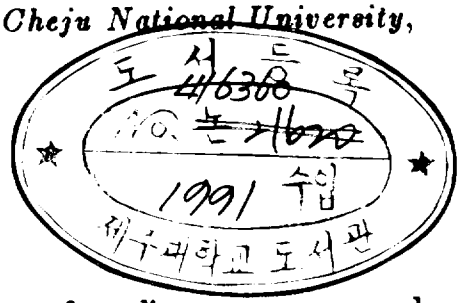
Theory of Nonlinear Transport for Electron–Impurity Systems in Very High Fields

Jai Yon Ryu, Nam Kyu Hyun, and Jeong Dae Ko
Department of Physics, Cheju National University, Cheju 690 – 756



ABSTRACT

Starting with Tani's theory of nonlinear response and using the operator method introduced by Argyres and Sigel, the field–dependent self–energy for a weak electron–impurity coupling is derived. The result in the lowest order approximation is identical with that of Suzuki.

1. INTRODUCTION

In recent years the behavior of electrons in very high electric (and magnetic) fields has received considerable attention in connection with the remarkable advance in technology of crystal growth and device processing. Therefore, the study on this problem has become one of the subjects of active theoretical and experimental investigations[1–14].

Theoretically, many analytical[4–11] and numerical[12–14] attempts have been made in order to develop the theories which would be capable of including a variety of high field effects. Through these intense studies, some new transport phenomena, such as collisional broadening and intracollisional field effects, have been predicted[3]. These phenomena are closely related with the field dependence of the conductivity or the self–energy. In this sense the transport is refered to as "nonlinear".

Almost all the theories reported so far on the nonlinear phenomena are of lowest order in the scattering strength. It is to be noted that the lowest order approximation cannot yield correct interpretation in general. In the present article we derive a field–dependent self–energy

general. In the present article we derive a field-dependent self-energy operator using the projection operator method introduced by Argyres and Sigel[15].

2. NONLINEAR CONDUCTIVITY TENSOR

If a dc electric field $\vec{E}$ is applied adiabatically to a system of non-interacting electrons in a impurity field, the spectral density is characterized by Tani's field-dependent conductivity tensor[4,11]

$$\sigma_{kl}(E_l) = \lim_{\epsilon\to 0^+}(1/\Omega)\int_0^\infty dt\ exp(-\epsilon t) < tr\{\lim_{u_l\to 0}[\frac{\partial \bar{f}}{\partial u_l}]j_k(t)\} >_{imp} \quad (1)$$

for $k,l \equiv x,y,z$. Here Ω is the volume of the system, $< \cdots >_{imp}$ denotes the averaging over the impurity background, "tr" means the single electron trace. In Eq.(1) $j_k(t)$ is given by

$$j_k(t) \equiv exp(iLt/\hbar)j_k, \quad (2)$$

where $\vec{j}$ is the electron current operator and L is the Liouville operator corresponding to the total Hamiltonian h_T, and $\bar{f}$ is given by

$$\bar{f} = \{exp[\beta'(h_e + V + \vec{u}\cdot\vec{j} - \varsigma)]\}^{-1}, \quad (3)$$

where $\beta' \equiv (k_B T_e)^{-1}$, T_e being the electron temperature, ς is the chemical potential, $\vec{u}$ is a constant vector, and h_e and V shall be defined in detail in the following.

The total Hamiltonian h_T is defined by

$$h_T = h_{eE} + V \quad (4)$$

which corresponds to $L = L_{eE} + L_1$. Here

$$h_{eE} = h_e + e\vec{r}\cdot\vec{E}, \quad (5)$$

$$V = \sum_{\vec{q}} V_q exp(i\vec{q}\cdot\vec{r}), \quad (6)$$

where $e\vec{r}$ is the electron polarization operator, h_e the single electron Hamiltonian and V_q the Fourier transform of an impurity potential.

The interaction term in the impurity average given by Eq.(1) can be rewritten, by utilizing the residue theorem, as

$$tr\{\lim_{u_l\to 0}[\frac{\partial \bar{f}}{\partial u_l}]j_k(t)\} \equiv \sum_{\alpha_1,\alpha_2}\frac{1}{2\pi}\oint dz f(z) < \alpha_1 \mid R_z j_l R_z \mid \alpha_2 > \times < \alpha_2 \mid j_k(t) \mid \alpha_1 >, \tag{7}$$

where

$$f(z) = [exp\{\beta'(z-\zeta)\}+1]^{-1}, \tag{8}$$

$$R_z = (h_e + V - z)^{-1}, \tag{9}$$

and $\alpha(\equiv \alpha_1, \alpha_2)$ is the electron state index, the corresponding eigenstate and eigenvalue being given by[11]

$$h_e \mid \alpha >= \varepsilon_\alpha \mid \alpha >, \tag{10}$$

$$h_{eE} \mid \alpha >= E_\alpha \mid \alpha > \tag{11}$$

in approximation. This approximation is acceptable for weak fields although the correct eigenstate corresponding to E_α depends on the field.

For weakly interacting systems, we can expand R_z as

$$R_z = \sum_{m=0} R_{0z}(-VR_{0z})^m, \tag{12}$$

where

$$R_{0z} = (h_e - z)^{-1}. \tag{13}$$

Then, making an approximation[11] R_z as R_{0z} and considering Eqs.(1) and (7), we have

$$\sigma_{kl}(E_l) = -i\hbar \lim_{\epsilon \to 0^+} (1/\Omega) \sum_{\alpha_1,\alpha_2} \frac{f(\varepsilon_{\alpha_1}) - f(\varepsilon_{\alpha_2})}{\varepsilon_{\alpha_1} - \varepsilon_{\alpha_2}} j_{l\alpha_1\alpha_2} Y_{k\alpha_2\alpha_1}(E_l), \quad (14)$$

where $X_{\alpha_1\alpha_2} = < \alpha_1 \mid X \mid \alpha_2 >$ and

$$Y_k(E_l) = (-i\hbar\epsilon - L)^{-1} j_k. \quad (15)$$

3. FIELD-DEPENDENT SELF-ENERGY OPERATOR

Now it suffices to calculate $Y_k(E_l)$ in Eq.(14) properly.

With the use of the projection operators P and P' defined by Argyres and Sigel[15,16] as

$$PX = [X_{\alpha_2\alpha_1}/j_{k\alpha_2\alpha_1}]j_k, \quad (16)$$

$$P' = 1 - P, \quad (17)$$

we obtain

$$(L_{\epsilon E} P' X)_{\alpha_2\alpha_1} = 0, \quad (18)$$

$$\sum_{\alpha_3} (P'X)_{\alpha_3\alpha_1} = \sum_{\alpha_3 \neq \alpha_2} X_{\alpha_3\alpha_1}, \quad (19)$$

$$\sum_{\alpha_3} (P'X)_{\alpha_2\alpha_3} = \sum_{\alpha_3 \neq \alpha_1} X_{\alpha_2\alpha_3}, \quad (20)$$

$$(L_{\epsilon E} j_k)_{\alpha_2\alpha_1} = (E_{\alpha_2} - E_{\alpha_1}) j_{k\alpha_2\alpha_1}, \quad (21)$$

$$PL_{\epsilon E}P'X = 0. \tag{22}$$

Considering all these relations and following the procedure adotped in ref.[16] we obtain from Eq.(15)

$$Y_{k\alpha_2\alpha_1}(E_l) = \frac{j_{k\alpha_2\alpha_1}}{-i\hbar\epsilon - E_{\alpha_2} + E_{\alpha_1} - B_{k\alpha_2\alpha_1}(E_l)}. \tag{23}$$

Here $B_{k\alpha_2\alpha_1}(E_l)$ is the field-dependent self-energy operator given by

$$B_{k\alpha_2\alpha_1}(E_l) = (j_{k\alpha_2\alpha_1})^{-1} < \sum_{N=1}^{\infty} [L_1\{G_0P'L_1\}^N j_k]_{\alpha_2\alpha_1} >_{imp}, \tag{24}$$

$$G_0 \equiv (-i\hbar\epsilon - L_{\epsilon E})^{-1}, \tag{25}$$

where we have used Eqs.(18) and (22), taken into account the relation $PL_{\epsilon E}G_0P'X = (L_{\epsilon E}G_0P'X)_{\alpha_2\alpha_1} = 0$, and utilized the identity $(A - B)^{-1} \equiv A^{-1}\sum_{m=0}(BA^{-1})^m$. It is to be noted that the self-energy operator $B_{k\alpha_2\alpha_1}(E_l)$ has been expanded with respect to L_1 or V, the scattering potential.

The lowest order approximation is given, by taking N=1, as

$$B_{k\alpha_2\alpha_1}(E_l) = \sum_{\alpha_3} < \frac{|V_{\alpha_2\alpha_3}|^2}{E_{\alpha_1} - E_{\alpha_3} - i\hbar\epsilon} + \frac{|V_{\alpha_3\alpha_1}|^2}{E_{\alpha_3} - E_{\alpha_2} - i\hbar\epsilon} >_{imp}, \tag{26}$$

where we have used Eqs.(21), (22) and (23), taken into account the following relation:

$$(G_0X)_{\alpha_i\alpha_j} = (-i\hbar\epsilon - E_{\alpha_i} + E_{\alpha_j})^{-1}X_{\alpha_i\alpha_j}, \tag{27}$$

and dropped the vertex correction terms involving $V_{\alpha_i\alpha_i}$[11,17]. We see that Eq.(26) is identical with Suzuki's result.

The collision broadening by scattering can be examined by calculating the real part of the dc conductivity, i.e.

$$Re\{\sigma_{kl}(E_l)\} = \frac{\hbar}{\Omega}\sum_{\alpha_1,\alpha_2} j_{l\alpha_1\alpha_2} j_{k\alpha_2\alpha_1} \frac{f(\varepsilon_{\alpha_1}) - f(\varepsilon_{\alpha_2})}{\varepsilon_{\alpha_1} - \varepsilon_{\alpha_2}} \times \frac{\Gamma_{k\alpha_2\alpha_1}(E_l)}{\{E_{\alpha_1} - E_{\alpha_2} - \Delta_{k\alpha_2\alpha_1}(E_l)\}^2 + \Gamma^2_{k\alpha_2\alpha_1}(E_l)}, \tag{28}$$

where the linewidth $\Gamma_{k\alpha_2\alpha_1}(E_l)$ and lineshift $\Delta_{k\alpha_2\alpha_1}(E_l)$ for the transition between $|\alpha_1>$ and $|\alpha_2>$, respectively, are the imaginary part and real part of the self-energy $B_{k\alpha_2\alpha_1}(E_l)$ in Eq.(26), which are

$$\Gamma_{k\alpha_2\alpha_1}(E_l) = \pi\sum_{\alpha_3} < |V_{\alpha_2\alpha_3}|^2 \delta(E_{\alpha_1} - E_{\alpha_3}) + |V_{\alpha_3\alpha_1}|^2 \delta(E_{\alpha_3} - E_{\alpha_2}) >_{imp}, \tag{29}$$

$$\Delta_{k\alpha_2\alpha_1}(E_l) = \sum_{\alpha_3} <|V_{\alpha_2\alpha_3}|^2 P\frac{1}{E_{\alpha_1} - E_{\alpha_3}} + |V_{\alpha_3\alpha_1}|^2 P\frac{1}{E_{\alpha_3} - E_{\alpha_2}} >_{imp}, \tag{30}$$

where P denotes Cauchy's principal-value integral.

So far we have derived the electric field-dependent self-energy operator for the electron in a impurity field. The result in the lowest order approximation is identical with that of Suzuki[11]. If we include higher order terms, we expect to get more precise results.

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