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# Ultrasonic attenuation by impurities in semiconductors

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We have calculated the ultrasonic attenuation by donors and acceptors in semiconductors by solving the equation of motion for one-particle density matrix and the equation of sound. Explicit expressions of the attenuation coefficient are given for *n*-Ge and *p*-Si. The crucial point in our theory is to take account of the relaxation of the system into an instantaneous local thermal equilibrium. In contrast to the theories for *n*-Ge by Kwok and for *p*-Si by Suzuki and Mikoshiba, who calculated the attenuation from the self-energy function in the Green's-function method, our formula is written as the sum of three terms: the *classical* Zener relaxation term and the *usual* resonance and antiresonance terms with the Lorentzian line shape. It is pointed out that the diagram technique used by Kowk is not justified for the impurity system. Our theory seems to be valid when the angular frequency of ultrasonic waves is smaller than the inverse of the relaxation time of the system.

## I. INTRODUCTION

Ultrasonic attenuations by isolated, neutral donors and acceptors in Ge and Si have been experimentally investigated at low temperatures by many workers. They have measured (i) the temperature dependence of the attenuation in *n*-Ge,[1-3] *n*-Si,[2] *p*-Si,[4-6] and *p*-Ge,[5] (ii) the uniaxial stress dependence of the attenuation in *p*-Si,[7] and (iii) the magnetic-field dependence of the attenuation in *n*-Ge,[8,9] *p*-Si,[6,10,11] and *p*-Ge.[12]

The experimental results have been analyzed fairly well by using the following two types of theories. The first theory[5,7,13] was developed based on the classical consideration that the ultrasonic attenuation by neutral donors and acceptors is caused by the relaxation of the system into an instantaneous, local thermal equilibrium when the impurity levels are modulated by strains associated with ultrasonic waves. The theoretical formula has the form of a classical Zener relaxation attenuation. The second theory, which takes into account quantum mechanically not only the relaxation attenuation but also the resonance and antiresonance attenuation, has been developed by Kwok[14] for *n*-Ge and by Suzuki and Mikoshiba[15] (hereafter referred to as SM) for *p*-Si. They have calculated the attenuation from the self-energy function in the Green's-function method.

Recently, Schad and Lassmann[16] criticized the calculation by SM in the sense that the SM formula for *p*-Si does not agree with the classical Zener relaxation formula in the low-frequency limit. Here, we remark also that the resonance and antiresonance terms in the SM model do not have the same form as the usual resonance absorption with the Lorentzian line shape. We believe that the relaxation of the system into the instantaneous, local equilibrium is essentially important in the low-frequency range as is shown in the theories of ultrasonic attenuation by conduction electrons in metals[17,18] and by thermal phonons in dielectrics,[19] and it is not properly taken into account in the theories by Kwok[14] and SM.

The purpose of this paper is to give a theory which might be valid in the low-frequency range. In Sec. II, we solve, up to first order in the amplitude of the ultrasonic waves, the dynamical equation for the one-particle density matrix for donor electrons (acceptor holes) by introducing phenomenologically a term which represents the relaxation to the instantaneous, local thermal equilibrium. General expressions for the change in elastic constants due to impurities and for attenuation coefficients are derived in Sec. III.

In Sec. IV, explicit expressions for the attenuation coefficients in *n*-Ge are given for shear and longitudinal waves propagated along the [100] direction. It is pointed out that the attenuation coefficient for shear waves has a relaxation attenuation term which is proportional to the upper-level population in the donor ground states and is the same as that derived classically by Suzuki and Mikoshiba[13] and by Pomerantz.[2,5] In Sec. V, the attenuation coefficients in *p*-Si, where internal random strains give rise to the level splitting of acceptor ground states, are calculated for shear and longitudinal waves propagated along the [100] direction. Explicit expressions are given for particular cases of the internal uniaxial strain along the [111] direction. It is shown that our relaxation attenuation term is proportional to the product of the upper-level and lower-level population and is the same as that derived classically by Ishiguro *et al.*[7]

In Sec. VI, we compare our results for *p*-Si with those in the SM model. First, it is pointed out that the diagram technique in the Green's-function method used by Kwok and SM is not justified for the impurity problem. In fact, the relaxation attenuation in the SM model is given by the sum of two terms proportional to the upper-level and lower-level population in contrast to our result. It seems at first sight that the relaxation attenuation for $n$-Ge derived by Kwok is the same as that[2,5,13] derived classically. However, this agreement is an accidental coincidence which is caused by the particular form of the deformation-potential matrix elements in $n$-Ge.

## II. INTERACTION BETWEEN ULTRASONIC WAVES AND DONOR ELECTRONS (ACCEPTOR HOLES)

Let us consider the interaction of ultrasonic waves with donor electrons (acceptor holes). The total Hamiltonian is given by

$$H = H_0 + H' = \sum_i H_i = \sum_i (H_{0i} + H_i'). \tag{1}$$

In the notation of the second quantization, we have the expressions

$$H_0 = \sum_i H_{0i} = \sum_{i\mu_i} \epsilon_{\mu_i} c^\dagger_{\mu_i} c_{\mu_i}. \tag{2a}$$

$$H' = \sum_i H_i' = \sum_{\substack{i\vec{q}\lambda \\ \mu_i\nu_i}} \left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)^{1/2} \times C_{q\lambda}^{\mu_i\nu_i} e^{i\vec{q}\cdot\vec{R}_i} f(q)(a_{q\lambda} + a^*_{-q\lambda}) c^\dagger_{\mu_i} c_{\nu_i} \tag{2b}$$

[see Appendix A for the derivation of Eq. (2)], where $c_{\mu_i}$ and $c^\dagger_{\mu_i}$ are the annihilation and creation operators for the electron (hole) on the level $\mu_i$ with energy $\epsilon_{\mu_i}$ at the $i$th donor (acceptor), $a_{q\lambda}$ is the amplitude of ultrasonic waves in the $\lambda$ branch with wave vector $\vec{q}$, sound velocity $v_{q\lambda}$, and the angular frequency $\omega_{q\lambda} = qv_{q\lambda}$, $\rho_0$ is the mass density, $V$ is the volume of the sample, $f(q)$ is the cutoff function[20] which characterizes the spread of donor (acceptor) wave functions, $C_{q\lambda}^{\mu_i\nu_i}$ is the deformation-potential matrix element given by

$$C_{q\lambda}^{\mu_i\nu_i} = \frac{i}{2}\sum_{\alpha\beta l} [(\hat{e}_{q\lambda})_\alpha(\hat{q})_\beta + (\hat{e}_{q\lambda})_\beta(\hat{q})_\alpha]\, \Xi_{\alpha\beta}(l)\, \alpha^{(l)}_{\mu_i}\alpha^{(l)}_{\nu_i}. \tag{3}$$

Here, $\hat{e}_{q\lambda}$ is the polarization vector of the ultrasonic wave in the $(\vec{q},\lambda)$ mode, $\hat{q}$ is the unit vector along the direction of $\vec{q}$, $\Xi_{\alpha\beta}(l)$ is the $(\alpha,\beta)$ component of the deformation potential, $\alpha^{(l)}_{\mu_i}$ is the quantity[20] introduced to represent the symmetry of the band structure, and $\vec{R}_i$ is the position vector of the $i$th impurity.

Since $a_{q\lambda}$ is a $c$ number in our treatment, $H_i$ and $H_j$ commute. Therefore, we get the following dynamical equation for the one-particle density matrix for the $i$th donor electron (acceptor hole):

$$i\hbar\frac{\partial\rho_i}{\partial t} = [H_i, \rho_i] - i\hbar\left(\frac{\partial\rho_i}{\partial t}\right)_{\text{relax}}, \tag{4}$$

$$\left(\frac{\partial\rho_i}{\partial t}\right)_{\text{relax},\mu\nu} = \frac{1}{\tau_{\mu\nu}}\left(\rho_{i,\mu\nu} - \frac{e^{-\beta H_i}}{\mathrm{Tr}(e^{-\beta H_i})}\right), \tag{5}$$

where $\beta \equiv 1/k_B T$ and $\tau_{\mu\nu}(=\tau_{\nu\mu})$ is the relaxation time between the $\mu$ and $\nu$ states caused by the interaction with thermal phonons. A method to obtain explicit expressions for $\tau_{\mu\nu}$ in the two-level system is given in Appendix B. In Eq. (4) we have introduced phenomologically the term by which $\rho_i$ relaxes not into the complete thermal equilibrium, $\rho_{i0} = \exp(-\beta H_{0i})/\mathrm{Tr}[\exp(-\beta H_{0i})]$, but into the instantaneous, local thermal equilibrium, $\exp(-\beta H_i)/\mathrm{Tr}[\exp(-\beta H_i)]$. It is noted that Eqs. (4) and (5) cannot be justified in the case of $\omega\tau > 1$, and we have neglected the change in local temperature caused by ultrasonic waves.

In order to satisfy the normalization condition

$$\mathrm{Tr}(\rho_i) = 1, \tag{6}$$

we take, for simplicity, all the diagonal relaxation times to be equal, i.e., $\tau_{\mu\mu} = \tau$. We now expand $\rho_i$ as

$$\rho_i = \rho_{i0} + \rho_{i1}, \tag{7}$$

where $\rho_{i1}$ is the term proportional to the amplitude of ultrasonic waves. Using the well-known formula[21]

$$e^{-\beta(H_{0i}+H_i')} = e^{-\beta H_{0i}}\left(1 - \int_0^\beta ds\, e^{sH_{0i}} H_i' e^{-sH_{0i}} + \cdots\right), \tag{8}$$

we obtain the expression for $\rho_{i1}$:

$$\rho_{i1}(t) = \sum_{q\lambda}[\rho_{i1}(\omega_{q\lambda})e^{-i\omega_{q\lambda}t} + \rho^*_{i1}(\omega_{q\lambda})e^{i\omega_{q\lambda}t}], \tag{9}$$

$$[\rho_{i1}(\omega_{q\lambda})]_{\mu\nu} = \sum_{\Omega_q} \frac{(\hbar\omega_{q\lambda}/2\rho_0 V v_{q\lambda}^2)^{1/2} f(q)}{\hbar(\omega_{q\lambda} + \omega_{\nu\mu_i} + i/\tau_{\mu\nu})} \times\left[(n_{\nu_i} - n_{\mu_i})\left(1 + \frac{i}{\tau_{\mu\nu}\omega_{\nu\mu_i}}\right)C^{\mu\nu}_{q\lambda} + \frac{i}{\tau_{\mu\nu}}\hbar\beta\delta_{\mu\nu}\sum_{\mu'} n_{\mu_i'} C^{\mu'\mu'}_{q\lambda}\right]\tilde{a}_{q\lambda} e^{i\vec{q}\cdot\vec{R}_i}, \tag{10}$$

where the sum in Eq. (10) represents the sum over the direction of $\hat{q}$ and we used the relations

$$n_{\mu_i} \equiv (\rho_{i0})_{\mu_i\mu_i} = e^{-\beta\epsilon_{\mu_i}} \Big/ \sum_{\mu_i'} e^{-\beta\epsilon_{\mu_i'}},$$

$$H_{0i}\varphi_{\mu_i} = \epsilon_{\mu_i}\varphi_{\mu_i}, \quad \hbar\omega_{\nu\mu_i} \equiv \epsilon_{\nu_i} - \epsilon_{\mu_i}, \quad a_{q\lambda} \equiv \tilde{a}_{q\lambda} e^{-i\omega_{q\lambda}t}. \tag{11}$$

## III. DERIVATION OF ULTRASONIC ATTENUATION COEFFICIENT

Let us denote the $(q,\omega)$ components of stress and strain tensor by $\sigma_{\alpha\beta}(q,\omega)$ and $\epsilon_{\alpha\beta}(q,\omega)$, respectively. Then, the elastic constants are defined by the equation

$$\sigma_{\alpha\beta}(q,\omega)=c_{\alpha\beta\gamma\delta}(q,\omega)\epsilon_{\gamma\delta}(q,\omega), \quad (12)$$

$$c_{\alpha\beta\gamma\delta}(q,\omega)=c^{(0)}_{\alpha\beta\gamma\delta}(q,\omega)+c^{(1)}_{\alpha\beta\gamma\delta}(q,\omega), \quad (13)$$

where $c^{(0)}_{\alpha\beta\gamma\delta}(q,\omega)$ is the elastic constant of semiconductors with no impurity and $c^{(1)}_{\alpha\beta\gamma\delta}(q,\omega)$ is the change in elastic constants caused by impurities.

Using the dynamical equation of sound,[22] we obtain the determinantal equation,

$$|q_\beta q_\gamma c_{\alpha\beta\gamma\delta}(q,\omega)-\rho_0\omega^2\delta_{\alpha\delta}|=0. \quad (14)$$

In the case of ultrasonic waves propagated along the [100] direction in cubic crystals, the solution of Eq. (14) is given for the transverse wave by

$$q=(\rho_0\omega^2/c_{ll})^{1/2}, \quad l=5,6, \quad (15)$$

and for the longitudinal wave by

$$q=(\rho_0\omega^2/c_{11})^{1/2}, \quad (16)$$

where $c_{11}$ and $c_{ll}=c_{44}(l=5,6)$ are the well-known matrix notation for the elastic constants.[23] Since the ultrasonic (amplitude) attenuation coefficient $\alpha$ is given by the imaginary part of $q$, we obtain for the transverse wave

$$\alpha=\rho_0^{1/2}\omega\,\mathrm{Im}(c^{(0)}_{ll}+c^{(1)}_{ll})^{-1/2}$$
$$\cong-\tfrac{1}{2}\rho_0^{1/2}\omega(c^{(0)}_{ll})^{-3/2}\,\mathrm{Im}(c^{(1)}_{ll}), \quad (17)$$

and for the longitudinal wave

$$\alpha\cong-\tfrac{1}{2}\rho_0^{1/2}\omega(c^{(0)}_{11})^{-3/2}\,\mathrm{Im}(c^{(1)}_{11}). \quad (18)$$

As is shown in Appendix C, the contribution of impurities to the stress tensor is given by

$$\sigma_{\alpha\beta}(q,t)=\mathrm{Tr}\left(\rho V^{-1/2}\sum_{il\mu_i\nu_i}f(-q)\Xi_{\alpha\beta}(l)\times e^{-i\vec{q}\cdot\vec{R}_i}\alpha^{(l)}_{\mu_i}\alpha^{(l)}_{\nu_i}c^\dagger_{\mu_i}c_{\nu_i}\right). \quad (19)$$

On the other hand, the $(q,\lambda)$ component of the strain tensor associated with ultrasonic waves is given by

$$\epsilon_{\alpha\beta}(q\lambda,t)=(\tfrac{1}{2}i)(\hbar\omega_{q\lambda}/2\rho_0v^2_{q\lambda})^{1/2}\times[(\hat{e}_{q\lambda})_\alpha(\hat{q})_\beta+(\hat{e}_{q\lambda})_\beta(\hat{q})_\alpha](a_{q\lambda}+a^*_{-q\lambda}). \quad (20)$$

Inserting the expression for the density matrix

$$\rho=\prod_i^N(\rho_{i0}+\rho_{i1}) \quad (21)$$

($N$: total number of impurities) into Eq. (19), we obtain

$$\sigma_{\alpha\beta}(q\lambda,\omega_{q'\lambda})=V^{-1/2}\sum_{i\mu_i\nu_il}f(-q)\Xi_{\alpha\beta}(l)\times\alpha^{(l)}_{\mu_i}\alpha^{(l)}_{\nu_i}e^{-i\vec{q}\cdot\vec{R}_i}[\rho_{i1}(\omega_{q'\lambda})]_{\nu_i\mu_i}. \quad (22)$$

It should be noted that in addition to Eq. (22) there is a static component of stress tensor given by

$$\sigma_{\alpha\beta}(q,0)=\sum_{i\mu_il}f(-q)V^{-1/2}n_{\mu_i}\Xi_{\alpha\beta}(l)\alpha^{(l)}_{\mu_i}\alpha^{(l)}_{\mu_i}, \quad (23)$$

which is irrelevant to the present problem and is neglected hereafter.

We now assume that the distribution of impurities is at random so that

$$\sum_i^N\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_i]=N\delta_{\vec{q}\vec{q}'},$$

and the energy levels $\epsilon_{\mu_i}$ are equal for all impurities. Then, inserting Eq. (10) into Eq. (22), we obtain

$$\sigma_{\alpha\beta}(q\lambda,\omega_{q\lambda})=NV^{-1/2}\sum_{\mu\nu}f(-q)\tilde{\Xi}^{\mu\nu}_{\alpha\beta}\frac{(\hbar\omega_{q\lambda}/2\rho_0Vv^2_{q\lambda})^{1/2}f(q)}{\hbar(\omega_{q\lambda}+\omega_{\mu\nu}+i/\tau_{\mu\nu})}\left[(n_\mu-n_\nu)\left(1+\frac{i}{\tau_{\mu\nu}\omega_{\mu\nu}}\right)C^{\mu\nu}_{q\lambda}+\frac{i\hbar\beta}{\tau_{\mu\nu}}\delta_{\mu\nu}\sum_{\mu'}n_{\mu'}C^{\mu'\mu'}_{q\lambda}\right]\tilde{a}_{q\lambda}, \quad (24)$$

where

$$\tilde{\Xi}^{\mu\nu}_{\alpha\beta}=\sum_l\Xi_{\alpha\beta}(l)\alpha^{(l)}_\mu\alpha^{(l)}_\nu. \quad (25)$$

With the help of Eqs. (3) and (20), we obtain the final expression for the contribution of impurities to the elastic constant:

$$c^{(1)}_{\alpha\beta\gamma\delta}(q\lambda,\omega_{q\lambda})=\frac{N}{V}|f(q)|^2\sum_{\mu\neq\nu}\left(\frac{(n_\mu-n_\nu)(\omega_{\mu\nu}+i/\tau_{\mu\nu})}{\hbar\omega_{\mu\nu}(\omega_{q\lambda}+\omega_{\mu\nu}+i/\tau_{\mu\nu})}\tilde{\Xi}^{\mu\nu}_{\alpha\beta}\tilde{\Xi}^{\nu\mu}_{\gamma\delta}-\frac{1}{2}\frac{\beta n_\mu n_\nu}{(1-i\omega_{q\lambda}\tau)}(\tilde{\Xi}^{\nu\nu}_{\alpha\beta}-\tilde{\Xi}^{\mu\mu}_{\alpha\beta})(\tilde{\Xi}^{\nu\nu}_{\gamma\delta}-\tilde{\Xi}^{\mu\mu}_{\gamma\delta})\right). \quad (26)$$

The effects of the relaxation into the instantaneous, local equilibrium appear in the term $i/\tau_{\mu\nu}$ in the numerator of the first term and in the second term of Eq. (26). Inserting Eq. (26) into Eqs. (17) and (18), we obtain the formulas for attenuation coefficients of ultrasonic waves propagated along the [100] direction in cubic crystals:

$$\alpha_t(q,\omega_{q\lambda})=\frac{n\omega_{q\lambda}|f(q)|^2}{2\rho_0 v_{q\lambda}^2}\sum_{\mu\neq\nu}\mathrm{Im}\left(\frac{(n_\nu-n_\mu)(\omega_{\mu\nu}+i/\tau_{\mu\nu})}{\hbar\omega_{\mu\nu}(\omega_{q\lambda}+\omega_{\mu\nu}+i/\tau_{\mu\nu})}\tilde{\Xi}^{\mu\nu}_{mk}\tilde{\Xi}^{\nu\mu}_{mk}+\frac{\beta n_\mu n_\nu}{2(1-i\omega_{q\lambda}\tau)}(\tilde{\Xi}^{\nu\nu}_{mk}-\tilde{\Xi}^{\mu\mu}_{mk})^2\right),\tag{27a}$$

$$n\equiv N/V,\quad v_{q\lambda}^2=c_{ll}^{(0)}/\rho_0\tag{27b}$$

for transverse waves, where $(m,k)=(1,3)$ for $l=5$ $(\lambda=3)$ and $(m,k)=(1,2)$ for $l=6$ $(\lambda=2)$. The attenuation coefficient $\alpha_l(q,\omega_{ql})$ for longitudinal wave is obtained by replacing $\omega_{q\lambda}, c_{ll}^{(0)}, v_{q\lambda}$ by $\omega_{ql}$, $c_{11}^{(0)}, v_{ql}$ and taking $(m,k)=(1,1)$ in Eq. (27).

## IV. ULTRASONIC ATTENUATION BY NEUTRAL DONORS IN Ge

Let us now derive the explicit expressions for the attenuation coefficients in $n$-Ge. In Fig. 1 is shown the schematic diagram of energy levels of donor ground states in $n$-Ge.

According to Hasegawa,[20] the relation

$$\tilde{\Xi}^{\mu\nu}_{\alpha\beta}=\tfrac{1}{3}\Xi_u D^{\mu\nu}_{\alpha\beta}+\Xi_d\delta_{\mu\nu}\delta_{\alpha\beta}\tag{28}$$

holds in $n$-Ge, where the tensor $D^{\mu\nu}$ is defined by

$$D^{\mu\nu}=\sum_l \alpha_\mu^{(l)}\alpha_\nu^{(l)}U^{(l)}.\tag{29}$$

We can choose the following set of values[24] for $\alpha_\mu^{(l)}$ and $U^{(l)}$:

$$\begin{aligned}&\alpha_0=\tfrac{1}{2}(1,1,1,1)\ (s\text{-like}),\ A_1\ (\text{singlet}),\\&\left.\begin{aligned}\alpha_1&=\tfrac{1}{2}(1,1,-1,-1)\ (p_x\text{-like})\\\alpha_2&=\tfrac{1}{2}(1,-1,1,-1)\ (p_y\text{-like})\\\alpha_3&=\tfrac{1}{2}(1,-1,-1,1)\ (p_z\text{-like})\end{aligned}\right\}T_2\ (\text{triplet}),\end{aligned}\tag{30}$$

$$U^{(1)}=\begin{bmatrix}1&1&1\\1&1&1\\1&1&1\end{bmatrix},\quad U^{(2)}=\begin{bmatrix}1&-1&-1\\-1&1&1\\-1&1&1\end{bmatrix},\quad U^{(3)}=\begin{bmatrix}1&-1&1\\-1&1&-1\\1&-1&1\end{bmatrix},\quad U^{(4)}=\begin{bmatrix}1&1&-1\\1&1&-1\\-1&-1&1\end{bmatrix},\tag{31}$$

$$\begin{aligned}&D^{00}=D^{11}=D^{22}=D^{33}=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix},\quad D^{01}=D^{23}=\begin{bmatrix}0&0&0\\0&0&1\\0&1&0\end{bmatrix},\\&D^{02}=D^{13}=\begin{bmatrix}0&0&1\\0&0&0\\1&0&0\end{bmatrix},\quad D^{03}=D^{12}=\begin{bmatrix}0&1&0\\1&0&0\\0&0&0\end{bmatrix},\quad D^{ij}=D^{ji}.\end{aligned}\tag{32}$$

Thus, we obtain the following explicit expressions for the attenuation coefficients:

(i) Shear wave; $\hat{q}\parallel[100], \hat{e}_q\parallel[010]$:

$$\alpha_t(q,\omega)=\frac{n\omega^2\Xi_u^2|f(q)|^2}{18\rho_0 v_t^3(3+e^{4\Delta\beta})}\left[\frac{e^{4\Delta\beta}-1}{4\Delta}\left(\frac{1/\tau_{03}}{(\omega+4\Delta/\hbar)^2+1/\tau_{03}^2}+\frac{1/\tau_{30}}{(\omega-4\Delta/\hbar)^2+1/\tau_{30}^2}\right)+2\beta\frac{1/\tau_{12}}{\omega^2+1/\tau_{12}^2}\right].\tag{33}$$

The last term is the same as that derived classically by Suzuki and Mikoshiba[13] and by Pomerantz[2,5] when $|f(q)|=1$.

(ii) Shear wave; $\hat{q}\parallel[100]$, $\hat{e}_q\parallel[001]$: The expression for $\alpha_t(q,\omega)$ is the same as Eq. (33) except that $\tau_{12}$ is replaced by $\tau_{13}$.

(iii) Longitudinal wave; $\hat{q}\parallel[100]$, $\hat{e}_q\parallel[100]$:

$$\alpha_l(q,\omega)=0.\tag{34}$$

We note that the set of values in Eqs. (30)–(32) is different from that used by Kwok.[14] The attenuation coefficients, when Kwok's matrix elements are used, are discussed in Appendix D.

## V. ULTRASONIC ATTENUATION BY NEUTRAL ACCEPTORS IN Si

The ground state of acceptor holes in $p$-Si is fourfold degenerate when there is no strain in crystals. We denote these degenerate states by

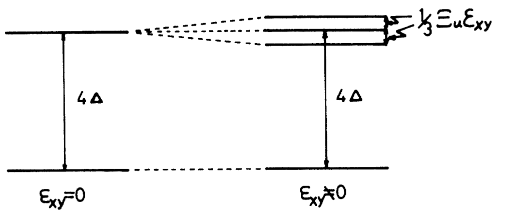


FIG. 1. Schematic diagram of ground-state energy levels of a donor electron in $n$-Ge. When there is no strain (e.g., $\epsilon_{xy}=0$), the upper levels are threefold degenerate (triplet). The separation between the singlet and the triplet is denoted by $4\Delta$ and is called the valley-orbit splitting. To first order in $\epsilon_{xy}$, the triplet states split into three different energy levels of equal spacing, $(1/3)\,\Xi_u\epsilon_{xy}$, with the center level unshifted, while the singlet remains unchanged.

$|n\rangle$ ($n=1,2,3,4$) corresponding to the quantum number $M_J(=\frac{3}{2},\frac{1}{2},-\frac{1}{2},-\frac{3}{2})$. SM first pointed out that the fourfold-degenerate ground states split into two energy levels by the interaction of acceptor holes with an internal random strain $\epsilon^{(r)}$, and this splitting is essentially important to explain the experiments of ultrasonic attenuation. The schematic diagram of energy levels of acceptor ground state in $p$-Si is shown in Fig. 2. The hole-strain interaction[25,26] is given by

$$H^{(r)}_{\text{h-s}}=\tfrac{2}{3}D^a_u\left[(J_x^2-\tfrac{1}{3}J^2)\epsilon^{(r)}_{xx}+\text{c.p.}\right]+\tfrac{1}{3}D^a_{u'}\left[(J_xJ_y+J_yJ_x)\epsilon^{(r)}_{xy}+\text{c.p.}\right], \tag{35}$$

where $J_\alpha$ is the $\alpha$th component of angular momentum $J=\frac{3}{2}$ and c.p. denotes cyclic permutation.

Let us calculate the ultrasonic attenuation by acceptor holes when the internal strain $\epsilon^{(r)}$ exists. The unperturbed state $\Psi_\mu$ and energy splittings when $\epsilon^{(r)}\neq 0$ are calculated in Appendix E. The interaction Hamiltonian with ultrasonic waves is given by

$$H'=\sum_{\substack{iq\lambda\\ \mu_i\nu_i}}\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)^{1/2} f(q)\,C^{\mu_i\nu_i}_{q\lambda}e^{i\vec{q}\cdot\vec{R}_i}(a_{q\lambda}+a^*_{-q\lambda})\,c^\dagger_{\mu_i}c_{\nu_i}\,. \tag{36}$$

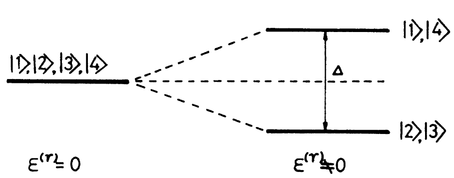


FIG. 2. Schematic diagram of ground-state energy levels of an acceptor hole in $p$-Si. When there is no strain ($\epsilon^{(r)}=0$), the ground state are fourfold degenerate. When there is a strain $\epsilon^{(r)}$, the ground states split into two levels with the energy splitting $\Delta$.

Here, $C^{\mu_i\nu_i}_{q\lambda}$ can be expressed in terms of $\tilde{C}^{nn'}_{q\lambda}$ by using the unitary transformation $\tilde{v}$ from the $|n\rangle$ states to the $\Psi_\mu$ states:

$$C^{\mu_i\nu_i}_{q\lambda}=\sum_{nn'} i\tilde{C}^{nn'}_{q\lambda}v^*_{n\mu_i}v_{n'\nu_i}\,, \tag{37}$$

where

$$\tilde{v}=\{v_{n\mu_i}\}=\frac{1}{[A(\epsilon)]^{1/2}}\begin{bmatrix} a_i+\epsilon_i & b_i & c_i & 0\\ b_i^* & -a_i-\epsilon_i & 0 & c_i\\ c_i^* & 0 & -a_i-\epsilon_i & -b_i\\ 0 & c_i^* & -b_i & a_i+\epsilon_i\end{bmatrix} \tag{38}$$

is an hermitian unitary matrix and $a,b,c,\epsilon,A(\epsilon)$ are given in Appendix E.

Let us define $\Xi^{nn'}_{\alpha\beta}$ by

$$\tilde{C}^{nn'}_{q\lambda}=\tfrac{1}{2}\sum_{\alpha\beta}\left[(\hat{e}_{q\lambda})_\alpha(\hat{q})_\beta+(\hat{e}_{q\lambda})_\beta(\hat{q})_\alpha\right]\Xi^{nn'}_{\alpha\beta}, \tag{39}$$

where the explicit expressions of $\Xi^{nn'}_{\alpha\beta}$ are given in Appendix F. From Eqs. (37) and (39), we obtain

$$C^{\mu_i\nu_i}_{q\lambda}=\sum_{nn'}\frac{i}{2}\left[(\hat{e}_{q\lambda})_\alpha(\hat{q})_\beta+(\hat{e}_{q\lambda})_\beta(\hat{q})_\alpha\right]\Xi^{nn'}_{\alpha\beta}v^*_{n\mu_i}v_{n'\nu_i}. \tag{40}$$

Let $\tilde{\Xi}^{\mu\nu}_{\alpha\beta}$ be the quantity given by

$$\tilde{\Xi}^{\mu\nu}_{\alpha\beta}=\sum_{nn'}v^*_{n\mu}v_{n'\nu}\Xi^{nn'}_{\alpha\beta}, \tag{41}$$

i.e.,

$$\tilde{\Xi}_{\alpha\beta}=\tilde{v}^\dagger\,\Xi_{\alpha\beta}\tilde{v} \tag{42}$$

in the matrix notation. Then we obtain the formula

$$C^{\mu\nu}_{q\lambda}=\sum_{\alpha\beta}\frac{i}{2}\left[(\hat{e}_{q\lambda})_\alpha(\hat{q})_\beta+(\hat{e}_{q\lambda})_\beta(\hat{q})_\alpha\right]\tilde{\Xi}^{\mu\nu}_{\alpha\beta}, \tag{43}$$

which has the same form as Eq. (3) [see also Eq. (25)], so that the elastic constant $c^{(1)}_{\alpha\beta\gamma\delta}(q,\omega_{q\lambda})$ due to acceptor holes under the random strain is given by the general expression (26) with $\tilde{\Xi}^{\mu\nu}_{\alpha\beta}$ in Eq. (41).

General expressions for $\tilde{\Xi}^{\mu\nu}_{\alpha\beta}$ and the attenuation coefficients in $p$-Si under the arbitrary strain are rather complicated and are given in Appendix G. Here, we shall confine ourselves to the case considered by SM, i.e., the case where the uniaxial stress exists along the [111] direction. In this case we have the relations

$$\text{Im}(c)=\text{Im}(b)=-\text{Re}(b),\quad \text{Re}(c)=0, \tag{44}$$

so that the effect of the strain appears only through the level splitting $\Delta$. The explicit expressions for the attenuation coefficients are given as follows:

(i) Shear wave; $\hat{q} \parallel [100], \hat{e}_q \parallel [010]$:

$$\alpha_t = \frac{n(n_2 - n_1) D_{u'}^{a2} |f(q)|^2 \omega^2}{27 \rho_0 v_t^3 \Delta} \left[ 2 \left( \frac{1/\tau_{31}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{31}^2} + \frac{1/\tau_{13}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{13}^2} + \frac{1/\tau_{24}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{24}^2} + \frac{1/\tau_{42}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{42}^2} \right) \right.$$
$$\left. + \left( \frac{1/\tau_{21}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{21}^2} + \frac{1/\tau_{12}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{12}^2} + \frac{1/\tau_{34}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{34}^2} + \frac{1/\tau_{43}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{43}^2} \right) \right]$$
$$+ \frac{8 n \beta n_1 n_2 D_{u'}^{a2} |f(q)|^2 \omega^2 \tau}{9 \rho_0 v_t^3 (1 + \omega^2 \tau^2)} , \tag{45}$$

where

$$n_1 = 1/2(1 + e^{\beta\Delta}), \quad n_2 = e^{\beta\Delta}/2(1 + e^{\beta\Delta}). \tag{46}$$

We note that the relaxation term (last term) is of the same form as that derived classically by Ishiguro *et al.*[7]

(ii) Shear wave; $\hat{q} \parallel [100], \hat{e}_q \parallel [001]$:

$$\alpha_t = \frac{n(n_2 - n_1) D_{u'}^{a2} |f(q)|^2 \omega^2}{54 \rho_0 v_t^3 \Delta} \left[ 5 \left( \frac{1/\tau_{21}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{21}^2} + \frac{1/\tau_{12}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{12}^2} + \frac{1/\tau_{34}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{34}^2} + \frac{1/\tau_{43}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{43}^2} \right) \right.$$
$$\left. + \left( \frac{1/\tau_{31}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{31}^2} + \frac{1/\tau_{13}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{13}^2} + \frac{1/\tau_{24}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{24}^2} + \frac{1/\tau_{42}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{42}^2} \right) \right]$$
$$+ \frac{8 n \beta n_1 n_2 D_{u'}^{a2} |f(q)|^2 \omega^2 \tau}{9 \rho_0 v_t^3 (1 + \omega^2 \tau^2)} . \tag{47}$$

(iii) Longitudinal wave; $\hat{q} \parallel [100], \hat{e}_q \parallel [100]$:

$$\alpha_l = \frac{n(n_2 - n_1) D_{u}^{a2} |f(q)|^2 \omega^2}{27 \rho_0 v_l^3 \Delta} \left[ \left( \frac{1/\tau_{21}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{21}^2} + \frac{1/\tau_{12}}{(\omega - \Delta/\hbar)^2 + 1\tau_{12}^2} + \frac{1/\tau_{34}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{34}^2} + \frac{1/\tau_{43}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{43}^2} \right) \right.$$
$$\left. + 5 \left( \frac{1/\tau_{31}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{31}^2} + \frac{1/\tau_{13}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{13}^2} + \frac{1/\tau_{24}}{(\omega + \Delta/\hbar)^2 + 1/\tau_{24}^2} \; \frac{1/\tau_{42}}{(\omega - \Delta/\hbar)^2 + 1/\tau_{42}^2} \right) \right] . \tag{48}$$

## VI. COMPARISON WITH THE RESULTS OF SM

SM applied the attenuation formula obtained by Kwok[14] for $n$-Ge to $p$-Si assuming that the internal strain exists along the [111] direction and showed a good agreement with experiments. In terms of the notations used in this paper, the SM formula is given by

$$\alpha(q, \omega_{q\lambda}) = \frac{\hbar \omega_{q\lambda}^2 \beta n}{\rho_0 v_{q\lambda}^3} \times \sum_{\mu, \nu} n_\mu |C_{q\lambda}^{\mu\nu}|^2 \frac{\Gamma_\nu + \Gamma_\mu}{\hbar^2 (\omega_{q\lambda} - \omega_{\nu\mu})^2 + (\Gamma_\mu + \Gamma_\nu)^2} , \tag{49}$$

where $\Gamma_\mu$ is the level width of the $\mu$ state.

We shall now point out that the diagram technique of the Green's-function method used by Kwok is not justified for the impurity problem for the following reasons. The condition that one impurity has neccessarily one and only one electron (hole) in the discrete energy levels, i.e., $\sum_\mu c_\mu^\dagger c_\mu = 1$, is not taken into account in deriving Eq. (49). As shown in Appendix H, a recalculation of the contribution of impurities to the elastic constant by the Green's-function method does not lead to Kwok's result.

However, since many experiments were analyzed by using the SM formula (49), we shall compare in more detail the attenuation coefficient $\alpha_{\text{ITM}}$ obtained in this paper with $\alpha_{\text{SM}}$ obtained by SM. The SM formulas corresponding to Eqs. (45), (47), and (48) are written as follows:

(i) Shear wave; $\hat{q} \parallel [100], \hat{e}_q \parallel [010]$:

$$\alpha_t = \frac{n\beta D_u^{a2}\hbar\omega^2}{9\rho_0 v_t^3}\left[n_2\left(\frac{2\Gamma_2}{(\hbar\omega)^2+(2\Gamma_2)^2}+\frac{2\Gamma_3}{(\hbar\omega)^2+(2\Gamma_3)^2}\right)+n_1\left(\frac{2\Gamma_1}{(\hbar\omega)^2+(2\Gamma_1)^2}+\frac{2\Gamma_4}{(\hbar\omega)^2+(2\Gamma_4)^2}\right)\right.$$
$$+\tfrac{2}{3}n_1\left(\frac{\Gamma_1+\Gamma_2}{(\hbar\omega+\Delta)^2+(\Gamma_1+\Gamma_2)^2}+\frac{2(\Gamma_1+\Gamma_3)}{(\hbar\omega+\Delta)^2+(\Gamma_1+\Gamma_3)^2}+\frac{2(\Gamma_2+\Gamma_4)}{(\hbar\omega+\Delta)^2+(\Gamma_2+\Gamma_4)^2}+\frac{\Gamma_3+\Gamma_4}{(\hbar\omega+\Delta)^2+(\Gamma_3+\Gamma_4)^2}\right)$$
$$\left.+\tfrac{2}{3}n_2\left(\frac{\Gamma_1+\Gamma_2}{(\hbar\omega-\Delta)^2+(\Gamma_1+\Gamma_2)^2}+\frac{2(\Gamma_1+\Gamma_3)}{(\hbar\omega-\Delta)^2+(\Gamma_1+\Gamma_3)^2}+\frac{2(\Gamma_2+\Gamma_4)}{(\hbar\omega-\Delta)^2+(\Gamma_2+\Gamma_4)^2}+\frac{\Gamma_3+\Gamma_4}{(\hbar\omega-\Delta)^2+(\Gamma_3+\Gamma_4)^2}\right)\right]. \tag{50}$$

(ii) Shear wave; $\hat{q}\parallel[100], \hat{e}_q\parallel[001]$: The expression for $\alpha_t$ is not identical with Eq. (50) but becomes identical when we put $\Gamma_1=\Gamma_4$ and $\Gamma_2=\Gamma_3$.

(iii) Longitudinal wave; $\hat{q}\parallel[100], \hat{e}_q\parallel[100]$:

$$\alpha_l = \frac{2n\beta D_u^{a2}\hbar\omega^2}{27\rho v_l^3}\left[n_1\left(\frac{\Gamma_1+\Gamma_2}{(\hbar\omega+\Delta)^2+(\Gamma_1+\Gamma_2)^2}+\frac{\Gamma_3+\Gamma_4}{(\hbar\omega+\Delta)^2+(\Gamma_3+\Gamma_4)^2}+\frac{5(\Gamma_1+\Gamma_3)}{(\hbar\omega+\Delta)^2+(\Gamma_1+\Gamma_3)^2}+\frac{5(\Gamma_2+\Gamma_4)}{(\hbar\omega+\Delta)^2+(\Gamma_2+\Gamma_4)^2}\right)\right.$$
$$\left.+n_2\left(\frac{\Gamma_1+\Gamma_2}{(\hbar\omega-\Delta)^2+(\Gamma_1+\Gamma_2)^2}+\frac{\Gamma_3+\Gamma_4}{(\hbar\omega-\Delta)^2+(\Gamma_3+\Gamma_4)^2}+\frac{5(\Gamma_1+\Gamma_3)}{(\hbar\omega-\Delta)^2+(\Gamma_1+\Gamma_3)^2}+\frac{5(\Gamma_2+\Gamma_4)^2}{(\hbar\omega-\Delta)^2+(\Gamma_2+\Gamma_4)^2}\right)\right]. \tag{51}$$

Let us now discuss the difference between $\alpha_{\rm ITM}$ and $\alpha_{\rm SM}$.

### A. Resonance and antiresonance terms

We have the relations

$$\alpha_{\rm ITM} \propto \frac{n_2-n_1}{\Delta}\left(\frac{\hbar/\tau_{12}}{(\hbar\omega-\Delta)^2+(\hbar/\tau_{12})^2}+\frac{\hbar/\tau_{21}}{(\hbar\omega+\Delta)^2+(\hbar/\tau_{21})^2}+\cdots\right), \tag{52}$$

$$\alpha_{\rm SM} \propto \beta\left[n_2\left(\frac{\Gamma_1+\Gamma_2}{(\hbar\omega-\Delta)^2+(\Gamma_1+\Gamma_2)^2}+\cdots\right)+n_1\left(\frac{\Gamma_1+\Gamma_2}{(\hbar\omega+\Delta)^2+(\Gamma_1+\Gamma_2)^2}+\cdots\right)\right], \tag{53}$$

where $n_1$ and $n_2$ are given in Eq. (46). When $\beta\Delta \ll 1$, $\alpha_{\rm ITM}$ becomes of the same form as $\alpha_{\rm SM}$ except for a numerical factor, if we assume

$$\hbar/\tau_{ij} = \Gamma_i + \Gamma_j. \tag{54}$$

On the other hand, when $\beta\Delta \gg 1$, the resonance term of $\alpha_{\rm ITM}$ becomes much smaller than that of $\alpha_{\rm SM}$. It is noted that $\alpha_{\rm ITM}$ is proportional to $n_2 - n_1$ as in the usual resonance term.

### B. Relaxation term

If we assume

$$\Gamma_i = \Gamma_j = \hbar/2\tau, \tag{55}$$

we obtain the relations

$$\alpha_{\rm ITM} \propto \{\omega^2\tau/[1+(\omega\tau)^2]\} n_1 n_2, \tag{56}$$

$$\alpha_{\rm SM} \propto \{\omega^2\tau/[1+(\omega\tau)^2]\}(n_1+n_2). \tag{57}$$

When $\beta\Delta \ll 1$, $\alpha_{\rm ITM}$ has the same form as $\alpha_{\rm SM}$ except for a numerical factor. When $\beta\Delta \gg 1$, $\alpha_{\rm ITM}$ is much smaller than $\alpha_{\rm SM}$.

It is important to note that Eq. (49) in $n$-Ge gives the same formula for the relaxation attenuation as that[2,5,13] derived classically. However, this agreement is an accidental coincidence because Eq. (49) in $p$-Si does not give th classical relaxation attenuation.

## VII. CONCLUSION

We have calculated the ultrasonic attenuation by impurities in semiconductors by solving the dynamical equation for the one-particle density matrix with the phenomenologically introduced term which represents the relaxation to the instantaneous, local thermal equilibrium. Our theory corresponds in a sense to the Pippard theory[17,18] for the ultrasonic attenuation by conduction electrons in metals and to the Maris theory[19] for the ultrasonic attenuation by thermal phonons in dielectrics.

Although the SM model for the attenuation by holes has been successfully employed for the analysis of experiments, the derivation of the SM formula is not justified as shown in Sec. VI. We believe that our formula gives a better agreement with experiments, especially in the temperature dependence of attenuation.

There still remains one problem in the ultrasonic attenuation by acceptor holes even when $\omega\tau < 1$:

In what circumstance does the relaxation-time approximation break down? In this connection, we shall make a remark that the use of the relaxation-time approximation is questioned for the ultrasonic attenuation by conduction electrons in strong magnetic fields.[27,28]

Finally, we shall make a brief comment on the interaction of phonons with donor electrons (acceptor holes) when the condition $\omega\tau > 1$ is satisfied. In this situation the Kwok formulation for the elastic scattering of phonons based on the Born approximation[14] is valid. In fact, Suzuki and Mikoshiba applied this formulation to calculate the thermal conductivity of $n$-Ge,[29] and $p$-Ge and $p$-Si,[26] and obtained quantitative agreements with experiments.

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## APPENDIX A: DERIVATION OF INTERACTION HAMILTONIAN $H'$

We denote the wave function of the $\mu_i$ state of the $i$th donor electron (acceptor hole) by $\varphi_{\mu_i}(\vec{r}_i)$. If the set of functions $\{\varphi_{\mu_i}(\vec{r}_i)\}$ are orthonormal and complete, the field operators $\Psi(\vec{r}_i)$ and $\Psi^\dagger(\vec{r}_i)$ of the electron (hole) are given by

$$\Psi(\vec{r}_i) = \sum_{\mu_i} c_{\mu_i}\varphi_{\mu_i}(\vec{r}_i), \quad \Psi^\dagger(\vec{r}_i) = \sum_{\mu_i} c^\dagger_{\mu_i}\varphi^*_{\mu_i}(\vec{r}_i), \tag{A1}$$

where $c_{\mu_i}$ and $c^\dagger_{\mu_i}$ are the annihilation and creation operators for the $\mu_i$ state and satisfy the relation

$$c_{\mu_i}c^\dagger_{\nu_i} + c^\dagger_{\nu_i}c_{\mu_i} = \delta_{\mu_i\nu_i}. \tag{A2}$$

When the overlap of different donor electron (acceptor hole) wave functions can be neglected, the following relations hold:

$$\sum_{\mu_i} c^\dagger_{\mu_i}c_{\mu_i} = 1, \tag{A3}$$

$$c^\dagger_{\mu_i}c_{\nu_j} = c_{\nu_j}c^\dagger_{\mu_i}, \quad c_{\mu_i}c_{\nu_j} = c_{\nu_j}c_{\mu_i} \quad (i \neq j). \tag{A4}$$

The interaction Hamiltonian between electrons (holes) and ultrasonic waves takes the form of

$$\mathcal{H}' = \sum_i \Xi : \epsilon(\vec{r}_i, t), \tag{A5}$$

where $\Xi$ is the deformation potential and $\epsilon(\vec{r}_i, t)$ is the strain tensor at the position of the $i$th electron (hole). In the notation of the second quantization, $H'$ can be written

$$H' = \int \prod_i d\vec{r}_i \prod_j \Psi^\dagger(\vec{r}_j)\mathcal{H}'\prod_l \Psi(\vec{r}_l), \tag{A6}$$

$$H' = \sum_{i\mu_i\nu_i} \int d\vec{r}_i\, \varphi^*_{\mu_i}(\vec{r}_i)\Xi{:}\epsilon(\vec{r}_i, t)\varphi_{\nu_i}(\vec{r}_i)c^\dagger_{\mu_i}c_{\nu_i}. \tag{A7}$$

The strain tensor is written by the normal-mode expansion as

$$\epsilon_{\alpha\beta}(\vec{r}_i, t) = \sum_{q,\lambda}\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v^2_{q\lambda}}\right)^{1/2} \tfrac{1}{2}i[(\hat{e}_{q\lambda})_\alpha(\hat{q})_\beta + (\hat{e}_{q\lambda})_\beta(\hat{q})_\alpha] \times (a_{q\lambda} + a^*_{-q\lambda})e^{i\vec{q}\cdot\vec{r}_i} \tag{A8}$$

(see the text for the meaning of notations). Inserting Eq. (A8) into Eq. (A7), we obtain

$$H' = \sum_{\substack{i\mu_i\nu_i\\ \alpha\beta\\ q\lambda}} \left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v^2_{q\lambda}}\right)^{1/2} \tfrac{1}{2}i[(\hat{e}_{q\lambda})_\alpha(\hat{q})_\beta + (\hat{e}_{q\lambda})_\beta(\hat{q})_\alpha](a_{q\lambda} + a^*_{-q\lambda})c^\dagger_{\mu_i}c_{\nu_i} \int d\vec{r}_i \varphi^*_{\mu_i}(\vec{r}_i)e^{i\vec{q}\cdot\vec{r}_i}\Xi_{\alpha\beta}\varphi_{\nu_i}(\vec{r}_i). \tag{A9}$$

The wave function for the ground state of a donor electron (acceptor hole) can be written[20]

$$\varphi_{\mu_i}(\vec{r}_i) = \sum_l \alpha^{(l)}_{\mu_i}\tilde{\varphi}^{(l)}(\vec{r}_i - \vec{R}_i), \tag{A10}$$

where the superscript $(l)$ represents the location of an energy valley in the conduction (valence) band. Now we assume the relation

$$\Xi\,\tilde{\varphi}^{(l)}(\vec{r}_i - \vec{R}_i) = \Xi(l)\tilde{\varphi}^{(l)}(\vec{r}_i - \vec{R}_i), \tag{A11}$$

where $\Xi(l)$ is the $l$th valley deformation potential. Following the procedure similar to that employed by Hasegawa,[20] we obtain the final form of $H'$:

$$H' = \sum_{\substack{iq\lambda\\ \mu_i\nu_i}} \left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v^2_{q\lambda}}\right)^{1/2} C^{\mu_i\nu_i}_{q\lambda} f(q) e^{i\vec{q}\cdot\vec{R}_i} \times (a_{q\lambda} + a^*_{-q\lambda})c^\dagger_{\mu_i}c_{\nu_i}, \tag{A12}$$

where

$$C^{\mu\nu}_{q\lambda} = \sum_{\alpha\beta l} \frac{i}{2}[(\hat{e}_{q\lambda})_\alpha(\hat{q})_\beta + (\hat{e}_{q\lambda})_\beta(\hat{q})_\alpha]\ \Xi_{\alpha\beta}(l)\,\alpha^{(l)}_\mu\alpha^{(l)}_\nu. \tag{A13}$$

At sufficiently low frequencies where $1/q \gg a^*_B$ [$a^*_B$ is the effective Bohr radius of electrons (holes)], we can put $f(q) = 1$ and Eq. (A12) can be rewritten

$$H' = \sum_{i\alpha\beta} \tilde{\Xi}_{\alpha\beta}^{\mu_i\nu_i} \epsilon_{\alpha\beta}(\vec{R}_i, t) c_{\mu_i}^\dagger c_{\nu_i}, \tag{A14}$$

where

$$\Xi_{\alpha\beta}^{\mu_i\nu_i} = \sum_l \Xi_{\alpha\beta}(l)\alpha_{\mu_i}(l)\alpha_{\nu_i}(l). \tag{A15}$$

### APPENDIX B: A METHOD TO OBTAIN EXPLICIT EXPRESSIONS FOR $\tau_{\mu\nu}$

Explicit expressions for $\tau_{\mu\nu}$ can be obtained by assuming that the relaxation time $\tau_{\mu\nu}$ in Eq. (5) is equal to that of donor electrons (acceptor holes) due to the interaction with thermal phonons in the absence of external ultrasonic waves. The Hamiltonian for one donor electron (acceptor hole) interacting with thermal phonons can be written

$$H = H_0 + H', \tag{B1}$$

$$H_0 = \sum_\mu \epsilon_\mu c_\mu^\dagger c_\mu + \sum_{\vec{q}\lambda} \hbar\omega_{q\lambda} a_{q\lambda}^\dagger a_{q\lambda}, \tag{B2}$$

$$H' = \sum_{\substack{\vec{q}\lambda \\ \mu\nu}} \left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)^{1/2} C_{q\lambda}^{\mu\nu} e^{i\vec{q}\cdot\vec{R}} f(q)(a_{q\lambda} + a_{-q\lambda}^\dagger) c_\mu^\dagger c_\nu, \tag{B3}$$

where $a_{q\lambda}$ and $a_{q\lambda}^\dagger$ are the annihilation and creation operators for the $(\vec{q}, \lambda)$ mode of thermal phonons and other notations have the same meanings as those in the text. In the dynamical equation for the density matrix

$$i\hbar\frac{\partial\rho}{\partial t} = [H, \rho] \tag{B4}$$

we introduce $\tilde{\rho}$ in the interaction representation

$$\tilde{\rho} = e^{iH_0t/\hbar}\rho e^{-iH_0t/\hbar}. \tag{B5}$$

Then, Eq. (B4) can be rewritten

$$i\hbar\frac{\partial\tilde{\rho}}{\partial t} = [\tilde{H}'(t), \tilde{\rho}], \tag{B6}$$

where

$$\tilde{H}'(t) = e^{iH_0t/\hbar}H'e^{-iH_0t/\hbar}. \tag{B7}$$

The solution of Eq. (B6) is given by

$$\tilde{\rho}(t) = \tilde{\rho}(0) - \frac{i}{\hbar}\int_0^t d\tau\,[\tilde{H}'(\tau), \rho(0)] - \frac{1}{\hbar^2}\int_0^t d\tau \int_0^\tau d\tau'\,[\tilde{H}'(\tau), [\tilde{H}'(\tau'), \tilde{\rho}(\tau')]]. \tag{B8}$$

Up to the second-order approximation, the density matrix $\tilde{\rho}_D$ for the donor (acceptor) is then given by

$$\begin{aligned}\tilde{\rho}_D(t) &= \mathrm{Tr}_{(\mathrm{phonon})}\tilde{\rho}(t) \\ &= \mathrm{Tr}_{(\mathrm{phonon})}\tilde{\rho}(0) - \frac{i}{\hbar}\int_0^t d\tau\,\mathrm{Tr}_{(\mathrm{phonon})}[\tilde{H}'(\tau), \tilde{\rho}(0)] - \frac{1}{\hbar^2}\int_0^t d\tau\int_0^\tau d\tau'\,\mathrm{Tr}_{(\mathrm{phonon})}[\tilde{H}'(\tau), [\tilde{H}'(\tau'), \tilde{\rho}(0)]],\end{aligned} \tag{B9}$$

where $\mathrm{Tr}_{(\mathrm{phonon})}$ means to take the trace over the phonon system. If we assume that at $t = 0$ there is no correlation between the donor (acceptor) and the phonon system and the phonon system is in thermal equilibrium, i.e.,

$$\rho(0) = \rho_D(0) \otimes \rho_{\mathrm{ph}}^{(0)}, \tag{B10}$$

$$\rho_{\mathrm{ph}}^{(0)} = \exp\left(-\beta\sum_{\vec{q}\lambda}\hbar\omega_{q\lambda}a_{q\lambda}^\dagger a_{q\lambda}\right)\Big/\mathrm{Tr}\left[\exp\left(-\beta\sum_{\vec{q}\lambda}\hbar\omega_{q\lambda}a_{q\lambda}^\dagger a_{q\lambda}\right)\right], \tag{B11}$$

then the second term in Eq. (B9) vanishes. By using the formula[30]

$$\int_0^t d\tau\int_0^\tau d\tau'\,e^{i\omega_1(q)\tau + i\omega_2(q)\tau'} \cong \delta_{\omega_1(q)+\omega_2(q),0}\left(-iP\frac{1}{\omega_2(q)} + \pi\delta(\omega_2(q))\right)t, \tag{B12}$$

when $\omega_1(q) + \omega_2(q)$ is $q$ independent, (B13)

we can rewrite Eq. (B9) as

$$\tilde{\rho}_D(t)-\tilde{\rho}_D(0)=-\frac{t}{\hbar^2}\sum_{\substack{q\lambda\\ \mu\nu\mu'\nu'}}\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)C_{q\lambda}^{\mu\nu}C_{-q\lambda}^{\mu'\nu'}f(q)f(-q)\delta_{\epsilon_{\mu\nu}+\epsilon_{\mu'\nu'},0}$$

$$\Bigg(\left\{\left[-\frac{iP}{\omega_{q\lambda}+(1/\hbar)\epsilon_{\mu'\nu'}}+\pi\delta\left(\omega_{q\lambda}+\frac{1}{\hbar}\epsilon_{\mu'\nu'}\right)\right](n_{q\lambda}+1)+\left[-\frac{iP}{-\omega_{q\lambda}+(1/\hbar)\epsilon_{\mu'\nu'}}+\pi\delta\left(-\omega_{q\lambda}+\frac{1}{\hbar}\epsilon_{\mu'\nu'}\right)\right]n_{q\lambda}\right\}c_\mu^\dagger c_\nu c_{\mu'}^\dagger c_{\nu'}\tilde{\rho}_D(0)$$

$$-\left\{\left[-\frac{iP}{\omega_{q\lambda}+(1/\hbar)\epsilon_{\mu'\nu'}}+\pi\delta\left(\omega_{q\lambda}+\frac{1}{\hbar}\epsilon_{\mu'\nu'}\right)\right]n_{q\lambda}+\left[-\frac{iP}{-\omega_{q\lambda}+(1/\hbar)\epsilon_{\mu'\nu'}}+\pi\delta\left(-\omega_{q\lambda}+\frac{1}{\hbar}\epsilon_{\mu'\nu'}\right)\right](n_{q\lambda}+1)\right\}c_\mu^\dagger c_\nu\tilde{\rho}_D(0)c_{\mu'}^\dagger c_{\nu'}$$

$$-\left\{\left[-\frac{iP}{-\omega_{q\lambda}+(1/\hbar)\epsilon_{\mu'\nu'}}+\pi\delta\left(-\omega_{q\lambda}+\frac{1}{\hbar}\epsilon_{\mu'\nu'}\right)\right]n_{q\lambda}+\left[-\frac{iP}{\omega_{q\lambda}+(1/\hbar)\epsilon_{\mu'\nu'}}+\pi\delta\left(\omega_{q\lambda}+\frac{1}{\hbar}\epsilon_{\mu'\nu'}\right)\right](n_{q\lambda}+1)\right\}c_{\mu'}^\dagger c_{\nu'}\tilde{\rho}_D(0)c_\mu^\dagger c_\nu$$

$$+\left\{\left[-\frac{iP}{\omega_{q\lambda}+(1/\hbar)\epsilon_{\mu'\nu'}}+\pi\delta\left(\omega_{q\lambda}+\frac{1}{\hbar}\epsilon_{\mu'\nu'}\right)\right]n_{q\lambda}+\left[-\frac{iP}{-\omega_{q\lambda}+(1/\hbar)\epsilon_{\mu'\nu'}}+\pi\delta\left(-\omega_{q\lambda}+\frac{1}{\hbar}\epsilon_{\mu'\nu'}\right)\right](n_{q\lambda}+1)\right\}\tilde{\rho}_D(0)c_{\mu'}^\dagger c_{\nu'}c_\mu^\dagger c_\nu\Bigg), \quad \text{(B14)}$$

$$n_{q\lambda}\equiv 1/(e^{\beta\hbar\omega_{q\lambda}}-1),\quad \epsilon_{\mu\nu}\equiv\epsilon_\mu-\epsilon_\nu. \quad \text{(B15)}$$

For simplicity, we consider the two-level system ($\epsilon_2>\epsilon_1$) where the simple explicit expressions for $\tau_{\mu\nu}$ are obtained. Neglecting the energy shift [the imaginary parts in Eq. (B14)] and assuming the time $t$ to be sufficiently small, we obtain

$$\frac{\partial\tilde{\rho}_D(t)}{\partial t}=-\frac{1}{\hbar^2}\sum_{\vec{q}\lambda}\pi\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)|f(q)|^2|C_{q\lambda}^{12}|^2[(n_{q\lambda}+1)c_2^\dagger c_2\tilde{\rho}_D+(n_{q\lambda}+1)\tilde{\rho}_D c_2^\dagger c_2+n_{q\lambda}c_1^\dagger c_1\tilde{\rho}_D$$
$$+n_{q\lambda}\tilde{\rho}_D c_1^\dagger c_1-2n_{q\lambda}c_2^\dagger c_1\tilde{\rho}_D c_1^\dagger c_2-2(n_{q\lambda}+1)c_1^\dagger c_2\tilde{\rho}_D c_2^\dagger c_1]. \quad \text{(B16)}$$

The matrix elements of $\tilde{\rho}_D$ are then given by

$$\left(\frac{\partial\tilde{\rho}_D}{\partial t}\right)_{11}=-\frac{2\pi}{\hbar^2}\sum_{\vec{q}\lambda}\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)\times|C_{q\lambda}^{12}|^2[n_{q\lambda}(\tilde{\rho}_D)_{11}-(n_{q\lambda}+1)(\tilde{\rho}_D)_{22}], \quad \text{(B17a)}$$

$$\left(\frac{\partial\tilde{\rho}_D}{\partial t}\right)_{22}=-\frac{2\pi}{\hbar^2}\sum_{\vec{q}\lambda}\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)\times|C_{q\lambda}^{12}|^2[(n_{q\lambda}+1)(\tilde{\rho}_D)_{22}-n_{q\lambda}(\tilde{\rho}_D)_{11}], \quad \text{(B17b)}$$

$$\left(\frac{\partial\tilde{\rho}_D}{\partial t}\right)_{12}=-\frac{\pi}{\hbar^2}\sum_{\vec{q}\lambda}\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)\times|C_{q\lambda}^{12}|^2(2n_{q\lambda}+1)(\tilde{\rho}_D)_{12}, \quad \text{(B17c)}$$

$$\left(\frac{\partial\tilde{\rho}_D}{\partial t}\right)_{21}=-\frac{\pi}{\hbar^2}\sum_{\vec{q}\lambda}\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)\times|C_{q\lambda}^{12}|^2(2n_{q\lambda}+1)(\tilde{\rho}_D)_{21}. \quad \text{(B17d)}$$

Using the normalization condition

$$(\tilde{\rho}_D)_{11}+(\tilde{\rho}_D)_{22}=1 \quad \text{(B18)}$$

we obtain the final expressions for $\partial\rho_D/\partial t$ in the Schrödinger representation:

$$\left(\frac{\partial\rho_D}{\partial t}\right)_{11}=-\frac{[(\rho_D)_{11}-(\rho_D^{(0)})_{11}]}{\tau}, \quad \text{(B19a)}$$

$$\left(\frac{\partial\rho_D}{\partial t}\right)_{22}=-\frac{[(\rho_D)_{22}-(\rho_D^{(0)})_{22}]}{\tau}, \quad \text{(B19b)}$$

$$\left(\frac{\partial\rho_D}{\partial t}\right)_{12}=i\left(\frac{\epsilon_{21}}{\hbar}\right)(\rho_D)_{12}-\frac{(\rho_D)_{12}}{\tau_{12}}, \quad \text{(B19c)}$$

$$\left(\frac{\partial\rho_D}{\partial t}\right)_{21}=-i\left(\frac{\epsilon_{21}}{\hbar}\right)(\rho_D)_{21}-\frac{(\rho_D)_{21}}{\tau_{21}}, \quad \text{(B19d)}$$

where the relaxation times $\tau$ and $\tau_{12}$ ($=\tau_{21}$) are given by

$$\frac{1}{\tau}=\frac{2\pi}{\hbar^2}\sum_{\vec{q}\lambda}\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)\times|C_{q\lambda}^{12}|^2(2n_{q\lambda}+1)\,, \tag{B20a}$$

$$\frac{1}{\tau_{12}}=\frac{\pi}{\hbar^2}\sum_{\vec{q}\lambda}\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)\times|C_{q\lambda}^{12}|^2(2n_{q\lambda}+1)=\frac{1}{2\tau}, \tag{B20b}$$

$$\frac{(\rho_D^{(0)})_{11}}{\tau}=\frac{2\pi}{\hbar^2}\sum_{\vec{q}\lambda}\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)\times|C_{q\lambda}^{12}|^2(n_{q\lambda}+1)\,, \tag{B20c}$$

$$\frac{(\rho_D^{(0)})_{22}}{\tau}=\frac{2\pi}{\hbar^2}\sum_{\vec{q}\lambda}\delta\left(\omega_{q\lambda}-\frac{1}{\hbar}\epsilon_{21}\right)\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)\times|C_{q\lambda}^{12}|^2 n_{q\lambda}. \tag{B20d}$$

It is noted that $\tau$ and $\tau_{12}(=\tau_{21})$ correspond to the longitudinal ($T_1$) and transverse ($T_2$) relaxation time in general relaxation phenomena.

## APPENDIX C: DERIVATION OF MICROSCOPIC EXPRESSION FOR STRESS TENSOR

Let us first derive the microscopic expression for the stress tensor in thermal equilibrium. From the thermodynamical formula, the free energy is given by

$$dF=-S\,dT+\int d^3r\,\sigma_{\alpha\beta}(\vec{r})\,d\epsilon_{\alpha\beta}(\vec{r}). \tag{C1}$$

Inserting the Fourier expansions

$$\sigma_{\alpha\beta}(\vec{r})=\frac{1}{(V)^{1/2}}\sum_{\vec{q}}\sigma_{\alpha\beta}(q)e^{i\vec{q}\cdot\vec{r}},\qquad \epsilon_{\alpha\beta}(\vec{r})=\frac{1}{(V)^{1/2}}\sum_{\vec{q}\lambda}\epsilon_{\alpha\beta}(q\lambda)e^{i\vec{q}\cdot\vec{r}} \tag{C2}$$

into Eq. (C1), we obtain

$$dF=-S\,dT+\sum_{\vec{q}\lambda}\sigma_{\alpha\beta}(q)d\epsilon_{\alpha\beta}(-q\lambda). \tag{C3}$$

Thus, we get

$$\sigma_{\alpha\beta}(q)=\left(\frac{\partial F}{\partial\epsilon_{\alpha\beta}(-q\lambda)}\right)_{T,\{\epsilon_{\alpha\beta}(-q',\lambda')\}(q'\neq q\text{ or }\lambda'\neq\lambda)} \tag{C4}$$

On the other hand, the free energy in statistical mechanics is given by

$$F=-\beta^{-1}\ln(\mathrm{Tr}e^{-\beta H}),\quad H=H_0+H'. \tag{C5}$$

Inserting Eq. (C5) into Eq. (C4), we obtain

$$\sigma_{\alpha\beta}(q)=\mathrm{Tr}\left[e^{-\beta H}\left(\frac{\partial H'}{\partial\epsilon_{\alpha\beta}(-q\lambda)}\right)\right]\Big/\mathrm{Tr}e^{-\beta H}. \tag{C6}$$

Using the expression (A12) for $H'$, $\sigma_{\alpha\beta}(q)$ is now given by

$$\sigma_{\alpha\beta}(q)=\mathrm{Tr}[\rho\hat{\sigma}_{\alpha\beta}(q)], \tag{C7}$$

where

$$\hat{\sigma}_{\alpha\beta}(q)\equiv\frac{\partial H'}{\partial\epsilon_{\alpha\beta}(-q\lambda)}=\sum_{\substack{il\\ \mu_i\nu_i}}f(-q)\Xi_{\alpha\beta}(l)e^{-i\vec{q}\cdot\vec{R}_i}\alpha_{\mu_i}^{(l)}\alpha_{\nu_i}^{(l)}c_{\mu_i}^{\dagger}c_{\nu_i}V^{-1/2}, \tag{C8}$$

$$\rho=e^{-\beta H}/\mathrm{Tr}e^{-\beta H}. \tag{C9}$$

Equation (C7) is the microscopic expression for stress tensor in thermal equilibrium.

Even when the system is not in thermal equilibrium, the dynamical stress tensor $\sigma_{\alpha\beta}(q,t)$ will be given by

$$\sigma_{\alpha\beta}(q,t)=\mathrm{Tr}[\rho(t)\hat{\sigma}_{\alpha\beta}(q)], \tag{C10}$$

where $\rho(t)$ is the solution of the dynamical equation for density matrix. The justification of Eq. (C10) is as follows. First, the operator in the Schrödinger representation which is independent of the time evolution has the identical expression irrespective of whether the system is in thermal equilibrium or not. Second, the expectation value of an arbitrary observable is given by the trace of $\rho(t)$ multiplied by an operator corresponding to the observable in the Schrödinger representation. It is noted that this justification is not necessarily valid for a quantity which is not observable. For example, the correlation function cannot be expressed by the method described above.

## APPENDIX D: ATTENUATION COEFFICIENT IN n-Ge WHEN KWOK'S MATRIX ELEMENTS ARE USED

We discuss the attenuation coefficients in $n$-Ge when we use the matrix elements $D_{\alpha\beta}^{\mu\nu}$ of Table II in Kwok's paper[14]:

(i) Shear wave; $\hat{q}\parallel[100]$, $\hat{e}_q\parallel[010]$: The attenuation coefficient is the same as Eq. (33) except that $\tau_{12}$ is replaced by $\tau$.

(ii) Shear wave; $\hat{q}\parallel[100]$, $\hat{e}_q\parallel[001]$: The attenuation coefficient is the same as Eq. (33) except that the terms including $\tau_{03}$ are replaced by the terms including $\tau_{01}$ and $\tau_{02}$.

## APPENDIX E: ENERGY-LEVEL SPLITTING OF ACCEPTOR-HOLE GROUND STATE CAUSED BY INTERNAL STRAINS

Let the $(q\lambda)$ component of the internal strain in the normal-mode expansion be $a_{q\lambda}^{(r)}$. The matrix elements of $H_{h-s}^{(r)}$ between the $|n\rangle$ states are given by[26]

$$\langle n|H_{\text{h-s}}^{(r)}|n'\rangle=\sum_{q\lambda}\left(\frac{\hbar\omega_{q\lambda}}{2\rho_0 V v_{q\lambda}^2}\right)^{1/2} i f(q)\tilde{C}_{q\lambda}^{nn'}(a_{q\lambda}^{(r)}+a_{-q\lambda}^{(r)*}), \tag{E1}$$

where

$$\begin{aligned}
&\tilde{C}_{q\lambda}^{11}=\tilde{C}_{q\lambda}^{44}=-\tilde{C}_{q\lambda}^{22}=-\tilde{C}_{q\lambda}^{33}=\tfrac{1}{3}D_u^a[2(\hat{q})_z(\hat{e}_{q\lambda})_z-(\hat{q})_x(\hat{e}_{q\lambda})_x-(\hat{q})_y(\hat{e}_{q\lambda})_y],\\
&\tilde{C}_{q\lambda}^{12}=-\tilde{C}_{q\lambda}^{34}=(1/\sqrt{3})D_{u'}^a\{(\hat{q})_z(\hat{e}_{q\lambda})_x+(\hat{q})_x(\hat{e}_{q\lambda})_z-i[(\hat{q})_z(\hat{e}_{q\lambda})_y+(\hat{q})_y(\hat{e}_{q\lambda})_z]\},\\
&\tilde{C}_{q\lambda}^{13}=-\tilde{C}_{q\lambda}^{24}=(1/\sqrt{3})D_u^a[(\hat{q})_x(\hat{e}_{q\lambda})_x-(\hat{q})_y(\hat{e}_{q\lambda})_y]-(i/\sqrt{3})D_{u'}^a[(\hat{q})_x(\hat{e}_{q\lambda})_y+(\hat{q})_y(\hat{e}_{q\lambda})_x],\\
&\tilde{C}_{q\lambda}^{14}=\tilde{C}_{q\lambda}^{23}=0,\quad \tilde{C}_{q\lambda}^{nn'}=\tilde{C}_{-q\lambda}^{n'n},\quad f(q)=(1+\tfrac{1}{4}a_B^{*}q^2)^{-1/2}.
\end{aligned} \tag{E2}$$

The eigenvalue $\epsilon$ and the eigenfunction $\Psi_\mu$ of $H_{\text{h-s}}^{(r)}$ are easily calculated:

$$\epsilon=\pm(|a|^2+|b|^2+|c|^2)^{1/2}, \tag{E3}$$

where

$$\begin{aligned}
&a\equiv\langle 1|H_{\text{h-s}}^{(r)}|1\rangle=\langle 4|H_{\text{h-s}}^{(r)}|4\rangle=-\langle 2|H_{\text{h-s}}^{(r)}|2\rangle=-\langle 3|H_{\text{h-s}}^{(r)}|3\rangle,\\
&b\equiv\langle 1|H_{\text{h-s}}^{(r)}|2\rangle=-\langle 3|H_{\text{h-s}}^{(r)}|4\rangle,\\
&c\equiv\langle 1|H_{\text{h-s}}^{(r)}|3\rangle=\langle 2|H_{\text{h-s}}^{(r)}|4\rangle,\quad \langle 1|H_{\text{h-s}}^{(r)}|4\rangle=\langle 2|H_{\text{h-s}}^{(r)}|3\rangle=0,
\end{aligned} \tag{E4}$$

and

$$\begin{pmatrix}\Psi_1\\ \Psi_2\\ \Psi_3\\ \Psi_4\end{pmatrix}=\frac{1}{A(\epsilon)}\begin{pmatrix}a+\epsilon & b & c & 0\\ b^* & -a-\epsilon & 0 & c\\ c^* & 0 & -a-\epsilon & -b\\ 0 & c^* & -b & a+\epsilon\end{pmatrix}\begin{pmatrix}|1\rangle\\ |2\rangle\\ |3\rangle\\ |4\rangle\end{pmatrix},\quad A(\epsilon)\equiv[2\epsilon(\epsilon+a)]^{1/2}. \tag{E5}$$

Therefore, the energy splitting $\Delta$ between two twofold-degenerate states (1,4; 2,3) is given by

$$\Delta=2(|a|^2+|b|^2+|c|^2)^{1/2}. \tag{E6}$$

## APPENDIX F: EXPRESSIONS FOR $\Xi_{\alpha\beta}^{nn}$ IN $p$-Si

$$\Xi_{11}=\frac{D_u^a}{3}\begin{pmatrix}-1 & 0 & \sqrt{3} & 0\\ 0 & 1 & 0 & \sqrt{3}\\ \sqrt{3} & 0 & 1 & 0\\ 0 & \sqrt{3} & 0 & -1\end{pmatrix},\quad \Xi_{12}=\frac{iD_{u'}^a}{\sqrt{3}}\begin{pmatrix}0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\\ 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\end{pmatrix},\quad \Xi_{13}=\frac{D_{u'}^a}{\sqrt{3}}\begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix},$$

$$\Xi_{22}=\frac{D_u^a}{3}\begin{pmatrix}-1 & 0 & -\sqrt{3} & 0\\ 0 & 1 & 0 & -\sqrt{3}\\ -\sqrt{3} & 0 & 1 & 0\\ 0 & -\sqrt{3} & 0 & -1\end{pmatrix},\quad \Xi_{23}=\frac{iD_{u'}^a}{\sqrt{3}}\begin{pmatrix}0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\end{pmatrix},\quad \Xi_{33}=\frac{2D_u^a}{3}\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

## APPENDIX G: GENERAL EXPRESSION OF ATTENUATION COEFFECIENT IN $p$-Si UNDER ARBITRARY STRAIN

(i) Shear wave; $\hat{q}\parallel[100]$, $\hat{e}_q\parallel[010]$:

$$\tilde{\Xi}_{12}=\frac{iD_{u'}^a}{\sqrt{3}A(\epsilon)^2}\begin{pmatrix}(a+\epsilon)(c-c^*) & b(c-c^*) & (a+\epsilon)^2+|b|^2+c^2 & 0\\ b^*(c-c^*) & -(c-c^*)(a+\epsilon) & 0 & (a+\epsilon)^2+|b|^2+c^2\\ -(a+\epsilon)^2-|b|^2-c^{*2} & 0 & -(c-c^*)(a+\epsilon) & -b(c-c^*)\\ 0 & -(a+\epsilon)^2-|b|^2-c^{*2} & -b^*(c-c^*) & (a+\epsilon)(c-c^*)\end{pmatrix}, \tag{G1}$$

$$\alpha_t(q,\omega)=\frac{n(n_2-n_1)D_{u'}^{a2}|f(q)|^2\omega^2}{6\rho_0 v_t^3\Delta A(\epsilon)^4}$$
$$\times\Bigg[\big|(a+\epsilon)^2+|b|^2+c^2\big|^2\left(\frac{1/\tau_{31}}{(\omega+\Delta/\hbar)^2+1/\tau_{31}^2}+\frac{1/\tau_{13}}{(\omega-\Delta/\hbar)^2+1/\tau_{13}^2}+\frac{1/\tau_{24}}{(\omega+\Delta/\hbar)^2+1/\tau_{24}^2}+\frac{1/\tau_{42}}{(\omega-\Delta/\hbar)^2+1/\tau_{42}^2}\right)$$
$$+|b|^2|c-c^*|^2\left(\frac{1/\tau_{21}}{(\omega+\Delta/\hbar)^2+1/\tau_{21}^2}+\frac{1/\tau_{12}}{(\omega-\Delta/\hbar)^2+1/\tau_{12}^2}+\frac{1/\tau_{34}}{(\omega+\Delta/\hbar)^2+1/\tau_{34}^2}+\frac{1/\tau_{43}}{(\omega-\Delta/\hbar)^2+1/\tau_{43}^2}\right)\Bigg]$$
$$+\frac{8n\beta n_1 n_2 D_{u'}^{a2}(a+\epsilon)|c-c^*|^2|f(q)|^2\omega^2\tau}{3\rho_0 v_t^3 A(\epsilon)^4(1+\omega^2\tau^2)}\,. \qquad \text{(G2)}$$

(ii) Shear wave; $\hat{q}\parallel[100]$, $\hat{e}_q\parallel[001]$:

$$\tilde{\Xi}_{13}=\frac{D_{u'}^{a}}{\sqrt{3}\,A(\epsilon)^2}\begin{bmatrix}(a+\epsilon)(b+b^*) & -(a+\epsilon)^2+b^2-|c|^2 & c(b+b^*) & 0\\ -(a+\epsilon)^2+b^{*2}-|c|^2 & -(a+\epsilon)(b+b^*) & 0 & c(b+b^*)\\ c^*(b+b^*) & 0 & -(a+\epsilon)(b+b^*) & (a+\epsilon)^2-b^2+|c|^2\\ 0 & c^*(b+b^*) & (a+\epsilon)^2-b^{*2}+|c|^2 & (a+\epsilon)(b+b^*)\end{bmatrix}, \qquad \text{(G3)}$$

$$\alpha_t(q,\omega)=\frac{n(n_2-n_1)D_{u'}^{a2}|f(q)|^2\omega^2}{6\rho_0 v_t^3\Delta A(\epsilon)^4}\Bigg[\big|(a+\epsilon)^2-b^2+|c|^2\big|^2\left(\frac{1/\tau_{21}}{(\omega+\Delta/\hbar)^2+1/\tau_{21}^2}+\frac{1/\tau_{12}}{(\omega-\Delta/\hbar)^2+1/\tau_{12}^2}\right.$$
$$\left.+\frac{1/\tau_{34}}{(\omega+\Delta/\hbar)^2+1/\tau_{34}^2}+\frac{1/\tau_{43}}{(\omega-\Delta/\hbar)^2+1/\tau_{43}^2}\right)+|c|^2|b+b^*|^2\left(\frac{1/\tau_{31}}{(\omega+\Delta/\hbar)^2+1/\tau_{31}^2}+\frac{1/\tau_{13}}{(\omega-\Delta/\hbar)^2+1/\tau_{13}^2}\right.$$
$$\left.+\frac{1/\tau_{24}}{(\omega+\Delta/\hbar)^2+1/\tau_{24}^2}+\frac{1/\tau_{42}}{(\omega-\Delta/\hbar)^2+1/\tau_{42}^2}\right)\Bigg]+\frac{8n\beta n_1 n_2 D_{u'}^{a2}(a+\epsilon)^2(b+b^*)^2|f(q)|^2\omega^2\tau}{3\rho_0 v_t^3 A(\epsilon)^4(1+\omega^2\tau^2)}\,. \qquad \text{(G4)}$$

(iii) Longitudinal wave; $\hat{q}\parallel[100]$, $\hat{e}_q\parallel[100]$:

$$\tilde{\Xi}_{11}=\frac{D_u^{a2}}{3A(\epsilon)^2}\begin{bmatrix}-(a+\epsilon)^2+|b|^2+|c|^2+\sqrt{3}(a+\epsilon)(c+c^*) & b[\sqrt{3}(c+c^*)-2(a+\epsilon)] & -\sqrt{3}[(a+\epsilon)^2+|b|^2-c^2]-2c(a+\epsilon) & 0\\ b^*[\sqrt{3}(c+c^*)-2(a+\epsilon)] & (a+\epsilon)^2-|b|^2-|c|^2-\sqrt{3}(a+\epsilon)(c+c^*) & 0 & -\sqrt{3}[(a+\epsilon)^2+|b|^2-c^2]-2c(a+\epsilon)\\ -\sqrt{3}[(a+\epsilon)^2+|b|^2-c^{*2}]-2c^*(a+\epsilon) & 0 & (a+\epsilon)^2-|b|^2-|c|^2-\sqrt{3}(a+\epsilon)(c+c^*) & -b[\sqrt{3}(c+c^*)-2(a+\epsilon)]\\ 0 & -\sqrt{3}[(a+\epsilon)^2+|b|^2-c^{*2}]-2c^*(a+\epsilon) & -b^*[\sqrt{3}(c+c^*)-2(a+\epsilon)] & -(a+\epsilon)^2+|b|^2+|c|^2+\sqrt{3}(a+\epsilon)(c+c^*)\end{bmatrix}, \qquad \text{(G5)}$$

$$\alpha_l(q,\omega)=\frac{n(n_2-n_1)D_u^{a2}|f(q)|^2\omega^2}{18\rho_0 v_l^3\Delta A(\epsilon)^4}\Bigg[|b|^2\big|\sqrt{3}(c+c^*)-2(a+\epsilon)\big|^2$$
$$\times\left(\frac{1/\tau_{21}}{(\omega+\Delta/\hbar)^2+1/\tau_{21}^2}+\frac{1/\tau_{12}}{(\omega-\Delta/\hbar)^2+1/\tau_{12}^2}+\frac{1/\tau_{34}}{(\omega+\Delta/\hbar)^2+1/\tau_{34}^2}+\frac{1/\tau_{43}}{(\omega-\Delta/\hbar)^2+1/\tau_{43}^2}\right)$$
$$+\big|\sqrt{3}[(a+\epsilon)^2+|b|^2-c^2]+2c(a+\epsilon)\big|^2\left(\frac{1/\tau_{31}}{(\omega+\Delta/\hbar)^2+1/\tau_{31}^2}+\frac{1/\tau_{13}}{(\omega-\Delta/\hbar)^2+1/\tau_{13}^2}\right.$$
$$\left.+\frac{1/\tau_{24}}{(\omega+\Delta/\hbar)^2+1/\tau_{24}^2}+\frac{1/\tau_{42}}{(\omega-\Delta/\hbar)^2+1/\tau_{42}^2}\right)\Bigg]$$
$$+\frac{8n\beta n_1 n_2 D_u^{a2}|f(q)|^2\omega^2\tau}{9\rho_0 v_l^3 A(\epsilon)^4(1+\omega^2\tau^2)}\big|(a+\epsilon)^2-|b|^2-|c|^2-\sqrt{3}(a+\epsilon)(c+c^*)\big|^2\,. \qquad \text{(G6)}$$

## APPENDIX H: CALCULATION OF THE CONTRIBUTION OF IMPURITIES TO THE ELASTIC CONSTANT BY THE GREEN'S FUNCTION METHOD

A method given in a standard textbook[31] on the Green's function cannot be used for spin and impurity systems where one atom has one and only one electron (hole). The reason is that $c_{\mu_i}$ and $c_{\mu_i}^\dagger$ defined in Appendix A are not the Fermion operators because of the condition (A3). To avoid this difficulty, we impose the constraint on the state $|\alpha\rangle$:

$$\sum_{\mu_i} c_{\mu_i}^\dagger c_{\mu_i}|\alpha\rangle=|\alpha\rangle\,, \qquad \text{(H1)}$$

regarding $c_{\mu_i}$ and $c_{\mu_i}^\dagger$ to be the Fermion operators. Hence, the trace in Eq. (19) must be taken over the states $|\alpha\rangle$ which satisfy Eq. (H1) and are not the complete set of states for Fermion operators. We denote such a trace by Tr′.

The component of the stress tensor $\sigma_{\alpha\beta}^{(1)}(q,t)$ proportional to the amplitude of ultrasonic waves is then given by

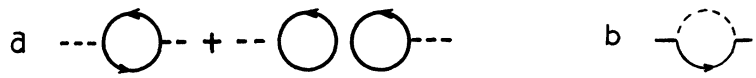

FIG. 3. (a) Lowest-order diagrams for $\pi$. The directional line is the complete one-particle Green's function. (b) Lowest-order diagram for self-energy part of the one-particle Green's function. The dashed line is the free phonon Green's function, the directional line is the free one-particle Green's function.

$$\sigma^{(1)}_{\alpha\beta}(q,t)=\frac{1}{V}\sum_{\substack{ij\mu_i\nu_i\\ \mu_j'\nu_j'\gamma\delta\\ q'\lambda}} f(-q)f(q')\Xi^{\mu_i\nu_i}_{\alpha\beta}\,\Xi^{\mu_j'\nu_j'}_{\gamma\delta}\,e^{i\vec{q}'\cdot\vec{R}_j-i\vec{q}\cdot\vec{R}_i}\int_{-\infty}^{t}dt'\,P^{(R)}_{\mu_i\nu_i\mu_j'\nu_j'}(t-t')\epsilon_{\gamma\delta}(q'\lambda,t')\,, \tag{H2a}$$

where

$$P^{(R)}_{\mu_i\nu_i\mu_j'\nu_j'}(t-t')\equiv\begin{cases}-i\,\mathrm{Tr}'\rho(-\infty)\,(e^{iH(t-t')}c^\dagger_{\mu_i}c_{\nu_i}e^{-iH(t-t')},\,c^\dagger_{\mu_j'}c_{\nu_j'}), & t>t'\,,\\ 0 & t<t'\,,\end{cases} \tag{H2b}$$

$$\rho(-\infty)\equiv e^{-\beta H}/\mathrm{Tr}'e^{-\beta H}\,. \tag{H2c}$$

The notations used have the same meanings as those in the text except for $k_B=\hbar=1$ in this Appendix.

We now introduce a thermal Green's function $\mathcal{P}_{\mu_i\nu_i\mu_j'\nu_j'}(\tau-\tau')$ in order to calculate Eq. (H2b):

$$\begin{aligned}\mathcal{P}_{\mu_i\nu_i\mu_j'\nu_j'}(\tau-\tau') &= -\mathrm{Tr}'\rho(-\infty)\,\mathrm{Tr}(e^{H\tau}c^\dagger_{\mu_i}c_{\nu_i}e^{-H\tau}-\langle c^\dagger_{\mu_i}c_{\nu_i}\rangle)\\ &\quad\times(e^{H\tau'}c^\dagger_{\mu_j'}c_{\nu_j'}e^{-H\tau'}-\langle c^\dagger_{\mu_j'}c_{\nu_j'}\rangle)\,,\end{aligned} \tag{H3a}$$

where

$$\langle c^\dagger_{\mu_i}c_{\nu_i}\rangle=\mathrm{Tr}'\rho(-\infty)c^\dagger_{\mu_i}c_{\nu_i}\,. \tag{H3b}$$

Then, we obtain the elastic constant $c^{(1)}_{\alpha\beta\gamma\delta}(\vec{q},\vec{q}',\lambda\omega)$:

$$\begin{aligned}c^{(1)}_{\alpha\beta\gamma\delta}(\vec{q},\vec{q}',\lambda,\omega) &=\frac{1}{V}\sum_{\substack{ij\mu_i\nu_i\\ \mu_j'\nu_j'}} f(-q)f(q')\\ &\quad\times\Xi^{\mu_i\nu_i}_{\alpha\beta}\Xi^{\mu_j'\nu_j'}_{\gamma\delta}\,e^{i\vec{q}\cdot\vec{R}_j-\vec{q}'\cdot\vec{R}_i}P^{(R)}_{\mu_i\nu_i\mu_j'\nu_j'}(\omega)\,,\end{aligned} \tag{H4a}$$

where

$$P^{(R)}_{\mu_i\nu_i\mu_j'\nu_j'}(\omega)=\mathcal{P}_{\mu_i\nu_i\mu_j'\nu_j'}\;(i\omega_n\to\omega+i\delta)\,, \tag{H4b}$$

$$\mathcal{P}_{\mu_i\nu_i\mu_j'\nu_j'}(i\omega_n)=-\int_0^\beta d\tau\,e^{i\omega_n\tau}\mathcal{P}_{\mu_i\nu_i\mu_j'\nu_j'}(\tau),\qquad(\omega_n=2n\pi T)\,. \tag{H4c}$$

In order to apply the diagram technique to calculate $\mathcal{P}_{\mu_i\nu_i\mu_j'\nu_j'}(i\omega_n)$, we eliminate the constraint Eq. (H1) by using the relation $\int_C dz\,(1/2\pi i z^n)=\delta_{n,1}$ ($n$ is an integer; $C$ is any closed path encircling $z=0$ counterclockwise). Thus, using the relations

$$\Big[H,\sum_{\mu_i}c^\dagger_{\mu_i}c_{\mu_i}\Big]=0\quad\text{and}\quad\Big[c^\dagger_{\mu_i}c_{\nu_i},\sum_{\mu_j}c^\dagger_{\mu_j}c_{\mu_j}\Big]=0\,,$$

we obtain

$$\begin{aligned}\mathcal{P}_{\mu_i\nu_i\mu_j'\nu_j'}(i\omega_n) &=\Big(\prod_i\frac{1}{2\pi i}\int_C dz_i\Big)\frac{\mathrm{Tr}(e^{-\beta H(z)})}{\mathrm{Tr}'(e^{-\beta H})}\\ &\quad\times K_{\mu_i\nu_i\mu_j'\nu_j'}(i\omega_n)\\ &\quad+\beta\delta(\omega_n)g_{\nu_i\mu_i}(\tau=-0)g_{\nu_j'\mu_j'}(\tau=-0)\,,\end{aligned} \tag{H5a}$$

$$H(z)=H+\beta^{-1}\sum_{i\mu_i}(\ln z_i)c^\dagger_{\mu_i}c_{\mu_i}\,, \tag{H5b}$$

$$\mathrm{Tr}'(e^{-\beta H})=\Big(\prod_i\frac{1}{2\pi i}\int_C dz_i\Big)\mathrm{Tr}(e^{-\beta H(z)})\,, \tag{H5c}$$

$$K_{\mu_i\nu_i\mu_j'\nu_j'}(i\omega_n)=-\int_0^\beta d\tau\,e^{i\omega_n\tau}\frac{\mathrm{Tr}e^{-\beta H(z)+\tau H(z)}c^\dagger_{\mu_i}c_{\nu_i}e^{-\tau H(z)}c^\dagger_{\mu_j'}c_{\nu_j'}}{\mathrm{Tr}e^{-\beta H(z)}}\,, \tag{H5d}$$

$$g_{\nu_i\mu_i}(\tau)=\Big(\prod_j\frac{1}{2\pi i}\int_C dz_j\Big)e^{\tau\ln z_i/\beta}\,\frac{\mathrm{Tr}e^{-\beta H(z)}}{\mathrm{Tr}'e^{-\beta H}}\,G_{\nu_i\mu_i}(\tau)\,, \tag{H5e}$$

$$G_{\nu_i\mu_i}(\tau)=-\mathrm{Tr}e^{-\beta H(z)}\,\mathrm{Tr}(e^{\tau H(z)}c_{\nu_i}e^{-\tau H(z)}c^\dagger_{\mu_i})/\mathrm{Tr}e^{-\beta H(z)}\,. \tag{H5f}$$

The trace (Tr) in Eqs. (H5a)–(H5b) must be taken over the complete set of states for the Fermion operators.

In order to calculate $\mathcal{P}(i\omega_n)$ for donors (acceptors) interacting with thermal phonons, we use the following approximations. First, we approximate $K$ by $\pi$ which is the irreducible part of diagrams for $K$ and calculate $\pi$ by its lowest-order diagrams shown in Fig. 3(a). Moreover, for the self-energy part of one-particle Green's functions we use the lowest-order diagram in Fig. 3(b). Thus, we obtain

$$\pi_{\mu_i\nu_i\mu_j\nu_j'}(i\omega_n\to\omega+i\delta)=-\tfrac{1}{2}\delta_{ij}\delta_{\mu_i'\nu_i}\delta_{\mu_i\nu_i'}\int\frac{d\omega_1}{\pi}\frac{d\omega_2}{\pi}A_{\mu_i}(\omega_1)A_{\mu_i'}(\omega_2)$$
$$\times\frac{\tanh(\omega_1/2T)-\tanh(\omega_2/2T)}{\omega+\omega_1-\omega_2+i\delta}-\frac{\beta\delta(\omega_n)\delta_{\mu_i\nu_i}\delta_{\mu_j'\nu_j'}}{(e^{\beta\bar\epsilon_{\mu_i}}+1)(e^{\beta\bar\epsilon_{\mu_j'}}+1)},\qquad\text{(H6a)}$$

$$A_{\mu_i}(\omega)=\Big(\Gamma_{\mu_i}+\sum_{\nu_i'}\bar n_{\nu_i'}\,\mathrm{Im}w_{\nu_i'\mu_i}\Big)\Big[\Big(\omega-\bar\epsilon_{\mu_i}+\sum_{\nu_i'}\bar n_{\nu_i'}\,\mathrm{Re}w_{\nu_i'\mu_i}\Big)^2+\Big(\Gamma_{\mu_i}+\sum_{\nu_i'}\bar n_{\nu_i'}\,\mathrm{Im}w_{\nu_i'\mu_i}\Big)^2\Big]^{-1},\qquad\text{(H6b)}$$

$$\Gamma_{\mu_i}=\sum_{q\lambda\nu_i'}(x_{q\lambda})_{\mu_i\nu_i'}(x_{-q\lambda})_{\nu_i'\mu_i}\frac{\omega_{q\lambda}}{2}\pi[(n_{q\lambda}+1)\delta(\epsilon_{\mu_i}-\epsilon_{\nu_i'}-\omega_{q\lambda})+n_{q\lambda}\delta(\epsilon_{\mu_i}-\epsilon_{\nu_i'}+\omega_{q\lambda})],\qquad\text{(H6c)}$$

$$w_{\nu_i'\mu_i}=\sum_{q\lambda}(x_{q\lambda})_{\mu_i\nu_i'}(x_{-q\lambda})_{\nu_i'\mu_i}\frac{\omega_{q\lambda}}{2}\Big(\frac{1}{\epsilon_{\mu_i}-\epsilon_{\nu_i'}-\omega_{q\lambda}+i\delta}-\frac{1}{\epsilon_{\mu_i}-\epsilon_{\nu_i'}+\omega_{q\lambda}+i\delta}\Big),\qquad\text{(H6d)}$$

$$\bar\epsilon_{\mu_i}=\epsilon_{\mu_i}+\beta^{-1}\ln z_i,\quad\tilde\epsilon_{\mu_i}=\bar\epsilon_{\mu_i}-\sum_{\nu_i}\bar n_{\nu_i}\,\mathrm{Re}w_{\nu_i\mu_i},\qquad\text{(H6e)}$$

$$(x_{q\lambda})_{\mu_i\nu_i}=\Big(\frac{1}{\rho_0Vv_{q\lambda}^2}\Big)^{1/2}C_{q\lambda}^{\mu_i\nu_i}e^{i\vec q\cdot\vec R_i}f(q),\qquad\text{(H6f)}$$

$$n_{q\lambda}=1/(e^{\beta\omega_{q\lambda}}-1),\quad\bar n_{\nu_i}=1/(e^{\beta\bar\epsilon_{\nu_i}}+1),\qquad\text{(H6g)}$$

$$G_{\nu_i\mu_i}(\tau=-0)=\tfrac{1}{2}\delta_{\mu_i\nu_i}[1-\tanh(\tilde\epsilon_{\mu_i}/2T)],\qquad\text{(H7)}$$

where we assume the condition that $T=\beta^{-1}$ is much greater than the width of the spectral weight $A_\mu(\omega)$.

Second, we calculate $\ln\mathrm{Tr}\exp[-\beta H(z)]$ up to the second-order perturbation neglecting the self-energy shift and taking the integral over $z$ into account. It is concluded that $\mathrm{Tr}\exp[-\beta H(z)]/\mathrm{Tr}'\exp(-\beta H)$ can be replaced by one in this approximation.

In order to obtain explicit expressions for the elastic constant, we use the following two different approximations:

(a) We rewrite $\pi^{(1)}_{\mu_i\nu_i\nu_i\mu_i}$ [the first term in Eq. (H6a)] in the form

$$\pi^{(1)}_{\mu_i\nu_i\nu_i\mu_i}(i\omega_n\to\omega+i\delta)=-\tfrac{1}{2}\int\frac{d\omega_1d\omega_2}{\pi^2}\frac{\omega A_{\mu_i}(\omega_1)A_{\nu_i}(\omega_2)[\tanh(\omega_1/2T)-\tanh(\omega_2/2T)]}{(\omega+\omega_1-\omega_2+i\delta)(\omega_1-\omega_2)}$$
$$-\tfrac{1}{2}\int\frac{d\omega_1d\omega_2}{\pi^2}A_{\mu_i}(\omega_1)A_{\nu_i}(\omega_2)\frac{\tanh(\omega_1/2T)-\tanh(\omega_2/2T)}{\omega_1-\omega_2}\qquad\text{(H8)}$$

and replace

$[\tanh(\omega_1/2T)-\tanh(\omega_2/2T)]/(\omega_1-\omega_2)$ by $[\tanh(\tilde\epsilon_{\mu_i}/2T)-\tanh(\tilde\epsilon_{\nu_i}/2T)]/(\tilde\epsilon_{\mu_i}-\tilde\epsilon_{\nu_i})$.

Then, we obtain

$$\pi^{(1)}_{\mu_i\nu_i\nu_i\mu_i}(i\omega_n\to\omega+i\delta)=\frac{[\tanh(\tilde\epsilon_{\mu_i}/2T)-\tanh(\tilde\epsilon_{\nu_i}/2T)][\tilde\epsilon_{\mu_i}-\tilde\epsilon_{\nu_i}+i(\Gamma_{\mu_i}+\Gamma_{\nu_i})+i\sum_{\nu_i'}\bar n_{\nu_i'}\,\mathrm{Im}(w_{\nu_i'\nu_i}+w_{\nu_i'\nu_i})]}{2(\tilde\epsilon_{\mu_i}-\tilde\epsilon_{\nu_i})[\omega+\tilde\epsilon_{\mu_i}-\tilde\epsilon_{\nu_i}+i(\Gamma_{\mu_i}+\Gamma_{\nu_i})+i\sum_{\nu_i'}\bar n_{\nu_i'}\,\mathrm{Im}(w_{\nu_i'\mu_i}+w_{\nu_i'\nu_i})]},\qquad\text{(H9)}$$

$$c^{(1)}_{\alpha\beta\gamma\delta}(qq'\lambda\omega)=\delta_{q,q'}\frac{N}{V}|f(q)|^2\sum_{\mu,\nu}\Big(\frac{(n_\mu-n_\nu)[\epsilon_\mu-\epsilon_\nu+i(\Gamma_\mu+\Gamma_\nu)]\Xi^{\mu\nu}_{\alpha\beta}\Xi^{\nu\mu}_{\gamma\delta}}{(\epsilon_\mu-\epsilon_\nu)[\omega+\epsilon_\mu-\epsilon_\nu+i(\Gamma_\mu+\Gamma_\nu)]}+\beta\delta(\omega)n_\mu n_\nu\Xi^{\mu\mu}_{\alpha\beta}\Xi^{\nu\nu}_{\gamma\delta}\Big).\qquad\text{(H10)}$$

The first term in Eq. (H10) is the same as the first term in Eq. (26) in the text if we put $\Gamma_\mu+\Gamma_\nu=1/\tau_{\mu\nu}$, while the second term in Eq. (H10) is not identical with the relaxation (second) term in Eq. (26). It should be remarked, however, that the approximation to derive Eq. (H10) is different from the usual calculation of the Green's function in the treatment of δ function.

(b) We calculate the real and imaginary parts of $\pi^{(1)}$ independently by using the usual treatment of δ function. Then, we obtain

$$\pi^{(1)}_{\mu_i\nu_i\nu_i\mu_i}(i\omega_n\to\omega+i\delta)=\frac{\tanh(\tilde\epsilon_{\mu_i}/2T)-\tanh(\tilde\epsilon_{\nu_i}/2T)}{2(\tilde\epsilon_{\mu_i}-\tilde\epsilon_{\nu_i})}\Big(-1+\frac{\omega(\omega+\tilde\epsilon_{\mu_i\nu_i})}{(\omega+\tilde\epsilon_{\mu_i\nu_i})^2+(\tilde\Gamma_{\mu_i}+\tilde\Gamma_{\nu_i})^2}\Big)$$
$$+i\frac{\tilde\Gamma_{\mu_i}+\tilde\Gamma_{\nu_i}}{(\omega+\tilde\epsilon_{\mu_i\nu_i})^2+(\tilde\Gamma_{\mu_i}+\tilde\Gamma_{\nu_i})^2}\frac{(e^{-\beta\omega}-1)e^{-\beta\tilde\epsilon_{\mu_i}}}{(1+e^{-\beta\tilde\epsilon_{\mu_i}})(1+e^{-\beta(\omega+\tilde\epsilon_{\mu_i})})},\qquad\text{(H11)}$$

where

$$T=\beta^{-1} \gg \Gamma_{\nu_i} > \Gamma_{\mu_i}, \quad \bar{\Gamma}_{\mu_i} = \Gamma_{\mu_i} + \sum_{\nu_i'} \bar{n}_{\nu_i'} \operatorname{Im} w_{\nu_i' \mu_i},$$

$$c^{(1)}_{\alpha\beta\gamma\delta}(q, q'\lambda, \omega) = \delta_{q,q'} \frac{N}{V} |f(q)|^2 \sum_{\mu,\nu} \left[ \frac{n_\mu - n_\nu}{\epsilon_{\mu\nu}} \left( 1 - \frac{\omega(\omega+\epsilon_{\mu\nu})}{(\omega+\epsilon_{\mu\nu})^2 + (\Gamma_\mu + \Gamma_\nu)^2} \right) \tilde{\Xi}^{\mu\nu}_{\alpha\beta} \tilde{\Xi}^{\nu\mu}_{\gamma\delta} \right.$$
$$+ i(e^{-\beta\omega} - 1)[n_\mu \Theta(\Gamma_\nu - \Gamma_\mu) + n_\nu \Theta(\Gamma_\mu - \Gamma_\nu)] \frac{(\Gamma_\mu + \Gamma_\nu) \tilde{\Xi}^{\mu\nu}_{\alpha\beta} \tilde{\Xi}^{\nu\mu}_{\gamma\delta}}{(\omega+\epsilon_{\mu\nu})^2 + (\Gamma_\mu + \Gamma_\nu)^2}$$
$$\left. + \beta\delta(\omega) n_\mu n_\nu \tilde{\Xi}^{\mu\mu}_{\alpha\beta} \tilde{\Xi}^{\nu\nu}_{\gamma\delta} \right], \quad \text{(H12)}$$

where

$$\Theta(x) = \begin{cases} 1, & x>0, \\ 0, & x<0. \end{cases}$$

Equation (H11) with $\tilde{\epsilon}_{\mu_i}$, $\tilde{\Gamma}_{\mu_i}$ replaced by $\epsilon_{\mu_i}$, $\Gamma_{\mu_i}$ should be compared with Eq. (52) in Kwok's paper.[14] It is noted that Eq. (H11) becomes identical with Eq. (52) in Kwok's paper if we can replace $e^{-\beta\omega_1}/(1+e^{-\beta\omega_1})(1+e^{-\beta(\omega+\omega_1)})$ by $f_{\omega_1}(T) = Ae^{-\omega_1\beta}$, where $A$ is the normalization constant and is independent of $\omega, \omega_1$. However, this replacement is not possible and therefore Kwok's result cannot be justified. It is seen from Eq. (H11) that the both real and imaginary parts of $c^{(1)}$ calculated in this approximation are different from those in Eq. (26) in the text. In particular, the imaginary part of $c^{(1)}$ in Eq. (H12) is not proportional to $n_\mu - n_\nu$. This type of discrepancy between the results by the kinetic equation method and those by the Green's-function method appears in other problems, for example, in the ultrasonic attenuation by conduction electrons in metals in strong magnetic fields.[27]

At present, it is not clear whether the calculation of the Green's function up to higher orders by using the method of (b) gives the same result as Eq. (H10) or Eq. (26).


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