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Theory of Direct–Interband–Transition Line Shapes Based on Mori's Method

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Summary A theory of direct interband optical transitions in the electron phonon system is introduced on the basis of the Kubo formalism and by using Mori's method of calculation. The line shape functions are introduced in two different ways and are compared wuth those obtained by Choi and Chung based on Argyres and Sigel's projection technique.

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1. Introduction.

Electron motion in solids is usually affected by some scattering mechanisms including electron-electron, electron-phonon and electron-impurity interactions.But if the number density of electron is very low, the electron-electron interaction may be neglected. The other background interactions may be dealt with as perturbation.

In the presence of a constant magnetic field, the noninteracting electrons perform undisturbed cyclotron motion. The electron energy is made up of the kinetic energy of the original motion in the field direction, together with the quantized energy of the oscillatory motion in the plane perpendicular to the field direction. This results in the Landau splittings in both conduction and valence bands in solids.

In the process of absorption of photons the electrons change their energies and momenta to make optical transitions to higher sublevels. The transitions are classified into two categories in general. The first of there is the case of intraband transitions including direct and indirect cyclotron transitions. The second is the case of interband transitions including direct and indirect transitions(1).

If there is no background scattering, the absorption line shape will be like a delta-function. But if the electrons are scattered by the background interactions, the shape will be broadened. Thus we see that studies of optical transitions are useful in examining the transport behaviour of electrons as well as the band structure of solids. Quite many theoretical(2−25) and experimental(26−42) studies on the interband optical transitions have appeared. Here we are interested in Choi and Chung's line shape formula for the electron-phonon systems.

In dealing with the scattering responsible for the line broadening, many approaches were utilized. Ohta et al.(4) used the kinetic theoretical formalism and Choi et al.(23,24) made use of Argyres and Sigel's projection technique(43).

On the other hand, Ryu et al.(44,45) showed that Mori's method(46) and Argyres and Sigel's technique gave the same result in a theory of phonon-induced cyclotron resonance line shapes. In view of this fact we may guess that Mori's method can also yield the same formula obtained by Choi and Chung(24) for the interband absorption line shapes. In this paper we shall show the work.

2. Theory of interband transition.

When a circularly polarized electromagnetic wave of amplitude F and frequency ω given by

$$F_x = F\cos\omega t, \qquad F_y = F\sin\omega t, \qquad F_z = 0 \tag{2.1}$$

is applied along the z-axis in a semiconductor, the average absorption power delivered to the system is[47]

(2.2)
$$P = (F^2/2)\mathrm{Re}\sigma_{+-}(\omega),$$

where the symbol Re means ¡¡the real part of¿¿ and the conductivity tensor, $\sigma_{+-}(\omega)$, is given in the Kubo formalism by

(2.3)
$$\sigma_{+-}(\omega) = \frac{\beta}{\Omega} \lim_{\eta \to O+} \int_0^\infty dt \, \exp[-i\omega t - \eta t](< J^-; J^+(t) >),$$

(2.4)
$$< A; B > \equiv \frac{1}{\beta} \int_0^\beta < A(-i\lambda)B > d\lambda,$$

(2.5)
$$J^\pm \equiv J_x \pm i J_y.$$

Here Ω is the volume of the system, $\beta = (k_B T)^{-1}$ for the temperature T, $J(t)$ is the time-dependent total current operator in the Heisenberg representation, $< A >$ denotes the grand canonical ensemble average of A, and we use units in which $h = 1$. It should be noted that the conductivity tensor is expressed in the many-body formalism.

We assume that the majority carriers are noninteracting electrons and consider only the phonon background. Then the Hamiltonian of the system, H, can be given in terms of the unperturbed single-electron Hamiltonian h_0, the electron-phonon interaction potential V and the phonon Hamiltonian H_p:

(2.6)
$$H = \sum_n h^{(n)} + H_p,$$

(2.7)
$$h = h_0 + V,$$

(2.8) $$V = \sum_q (\gamma_q b_q + \gamma_q^+ b_q^+),$$

(2.9) $$\gamma_q = C_q \exp[iq \cdot r],$$

(2.10) $$H_p = \sum_q \omega_q b_q^+ b_q,$$

where n denotes the single-electron index. b_q^+ and b_q are, respectively, the creation and annihilation operators of the phonon with momentum q and energy ω_q. C_q is the electron-phonon interaction matrix and $r(\equiv (x, y, z))$ is the electron position vector.

The total current operator can also be written in terms of the single-electron current j as[24]

(2.11) $$J = \sum_{\alpha,\beta} < \beta \mid j \mid \alpha > a_\beta^+ a_\alpha,$$

a_α^+ and a_α, respectively, being the creation and annihilation operators for the single electron. Therefore, the total system can now be expressed in the single-electron formalism.

In the presence of a constant magnetic field B characterized by the vector potential $A = (0, Bx, 0)$ the unperturned Hamiltonian becomes

(2.12) $$h_0 = [p_x^2 + (p_y + m\omega_0 x)^2 + p_z^2]/2m,$$

where the cyclotron frequency $\omega_0(\equiv eB/m)$ and the effective mass m should be replaced by $\omega_c(\omega_V)$ and $m_c(m_V)$, respectively, for the electrons in the conduction (valence) band.

The energy eigenvalues and eigenstates are characterized by the Landau index N, the electron wave vector k and the corresponding Bloch functions in the parabolic-band formalism:

(2.13)
$$E_{\alpha}^{c} = E_{N,k}^{c} = E_g + (N + \frac{1}{2})\omega_c + k_z^2/2m_c,$$

(2.14)
$$E_{\alpha'}^{V} = E_{N',k'}^{V} = -(N' + \frac{1}{2})\omega_V - (k_z')^2/2m_V,$$

(2.15)
$$\mid \alpha_c > \equiv \mid \alpha; c > = \Psi_{N.k}^{c}(r) \mid U_c >,$$

(2.16)
$$\mid \alpha_V' > \equiv \mid \alpha'; v > = \Psi_{N'.k'}^{V}(r) \mid U_V > .$$

Here E_g is the energy gap. The Greek letters α and α' denote, respectively, the states (N, k) and (N', k'), $\mid U_c > \mid (U_v >)$ are the Bloch functions for the conduction (valence) band, and $\Phi_{N,k}(r)$ are the wave functions of the electrons corresponding to N and k.

If we restrict ourselves to the direct transition, we may adopt the following selection rule (24):

(2.17)
$$< \alpha_c \mid j^+ \mid \beta_V > = j_{\alpha}^{+}\delta_{\alpha\beta}.$$

where $j_{\alpha}^{+} \equiv < \alpha_c \mid j^+ \mid \alpha_V >$. $\sigma_{+-}(\omega)$ can now be written in the single-electron expression

(2.18)
$$\sigma_{+-}(\omega) = \frac{1 - \exp[-\beta E_g']}{\Omega E_g'} \sum_{\alpha_V, \alpha_c} f(E_{\alpha}^{V})\{1 - f(E_{\alpha}^{c})\}(j_{\alpha}^{+})^* < \widetilde{F}_{\alpha}(\omega) >_p,$$

$$\widetilde{F}_\alpha(\omega) = \lim_{\eta\to 0+} \int_0^\infty dt \exp[-i\omega t - \eta t](< \alpha_c \mid j^+(t) \mid \alpha_V >), \tag{2.19}$$

which is equivalent, respectively, to eqs. (3.15) and (3.16) in ref.([24]). Here $E_g' = E_\alpha^c - E_\alpha^V$, $f(E)$ stands for the Fermi distribution function, and $< \ldots >_p$ denotes the average over the phonon distribution.

3. Line shape function.

Let us define two projection operators P_α and P_α' by ([46])

$$P_\alpha B = \frac{(A_\alpha, B)}{(A_\alpha, j^+)} j^+, \tag{3.1}$$

$$P_\alpha' B = \frac{(B, j^+)}{(A_\alpha, j^+)} A_\alpha, \tag{3.2}$$

where

$$(A, B) \equiv \mathrm{tr}(AB) \tag{3.3}$$

for two operators A and B, tr representing the trace in the single-electron expression, and $A_\alpha = a_{\alpha_V}^+ a_{\alpha_c}$ is an operator satisfying

$$(A_\alpha, B) = < \alpha_V \mid A_\alpha \mid \alpha_c >< \alpha_c \mid B \mid \alpha_V > . \tag{3.4}$$

After some simple manipulations using the projection operators (see eq. (3.10) through eq. (3.26) in ref. ([44])), we obtain from eq. (2.19)

$$\widetilde{F}_\alpha(\omega) = \frac{(A_\alpha, j^+)}{i(\omega^- - \omega_\alpha) + \widetilde{\Gamma}_\alpha(\omega)}, \tag{3.5}$$

where $\omega^- \equiv \omega - i\eta$, $\omega_\alpha = (E^c_\alpha - E^V_\alpha) + < \alpha_c \mid V \mid \alpha_c > - < \alpha_V \mid V \mid \alpha_V >$ and $\widetilde{\Gamma}_\alpha(\omega)$ is the Fourier-Laplace transform of

$$\Gamma_\alpha(t) = \frac{(Q_\alpha, R_\alpha(t))}{(A_\alpha, j^+)}. \tag{3.6}$$

Here

$$Q_\alpha = (1 - P'_\alpha) i L A_\alpha, \tag{3.7a}$$

$$Q_\alpha = i(1 - P'_\alpha)[V, A_\alpha], \tag{3.7b}$$

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

$$R_\alpha = i(1 - P_\alpha)Lj^+, \tag{3.9}$$

$$L \equiv L_0 + L_p + L_1, \tag{3.10}$$

L_0, L_p and L_1 being, respectively, the Liouville opertors corresponding to h_0, H_p and V. $[A, B]$ is the commutator of operators A and B.

We see from eqs. (2.18) and (3.5) that $\widetilde{\Gamma}_\alpha(\omega)$ gives information about line width and frequency shift. Thus we will call $\widetilde{\Gamma}_\alpha(\omega)$ the line shape function for the optical transition between the states $\mid \alpha_V >$ and $\mid \alpha_c >$. Since $\widetilde{\Gamma}_\alpha(\omega)$ in eq. (3.5) can be obtained via $(Q_\alpha, R_\alpha(t),)$ substituting eqs. (3.7b) and (3.8) into the numerator of eq. (3.6) and considering the perturbation only up to the second order in V, we have

$$(3.11) \qquad (Q_x, R_x(t)) = \Big(i[V, A_x], i(1-P_x)\Big\{[V, j^\dagger] + [it(h_0+H_p), [V, j^\dagger]] + \frac{1}{2}[it(h_0+H_p), [it(h_0+H_p), [V, j^\dagger]]] + \dots\Big\}\Big)$$

$$\begin{aligned}
&\simeq -\{(VA_x, Vj^\dagger) - (VA_x, j^\dagger V) - (A_xV, Vj^\dagger) + (A_xV, j^\dagger V) \\
&- (VA_x, P_xVj^\dagger) + (VA_x, P_xj^\dagger V) + (A_xV, P_xVj^\dagger) - (A_xV, P_xj^\dagger V)\} \\
&- it\{(VA_x, h_0Vj^\dagger) - (VA_x, h_0j^\dagger V) - (VA_x, Vj^\dagger h_0) + (VA_x, j^\dagger Vh_0) \\
&- (A_xV, h_0Vj^\dagger) + (A_xV, h_0j^\dagger V) + (A_xV, Vj^\dagger h_0) - (A_xV, j^\dagger Vh_0) \\
&- (VA_x, P_xh_0Vj^\dagger) + (VA_x, P_xh_0j^\dagger V) + (VA_x, P_xVj^\dagger h_0) - (VA_x, P_xj^\dagger Vh_0) \\
&+ (A_xV, P_xh_0Vj^\dagger) - (A_xV, P_xh_0j^\dagger V) - (A_xV, P_xVj^\dagger h_0) - (A_xV, P_xj^\dagger Vh_0) \\
&+ (VA_x, H_pVj^\dagger) - (VA_x, H_pj^\dagger V) - (VA_x, Vj^\dagger H_p) + (VA_x, j^\dagger VH_p) \\
&- (A_xV, H_pVj^\dagger) + (A_xV, H_pj^\dagger V) + (A_xV, Vj^\dagger H_p) - (A_xV, j^\dagger VH_p) \\
&- (VA_x, P_xH_pVj^\dagger) + (VA_x, P_xH_pj^\dagger V) + (VA_x, P_xVj^\dagger H_p) - (VA_x, P_xj^\dagger VH_p) \\
&+ (A_xV, P_xH_pVj^\dagger) - (A_xV, P_xH_pj^\dagger V) - (A_xV, P_xVj^\dagger H_p) + (A_xV, P_xj^\dagger VH_p)\} - \frac{1}{2}(it)^2 \\
&\cdot\{(VA_x, h_0h_0Vj^\dagger) - (VA_x, h_0h_0j^\dagger V) + (VA_x, h_0H_pVj^\dagger) - (VA_x, h_0H_pj^\dagger V) \\
&- (VA_x, h_0Vj^\dagger h_0) - (VA_x, h_0Vj^\dagger H_p) + (VA_x, h_0j^\dagger Vh_0) + (VA_x, h_0j^\dagger VH_p) \\
&+ (VA_x, H_ph_0Vj^\dagger) - (VA_x, H_ph_0j^\dagger V) + (VA_x, H_pH_pVj^\dagger) - (VA_x, H_pH_pj^\dagger V) \\
&- (VA_x, H_pVj^\dagger h_0) - (VA_x, H_pVj^\dagger H_p) + (VA_x, H_pj^\dagger Vh_0) + (VA_x, H_pj^\dagger VH_p) \\
&- (VA_x, h_0Vj^\dagger h_0) + (VA_x, h_0j^\dagger Vh_0) - (VA_x, H_pVj^\dagger h_0) + (VA_x, H_pj^\dagger Vh_0) \\
&+ (VA_x, Vj^\dagger h_0h_0) + (VA_x, Vj^\dagger H_ph_0) - (VA_x, j^\dagger Vh_0h_0) - (VA_x, j^\dagger VH_ph_0) \\
&- (VA_x, h_0Vj^\dagger H_p) + (VA_x, h_0j^\dagger VH_p) - (VA_x, H_pVj^\dagger H_p) + (VA_x, H_pj^\dagger VH_p) \\
&+ (VA_x, Vj^\dagger h_0H_p) + (VA_x, Vj^\dagger H_pH_p) - (VA_x, j^\dagger Vh_0H_p) - (VA_x, j^\dagger VH_pH_p) \\
&- (VA_x, P_xh_0h_0Vj^\dagger) + (VA_x, P_xh_0h_0j^\dagger V) - (VA_x, P_xh_0H_pVj^\dagger) + (VA_x, P_xh_0H_pj^\dagger V) \\
&+ (VA_x, P_xh_0Vj^\dagger h_0) + (VA_x, P_xh_0Vj^\dagger H_p) - (VA_x, P_xh_0j^\dagger Vh_0) - (VA_x, P_xh_0j^\dagger VH_p) \\
&- (VA_x, P_xH_ph_0Vj^\dagger) + (VA_x, P_xH_ph_0j^\dagger V) - (VA_x, P_xH_pH_pVj^\dagger) + (VA_x, P_xH_pH_pj^\dagger V) \\
&+ (VA_x, P_xH_pVj^\dagger h_0) + (VA_x, P_xH_pVj^\dagger H_p) - (VA_x, P_xH_pj^\dagger Vh_0) - (VA_x, P_xH_pj^\dagger VH_p)
\end{aligned}$$

$$
\begin{aligned}
&+(VA_z,\ P_z h_0 V j^{\dagger} h_0) - (VA_z,\ P_z h_0 j^{\dagger} V h_0) + (VA_z,\ P_z H_p V j^{\dagger} h_0) - (VA_z,\ P_z H_p j^{\dagger} V h_0) \\
&- (VA_z,\ P_z V j^{\dagger} h_0 h_0) - (VA_z,\ P_z V j^{\dagger} H_p h_0) + (VA_z,\ P_z j^{\dagger} V h_0 h_0) + (VA_z,\ P_z j^{\dagger} V H_p h_0) \\
&+ (VA_z,\ P_z h_0 V j^{\dagger} H_p) - (VA_z,\ P_z h_0 j^{\dagger} V H_p) + (VA_z,\ P_z H_p V j^{\dagger} H_p) - (VA_z,\ P_z H_p j^{\dagger} V H_p) \\
&- (VA_z,\ P_z V j^{\dagger} h_0 H_p) - (VA_z,\ P_z V j^{\dagger} H_p H_p) + (VA_z,\ P_z j^{\dagger} V h_0 H_p) + (VA_z,\ P_z j^{\dagger} V H_p H_p) \\
&- (A_z V,\ h_0 h_0 V j^{\dagger}) + (A_z V,\ h_0 h_0 j^{\dagger} V) - (A_z V,\ h_0 H_p V j^{\dagger}) + (A_z V,\ h_0 H_p j^{\dagger} V) \\
&+ (A_z V,\ h_0 V j^{\dagger} h_0) + (A_z V,\ h_0 V j^{\dagger} H_p) - (A_z V,\ h_0 j^{\dagger} V h_0) - (A_z V,\ h_0 j^{\dagger} V H_p) \\
&- (A_z V,\ H_p h_0 V j^{\dagger}) + (A_z V,\ H_p h_0 j^{\dagger} V) - (A_z V,\ H_p H_p V j^{\dagger}) + (A_z V,\ H_p H_p j^{\dagger} V) \\
&+ (A_z V,\ H_p V j^{\dagger} h_0) + (A_z V,\ H_p V j^{\dagger} \mathrm{H}_p) - (A_z V,\ H_p j^{\dagger} V h_0) - (A_z V,\ H_p j^{\dagger} V H_p) \\
&+ (A_z V,\ h_0 V j^{\dagger} h_0) - (A_z V,\ h_0 j^{\dagger} V h_0) + (A_z V,\ H_p V j^{\dagger} h_0) - (A_z V,\ H_p j^{\dagger} V h_0) \\
&- (A_z V,\ V j^{\dagger} h_0 h_0) - (A_z V,\ V j^{\dagger} H_p h_0) + (A_z V,\ j^{\dagger} V h_0 h_0) + (A_z V,\ j^{\dagger} V H_p h_0) \\
&+ (A_z V,\ h_0 V j^{\dagger} H_p) - (A_z V,\ h_0 j^{\dagger} V H_p) + (A_z V,\ H_p V j^{\dagger} H_p) - (A_z V,\ H_p j^{\dagger} V H_p) \\
&- (A_z V,\ V j^{\dagger} h_0 H_p) - (A_z V,\ V j^{\dagger} H_p H_p) + (A_z V,\ j^{\dagger} V h_0 H_p) + (A_z V,\ j^{\dagger} V H_p H_p) \\
&+ (A_z V,\ P_z h_0 h_0 V j^{\dagger}) - (A_z V,\ P_z h_0 h_0 j^{\dagger} V) + (A_z V,\ P_z h_0 H_p V j^{\dagger}) - (A_z V,\ P_z h_0 H_p j^{\dagger} V) \\
&- (A_z V,\ P_z h_0 V j^{\dagger} h_0) - (A_z V,\ P_z h_0 V j^{\dagger} H_p) + (A_z V,\ P_z h_0 j^{\dagger} V h_0) + (A_z V,\ P_z h_0 j^{\dagger} V H_p) \\
&+ (A_z V,\ P_z H_p h_0 V j^{\dagger}) - (A_z V,\ P_z H_p h_0 j^{\dagger} V) + (A_z V,\ P_z H_p H_p V j^{\dagger}) - (A_z V,\ P_z H_p H_p j^{\dagger} V) \\
&- (A_z V,\ P_z H_p V j^{\dagger} h_0) - (A_z V,\ P_z H_p V j^{\dagger} H_p) + (A_z V,\ P_z H_p j^{\dagger} V h_0) + (A_z V,\ P_z H_p j^{\dagger} V H_p) \\
&- (A_z V,\ P_z h_0 V j^{\dagger} h_0) + (A_z V,\ P_z h_0 j^{\dagger} V h_0) - (A_z V,\ P_z H_p V j^{\dagger} h_0) + (A_z V,\ P_z H_p j^{\dagger} V h_0) \\
&+ (A_z V,\ P_z V j^{\dagger} h_0 h_0) + (A_z V,\ P_z V j^{\dagger} H_p h_0) - (A_z V,\ P_z j^{\dagger} V h_0 h_0) - (A_z V,\ P_z j^{\dagger} V H_p h_0) \\
&- (A_z V,\ P_z h_0 V j^{\dagger} H_p) + (A_z V,\ P_z h_0 j^{\dagger} V H_p) - (A_z V,\ P_z H_p V j^{\dagger} H_p) + (A_z V,\ P_z H_p j^{\dagger} V H_p) \\
&+ (A_z V,\ P_z V j^{\dagger} h_0 H_p) + (A_z V,\ P_z V j^{\dagger} H_p H_p) - (A_z V,\ P_z j^{\dagger} V h_0 H_p) - (A_z V,\ P_z j^{\dagger} V H_p H_p) \} \ .
\end{aligned}
$$

The terms of higer order in time may not be considered since these 168 terms are enough for our formal expression. It is convenient to divide the 168 terms in eq. (3.11) into four parts. By doing so we will calculate $(Q_\alpha, R_\alpha(t))$,

$\Gamma_\alpha(t)$ and $\widetilde{\Gamma}_\alpha(\omega)$ in the next section.

4. Calculation in the two coupling schemes.

In carrying out the calculation with respect to the electron states and the phonon averaging, we may adopt the following two ways.

4.1. MWC. If the electron state calculation is performed prior to the phonon averaging, we may use the trace property

$$
\begin{aligned}
(4.1) \qquad & < \mathrm{tr}(BA_\alpha C) >_p = < \mathrm{tr}(A_\alpha CB) >_p \\
& = < \alpha_V \mid A_\alpha \mid \alpha_c > \sum_\beta (< \alpha_c \mid C \mid \beta_V >< \beta_V \mid B \mid \alpha_V >)_p
\end{aligned}
$$

for arbitrary operators B and C.

Part I of eq. (3.11) is calculated in this scheme as

$$
\begin{aligned}
(4.2) \qquad 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}) + (41\mathrm{st} + 73\mathrm{rd}) + \{(43\mathrm{rd} + 49\mathrm{th}) + (75\mathrm{th} + 81\mathrm{st})\} \\
& + \{(46\mathrm{th} + 65\mathrm{th}) + (78\mathrm{th} + 97\mathrm{th})\} + (51\mathrm{st} + 83\mathrm{rd}) + (70\mathrm{th} + 102\mathrm{nd}) \\
& + \{(54\mathrm{th} + 67\mathrm{th}) + (86\mathrm{th} + 99\mathrm{th})\} + (61\mathrm{st} + 93\mathrm{rd}) + \{(62\mathrm{nd} + 69\mathrm{th}) \\
& + (94\mathrm{th} + 101\mathrm{st})\} + \{(53\mathrm{rd} + 59\mathrm{th}) + (85\mathrm{th} + 91\mathrm{st})\} \\
& \qquad + \{(45\mathrm{th} + 57\mathrm{th}) + (77\mathrm{th} + 89\mathrm{th})\} \\
= & - \langle \alpha_v | A_\alpha | \alpha_c \rangle [\{ \sum_\beta j_\beta^\dagger \langle \alpha_c | V | \beta_c \rangle \langle \beta_v | V | \alpha_v \rangle - j_\alpha^\dagger \langle \alpha_c | V | \alpha_c \rangle \langle \alpha_v | V | \alpha_v \rangle \} \\
& + it \{ \sum_\beta j_\beta^\dagger E_\alpha^c \langle \alpha_c | V | \beta_c \rangle \langle \beta_v | V | \alpha_v \rangle - j_\alpha^\dagger E_\alpha^c \langle \alpha_c | V | \alpha_c \rangle \langle \alpha_v | V | \alpha_v \rangle \\
& - \sum_\beta j_\beta^\dagger E_\beta^v \langle \alpha_c | V | \beta_c \rangle \langle \beta_v | V | \alpha_v \rangle + j_\alpha^\dagger E_\alpha^v \langle \alpha_c | V | \alpha_c \rangle \langle \alpha_v | V | \alpha_v \rangle \\
& + \sum_\beta j_\beta^\dagger H_p \langle \alpha_c | V | \beta_c \rangle \langle \beta_v | V | \alpha_v \rangle - j_\alpha^\dagger H_p \langle \alpha_c | V | \alpha_c \rangle \langle \alpha_v | V | \alpha_v \rangle \\
& - \sum_\beta j_\beta^\dagger \langle \alpha_c | V | \beta_c \rangle H_p \langle \beta_v | V | \alpha_v \rangle + j_\alpha^\dagger \langle \alpha_c | V | \alpha_c \rangle H_p \langle \alpha_v | V | \alpha_v \rangle \} \\
& + (it)^2 \{ \sum_\beta j_\beta^\dagger (E_\alpha^c)^2 \langle \alpha_c | V | \beta_c \rangle \langle \beta_v | V | \alpha_v \rangle - j_\alpha^\dagger (E_\alpha^c)^2 \langle \alpha_c | V | \alpha_c \rangle \langle \alpha_v | V | \alpha_v \rangle
\end{aligned}
$$

$$+\sum_{\beta} 2j_{\beta}^{+} E_{\alpha}^{c} H_{p} \langle \alpha_{c} |V| \beta_{c} \rangle \langle \beta_{v} |V| \alpha_{v} \rangle - 2j_{\alpha}^{+} E_{\alpha}^{c} H_{p} \langle \alpha_{c} |V| \alpha_{c} \rangle \langle \alpha_{v} |V| \alpha_{v} \rangle$$

$$-\sum_{\beta} 2j_{\beta}^{+} E_{\alpha}^{c} \langle \alpha_{c} |V| \beta_{c} \rangle H_{p} \langle \beta_{v} |V| \alpha_{v} \rangle + 2j_{\alpha}^{+} E_{\alpha}^{c} \langle \alpha_{c} |V| \alpha_{c} \rangle H_{p} \langle \alpha_{v} |V| \alpha_{v} \rangle$$

$$+\sum_{\beta} j_{\beta}^{+} H_{p} H_{p} \langle \alpha_{c} |V| \beta_{c} \rangle \langle \beta_{v} |V| \alpha_{v} \rangle - j_{\alpha}^{+} H_{p} H_{p} \langle \alpha_{c} |V| \alpha_{c} \rangle \langle \alpha_{v} |V| \alpha_{v} \rangle$$

$$+\sum_{\beta} j_{\beta}^{+} \langle \alpha_{c} |V| \beta_{c} \rangle H_{p} H_{p} \langle \beta_{v} |V| \alpha_{v} \rangle - j_{\alpha}^{+} \langle \alpha_{c} |V| \alpha_{c} \rangle H_{p} H_{p} \langle \alpha_{v} |V| \alpha_{v} \rangle$$

$$-\sum_{\beta} 2j_{\beta}^{+} H_{p} \langle \alpha_{c} |V| \beta_{c} \rangle H_{p} \langle \beta_{v} |V| \alpha_{v} \rangle + 2j_{\alpha}^{+} H_{p} \langle \alpha_{c} |V| \alpha_{c} \rangle H_{p} \langle \alpha_{v} |V| \alpha_{v} \rangle$$

$$+\sum_{\beta} j_{\beta}^{+} (E_{\beta}^{v})^{2} \langle \alpha_{c} |V| \beta_{c} \rangle \langle \beta_{v} |V| \alpha_{v} \rangle - j_{\alpha}^{+} (E_{\alpha}^{v})^{2} \langle \alpha_{c} |V| \alpha_{c} \rangle \langle \alpha_{v} |V| \alpha_{v} \rangle$$

$$+\sum_{\beta} 2j_{\beta}^{+} E_{\beta}^{v} \langle \alpha_{c} |V| \beta_{c} \rangle H_{p} \langle \beta_{v} |V| \alpha_{v} \rangle - 2j_{\alpha}^{+} E_{\alpha}^{v} \langle \alpha_{c} |V| \alpha_{c} \rangle H_{p} \langle \alpha_{v} |V| \alpha_{v} \rangle$$

$$-\sum_{\beta} 2j_{\beta}^{+} E_{\beta}^{v} H_{p} \langle \alpha_{c} |V| \beta_{c} \rangle \langle \beta_{v} |V| \alpha_{v} \rangle + 2j_{\alpha}^{+} E_{\alpha}^{v} H_{p} \langle \alpha_{c} |V| \alpha_{c} \rangle \langle \alpha_{v} |V| \alpha_{v} \rangle$$

$$-\sum_{\beta} j_{\beta}^{+} 2E_{\alpha}^{c} E_{\beta}^{v} \langle \alpha_{c} |V| \beta_{c} \rangle \langle \beta_{v} |V| \alpha_{v} \rangle + 2j_{\alpha}^{+} E_{\alpha}^{c} E_{\alpha}^{v} \langle \alpha_{c} |V| \alpha_{c} \rangle \langle \alpha_{v} |V| \alpha_{v} \rangle \}] \,.$$

Here we see that the terms corresponding to $\beta = \alpha$ are excluded in the summations. Averaging over the phonon distribution can be carried out by virtue of

$$(4.3) \qquad < b_q^{+} b_{q'} >_q = n_q \delta_{qq'},$$

$$(4.4) \qquad < b_q b_{q'}^{+} >_q = (1 + n_q) \delta_{qq'},$$

n_q being the Planck distribution function. As a result, we have

$$(4.5) \qquad < P(I) >_p$$

$$= - < \alpha_V | A_\alpha | \alpha_c > \sum_{\beta(\neq\alpha)} \sum_q j_\beta^{+} [(1 + n_q) < \alpha_c | \gamma_q | \beta_c >$$

$$< \beta_V | \gamma_q^{+} | \alpha_V > \exp[it(E_\alpha^c - E_\beta^V - \omega_q)]$$

$$+ n_q < \alpha_c | \gamma_q^{+} | \beta_c >< \beta_V | \gamma_q | \alpha_V > \exp[it(E_\alpha^c - E_\beta^V + \omega_q)]],$$

where we have used the formal expression that $1 + itE_\alpha + (itE_\alpha)^2/2! = \exp[itE_\alpha]$. Similarly we have

(4.6)
$$\begin{aligned}\langle P(\mathrm{II})\rangle_{\mathrm{p}} = \langle &(2\mathrm{nd}+6\mathrm{th}) + (10\mathrm{th}+18\mathrm{th}) + (12\mathrm{th}+20\mathrm{th}) + (26\mathrm{th}+34\mathrm{th}) \\ &+ (28\mathrm{th}+36\mathrm{th}) + (42\mathrm{nd}+74\mathrm{th}) + \{(44\mathrm{th}+40\mathrm{th}+76\mathrm{th}+82\mathrm{nd}) \\ &+ (48\mathrm{th}+66\mathrm{th}+80\mathrm{th}+90\mathrm{th})\} + \{(52\mathrm{nd}+84\mathrm{th}) + (72\mathrm{nd}+104\mathrm{th}) \\ &+ (56\mathrm{th}+68\mathrm{th}+88\mathrm{th}+100\mathrm{th})\} + (63\mathrm{rd}+95\mathrm{th}) \\ &+ \{(64\mathrm{th}+71\mathrm{th}+106\mathrm{th}+103\mathrm{th}) + (55\mathrm{th}+60\mathrm{th}+87\mathrm{th}+92\mathrm{nd})\} \\ &\qquad + (47\mathrm{th}+58\mathrm{th}+79\mathrm{th}+90\mathrm{th})\rangle_{\mathrm{p}} \\ = \langle\alpha_{\mathrm{v}}|A_\alpha|\alpha_{\mathrm{c}}\rangle j_\alpha^{\dagger} &\sum_{\beta(\neq\alpha)}\sum_q [(1+n_q)\langle\alpha_{\mathrm{v}}|\gamma_q|\beta_{\mathrm{v}}\rangle\langle\beta_{\mathrm{v}}|\gamma_q^{\dagger}|\alpha_{\mathrm{v}}\rangle \exp[it(E_\alpha^{\mathrm{c}} - E_\beta^{\mathrm{v}} - \omega_q)] \\ &\qquad + n_q\langle\alpha_{\mathrm{v}}|\gamma_q^{\dagger}|\beta_{\mathrm{v}}\rangle\langle\beta_{\mathrm{v}}|\gamma_q|\alpha_{\mathrm{v}}\rangle \exp[it(E_\alpha^{\mathrm{c}} - E_\beta^{\mathrm{v}} + \omega_q)]]\,,\end{aligned}$$

(4.7)
$$\begin{aligned}\langle P(\mathrm{III})\rangle_{\mathrm{p}} = \langle &(3\mathrm{rd}+7\mathrm{th}) + (13\mathrm{th}+21\mathrm{st}) + (15\mathrm{th}+23\mathrm{rd}) + (29\mathrm{th}+37\mathrm{th}) \\ &+ (31\mathrm{st}+39\mathrm{th}) + (105\mathrm{th}+137\mathrm{th}) + \{(107\mathrm{th}+113\mathrm{th}+139\mathrm{th}+145\mathrm{th}) \\ &+ (110\mathrm{th}+129\mathrm{th}+142\mathrm{nd}+161\mathrm{st})\} + \{(115\mathrm{th}+147\mathrm{th}) + (134\mathrm{th}+166\mathrm{th}) \\ &+ (118\mathrm{th}+131\mathrm{st}+150\mathrm{th}+163\mathrm{rd})\} + (125\mathrm{th}+157\mathrm{th}) \\ &+ \{(126\mathrm{th}+133\mathrm{rd}+158\mathrm{th}+165\mathrm{th}) + (117\mathrm{th}+123\mathrm{rd}+149\mathrm{th}+155\mathrm{th})\} \\ &\qquad + (109\mathrm{th}+121\mathrm{st}+141\mathrm{st}+153\mathrm{rd})\rangle_{\mathrm{p}} \\ = \langle\alpha_{\mathrm{v}}|A_\alpha|\alpha_{\mathrm{c}}\rangle j_\alpha^{\dagger} &\sum_{\beta(\neq\alpha)}\sum_q [(1+n_q)\langle\alpha_{\mathrm{c}}|\gamma_q|\beta_{\mathrm{c}}\rangle\langle\beta_{\mathrm{c}}|\gamma_q^{\dagger}|\alpha_{\mathrm{c}}\rangle \exp[it(E_\beta^{\mathrm{c}} - E_\alpha^{\mathrm{v}} + \omega_q)] \\ &\qquad + n_q\langle\alpha_{\mathrm{c}}|\gamma_q^{\dagger}|\beta_{\mathrm{c}}\rangle\langle\beta_{\mathrm{c}}|\gamma_q|\alpha_{\mathrm{c}}\rangle \exp[it(E_\beta^{\mathrm{c}} - E_\alpha^{\mathrm{v}} - \omega_q)]]\,,\end{aligned}$$

(4.8)
$$\begin{aligned}\langle P(\mathrm{IV})\rangle_{\mathrm{p}} = \langle &(4\mathrm{th}+8\mathrm{th}) + (14\mathrm{th}+22\mathrm{nd}) + (16\mathrm{th}+24\mathrm{th}) + (30\mathrm{th}+38\mathrm{th}) \\ &+ (32\mathrm{nd}+40\mathrm{th}) + (106\mathrm{th}+138\mathrm{th}) + \{(108\mathrm{th}+114\mathrm{th}+140\mathrm{th}+146\mathrm{th}) \\ &+ (112\mathrm{th}+130\mathrm{th}+144\mathrm{th}+162\mathrm{nd})\} + \{(116\mathrm{th}+159\mathrm{th}) + (136\mathrm{th}+168\mathrm{th}) \\ &+ (120\mathrm{th}+132\mathrm{nd}+152\mathrm{nd}+164\mathrm{th})\} + (127\mathrm{th}+159\mathrm{th}) \\ &+ \{(128\mathrm{th}+135\mathrm{th}+160\mathrm{th}+167\mathrm{th}) + (119\mathrm{th}+124\mathrm{th}+151\mathrm{st}+156\mathrm{th})\} \\ &\qquad + (111\mathrm{th}+122\mathrm{nd}+143\mathrm{rd}+154\mathrm{th})\rangle_{\mathrm{p}} \\ = -\langle\alpha_{\mathrm{v}}|A_\alpha|\alpha_{\mathrm{c}}\rangle &\sum_{\beta(\neq\alpha)}\sum_q j_\beta^{\dagger}[(1+n_q)\langle\alpha_{\mathrm{c}}|\gamma_q|\beta_{\mathrm{c}}\rangle\langle\beta_{\mathrm{v}}|\gamma_q^{\dagger}|\alpha_{\mathrm{v}}\rangle \exp[it(E_\beta^{\mathrm{c}} - E_\alpha^{\mathrm{v}} + \omega_q)] \\ &\qquad + n_q\langle\alpha_{\mathrm{c}}|\gamma_q^{\dagger}|\beta_{\mathrm{c}}\rangle\langle\beta_{\mathrm{v}}|\gamma_q|\alpha_{\mathrm{v}}\rangle \exp[it(E_\beta^{\mathrm{c}} - E_\alpha^{\mathrm{v}} - \omega_q)]]\,.\end{aligned}$$

We now collect all the parts and divide them by $(A_\alpha, j^+) \equiv < \alpha_V | A_\alpha | \alpha_c >$ j_α^+ to get the average of $\Gamma_\alpha(t)$ over the phonon distribution. Consequently $\widetilde{\Gamma}_\alpha(\omega)$, the Fourier-Laplace transform of $\Gamma_\alpha(t)$, is obtained as

$$(4.9) \qquad [i\tilde{\Gamma}_\alpha(\omega)]_{\rm MWC} = \sum_q \sum_{\beta(\neq\alpha)} (1+n_q) \Bigg[\frac{\langle \alpha_c | \gamma_q | \beta_c \rangle \{ \langle \beta_c | \gamma_q^\dagger | \alpha_c \rangle - \langle \beta_v | \gamma_q^\dagger | \alpha_v \rangle j_\beta^+ / j_\alpha^+ \}}{\omega - E_\beta^c + E_\alpha^v - \omega_q - i\eta}$$

$$+ \frac{\{ \langle \alpha_v | \gamma_q | \beta_v \rangle - \langle \alpha_c | \gamma_q | \beta_c \rangle j_\beta^+ / j_\alpha^+ \} \langle \beta_v | \gamma_q^\dagger | \alpha_v \rangle}{\omega - E_\alpha^c + E_\beta^v + \omega_q - i\eta} \Bigg]$$

$$+ \sum_q \sum_{\beta(\neq\alpha)} n_q \Bigg[\frac{\langle \alpha_c | \gamma_q^\dagger | \beta_c \rangle \{ \langle \beta_c | \gamma_q | \alpha_c \rangle - \langle \beta_v | \gamma_q | \alpha_v \rangle j_\beta^+ / j_\alpha^+ \}}{\omega - E_\beta^c + E_\alpha^v + \omega_q - i\eta}$$

$$+ \frac{\{ \langle \alpha_v | \gamma_q^\dagger | \beta_v \rangle - \langle \alpha_c | \gamma_q^\dagger | \beta_c \rangle j_\beta^+ / j_\alpha^+ \} \langle \beta_v | \gamma_q | \alpha_v \rangle}{\omega - E_\alpha^c + E_\beta^v - \omega_q - i\eta} \Bigg],$$

where $\eta \to 0^+$. This is identical with Choi and Chung's MWC scheme result (see eq. (18) in ref.[23]. The parts with $n_q + 1$ and n_q are known as emission and absorption terms, respertively. But this does not imply that each part plays a major role only in the emission or absorption of a phonon. In other words, the two parts should be combined in yielding the line shape. We should also note both positive and negative signs appear on ω_q in the energy denominators of each part.

4.2. EWC. On the other hand, if the phonon averaging is performed prior to the electron state calculation, we have

$$(4.10) \quad < {\rm tr}(B A_\alpha C) >_p = < \alpha_V | A_\alpha \mid \alpha_c > \sum_\beta << \beta_V \mid B \mid \alpha_V >< \alpha_c \mid C \mid \beta_V >>_p .$$

In this scheme we obtain

$$
\begin{aligned}
(4.11)\qquad [i\bar{\Gamma}_{\alpha}(\omega)]_{\mathrm{EWC}} = \sum_{q}\sum_{\beta(\neq\alpha)}(1+n_q)\Bigg[& \frac{\langle \alpha_c|\gamma_q|\beta_c\rangle\{\langle\beta_c|\gamma_q^{\dagger}|\alpha_c\rangle - \langle\beta_v|\gamma_q^{\dagger}|\alpha_v\rangle j_{\beta}^{\dagger}/j_{\alpha}^{\dagger}\}}{\omega - E_{\beta}^{c} + E_{\alpha}^{v} - \omega_q - i\eta} \\
& + \frac{\{\langle\alpha_v|\gamma_q^{\dagger}|\beta_v\rangle - \langle\alpha_c|\gamma_q^{\dagger}|\beta_c\rangle j_{\beta}^{\dagger}/j_{\alpha}^{\dagger}\}\langle\beta_v|\gamma_q|\alpha_v\rangle}{\omega - E_{\alpha}^{c} + E_{\beta}^{v} - \omega_q - i\eta}\Bigg] \\
+\sum_{q}\sum_{\beta(\neq\alpha)} n_q \Bigg[& \frac{\langle\alpha_c|\gamma_q^{\dagger}|\beta_c\rangle\{\langle\beta_c|\gamma_q|\alpha_c\rangle - \langle\beta_v|\gamma_q|\alpha_v\rangle j_{\beta}^{\dagger}/j_{\alpha}^{\dagger}\}}{\omega - E_{\beta}^{c} + E_{\alpha}^{v} + \omega_q - i\eta} \\
& + \frac{\{\langle\alpha_v|\gamma_q|\beta_v\rangle - \langle\alpha_c|\gamma_q|\beta_c\rangle j_{\beta}^{\dagger}/j_{\alpha}^{\dagger}\}\langle\beta_v|\gamma_q^{\dagger}|\alpha_v\rangle}{\omega - E_{\alpha}^{c} + E_{\beta}^{v} + \omega_q - i\eta}\Bigg],
\end{aligned}
$$

where $\eta \to 0^{+}$. This is identical with Choi and Chung's EWC scheme result(see eq. (19) in ref.[(23)]. The energy denominators of the emision and absorption parts contain ω_q with the negative and positive signs, respetively. This point is the main difference between the two–scheme results.

5. Discussion

So far we have derived two different functions for the phonon-induced direct interband transition line shapes. These are identical with the corresponding formulae of choi and Chung introduced in ref.[(23)]. The results of MWC and EWC were based on eqs. (4.1) and (4.10). These two ways gave different values since $< b_q^{+} b_q >_p = n_q$ and $< b_q b_q^{+} >_p = 1 + n_q$. It should be noted that the method adopted in this paper and that used in ref.([(23)] are apparently different, but yield identical results.

In deriving the line shape functions we have made some approximations. Furthermore the linewidth and frequency shift depend on the arbitrary infinitesimal η. In order to make the present theory better, these points should be improved. This work is to justify that Mori's method is a good one.

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