Optical Conductivity in a Two Dimensional Quantum Well System with Impurity Scattering

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The conductivity of Kubo linear response theory for a quantum well system of many electrons interacting with impurities and confined by a parabolic potential is formulated via a projection operator technique. A line-width function of the optical absorption spectrum is explicitly obtained in the weak coupling approximation up to the second order of the interaction.

KEYWORDS: conductivity, relaxation and scattering, quasi-two dimensional system

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1. Introduction

Recently, considerable attention has been focused on a study of quantum transport and optical properties of low-dimensional electron systems. Furthermore, due to rapid progress in technology, the properties of electrons confined in a quantum-well potential have been the interesting and important subject of experimental and theoretical investigations in condensed matter physics. The investigations of the optical transition occurring between quantized energy spectrum provide valuable information on relaxation and scattering mechanism as well as on many-body effect. Physically relevant quantity such as the optical absorption power can be obtained from the conductivity tensor. It is, therefore, of considerable importance to obtain an explicit expression of the conductivity for a given confining potential system. Here the central quantity is the line-width function that measures optical spectrum’s width in the transition process.

The objective of this paper is twofolds: first, to present an explicit result of the line-width function for a confining potential system, second, to give a theoretical formulation which facilitates conductivity calculation by making use of a standard projection operator technique. The system we want to study in this work is a quasi-two dimensional quantum-well system in which the electrons are restricted in a parabolic potential along the z-direction in the absence of external magnetic field and thus energy levels are formed only in this z-direction. The scattering situation of interest is that the electrons are assumed to be mostly scattered by impurities, which may be valid in the low-temperature limit as well as in the limit where the electron-electron interaction is not important. More specifically the valid region is such that the kinetic energy is larger than the impurity scattering process. The weak scattering approximation can be thus made.

In this work, we focus on the electron-impurity interaction which mainly influences optical transitions between energy levels. Starting from Kubo conductivity formula, we use a many-body projection operator technique to formulate the conductivity in the weak coupling approximation with respect to the scattering interaction. Then we obtain an explicit expression of the line-width function that determines the optical spectrum properties. It is shown in this expression that the transitions between energy states are explicitly described by the interaction coupling functions and by the Fermi–Dirac distribution functions for electrons and also relaxations between the transitions are properly explained. Finally, our discussion is given in the last section.

2. System and Problem

The Hamiltonian of our electron–impurity system is given by

\[ H = H_\text{el} + H_\text{el-imp}, \]

\[ H_\text{el} = \sum_\alpha \varepsilon_\alpha a_\alpha^\dagger a_\alpha, \]

\[ H_\text{el-imp} = \sum_q \sum_{\alpha, \beta} C_{\alpha, \beta}(q) a_\alpha^\dagger a_\beta. \]

Here \( H_\text{el} \) represents the Hamiltonian of dynamically independent electrons, and \( H_\text{el-imp} \) the interaction potential between these electrons and impurities, which is responsible for scattering effects. \( a_\alpha^\dagger \) (\( a_\alpha \)) denotes the creation (annihilation) operator for the electron in a state \( |\alpha\rangle \), which satisfies the fermion anticommutation relation, \( \{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha, \beta} \). The interaction function \( C_{\alpha, \beta}(q) \) in eq. (3) describes the coupling of an electron with the impurities, which is defined as matrix elements characterized by electron states (i.e., \( C_{\alpha, \beta}(q) \equiv \langle \alpha | c(q) | \beta \rangle \)). In general this coupling function depends on types of systems.

We will now find the state \( |\alpha\rangle \). Our quasi-two dimensional system is confined in a z-directional parabolic potential so that it is quantized only in this direction. For this potential, solving the Schrödinger equation for the single electron Hamiltonian given by

\[ \hbar_\text{el} = -\frac{\hbar^2 \nabla^2}{2m_0} + m_0 \omega_0^2 z^2, \]

yields the following energy \( \varepsilon_\alpha \) and state \( |\alpha\rangle \):

\[ \varepsilon_\alpha = \varepsilon_{n,k_z} = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\hbar^2}{2m_0} (k_x^2 + k_y^2) \]

\[ |\alpha\rangle = |n, k_z\rangle = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \exp(i k_x x + i k_y y) \times \exp \left( -\frac{m_0 \omega_0^2 z^2}{2\hbar} \right), \]

where \( \varepsilon_{n,k_z} = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\hbar^2}{2m_0} (k_x^2 + k_y^2) \), \( m_0 = \frac{\hbar^2}{2\epsilon_0} \), \( \epsilon_0 = \frac{\hbar^2}{2m_0} \), and \( \omega_0 = \sqrt{\frac{2m_0}{\hbar^2}} \).
where $\omega_0$ is the characteristic frequency of potential, $m_0$ is the mass of an electron, $H_0(z)$ is the Hamiltonian, and $k_d$ denotes $k_d \equiv (k_x, k_y)$. Here and in what follows, $\epsilon_{n+1} \alpha$ and $|\alpha + 1|$ imply $\epsilon_{n+1} \alpha$ and $|n + 1, \alpha|$, respectively.

To probe the optical transition in our quasi-two-dimensional system, we suppose that an electric field of amplitude $E_0$ and frequency $\omega$ is applied to the system along the $z$-direction, which is linearly polarized in this direction. Then the absorption power delivered to the system can be expressed as

$$P(\omega) = \frac{1}{2} E_0^2 \text{Re} \sigma_{zz}(\omega), \quad (7)$$

where $\text{Re}$ means “the real part of”. The conductivity $\sigma_{zz}(\omega)$ in eq. (7) can be obtained from Kubo theory that we will adopt in this work. According to Kubo theory, the weak-external electric field the absorption of energy by an electron can be properly described by linear response theory, where the absorption power delivered to the system can be expressed as

$$\left\langle \sigma_{zz}(\omega) \right\rangle = \frac{ie}{\hbar} \left\langle J_z^2 \right\rangle \left( \frac{1}{\hbar^2 - L} \right), \quad (8)$$

where $j_0 = ie\sqrt{\hbar \omega/2m_0}$, $e$ being electric charge. In the following section, the conductivity $\sigma_{zz}$ with the current operator $J_z$ above will be expressed in terms of the line-width function, which will be subsequently calculated.

3. Formulation and Calculation

3.1 Conductivity and line-width function

Following Kubo’s conductivity formula, the conductivity $\sigma_{zz}(\omega)$ may be expressed as

$$\text{Re}\sigma_{zz}(\omega) = \frac{1}{\omega} \sum \alpha \left[ \left( \frac{1}{\hbar \omega - L} J_z \right)^{\alpha} \right], \quad (9)$$

Here the unit volume system is taken, $\omega = \omega - i\eta$ and $\eta \to 0^+$ will be taken in the final stage, $L$ is the quantum Liouville operator defined as $L \equiv [H, A]$ for an operator $A$, $J_\alpha$ implies $J_\alpha$ for state $\alpha$, and the ensemble average $\langle \cdots \rangle$ means the grand-canonical distribution, $\text{Tr}$ denoting the many-body trace, with the grand-canonical density operator $\rho(H)$ given by

$$\rho(H) = \frac{\exp[-\beta(H - \mu N)]}{\text{Tr}[\exp[-\beta(H - \mu N)]],} \quad (10)$$

where $\mu$ is the chemical potential, $N$ the total number of electrons, $H$ the Hamiltonian of the system.

We are not able to evaluate eq. (9) exactly because of the many-body interaction due to the term $H_{\text{el-imp}}$ in eq. (3). This fact requires a reasonable approximation. To this end, we consider the projection operator $P$ onto a subspace of the space of states defined by eigenstates of $H_0 \equiv H_{\text{el}}$ (assuming a full space is defined on $H$) in which the operators $P$ and $Q = 1 - P$ satisfy the relations, $P^2 = P$ and $Q^2 = Q$, and the Liouville operator $L_{\text{el}} \equiv [H_0, A]$. In this subspace, $\rho(H)$ may be chosen to be $\rho(H_0)$, which will be valid in the weak coupling approximation, and the interaction $H_{\text{el-imp}} \equiv H_1$ or the Liouville operator $L_1 A = [H_1, A]$ can be treated in a perturbative way. The projection operator $P$ is then defined as

$$P = \left\langle \langle A \rangle J_z / \langle \langle J_z \rangle \right\rangle, \quad (11)$$

where $\langle \langle A \rangle \rangle \equiv \text{Tr}[\rho(H_0)[A, J_z^{\alpha}]]$ for arbitrary operator $A$. It should be noted that the notation $\langle \langle \cdots \rangle \rangle$ is not the very average $\langle \cdots \rangle$. We now use the operator identity $(A + B)^{-1} = A^{-1} - A^{-1}B(A + B)^{-1}$ to make the decomposition of $L = L_0 + L_1$ and expand it in terms of $L_1$. First, we rewrite, using the identity, the terms $(\hbar \omega - L)^{-1} J_z$ appearing in the conductivity eq. (9) as

$$\begin{align*}
(\hbar \omega - L)^{-1} J_z &= (\hbar \omega - LQ)^{-1} J_z \\
&= (\hbar \omega - LQ)^{-1} L \left( \hbar \omega - L \right)^{-1} J_z,
\end{align*} \quad (12)$$

where we note that $Q J_z = 0$ and $P J_z = J_z$, and $(\hbar \omega - LQ)^{-1} J_z = J_z / \hbar \omega$. Second, we substitute $L = L_0 + L_1$ into the second term in eq. (12) and then use the operator identity again to make the expansion up to the second order of $L_1$. Then we find that the conductivity is given by

$$\text{Re}\sigma_{zz}(\omega) = \frac{1}{\omega} \sum \alpha \left[ \left( \frac{1}{\hbar \omega - L} J_z \right)^{\alpha} \right], \quad (13)$$

where $\Omega = \langle \langle L J_z \rangle \rangle / \langle \langle J_z \rangle \rangle$ and the line-width function $\Gamma(\omega)$ is given by

$$\Gamma(\omega) = \left( \langle \left( \hbar \omega - L_0 \right)^{-1} L_1 J_z, L_1 J_z^{\alpha} \rangle / \langle \langle J_z \rangle \rangle \right). \quad (14)$$

The present second order expansion carried out in this work is the lowest order approximation. It should be noted that the above formal results eqs. (13) and (14) are exact as far as the weak coupling approximation is concerned.

3.2 Explicit results

Now we further calculate the conductivity eq. (13) together with the line-width function eq. (14). To accomplish this calculation, we note the following. $\text{Tr}[\rho(H_0)a_\alpha^\dagger a_\beta] = f_{\alpha, \beta}$ where $f_{\alpha, \beta}$ denotes the Fermi–Dirac distribution for electrons with energy $\epsilon_a$ at a temperature $T = 1/k_B \beta$. Since $\text{Tr}[\rho(H_0)L_1 a_\alpha^\dagger a_\beta] = 0$ due to the average over the (random) impurity distribution it follows that $\langle L_{\text{el}} \rangle = \langle L_1 J_z \rangle$. Also, since the operator term $(\hbar \omega - L_0)$ in eq. (14) is represented in the eigenstate of the subspace, applying $(\hbar \omega - L_0)^{-1}$ to $a_\alpha^\dagger a_\beta$ yields $(\hbar \omega - \epsilon_{\alpha, \beta})^{-1}$ as an eigenvalue. The notation $\epsilon_{\alpha, \beta} = \epsilon_\alpha - \bar{\epsilon}$. Using the above mathematical points and doing some algebra, we finally obtain that $\langle \langle J_z \rangle \rangle = \left| j_0 \right|^2 j_{a, +1}^\dagger j_{a, +1} + \left| j_{a, -1} \right|^2 j_{a, -1}^\dagger j_{a, -1}$ with the notation $f_{a, \beta} = f_{\alpha, \beta}$ and

$$\langle \langle J_z \rangle \rangle \Omega = \left| j_0 \right|^2 \epsilon_{a, +1}^\dagger j_{a, +1} + \left| j_{a, -1} \right|^2 \epsilon_{a, -1}^\dagger j_{a, -1}, \quad (15)$$

$$\langle \langle J_z \rangle \rangle \Gamma(\omega) = \Gamma_1(\omega) + \Gamma_2(\omega) + \Gamma_3(\omega). \quad (16)$$

Here
\[ \Gamma_1(\omega) = \sum_q \sum_{\beta} \epsilon_a^{\dagger} c_{\beta a}^* j_{\beta-1} c_{\alpha+1, \beta} - j_{\alpha+1} c_{\alpha+2, \beta} + j_{\alpha} c_{\alpha, \beta} - j_{\beta} c_{\alpha+1, \beta+1} \]
\[ \times \left[ \frac{f_{\alpha+1}(1 - f_{\beta}) - f_{\beta}(1 - f_{\alpha+1})}{\hbar \omega - (\epsilon_{\alpha+1} - \epsilon_{\beta})} \right] \]
\[ \Gamma_2(\omega) = \sum_q \sum_{\beta} \epsilon_a^{\dagger} c_{\beta a}^* (j_{\beta-1} c_{\alpha+1, \beta} - j_{\alpha+1} c_{\beta+1, \alpha} + j_{\beta-1} c_{\beta-1, \alpha} - j_{\alpha} c_{\beta, \alpha+1}) \]
\[ \times \left[ \frac{f_{\beta}(1 - f_{\alpha}) - f_{\alpha}(1 - f_{\beta})}{\hbar \omega - (\epsilon_{\beta} - \epsilon_{\alpha})} \right], \]
\[ \Gamma_3(\omega) = \sum_q \sum_{\beta} \epsilon_a^{\dagger} c_{\beta a}^* (j_{\beta-1} c_{\alpha+1, \beta} - j_{\alpha+1} c_{\beta+1, \alpha} + j_{\beta+1} c_{\alpha-1, \beta} - j_{\alpha-2} c_{\alpha-2, \beta}) \]
\[ \times \left[ \frac{f_{\alpha+1}(1 - f_{\beta}) - f_{\beta}(1 - f_{\alpha+1})}{\hbar \omega - (\epsilon_{\alpha+1} - \epsilon_{\beta})} \right]. \]  

Here \( j_\beta = j_0 \sqrt{\alpha + 1}, C_{\alpha, \beta} \equiv C_{\alpha, \beta}(q), \) and * and \( \dagger \) stand for complex conjugate and Hermitian conjugate, respectively.

We now specify the electron-impurity-interaction matrix elements \( C_{\alpha, \beta} \). This matrix element \( C_{\alpha, \beta} \) is given by \( V_q(\alpha) \exp(iq \cdot r)|\beta\rangle \) where \( V_q \) is the interaction factor and \( r \) the electron position vector. Using the state \( |\alpha\rangle \) in eq. (6), we obtain
\[ C_{\alpha, \beta}(q) = V_q \sqrt{\frac{n_{\alpha+1}}{n_{\beta+1}}} \sqrt{\frac{\hbar}{2m_0 \omega_0}} e^{-\frac{\hbar}{2m_0 \omega_0}(\langle \mathbf{q}\rangle \cdot \mathbf{q}_1)^2} L_n^{m_{\alpha+1}}(\mathbf{q}_1) \delta_{\mathbf{q}_1+q_1 \mathbf{q}_2} \delta_{\mathbf{q}_1+q_2 \mathbf{q}_2}, \]
where \( \mathbf{q}_1 = \frac{\hbar}{m_0 \omega_0} \mathbf{q}_1 \) and \( L_n^{m}(\mathbf{x}) \) is the Laguerre polynomial defined by
\[ L_n^{m}(\mathbf{x}) = (n!)^{-1} \exp(x) x^{-m} \frac{d^n}{dx^n}(x^{m+n} \exp(-x)). \]  

Therefore, if \( V_q \) is given, one can calculate the line-width function eq. (16) for a given system.

4. Discussion

It is found that the line-width function eq. (16) with eqs. (17)–(19) describing the optical transition process between the states \( \alpha \)'s in the quantum well of the parabolic potential is expressed in terms of the electron–impurity-interaction matrix elements \( C_{\alpha, \beta} \) and the energy denominators [see \( [\cdot \cdot \cdot ] \) in eqs. (17)–(19)] implying the energy conservation in the transition. In this process, the electron absorbs energy from the applied field (photon energy) and makes the transition to an excited state, and then it goes to a state of lower energy by emitting a photon. The electron–impurity-interaction affects the scattering processes. The appearance of the Fermi–Dirac distributions in the line-width function eq. (16) can be interpreted as follows. The process of the first term \( \Gamma_1(\omega) \) in eq. (17) implies that the relaxation for the transition from \( \alpha + 1 \) to \( \beta \) (\( \alpha + 1 \rightarrow \beta \)) minus that for the inverse transition. In the same way, the processes of the second term \( \Gamma_2(\omega) \) in eq. (18) and the third term \( \Gamma_3(\omega) \) in eq. (19) imply that the relaxations for the transitions \( \beta \rightarrow \alpha \) and \( \alpha - 1 \rightarrow \beta \) minus those for their inverse transitions, respectively. During the transition processes the state \( \beta \) plays a role of intermediate state for given initial or final state \( \alpha \)'s. The present result fully gives a general description of the optical transitions. It is to be noted that the relaxations are derived from the Liouville equation of motion not from phenomenological assumptions so that the description above is properly established.

In this work, staring from Kubo's theory and using a many-body projection operator technique we have made a theoretical formulation of the optical transition for a quantum well system in which the impurity scattering is dominant but considered in the weak coupling approximation. We have presented the explicitly analytical expression of the optical conductivity. Apparently, the z-component current operator depends on types of confining potentials since their wave functions and energy states are different. Their general expressions of conductivities seem to involve all relevant but perhaps complicated transition processes which is to be analyzed explicitly, which requires a reasonable theoretical approach and evaluation. In this aspect, the present explicit results in this work are expected to be useful for a study of optical transitions in quasi-two dimensional systems.

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