# Theory of cyclotron-resonance line shapes based on the isolation-projection technique

Yong Jai Cho and Sang Don Choi

Department of Physics, Kyungpook National University, Taegu 702-701, South Korea

(Received 9 November 1992)

The density operator for a system of many electrons in interaction with the background is expressed in a diagonal-plus-nondiagonal form, which is useful for calculation of the ensemble average of physical quantities. Starting with this form and with the help of the isolation-projection technique, the cyclotron-resonance-line-shape function for electron-phonon systems is derived. The dominant part is shown to reduce to the expression of Badjou and Argyres [Phys. Rev. 8 35, 5964 (1987)] for quite weak interactions.

## I. INTRODUCTION

The study of cyclotron-resonance line shapes is known to be a powerful tool for investigating the electronic structure of solids, since absorption line shapes are very sensitive to the type of scattering mechanisms afFecting the behavior of the carriers. So far, various theoretical studies<sup>1-33</sup> have appeared regarding the dependence of the absorption line shapes on the magnetic field and the temperature in three-dimensional<sup>1-22</sup> and twothree-dimensional<sup> $1^{1-22}$ </sup> and twodimensional systems. $23-33$ 

To our knowledge, most of the theories presented so far are based on the well-known relation that the absorption coefficient is proportional to the transition probability,<sup>1-9</sup> the imaginary part of the dielectric constant,<sup>10</sup> or ty,<sup>1-9</sup> the imaginary part of the dielectric constant,<sup>10</sup> or<br>the real part of the electric conductivity.<sup>11-33</sup> In these formalisms, with extremely few exceptions, the absorption coefficient is given by

$$
\mu(\omega - i\eta) \propto \sum_{\alpha} A(\alpha) [i(\omega - \omega_c) + \Gamma_{\alpha}(\omega - i\eta) - i\eta]^{-1},
$$
\n(1.1)

where  $A(\alpha)$  is a function of the one-electron state index  $\alpha$ ,  $\omega$  is the microwave frequency,  $\omega_c$  is the cyclotron frequency,  $\Gamma_{\alpha}(\omega - i\eta)$  is the complex line-shape function,  $\eta$ is an arbitrary positive infinitesimal constant which is taken to be zero in the final stage, and  $\hbar$  is taken equal to 1. For weak interactions, the line-shape functions are usually expanded in powers of the scattering strength  $\lambda$ as

$$
\Gamma_{\alpha}(\omega - i\eta) \propto -i\Delta(\alpha) + \sum_{n=2}^{n=\infty} \lambda^{n} \Gamma_{\alpha}^{(n)}(\omega - i\eta) , \qquad (1.2)
$$

where  $\Delta(\alpha)$  is the line shift due to the self-energy of the system which contains the electron-phonon or the electron-impurity interactions and  $\Gamma_{\alpha}^{(n)}(\omega - i\eta)$  is thenth-order line-shape function in powers of  $\lambda$ . The functions obtained in most theories are given up to only  $\lambda^2$  for extremely weak interactions.

These theories, however, have some controversial points on the validity of the expansion. Argyres and These theories, however, have some controversial<br>points on the validity of the expansion. Argyres and<br>Sigel<sup>18(c)</sup> showed that the correct expression for the lineshape function cannot be given in powers of  $\lambda$  and obtained the function to order of  $\lambda^2$  by means of the integral equation with an infinite subset of divergent terms. Furthermore, most theories have adopted the approximation that the total Hamiltonian of the system is replaced by the noninteraeting part in calculating the trace for the scattering potential in the exponential form, which contains nondiagonal elements. This approximation results in ignoring the line shift of the absorption spectrum due to the self-energy of the electron-phonon system.

In this paper, we will derive a general line-shape function for electron-phonon systems by utilizing the socalled isolation-projection technique. In Sec. II, we first present a diagonal-plus-nondiagonal form of the density operator using the integral equation. This transformed density operator has the nondiagonal part including the scattering potential, which is separated from the exponential form, so that we can calculate straightforwardly the ensemble average and also make a suitable approximation based on our condition for the scattering potential. In Sec. III, we derive the general form of the lineshape function for electron-phonon systems by using the isolation-projection technique, which combines the isolation operators and the projection operators. Then we show that the line-shape function cannot be expanded in powers of  $\lambda$ , although the scattering interaction is weak. Finally, we make a careful approximation for small  $\lambda$  and obtain the dominant terms of the line-shape function without taking the usual expansion. We also show that the transformed density operator recovers the line shift due to the self-energy. The last section is devoted to the conclusion.

# II. CYCLOTRON-RESONANCE ABSORPTION POWER FOR THE ELECTRON-PHONON SYSTEMS

When a time-independent magnetic field **B** is applied along the z axis the Hamiltonian of the system of many electrons in interaction with phonons in equilibrium is given by

$$
H_{\text{eq}} = H_0 + V \tag{2.1}
$$

$$
H_0 = H_e + H_p \tag{2.2}
$$

where  $H_e$ ,  $H_p$ , and V, respectively, are the Hamiltonians

(2.14)

corresponding to the dynamically independent electrons, the background phonon field, and the scattering potential due to the electron-phonon interaction given by

$$
H_e = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} , \qquad (2.3)
$$

$$
H_p = \sum_q \omega_q b_q^{\dagger} b_q \tag{2.4}
$$

$$
V = \sum_{q} \sum_{\alpha,\beta} C_{\alpha,\beta}(q) a_{\alpha}^{\dagger} a_{\beta} (b_q + b_{-q}^{\dagger}) \tag{2.5}
$$

Here  $a_{\alpha}^{\dagger}$  ( $a_{\alpha}$ ) is the creation (annihilation) operator for an electron in the state  $|\alpha\rangle$  with energy  $\epsilon_{\alpha}$  given by

$$
|\alpha\rangle \equiv |N, k_y, k_z\rangle = (L_y L_z)^{-1/2} \phi_N(x + k_y / m^* \omega_c)
$$
  
× $\exp(i y k_y + iz k_z)$ , (2.6)

$$
\epsilon_{\alpha} = (N + 1/2)\omega_c + k_z^2 / 2m^* , \qquad (2.7)
$$

where  $N$  is the Landau index,  $k$  the electron wave vector,  $m^*$  the effective mass of an electron, and  $\phi_N(x + k_y/m^* \omega_c)$  are the eigenfunctions of a harmonic  $\phi_N(x + \kappa_y/m \omega_c)$  are the eigenfunctions of a narmonic<br>oscillator of the cyclotron frequency  $\omega_c \equiv |e|B/m^*$ , cen-<br>tered at  $(-k_y/m^* \omega_c)$ .  $b_q^{\dagger} (b_q)$  in Eqs. (2.4) and (2.5) is<br>the creation (annihilation) operator for a p tered at  $(-k_y/m^*\omega_c)$ .  $b_q^{\dagger}$  ( $b_q$ ) in Eqs. (2.4) and (2.5) is the creation (annihilation) operator for a phonon with  $q \equiv (s, q)$ , where s is the polarization index and q the wave<br>vector of a phonon with energy  $\omega_q$ . In Eq. (2.5),  $C_{\alpha,\beta}(q) \equiv \langle \alpha | c(q) | \beta \rangle$  is the matrix element of the oneelectron operator  $c(q)$ , which describes the interaction of an electron with the vibrating lattices in a self-consistent approximation scheme. In the following,  $|\alpha+1\rangle$  shall denote the state  $|N+1, k_y, k_z\rangle$  if  $|\alpha\rangle = |N, k_y, k_z\rangle$ , and denote the state  $|N+1,\kappa_y,\kappa_z|$  in  $|\alpha\rangle = |N,\kappa_y,\kappa_z|$ , and  $C^{\dagger}(q) = C(-q)$ , where  $-q = (s, -q)$ , since V is Hermitian.

We suppose that the external time-dependent field is initially absent and the electron-phonon system is macroscopically in thermodynamic equilibrium with an ab-

solute temperature  $T$ . The system, then, can be described in terms of the grand-canonical density operator

$$
\rho_{\text{eq}}(H_{\text{eq}}) = \frac{\exp[-\beta(H_{\text{eq}} - \mu \overline{N})]}{T_R \{\exp[-\beta(H_{\text{eq}} - \mu \overline{N})]\}} \tag{2.8}
$$

Here  $\overline{N}$  is the total number of electrons in the system,  $\mu$ the chemical potential of an electron, and  $\beta \equiv (k_B T)^{-1}$ , where  $k_B$  is the Boltzmann constant.  $T_R$  denotes the many-body trace for the electron-phonon states.

Most theories have adopted the approximation that  $H_{eq} \simeq H_0$  in the density operator, since it is difficult to calculate the trace for  $V$  in the exponential form which contains nondiagonal elements. This approximation disregards the shift of the cyclotron-resonance absorption peak due to the self-energy of the electron-phonon system.

Now we present a diagonal-plus-nondiagonal form of the density operator. We first define the integralequation operator  $U(\lambda)$  given by

$$
U(\lambda) \equiv \exp[\lambda \beta (H_0 - \mu \overline{N})] \exp[-\lambda \beta (H_{\text{eq}} - \mu \overline{N})]. \quad (2.9)
$$

Differentiation with respect to  $\lambda$  gives

$$
\frac{\partial U(\lambda)}{\partial \lambda} = -\beta V(\lambda) U(\lambda) , \qquad (2.10)
$$

where  $V(\lambda)$  is defined as

$$
V(\lambda) \equiv \exp[\lambda \beta (H_0 - \mu \overline{N})] V \exp[-\lambda \beta (H_0 - \mu \overline{N})].
$$
\n(2.11)

The differential equation for the operator  $U(\lambda)$  in Eq. (2.10) can be solved by integration with respect to  $\lambda$ .

$$
U(\lambda) = 1 - \beta \int_0^{\lambda} V(\lambda_1) U(\lambda_1) d\lambda_1 . \qquad (2.12)
$$

If this manipulation is iteratively performed, we get

$$
U(\lambda) = 1 + \sum_{n=1}^{\infty} (-\beta)^n \int_0^{\lambda} d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \cdots \int_0^{\lambda_{n-1}} d\lambda_n V(\lambda_1) V(\lambda_2) \cdots V(\lambda_n) . \tag{2.13}
$$

Substituting 1 for  $\lambda$  in Eqs. (2.9) and (2.13), we have

$$
\exp[-\beta (H_{\text{eq}} - \mu \bar{N})] = \exp[-\beta (H_0 - \mu \bar{N})][1 + S(V)],
$$

where

$$
{}_{n=1}^{n=1}
$$
  
\n
$$
exp[-\beta(H_{eq} - \mu \overline{N})] = exp[-\beta(H_0 - \mu \overline{N})][1 + S(V)],
$$
  
\n
$$
S(V) = \sum_{n=1}^{\infty} (-\beta)^n \int_0^1 d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \cdots \int_0^{\lambda_{n-1}} d\lambda_n V(\lambda_1) V(\lambda_2) \cdots V(\lambda_n).
$$
  
\n
$$
F(C) = \sum_{n=1}^{\infty} (-\beta)^n \int_0^1 d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \cdots \int_0^{\lambda_{n-1}} d\lambda_n V(\lambda_1) V(\lambda_2) \cdots V(\lambda_n).
$$
  
\n
$$
F(C) = \sum_{n=1}^{\infty} (-\beta)^n \int_0^1 d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \cdots \int_0^{\lambda_{n-1}} d\lambda_n V(\lambda_1) V(\lambda_2) \cdots V(\lambda_n).
$$
  
\n
$$
F(C) = \sum_{n=1}^{\infty} (-\beta) \left( \frac{1}{n} \sum_{n=1}^{\infty} \left[ \frac{1}{n} \sum_{n=1}^{\infty} \left[ \frac{1}{n} \sum_{n=1}^{\infty} \frac{
$$

Therefore, we finally have a diagonal-plus-nondiagonal form of the density operator as

$$
\rho_{\text{eq}}(H_{\text{eq}}) = \rho_0(H_0)[1 + S(V)]/Z_r , \qquad (2.16)
$$

where

and

$$
Z_r \equiv 1 + T_R [\rho_0(H_0)S(V)] \tag{2.17}
$$

$$
\rho_0(H_0) \equiv \frac{\exp[-\beta(H_0 - \mu \overline{N})]}{T_R \{\exp[-\beta(H_0 - \mu \overline{N})]\}}.
$$
\n(2.18)

The transformed density operator expressed as Eq. (2.16) has the nondiagonal part including  $V$  separated from the exponential form, and thus we can calculate straightforwardly the ensemble average and also make a suitable approximation based on our condition for V.

When an applied electromagnetic field is very weak

compared with the internal field of the electrons and the ionized nuclei in the system and the wavelength is much larger than the atomic constant, the perturbation associated with the field can be taken to be uniform and grow adiabatically from the nonperturbed equilibrium state to the perturbed steady state in approximation. The component of the induced current density  $J_i$  for the electrons driven by the electric field is given by

$$
J_i = \sum_{\alpha,\beta} \langle \alpha | j_i | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} \quad (i = x, y, z) , \qquad (2.19)
$$

where  $j_i$  is the one-electron current operator. Then we can obtain the conductivity tensor for the induced current through the Kubo formalism. $3$ 

Especially for the electric field of amplitude  $E$  and angular frequency  $\omega$ , which is circularly polarized in the xy plane, the time-averaged absorption power per unit plane, the time-aver.<br>volume is given by<sup>5(a),:</sup>

$$
P(\omega) = \frac{1}{2} E^2 \text{Re} [\sigma_{+-}(\omega^{-})]. \qquad (2.20)
$$

Here  $\omega = \omega - i\eta$  ( $\eta \rightarrow 0^+$  in the final stage), the symbol Re means "the real part of," and, according to Ref.  $18(e)$ ,

$$
\sigma_{+-}(\omega^-) = \frac{i}{\omega_c} \sum_{\alpha} (j^+_{\alpha})^* \langle K(\omega^-) \rangle_{\alpha} . \tag{2.21}
$$

Here

$$
K(\omega^-) \equiv G(\omega^-)J^+ \t\t(2.22)
$$

 $\mathcal{L}$  (construction )  $\mathcal{L}$ 

$$
G(\omega^-) \equiv (\omega^- - L)^{-1} \;, \tag{2.23}
$$

$$
J^{\pm} \equiv J_x \pm iJ_y \tag{2.24}
$$

$$
j_{\alpha}^{+} \equiv \langle \alpha + 1 | j^{+} | \alpha \rangle , \qquad (2.25)
$$

$$
\langle X \rangle_{\alpha} \equiv T_R \{ \rho_{\text{eq}}(H_{\text{eq}}) [X, a_{\alpha}^{\dagger} a_{\alpha+1}] \}, \qquad (2.26)
$$

where  $L = L_0 + L_1$  is the Liouville operator correspond ing to  $H_{\text{eq}} = H_0 + V$ .

There have been some controversies on the validity of expansion of the line-shape function in powers of  $\lambda$ , as mentioned above. In the next section, we will show a different way of expansion, which is free from any divergence.

### III. LINE-SHAPE FUNCTION

We shall derive the general form of line-shape function by using the so-called isolation-projection technique and obtain the dominant terms for a sufficiently small  $V$ . First, following Argyres and Siegel,  $18(c)$  we define a set of operators  $\{\Delta, \Delta'\}$ , which are called the isolation operators, by

$$
\langle \beta | \Delta Y | \beta' \rangle \equiv \langle \beta | Y | \beta - 1 \rangle \delta_{\beta', \beta - 1}
$$
 (3.1)

and

$$
\Delta' \equiv 1 - \Delta \tag{3.2}
$$

If we split the function  $K(\omega^-)$  in Eq. (2.22) into  $K(\omega^-) = \Delta K(\omega^-) + \Delta' K(\omega^-)$ , then with  $\Delta$  and  $\Delta'$  applied to this expression separately, we have

$$
(\omega^- - \Delta L)\Delta K(\omega^-) - \Delta L\Delta' K(\omega^-) = \Delta J^+ = J^+ \quad , \qquad (3.3) \qquad \text{or}
$$

$$
\omega^- - \Delta' L \Delta' K (\omega^-) - \Delta' L \Delta K (\omega^-) = \Delta' J^+ = 0 \tag{3.4}
$$

Making use of 
$$
\Delta L_0 = L_0 \Delta = (\omega_c + L_p) \Delta
$$
 and  
 $\Delta L_0 \Delta' = \Delta' L_0 \Delta = 0$ , we obtain

$$
(\omega^- - L_0 - \Delta L_1) \Delta K(\omega^-) - \Delta L_1 \Delta' K(\omega^-) = J^+ \,, \qquad (3.5)
$$

$$
(\omega^- - L_0 - \Delta' L_1) \Delta' K(\omega^-) - \Delta' L_1 \Delta K(\omega^-) = 0.
$$
 (3.6)

Solving Eq. (3.6) for  $\Delta' K(\omega^-)$  in terms of  $\Delta K(\omega^-)$ , we get

$$
\Delta' K(\omega^-) = G'(\omega^-) \Delta' L_1 \Delta K(\omega^-) , \qquad (3.7)
$$

where

$$
G'(\omega^-) \equiv \frac{1}{\omega^- - L_0 - \Delta' L_1} \tag{3.8}
$$

when  $\Delta' K(\omega^-)$  in Eq. (3.7) is substituted into Eq. (3.5), we find a new form of  $K(\omega^-)$  given by

$$
K(\omega^{-}) = \frac{1}{\omega^{-} - L_0 - Q(\omega^{-})} J^{+} , \qquad (3.9)
$$

where

$$
Q(\omega^{-}) \equiv L_1 \Delta + L_1 G'(\omega^{-}) \Delta' L_1 \Delta . \qquad (3.10)
$$

Equation (3.9) is similar to the result of Argyres and Sigel obtained by using integral-equation method in Ref. 18(c).

Second, we shall transform the propagator in Eq. (3.9) into the Lorentzian form by which we can define the shift and the linewidth of the absorption power spectrum. We define another set of operators  $\{P, P'\}$ , which are called the projection operators, by

$$
PY \equiv \langle Y \rangle_{\alpha} J^{+} / \langle J^{+} \rangle_{\alpha} , \qquad (3.11)
$$

$$
P' \equiv 1 - P \tag{3.12}
$$

With P and P' applied to  $K(\omega^-)$  as  $K(\omega^-)$  $=PK(\omega^-)+P'K(\omega^-)$ , we obtain

$$
[\omega^{+} - \omega_{c} - PQ(\omega^{-})]PK(\omega^{-}) - PQ(\omega^{-})P'K(\omega^{-}) = J^{+},
$$
\n(3.13)

$$
[\omega^- - L_0 - P'Q(\omega^-)]P'K(\omega^-) - P'Q(\omega^-)PK(\omega^-) = 0.
$$
\n(3.14)

Solving Eq. (3.14) for  $P'K(\omega^-)$  in terms of  $PK(\omega^-)$ , we get

$$
P'K(\omega^-) = G''(\omega^-)P'Q(\omega^-)PK(\omega^-) , \qquad (3.15)
$$

where

$$
G''(\omega^{-}) \equiv \frac{1}{\omega^{-} - L_0 - P'Q(\omega^{-})} \ . \tag{3.16}
$$

We now substitute Eq. (3.15) into Eq. (3.13) and obtain

 $[\omega^--\omega_c - PQ(\omega^-) - PQ(\omega^-)G''(\omega^-)P'Q(\omega^-)]PK(\omega^-)$  $=J^+$ , (3.17)

(3.28)

$$
\langle K(\omega^-) \rangle_a = \frac{i \langle J^+ \rangle_a}{i(\omega^- - \omega_c) + \Gamma_a(\omega^-)} , \qquad (3.18)
$$

where the complex line-shape function  $\Gamma_{\alpha}(\omega^{-})$  is defined by

$$
\Gamma_{\alpha}(\omega^{-}) \equiv \frac{1}{i \langle J^{+} \rangle_{\alpha}}
$$
  
 
$$
\times \langle [Q(\omega^{-}) + Q(\omega^{-})G''(\omega^{-})P'Q(\omega^{-})]J^{+} \rangle_{\alpha}.
$$
  
(3.19)

If we expand the above function in powers of  $V$  or  $L_1$ , the first term is expressed in terms of  $G_0(\omega^-)\Delta'$ , where  $G_0(\omega^-) \equiv (\omega^- - L_0)^{-1}$ . This term gives rise to regular terms, since

$$
\langle \beta | G_0(\omega^-) \Delta' Y | \beta' \rangle = \frac{\langle \beta | Y | \beta' \rangle}{\omega - \omega_{\beta, \beta} - i \eta} \quad (\beta' \neq \beta - 1) ,
$$
\n(3.20)

where  $\omega_{\beta,\beta} \equiv \epsilon_{\beta} - \epsilon_{\beta}$ . On the other hand, if the second where  $\omega_{\beta,\beta} = \epsilon_{\beta} - \epsilon_{\beta}$ . On the other hand, if the second<br>term in Eq. (3.19) is expanded in powers of V or  $L_1$ , then this part includes the terms with  $G_0(\omega^-)P'$ . We easily see that the terms containing  $G_0(\omega^-)P'$  diverge near the cyclotron frequency [for details, see Ref. 18(c)]. If we leave the expression in Eq. (3.19) as is, without expansion with respect to  $V$  or  $L_1$ , no danger of divergence arises.

Fortunately, for a sufficiently weak scattering potential  $V$ , we can ignore the second term of Eq.  $(3.19)$ , which is composed of higher orders of V, and then  $Q(\omega^{-})$  can be replaced by  $[L_1+L_1G_0(\omega^-)\Delta'L_1]\Delta$  in approximation. Thus the dominant part of the line-shape function is given by

$$
\Gamma_{\alpha}(\omega^{-}) \simeq -i\,\Delta(\alpha) + \widetilde{\Gamma}_{\alpha}(\omega^{-}) \;, \tag{3.21}
$$

$$
\Delta(\alpha) \equiv \langle L_1 J^+ \rangle_{\alpha} / \langle J^+ \rangle_{\alpha} \tag{3.22}
$$

and

$$
\widetilde{\Gamma}_a(\omega^-) \equiv -i \left\langle L_1 G_0(\omega^-) \Delta' L_1 J^+ \right\rangle_a / \left\langle J^+ \right\rangle_a . \tag{3.23}
$$

Here we will see soon that  $\Delta(\alpha)$  is the line shift due to the self-energy and  $\tilde{\Gamma}_\alpha(\omega^-)$  is the  $\omega$ -dependent part of the line-shape function. If  $\Delta'$  in  $\tilde{\Gamma}_\alpha(\omega^-)$  given by Eq. (3.23) is line-shape function. If  $\Delta'$  in  $\Gamma_{\alpha}(\omega)$  given by Eq. (3.23) is replaced by P', this part is identical to the result of Bad-<br>jou and Argyres.<sup>18(e)</sup>

For the calculation of the ensemble average, we shall take the dominant part of the density operator in Eq. (2.16) with  $Z_{r} \simeq 1$  in approximation. Then for each part in Eqs. (3.22) and (3.23), we have

$$
\langle J^+ \rangle_a \simeq T_R \{ \rho_0(H_0) [J^+, a^\dagger_a a_{\alpha+1}] \} , \qquad (3.24)
$$

$$
\langle L_1 J^+ \rangle_{\alpha} \simeq -\beta \int_0^1 d\lambda T_R \{ \rho_0(H_0) V(\lambda) [L_1 J^+, a_{\alpha}^\dagger a_{\alpha+1}] \},
$$
\n(3.25)

$$
\langle L_1 G_0(\omega^-) \Delta' L_1 J^+ \rangle_{\alpha}
$$
  
\n
$$
\simeq T_R \{ \rho_0(H_0) [L_1 G_0(\omega^-) \Delta' L_1 J^+, a_{\alpha}^\dagger a_{\alpha+1}] \} .
$$
\n(3.26)

For the electron-phonon systems,  $\Delta(\alpha)$  disappears in some other theories,  $14(a)$ ,  $15(a)$ ,  $18(e)$ ,  $21$  since they made the approximation that  $\rho_{\rm eq}(H_{\rm eq}) \simeq \rho_0(H_0)$ . But in the present theory we have recovered it, as shown in Eqs. (3.22) and (3.25). Finally, in the one-electron representation, we have

$$
\sigma_{+-}(\omega^{-}) = \frac{1}{\omega_c} \sum_{\alpha} \frac{[f(\epsilon_{\alpha}) - f(\epsilon_{\alpha+1})]|j_{\alpha}^{+}|^2}{i[\omega^{-} - \omega_c - \Delta(\alpha)] + \tilde{\Gamma}_{\alpha}(\omega^{-})}.
$$
\n(3.27)

where **Here**  $\Delta(\alpha)$  and  $\tilde{\Gamma}_\alpha(\omega^-)$  are given by

$$
\Delta(\alpha) \approx \sum_{q} \sum_{\beta} \frac{f_{\alpha+1}(1-f_{\beta})}{f_{\alpha+1}-f_{\alpha}} C_{\alpha+1,\beta}^{\dagger} (C_{\beta,\alpha+1}-C_{\beta-1,\alpha}j_{\beta-1}^{+}/j_{\alpha}^{+})
$$
\n
$$
\times \left[ \frac{N_q \{1-\exp[\beta(\omega_{\alpha+1,\beta}+\omega_q)]\}}{\omega_{\alpha+1,\beta}+\omega_q} + \frac{(N_q+1)\{1-\exp[\beta(\omega_{\alpha+1,\beta}-\omega_q)]\}}{\omega_{\alpha+1,\beta}-\omega_q} \right]
$$
\n
$$
+ \sum_{q} \sum_{\beta} \frac{f_{\beta}(1-f_{\alpha})}{f_{\alpha+1}-f_{\alpha}} C_{\beta,\alpha}^{\dagger} (C_{\alpha,\beta}-C_{\alpha+1,\beta+1}j_{\beta}^{+}/j_{\alpha}^{+})
$$
\n
$$
\times \left[ \frac{N_q \{1-\exp[\beta(\omega_{\beta,\alpha}+\omega_q)]\}}{\omega_{\beta,\alpha}+\omega_q} + \frac{(N_q+1)\{1-\exp[\beta(\omega_{\beta,\alpha}-\omega_q)]\}}{\omega_{\beta,\alpha}-\omega_q} \right]
$$
\n
$$
+ \sum_{q} \sum_{\beta} \frac{f_{\beta}}{\omega_q} C_{\beta,\beta}^{\dagger} (C_{\alpha,\alpha}-C_{\alpha+1,\alpha+1}) \left[ 2N_q \sinh(\beta\omega_q) + 1 - \exp(-\beta\omega_q) \right]
$$

and

$$
i\tilde{\Gamma}_{\alpha}(\omega^{-}) \approx \sum_{q} \sum_{\beta \neq \alpha+1} C^{\dagger}_{\alpha+1,\beta}(C_{\beta,\alpha+1} - C_{\beta-1,\alpha}j^{\dagger}_{\beta-1}/j^{\dagger}_{\alpha}) \left[ \frac{1+N_{q}-f_{\beta}}{\omega^{-}-\omega_{\beta,\alpha}-\omega_{q}} + \frac{N_{q}+f_{\beta}}{\omega^{-}-\omega_{\beta,\alpha}+\omega_{q}} \right]
$$
  
+ 
$$
\sum_{q} \sum_{\beta \neq \alpha} C^{\dagger}_{\beta,\alpha}(C_{\alpha,\beta}-C_{\alpha+1,\beta+1}j^{\dagger}_{\beta}/j^{\dagger}_{\alpha}) \left[ \frac{1+N_{q}-f_{\beta}}{\omega^{-}-\omega_{\alpha+1,\beta}+\omega_{q}} + \frac{N_{q}+f_{\beta}}{\omega^{-}-\omega_{\alpha+1,\beta}-\omega_{q}} \right]
$$
  
+ 
$$
\sum_{q} \sum_{\beta} f_{\beta}(C^{\dagger}_{\alpha+1,\alpha}/j^{\dagger}_{\alpha})(j^{\dagger}_{\beta}C_{\beta,\beta+1}-j^{\dagger}_{\beta-1}C_{\beta-1,\beta}) \left[ \frac{1}{\omega^{-}-\omega_{q}} - \frac{1}{\omega^{-}+\omega_{q}} \right],
$$
(3.29)

where we have written the electron-phonon interaction matrix element as  $C_{\alpha,\beta}$  instead of  $C_{\alpha,\beta}(q)$  for brevity,<br>  $N_q \equiv [\exp(\beta(\epsilon_\alpha - \mu))] + 1]^{-1}$  is the Fermi-Dirac distribu-<br>  $f_\alpha \equiv [\exp(\beta(\epsilon_\alpha - \mu))] + 1]^{-1}$  is the Fermi-Dirac distribution function. The  $\omega$ -dependent part of the line-shape tion function. The  $\omega$ -dependent part of the line-shape<br>function shown in Eq. (3.29) is similar to the result of<br>Badjou and Argyres.<sup>18(e)</sup> It is to be noted that the present theory and the theory of Badjou and Argyres include the effects of exchange among moving electrons in the field of vibrating nuclei. Thus the Fermi-Dirac distribution funcviorating nuclei. Thus the Fermi-Dirac distribution func-<br>tion  $f_\beta$  is contained in the final results. If we put  $f_\beta=0$ , Eq. (3.29) is similar to the results of Ref. 21.

### IV. CONCLUSION

In the preceding section, starting with the diagonalplus-nondiagonal form of the density operator given in Eq. (2.16) and utilizing the isolation-projection technique, we obtained the dominant part of the line-shape function, which is free from divergence. The diagonal-plusnondiagonal form of the density operator was obtained by using the integral equation. The transformed density operator has the nondiagonal part, including the electron-phonon scattering potential, which is separated from the exponential form. This enables us to calculate straightforwardly the ensemble average of any operators for the system and make a suitable approximation based on our condition for the scattering potential. It is also to be noted that for the electron-phonon systems, the line shift  $\Delta(\alpha)$  due to the self-energy given in Eq. (3.28) is recovered through the transformed density operator.

The final result, the dominant part of the line-shape function given in Eq. (3.21), was obtained from Eq. (3.19), which is a more explicit form than our previous one.<sup>21</sup> For extremely weak interactions, if  $\Delta'$  of  $\tilde{\Gamma}_a (\omega^-)$  in Eq.  $(3.23)$  is replaced by  $P'$ , this part is identical to the expression of Badjou and Argyres.

It is expected that the present formalism can be applied to the system of electron-impurity interactions, if the electron-phonon scattering potential  $V$  is replaced by the electron-impurity scattering potential, and also the forced-balanced theory of resistivity, which has been recently issued.<sup>35,36</sup> We will leave these problems for future studies.

### ACKNOWLEDGMENTS

This research has been supported in part by the Korea Science and Engineering Foundation and the Center for Thermal and Statistical Physics at Korea University.

- <sup>1</sup>H. J. G. Meyer, Phys. Lett. 2, 259 (1962).
- <sup>2</sup>G. D. Mahan and J. J. Hopfield, Phys. Rev. Lett. 12, 241 (1964).
- <sup>3</sup>G. M. Larsen, Phys. Rev. 142, 428 (1966); D. H. Dickey, E. J. Johnson, and G. M. Larsen, Phys. Rev. Lett. 18, 599 (1967); G. M. Larsen, J. Phys. C 7, 2877 (1974); 7, 2890 (1974); Phys. Rev. 8 30, 4595 (1984).
- 4H. Scher and T. Holstein, Phys. Rev. 148, 598 (1966).
- 5(a) S.J. Miyake, J. Phys. Soc.Jpn. 20, 412 (1965);(b) Phys. Rev. 170, 726 (1968).
- ${}^{6}R$ . C. Enck, A. S. Saleyh, and H. Y. Fan, Phys. Rev. 182, 790 (1969).
- 7E. E. H. Shin, P. N. Argyres, and B. Lax, Phys. Rev. 8 7, 3572 (1973); E. E. H. Shin, P. N. Argyres, N. J. Horring, and B. Lax, ibid. 7, 5408 (1973).
- <sup>8</sup>J. P. Vigneron, R. Evrard, and E. Kartheuser, Phys. Rev. B 18, 6930 (1978); J. P. Vigneron, Solid State Commun. 32, 595 (1979).
- $9H$ . W. Goodwin and D. G. Seiler, Phys. Rev. B 27, 3451 (1983).
- <sup>10</sup>P. G. Harper, Proc. Phys. Soc. London 92, 793 (1967); C. J.

Summers, R. B. Dennis, B. S. Wherrett, P. G. Haper, and S. D. Smith, Phys. Rev. 170, 755 (1968).

- <sup>11</sup>C. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev. 98, 368 (1955).
- $^{12}$ M. Fukai, H. Kawamura, K. Sekido, and I. Imai, J. Phys. Soc. Jpn. 19, 30 (1964); O. Matsuda and E. Otsuka, J. Phys. Chem. Solids 40, 809 (1979); 40, 819 (1979).
- <sup>13</sup>A. Kawabata, J. Phys. Soc. Jpn. 23, 999 (1967); M. Saitoh and A. Kawabata, ibid. 23, 1006 (1967).
- $14(a)$  A. Lodder and S. Fujita, J. Phys. Soc. Jpn. 25, 774 (1968); {b) C. Raju and S. Fujita, Acta Phys. Austriaca 43, <sup>1</sup> (1975); (c) S. Fujita and A. Lodder, Physica 83B, 117 (1976); (d) A. Suzuki, S. D. Choi, and S. Fujita, J. Phys. Chem. Solids 41, 735 (1980); (e) S. D. Choi and S. Fujita, Solid State Commun. 37, 293 (1981).
- $15(a)$  A. Suzuki and D. Dunn, Phys. Rev. A 25, 2247 (1982); (b) Phys. Rev. 8 25, 7754 (1982); (c) D. Dunn and A. Suzuki, ibid. 29, 942 (1984); (d) A. Suzuki, ibid. 33, 1047 (1986); (e) Prog. Theor. Phys. 79, 343 (1988).
- W. G. Tam, Phys. Lett. 30A, 30 (1969).
- <sup>17</sup>V. M. Kenkre, Phys. Rev. A 7, 772 (1973).
- $18(a)$  P. N. Argyres and J. L. Sigel, Phys. Rev. Lett. 31, 1397 (1973); (b) Phys. Rev. B 9, 3197 (1974); (c) 10, 1139 (1974); (d) P. N. Argyres, Solid State Commun. 50, 297 (1984); (e) S. Badjou and P. N. Argyres, Phys. Rev. B 35, 5964 (1987).
- <sup>19</sup>R. Danzer and M. Kriechbaum, Acta Phys. Austriaca 49, 27 (1978).
- $20V$ . K. Arora, Phys. Rev. B 14, 679 (1976); V. K. Arora and H. N. Spector, Phys. Status Solidi B 94, 701 (1979); V. K. Arora, M. A. Al-Mass'ari, and M. Prasad, Phys. Rev. B 23, 5619 (1981).
- <sup>21</sup>S. D. Choi and O. H. Chung, Solid State Commun. 46, 717 (1983); J. Y. Ryu and S. D. Choi, Prog. Theor. Phys. 72, 429 (1984);J. Y. Ryu, Y. C. Chung, and S. D. Choi, Phys. Rev. B 32, 7769 (1985); S. N. Yi, O. H. Chung, and S. D. Choi, Prog. Theor. Phys. 77, 429 (1987); S. N. Yi, J. Y. Ryu, and S. D. Choi, ibid. 823, 299 (1989); J. Y. Ryu, S. N. Yi, and S. D. Choi, J. Phys. C 2, 3515 (1990).
- <sup>22</sup>J. V. Royen, J. D. Sitter, and J. T. Devreese, Phys. Rev. B 30, 7154 (1984).
- $23$ T. Ando and Y. Uemura, J. Phys. Soc. Jpn. 36, 959 (1974); T. Ando, ibid. 38, 989 (1975).
- <sup>24</sup>M. I. Dykman, Fiz. Tverd. Tela (Leningrad) 17, 3295 (1976) [Sov. Phys. Solid State 17, 2163 (1976)]; Phys. Status Solidi B

74, 547 (1976);88, 463 (1978).

- $25$ M. Prasad and S. Fujita, Solid State Commun. 21, 1105 (1977); M. Prasad, T. K. Srinivas, and S. Fujita, ibid. 24, 439 (1977).
- $^{26}$ C. S. Ting, S. C. Ying, and J. J. Quinn, Phys. Rev. Lett. 37, 215 (1976); Phys. Rev. B 16, 5394 (1977); K. S. Yi and J. J. Quinn, ibid. 27, 1184 (1983).
- $27A$ . Ishihara, M. Mukai, and S. J. Lee, Phys. Rev. B 26, 3279 (1982); Y. Shiwa and A. Ishihara, Solid State Commun. 53, 519 (1985)<sup>~</sup>
- M. Zaluzny, Phys. Rev. B 40, 8495 (1989).
- $29$ F. M. Peeters, Phys. Rev. Lett. 63, 2120 (1989); Xiaoguang Wu and F. M. Peeters, Phys. Rev. B41, 3109 (1990).
- <sup>30</sup>G. Y. Hu and R. F. O' Connell, Phys. Rev. B 40, 11 701 (1989).
- M. Singh, Phys. Rev. B 36, 5062 (1987); M. Singh and B. Tanatar, ibid. 41, 12781 (1990); B. Tanatar and M. Singh, ibid. 42, 3077 (1990).
- 32J. S. Bhat, S. S. Kubakaddi, and B. G. Mulimani, J. Appl. Phys. 70, 2216 (1991).
- 33K. D. Zhu and S. W. Gu, Phys. Lett. A 164, 465 (1992).
- <sup>34</sup>R. Kubo, J. Phys. Soc. Jpn. 12, 570 (1957).
- 35P. N. Argyres, Phys. Rev. B 39, 2982 (1989).
- $36R$ . S. Fishmann and G. D. Mahan, Phys. Rev. B 39, 2990  $(1989).$