mA_a^\lambda A_b^{\lambda'}R^{\lambda'}(4) ,$$

$$n_{13}(\omega)=\omega^2\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(24)}_{jablm}\widetilde{S}^{\lambda}(\omega,3)+\omega^3N^{(25)}_{jablm}\widetilde{V}^{\lambda}(\omega,3)]K_lK_mA_a^\lambda A_b^{\lambda'}R^{\lambda'}(4) ,$$

$$n_{14}(\omega)=\omega^2\sum_{q,\lambda}\sum_{q',\lambda'}\gamma_\lambda\gamma_{\lambda'}[N^{(26)}_{jablm}S^{\lambda}(\omega,4)+\omega^2N^{(27)}_{jablm}V^{\lambda}(\omega,4)]K_lK_mA_A^\lambda A_b^{\lambda'}\widetilde{R}^{\lambda'}(3) ,$$

and the denominator terms

$$Z_1(\omega)=\omega^2 Z^{(1)}_{jkl}K_k\langle\xi_l\rangle_T\ ,$$

$$Z_2(\omega)=\omega^4\sum_{q,\lambda}\gamma_\lambda[Z^{(2)}_{ja}S^\lambda(\omega,4)+Z^{(3)}_{jalm}V^\lambda(\omega,4)K_lK_m]A^\lambda_a\ ,$$

$$Z_3(\omega)=\omega^4\sum_{q,\lambda}\gamma_\lambda[Z^{(4)}_{jalm}\widetilde{S}^\lambda(\omega,3)+Z^{(5)}_{jalm}\widetilde{V}^\lambda(\omega,5)]K_l\langle\xi_m\rangle_T A^\lambda_a\ ,$$

$$Z_4(\omega)=\omega^4\sum_{q,\lambda}\gamma_\lambda[Z^{(6)}_{jalm}S^\lambda(\omega,4)K_m+Z^{(7)}_{jalm}\widetilde{S}^\lambda(\omega,5)\langle\xi_m\rangle_T]K_lA^\lambda_a\ ,$$

$$Z_5(\omega)=\omega^2\sum_{q,\lambda}\gamma_\lambda[Z^{(8)}_{jalm}\widetilde{S}^\lambda(\omega,5)+\omega^2 Z^{(9)}_{jalm}\widetilde{V}^\lambda(\omega,5)]K_l\langle\xi_m\rangle_T A^\lambda_a\ ,$$

$$Z_6(\omega)=\omega\sum_{q,\lambda}\sum_{q',\lambda'}[Z^{(10)}_{jab}S^\lambda(\omega,6)+Z^{(11)}_{jablm}V^\lambda(\omega,6)K_lK_m]A^\lambda_a A^{\lambda'}_b R^{\lambda'}(4)\ ,$$

$$Z_7(\omega)=\omega\sum_{q,\lambda}\sum_{q',\lambda'}[Z^{(12)}_{jablm}S^\lambda(\omega,6)+Z^{(13)}_{jablmkp}V^\lambda(\omega,6)K_kK_p]A^\lambda_a A^{\lambda'}_b \widetilde{R}^{\lambda'}(3)K_l\langle\xi_m\rangle_T\ .$$

The values of the coefficients $N^{(i)}$ and $Z^{(i)}$ are not given explicitly. They contain the algebraic properties of SU(4) through different kinds of commutators. In our case they were determined numerically.

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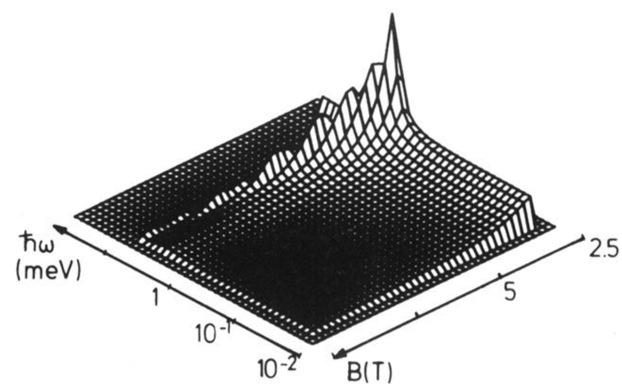

FIG. 5. Phonon relaxation rate plotted against magnetic field strength and phonon energy. The energy scale is logarithmic, the magnetic field scale is linear.

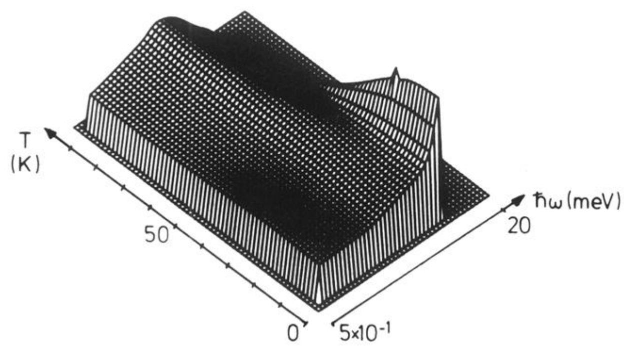

FIG. 6. Temperature dependence of the relaxation rate for an applied elastic field with $\Delta\epsilon=4$ meV. The energy scale is logarithmic, the temperature scale is linear.