Progress of Theoretical Physics, Vol. 77, No. 4, April 1987

Theory of Cyclotron Resonance Lineshape Revisited

Sam Nyung YI, Ok Hee CHUNG and Sang Don CHOI

Department of Physics, Kyungpook National University, Taegu

(Received July 16, 1986)

Validity of the exponential expression in the theory of cyclotron resonance lineshapes for electron-phonon systems reported by the present group [Prog. Theor. Phys. **72** (1984), 429] is discussed. The expansion up to the second order in time is justified.

§ 1. Introduction

Quite many theories have been reported so far on cyclotron resonance lineshapes (CRLS) for electron-phonon systems in solids.[1)~12)] As pointed out in Ref. 12), the theories may be classified into several categories. Among them combinations of the Kubo formalism[15)] and projection techniques, such as Mori's[14)] and Argyres and Sigel's,[13)] have called attention of the present authors.

In 1983 Choi and Chung presented a theory of CRLS by using Argyres and Sigel's technique. In deriving the lineshape formula, they introduced two calculation schemes called EWC and MWC schemes.

In 1984 Ryu and Choi[12)] obtained the EWC scheme result by the methods of Mori and Kawabata. However, the theory introduced has been followed by some critiques. Among them is validity of the exponential expansion adopted in deriving the lineshape formula. Of course, perfect proof of the validity should be investigated via the well-known expression

$$\sum_{n=0}^{\infty}(itE)^n/n!=\exp(itE)\,. \tag{1·1}$$

However, only the terms corresponding to $n=0$ and $n=1$ were contained in Ref. 12). In order to check the validity of the exponential expression up to $n=\infty$ in Eq. (1·1), the infinite amount of calculation will be required, which is actually impossible. Thus we will demonstrate only the terms up to $n=2$. Prior to examining the validity we will briefly summarize the work of Ryu and Choi. Here the unit system in which $\hbar=1$ is adopted.

The power absorption delivered for a circularly polarized microwave of frequency ω applied along the z-axis is proportional to the conductivity tensor, which is given by

$$\sigma_{+-}(\omega)=\frac{1-\exp(-\beta\omega_0)}{\omega_0\Omega}\sum_{\alpha}f(E_\alpha)(1-f(E_\alpha+\omega_0))j^-_{\alpha,\alpha+1}\frac{(A_\alpha, j^+)}{i(\omega-\omega_\alpha)+\tilde{\Gamma}_\alpha(\omega)} \tag{1·2}$$

for the system with a static magnetic field B applied in the z-direction. Here, Ω is 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, and $\beta=(k_B T)^{-1}$ for the temperature T. E_α is the energy eigenvalue corresponding to the eigenstate $|\alpha\rangle \equiv |N, \boldsymbol{k}\rangle$ in the parabolic-band approximation, where N is the Landau index and $\boldsymbol{k}$ is the electron wave vector. For the single electron current vector $\boldsymbol{j}$, $j^{\pm} \equiv j_x \pm i j_y$, and $j_\alpha{}^{+} \equiv j^{+}_{\alpha+1,\alpha} = \langle \alpha+1|j^{+}|\alpha\rangle$, where $|\alpha+1\rangle \equiv |N+1, \boldsymbol{k}\rangle$. ω_α is the characteristic frequency of the system in the state $|\alpha\rangle$ which is reduced to ω_0 for materials with good symmetricity [see Eq. (3·18) in Ref. 12)]. (A, B) is identical with trace (AB) and A_α is defined as $A_\alpha \equiv a_\alpha{}^{\dagger} a_{\alpha+1}$, $a_\alpha{}^{\dagger}(a_\alpha)$ being the creation (annihilation) operator corresponding to the state $|\alpha\rangle$. $\tilde{\Gamma}_\alpha(\omega)$ is the Fourier-Laplace transform(FLT) of the phonon average of

$$\Gamma_\alpha(t) \simeq \frac{1}{(A_\alpha, j^{+})}(i[V, A_\alpha], i(1-P_\alpha)\{[V, j^{+}] + [it(h_0+H_p), [V, j^{+}]] + \frac{1}{2}[it(h_0+H_p), [it(h_0+H_p), [V, j^{+}]]]\}), \tag{1·3}$$

which has been approximated to the second order in time t. Here $[A, B]$ is the commutator of operators A and B. P_α is the projection operator defined by

$$P_\alpha B = \frac{(A_\alpha, B)}{(A_\alpha, j^{+})} j^{+} \tag{1·4}$$

for arbitrary operator B. h_0 is the unperturbed single-electron Hamiltonian, and H_p and V are the phonon Hamiltonian and scattering potential respectively given by

$$H_p = \sum_q \omega_q b_q{}^{\dagger} b_q, \tag{1·5}$$

$$V = \sum_q (\gamma_q b_q + \gamma_q{}^{\dagger} b_q{}^{\dagger}) \tag{1·6}$$

for the phonon with energy ω_q and momentum $\boldsymbol{q}$, $b_q{}^{\dagger}(b_q)$ being the creation (annihilation) operator.

The zeroth and first order terms of the numerator in Eq. (1·3) can be calculated in four parts. After averaging over the phonon distribution by considering $\langle b_q{}^{\dagger} b_q\rangle_p = n_q$, n_q being the Planck distribution function, we have

$$\langle \mathrm{Part(I)}\rangle_p = -(A_\alpha)_{\alpha,\alpha+1} \sum_{\beta(\neq\alpha)} \sum_q j_\beta{}^{+}[(1+n_q)(\gamma_q)_{\beta\alpha}(\gamma_q{}^{\dagger})_{\alpha+1,\beta+1}\{1+it(E_{\alpha+1}-E_\beta+\omega_q)\} + n_q(\gamma_q{}^{\dagger})_{\beta\alpha}(\gamma_q)_{\alpha+1,\beta+1}\{1+it(E_{\alpha+1}-E_\beta-\omega_q)\}], \tag{1·7}$$

which is identical with the expression preceding Eq. (4·2) in Ref. 12). The other parts can be obtained in a similar manner:

$$\langle \mathrm{Part\ (II)}\rangle_p = (A_\alpha)_{\alpha,\alpha+1} j_\alpha{}^{+} \sum_{\beta(\neq\alpha)} \sum_q [(1+n_q)(\gamma_q)_{\beta\alpha}(\gamma_q{}^{\dagger})_{\alpha\beta}\{1+it(E_{\alpha+1}-E_\beta+\omega_q)\} + n_q(\gamma_q{}^{\dagger})_{\beta\alpha}(\gamma_q)_{\alpha\beta}\{1+it(E_{\alpha+1}-E_\beta-\omega_q)\}], \tag{1·8}$$

$$\langle \text{Part (III)} \rangle_p = (A_\alpha)_{\alpha,\alpha+1} j_\alpha{}^+$$

$$\times \sum_{\beta(\neq\alpha+1)} \sum_q [(1+n_q)(\gamma_q)_{\alpha+1,\beta}(\gamma_q{}^\dagger)_{\beta,\alpha+1}\{1+it(E_\beta - E_\alpha + \omega_q)\}$$

$$+ n_q(\gamma_q{}^\dagger)_{\alpha+1,\beta}(\gamma_q)_{\beta,\alpha+1}\{1+it(E_\beta - E_\alpha - \omega_q)\}] , \qquad (1\cdot 9)$$

$$\langle \text{Part (IV)} \rangle_p = -(A_\alpha)_{\alpha,\alpha+1}$$

$$\times \sum_{\beta(\neq\alpha+1)} \sum_q j_{\beta-1}^+ [(1+n_q)(\gamma_q)_{\alpha+1,\beta}(\gamma_q{}^\dagger)_{\beta-1,\alpha}\{1+it(E_\beta - E_\alpha + \omega_q)\}$$

$$+ n_q(\gamma_q{}^\dagger)_{\alpha+1,\beta}(\gamma_q)_{\beta-1,\alpha}\{1+it(E_\beta - E_\alpha - \omega_q)\}] . \qquad (1\cdot 10)$$

These terms are of zeroth and first order in time. So far we have summarized the work of Ryu and Choi. In the next section, we will calculate the second order terms to see whether the exponential expression may be used.

§ 2. Validity of the exponential expression revisited

The second order terms of the numerator in Eq. (1·3) is expanded as

$$-\frac{1}{2}(it)^2[([V, A_\alpha], [h_0+H_p, [h_0+H_p, [V, j^+]]])$$

$$-([V, A_\alpha], P_\alpha[h_0+H_p, [h_0+H_p, [V, j^+]]])] \qquad (2\cdot 1)$$

$$= -\frac{1}{2}(it)^2[(VA_\alpha, h_0h_0Vj^+) - (VA_\alpha, h_0h_0j^+V) + (VA_\alpha, h_0H_pVj^+)$$

$$-(VA_\alpha, h_0H_pj^+V) - (VA_\alpha, h_0Vj^+h_0) - (VA_\alpha, h_0Vj^+H_p) + (VA_\alpha, h_0j^+Vh_0)$$

$$+(VA_\alpha, h_0j^+VH_p) + (VA_\alpha, H_ph_0Vj^+) - (VA_\alpha, H_ph_0j^+V) + (VA_\alpha, H_pH_pVj^+)$$

$$-(VA_\alpha, H_pH_pj^+V) - (VA_\alpha, H_pVj^+h_0) - (VA_\alpha, H_pVj^+H_p) + (VA_\alpha, H_pj^+Vh_0)$$

$$+(VA_\alpha, H_pj^+VH_p) - (VA_\alpha, h_0Vj^+h_0) + (VA_\alpha, h_0j^+Vh_0) - (VA_\alpha, H_pVj^+h_0)$$

$$+(VA_\alpha, H_pj^+Vh_0) + (VA_\alpha, Vj^+h_0h_0) + (VA_\alpha, Vj^+H_ph_0) - (VA_\alpha, j^+Vh_0h_0)$$

$$-(VA_\alpha, j^+VH_ph_0) - (VA_\alpha, h_0Vj^+H_p) + (VA_\alpha, h_0j^+VH_p) - (VA_\alpha, H_pVj^+H_p)$$

$$+(VA_\alpha, H_pj^+VH_p) + (VA_\alpha, Vj^+h_0H_p) + (VA_\alpha, Vj^+H_pH_p) - (VA_\alpha, j^+Vh_0H_p)$$

$$-(VA_\alpha, j^+VH_pH_p) - (VA_\alpha, P_\alpha h_0h_0Vj^+) + (VA_\alpha, P_\alpha h_0h_0j^+V)$$

$$-(VA_\alpha, P_\alpha h_0H_pVj^+) + (VA_\alpha, P_\alpha h_0H_pj^+V) + (VA_\alpha, P_\alpha h_0Vj^+h_0)$$

$$+(VA_\alpha, P_\alpha h_0Vj^+H_p) - (VA_\alpha, P_\alpha h_0j^+Vh_0) - (VA_\alpha, P_\alpha h_0j^+VH_p)$$

$$-(VA_\alpha, P_\alpha H_ph_0Vj^+) + (VA_\alpha, P_\alpha H_ph_0j^+V) - (VA_\alpha, P_\alpha H_pH_pVj^+)$$

$$+(VA_\alpha, P_\alpha H_pH_pj^+V) + (VA_\alpha, P_\alpha H_pVj^+h_0) + (VA_\alpha, P_\alpha H_pVj^+H_p)$$

$$-(VA_\alpha, P_\alpha H_pj^+Vh_0) - (VA_\alpha, P_\alpha H_pj^+VH_p) + (VA_\alpha, P_\alpha h_0Vj^+h_0)$$

$$
\begin{aligned}
&-(VA_\alpha,\ P_\alpha h_0 j^+ Vh_0)+(VA_\alpha,\ P_\alpha H_p Vj^+ h_0)-(VA_\alpha,\ P_\alpha H_p j^+ Vh_0)\\
&-(VA_\alpha,\ P_\alpha Vj^+ h_0 h_0)-(VA_\alpha,\ P_\alpha Vj^+ H_p h_0)+(VA_\alpha,\ P_\alpha j^+ Vh_0 h_0)\\
&+(VA_\alpha,\ P_\alpha j^+ VH_p h_0)+(VA_\alpha,\ P_\alpha h_0 Vj^+ H_p)-(VA_\alpha,\ P_\alpha h_0 j^+ VH_p)\\
&+(VA_\alpha,\ P_\alpha H_p Vj^+ H_p)-(VA_\alpha,\ P_\alpha H_p j^+ VH_p)-(VA_\alpha,\ P_\alpha Vj^+ h_0 H_p)\\
&-(VA_\alpha,\ P_\alpha Vj^+ H_p H_p)+(VA_\alpha,\ P_\alpha j^+ Vh_0 H_p)+(VA_\alpha,\ P_\alpha j^+ VH_p H_p)\\
&-(A_\alpha V,\ h_0 h_0 Vj^+)+(A_\alpha V,\ h_0 h_0 j^+ V)-(A_\alpha V,\ h_0 H_p Vj^+)+(A_\alpha V,\ h_0 H_p j^+ V)\\
&+(A_\alpha V,\ h_0 Vj^+ h_0)+(A_\alpha V,\ h_0 Vj^+ H_p)-(A_\alpha V,\ h_0 j^+ Vh_0)-(A_\alpha V,\ h_0 j^+ VH_p)\\
&-(A_\alpha V,\ H_p h_0 Vj^+)+(A_\alpha V,\ H_p h_0 j^+ V)-(A_\alpha V,\ H_p H_p Vj^+)\\
&+(A_\alpha V,\ H_p H_p j^+ V)+(A_\alpha V,\ H_p Vj^+ h_0)+(A_\alpha V,\ H_p Vj^+ H_p)-(A_\alpha V,\ H_p j^+ Vh_0)\\
&-(A_\alpha V,\ H_p j^+ VH_p)+(A_\alpha V,\ h_0 Vj^+ h_0)-(A_\alpha V,\ h_0 j^+ Vh_0)+(A_\alpha V,\ H_p Vj^+ h_0)\\
&-(A_\alpha V,\ H_p j^+ Vh_0)-(A_\alpha V,\ Vj^+ h_0 h_0)-(A_\alpha V,\ Vj^+ H_p h_0)+(A_\alpha V,\ j^+ Vh_0 h_0)\\
&+(A_\alpha V,\ j^+ VH_p h_0)+(A_\alpha V,\ h_0 Vj^+ H_p)-(A_\alpha V,\ h_0 j^+ VH_p)+(A_\alpha V,\ H_p Vj^+ H_p)\\
&-(A_\alpha V,\ H_p j^+ VH_p)-(A_\alpha V,\ Vj^+ h_0 H_p)-(A_\alpha V,\ Vj^+ H_p H_p)+(A_\alpha V,\ j^+ Vh_0 H_p)\\
&+(A_\alpha V,\ j^+ VH_p H_p)+(A_\alpha V,\ P_\alpha h_0 h_0 Vj^+)-(A_\alpha V,\ P_\alpha h_0 h_0 j^+ V)\\
&+(A_\alpha V,\ P_\alpha h_0 H_p Vj^+)-(A_\alpha V,\ P_\alpha h_0 H_p j^+ V)-(A_\alpha V,\ P_\alpha h_0 Vj^+ h_0)\\
&-(A_\alpha V,\ P_\alpha h_0 Vj^+ H_p)+(A_\alpha V,\ P_\alpha h_0 j^+ Vh_0)+(A_\alpha V,\ P_\alpha h_0 j^+ VH_p)\\
&+(A_\alpha V,\ P_\alpha H_p h_0 Vj^+)-(A_\alpha V,\ P_\alpha H_p h_0 j^+ V)+(A_\alpha V,\ P_\alpha H_p H_p Vj^+)\\
&-(A_\alpha V,\ P_\alpha H_p H_p j^+ V)-(A_\alpha V,\ P_\alpha H_p Vj^+ h_0)-(A_\alpha V,\ P_\alpha H_p Vj^+ H_p)\\
&+(A_\alpha V,\ P_\alpha H_p j^+ Vh_0)+(A_\alpha V,\ P_\alpha H_p j^+ VH_p)-(A_\alpha V,\ P_\alpha h_0 Vj^+ h_0)\\
&+(A_\alpha V,\ P_\alpha h_0 j^+ Vh_0)-(A_\alpha V,\ P_\alpha H_p Vj^+ h_0)+(A_\alpha V,\ P_\alpha H_p j^+ Vh_0)\\
&+(A_\alpha V,\ P_\alpha Vj^+ h_0 h_0)+(A_\alpha V,\ P_\alpha Vj^+ H_p h_0)-(A_\alpha V,\ P_\alpha j^+ Vh_0 h_0)\\
&-(A_\alpha V,\ P_\alpha j^+ VH_p h_0)-(A_\alpha V,\ P_\alpha h_0 Vj^+ H_p)+(A_\alpha V,\ P_\alpha h_0 j^+ VH_p)\\
&-(A_\alpha V,\ P_\alpha H_p Vj^+ H_p)+(A_\alpha V,\ P_\alpha H_p j^+ VH_p)+(A_\alpha V,\ P_\alpha Vj^+ h_0 H_p)\\
&+(A_\alpha V,\ P_\alpha Vj^+ H_p H_p)-(A_\alpha V,\ P_\alpha j^+ Vh_0 H_p)-(A_\alpha V,\ P_\alpha j^+ VH_p H_p)]\,. \qquad (2\cdot 2)
\end{aligned}
$$

Thus we have 128 terms in total. For the same reason as that in Ref. 12), we divide all the terms into four parts. The parts to be matched with Eq. (1·7) through Eq. (1·10) will be called the companions of part one through four and will be denoted by Part(IC), Part(IIC), Part(IIIC) and Part(IVC) respectively. After performing the trace calculations based on the EWC scheme as $(B,\ A_\alpha C)\equiv \mathrm{tr}(BA_\alpha C)=(A_\alpha)_{\alpha,\alpha+1}\sum_\beta B_{\beta\alpha}C_{\alpha+1,\beta}$, we have

$$\mathrm{Part(IC)}=(1\mathrm{st}+33\mathrm{rd})+\{(3\mathrm{rd}+9\mathrm{th}+35\mathrm{th}+41\mathrm{st})+(6\mathrm{th}+25\mathrm{th}+38\mathrm{th}+57\mathrm{th})\}$$

$$+\{(11\text{th}+43\text{rd})+(30\text{th}+62\text{nd})+(14\text{th}+27\text{th}+46\text{th}+59\text{th})\}$$
$$+(21\text{st}+53\text{rd})+\{(22\text{nd}+29\text{th}+54\text{th}+61\text{st})$$
$$+(13\text{th}+19\text{th}+45\text{th}+51\text{st})\}$$
$$+(5\text{th}+17\text{th}+37\text{th}+49\text{th})$$

$$=-\frac{1}{2}(it)^2(A_\alpha)_{\alpha,\alpha+1}[\{\sum_\beta j_\beta{}^+(E_{\alpha+1})^2 V_{\beta\alpha}V_{\alpha+1,\beta+1}-j_\alpha{}^+(E_{\alpha+1})^2 V_{\alpha\alpha}V_{\alpha+1,\alpha+1}\}$$
$$+\{\sum_\beta j_\beta{}^+2E_{\alpha+1}V_{\beta\alpha}H_pV_{\alpha+1,\beta+1}-j_\alpha{}^+2E_{\alpha+1}V_{\alpha\alpha}H_pV_{\alpha+1,\alpha+1}\}$$
$$+\{-\sum_\beta j_\beta{}^+2E_{\alpha+1}V_{\beta\alpha}V_{\alpha+1,\beta+1}H_p+j_\alpha{}^+2E_{\alpha+1}V_{\alpha\alpha}V_{\alpha+1,\alpha+1}H_p\}$$
$$+\{\sum_\beta j_\beta{}^+V_{\beta\alpha}H_pH_pV_{\alpha+1,\beta+1}-j_\alpha{}^+V_{\alpha\alpha}H_pH_pV_{\alpha+1,\alpha+1}\}$$
$$+\{\sum_\beta j_\beta{}^+V_{\beta\alpha}V_{\alpha+1,\beta+1}H_pH_p-j_\alpha{}^+V_{\alpha\alpha}V_{\alpha+1,\alpha+1}H_pH_p\}$$
$$+\{-\sum_\beta j_\beta{}^+2V_{\beta\alpha}H_pV_{\alpha+1,\beta+1}H_p+j_\alpha{}^+2V_{\alpha\alpha}H_pV_{\alpha+1,\alpha+1}H_p\}$$
$$+\{\sum_\beta j_\beta{}^+(E_\beta)^2V_{\beta\alpha}V_{\alpha+1,\beta+1}-j_\alpha{}^+(E_\alpha)^2V_{\alpha\alpha}V_{\alpha+1,\alpha+1}\}$$
$$+\{\sum_\beta j_\beta{}^+2E_\beta V_{\beta\alpha}V_{\alpha+1,\beta+1}H_p-j_\alpha{}^+2E_\alpha V_{\alpha\alpha}V_{\alpha+1,\alpha+1}H_p\}$$
$$+\{-\sum_\beta j_\beta{}^+2E_\beta V_{\beta\alpha}H_pV_{\alpha+1,\beta+1}+j_\alpha{}^+2E_\alpha V_{\alpha\alpha}H_pV_{\alpha+1,\alpha+1}\}$$
$$+\{-\sum_\beta j_\beta{}^+2E_{\alpha+1}E_\beta V_{\beta\alpha}V_{\alpha+1,\beta+1}+j_\alpha{}^+2E_{\alpha+1}E_\alpha V_{\alpha\alpha}V_{\alpha+1,\alpha+1}\}], \tag{2·3}$$

where the ordinal numbers refer to the terms in Eq. (2·2). Here we see that the terms corresponding to $\beta=\alpha$ are excluded in the summations. Carrying out the phonon averaging, we obtain

$$\langle \text{Part(IC)}\rangle_p=-(A_\alpha)_{\alpha,\alpha+1}$$
$$\times\sum_{\beta(\neq\alpha)}\sum_q j_\beta{}^+\Big[(1+n_q)(\gamma_q)_{\beta\alpha}(\gamma_q{}^\dagger)_{\alpha+1,\beta+1}\frac{1}{2}(it)^2(E_{\alpha+1}-E_\beta+\omega_q)^2$$
$$+n_q(\gamma_q{}^\dagger)_{\beta\alpha}(\gamma_q)_{\alpha+1,\beta+1}\frac{1}{2}(it)^2(E_{\alpha+1}-E_\beta-\omega_q)^2\Big]. \tag{2·4}$$

We now combine this with Eq. (1·7). Then we feel freer to adopt the exponential expression than in Ref. 12). Using $1+itE+(itE)^2/2!=\exp(itE)$, we obtain

$$\langle \text{Part(I)}+\text{Part(IC)}\rangle_p=-(A_\alpha)_{\alpha,\alpha+1}$$
$$\times\sum_{\beta(\neq\alpha)}\sum_q j_\beta{}^+[(1+n_q)(\gamma_q)_{\beta\alpha}(\gamma_q{}^\dagger)_{\alpha+1,\beta+1}\exp\{it(E_{\alpha+1}-E_\beta+\omega_q)\}$$
$$+n_q(\gamma_q{}^\dagger)_{\beta\alpha}(\gamma_q)_{\alpha+1,\beta+1}\exp\{it(E_{\alpha+1}-E_\beta-\omega_q)\}]. \tag{2·5}$$

In the same manner, for Part(IIC) we have

$$\begin{aligned}
\langle \text{Part(IIC)}\rangle_p =& \langle (\text{2nd}+\text{34th})+\{(\text{4th}+\text{10th}+\text{36th}+\text{42nd}) \\
&+(\text{8th}+\text{26th}+\text{40th}+\text{50th})\}+\{(\text{12th}+\text{44th})+(\text{32nd}+\text{64th}) \\
&+(\text{16th}+\text{28th}+\text{48th}+\text{60th})\}+(\text{23rd}+\text{55th}) \\
&+\{(\text{24th}+\text{31st}+\text{56th}+\text{63rd})+(\text{15th}+\text{20th}+\text{47th}+\text{52nd})\} \\
&+(\text{7th}+\text{18th}+\text{39th}+\text{50th})\rangle_p \\
=& (A_\alpha)_{\alpha,\alpha+1} j_\alpha^{\ +} \\
&\times \sum_{\beta(\neq\alpha)} \sum_q \Big[(1+n_q)(\gamma_q)_{\beta\alpha}(\gamma_q^{\ \dagger})_{\alpha\beta} \frac{1}{2}(it)^2 (E_{\alpha+1}-E_\beta+\omega_q)^2 \\
&+ n_q(\gamma_q^{\ \dagger})_{\beta\alpha}(\gamma_q)_{\alpha\beta} \frac{1}{2}(it)^2 (E_{\alpha+1}-E_\beta-\omega_q)^2 \Big] . \qquad (2\cdot6)
\end{aligned}$$

Combining this with Eq. (1·8) we obtain

$$\begin{aligned}
\langle \text{Part(II)}+\text{Part(IIC)}\rangle_p =& (A_\alpha)_{\alpha,\alpha+1} j_\alpha^{\ +} \\
&\times \sum_{\beta(\neq\alpha)} \sum_q [(1+n_q)(\gamma_q)_{\beta\alpha}(\gamma_q^{\ \dagger})_{\alpha\beta} \exp\{it(E_{\alpha+1}-E_\beta+\omega_q)\} \\
&+ n_q(\gamma_q^{\ \dagger})_{\beta\alpha}(\gamma_q)_{\alpha\beta} \exp\{it(E_{\alpha+1}-E_\beta-\omega_q)\}] . \qquad (2\cdot7)
\end{aligned}$$

For Part(IIIC) we have

$$\begin{aligned}
&\langle \text{Part(IIIC)}\rangle_p \\
&= \langle (\text{65th}+\text{97th})+\{(\text{67th}+\text{73rd}+\text{99th}+\text{105th})+(\text{70th}+\text{89th}+\text{102nd}+\text{121st})\} \\
&\quad +\{(\text{75th}+\text{107th})+(\text{94th}+\text{126th})+(\text{78th}+\text{91st}+\text{110th}+\text{123rd})\} \\
&\quad +(\text{85th}+\text{117th})+\{(\text{86th}+\text{93rd}+\text{118th}+\text{125th}) \\
&\quad +(\text{77th}+\text{83rd}+\text{109th}+\text{115th})\}+(\text{69th}+\text{81st}+\text{101st}+\text{113th})\rangle_p \\
&= (A_\alpha)_{\alpha,\alpha+1} j_\alpha^{\ +} \\
&\quad \times \sum_{\beta(\neq\alpha+1)} \sum_q \Big[(1+n_q)(\gamma_q)_{\alpha+1,\beta}(\gamma_q^{\ \dagger})_{\beta,\alpha+1} \frac{1}{2}(it)^2 (E_\beta-E_\alpha+\omega_q)^2 \\
&\quad + n_q(\gamma_q^{\ \dagger})_{\alpha+1,\beta}(\gamma_q)_{\beta,\alpha+1} \frac{1}{2}(it)^2 (E_\beta-E_\alpha-\omega_q)^2 \Big] \qquad (2\cdot8)
\end{aligned}$$

and

$$\begin{aligned}
&\langle \text{Part(III)}+\text{Part(IIIC)}\rangle_p \\
&= (A_\alpha)_{\alpha,\alpha+1} j_\alpha^{\ +} \sum_{\beta(\neq\alpha+1)} \sum_q [(1+n_q)(\gamma_q)_{\alpha+1,\beta}(\gamma_q^{\ \dagger})_{\beta,\alpha+1} \exp\{it(E_\beta-E_\alpha+\omega_q)\} \\
&\quad + n_q(\gamma_q^{\ \dagger})_{\alpha+1,\beta}(\gamma_q)_{\beta,\alpha+1} \exp\{it(E_\beta-E_\alpha-\omega_q)\}] . \qquad (2\cdot9)
\end{aligned}$$

For Part (IVC) we have

$$\langle \text{Part(IVC)} \rangle_p$$

$$=\langle(66\text{th}+98\text{th})+\{(68\text{th}+74\text{th}+100\text{th}+106\text{th})+(72\text{nd}+90\text{th}+104\text{th}+122\text{nd})\}$$

$$+\{(76\text{th}+119\text{th})+(96\text{th}+128\text{th})+(80\text{th}+92\text{nd}+112\text{th}+124\text{th})\}$$

$$+(87\text{th}+119\text{th})+\{(88\text{th}+95\text{th}+120\text{th}+127\text{th})$$

$$+(79\text{th}+84\text{th}+111\text{th}+116\text{th})\}+(71\text{st}+82\text{nd}+103\text{rd}+114\text{th})\rangle_p$$

$$=-(A_\alpha)_{\alpha,\alpha+1}\sum_{\beta(\neq\alpha+1)}\sum_q j^+_{\beta-1}\Big[(1+n_q)(\gamma_q)_{\alpha+1,\beta}(\gamma_q{}^\dagger)_{\beta-1,\alpha}\frac{1}{2}(it)^2(E_\beta-E_\alpha+\omega_q)^2$$

$$+n_q(\gamma_q{}^\dagger)_{\alpha+1,\beta}(\gamma_q)_{\beta-1,\alpha}\frac{1}{2}(it)^2(E_\beta-E_\alpha-\omega_q)^2\Big] \tag{2·10}$$

and

$$\langle \text{Part(IV)}+\text{Part(IVC)} \rangle_p$$

$$=-(A_\alpha)_{\alpha,\alpha+1}\sum_{\beta(\neq\alpha+1)}\sum_q j^+_{\beta-1}[(1+n_q)(\gamma_q)_{\alpha+1,\beta}(\gamma_q{}^\dagger)_{\beta-1,\alpha}\exp\{it(E_\beta-E_\alpha+\omega_q)\}$$

$$+n_q(\gamma_q{}^\dagger)_{\alpha+1,\beta}(\gamma_q)_{\beta-1,\alpha}\exp\{it(E_\beta-E_\alpha-\omega_q)\}]\,. \tag{2·11}$$

Now collecting all the parts and dividing them by $(A_\alpha, j^+)=(A_\alpha)_{\alpha,\alpha+1}j_\alpha{}^+$, we can obtain the lineshape function which is the FLT of the phonon average of $\Gamma_\alpha(t)$ given in Eq. (1·3). The result is as follows:

$$[i\tilde{\Gamma}_\alpha(\omega)]_{\text{EWC}}=\int_0^\infty dt\langle i\Gamma_\alpha(t)\rangle_p\exp(-i\omega t-\eta t) \tag{2·12}$$

$$=\sum_q(1+n_q)\Big[\sum_{\beta(\neq\alpha+1)}\frac{(\gamma_q)_{\alpha+1,\beta}\{(\gamma_q{}^\dagger)_{\beta,\alpha+1}-j^+_{\beta-1}/j_\alpha{}^+(\gamma_q{}^\dagger)_{\beta-1,\alpha}\}}{\omega^--E_\beta+E_\alpha-\omega_q}$$

$$+\sum_{\beta(\neq\alpha)}\frac{(\gamma_q)_{\beta\alpha}\{(\gamma_q{}^\dagger)_{\alpha\beta}-j_\beta{}^+/j_\alpha{}^+(\gamma_q{}^\dagger)_{\alpha+1,\beta+1}\}}{\omega^--E_{\alpha+1}+E_\beta-\omega_q}\Big]$$

$$+\sum_q n_q\Big[\sum_{\beta(\neq\alpha+1)}\frac{(\gamma_q{}^\dagger)_{\alpha+1,\beta}\{(\gamma_q)_{\beta,\alpha+1}-j^+_{\beta-1}/j_\alpha{}^+(\gamma_q)_{\beta-1,\alpha}\}}{\omega^--E_\beta+E_\alpha+\omega_q}$$

$$+\sum_{\beta(\neq\alpha)}\frac{(\gamma_q{}^\dagger)_{\beta\alpha}\{(\gamma_q)_{\alpha\beta}-j_\beta{}^+/j_\alpha{}^+(\gamma_q)_{\alpha+1,\beta+1}\}}{\omega^--E_{\alpha+1}+E_\beta+\omega_q}\Big], \tag{2·13}$$

where $\omega^-\equiv\omega-i\eta(\eta\to0^+)$. This expression is just Eq. (4·6) in Ref. 12).

§ 3. Conclusion

So far we have proved that the exponential expression in the lineshape formula in the EWC scheme is valid up to second order in time. If all the higher order perturbative terms are included, the expression will be more precisely justified.

Accepting that, we conclude that the lineshape function derived in the EWC scheme on the basis of Mori and Kawabata's method is the same as that obtained by using Argyres and Sigel's technique.

The same technique may be applied to the MWC scheme formula derived by Ryu, Chung and Choi in 1985. The only difference is that the MWC scheme calculation is based on

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

[For details, see Ref. 16).] The detailed work on this scheme will be reported elsewhere.

Acknowledgements

We thank Professors J. Hong, S. Lee, A. Fortini, B. Goodman, M. H. Lee, E. Otsuka, and N. Q. Khanh for helpful discussions and concerns. This research has been supported by the Korean Science and Engineering Foundation.

References

1) H. J. G. Meyer, Phys. Lett. **2** (1962), 259.
2) G. D. Mahan and J. J. Hopfield, Phys. Rev. Lett. **12** (1964), 241.
3) R. C. Enck, A. S. Saleh and H. Y. Fan, Phys. Rev. **182** (1969), 790.
4) J. P. Vigneron, R. Evrard and E. Kartheuser, Phys. Rev. **B18** (1978), 6930.
J. P. Vigneron, Solid State Commun. **32** (1979), 595.
5) P. G. Harper, Proc. Phys. Soc. London **92** (1967), 793.
C. J. Summers, R. B. Dennis, B. S. Wherrett, P. G. Harper and S. D. Smith, Phys. Rev. **170** (1968), 755.
6) O. Matsuda and E. Otsuka, J. Phys. Chem. Solids **40** (1979), 819.
7) M. Saitoh and A. Kawabata, J. Phys. Soc. Jpn. **23** (1967), 1006.
8) C. S. Raju and S. Fujita, Acta Phys. Austriaca **43** (1975), 1.
A. Suzuki, S. D. Choi and S. Fujita, J. Phys. Chem. Solids **41** (1980), 735.
S. D. Choi, and S. Fujita, Solid State Commun. **37** (1981), 293.
A. Suzuki and D. Dunn, Phys. Rev. **B25** (1982), 7754.
D. Dunn and A. Suzuki, Phys. Rev. **B29** (1984), 942.
9) W. G. Tam, Phys. Lett. **30A** (1969), 43.
10) Y. A. Gurvich and M. D. Cherepanov, Fiz. Tekh. Poluprovodn. **10** (1976), 958 [Sov. Phys. Semicond. **10** (1976), 565].
11) S. D. Choi and O. H. Chung, Solid State Commun. **46** (1983), 717.
12) J. Y. Ryu and S. D. Choi, Prog. Theor. Phys. **72** (1984), 429.
13) P. N. Argyres and J. L. Sigel, Phys. Rev. **B10** (1974), 1139; Phys. Rev. Lett. **31** (1973), 1397.
14) H. Mori, Prog. Theor. Phys. **34** (1965), 399.
15) R. Kubo, J. Phys. Soc. Jpn. **12** (1957), 570.
16) J. Y. Ryu, Y. C. Chung and S. D. Choi, Phys. Rev. **B32** (1985), 7769.