Comparison of two techniques in the theory of phonon-induced cyclotron resonance line shapes

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Two perturbation methods are compared for the theories of the cyclotron resonance line shape for electron-phonon systems. The line-shape functions in schemes designated as "moderately weak coupling" and "extremely weak coupling" by Choi and Chung are obtained using Mori's method of calculation. The results agree exactly with the functions Choi and Chung derived using Argyres and Sigel's projection technique.

I. INTRODUCTION

Studies of cyclotron resonance line shapes (CRLS) are of importance in investigating the electronic band structure of solids. Much theoretical work on this topic has been published since the 1950s. Most of the studies, however, are restricted to the investigation of three-dimensional electron systems,[1–24] although some work on two-dimensional systems[25–28] has been reported.

To the authors' knowledge, most of the theories presented start with the assumption that the absorption coefficient is proportional to the transition probability,[1–10] the imaginary part of the dielectric constant,[11] or the real part of the electric conductivity.[12–28] In these formalisms, with extremely few exceptions, the absorption coefficient is given by

$$\mu \propto \sum_{\alpha} A(\alpha)[(\omega-\omega_0)-i\tilde{\Gamma}_{\alpha}(\omega)]^{-1} , \tag{1.1}$$

where $A(\alpha)$ is a function of the state index α, ω is the microwave frequency, ω_0 is the cyclotron frequency, and $\tilde{\Gamma}_{\alpha}(\omega)$, which is equivalent to $B_{\alpha}(\omega)$ in the paper of Choi and Chung,[22(a)] is the line-shape function.[29] The line-shape function depends in general on the electron momentum, and thus its real and imaginary parts of themselves do not give the width and shift characteristics, respectively. The line-shape function appears as a result of the electron-background interactions. Among the many kinds of interactions available, impurity [Refs. 8, 13(b), 14(a), 15(a), 15(c), 18(a), 19, 20, and 24] and phonon scatterings [Refs. 1, 3–7, 9–11, 13(c), 14(b), 15(b), 15(d)–15(g), 16, 18(b), 18(c), 22, and 23] have been dealt with quite frequently in the theoretical papers.

The present work is concerned with the third formalism for the absorption coefficient, namely, the conductivity tensor formalism, and with three-dimensional electron-phonon systems. Many theories based on this formalism have appeared, but here we will discuss only a few, such as those of Kawabata,[14(a)] Lodder and Fujita,[15(a)] Argyres and Sigel,[19] and Choi and Chung.[22(a)] In dealing with the scattering, they made use of different methods. In most of the theories[14(a),15(a),22(a)] the line-shape function is given in the following form:

$$\tilde{\Gamma}_{\alpha}(\omega) \propto \sum_{\beta} B(\alpha,\beta)[\omega-\Delta_1(\alpha,\beta)-i\tilde{\Gamma}'(\alpha,\beta)-i\eta]^{-1} + \tilde{\Gamma}_{\alpha}^{\text{higher}} , \tag{1.2}$$

$$\tilde{\Gamma}'(\alpha,\beta) \propto \sum_{\gamma} C(\alpha,\beta,\gamma)[\omega-\Delta_2(\alpha,\beta,\gamma) - i\tilde{\Gamma}''(\alpha,\beta,\gamma)-i\eta]^{-1} + \tilde{\Gamma}'(\alpha,\beta)^{\text{higher}} \tag{1.3}$$

where $\eta\rightarrow 0^+$; $\tilde{\Gamma}_{\alpha}^{\text{higher}}, \tilde{\Gamma}'(\alpha,\beta)^{\text{higher}}, \ldots$ are the higher-order perturbation terms usually neglected for the weak interactions, $B(\alpha,\beta), C(\alpha,\beta,\gamma), \ldots$ are functions of the state indices $\alpha,\beta,\gamma,\ldots$; and $\Delta_1(\alpha,\beta)$, $\Delta_2(\alpha,\beta,\gamma), \ldots$ are energy factors corresponding to $\alpha,\beta,\gamma,\ldots$. $\tilde{\Gamma}', \tilde{\Gamma}'', \ldots$, often called the collision factors, appear iteratively and their structures are all similar.

In 1967 Kawabata introduced a theory based on the Kubo formalism and Mori's method of calculation.[30] In the parabolic-band formalism, the line-shape function is given by

$$\tilde{\Gamma}_{\alpha}(\omega) \propto \sum_{\beta'} B(\alpha,\beta)[\omega-n\omega_0-E(\mathbf{k}_{\alpha},\mathbf{k}_{\beta})-i\eta]^{-1} + \tilde{\Gamma}_{\alpha}^{\text{higher}} , \tag{1.4}$$

$$\tilde{\Gamma}'_{\alpha}=0 , \tag{1.5}$$

where β' implies that $n\neq 1$ and $E(\mathbf{k}_{\alpha},\mathbf{k}_{\beta})$ is the energy in terms of the electron momenta $\mathbf{k}_{\alpha}$ and $\mathbf{k}_{\beta}$. $E(\mathbf{k}_{\alpha},\mathbf{k}_{\beta})$ is negligible compared with $\omega-n\omega_0$ at low temperatures, but the first term of $\tilde{\Gamma}_{\alpha}(\omega)$ is finite at the resonance peak ($\omega=\omega_0$) since $n\neq 1$. This formula does not include the phonon energy in the energy denominators and cannot successfully reproduce the electron-phonon interactions, although an approximate solution for the acoustic phonon scattering could be obtained on the basis of it.[14(b)] Furthermore, the theory could not survive the critique of Argyres and Sigel (AS) that a line-shape function of this type does not give the correct line shape since the higher-order terms ($\tilde{\Gamma}_{\alpha}^{\text{higher}}$) neglected in the perturbative expansion

blow up at the resonance peaks. Choi and Chung[31] recently claimed that the higher-order terms were finite at the peaks, but soon their claim turned out to be erroneous (see the calculation carried out by Argyres in Ref. 32). In conclusion, the line-shape function obtained in this way does not adequately reflect the impurity or elastic phonon scattering where the phonon energy terms are not included.

In 1968 Lodder and Fujita obtained a line-shape function making use of Fujita's connected-diagram method.[15(a)] The line-shape function for the electron-phonon interactions derived in this way contains not only the phonon energy (ω_q) but also the collision factors $\tilde{\Gamma}'(\alpha,\beta)$ in the denominators:

$$\tilde{\Gamma}_\alpha(\omega) \propto \sum_\beta B(\alpha,\beta)[\omega - n\omega_0 - E(\mathbf{k}_\alpha,\mathbf{k}_\beta) \pm \omega_q - i\tilde{\Gamma}'(\alpha,\beta)]^{-1} + \tilde{\Gamma}_\alpha^{\text{higher}}, \tag{1.6}$$

$$\tilde{\Gamma}'(\alpha,\beta) \neq 0 . \tag{1.7}$$

The collision factors appear iteratively and the structure is similar to that of $\tilde{\Gamma}_\alpha(\omega)$. It can be stated that the expansion in this case does not break down. But the formula has been applied to some impurity scatterings[15(c)] by simply dropping the phonon energy terms and also neglecting the collision factors for the sake of mathematical simplicity. In that case the formula is very similar to Kawabata's expression and is subject to the same critique.

In 1974 Argyres and Sigel presented a theory starting with the kinetic equation, using their own projection technique.[33] Their theory seems to be quite general in the sense that it is based on rigorous formalism and the self-consistent projection technique and does not suffer from the break down of the expansion. Granting that it is true, their formula looks somewhat complicated. Hence, in order that it may be applied to real systems some simplifications are advisable.

In 1983 Choi and Chung presented a theory for electron-phonon systems. The projection technique of Argyres and Sigel was made use of in the theory. The line-shape function is given as

$$\tilde{\Gamma}_\alpha(\omega) \propto \sum_{\beta'} B(\alpha,\beta)[\omega - n\omega_0 - E(\mathbf{k}_\alpha,\mathbf{k}_\beta) \pm \omega_q - i\eta]^{-1} + \tilde{\Gamma}_\alpha^{\text{higher}}, \tag{1.8}$$

$$\tilde{\Gamma}'(\alpha,\beta) = 0 . \tag{1.9}$$

The line-shape function obtained is more or less similar to the formula of Lodder and Fujita, the difference being that collision factors are not included and summation over some specific Landau indices are excluded. The disappearance of the collision factors seems to be due to the neglect of the scattering potential against the unperturbed electron Hamiltonian in a middle step of the calculation. Therefore, the line-shape function of Choi and Chung is given in closed form, failing to give the iterative behavior. Furthermore, they introduced two coupling schemes in dealing with the calculations. According to them, the electron-phonon interactions may belong to the moderately weak coupling (MWC) or the extremely weak coupling (EWC) schemes, depending on the coupling strength. Usually the electron-state calculation precedes the phonon averaging, but if the coupling is extremely weak the reverse order seems acceptable. The authors called the former coupling MWC and the latter EWC. This classification is rather mathematical, and thus its exact criteria are not available in the present situation. They calculated the line shape for the electron-phonon interaction in InSb in the extreme quantum limit,[22(b)] where only the ground level was occupied. The result showed the disappearance of the width for photon energy smaller than the phonon energy, supporting the experimental result of Summers *et al.*[11(b)] Furthermore, the prediction of Raju and Fujita of anomalous broadening in the system[15(b)] was not supported by this theory. Although Choi and Chung utilized the same perturbative expansion, their line-shape function is not subject to the AS critique since the phonon energy is included in the energy denominators.

In 1984 Ryu and Choi[23] obtained the same function by the use of Kawabata's approach based on Mori's method. Their calculation, however, confined itself to the EWC scheme. The question of why only the EWC result appeared was not addressed in their paper.

In this paper we shall first summarize the theory of CRLS for the electron-phonon systems originally introduced by the other authors and discuss a procedure which enables us to derive the respective line-shape function for the two coupling schemes. We shall then briefly discuss the results.

II. CONDUCTIVITY

When a circularly polarized microwave of amplitude F and frequency ω is applied along the z axis in a semiconductor, the average absorption power[15(a)]

$$P = (F^2/2)\,\mathrm{Re}\sigma_{+-}(\omega) \tag{2.1}$$

is delivered to the system, where the symbol Re means "the real part of " and the conductivity tensor $\sigma_{+-}(\omega)$, in units in which $\hbar = 1$, and with a static magnetic field $\mathbf{B}$ applied in the z direction, is given by

$$\sigma_{+-}(\omega) = \frac{1-\exp(-\beta\omega_0)}{\omega_0\Omega} \sum_\alpha f(E_\alpha)(1-f(E_\alpha+\omega_0)) \times j^-_{\alpha,\alpha+1}\langle \tilde{F}_\alpha(\omega)\rangle_p , \tag{2.2}$$

which is equivalent to the Choi-Chung expression[22(a)]

$$\sigma_{+-}(\omega) = \frac{1}{i\omega_0\Omega} \sum_\alpha [f(E_\alpha) - f(E_\alpha+\omega_0)](j^+_\alpha)^* \langle R_\alpha(\omega)\rangle_p . \tag{2.3}$$

Here, Ω is the volume of the system, $f(E)$ stands for the Fermi distribution function, $\omega_0 \equiv eB/m$ is the cyclotron frequency for the electron of effective mass m, $j^\pm \equiv j_x \pm i j_y$, $\mathbf{j}$ being the single-electron current vector, $j^+_\alpha \equiv j^+_{\alpha+1,\alpha} = \langle \alpha+1 \,|\, j^+ \,|\, \alpha\rangle$, $\beta \equiv (k_B T)^{-1}$ for the temperature T, and E_α is the energy eigenvalue correspond-

ing to the eigenstate $|\alpha\rangle \equiv |N,\mathbf{k}\rangle$ in the parabolic-band approximation, N is the Landau index, $\mathbf{k}$ is the electron wave vector, $\langle A \rangle_p$ denotes the average of quantity A over the phonon distribution, $\tilde{F}_\alpha(\omega)$ is the Fourier-Laplace transform (FLT) of $\langle \alpha+1 | j^+(t) | \alpha \rangle$ defined by

$$\tilde{F}_\alpha(\omega)=\int_0^\infty dt \langle \alpha+1 | j^+(t) | \alpha \rangle \exp(-i\omega t-\eta t) , \quad (2.4)$$

which corresponds to

$$R_\alpha(\omega)=\langle \alpha+1 | (\omega-i\eta-L)^{-1} j^+ | \alpha \rangle , \quad (2.5)$$

where $\eta \to 0^+$, $A(t)$ is the operator A in the Heisenberg representation, and

$$L=L_0+L_p+L_1 , \quad (2.6)$$

where L_0, L_p, and L_1, respectively, are the Liouville operators corresponding to the unperturbed single-electron Hamiltonian h_0, the phonon Hamiltonian H_p, and the scattering potential V given by

$$H_p=\sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} , \quad (2.7)$$

$$V=\sum_{\mathbf{q}} (\gamma_{\mathbf{q}} b_{\mathbf{q}}+\gamma_{\mathbf{q}}^\dagger b_{\mathbf{q}}^\dagger) , \quad (2.8)$$

$$\gamma_{\mathbf{q}}=C_{\mathbf{q}} \exp(i\mathbf{q}\cdot\mathbf{r}) \quad (2.9)$$

for the phonon with energy $\omega_{\mathbf{q}}$ and momentum $\mathbf{q}$, $b_{\mathbf{q}}^\dagger$ and $b_{\mathbf{q}}$, respectively, being the creation and annihilation operators. It should be noted that

$$j^+_{\alpha\beta} \equiv \langle \alpha | j^+ | \beta \rangle = (\langle \beta | j^{-1} | \alpha \rangle)^* = j^+_\beta \delta_{\alpha,\beta+1} \quad (2.10)$$

holds for arbitrary-state indicates α and β, where the states α, $\alpha+1$, and β, respectively, denote $(N,\mathbf{k})$, $(N+1,\mathbf{k})$, and $(N',\mathbf{k}')$.

III. LINE-SHAPE FUNCTION

Following Ref. 14(a), we define two projection operators P_α and P'_α by

$$P_\alpha B=\frac{(A_\alpha,B)}{(A_\alpha,j^+)} j^+ = j^+ (B_{\alpha+1,\alpha}/j^+_{\alpha+1,\alpha}) , \quad (3.1)$$

$$P'_\alpha B=\frac{(B,j^+)}{(A_\alpha,j^+)} A_\alpha , \quad (3.2)$$

where B is an arbitrary operator,

$$(A,B)=\mathrm{Tr}(AB) , \quad (3.3)$$

and $A_\alpha=a_\alpha^\dagger a_{\alpha+1}$ is a projection operator satisfying

$$(A_\alpha,B)=(A_\alpha)_{\alpha,\alpha+1} B_{\alpha+1,\alpha} , \quad (3.4)$$

$a_\alpha^\dagger$ (a_α) being the creation (annihilation) operator for the electron state $|\alpha\rangle$ and Tr representing the trace in the single-electron expression. After some simple manipulation using the projection operators, we obtain from Eq. (2.4)

$$\langle \tilde{F}_\alpha(\omega) \rangle_p = \frac{(A_\alpha,j^+)}{i(\omega-\omega_\alpha)+\tilde{\Gamma}_\alpha(\omega)} , \quad (3.5)$$

where

$$i\omega_\alpha = \left\langle \frac{(A_\alpha,iLj^+)}{(A_\alpha,j^+)} \right\rangle_p = \langle i\omega_0 + i(V_{\alpha+1,\alpha+1}-V_{\alpha\alpha}) \rangle_p , \quad (3.6)$$

which yields $\omega_\alpha=\omega_0$ if $\langle V_{\alpha\alpha} \rangle_p=0$ is assumed, and $\tilde{\Gamma}_\alpha(\omega)$ or $B_\alpha(\omega)$ in the notation of Choi and Chung, called the line-shape function, is the FLT of

$$\langle \Gamma_\alpha(t) \rangle_p = \left\langle \frac{(Q_\alpha,R_\alpha(t))}{(A_\alpha,j^+)} \right\rangle_p , \quad (3.7)$$

where

$$R_\alpha(t)=\exp[it(1-P_\alpha)L]R_\alpha , \quad (3.8)$$

$$R_\alpha = i(1-P_\alpha)Lj^+ \quad (3.9a)$$

$$= i(1-P_\alpha)[V,j^+] , \quad (3.9b)$$

$$Q_\alpha = (1-P'_\alpha)iLA_\alpha \quad (3.10a)$$

$$= i(1-P'_\alpha)[V,A_\alpha] , \quad (3.10b)$$

$[A,B]$ being the commutator of operators A and B. Combining Eqs. (2.1), (2.2), and (3.5), we have Eq. (1.1). In order to calculate $\tilde{\Gamma}_\alpha(\omega)$, we make use of the following relations:

$$[h_0+H_p,j^+]=\omega_0 j^+ , \quad (3.11)$$

$$(1-P'_\alpha)[h_0+H_p,A_\alpha]=0 , \quad (3.12)$$

$$(1-P_\alpha)(L_0+L_p)P_\alpha B=0 , \quad (3.13)$$

$$(P'_\alpha A,(1-P_\alpha)B)=0 , \quad (3.14)$$

$$[(1-P_\alpha)(L_0+L_p)]^n(1-P_\alpha)B=(1-P_\alpha)[(L_0+L_p)^n]B . \quad (3.15)$$

By taking into account Eqs. (3.8), (3.9), (3.10), (3.14), and (3.15) and considering the perturbation only up to second order in the scattering, the numerator of Eq. (3.7) then becomes

$$
\begin{aligned}
(Q_\alpha,R_\alpha(t))&=(i[V,A_\alpha],i(1-P_\alpha)[[V,j^+]+it[h_0+H_p,[V,j^+]])\\
&=-[(VA_\alpha,Vj^+)-(VA_\alpha,j^+V)-(A_\alpha V,Vj^+)+(A_\alpha V,j^+V)-(VA_\alpha,P_\alpha Vj^+)+(VA_\alpha,P_\alpha j^+V)+(A_\alpha V,P_\alpha Vj^+)\\
&\quad-(A_\alpha V,P_\alpha j^+V)]-it[(VA_\alpha,h_0Vj^+)-(VA_\alpha,h_0j^+V)-(VA_\alpha,Vj^+h_0)+(VA_\alpha,j^+Vh_0)\\
&\quad-(A_\alpha V,h_0Vj^+)+(A_\alpha V,h_0j^+V)+(A_\alpha V,Vj^+h_0)-(A_\alpha V,j^+Vh_0)\\
&\quad-(VA_\alpha,P_\alpha h_0Vj^+)+(VA_\alpha,P_\alpha h_0j^+V)+(VA_\alpha,P_\alpha Vj^+h_0)-(VA_\alpha,P_\alpha j^+Vh_0)\\
&\quad+(A_\alpha V,P_\alpha h_0Vj^+)-(A_\alpha V,P_\alpha h_0j^+V)-(A_\alpha V,P_\alpha Vj^+h_0)+(A_\alpha V,P_\alpha j^+Vh_0)\\
&\quad+(VA_\alpha,H_pVj^+)-(VA_\alpha,H_pj^+V)-(VA_\alpha,Vj^+H_p)+(VA_\alpha,j^+VH_p)\\
&\quad-(A_\alpha V,H_pVj^+)+(A_\alpha V,H_pj^+V)+(A_\alpha V,Vj^+H_p)-(A_\alpha V,j^+VH_p)\\
&\quad-(VA_\alpha,P_\alpha H_pVj^+)+(VA_\alpha,P_\alpha H_pj^+V)+(VA_\alpha,P_\alpha Vj^+H_p)-(VA_\alpha,P_\alpha j^+VH_p)\\
&\quad+(A_\alpha V,P_\alpha H_pVj^+)-(A_\alpha V,P_\alpha H_pj^+V)-(A_\alpha V,P_\alpha Vj^+H_p)\\
&\quad+(A_\alpha V,P_\alpha j^+VH_p)]\ . \qquad (3.16)
\end{aligned}
$$

Dividing the forty terms in Eq. (3.16) into four parts, we can calculate $\Gamma_\alpha(t)$ and $\tilde{\Gamma}_\alpha(\omega)$ in succession.

IV. CALCULATIONS IN THE TWO COUPLING SCHEMES

In performing the calculation with respect to the electron states and the phonon averaging, the following two ways are possible. If the electron-state calculation is carried out first, we may use the trace property

$$\langle \mathrm{Tr}(BA_\alpha C)\rangle_p=\langle \mathrm{Tr}(A_\alpha CB)\rangle_p=(A_\alpha)_{\alpha,\alpha+1}\sum_\beta \langle C_{\alpha+1,\beta}B_{\beta\alpha}\rangle_p$$

for arbitrary operators B and C. We will call this scheme of calculation the MWC scheme after Ref. 22(a). In this scheme we then have [where the numbers refer to the terms in Eq. (3.16)]

$$
\begin{aligned}
\mathscr{P}(\mathrm{I})&=(1\mathrm{st}+5\mathrm{th})+(9\mathrm{th}+17\mathrm{th})+(11\mathrm{th}+19\mathrm{th})+(25\mathrm{th}+33\mathrm{rd})+(27\mathrm{th}+35\mathrm{th})\\
&=-(A_\alpha)_{\alpha,\alpha+1}\left[\left[\sum_\beta j_\beta^+V_{\alpha+1,\beta+1}V_{\beta\alpha}-j_\alpha^+V_{\alpha+1,\alpha+1}V_{\alpha\alpha}\right]\right.\\
&\quad+it\left[\sum_\beta j_\beta^+E_{\alpha+1}V_{\alpha+1,\beta+1}V_{\beta\alpha}-j_\alpha^+E_{\alpha+1}V_{\alpha+1,\alpha+1}V_{\alpha\alpha}-\sum_\beta j_\beta^+E_\beta V_{\alpha+1,\beta+1}V_{\beta\alpha}+j_\alpha^+E_\alpha V_{\alpha+1,\alpha+1}V_{\alpha\alpha}\right.\\
&\quad\left.\left.+\sum_\beta j_\beta^+H_pV_{\alpha+1,\beta+1}V_{\beta\alpha}-j_\alpha^+H_pV_{\alpha+1,\alpha+1}V_{\alpha\alpha}-\sum_\beta j_\beta^+V_{\alpha+1,\beta+1}H_pV_{\beta\alpha}+j_\alpha^+V_{\alpha+1,\alpha+1}H_pV_{\alpha\alpha}\right]\right]. \qquad (4.1)
\end{aligned}
$$

With a close look at each pair in the small brackets, we see that the terms corresponding to $\beta=\alpha$ are excluded in the summations. Averaging over the phonon distribution can be carried out by considering $\langle b_q^\dagger b_{q'}\rangle_p=n_q\delta_{qq'}$ and $\langle b_q b_{q'}^\dagger\rangle_p=(1+n_q)\delta_{qq'}$, n_q being the Planck distribution function. As a result, we have

$$
\begin{aligned}
\langle\mathscr{P}(\mathrm{I})\rangle_p=-(A_\alpha)_{\alpha,\alpha+1}\sum_{\beta(\neq\alpha)}\sum_q j_\beta^+\{&(1+n_q)(\gamma_q)_{\alpha+1,\beta+1}(\gamma_q^\dagger)_{\beta\alpha}\exp[it(E_{\alpha+1}-E_\beta-\omega_q)]\\
&+n_q(\gamma_q^\dagger)_{\alpha+1,\beta+1}(\gamma_q)_{\beta\alpha}\exp[it(E_{\alpha+1}-E_\beta+\omega_q)]\}\ , \qquad (4.2)
\end{aligned}
$$

where we have used the formal expression $1+itE_\alpha=\exp(itE_\alpha)$. This looks unreasonable, but if all the higher-order perturbative terms excluded here are considered, this expression will be justified. Similarly, we have

$$
\begin{aligned}
\langle\mathscr{P}(\mathrm{II})\rangle_p&=\langle(2\mathrm{nd}+6\mathrm{th})+(10\mathrm{th}+18\mathrm{th})+(12\mathrm{th}+20\mathrm{th})+(26\mathrm{th}+34\mathrm{th})+(28\mathrm{th}+36\mathrm{th})\rangle_p\\
&=(A_\alpha)_{\alpha,\alpha+1}\sum_{\beta(\neq\alpha)}\sum_q j_\alpha^+\{(1+n_q)(\gamma_q)_{\alpha\beta}(\gamma_q^\dagger)_{\beta\alpha}\exp[it(E_{\alpha+1}-E_\beta-\omega_q)]\\
&\quad+n_q(\gamma_q^\dagger)_{\alpha\beta}(\gamma_q)_{\beta\alpha}\exp[it(E_{\alpha+1}-E_\beta+\omega_q)]\}\ , \qquad (4.3)
\end{aligned}
$$

$$\langle \mathscr{P}(\mathrm{III})\rangle_p=\langle(3\mathrm{rd}+7\mathrm{th})+(13\mathrm{th}+21\mathrm{st})+(15\mathrm{th}+23\mathrm{rd})+(29\mathrm{th}+37\mathrm{th})+(31\mathrm{st}+37\mathrm{th})\rangle_p$$
$$=(A_\alpha)_{\alpha,\alpha+1}j_\alpha^+\sum_{\beta(\neq\alpha+1)}\sum_{\mathbf{q}}\{(1+n_{\mathbf{q}})(\gamma_{\mathbf{q}})_{\alpha+1,\beta}(\gamma_{\mathbf{q}}^\dagger)_{\beta,\alpha+1}\exp[it(E_\beta-E_\alpha+\omega_{\mathbf{q}})]$$
$$+n_{\mathbf{q}}(\gamma_{\mathbf{q}}^\dagger)_{\alpha+1,\beta}(\gamma_{\mathbf{q}})_{\beta,\alpha+1}\exp[it(E_\beta-E_\alpha-\omega_{\mathbf{q}})]\}\ , \tag{4.4}$$

$$\langle \mathscr{P}(\mathrm{IV})\rangle_p=\langle(4\mathrm{th}+8\mathrm{th})+(14\mathrm{th}+22\mathrm{nd})+(16\mathrm{th}+24\mathrm{th})+(30\mathrm{th}+38\mathrm{th})+(32\mathrm{nd}+40\mathrm{th})\rangle_p$$
$$=-(A_\alpha)_{\alpha,\alpha+1}\sum_{\beta(\neq\alpha+1)}\sum_{\mathbf{q}}j_{\beta-1}^+\{(1+n_{\mathbf{q}})(\gamma_{\mathbf{q}})_{\alpha+1,\beta}(\gamma_{\mathbf{q}}^\dagger)_{\beta-1,\alpha}\exp[it(E_\beta-E_\alpha+\omega_{\mathbf{q}})]$$
$$+n_{\mathbf{q}}(\gamma_{\mathbf{q}}^\dagger)_{\alpha+1,\beta}(\gamma_{\mathbf{q}})_{\beta-1,\alpha}\exp[it(E_\beta-E_\alpha-\omega_{\mathbf{q}})]\}\ . \tag{4.5}$$

Collecting all the parts and dividing them by $(A_\alpha,j^+)=(A_\alpha)_{\alpha,\alpha+1}j_\alpha^+$, we get the average of $\Gamma_\alpha(t)$ over the phonon distribution. Consequently, $\langle\tilde{\Gamma}_\alpha(\omega)\rangle_p$, the FLT of $\langle\Gamma_\alpha(t)\rangle_p$, can be obtained:

$$[i\tilde{\Gamma}_\alpha(\omega)]_{\mathrm{MWC}}=\sum_{\mathbf{q}}(n_{\mathbf{q}}+1)\left[\sum_{\beta(\neq\alpha+1)}\frac{(\gamma_{\mathbf{q}})_{\alpha+1,\beta}[(\gamma_{\mathbf{q}}^\dagger)_{\beta,\alpha+1}-(\gamma_{\mathbf{q}}^\dagger)_{\beta-1,\alpha}j_{\beta-1}^+/j_\alpha^+]}{\omega-E_\beta+E_\alpha-\omega_{\mathbf{q}}-i\eta}\right.$$
$$\left.+\sum_{\beta(\neq\alpha)}\frac{[(\gamma_{\mathbf{q}})_{\alpha\beta}-(\gamma_{\mathbf{q}})_{\alpha+1,\beta+1}j_\beta^+/j_\alpha^+](\gamma_{\mathbf{q}}^\dagger)_{\beta\alpha}}{\omega-E_{\alpha+1}+E_\beta+\omega_{\mathbf{q}}-i\eta}\right]$$
$$+\sum_{\mathbf{q}}n_{\mathbf{q}}\left[\sum_{\beta(\neq\alpha+1)}\frac{(\gamma_{\mathbf{q}}^\dagger)_{\alpha+1,\beta}[(\gamma_{\mathbf{q}})_{\beta,\alpha+1}-(\gamma_{\mathbf{q}})_{\beta-1,\alpha}j_{\beta-1}^+/j_\alpha^+]}{\omega-E_\beta+E_\alpha+\omega_{\mathbf{q}}-i\eta}\right.$$
$$\left.+\sum_{\beta(\neq\alpha)}\frac{[(\gamma_{\mathbf{q}}^\dagger)_{\alpha\beta}-(\gamma_{\mathbf{q}}^\dagger)_{\alpha+1,\beta+1}j_\beta^+/j_\alpha^+](\gamma_{\mathbf{q}})_{\beta\alpha}}{\omega-E_{\alpha+1}+E_\beta-\omega_{\mathbf{q}}-i\eta}\right]\ , \tag{4.6}$$

which is identical to the result of Choi and Chung [Eq. (1.8)]. The parts with $n_{\mathbf{q}}+1$ and $n_{\mathbf{q}}$ are known as emission and absorption terms, respectively. Note that both positive and negative signs appear on $\omega_{\mathbf{q}}$ in the energy denominators of each part.

On the other hand, if the phonon averaging is carried out first in

$$\langle\mathrm{Tr}(BA_\alpha C)\rangle_p=(A_\alpha)_{\alpha,\alpha+1}\sum_\beta\langle B_{\beta\alpha}C_{\alpha+1,\beta}\rangle_p\ ,$$

we will have a different result. It should be noted that both B and C contain $b_{\mathbf{q}}^\dagger$ and $b_{\mathbf{q}}$. The details of the evaluation are given in Ref. 23. We will call this scheme of calculation the EWC scheme, also after Ref. 22(a) (this name may not be appropriate). In this scheme we have

$$[i\tilde{\Gamma}_\alpha(\omega)]_{\mathrm{EWC}}=\sum_{\mathbf{q}}(1+n_{\mathbf{q}})\left[\sum_{\beta(\neq\alpha+1)}\frac{(\gamma_{\mathbf{q}})_{\alpha+1,\beta}[(\gamma_{\mathbf{q}}^\dagger)_{\beta,\alpha+1}-(\gamma_{\mathbf{q}}^\dagger)_{\beta-1,\alpha}j_{\beta-1}^+/j_\alpha^+]}{\omega-E_\beta+E_\alpha-\omega_{\mathbf{q}}-i\eta}\right.$$
$$\left.+\sum_{\beta(\neq\alpha)}\frac{[(\gamma_{\mathbf{q}}^\dagger)_{\alpha\beta}-(\gamma_{\mathbf{q}}^\dagger)_{\alpha+1,\beta+1}j_\beta^+/j_\alpha^+](\gamma_{\mathbf{q}})_{\beta\alpha}}{\omega-E_{\alpha+1}+E_\beta-\omega_{\mathbf{q}}-i\eta}\right]$$
$$+\sum_{\mathbf{q}}n_{\mathbf{q}}\left[\sum_{\beta(\neq\alpha+1)}\frac{(\gamma_{\mathbf{q}}^\dagger)_{\alpha+1,\beta}[(\gamma_{\mathbf{q}})_{\beta,\alpha+1}-(\gamma_{\mathbf{q}})_{\beta-1,\alpha}j_{\beta-1}^+/j_\alpha^+]}{\omega-E_\beta+E_\alpha+\omega_{\mathbf{q}}-i\eta}\right.$$
$$\left.+\sum_{\beta(\neq\alpha)}\frac{[(\gamma_{\mathbf{q}})_{\alpha\beta}-(\gamma_{\mathbf{q}})_{\alpha+1,\beta+1}j_\beta^+/j_\alpha^+](\gamma_{\mathbf{q}}^\dagger)_{\beta\alpha}}{\omega-E_{\alpha+1}+E_\beta+\omega_{\mathbf{q}}-i\eta}\right]\ , \tag{4.7}$$

which is also identical to the result of Choi and Chung. We see that the energy denominators of the emission and absorption parts contain $\omega_{\mathbf{q}}$ with negative and positive signs, respectively.

V. CONCLUSION

In the preceding section, we obtained two different line-shape functions that are identical with the corresponding expressions derived by Choi and Chung. The MWC and EWC calculations are based on

$$\langle\mathrm{Tr}(BA_\alpha C)\rangle_p=(A_\alpha)_{\alpha,\alpha+1}\sum_\beta\langle C_{\alpha+1,\beta}B_{\beta\alpha}\rangle_p$$

and

$$\langle\mathrm{Tr}(BA_\alpha C)\rangle_p=(A_\alpha)_{\alpha,\alpha+1}\sum_\beta\langle B_{\beta\alpha}C_{\alpha+1,\beta}\rangle_p\ ,$$

respectively. These two ways yielded different values in the calculations involving $b_{\mathbf{q}}^\dagger$ and $b_{\mathbf{q}}$ since $b_{\mathbf{q}}^\dagger b_{\mathbf{q}}\neq b_{\mathbf{q}}b_{\mathbf{q}}^\dagger$.

The energy denominators contain ω_q differently in the two schemes. As far as only this behavior is concerned, our MWC-scheme result agrees with the formulas of many other authors.[15(a),18(a),21(b)] It is fairly similar to the formula of Lodder and Fujita, the critical difference being that $\beta=\alpha+1$ and $\beta=\alpha$, respectively, are excluded in the first and second parts of each term.

The EWC-scheme result looks unphysical. But as pointed out in Ref. 22(a), this function is well explained in a formal sense in connection with the effect of scattering on the line broadening. If the momentum dependence of the electron energy is disregarded, the emission in this scheme is maximum at $\omega=n\omega_0+\omega_q$, while the absorption is maximum at $\omega=n\omega_0-\omega_q$, n ($\neq 1$) being the appropriate integers. This implies that the broadening increases as a phonon is emitted or absorbed.

In deriving the functions, we adopted the parabolic-band approximation and neglected the scattering potential against the unperturbed electron energy at a stage of calculating the function in each scheme. As a result, the width, the real part of $\tilde{\Gamma}(\omega)$, comes from the arbitrary infinitesimal η. If these points are improved, more accurate results will be obtained. In addition, the technique used by Argyres and Sigel[19] in working out their general theory will also be helpful in improving the present theory. We will leave this for a further study.

In conclusion, we do not claim that our theory is quite general. The main purpose of this paper is to recall that the two different methodologies can yield identical results as far as both are valid. Thus it is not strange that both methods are still widely adopted in many theoretical papers.[34(a),34(b),35,36]

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