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Theory of impurity-doping effect on electronic states in a quasi-one-dimensional-structure semiconductor

Masumi Takeshima
Semiconductor Laboratory, Matsushita Electronics Corporation, Takatsuki, Osaka 569, Japan

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A theory is presented of the impurity-doping effect on the electronic states in a quasi-one-dimensional-structure semiconductor using Green's-function formalism. The theory is applied to a single quantum well made of *n*-type GaAs. It is shown that the density of states is strongly modulated by the doping as compared with the cases of a quasi-two-dimensional structure and a three-dimensional structure. A strong dependence of the screening on the free-carrier concentration is the cause of the strong modulation through rapid shift and broadening of the density of states toward a higher energy range and a lower energy range, respectively.

I. INTRODUCTION

Recent progress in epitaxial growth techniques has stimulated the study of quasi-two-dimensional-structure (Q2DS) semiconductors such as quantum wells and superlattices. Especially, the optical properties of Q2DS's have received much attention in the fields of fundamental physics[1,2] and device physics[3,4] represented by a quantum-well laser. Due to a step-function shape of the density of states (DOS) for an undoped well, laser operations in Q2DS's are known to show excellent characteristics, e.g., low threshold current and weak temperature dependence.[5-8] This result leads us to the suggestion that a quasi-one-dimensional structure (Q1DS) is more favorable for obtaining excellent laser operations.

In practice, intentional or unintentional doping is often inevitable. Previously, the present author has discussed[9] the doping effect on the electronic states in Q2DS's and has shown that the doping leads to strong modification of the DOS especially in the intraband region. If a well is undoped but electrons and holes are injected as in the case of laser operations, strong modification may also occur for the conduction band since the holes may scatter electrons in practically the same way as the donor impurities. Thus the modification of the DOS is of practical importance in various cases.

In a Q2DS, the DOS for an undoped well is a step function, which is modified into a gradual function under doping. In a three-dimensional structure (3DS), the DOS for an undoped crystal is a square-root function, whose modification, especially in the intraband states, under doping is very small as compared with the case of a Q2DS. In a Q1DS, on the other hand, the DOS for an undoped well is an inverse square-root function, which is infinite at a subband edge. From the above trend, i.e., 3DS, Q2DS, and Q1DS, it is expected that modification of the DOS in a Q1DS under doping is stronger than in a Q2DS. The doping effect of a Q1DS is quite important from both fundamental physics and device physics viewpoints.

In this paper we derive a method of calculating the DOS in a Q1DS using Green's function formalism. We use the Bonch-Bruevich assumption[10] that the impurity potential varies slowly; then fluctuations in the state energies closely mirror those in the potential energies. With the use of that assumption, the present author has previously performed calculations based on the diagram technique for 3DS's.[11] He has recently modified this approach[9] so as to be useful for Q2DS's. In this paper we extend this approach to include Q1DS's. A basic concept with which the present theory is developed is similar to that used for the theory of Auger recombination in Q1DS's by the present author.[12] Characteristic features of Q1DS's with respect to the doping effect are revealed in comparison with the cases of Q2DS's and 3DS's.

II. THEORY

Considering carrier confinement in the y and z directions, we define the two-dimensional position vector $\mathbf{r}=(y,z)$ in the confinement directions, the three-dimensional position vector $\mathbf{R}=(x,y,z)$, the two-dimensional wave vector $\mathbf{q}=(q_y,q_z)$, and the three-dimensional wave vector $\mathbf{Q}=(q_x,q_y,q_z)$. Let us consider the conduction band with the isotropic effective mass m^*. Confinement of a free electron produces subbands. Then the wave function for the electron is given within the framework of the effective-mass approach by

$$\phi_{lk_x}(\mathbf{R})=\frac{1}{(L_x)^{1/2}}\exp(jk_x x)u_l(\mathbf{r}) , \tag{2.1}$$

where L_x is the length of a crystal in the x direction, k_x the wave vector in one dimension, l the subband index, and $u_l(\mathbf{r})$ the wave function describing the bound state.

Let us consider a single two-dimensional quantum well, which is bounded by four heterobarriers lying at $y=0$ and L_y and $z=0$ and L_z; L_y and L_z are the well widths in the y and z directions, respectively. It is assumed that hydrogenic donor impurities are randomly distributed only in the well and there are no impurities outside. Starting with Eq. (2.1), we define our model by writing down the Hamiltonian

$$H=H_e+H_{e\text{-}i}+H_{e\text{-}e} , \tag{2.2}$$

where H_e, $H_{e\text{-}i}$, and $H_{e\text{-}e}$ are the Hamiltonians for the unperturbed subbands, the electron-impurity interaction, and the electron-electron interaction, respectively; $H_{e\text{-}i}$ and $H_{e\text{-}e}$ are considered to be perturbations. The explicit forms of the Hamiltonians are

$$H_e=\sum_{lk_x\sigma} E_l(k_x)a^{\dagger}_{lk_x\sigma}a_{lk_x\sigma} , \tag{2.3}$$

$$H_{e\text{-}i}=\frac{1}{V}\sum_{l'lk_x\mathbf{Q}\sigma} \overline{\Gamma}(\mathbf{Q})\gamma_{l'l}(\mathbf{q})a^{\dagger}_{l'k_x+q_x\sigma}a_{lk_x\sigma} , \tag{2.4}$$

$$H_{e\text{-}e}=\frac{1}{2V}\sum_{\substack{l_1l_2l_3l_4\\ k_xk_x'\sigma\sigma'\mathbf{Q}}} \overline{U}(\mathbf{Q})\gamma_{l_1l_4}(\mathbf{q})\gamma_{l_2l_3}(-\mathbf{q})a^{\dagger}_{l_1k_x+q_x\sigma} \times a^{\dagger}_{l_2k_x'-q_x\sigma'}a_{l_3k_x'\sigma'}a_{l_4k_x\sigma} . \tag{2.5}$$

Here $a^{\dagger}_{lk_x\sigma}$, $a_{lk_x\sigma}$, and $E_l(k_x)$ are the creation operator, the annihilation operator, and the unperturbed subband energy, respectively, for the electron with the subband index l, the one-dimensional wave vector k_x, and the spin σ. $\overline{\Gamma}(\mathbf{Q})$ is the Fourier transform of the potential $\Gamma(\mathbf{R})$ due to all the impurities

$$\Gamma(\mathbf{R})=\sum_{n=1}^{N_i} U_i(\mathbf{R}-\mathbf{R}_n) =\frac{1}{V}\sum_{\mathbf{Q}}\overline{\Gamma}(\mathbf{Q})\exp(j\mathbf{Q}\cdot\mathbf{R}) , \tag{2.6}$$

where $U_i(\mathbf{R}-\mathbf{R}_n)$ is the potential due to an impurity at $\mathbf{R}=\mathbf{R}_n$, N_i the total number of the impurities, and V the crystal volume defined later. $\overline{U}(\mathbf{Q})$ is the Fourier transform of the interaction $U(\mathbf{R}_1-\mathbf{R}_2)$ between the electrons at $\mathbf{R}_1$ and $\mathbf{R}_2$

$$U(\mathbf{R}_1-\mathbf{R}_2)=\frac{1}{V}\sum_{\mathbf{Q}}\overline{U}(\mathbf{Q})\exp[j\mathbf{Q}\cdot(\mathbf{R}_1-\mathbf{R}_2)] . \tag{2.7}$$

$\gamma_{l'l}(\mathbf{q})$ is an important parameter representing directly the effect of the electron confinement on the electron-impurity interaction and the electron-electron interaction, i.e.,

$$\gamma_{l'l}(\mathbf{q})=\int d\mathbf{r}\, u_{l'}^{*}(\mathbf{r})\exp(j\mathbf{q}\cdot\mathbf{r})u_l(\mathbf{r}) . \tag{2.8}$$

As for the potentials $U_i(\mathbf{R})$ and $U(\mathbf{R})$, we assume the free-carrier screening *a priori* with the inverse screening length λ. We have

$$U(\mathbf{R})=\frac{e^2}{\epsilon_0 R}\exp(-\lambda R) , \tag{2.9}$$

where e is the electronic charge and ϵ_0 is the dielectric constant of the host lattice. Assuming one species of ionic impurities we have

$$U_i(\mathbf{R})=ZU(\mathbf{R}) , \tag{2.10}$$

where Z is the minus of the valency of the impurity with respect to the host lattice. From Eqs. (2.9) and (2.10) we obtain

$$\overline{U}(\mathbf{Q})=\frac{4\pi e^2}{\epsilon_0}\frac{1}{Q^2+\lambda^2} \tag{2.11}$$

and

$$\overline{\Gamma}(\mathbf{Q})=\overline{U}_i(\mathbf{Q})h(\mathbf{Q}) . \tag{2.12}$$

Here $\overline{U}_i(\mathbf{Q})$ is the Fourier transform of the potential $U_i(\mathbf{R})$, i.e.,

$$\overline{U}_i(\mathbf{Q})=Z\overline{U}(\mathbf{Q}) , \tag{2.13}$$

and we define the phase factor

$$h(\mathbf{Q})=\sum_{n=1}^{N_i}\exp(-j\mathbf{Q}\cdot\mathbf{R}_n) . \tag{2.14}$$

Based on Eqs. (2.3)–(2.5), we consider the retarded Green's function which is a function of two subband indices l and l', two one-dimensional wave vectors k_x and k_x', one energy parameter ω, and the position vectors of the impurities $\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_{N_i}$. A diagram representing the impurity scattering is shown in Fig. 1 with the use of the free-particle Green's function

$$G_0^R(l\mathbf{k},\omega)=\frac{1}{\omega-E_l(\mathbf{k})+j0^+} . \tag{2.15}$$

Analogously to the case of a 3DS (Ref. 13) we obtain

$$G^R(lk_x,l'k_x')=G_0^R(lk_x)\left[\Delta(l-l')\Delta(k_x-k_x') +\sum_{l''\mathbf{Q}}\overline{\Gamma}(k_x-q_x,\mathbf{q})\gamma_{ll''}(\mathbf{q}) \times G^R(l''q_x,l'k_x')\right] , \tag{2.16}$$

where we have omitted the parameter ω and we define $\Delta(x)=1$ for $x=0$ and $\Delta(x)=0$ otherwise with x as a scalar or a vector. With the use of an expansion

$$G^R(l''q_x,l'k_x')=\sum_{m=0}^{\infty}\frac{1}{m!}\left[(q_x-k_x)\frac{\partial}{\partial k_x}\right]^m G^R(l''k_x,l'k_x') , \tag{2.17}$$

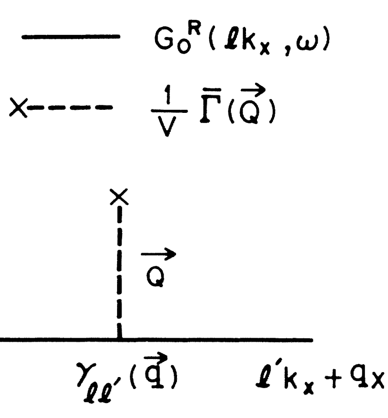

FIG. 1. Diagram representing the impurity scattering.

we can rewrite Eq. (2.16) as

$$G^R(lk_x,l'k_x')=G_0^R(lk_x)\left[\Delta(l-l')\Delta(k_x-k_x')+\sum_{l''}\tilde{\Gamma}_{ll''}\left[j\frac{\partial}{\partial k_x}\right]\times G^R(l''k_x,l'k_x')\right] . \qquad (2.18)$$

Here we define an operator

$$\tilde{\Gamma}_{ll''}\left[j\frac{\partial}{\partial k_x}\right]=\int d\mathbf{r}\,|u_l(\mathbf{r})|^2\Gamma\left[j\frac{\partial}{\partial k_x},\mathbf{r}\right] ; \qquad (2.19)$$

$\Gamma(j\partial/\partial k_x,\mathbf{r})$ is obtained from $\Gamma(\mathbf{R})$ by replacing $\mathbf{R}=(x,\mathbf{r})$ with $(j\partial/\partial k_x,\mathbf{r})$.

Equation (2.18) is easily rewritten for $l=l'$ as

$$G^R(lk_x,lk_x')=\frac{G_0^R(lk_x)\left[\Delta(k_x-k_x')+\sum_{l'(\neq l)}F\left[j\frac{\partial}{\partial k_x};l,l'\right]G^R(l'k_x,lk_x)\right]}{1-G_0^R(lk_x)\left[\tilde{\Gamma}_{ll}\left[j\frac{\partial}{\partial k_x}\right]+F\left[j\frac{\partial}{\partial k_x};l,l\right]\right]} , \qquad (2.20)$$

where

$$F\left[j\frac{\partial}{\partial k_x};l,l'\right]=\sum_{l''(\neq l,\neq l')}\tilde{\Gamma}_{ll''}\left[j\frac{\partial}{\partial k_x}\right]\frac{G_0^R(lk_x)}{1-G_0^R(lk_x)\tilde{\Gamma}_{l''l''}\left[j\frac{\partial}{\partial k_x}\right]}\tilde{\Gamma}_{l''l'}\left[j\frac{\partial}{\partial k_x}\right] . \qquad (2.21)$$

Note that $\tilde{\Gamma}_{ll'}(j\partial/\partial k_x)$ with $l\neq l'$ is an operator representing the intersubband interaction due to the impurity scattering. On the other hand, under $l\neq l'$ we have

$$G^R(lk_x,l'k_x')=\frac{G_0^R(lk_x)}{1-G_0^R(lk_x)\tilde{\Gamma}_{ll}\left[j\frac{\partial}{\partial k_x}\right]}\times\left[\tilde{\Gamma}_{ll'}\left[j\frac{\partial}{\partial k_x}\right]\Delta(k_x-k_x')G_0^R(lk_x)+\sum_{l''(\neq l)}\tilde{\Gamma}_{ll''}\left[j\frac{\partial}{\partial k_x}\right]G^R(l''k_x,l'k_x')\right] . \qquad (2.22)$$

Hereafter the discussion is restricted to the case where the energy difference between neighboring subbands is large enough to allow the neglect of the intersubband interaction due to the impurity scattering. This corresponds to assuming that $\tilde{\Gamma}_{ll'}(j\partial/\partial k_x)$ with $l\neq l'$ is small enough. Then $G^R(lk_x,l'k_x')$ with $l\neq l'$ is of first order in $\tilde{\Gamma}_{ll''}(j\partial/\partial k_x)$ with $l\neq l''$ so that we may consider only $G^R(lk_x,lk_x')$ given by Eq. (2.20). Furthermore, since $F(j\partial/\partial k_x;l,l')$ is of second order in $\Gamma_{l''l}(j\partial/\partial k_x)$ with $l''\neq l$, we obtain

$$G^R(lk_x,lk_x')=\frac{G^R(lk_x)}{1-G_0^R(lk_x)\tilde{\Gamma}_{ll}\left[j\frac{\partial}{\partial k_x}\right]}\Delta(k_x-k_x') \qquad (2.23)$$

by neglecting all F's in Eq. (2.20). This equation can be written in the form

$$G^R(lk_x,lk_x')=\frac{1}{L_x}\int dx\,\exp[j(k_x-k_x')x]\times\frac{1}{\omega-E_l\left[k_x+j\frac{\partial}{\partial x}\right]-\tilde{\Gamma}_{ll}(x)+j0^\dagger} , \qquad (2.24)$$

where $\tilde{\Gamma}_{ll}(x)$ is obtained from $\tilde{\Gamma}_{ll}(j\partial/\partial k_x)$ by replacing $j\partial/\partial k_x$ with x, i.e.,

$$\tilde{\Gamma}_{ll}(x)=\int d\mathbf{r}\,|u_l(\mathbf{r})|^2\Gamma(\mathbf{R}) =\frac{1}{V}\sum_{q_x}\bar{\bar{\Gamma}}_{ll}(q_x)\exp(jq_xx) \qquad (2.25)$$

with the definition of

$$\bar{\bar{\Gamma}}_{ll}(q_x)=\sum_{\mathbf{q}}\gamma_{ll}(\mathbf{q})\bar{\Gamma}(\mathbf{Q}) . \qquad (2.26)$$

After the Bonch-Bruevich approach[10] for 3DS's, it is assumed that the variation of $\tilde{\Gamma}_{ll}(x)$ with x is slow enough to allow approximating $E_l(k_x+j\partial/\partial x)$ as $E_l(k_x)$. We obtain

$$G^R(lk_x,lk_x') =\frac{1}{L_x}\int dx\,\exp[j(k_x-k_x')x]\frac{G_0^R(lk_x)}{1-G_0^R(lk_x)\tilde{\Gamma}_{ll}(x)} =G_0^R(lk_x)\sum_{m=0}^{\infty}[G_0^R(lk_x)]^m\frac{1}{L_x}\times\int dx[\tilde{\Gamma}_{ll}(x)]^m\exp[j(k_x-k_x')x] . \qquad (2.27)$$

With the use of Eqs. (2.12), (2.25), and (2.26) we have

$$\frac{1}{L_x}\int dx[\widetilde{\Gamma}_{ll}(x)]^m \exp[j(k_x-k_x')x] = \sum_{\mathbf{Q}_1,\mathbf{Q}_2,\dots,\mathbf{Q}_m} \Delta(q_{1x}+q_{2x}+\cdots+q_{mx}+k_x-k_x') \times\prod_{n=1}^{m}\left[\frac{1}{V}\widetilde{U}_i(\mathbf{Q}_n)h(\mathbf{Q}_n)\right], \tag{2.28}$$

where

$$\widetilde{U}_i(\mathbf{Q})=\gamma_{ll}(\mathbf{q})\overline{U}_i(\mathbf{Q}) . \tag{2.29}$$

Now we consider an ensemble average[10,13] of $G^R(lk_x,lk_x')$ over the impurity sites, which is defined as

$$\langle G^R(lk_x,lk_x')\rangle = \frac{1}{(L_xL_yL_z)^{N_i}}\int d\mathbf{R}_1 d\mathbf{R}_2\cdots d\mathbf{R}_{N_i} G^R(lk_x,lk_x') = G^R(lk_x)\Delta(k_x-k_x') . \tag{2.30}$$

Here L_y and L_z are the well widths in the y and z directions, respectively, assuming a wire structure with the rectangular cross section and the integrals are taken only over the layer where the impurities are distributed; in this paper this layer is considered to be just the well. The last step of Eq. (2.30) represents the fact that the space uniformity which is lost under the random distribution of the impurities, is restored under the averaged distribution giving the momentum conservation $k_x=k_x'$.

For convenience we define $\mathbf{q}$ such that the periodic boundary condition should be satisfied for a wave $\exp(j\mathbf{q}\cdot\mathbf{r})$ at both boundaries of the doped layer, i.e., the well. Then we have $q_y=2\pi n_y/L_y$ and $q_z=2\pi n_z/L_z$ with n_y and n_z as integers. We should take $V=L_xL_yL_z$ and we obtain

$$\frac{1}{V}\int d\mathbf{R}_n \exp(j\mathbf{Q}_s\cdot\mathbf{R}_n)=\Delta(\mathbf{Q}_s) \tag{2.31}$$

for $\mathbf{Q}_s$ which is a sum of an arbitrary combination of $\mathbf{Q}$'s picked out from $\mathbf{Q}_1,\mathbf{Q}_2,\dots,\mathbf{Q}_m$. After taking the ensemble average by noting $h(\mathbf{Q})$ in Eq. (2.14), $G^R(lk_x,\omega)$ is given as a sum of all the diagrams whose typical example is shown in Fig. 2. The diagram in this figure represents a term

$$S(m_1,m_2,\dots,m_p) = \frac{1}{G_0^R(lk_x)}\prod_{n=1}^{p}\{N_i[G_0^R(lk_x)]^{m_n}\}H_{m_n} , \tag{2.32}$$

where

$$H_m=\sum_{\mathbf{Q},\mathbf{Q}_2,\dots,\mathbf{Q}_m}\Delta(\mathbf{Q}_1+\mathbf{Q}_2+\cdots+\mathbf{Q}_m)\prod_{n=1}^{m}\left[\frac{1}{V}\widetilde{U}_i(\mathbf{Q}_n)\right]. \tag{2.33}$$

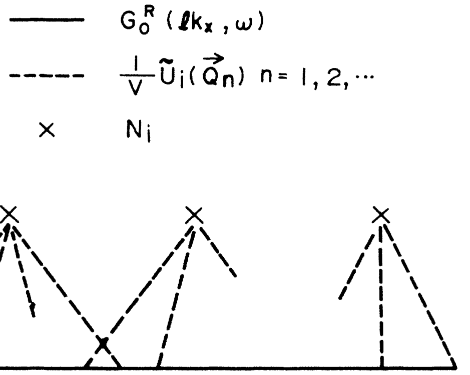

FIG. 2. Diagram representing the impurity scattering, which is obtained by taking an ensemble average over the impurity sites.

Let us define

$$U_i^e(\mathbf{R})=\frac{1}{V}\sum_{\mathbf{Q}}\widetilde{U}_i(\mathbf{Q})\exp(-j\mathbf{Q}\cdot\mathbf{R}) . \tag{2.34}$$

Then we obtain

$$H_m=\frac{1}{V}\int_{\text{layer}} d\mathbf{R}[U_i^e(\mathbf{R})]^m \tag{2.35}$$

and the final expression for S is

$$S(m_1,m_2,\dots,m_p) = \frac{n_i^p}{G_0^R(lk_x)}\prod_{n=1}^{p}\left[\int d\mathbf{R}[U_i^e(\mathbf{R})G_0^R(lk_x)]^{m_n}\right], \tag{2.36}$$

where n_i is the impurity concentration $n_i=N_i/V$. On the other hand we have

$$U_i^e(\mathbf{R})=\frac{1}{V}\sum_{\mathbf{Q}}\gamma_{ll}(\mathbf{q})\overline{U}_i(\mathbf{Q})\exp(-j\mathbf{Q}\cdot\mathbf{R}) = \frac{1}{V}\sum_{\mathbf{Q}}\int d\mathbf{r}'\,|u_l(\mathbf{r}')|^2\overline{U}_i(\mathbf{Q}) \times\exp[-jq_xx-j\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')] = \int d\mathbf{r}'\,|u_l(\mathbf{r}')|^2 U_i(x,\mathbf{r}-\mathbf{r}') . \tag{2.37}$$

This result evidently means that $U_i^e(\mathbf{R})$ is the potential at an impurity position $\mathbf{R}$ due to an electron in the well. Equation (2.37) in combination with Eq. (2.36) is of central importance in all the discussions above.

As for the electron-electron interaction we consider the Coulomb term. The self-energy as shown in Fig. 3 is considered and we obtain, as is done in Ref. 11 for 3DS's,

$$\Sigma_{e\text{-}e}^R(lk_x,\omega)=-\frac{2}{\pi V}\sum_{l'\mathbf{Q}}\frac{4\pi e^2}{\epsilon_0(q^2+\lambda^2)}\gamma_{ll}(q_z)\gamma_{l'l'}(-q_z) \times\int d\omega\,\mathrm{Im}G^R(l'q_x,\omega)\Theta(\omega) , \tag{2.38}$$

where $\Theta(\omega)$ is the Fermi-Dirac distribution function at an

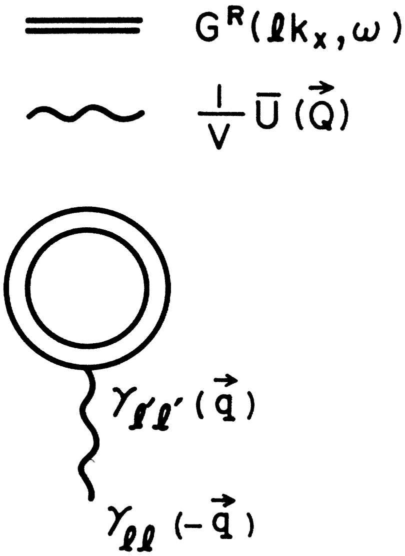

FIG. 3. Diagram representing the Coulomb term of the electron-electron interaction.

energy ω. On the other hand, the DOS $\rho(\omega)$ is given by

$$\rho(\omega)=-\frac{2}{\pi V}\sum_{l'q_x}\mathrm{Im}G^R(l'q_x,\omega)\ . \tag{2.39}$$

Then we obtain[11]

$$-Zn_i=\int d\omega\,\rho(\omega)\Theta(\omega)\ . \tag{2.40}$$

Restricting the discussion hereafter to the cases of sufficiently low temperature where almost all the electrons are in the lowest subband, we obtain

$$\Sigma^R_{e\text{-}e}(lk_x,\omega)=-\sum_{\mathbf{q}}\frac{4\pi e^2Zn_i}{\epsilon_0(q^2+\lambda^2)}\,|\gamma_{l_1l_1}(\mathbf{q})|^2\ , \tag{2.41}$$

where l_1 denotes the lowest subband.

For facility of the numerical calculation, we neglect the exchange energy. In fact, an estimation shows that the effect of this energy is significant but not so important.

With the use of Eqs. (2.36), (2.37) and (2.41), the calculation of $G^R(lk_x,\omega)$ is performed in perfectly the same way as in Ref. 11. We finally obtain

$$G^R(lk_x,\omega)=\frac{\epsilon_0}{|Z|e^2\lambda}\bar{G}^R(\Omega)\ , \tag{2.42}$$

$$\bar{G}^R(\Omega)=\frac{1}{j}\int_0^\infty d\xi\,\exp[j\xi\Omega+\gamma g(\xi)]\ , \tag{2.43}$$

$$\Omega=\frac{\epsilon_0}{|Z|e^2\lambda}[\omega-E_l(k_x)]\ , \tag{2.44}$$

$$g(\xi)=\int_{-\infty}^{\infty}dt_x\int_{\text{layer}}d\mathbf{t}\,\{\exp[-j\xi\bar{h}(t_x,\mathbf{t})]-1\}-j\xi\alpha\ , \tag{2.45}$$

$$\bar{h}(t_x,\mathbf{t})=\frac{Z}{|Z|}\int d\mathbf{r}'\,|u_l(\mathbf{r}')|^2\exp(-T)/T\ ;$$
$$T=(t_x^2+|\mathbf{t}-\lambda\mathbf{r}'|^2)^{1/2}\ , \tag{2.46}$$

$$\alpha=-\frac{Z}{|Z|}\sum_{\mathbf{q}}\frac{\lambda^2}{q^2+\lambda^2}\,|\gamma_{l_1l_1}(\mathbf{q})|^2\ , \tag{2.47}$$

$$\gamma=\frac{4\pi n_i}{\lambda^3}\ . \tag{2.48}$$

The integral of Eq. (2.45) comes from the integral $\int d\mathbf{R}\cdots$, which is transformed into $\lambda^{-3}\int dt_x\int d\mathbf{t}\cdots$ with $d\mathbf{t}=dt_y\,dt_z$. We have defined $t_x=\lambda x$ and $\mathbf{t}=\lambda\mathbf{r}$. $\bar{h}(t_x,\mathbf{t})$ comes from Eq. (2.37) and is the potential at an impurity. The integral over $\mathbf{t}$, i.e., $\mathbf{r}$, in $g(\xi)$ means averaging the contribution of this potential over the impurity site. It can be shown that we have $\mathrm{Im}\bar{G}^R(\Omega)\neq 0$ only in the range $\Omega<\gamma$. From Eq. (2.43) we obtain $\int_{-\infty}^{\infty}d\Omega\,\mathrm{Im}\bar{G}^R(\Omega)=-\pi$ which is used for correcting numerical error in a practical calculation.

The inverse screening length is calculated approximately by assuming that the screened potential of a point charge in a well is spherically symmetric. This is a good approximation under $\lambda^{-1}\ll L_y$ and L_z. Actually, this inequality holds only roughly in some cases of practical interest but an estimation shows that the above approximation is good. We use the Thomas-Fermi approach, giving

$$\lambda^2=-\frac{4\pi e^2}{\epsilon_0}\int d\omega\,\rho(\omega)\frac{d}{d\omega}\Theta(\omega)\ , \tag{2.49}$$

where $\rho(\omega)$ is calculated from Eq. (2.39). In practice, Eq. (2.49) is solved for λ noting that $\rho(\omega)$ depends on λ.

Now the criterion for the applicability of the present approach is discussed. We have used the assumption that the potential change within one wavelength of a quantum particle should be sufficiently small, i.e., $2\pi\lambda/|k_x|\ll 1$. As for k_x, we take a typical value k_F giving the Fermi level in the unperturbed band. Actually, the requirement $2\pi\lambda/|k_x|\ll 1$ seems to be too strong and we may use $2\pi\lambda/(4k_F)\ll 1$ instead. Considering degenerate statistics and the unperturbed subband, we approximately have $\lambda^2=4/[\pi a_B(L_yL_z)^2n_i]$ with a_B as the Bohr radius $\hbar^2\epsilon_0/(m^*e^2)$. We also use $k_F=L_yL_zn_i$. The criterion is

$$(\pi a_B)^{1/2}(L_yL_z)^2n_i^{3/2}\gtrsim 1\ . \tag{2.50}$$

This shows that the present approach is useful for a light-mass band under heavy doping.

For practical calculations in Sec. III, we assume a simple model that we have

$$u_l(\mathbf{r})=\frac{2}{(L_yL_z)^{1/2}}\sin\left[\frac{\pi l_y y}{L_y}\right]\sin\left[\frac{\pi l_z z}{L_z}\right] \tag{2.51}$$

for $0\le y\le L_y$ and $0\le z\le L_z$ and $u_l(\mathbf{r})=0$ otherwise with energy

$$E_l(k_x)=\frac{\hbar^2}{2m^*}\left[k_x^2+\left[\frac{\pi l_y}{L_y}\right]^2+\left[\frac{\pi l_z}{L_z}\right]^2\right] \tag{2.52}$$

as measured from the unperturbed band edge. Here l_y and l_z are integers larger than zero. The above model is applicable to the case where the well depth is infinite. With the use of Eq. (2.52), we examine a criterion under which the intersubband interaction is negligible. A spatial average of the impurity potential $\langle\lambda\Gamma\rangle$ is given by

$Ze^2\lambda\gamma/\epsilon_0$. The absolute magnitude of this value must be much smaller than at least the energy difference between the edges of the subbands with $(l_y,l_z)=(1,1)$ and $(1,2)$ for the lowest and the first excited subbands, respectively, assuming $L_y=L_z$ for simplicity.

With the use of $\lambda^2=4/[\pi a_B(L_yL_z)^2 n_i]$ we obtain the criterion $|Z|\,n_i^2(L_yL_z)^3 \ll 6$ and we tentatively give

$$|Z|\,n_i^2(L_yL_z)^3 \lesssim 1 \; . \tag{2.53}$$

The relations (2.50) and (2.53) give the range of n_i and L_yL_z where the present approach is useful.

From Eq. (2.51) and the restriction of **q** imposed just above Eq. (2.31), we obtain

$$|\gamma_{II}(\mathbf{q})|^2=\left\{\Delta(q_y)-\frac{1}{2}\left[\Delta\left(q_y+\frac{\pi l_y}{L_y}\right)+\Delta\left(q_y-\frac{\pi l_y}{L_y}\right)\right]\right\} \times\left\{\Delta(q_z)-\frac{1}{2}\left[\Delta\left(q_z+\frac{\pi l_z}{L_z}\right)+\Delta\left(q_z-\frac{\pi L_z}{L_z}\right)\right]\right\} . \tag{2.54}$$

From this relation, α in Eq. (2.47) is calculated to be

$$\alpha=1+\frac{1}{2}\left[\frac{\lambda^2}{\lambda^2+\left[\frac{2\pi}{L_y}\right]^2}+\frac{\lambda^2}{\lambda^2+\left[\frac{2\pi}{L_z}\right]^2}+\frac{1}{4}\frac{\lambda^2}{\lambda^2+\left[\frac{2\pi}{L_y}\right]^2+\left[\frac{2\pi}{L_z}\right]^2}\right] . \tag{2.55}$$

III. RESULTS AND DISCUSSIONS

The theory in Sec. II is applied to a single quantum well made of *n*-type GaAs at 0 K, whose conduction band is considered. Material parameters used are the effective mass 0.067 in unit of the electron mass in vacuo and $\epsilon_0=13.18$. We consider hydrogenic donor impurities with $Z=-1$ doped in a well region. The impurity concentration satisfying the criteria given in the preceding section should fall in a range $67(L_yL_z)^{-4/3} \lesssim n_i \lesssim (L_yL_z)^{-3/2}$ with L_y and L_z given in cm. However, for the sake of qualitative understanding the following calculations also include the cases of n_i outside the above range. All the calculations hereafter are done for the case of $L_y=L_z$ ($\equiv L$) only and for the lowest subband only.

Figure 4 shows the DOS's for the unperturbed (dashed line) and the perturbed (solid line) lowest subband ($l_y=l_z=1$) under $L=60$ Å as functions of energy ω measured from the unperturbed subband edge. The calculation for the perturbed subband has been done for $n_i=4\times10^{18}$ cm^{-3}. It is seen that the impurity doping not only gives rise to the band tail at the lower energy side of the peak but also pushes the peak up toward a higher energy. The modifications of the intraband states are seen also in the cases of a Q2DS and a 3DS, as shown in Figs. 5 and 6, respectively. Here the DOS's for the unperturbed (dashed lines) and the perturbed (solid lines) band are plotted for $n_i=4\times10^{18}$ cm^{-3}. Especially for the Q2DS we have considered the lowest subband under the well width 60 Å. It is seen that the modification is stronger in a lower dimensional structure. One reason is that the impurity scattering effect is larger on a lower energy particle

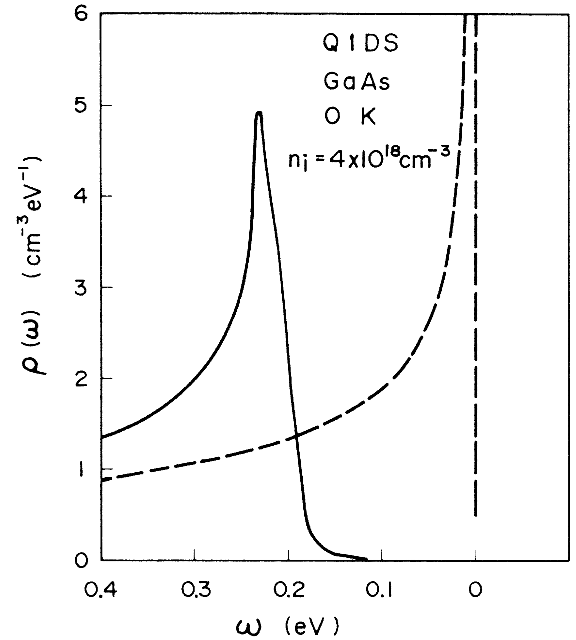

FIG. 4. DOS's for the unperturbed (dotted line) and the perturbed (solid line) lowest subband as functions of energy measured from the unperturbed subband edge under L ($=L_y=L_z$)$=60$ Å; $n_i=4\times10^{18}$ cm^{-3} is used for the perturbed subband.

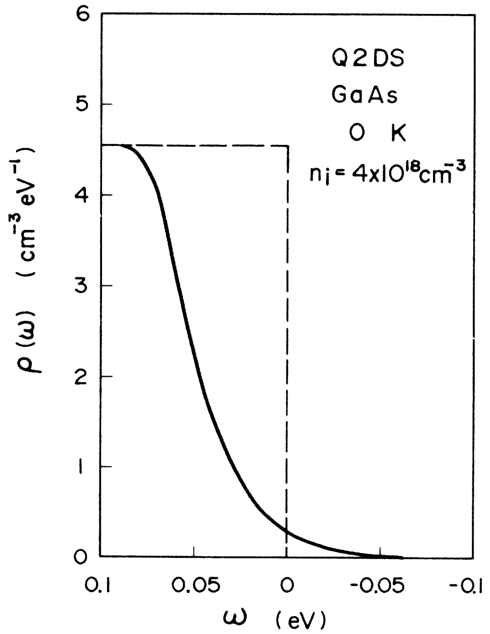

FIG. 5. DOS's for the unperturbed (dotted line) and the perturbed (solid line) lowest subband in a Q2DS as functions of energy measured from the unperturbed subband edge under the well width 60 Å; $n_i=4\times10^{18}$ cm^{-3} is used for the perturbed subband.

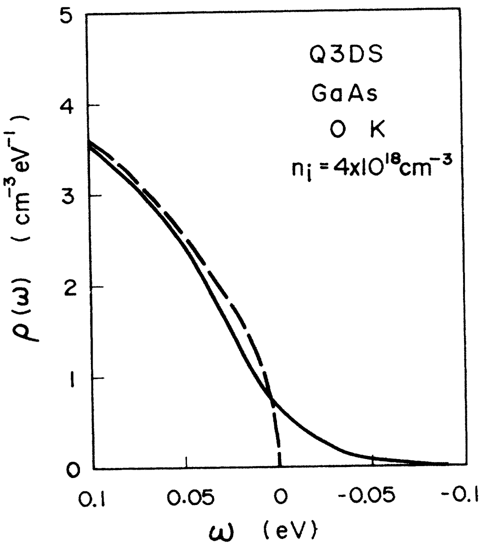

FIG. 6. DOS's for the unperturbed (dotted line) and the perturbed (solid line) band in a 3DS as functions of energy measured from the unperturbed band edge; $n_i = 4 \times 10^{18}$ cm^{-3} is used for the perturbed band.

and the DOS at the edge of the unperturbed band is larger in a lower dimension structure, i.e., zero for a 3DS, finite for a Q2DS, and infinite for a Q1DS. Another reason is that the screening is weaker in a lower dimension structure for the cases as considered in Figs. 4—6, i.e., a given carrier concentration and a given well width. In fact, the inverse screening length λ is calculated to be 1.54×10^6, and 2.41×10^6, and 2.50×10^6 cm^{-1} for the cases of Fig. 4 (Q1DS), 5 (Q2DS), and 6 (3DS), respectively.

In the following we consider only the perturbed band for Q1DS's. Figure 7 shows the DOS for the lowest subband as a function of energy measured from the unperturbed subband edge with n_i as a parameter for $L = 60$ Å. With increasing impurity concentration the peak of the DOS shifts toward a higher energy very rapidly together with the reduced height and the broadened width. The rapid shift of the peak is due largely to the rapid decrease of the inverse screening length λ with increasing n_i. In fact we have $\lambda = 2.16 \times 10^6$ and 1.38×10^6 cm^{-1} for $n_i = 2 \times 10^{18}$ and 5×10^{18} cm^{-3}, respectively. The shift of the DOS peak corresponds to that of the peak of $-\mathrm{Im}\bar{G}^R(\Omega)$ as shown in Fig. 8. It can be shown[11] that $-\mathrm{Im}\bar{G}^R(\Omega)$ is cut off at $\Omega = \gamma$ ($\equiv 4\pi n_i/\lambda^3$). The peak of $-\mathrm{Im}\bar{G}^R(\Omega)$ is located a little below this value and the DOS peak is nearly at $\omega = (-Ze^2\lambda/\epsilon_0)\gamma$ ($Z = -1$ here) as measured from the unperturbed subband edge. It should be noted that $Ze^2\lambda/\epsilon_0\gamma$ is just the spatially averaged electron-impurity interaction which is equal to the minus of the spatially averaged electron-electron interaction. The electron-impurity interaction pushes the DOS peak up toward a higher energy and broadens the width of the peak toward a lower energy region, as is seen in Figs. 7 and 8.

Figure 9 shows the DOS for the lowest subband as a function of energy measured from the unperturbed subband edge with L as a parameter under $n_i = 4 \times 10^{18}$ cm^{-3}. It is seen that the DOS approaches that for the unperturbed subband as the well width is decreased. The reason is that for a smaller well width the electron-electron and electron-impurity interactions become small with decreasing width due to increased λ. In fact, we have $\lambda = 1.13 \times 10^6$ and 3.47×10^6 cm^{-1} for $L = 70$ and 40 Å, respectively.

The relative importance of the DOS shift with respect to the growth of the band tail increases for a lower dimension structure, as is seen by comparing Figs. 4, 5, and 6. For example, in a 3DS only a small modification of the intraband DOS is observed with clear appearance of the band tail, as is in contrast with the cases of a Q1DS and a

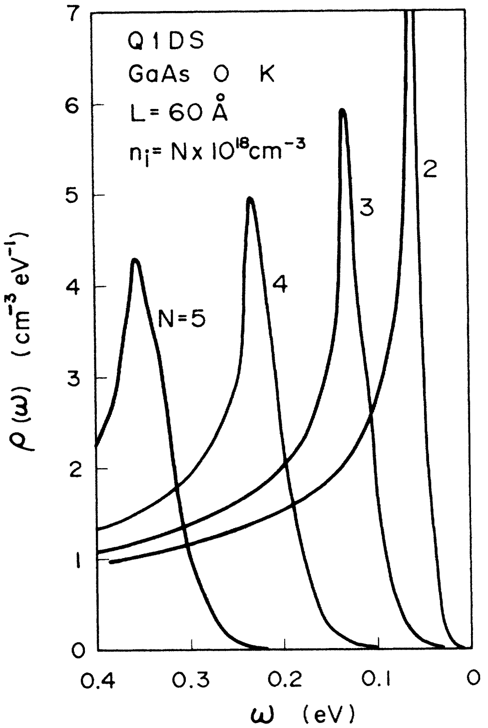

FIG. 7. DOS for the lowest subband as a function of energy measured from the unperturbed subband edge with n_i as a parameter under L ($= L_y = L_z$) $= 60$ Å.

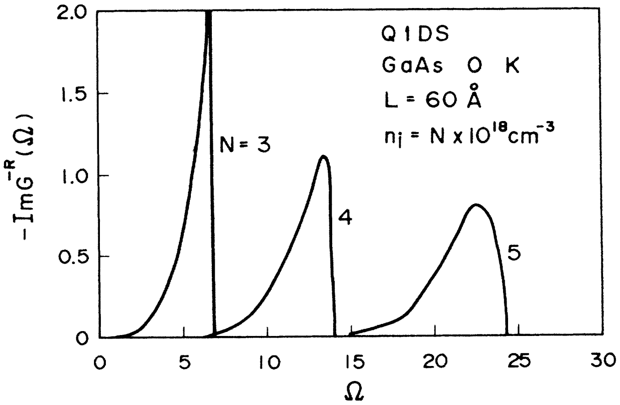

FIG. 8. $-\mathrm{Im}\bar{G}^R(\Omega)$ for the lowest subband as a function of Ω with n_i as a parameter under L ($= L_y = L_z$) $= 60$ Å.

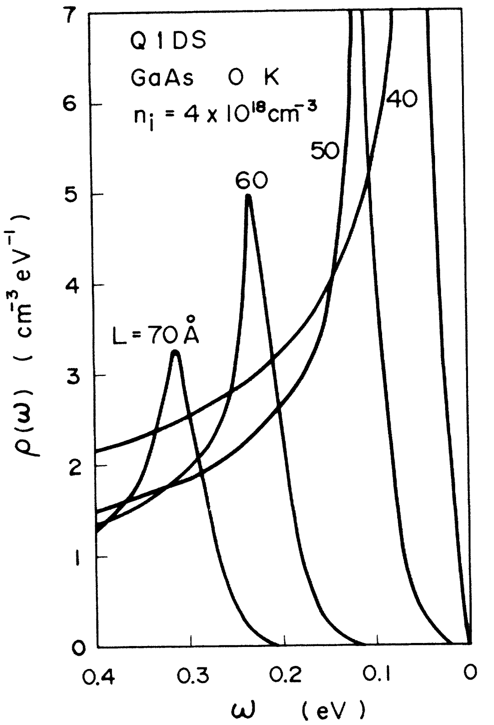

FIG. 9. DOS for the lowest subband as a function of energy measured from the unperturbed subband edge with L ($=L_y=L_z$) as a parameter under $n_i=4\times10^{18}$ cm^{-3}.

Q2DS. A rapid shift of the DOS peak with variation of n_i or L in a Q1DS is ascribed to the strong dependence of the inverse screening length λ on these parameters. Since the Fermi level ω_F is at a high energy for n_i under consideration, ω_F and λ are found to be given nearly the same values as those for the unperturbed band. In this approximation, the DOS at an energy ω measured from the unperturbed subband edge is given for sufficiently large ω by

$$\rho(\omega)=\frac{1}{2\pi L_y L_z}\left[\frac{2m^*}{\hbar^2}\right]^{1/2}\frac{1}{\sqrt{\omega}} . \tag{3.1}$$

On the other hand the Fermi level ω_F at 0 K is

$$\omega_F=\frac{\hbar^2}{2m^*}(\pi L_y L_z n_i)^2 . \tag{3.2}$$

With the use of

$$\lambda^2=\frac{4\pi e^2}{\epsilon_0}\rho(\omega_F) \tag{3.3}$$

we then have

$$\lambda^2=\frac{4}{\pi a_B (L_y L_z)^2 n_i} . \tag{3.4}$$

From the above equations we notice the remarkable facts that λ decreases with increasing Fermi level or increasing doping level and that λ is a rapidly decreasing function of the well width. The value of $(-Ze^2\lambda/\epsilon_0)\gamma$, which is a measure of pushing the DOS up toward a higher-energy region, is proportional to $n_i^2(L_yL_z)^2$ for a Q1DS, to n_iL (L being the well width) for a Q2DS, and to $n_i^{1/3}$ for a 3DS. Thus the dependence of the shift on the impurity concentration and the well width becomes important for a structure of lower dimension.

Because of the strong dependence of the peak height and position of the DOS on n_i, large elevation of the Fermi level is caused by the doping in a Q1DS. For example, the Fermi levels for $n_i=4\times10^{18}$ cm^{-3} are calculated on the perturbed band and the unperturbed band to be 0.3 and 0.12 eV, respectively, as measured from the lowest subband edge. On the other hand, the Fermi levels are nearly the same for both bands in a 3DS.

The situations discussed above, under the impurity doping may be nearly the same as those under high injection of electrons and holes since the holes are considered to scatter electrons in nearly the same way as the ionized impurities. A typical example is a wire structure laser. In addition to a well-known expectation that this laser can be operated under low threshold current with small sensitivity to temperature variation, a short-lasing-wavelength operation is expected under high injection and/or high doping due to large elevation of the Fermi level as discussed above. Strong dependence of the emission wavelength of a light-emitting diode on the injection level and the doping level is also expected. In those light-emitting devices above, carrier concentrations around 10^{18} cm^{-3} under the well widths from 50 to 100 Å may be typical operation conditions. These conditions almost satisfy the criteria (2.50) and (2.53) under which the present theory is useful. The Q1DS devices are attractive for both practical and academic purposes. Unfortunately, however, there seem to be few attempts[14] to fabricate such structure at the present stage.

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