Quantum transport theory based on the equilibrium density projection technique

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(Received 13 May 1996)

We introduce a projection technique, called the equilibrium density projection technique, which involves two schemes: the ensemble average projection scheme and the combined projection scheme. Using this technique directly on the Liouville equation, we derive the linear-nonlinear response formula. We also expand the scattering factors to a continued-fraction representation to avoid the danger of divergence, and expand again the continued-fraction representation formula in a series form. Finally, we introduce a simple example for the linear response term and compare the two schemes. [S1063-651X(97)13501-2]

PACS number(s): 02.50.−r, 05.40.+j

I. INTRODUCTION

Research in quantum transport theory is very important for investigation of microscopic phenomena of many-body systems. There are many theories in various methodologies, which are the Green function methods [3–10], the linear response formula from the quantum Liouville equation, [13–17], the quantum perturbation theories based on Boltzmann's transport equation [19], etc. Among those theories, many are based on the well known Kubo response theory [11–15]. Many of the theories use the projection technique to obtain a useful form of the scattering factor [12–18]. Although those theories are quite reasonable, the nonlinear behavior has been investigated in the limited scheme. Also, the problem of divergence in the expansion of the scattering factor has been discussed in some research [15]. On the other hand, by directly using a projection operator on the Liouville equation, Kenkre's group suggested a response function, which involves Kubo's theory as the lowest-order approximation [1]. Although their theory contains a nonlinear factor in the propagator, it is difficult to expand this term, since it is contained in the exponent.

Our group introduced a response function in many electron systems in which the nonlinear terms can be expanded by using the combined projection technique (CPT). We also suggested a continued fraction representation (CFR) of the scattering factor which is contained in the linear response function [2]. In this paper, we will derive a generalized linear-nonlinear response formula with the more compact symbols of elements, and expand the linear-nonlinear scattering factors to a CFR formula, which extend the former linear CFR formula to a nonlinear CFR formula. The projection operator used in this paper is different from Kenkre's, since it contains the mth order nonlinear index and the nth order CFR index. Futhermore, this technique involves two schemes, which are the ensemble average projection scheme (EAPS: the same as Kenkre's definition [1]) and the combined projection scheme (CPS) [2]. We call this the equilibrium density projection technique (EDPT) since it involves the equilibrium density operator as a projection direction. In Sec. II, we will derive the integrodifferential equation of a dynamic variable, and obtain a response function in Fourier-Laplace transformed space. In this first stage, the result contains a nonlinear response term which is not determined. In Sec. III, using the mth order nonlinear projection operator, we will obtain the nonlinear response terms in similar ways to Sec. II. In Sec. IV, we will expand the linear-nonlinear scattering factors to CFR [2,12–14,16] with the nth order projection operator to avoid any danger of divergence. And the CFR formula shall be expanded again in a series form for the sake of examining the convergence [20–23]. In Sec. V, we will introduce a simple example in an electron-impurity system, and compare the two schemes.

II. THE EXPECTATION VALUE OF A DYNAMIC VARIABLE BY A EQUILIBRIUM DENSITY PROJECTION TECHNIQUE (EDPT)

We consider a system of many-body systems which is subject to an oscillatory external field $\vec{E}(t)=\hat{\vec{e}}_l E_l \exp(-i\omega t)$, where $\hat{\vec{e}}_l$ is the unit vector in the external field direction ($l=x,y,z$, etc.) and ω is the angular frequency. Then the Hamiltonian $H(t)$ and the corresponding Liouville operator $L(t)$, respectively, are given by

$$H(t)=H_s+H'(t), \tag{2.1}$$

$$H'(t)\equiv R_l E_l(t)=R_l E_l \exp(-i\omega t) \tag{2.2}$$

and

$$L(t)=L_s+L_l'(t), \tag{2.3}$$

$$L_l'(t)=L_l' E_l(t), \tag{2.4}$$

where H_s and L_s are the time-independent part and L_l' corresponds to R_l, the response operator in the l direction ($l=x,y,z$, etc.), which implies that

$$L_l'(t)X=[R_l,X]E_l(t) \tag{2.5}$$

for an arbitrary operator X. The density operator for the system $\rho(t)$ can be written as

$$\rho(t)=\rho_s+\rho'(t), \tag{2.6}$$

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where ρ_s is the equilibrium density matrix. We can define the expectation value of arbitrary dynamic quantity R_k as

$$\overline{r_k}(t) \equiv \mathrm{Tr}\{R_k \rho(t)\} \equiv \sum_\alpha r_{k\alpha}(t), \tag{2.7}$$

where k is the direction index ($k=x,y,z$, etc.), Tr denotes the many-body trace, and

$$r_{k\alpha}(t) \equiv (R_k \rho(t))_{\alpha\alpha}. \tag{2.8}$$

In order to get a useful form of $\overline{r_k}(t)$ from the quantum Liouville equation, we define the projection operator in two types. The one is the ensemble average projection scheme (EAPS) introduced first by Kenkre [1] as

$$P_k^{\mathrm{tr}} X \equiv B_{kl}^{\mathrm{tr}} Tr\{R_k X\} \tag{2.9}$$

where

$$B_{kl}^{\mathrm{tr}} \equiv \frac{L_l' \rho_s}{Tr\{R_k L_l' \rho_s\}} \tag{2.10}$$

and using this we can obtain the expectation value of the dynamic quantity R_k as

$$\overline{r_k}(t) = P_k^{\mathrm{tr}} \rho(t) / B_{kl}^{\mathrm{tr}}. \tag{2.11}$$

The other type is the combined projection scheme (CPS) which was introduced by our group [2] as

$$P_k^\alpha X \equiv B_{kl}^\alpha (R_k X)_{\alpha\alpha}, \tag{2.12}$$

where

$$B_{kl}^\alpha \equiv \frac{L_l' \rho_s}{(R_k L_l' \rho_s)_{\alpha\alpha}} \tag{2.13}$$

and using this we can obtain

$$\overline{r_k}(t) = \sum_\alpha P_k^\alpha \rho(t) / B_{kl}^\alpha. \tag{2.14}$$

These two schemes are useful in a description of real systems and have some merits in calculating the scattering mechanism as shown in Sec. V. Here we will write the two projection schemes in a unified notation as

$$P_{k0} X \equiv B_{kl0}((R_k X)), \tag{2.15}$$

where the symbol (( )) is Tr { } in the EAPS scheme, and is $(\ )_{\alpha\alpha}$ in the CPS. This projection technique shall be called the equilibrium density projection technique (EDPT), since B_{kl0} includes ρ_s. We define the dynamic variable $r_k(t) \equiv ((R_k \rho(t))) = P_{k0}\rho(t)/B_{kl0}$, which can be $\overline{r_k}(t)$ in the EAPS and $r_{k\alpha}(t)$ in the CPS. We can obtain $r_k(t)$ by using P_{k0} and it's Abelian inverse $P_{k0}' \equiv 1 - P_{k0}$. From the Liouville equation we have

$$i\hbar \frac{\partial P_{k0}\rho'(t)}{\partial t} = P_{k0} L_s P_{k0} \rho'(t) + P_{k0} L_s P_0' \rho'(t) + \{P_{k0} D_0'(t) + P_{k0} D_0\} E_l(t), \tag{2.16}$$

$$i\hbar \frac{\partial P_{k0}'\rho'(t)}{\partial t} = P_{k0}' L_s P_{k0}' \rho'(t) + P_{k0}' L_s P_{k0} \rho'(t) + \{P_{k0}' D_0'(t) + P_{k0}' D_0\} E_l(t), \tag{2.17}$$

where

$$D_{l0} \equiv L_l' \rho_s \tag{2.18}$$

and

$$D_{l0}'(t) \equiv L_l' \rho'(t). \tag{2.19}$$

In order to expand the quantity in terms of the equilibrium density ρ_s and remove the fourth term in Eq. (2.17), we define the projection direction B_{kl0} as

$$B_{kl0} \equiv \frac{L_l' \rho_s}{\Lambda_{kl0}} \equiv \frac{D_{l0}}{\Lambda_{kl0}}, \tag{2.20}$$

where

$$\Lambda_{kl0} \equiv ((R_k D_{l0})). \tag{2.21}$$

It is to be noted that the direction of this projection is $L_l' \rho_s$ and the projection is time independent. We assume that the perturbation of the system may be expanded as [2]

$$D_{l0}'(t) \equiv D_{l0} \frac{((R_k D_{l0}'(t)))}{((R_k D_{l0}))}. \tag{2.22}$$

Thus the solution of Eq. (2.17) can be

$$P_{k0}'\rho'(t) = \left(\frac{-i}{\hbar}\right) \int_0^t ds G_{k0}(t-s) P_{k0}' L_s P_{k0} \rho'(s). \tag{2.23}$$

Here the propagator is

$$G_{k0}(\tau) = \exp(-i\tau P_{k0}' L_s / \hbar), \tag{2.24}$$

where $\tau \equiv t - s$. Substituting Eq. (2.23) into Eq. (2.16), we obtain an integrodifferential equation for $r_k(t)$ as

$$\frac{\partial r_k(t)}{\partial t} = A_{kl0} r_k(t) - \int_0^t Q_{kl0}(t-s) r_k(s) ds - (i/\hbar)\Lambda_{kl0} E_l(t) - (i/\hbar) r_k^1(t), \tag{2.25}$$

where $r_k(0) = 0$ for the initial condition and

$$A_{kl0} \equiv \frac{-i}{\hbar \Lambda_{kl0}} ((R_{k1} D_0)), \tag{2.26}$$

$$R_{k1} \equiv R_k L_s, \tag{2.27}$$

$$Q_{kl0}(\tau) \equiv \frac{1}{\hbar^2 \Lambda_{kl0}} ((R_{k1} f_1(\tau))), \tag{2.28}$$

$$f_1(\tau) \equiv G_{k0}(\tau) f_1, \tag{2.29}$$

$$f_1 \equiv L_1 D_0, \tag{2.30}$$

$$L_1 \equiv (1 - P_{k0}) L_s \equiv P'_{k0} L_s, \tag{2.31}$$

$$r_k^1(t) \equiv ((R_k^1 \rho'(t))) E_l(t), \tag{2.32}$$

$$R_k^1 \equiv R_k L'_l. \tag{2.33}$$

Equation (2.25) is the kinetic equation which shows the time evolution of the dynamical variable. The first three terms on the right hand side are of linear response, but the last term gives nonlinearity. We now express the behavior of the dynamical variable in the Fourier-Laplace transformed space. The Fourier-Laplace transform $\mathcal{T}_{\rm FL}$ of a time-dependent function $X(t)$ is defined as

$$\widetilde{X}(z) \equiv \mathcal{T}_{\rm FL}[X(t)] = \int_0^\infty \exp(-izt) X(t) dt.$$

Then by applying the convolution theorem, the $\tau_{\rm FL}$ of Eq. (2.25) turns out to be

$$\widetilde{r}_k(z) = \frac{-(i/\hbar)\Lambda_{kl0}\widetilde{E}_l(z)}{iz - A_{kl0} + \widetilde{Q}_{kl0}(z)} + \frac{-(i/\hbar)\widetilde{r}_k^1(z)}{iz - A_{kl0} + \widetilde{Q}_{kl0}(z)} \tag{2.34}$$

where $\widetilde{r}_k(z)$, $\widetilde{Q}_{kl0}(z)$, $\widetilde{E}_l(z)$ and $\widetilde{r}_k^1(z)$, respectively, are the $\mathcal{T}_{\rm FL}$ of $r_k(t)$, $Q_{kl0}(t)$, $E_l(t)$ and $r_k^1(t)$. The last term, which shows the nonlinearity, shall be dealt with in a similar way in Sec. III.

III. THE KINETICS OF THE *m*TH-ORDER NONLINEAR RESPONSE

We can reform Eq. (2.34) as

$$\widetilde{r}_k(z) = T_{kl0}^0 \Lambda_{kl0} \widetilde{E}_l(z) + T_{kl0}^0 \widetilde{r}_k^1(z), \tag{3.1}$$

where

$$T_{kl0}^0 \equiv \frac{-(i/\hbar)}{iz - A_{kl0} + \widetilde{Q}_{kl0}(z)} \tag{3.2}$$

and can guess that the nonlinear part can be expanded systematically further as in the previous papers [2]. In order to expand the nonlinear part , we define the mth-order nonlinear projection operator P_{k0}^m and it's Abelian inverse $P_{k0}^{m'}$ as

$$P_{k0}^m X \equiv B_{kl0}^m(t)((R_k^m (E_l(t))^m X)), \tag{3.3}$$

$$P_{k0}^{m'} \equiv 1 - P_{k0}^m, \tag{3.4}$$

where

$$R_k^m \equiv R_k (L'_l)^m; \tag{3.5}$$

and we choose $B_{kl0}^m(t)$ as

$$B_{kl0}^m(t) \equiv \frac{D_{l0}}{\Lambda_{kl0}^m (E_l(t))^m}, \tag{3.6}$$

where

$$\Lambda_{kl0}^m \equiv ((R_k^m D_{l0})). \tag{3.7}$$

In a similar way as Eq. (2.22), we assume that

$$D'_{l0}(t) = D_{l0} \frac{((R_k^m D'_{l0}(t)))}{((R_k^m D_{l0}))}. \tag{3.8}$$

Then with a similar procedure from Eq. (2.16) to Eq. (2.34), we have the expectation value of the mth order nonlinear response function in z space as

$$\widetilde{r}_k{}^m(z) = \frac{-(i/\hbar)\Lambda_{kl0}^m \widetilde{E}_l{}^{m+1}(z)}{iz - A_{kl0}^m + \widetilde{Q}_{kl0}^m(z)} + \frac{-(i/\hbar)\widetilde{r}_k{}^{m+1}(z)}{iz - A_{kl0}^m + \widetilde{Q}_{kl0}^m(z)}, \tag{3.9}$$

where

$$A_{kl0}^m \equiv m(i\omega) + \frac{-i}{\hbar \Lambda_{kl0}^m ((R_{k1}^m D_0))}, \tag{3.10}$$

$$R_{k1}^m \equiv R_k^m L_s \tag{3.11}$$

and $\widetilde{Q}_{kl0}^m(z)$ is the $\mathcal{T}_{\rm FL}$ of $Q_{kl0}^m(\tau_m)$, given as

$$Q_{kl0}^m(\tau_m) \equiv \frac{1}{\hbar^2 \Lambda_{kl0}^m} ((R_{k1}^m f_1^m(\tau_m))), \tag{3.12}$$

where $\tau_m = t - s_m$ and

$$f_1^m(\tau_m) \equiv G_{k0}^m(\tau_m) f_1^m, \tag{3.13}$$

$$G_{k0}^m(\tau_m) = \exp(-i\tau_m P_{k0}^{m'} L_s/\hbar) \tag{3.14}$$

$$f_1^m \equiv L_1^m D_0, \tag{3.15}$$

$$L_1^m \equiv (1 - P_{k0}^m) L_s \equiv P_{k0}^{m'} L_s, \tag{3.16}$$

$$r_k^{m+1}(t) \equiv ((R_k^{m+1} \rho'(t))) E_l^{m+1}(t), \tag{3.17}$$

$$R_k^{m+1} \equiv R_k (L'_l)^{m+1}. \tag{3.18}$$

Substituting successively Eq. (3.9) into Eq. (3.1), we have the linear-nonlinear response function in z space as

$$\widetilde{r}_k(z) = \sum_{m=0}^{\infty} \left\{ \left(\prod_{j=0}^{m} T_{kl0}^j \right) \Lambda_{kl0}^m \widetilde{E}_l^{m+1}(z) \right\}, \tag{3.19}$$

where

$$T_{kl0}^j \equiv \frac{-(i/\hbar)}{iz - A_{kl0}^j + \widetilde{Q}_{kl0}^j(z)}. \tag{3.20}$$

Here the first term, $m=0$, is the linear response. If the system is subject to an oscillatory external field $E(t) = E_l(0)\exp(-i\omega t)$, we have the $\mathcal{T}_{\rm FL}$ of $j+1$th degree of it, as

$$\widetilde{E}^{j+1}(z)=\left[1-\sum_{k=0}^{\infty}(-1)^k\{ij\omega(iz+i\omega)^{-1}\}^k\right]E_0^j\widetilde{E}(z), \tag{3.21}$$

and Eq. (3.19) can be rewritten as

$$\widetilde{r}_k(z)=\widetilde{\chi}_{kl}\widetilde{E}(z), \tag{3.22}$$

where

$$\widetilde{\chi}_{kl}(z)=\sum_{m=0}^{\infty}\left[\left(\prod_{j=0}^{m}T_{kl0}^j\right)\times\Lambda_{kl0}^m\left[1-\sum_{k=0}^{\infty}(-1)^k\{ij\omega(iz+i\omega)^{-1}\}^k\right]E_0^j\right], \tag{3.23}$$

which is the linear($m=0$) and nonlinear($m\geqslant 1$) susceptibility in the z space.

IV. THE CONTINUED FRACTION REPRESENTATION (CFR) OF THE LINEAR-NONLINEAR SCATTERING FACTORS, $\widetilde{Q}_{kl0}^m(Z)$

The time-independent Liouville operator L_s is composed of diagonal part L_d and nondiagonal part L_v as $L_s=L_d+L_v$. There are many studies to expand $\widetilde{G}_{kl0}^m(z)$ in series expansion for the diagonal propagator $\widetilde{G}_d\equiv(iz-L_d)^{-1}$, such as $\widetilde{G}\equiv\widetilde{G}_d\Sigma_n(\widetilde{G}_dP'L_v)^n$ [16]. But this manipulation may provoke danger of divergence at resonance peak, $\omega=\omega_0$ [15]. To avoid this danger we like to expand $\widetilde{G}$ in a continued fraction form [2,12–16]. We start with the equation of motion for $f_1^m(\tau_m)$ in Eq. (3.12)

$$\frac{\partial f_1^m(\tau_m)}{\partial\tau_m}=\left(\frac{-i}{\hbar}\right)L_1^mf_1^m(\tau_m), \tag{4.1}$$

with the definitions of Eqs. (3.13)–(3.18). We can separate it as

$$f_1^m(\tau_m)=f_1^m+f_1^{m'}(\tau_m) \tag{4.2}$$

and in order to obtain $\widetilde{Q}_{kl0}^m(z)$, we define the projection operator P_{k1}^m and it's Abelian inverse as

$$P_{k1}^mX=B_{kl1}^m((R_{k1}^mX)), \tag{4.3}$$

$$P_{k1}^{m'}X\equiv(1-P_{k1}^m)X, \tag{4.4}$$

such that

$$\hbar^2\Lambda_{kl0}^mQ_{kl0}^m(\tau_m)=((R_{k1}^mf_1^m(\tau_m)))=((R_{k1}^mf_1^m))+(1/B_{k1}^m)(P_{k1}^{m'}f_1^m(\tau_m)), \tag{4.5}$$

where we will choose the projection direction B_{kl1}^m later. We now separate Eq. (4.1) with help of this projection operator as

$$\frac{\partial P_{k1}^mf_1^{m'}(\tau_m)}{\partial\tau_m}=\left(\frac{-i}{\hbar}\right)P_{k1}^mD_{l1}^m+\left(\frac{-i}{\hbar}\right)P_{k1}^mL_1^mP_{k1}^mf_1^{m'}(\tau_m)+\left(\frac{-i}{\hbar}\right)P_{k1}^mL_1^mP_{k1}^{m'}f_1^{m'}(\tau_m), \tag{4.6}$$

$$\frac{\partial P_{k1}^{m'}f_1^{m'}(\tau_m)}{\partial\tau_m}=\left(\frac{-i}{\hbar}\right)P_{k1}^{m'}D_{l1}^m+\left(\frac{-i}{\hbar}\right)P_{k1}^{m'}L_1^mP_{k1}^{m'}f_1^{m'}(\tau_m)+\left(\frac{-i}{\hbar}\right)P_{k1}^{m'}L_1^mP_{k1}^mf_1^{m'}(\tau_m), \tag{4.7}$$

where

$$D_{l1}^m\equiv L_1^mf_1^m. \tag{4.8}$$

In order to expand with respect to the equilibrium density ρ_s through D_{l1}^m and to remove the first term of Eq. (4.7), we define the projection direction B_{kl1}^m as

$$B_{kl1}^m\equiv\frac{D_{l1}^m}{\Lambda_{kl1}^m}, \tag{4.9}$$

where

$$\Lambda_{kl1}^m\equiv((R_{k1}^mD_{l1}^m)). \tag{4.10}$$

So, we obtain from Eq. (4.7)

$$P_{k1}^{m'}f_1^{m'}(\tau_m)=-(i/\hbar)\int_0^{\tau_m}K_1^m(\tau_m-h)P_{k1}^{m'}L_1^mP_{k1}^mf_1^{m'}(\tau_m)dh, \tag{4.11}$$

where the new propagator is

$$K_1^m(\tau_m-h)=\exp(-i(\tau_m-h)P_{k1}^{m'}L_1^m/\hbar). \tag{4.12}$$

Substituting Eq. (4.11) into Eq. (4.6), we can obtain the integrodifferential equation as

$$\frac{\partial((R_{k1}^mf_1^{m'}(\tau_m)))}{\partial\tau_m}=-\left(\frac{i}{\hbar}\right)\Lambda_{kl1}^m-\left(\frac{i}{\hbar\Lambda_{kl1}^m}\right)((R_{k2}^mD_1^m))((R_{k1}^mf_1^{m'}(\tau_m)))-\left(\frac{1}{\hbar^2\Lambda_{kl1}^m}\right)\left(\left(R_{k2}^m\int_0^{\tau_m}f_2^m(\tau_m-h)dh\right)\right)\times((R_{k1}^mf_1^{m'}(\tau_m))), \tag{4.13}$$

where

$$R_{k2}^m\equiv R_{k1}^mL_1^m, \tag{4.14}$$

$$f_2^m(\tau_{m1})\equiv K_1^m(\tau_m-h)f_2^m, \tag{4.15}$$

$$f_2^m \equiv P_{k1}^{m'} L_1^m D_1^m \equiv L_2^m D_1^m, \tag{4.16}$$

$$L_2^m \equiv P_{k1}^{m'} L_1^m \tag{4.17}$$

and we can obtain the solution of Eq. (4.13) in the z space from $\mathcal{T}_{\mathrm{FL}}$ utilizing the convolution theorem, as

$$((R_{k1}^m \widetilde{f}_1^{m'}(z))) = \frac{-\left(\frac{1}{z\hbar}\right)\Lambda_{kl1}^m}{iz + \left(\frac{i}{\hbar\Lambda_{kl1}^m}\right)((R_{k2}^m D_1^m)) + \widetilde{Q}_{kl1}^m(z)}, \tag{4.18}$$

where

$$\widetilde{Q}_{kl1}^m(z) \equiv \left(\frac{1}{\hbar^2\Lambda_{kl1}^m}\right)((R_{k2}^m \widetilde{f}_2^m(z))), \tag{4.19}$$

so, we have

$$\widetilde{Q}_{kl0}^m(z) = \frac{-i}{z\hbar^2\Lambda_{kl0}^m}((R_{k1}^m f_1^m)) + \frac{\left(\frac{-1}{z\hbar^3\Lambda_{kl0}^m}\right)\Lambda_{kl1}^m}{iz + \left(\frac{i}{\hbar\Lambda_{kl1}^m}\right)((R_{k2}^m D_1^m)) + \widetilde{Q}_{kl1}^m(z)}, \tag{4.20}$$

since

$$\widetilde{f}_1{}^m(z) = \int_0^\infty e^{-izt}[f_1^m + f_1^{m'}(\tau)]dt = \frac{1}{iz} f_1^m + f_1^{m'}(z). \tag{4.21}$$

We can obtain a similar form of $\widetilde{Q}_{kl1}^m(z)$ by repeating the similar procedure. The $n-1$th-order CFR form is obtained as

$$\widetilde{Q}_{kl(n-1)}^m(z) \equiv \frac{1}{\hbar^2\Lambda_{kl(n-1)}^m}((R_{kn}^m \widetilde{f}_n^m(z))) = \frac{-i}{z\hbar^2\Lambda_{kl(n-1)}^m}((R_{kn}^m f_n^m)) + \frac{\left(\frac{-1}{z\hbar^3\Lambda_{kl(n-1)}^m}\right)\Lambda_{kln}^m}{iz + \left(\frac{i}{\hbar\Lambda_{kln}^m}\right)((R_{k(n+1)}^m D_n^m)) + \widetilde{Q}_{kln}^m(z)}, \tag{4.22}$$

with the definitions

$$P_{kn}^m X \equiv \frac{D_n^m}{\Lambda_{kln}^m}((R_{kn}^m X)), \tag{4.23}$$

$$D_n^m \equiv L_n^m f_n^m, \quad (n \geqslant 1) \tag{4.24}$$

$$\Lambda_{kln}^m \equiv ((R_{kn}^m D_n^m)), \quad (n \geqslant 1) \tag{4.25}$$

$$R_{kn}^m \equiv R_{k(n-1)}^m L_{n-1}^m, \quad (n \geqslant 2) \tag{4.26}$$

$$L_n^m \equiv P_{k(n-1)}^{m'} L_{n-1}^m, \quad (n \geqslant 2) \tag{4.27}$$

$$f_n^m \equiv L_n^m D_{n-1}^m, \quad (n \geqslant 2) \tag{4.28}$$

$$\widetilde{Q}_{kln}^m(z) \equiv \frac{1}{\hbar^2\Lambda_{kln}^m}((R_{k(n+1)}^m \widetilde{f}_{n+1}^m(z))), \quad (n \geqslant 1) \tag{4.29}$$

$$\widetilde{f}_n^m(z) = \frac{\hbar}{iz - iL_n^m} f_n^m, \quad (n \geqslant 2). \tag{4.30}$$

Substituting repeatedly nth order to $n-1$th order, we can expand the linear scattering factor $\widetilde{Q}_{kl0}(z)$, where $m=0$ and the nonlinear scattering factors $\widetilde{Q}_{kl0}^m(z)$, where $m \geqslant 1$, to compact CFR form as

$$\widetilde{Q}_{kl0}^m(z) = i\gamma_0^m + \cfrac{i\Delta_1^m}{iz + i\omega_1^m + i\gamma_1^m + \cfrac{i\Delta_2^m}{iz + i\omega_2^m + i\gamma_2^m + \cfrac{i\Delta_3^m}{iz + i\omega_3^m + i\gamma_3^m}}} \ddots + \cfrac{i\Delta_{n-2}^m}{iz + i\omega_{n-2}^m + i\gamma_{n-2}^m + \cfrac{i\Delta_{n-1}^m}{iz + i\omega_{n-1}^m + i\gamma_{n-1}^m + \cfrac{i\Delta_n^m}{iz + i\omega_n^m + \widetilde{Q}_{kln}^m(z)}}}, \tag{4.31}$$

where

$$\gamma_n^m \equiv \frac{-1}{z\hbar^2\Lambda_{kln}^m}((R_{k(n+1)}^m f_{n+1}^m)), \quad (n\geqslant 0) \tag{4.32}$$

$$\Delta_n^m \equiv \left(\frac{i}{z\hbar^3\Lambda_{kl(n-1)}^m}\right)\Lambda_{kln}^m, \quad (n\geqslant 1) \tag{4.33}$$

$$\omega_n^m \equiv \left(\frac{1}{\hbar\Lambda_{kln}^m}\right)((R_{k(n+1)}^m D_n^m)), \quad (n\geqslant 1). \tag{4.34}$$

In this expansion, since the diagonal propagator G_d is not included in the elements of $\tilde{Q}_{kl0}^m(z)$, we can expand this form to series of γ_n^m, Δ_n^m, and ω_n^m with no danger of divergency [23]. For series expansion, we define

$$\Gamma_n^m \equiv \frac{i\Delta_n^m}{iz+i\omega_n^m+i\gamma_n^m+\Gamma_{n+1}^m} \tag{4.35}$$

and

$$K_n^m = \frac{1}{iz+i\omega_n^m+i\gamma_n^m}, \tag{4.36}$$

so, we can expand Γ_n^m s, as

$$\Gamma_n^m = i\Delta_n^m K_n^m \sum_{s=0}^{\infty}(-1)^s(\Gamma_{n+1}^m K_n^m)^s. \tag{4.37}$$

Thus we can reform the scattering factor $\tilde{Q}_{kl0}^m(z)$ as

$$\begin{aligned}\tilde{Q}_{kl0}^m(z) = {} & i\gamma_0^m + (i\Delta_1^m)K_1^m \sum_{r=0}^{\infty}(-1)^r \Bigg[K_1^m (i\Delta_2^m) K_2^m \\ & \times \sum_{s=0}^{\infty}(-1)^s \Bigg\{ K_2^m (i\Delta_3^m) K_3^m \\ & \times \sum_{c=0}^{\infty}(-1)^c (K_3^m \Gamma_4)^c \Bigg\}^s \Bigg]^r \\ \approx {} & i\gamma_0^m + (i\Delta_1^m)K_1^m - \sum_{r=2}^{\infty}(-1)^r \Bigg\{ \Bigg[\prod_{s=1}^{r}(i\Delta_s^m) \Bigg] \\ & \times \Bigg[\prod_{s=1}^{r-1}(K_s^m)^2 \Bigg] K_r^m \Bigg\} + \cdots . \end{aligned} \tag{4.38}$$

In order words, we can expand the scattering factor $\tilde{Q}_{kl0}^m(z)$ in series form with Δ_n^m and K_n^m. We expect, in a weak perturbed system, that we can examine the convergency in the first several terms easily.

V. AN EXAMPLE AND DISCUSSION OF THE TWO SCHEMES

In order to illustrate and compare the two schemes, the CPS and EAPS, we consider a system of many electrons which is subject to an oscillatory electric field $\vec{E} = \hat{\vec{e}}_l E_l(0)\exp(-i\omega t)$, where $\hat{\vec{e}}_l$ is the unit vector in the electric field direction $l(l=x,y,z,$ etc.) and ω is the angular frequency. In this system the response operator R_l in Eq. (2.2) can be $-P_l$, where $-P_l \equiv \Sigma_i e_i r_{li}$ is the polarization, and the corresponding Liouville operator $L(t)$ in Eq. (2.5) is given by

$$L'(t)X = -[P_l, X]E_l(t) \tag{5.1}$$

for an arbitrary operator X. We consider a system of electrons in isotropic semiconductors which interact weakly with background impurities and assume that the electron-electron interaction is absent. For a static magnetic field $\vec{B}$ applied in the z axis, the electron energy is quantized. If, in addition, a microwave of angular frequency ω is applied along the z direction, the electromagnetic energy is absorbed at $\omega \approx \omega_c$, ω_c being the cyclotron frequency, i.e., the cyclotron transition arises. The Liouville operator L_s in Eq. (2.3) can be written as

$$L_s = L_e + L_v, \tag{5.2}$$

where L_e and L_v are the Liouville operators corresponding to the electron Hamiltonian H_e and the scattering potential V, respectively. If the microwave is circularly polarized, the absorption power is proportional to the real part of the conductivity tensor $\sigma_{kl}(\omega)$ with $k=-$ and $l=+$, for which the dynamic variable R_k in this system is the current J^-, as

$$(R_k)_{\alpha\beta} \equiv J^-_{\alpha,\alpha+1}\delta_{\beta,\alpha+1}. \tag{5.3}$$

And using the Kubo identity [2,13] we have

$$(L'\rho_s)_{\beta\alpha} \equiv (D_{l0})_{\beta\alpha} = -\Delta F_{\beta,\alpha} J^+_{\alpha+1,\alpha}\delta_{\beta,\alpha+1}. \tag{5.4}$$

Here $J^{\pm} = J_x \pm iJ_y$, $\Delta F_{\beta,\alpha} \equiv (F_\beta - F_\alpha)/\epsilon_{\beta\alpha}$ and $\epsilon_{\beta\alpha} \equiv \epsilon_\beta - \epsilon_\alpha$, where ϵ_α is the energy eigenvalue and F_α the Fermi-distribution function for the state $|\alpha\rangle \equiv |N,\vec{k}\rangle$, N being the Landau index and $\vec{k}$ the electron wave vector.

A. CPS

Applying the CPS, we obtain [2]

$$\Lambda_{kl0}^\alpha = -i\Delta F_{\alpha+1,\alpha} J^-_{\alpha,\alpha+1} J^+_{\alpha+1,\alpha}, \tag{5.5}$$

$$A_{kl0}^\alpha = -i\epsilon_{\alpha+1,\alpha} = -i\omega_c. \tag{5.6}$$

Thus we have the linear conductivity in the CPS as

$$\tilde{\sigma}_{kl}(\omega) = \sum_\alpha \tilde{\sigma}_{kl}^\alpha(\omega) = -i\hbar\sum_\alpha \frac{\Delta F_{\alpha+1,\alpha} J^-_{\alpha,\alpha+1} J^+_{\alpha+1,\alpha}}{(\hbar\omega - \hbar\omega_c) - i\hbar\tilde{Q}_{kl0}^\alpha(\omega)}, \tag{5.7}$$

where $\mathrm{Re}(\tilde{\sigma}_{kl}(\omega)) > 0$ since $\Delta F_{\alpha+1,\alpha} < 0$, and the scattering factor $\tilde{Q}_{kl0}^\alpha(\omega)$ with the definition of Eq. (2.28) is given as

$$\tilde{Q}_{kl0}^\alpha(\omega) \equiv \frac{1}{\hbar^2\Lambda_{kl0}^\alpha}[R_{k1}\tilde{f}_1(\omega)]_{\alpha\alpha} \equiv i\Delta(\alpha,\omega) + \gamma(\alpha,\omega), \tag{5.8}$$

which can be calculated further in a similar manner. In Eq. (5.8), the imaginary part $\Delta(\alpha,\omega)$ is the line shift and the real

part $\gamma(\alpha,\omega)$ is the half width of the broadening due to the scattering. We can obtain the absorption power, neglecting the line shift, as

$$P(\omega)=\frac{1}{2}\mathrm{Re}(\sigma E^2)\propto \mathrm{Re}(\sigma(\omega)) =\sum_{\alpha}\frac{|\Delta F_{\alpha+1,\alpha}||J^{+}_{\alpha+1,\alpha}|^2\gamma(\alpha,\omega)}{(\omega-\omega_c)^2+\gamma^2(\alpha,\omega)}, \tag{5.9}$$

where ''Re'' means the real part. In the quantum limit where $\hbar\omega_c \gg k_B T$, almost all the electrons are in the ground state, $|\alpha\rangle=|0,k_z\rangle$. Hence, the most important contribution to the absorption power comes from transition between the Landau level $N=0$ and $N=1$, so we can get the absorption power as

$$P(\omega)\propto\int dk_z\frac{|\Delta F_{\alpha+1,\alpha}||J^{+}_{\alpha+1,\alpha}|^2\gamma(0,k_z,\omega)}{(\omega-\omega_c)^2+\gamma^2(0,k_z,\omega)} \tag{5.10}$$

and thus in the CPS, we cannot obtain the half width directly, but can get it in the absorption power through integrating for k_z in Eq. (5.10). Even though the CPS has the merit of calculating the power in the feature, it is acompanied by the difficulty of integration.

B. EAPS

In the EAPS, the form of the conductivity is given by

$$\widetilde{\sigma}_{kl}(\omega)=\frac{-(i/\hbar)\Lambda^{\mathrm{tr}}_{kl0}}{iz-A^{\mathrm{tr}}_{kl0}+\widetilde{Q}^{\mathrm{tr}}_{kl0}(\omega)}\equiv\frac{-(i/\hbar)\sum_{\alpha}\Lambda^{\alpha'}_{kl0}}{iz-\sum_{\alpha}A^{\alpha'}_{kl0}+\sum_{\alpha}\widetilde{Q}^{\alpha'}_{kl0}(\omega)}, \tag{5.11}$$

where the prime indicates that the projection operator P^{tr}_k is used instead of P^{α}_k in the calculation of A^{α}_{kl} and $\widetilde{Q}^{\alpha}_{kl}(\omega)$. Note that the sum over the state $|\alpha\rangle$ appears separately in the numerator and the denominator. In this scheme, it is difficult to calculate each factor because P^{tr}_k includes the sum of the states. But in some appropriate systems, if the most considerable state can be fixed , as $|\alpha\rangle=|0,k_z\rangle$ in the quantum limit, the state calculation is reduced to CPS since the definition of P^{tr}_k is reduced to P^{α}_k in this case, while the form of conductivity is different. If $|\alpha\rangle=|0,k_z\rangle$ and the most important contribution to the absorption power comes from transition between the Landau level $N=0$ and $N=1$, the form of the conductivity in the EAPS is

$$\widetilde{\sigma}_{kl}(\omega)=\frac{i\int dk_z\Delta F(1,0,k_z)|J_{0,1}|^2}{(\omega-\omega_c)-i\int dk_z\widetilde{Q}^{\alpha'}_{kl0}(0,k_z,\omega)} \tag{5.12}$$

and so, in this scheme, the line shift $\Delta(\alpha,\omega)$ is the integration of the imaginary part of $\widetilde{Q}^{\alpha}_{kl}(\omega)$ and the half width $\gamma(\alpha,\omega)$ is the integration of the real part of $\widetilde{Q}^{\alpha}_{kl}(\omega)$, as

$$\int dk_z\widetilde{Q}^{\alpha'}_{kl0}(0,k_z,\omega)\equiv i\Delta(0,k_z,\omega)+\gamma(0,k_z,\omega). \tag{5.13}$$

If we neglect the shift, the absorption power is obtained as

$$P(\omega)\propto\frac{\gamma(0,k_z,\omega)\int dk_z|\Delta F_{1,0}||J^{+}_{1,0}|^2}{(\omega-\omega_c)^2+\gamma^2(0,k_z,\omega)}, \tag{5.14}$$

where

$$\gamma(0,k_z,\omega)\equiv\int dk_z\mathrm{Re}\widetilde{Q}^{\alpha'}_{kl0}(0,k_z,\omega) \tag{5.15}$$

so it is not necessary to calculate the absorption power to obtain the line width. The line width $\gamma(0,k_z,\omega)$ is merely the k_z integration of the real part of $\widetilde{Q}^{\alpha'}_{kl}(\omega)$ in Eq. (5.15). The sacttering factor $\widetilde{Q}^{\alpha}_{kl}(\omega)$ was introduced in the lowest- order CFR in our previous work. [2]

VI. CONCLUSION

In this paper, we have obtained the general response function using the EDPT which contains two schemes, the EADS and CPS, in Secs. II and III. The response function involves a linear response term and nonlinear response terms.

In Sec. IV, we have expanded the scattering factors, which are contained in the linear and nonlinear response functions, in a continued fraction representations(CFRs) using the more general projection operators. So, we could avoid any danger of divergence in expanding the propagators in series form, and we expanded the CFR again to a form useful for examining the convergence. Thus in real systems, we expect to be able to make a cutoff in the CFR with the proper degree of the strength of interactions. Finally, in Sec. V, we compared the two schemes in a simple interacting system, discussed their merits and difficulties in obtaining the absorption power and line broadening, and showed the simple result of $\widetilde{Q}^{\alpha}_{kl}(\omega)$ in two schemes.

ACKNOWLEDGEMENTS

This research has been supported by KOSEF (1996) and by Korea Ministry of Education (BSRI 96-2405).

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