PHYSICAL REVIEW B VOLUME 33, NUMBER 6 15 MARCH 1986

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

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(Received 14 June 1985)

A theory is presented of the effect of impurity doping on the electronic states in a quasi-two-dimensional—structure semiconductor on the basis of the Green's-function formalism. The theory is applied to a single quantum well of GaAs. It is shown that the states around the band edge are strongly modulated by the heavy doping as compared with the case of a three-dimensional structure. As the well width is decreased, the band tail becomes longer but the intraband density of states tends to that for an undoped well.

I. INTRODUCTION

Study of a quasi-two-dimensional—structure (Q2DS) semiconductor such as a quantum well and a superlattice is one of the current topics motivated by a recent progress of the epitaxial-growth techniques. Especially, optical properties of Q2DS have received much attention in the fields of fundamental physics[1,2] and device physics[3-8] represented by a quantum well laser. Owing to the strong confinement of the free carriers in the small size quantum well, size quantization produces subbands and plays an important role in determining the electrical and optical properties. One of the outstanding features of Q2DS is the density of states (DOS) which is a step function of energy. This is contrasted with a square root function in a usual three-dimensional structure (3DS). The step-function type of DOS has been found to result in excellent characteristics of laser operations in Q2DS, e.g., low threshold current and weak temperature dependence, as compared with those in 3DS. Thus the new feature of DOS plays various important roles in the Q2DS physics.

In practice, intentional or unintentional doping is often inevitable, leading to modification of DOS around the edges of the subbands. Recently, the calculation of the impurity-band tail in Q2DS has been carried out[9] on the basis of the minimum counting method developed by Halperin and Lax[10] for 3DS. This method is useful only for deep band-tail states. However, DOS around the band edge is more important in practical cases because device physics is often relevant to the intraband near-edge process as is in lasers and light-emitting diodes. Furthermore, the impurity scattering effect becomes important as one approaches to the band edge, where DOS for an unperturbed band in Q2DS is finite in contrast with that in 3DS. As a result, the modification of DOS around the band edge is considered to be more serious in Q2DS than in 3DS. Therefore the minimum counting method may not be powerful for understanding important aspects of device physics although useful for an academic purpose.

On the other hand, Bonch-Bruevich[11] has developed an approach for 3DS on the basis of an assumption that the potential varies slowly enough; then fluctuation in the energy of states mirrors closely that in the potential energy. The present author has discussed the approach in a different method,[12] i.e., a diagram method. The approach by Bonch-Bruevich and the present author is considered in this paper and is called hereafter as the Bonch-Bruevich—Takeshima (BT) approach. It has been shown[12,13] that the BT approach is useful for the intraband states and the states around the band edge especially in the case of a light mass band such as the conduction band at high doping levels.

In this paper we use the Bonch-Bruevich assumption also for the case of Q2DS. This approach is not only useful for a light mass band but also opens a way to analyzing the band tail in a heavy mass band on the basis of the pseudopotential approach.[13] Another advantage of the BT approach is the use of the Green's function formalism, which is well known to offer direct methods of calculating various physical parameters such as the conductivity,[12] the absorption constant,[14] and the Auger recombination lifetime.[15] Thus the extension of the BT approach for 3DS to the case of Q2DS offers a powerful method of analyzing various phenomena of practical interest.

II. THEORY

Considering carrier confinement in the z direction, we define notations for the two-dimensional position vector $\mathbf{r}=(x,y)$ in the confinement-free directions, the three-dimensional position vector $\mathbf{R}=(x,y,z)$, the two-dimensional wave vectors $\mathbf{q}=(q_x,q_y)$ and $\mathbf{k}=(k_x,k_y)$, 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. 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

$$\phi_{l\mathbf{k}}(\mathbf{R})=\frac{1}{(L_xL_y)^{1/2}}\exp(j\mathbf{k}\cdot\mathbf{r})u_l(z)\ , \tag{2.1}$$

where L_x and L_y are the lengths of the rectangular crystal in the x and y directions, respectively, and $u_l(z)$ the wave function for the subband l in the z direction.

Let us consider a single quantum well, where hydrogenic donor impurities are randomly distributed; outside the well no impurities are present. 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 perturbations. The explicit forms of the Hamiltonians are

$$H_e = \sum_{l,\mathbf{k},\sigma} E_l(\mathbf{k}) a^{\dagger}_{l\mathbf{k}\sigma} a_{l\mathbf{k}\sigma} \ , \tag{2.3}$$

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

$$H_{e\text{-}e} = \frac{1}{2V} \sum_{\substack{l_1,l_2,l_3,l_4, \\ \mathbf{k},\mathbf{k}',\sigma,\sigma',\mathbf{Q}}} \overline{U}(\mathbf{Q}) \gamma_{l_1 l_4}(q_z) \gamma_{l_2 l_3}(-q_z) \times a^{\dagger}_{l_1\mathbf{k}+\mathbf{q}\sigma} a^{\dagger}_{l_2\mathbf{k}'-\mathbf{q}\sigma'} a_{l_3\mathbf{k}'\sigma'} a_{l_4\mathbf{k}\sigma} \ . \tag{2.5}$$

Here $a^{\dagger}_{lk\sigma}$, $a_{lk\sigma}$, and $E_l(\mathbf{k})$ are the creation operator, the annihilation operator, and the unperturbed subband energy, respectively, for the electron with the subband index l, the two-dimensional wave vector $\mathbf{k}$, 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 the impurity at $\mathbf{R}=\mathbf{R}_n$, N_i the total number of 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 $\mathbf{R}_1$ and $\mathbf{R}_2$

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

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

$$\gamma_{l'l}(q_z) = \int dz \, u^{*}_{l'}(z) \exp(jq_z z) u_l(z) \ . \tag{2.8}$$

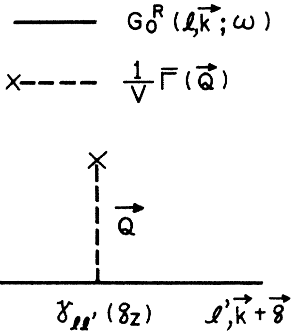

FIG. 1. Diagram representing the impurity scattering.

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. Derivation of the screened potential starting from an unscreened potential is given in Ref. 12 for 3DS. For Q2DS it is assumed that almost all of the electrons, which contribute to the screening, are in the lowest subband only so that the discussion is analogous to that for 3DS. Assuming one species of the impurities, we have

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

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

where e is the electronic charge, ϵ_0 the dielectric constant of the host lattice, and Z the minus of the valency of the impurity with respect to the host lattice. Then we have

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

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

where $U_i(\mathbf{Q})$ 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

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

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 wave vectors $\mathbf{k}$ and $\mathbf{k}'$, 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 an impurity scattering is shown in Fig. 1 with the use of the free-particle Green's function

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

under $\delta \to 0^+$. In a way analogous to the case of 3DS (Ref. 16) we obtain

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

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

$$G^R(l'',\mathbf{q};l',\mathbf{k}')=\sum_{m=0}^{\infty}\frac{1}{m!}[(\mathbf{q}-\mathbf{k})\cdot\nabla_k]^m G^R(l'',\mathbf{k};l',\mathbf{k}') \tag{2.17}$$

with ∇_k as $\partial/\partial\mathbf{k}$, we can rewrite Eq. (2.16) as

$$G^R(l,\mathbf{k};l',\mathbf{k}')=G_0^R(l,\mathbf{k})\left[\Delta(l-l')\Delta(\mathbf{k}-\mathbf{k}')+\sum_{l''}\widetilde{\Gamma}_{ll''}(j\nabla_k)G^R(l'',\mathbf{k};l',\mathbf{k}')\right]. \tag{2.18}$$

Here we define

$$\widetilde{\Gamma}_{ll''}(j\nabla_k)=\int dz\, u_l^*(z)u_{l''}(z)\overline{\Gamma}(j\nabla_k,z) \tag{2.19}$$

and $\overline{\Gamma}(j\nabla_k,z)$ is obtained from $\Gamma(\mathbf{R})$ by replacing x, y, and z with $j\partial/\partial k_x$, $j\partial/\partial k_y$, and z, respectively.

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

$$G^R(l,\mathbf{k};l,\mathbf{k}')=\frac{G_0^R(l,\mathbf{k})}{1-G_0^R(l\mathbf{k})[\widetilde{\Gamma}_{ll}(j\nabla_k)+F(j\nabla_k;l,l)]}\left[\Delta(\mathbf{k}-\mathbf{k}')+\sum_{l''}F(j\nabla_k;l,l'')G^R(l'',\mathbf{k};l,\mathbf{k}')\right], \tag{2.20}$$

where

$$F(j\nabla_k;l,l')=\sum_{l''\,(\neq l,l')}\widetilde{\Gamma}_{ll''}(j\nabla_k)\frac{G_0^R(l,\mathbf{k})}{1-G_0^R(l,\mathbf{k})\widetilde{\Gamma}_{l''l''}(j\nabla_k)}\widetilde{\Gamma}_{l''l'}(j\nabla_k). \tag{2.21}$$

Note that $\widetilde{\Gamma}_{ll'}(j\nabla_k)$ 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

$$G^R(l,\mathbf{k};l',\mathbf{k}')=\frac{G_0^R(l,\mathbf{k})}{1-G_0^R(l,\mathbf{k})\widetilde{\Gamma}_{ll}(j\nabla_k)}\left[\widetilde{\Gamma}_{ll'}(j\nabla_k)\Delta(\mathbf{k}-\mathbf{k}')G_0^R(l,\mathbf{k})+\sum_{l''\,(\neq l)}\widetilde{\Gamma}_{ll''}(j\nabla_k)G^R(l'',\mathbf{k};l',\mathbf{k}')\right]. \tag{2.22}$$

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

$$G^R(l,\mathbf{k};l,\mathbf{k}')=\frac{G_0^R(l,\mathbf{k})}{1-G_0^R(l,\mathbf{k})\widetilde{\Gamma}_{ll}(j\nabla_k)}\Delta(\mathbf{k}-\mathbf{k}') \tag{2.23}$$

by neglecting all F's in Eq. (2.20). This equation can be rewritten as

$$G^R(l,\mathbf{k};l,\mathbf{k}')=\int d\mathbf{r}\exp[j(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\times\frac{1}{\omega+j\delta-E_l(\mathbf{k}+j\nabla_r)-\widetilde{\Gamma}_{ll}(\mathbf{r})}1, \tag{2.24}$$

where $\nabla_r=\partial/\partial\mathbf{r}$ and $\widetilde{\Gamma}_{ll}(\mathbf{r})$ is obtained from $\widetilde{\Gamma}_{ll}(j\nabla_k)$ by replacing $j\nabla_k$ with $\mathbf{r}$, i.e.,

$$\widetilde{\Gamma}_{ll}(\mathbf{r})=\int dz\,|u_l(z)|^2\Gamma(\mathbf{R})=\frac{1}{V}\sum_{\mathbf{q}}\overline{\overline{\Gamma}}_{ll}(\mathbf{q})\exp(j\mathbf{q}\cdot\mathbf{r}), \tag{2.25}$$

with the definition of

$$\overline{\overline{\Gamma}}_{ll}(\mathbf{q})=\sum_{q_z}\gamma_{ll}(q_z)\overline{\Gamma}(\mathbf{Q}). \tag{2.26}$$

In Eq. (2.24) we define the operation

$$\{1/[\omega+j\delta-E_l(\mathbf{k}+j\nabla_r)-\widetilde{\Gamma}_{ll}(\mathbf{r})]\}1=[G_0^R(l,\mathbf{k})/(1-O_p)]1=G_0^R(l\mathbf{k})\sum_{n=0}^{\infty}O_p^n 1,$$

where $O_p=[E_l(\mathbf{k}+j\nabla_r)-E_l(\mathbf{k})+\widetilde{\Gamma}_{ll}(\mathbf{r})]G_0^R(l,\mathbf{k})$.

After the Bonch-Bruevich's approach[11] for 3DS it is assumed that in the xy plane the spatial variation of $\widetilde{\Gamma}_{ll}(\mathbf{r})$ within the de-Broglie wavelength is slow enough to allow neglecting the spatial derivatives of all orders of $\widetilde{\Gamma}_{ll}(\mathbf{r})$ contained in Eq. (2.23), i.e., $\nabla_r^n\widetilde{\Gamma}_{ll}(\mathbf{r})=0$ for $n\geq 1$. This approximation is completely equivalent to the standard method of the bent bands. For the present case this is valid only at sufficiently high doping levels, as will be discussed later, i.e., Eq. (2.50). We obtain

$$\begin{aligned}G^R(l,\mathbf{k};l,\mathbf{k}')&=\frac{1}{L_xL_y}\int d\mathbf{r}\exp[j(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\frac{G_0^R(l,\mathbf{k})}{1-G_0^R(l,\mathbf{k})\widetilde{\Gamma}_{ll}(\mathbf{r})}\\&=G_0^R(l,\mathbf{k})\sum_{m=0}^{\infty}[G_0^R(l,\mathbf{k})]^m\frac{1}{L_xL_y}\int d\mathbf{r}[\widetilde{\Gamma}_{ll}(\mathbf{r})]^m\exp[j(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}].\end{aligned} \tag{2.27}$$

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

$$\frac{1}{L_xL_y}\int d\mathbf{r}[\widetilde{\Gamma}_{ll}(\mathbf{r})]^m \exp[j(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}] = \sum_{\mathbf{Q}_1,\mathbf{Q}_2,\ldots,\mathbf{Q}_m} \Delta(\mathbf{q}_1+\mathbf{q}_2+\cdots+\mathbf{k}-\mathbf{k}') \prod_{n=1}^{m} \left[\frac{1}{V}\widetilde{U}_i(\mathbf{Q}_n)h(\mathbf{Q}_n)\right] , \tag{2.28}$$

where

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

Now we consider an ensemble average[11,16] of $G^R(l,\mathbf{k};l,\mathbf{k}')$ over the impurity sites, which is defined as

$$\begin{aligned}\langle G^R(l,\mathbf{k};l,\mathbf{k}')\rangle &= \frac{1}{(L_xL_yL_z)^{N_i}}\int d\mathbf{R}_1 \int d\mathbf{R}_2 \int \cdots \int d\mathbf{R}_{N_i} G^R(l,\mathbf{k};l,\mathbf{k}') \\ &= G^R(l,\mathbf{k};\omega)\Delta(\mathbf{k}-\mathbf{k}') ,\end{aligned} \tag{2.30}$$

where L_z is the well width. Here the integrals are taken only over a layer where the impurities are distributed; this layer is just the well in this paper. 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 average distribution giving the momentum conservation $\mathbf{k}=\mathbf{k}'$. For convenience we define q_z by proposing that the periodic boundary condition should be satisfied for a wave $\exp(jq_zz)$ at both boundaries of the doped layer, i.e., the well. Thus we should take $V=L_xL_yL_z$ and obtain

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

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

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

where

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

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 of S is

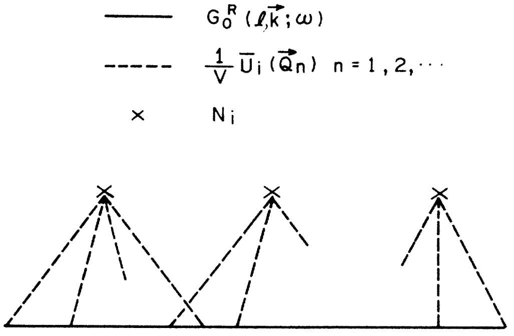

FIG. 2. Diagram representing the impurity scattering, which is obtained by taking an ensemble average over the impurity sites.

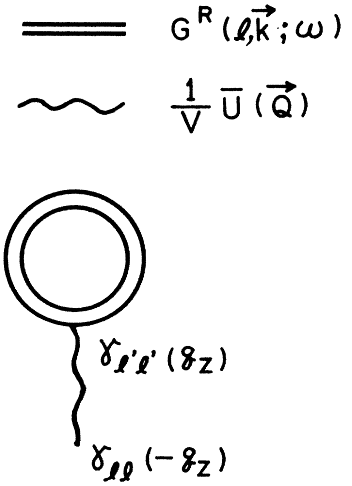

FIG. 3. Diagram representing the Coulomb term of the electron-electron interaction.

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

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

$$\begin{aligned}U_i^e(\mathbf{R})&=\frac{1}{V}\sum_{\mathbf{Q}}\gamma_{ll}(q_z)\overline{U}_i(\mathbf{Q})\exp(-j\mathbf{Q}\cdot\mathbf{R})\\&=\frac{1}{V}\sum_{\mathbf{Q}}\int dz'\,|u_l(z')|^2\overline{U}_i(\mathbf{Q})\exp[-j\mathbf{q}\cdot\mathbf{r}-jq_z(z-z')]=\int dz'\,|u_l(z')|^2U_i(\mathbf{r},z-z')\,.\end{aligned} \tag{2.37}$$

This result evidently means that $U_i^e(\mathbf{R})$ is the potential at an impurity position $\mathbf{R}$ due to an electron in a 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[12]

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

where $\theta(\omega)$ is the Fermi-Dirac distribution function at an energy ω. On the other hand, DOS $\rho(\omega)$ is given by

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

Then we have

$$|Z|\,n_i=\int d\omega\,\rho(\omega)\theta(\omega)\,. \tag{2.40}$$

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

$$\Sigma_{e\text{-}e}^R(l,\mathbf{k};\omega)=\sum_{q_z}\frac{4\pi e^2|Z|\,n_i}{\epsilon_0(q_z^2+\lambda^2)}|\gamma_{l_1l_1}(q_z)|^2\,, \tag{2.41}$$

where l_1 denotes the lowest subband.

For facility of the numerical calculation, we neglect the exchange energy in view of the present purpose that we investigate the impurity effect. In fact, an estimation shows that the effect of the exchange energy is significant but not so important.

With the use of Eqs. (2.36) and (2.41), the calculation of $G^R(l,\mathbf{k};\omega)$ is performed in perfectly the same way as in Ref. 12. In the calculation we take into account all the diagrams containing multisite and multiple impurity scatterings. Thus the present calculation goes beyond the single-site second-order Born approximation, which is not valid[12,17,18] for the de-Bloglie wavelength larger than the average separation of the impurities or for low energy states subject to strong impurity scattering. We finally obtain

$$G^R(l,\mathbf{k};\omega)=\frac{\epsilon_0}{|Z|e^2\lambda}G^R(\Omega)\,, \tag{2.42}$$

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

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

$$g(\xi)=\tfrac{1}{2}\int_0^\infty dt\,t\int_{\text{layer}}dt_z\{\exp[-j\xi\overline{h}(t,t_z)-1]-j\xi\alpha\}\,, \tag{2.45}$$

$$\begin{aligned}\overline{h}(t,t_z)&=\int dz'\,|u_l(z')|^2\exp(-T)/T,\\T&=[t^2+(t_z-\lambda z')^2]^{1/2}\,,\end{aligned} \tag{2.46}$$

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

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

The integral of Eq. (2.45) comes from the integral $\int d\mathbf{R}\cdots$, which is transformed into

$$(2\pi/\lambda^3)\int dt\,t\int dt_z\cdots$$

by using the cylindrical coordinates (r,z,θ) in place of the spherical coordinates (r,θ,ϕ) in Ref. 12 in the case of 3DS. We have defined $t=\lambda r$ and $t_z=\lambda z$. $\overline{h}(t,t_z)$ comes from Eq. (2.37) and is the potential at an impurity. The integral over t_z, i.e., z, in the layer region means averaging the contribution of this potential over the impurity site.

The inverse screening length λ is calculated approximately by assuming that the screened potential of an impurity is spherically symmetric. This is a good approximation under $\lambda^{-1}\ll L_z$. Actually, this inequality holds only roughly in some cases of practical calculations but we use the above approximation for simplicity. We use the Thomas-Fermi approach, which gives

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

where $\rho(\omega)$ is calculated from Eq. (2.39). Actually, λ is solved from Eq. (2.49) noting that $\rho(\omega)$ is a function of λ.

Now the criterion for the applicability of the present approach is discussed. This approach has used, after the BT approach for 3DS, the assumption that the potential change within one wavelength of a quantum particle should be sufficiently small, i.e., $2\pi\lambda/k\ll 1$. As for k we take a typical value k_F which is the magnitude of the Fermi wave vector in the unperturbed band. Actually, the requirement $2\pi\lambda/k_F \ll 1$ seems to be too strong and we may use $2\pi\lambda/(4k_F) \lesssim 1$ instead. Considering degenerate statistics, we approximately have $\lambda^2 = 4/(a_B L_z)$ with a_B as the Bohr radius $\hbar^2\epsilon_0/(m^* e^2)$, where m^* is the effective mass. We also use $k_F = (2\pi L_z n_i)^{1/2}$. As a result the criterion is

$$a_B L_z^2 n_i \geq \frac{\pi}{2} \ . \tag{2.50}$$

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

$$u_l(Z) = \left[\frac{2}{L_z}\right]^{1/2} \sin\left[\frac{\pi l_z}{L_z}\right] \tag{2.51}$$

for $0 \leq z \leq L_z$ and $u_l(z) = 0$ otherwise with energy

$$E_l(\mathbf{k}) = \frac{\hbar^2}{2m^*}\left[\frac{\pi l}{L_z}\right]^2 + \frac{\hbar^2}{2m^*}k^2 \tag{2.52}$$

as measured from the unperturbed band edge. Here l is an integer larger than zero. The above model is applicable to the case where the well depth is infinite. With the use of Eq. (2.51), we examine a criterion under which the intersubband interaction is negligible. A spatial average of the impurity potential $\langle \Gamma \rangle$ is roughly given by $e^2\lambda\gamma/\epsilon_0$. This value must be much smaller than at least the energy difference between the bottoms of the subbands with $l = 1$ and 2. With the use of $\lambda^2 = 4/(a_B L_z)$, we obtain the criterion $n_i L_z^3 \ll 6\pi$ and we tentatively give

$$n_i L_z^3 \lesssim 5 \ . \tag{2.53}$$

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

From Eq. (2.51) and the restriction on q_z given just above Eq. (2.31), we obtain

$$|\gamma_{ll}(q_z)|^2 = \Delta(q_z) + \frac{1}{4}\left[\Delta\left[q_z + \frac{2\pi l}{L_z}\right] + \Delta\left[q_z - \frac{2\pi l}{L_z}\right]\right] \ . \tag{2.54}$$

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

$$\alpha = 1 + \frac{1}{2}\frac{\lambda^2}{\lambda^2 + (2\pi/L_z)^2} \ . \tag{2.55}$$

III. RESULTS AND DISCUSSIONS

The theory in Sec. II is applied to a well made of n-type GaAs at 0 K. 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

$$1.3 \times 10^6/L_z^2 \lesssim n_i \lesssim 5/L_z^3$$

with L_z in cm. However, for obtaining a qualitative understanding the following calculations also include the cases of n_i outside the above range.

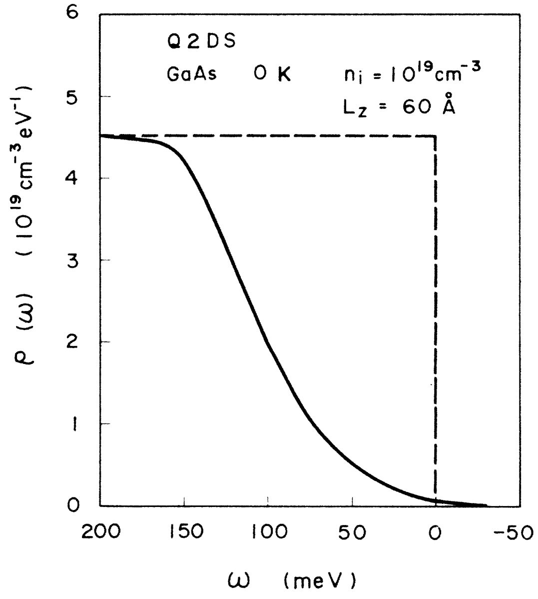

FIG. 4. DOS's for the unperturbed (dashed line) and the perturbed (solid line) lowest subband as functions of energy measured from the unperturbed subband edge under $L_z = 60$ Å; $n_i = 10^{19}$ cm^{-3} is used for the perturbed subband.

Figure 4 shows DOS's for the unperturbed (dashed line) and the perturbed (solid line) lowest subband under $L_z = 60$ Å as functions of energy ω measured from the unperturbed subband edge. The calculation for the per-

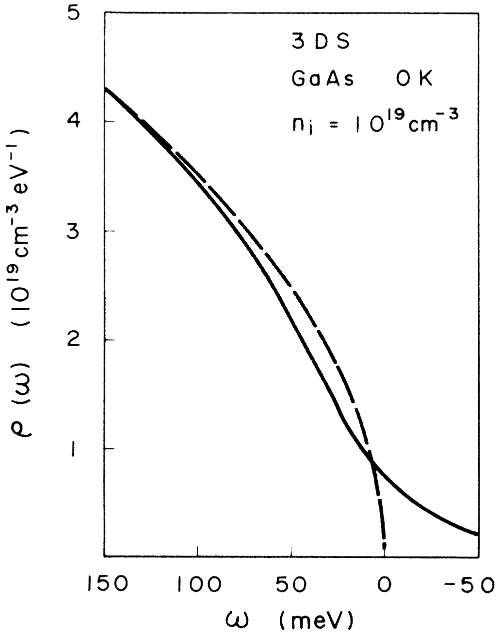

FIG. 5. DOS's for the unperturbed (dashed line) and the perturbed (solid line) band in 3DS as functions of energy measured from the unperturbed band edge. $n_i = 10^{19}$ cm^{-3} is used for the perturbed band.

turbed band has been done for $n_i = 10^{19}$ cm^{-3}. It is seen that the impurity doping not only gives rise to the band tail but also strongly modifies the intraband region. For comparison curves for 3DS under $n_i = 10^{19}$ cm^{-3} are shown in Fig. 5, where DOS's for the unperturbed (dashed line) and the perturbed (solid line) band are plotted. The method of the calculation is found in Ref. 12. An important point is that the intraband states are much more strongly modified for Q2DS than for 3DS. This is as a result that in Q2DS the impurity scattering effect becomes larger as the energy is decreased and DOS for the unperturbed subband is a constant in contrast to the case of 3DS, where DOS for the unperturbed band approaches zero as the energy is decreased toward the band edge.

In the following we consider only the perturbed subbands. Figure 6 shows DOS for the lowest subband as a function of energy measured from the unperturbed subband edge with L_z as a parameter under $n_i = 10^{19}$ cm^{-3}. It is seen that the band tail becomes long with decreasing well width. This result reflects the fact that an impurity level becomes deep with decreasing well width. Another observation is that the intraband DOS approaches that for the unperturbed band, i.e., a step function, as the well width is decreased. The reason is that for a smaller well width the electron-electron interaction, which pushes up the states to higher energies, becomes small due to increased λ.

Figure 7 shows DOS for the lowest subband as a function of energy measured from the unperturbed subband edge with n_i as a parameter under $L_z = 60$ Å. With increasing impurity concentration, DOS around the band edge is seen to be more and more modified. Amount of decrease of the intraband DOS is larger than that of the increase of the band tail states. Therefore the elevation of the Fermi level with increasing impurity concentration is not only caused by the increase of the concentration itself, but also enhanced by the decrease of the intraband DOS. In fact, the Fermi levels for the perturbed subband under $L_z = 60$ Å are calculated to be 0.055, 0.16, and 0.32 eV for $n_i = 2\times10^{18}$, 5×10^{18}, and 1×10^{19} cm^{-3}, respectively, while those for the unperturbed subband are 0.043, 0.11, and 0.21 eV for the respective values of n_i. Thus the elevation of the Fermi level due to the modification of

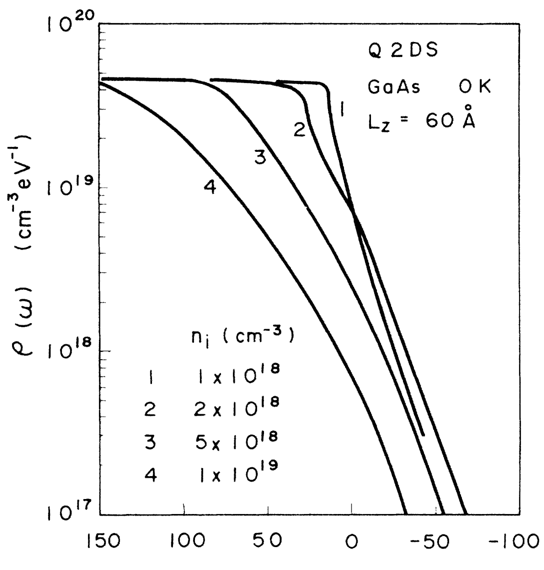

FIG. 7. DOS for the lowest subband as a function of energy measured from the unperturbed subband edge with n_i as a parameter under $L_z = 60$ Å.

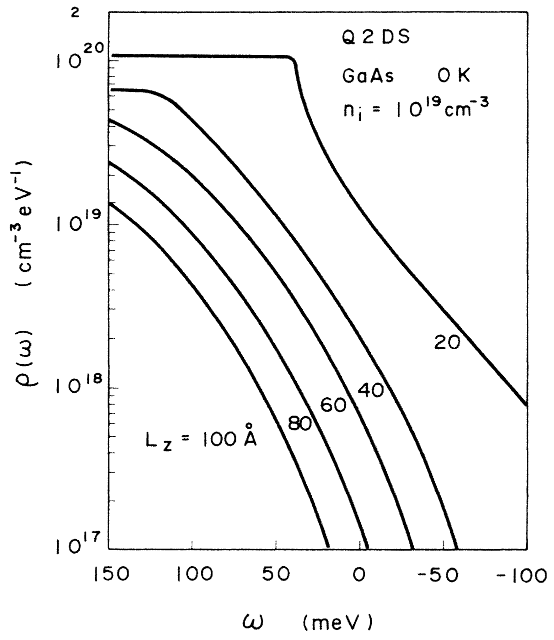

FIG. 6. DOS for the lowest subband as a function of energy measured from the unperturbed subband edge with L_z as a parameter under $n_i = 10^{19}$ cm^{-3}.

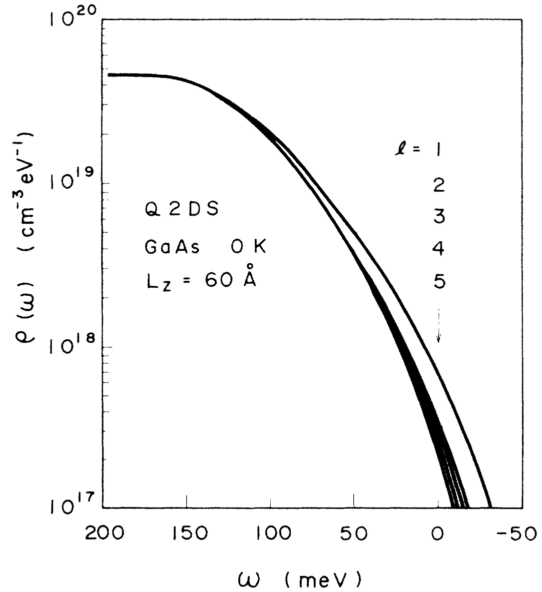

FIG. 8. DOS's for various subbands as functions of energies measured from the respective subband edges under $L_z = 60$ Å and $n_i = 10^{19}$ cm^{-3}.

DOS is large. In contrast, in 3DS the Fermi level for the perturbed band is calculated to be nearly the same as that for the unperturbed one. The strong modification of the intraband DOS in Q2DS may be very important in the fields of device physics as well as fundamental physics.

Figure 8 shows DOS's for various subbands as functions of energies measured from the respective subband edges. It is seen that DOS at a given relative energy is smaller for a higher subband especially in the band tail regions. This again reflects the fact that the impurity scattering effect is more important at lower energies. It should be pointed out here that DOS arising from all the subbands is practically the same as that for the lowest subband shown in Figs. 4—7. At energies exceeding those of some subband edges, contributions from higher subband DOS and the neglected effect of the intersubband scattering may be important. However, this does not matter, as far as the ranges of the energy and the well width considered in Figs. 4—7 are concerned. For example, the first excited subband ($l=2$) edge lies 0.17 eV higher than the lowest subband ($l=1$) under L_z as large as 100 Å. Therefore, the strong modification of the intraband DOS is a conclusive result and may play an important role in the fields of device physics as well as fundamental physics.

ACKNOWLEDGMENTS

The author wishes to express his appreciation to Dr. G. Kano, Dr. I. Teramoto, and Dr. H. Mizuno for their constant encouragement.

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