PHYSICAL REVIEW B, VOLUME 64, 125324

Effect of impurity correlation in modulation-doped quantum wires

Doan Nhat Quang
Center for Theoretical Physics, National Center for Natural Science and Technology, P. O. Box 429, Boho, Hanoi 10000, Vietnam

Nguyen Huyen Tung and Tran Doan Huan
Institute of Engineering Physics, Hanoi University of Technology, 1 Dai Co Viet Road, Hanoi, Vietnam

(Received 4 April 2000; revised manuscript received 28 June 2000; published 11 September 2001)

A theory is given of the electronic properties of modulation-doped quantum wires which undergo a thermal treatment, taking into account the Coulomb interaction among ionized impurities in the sample preparation. It is pointed out that the correlation among impurities weakens their field and is enhanced when elevating the doping level, lowering the freezing temperature for impurity diffusion, and reducing the size of the impurity system. The screening of the ionic correlation by charge carriers in the sample growth is of minor importance. In the limiting case of a one-dimensional impurity system, the correlation may totally suppress the random field at any doping level, so that a finite electron mobility is governed by other scattering mechanisms than impurity doping, e.g., interface roughness and alloying. It is found that the ionic correlation changes the electron mobility of quantum wires as regards not only its magnitude but its dependence on the doping conditions as well. For impurity systems of a small size, the mobility may be increased by up to more than one order of magnitude at a doping level of 10^6 cm^{-1}.

DOI: 10.1103/PhysRevB.64.125324 PACS number(s): 73.21.−b, 71.23.An

I. INTRODUCTION

Recently, there has been an increasing interest in semiconductor quantum wire (QWR) structures. These structures have opened up the potential for various device applications.[1] In practice, intentional or unintentional doping is often inevitable in a wire, which determines its quality. The quasi-one-dimensional electron gas (1DEG) in the wire is generally violently affected by disorder arising from impurity doping. The disorder has been shown to lead to remarkable changes in the observable properties of the wire, e.g., the electron mobility[1–5] and the density of states (DOS).[6–9]

It should be mentioned that all existing theories[1–9] of the disorder effect from impurity doping in QWR's were established by assuming that the ionized impurities are absolutely randomly distributed in the sample. Nevertheless, it is well known[10–12] that the assumption of the random impurity distribution fails to be valid at a high doping level, e.g., in heavily doped 3D (bulk) semiconductors, and in order to understand phenomena occurring in such a sample one has to invoke an impurity correlation. The effect is due to the Coulomb interaction among charged impurities in both the preparation of a sample and the measurement of its observable properties during whose course they could move freely and interact to each other. In the sample preparation, this develops during a sample growth and results in a correlation in realization of a given impurity configuration which is frozen after the growth. The effect is referred to as high-temperature ionic correlation. The situation is met when the sample undergoes a thermal treatment, e.g., prepared by molecular beam epitaxy[10–12] (MBE) or pulling from the melt.[13,14] Obviously, the correlation tends to drive the impurities to be uniformly distributed so that their configuration is of the lowest potential energy. Indeed, such ordered impurity distributions were experimentally observed by Headrick and co-workers[10] using x-ray diffraction. They reported correlated completely ordered $B\sqrt{3}\times\sqrt{3}$ two-dimensional structures at the interface between Si(111) and a-Si during MBE growth. Moreover, at a high doping level, the correlation effect is expected to significantly alter the doping profile as well as the characteristics of the impurity field seen by electrons. Experimentally, Schubert and co-workers[11,12] observed an apparent correlation-induced deviation from a δ doping profile of the sample GaAs:Be grown by MBE. The effect is to be distinguished from the low-temperature ionic correlation that develops during a sample measurement and was well studied in Refs. 15 and 16. There, the ionic correlation is related to the migration of electrons between impurities at low temperatures (changing the positions of charged impurities) if not all of the impurities are ionized.

So far, a number of theories of heavily doped bulk semiconductors have been established, starting from the assumption of the correlated impurity distribution. The theories were capable of explaining several experimental data, say, on the optical properties[13] and mobility.[14,17,18] In addition, the ionic correlation was shown to lead to an appreciable modification in the DOS of heavily doped materials.[19,20]

It is well known that with a reduction of the dimensionality of the electron system the effect of an interaction, e.g., disorder and many-body interactions, becomes generally stronger. So the influence of impurity correlation in a 1D structure is thought to likely be larger than that in 2D and 3D systems. Further, it is also believed that in the case of strictly one dimension, an interaction appears to exhibit some striking behavior which is often of great physical interest. Thus far, this has been theoretically proved for 1D electron systems. Indeed, in one dimension due to any small disorder all electronic states are exponentially Anderson localized,[21] whereas due to any small electron-electron interaction the 1D electrons make up a singular Tomonaga-Luttinger liquid.[22] So the ionic correlation in a 1D impurity system is thought to likely assume some peculiar property. Thus, the aim of this

 ©2001 The American Physical Society

paper is to supply an estimate of the effect from high-temperature ionic correlation in the sample preparation on the electronic properties of the 1D structure based on QWR's and to explore the behavior of correlated-impurity systems in one dimension.

II. AUTOCORRELATION FUNCTION FOR CORRELATED IMPURITIES

To start with, we derive the autocorrelation function for a random field created by correlated impurities. It has been pointed out that this plays the key role as the input function for disorder interaction in the calculation, e.g., of the mobility[4] and the DOS (Refs. 9 and 23) of QWR's. For that purpose, we need to specify our model by choosing a cylindrical QWR and confining the motion of electrons in the wire by an infinitely high potential barrier at its boundary. The wire has been so modulation doped that the impurities are chaotically located on an infinitely thin cylindrical tube coaxial with the wire. The motion of the electrons along the axis of the wire (chosen as the x axis) is affected by disorder due to a random field $U(x)$ created by fluctuations $\xi(\mathbf{r})$ in the impurity density. As usual, in what follows we assume that these fluctuations and, hence, their random field obey Gaussian statistics. Therefore, it may completely be characterized by an autocorrelation function, defined by

$$W(x-x')=\langle U(x)U(x')\rangle, \tag{1}$$

where the angular brackets denote averaging over all the configurations of the randomness. This function depends merely on the coordinate difference, the disordered electron system being macroscopically homogeneous.

It is well known that configuration averaging may be represented in terms of a Feynman path integral as

$$\langle O[\xi(\mathbf{r})]\rangle=\frac{\int \mathcal{D}\xi(\mathbf{r})\exp\{-\Omega[\xi(\mathbf{r})]\}O[\xi(\mathbf{r})]}{\int \mathcal{D}\xi(\mathbf{r})\exp\{-\Omega[\xi(\mathbf{r})]\}}, \tag{2}$$

in which $\mathcal{D}\xi(\mathbf{r})$ stands for the Feynman measure on the set of impurity density fluctuations, and $\exp\{-\Omega[\xi(\mathbf{r})]\}$ determines the probability for the realization of a given configuration $\xi(\mathbf{r})$. For Gaussian fluctuations, $\Omega[\xi(\mathbf{r})]$ must be a quadratic functional. Moreover, it is normally assumed[13,14] that the distribution of impurities after sample solidification is a snapshot of their distribution at the (high) freezing temperature T_0 for impurity diffusion. Thus, we may write

$$\Omega[\xi(\mathbf{r})]=\frac{1}{2N_{\mathrm{i}}}\int d\mathbf{r}\xi^2(\mathbf{r})+\frac{(Ze)^2}{2\epsilon_{\mathrm{L}}k_{\mathrm{B}}T_0}\times\int d\mathbf{r}\int d\mathbf{r}'\xi(\mathbf{r})\xi(\mathbf{r}')\frac{\exp(-|\mathbf{r}-\mathbf{r}'|/\lambda_{\mathrm{D}})}{|\mathbf{r}-\mathbf{r}'|}, \tag{3}$$

with the integrals being extended over the impurity tube. Here N_{i} means the impurity density per unit length along the wire axis and per unit circular arc on the impurity tube, Ze is the impurity charge, and ϵ_{L} the dielectric constant of the background lattice. The Debye screening radius is fixed by the charge carrier density N_e in the high-temperature plasma: $\lambda_{\mathrm{D}}=\sqrt{\epsilon_{\mathrm{L}}k_{\mathrm{B}}T_0/4\pi e^2N_e}$.

The first term on the right-hand side of Eq. (3) describes the random distribution of independent impurities, whereas the second one is connected with the minimum work to be done against the Coulomb attraction or repulsion between the charged impurities to realize the configuration $\xi(\mathbf{r})$. The second term clearly diminishes its probability and, hence, describes statistical screening of the random field. The probability functional (3) with $\lambda_{\mathrm{D}}\to\infty$ was first employed by Shklovskii and Efros[13,14] to estimate the effect from ionic correlation in 3D (bulk) semiconductors when ignoring the screening of the impurity-impurity interaction by charge carriers in the sample growth. The screening of ionic correlation was also neglected by Schubert and co-workers[11,12] when examining the correlation-induced deviation from a δ doping profile of the 2D sample GaAs:Be grown by MBE. In the present paper, we include explicitly the screening of the interimpurity interaction in the high-temperature plasma.

In order to perform the path integrals in Eq. (2), we must go over to discrete variables by means of a Fourier series expansion in cylindrical coordinates $\mathbf{r}=(\rho,\varphi,x)$. For impurity density fluctuations, on the tube of radius $\rho=a$, it holds that

$$\xi(\mathbf{r})=\sum_{\mathbf{k},m=-\infty}^{\infty}\xi_{km}e^{i(kx+m\varphi)}, \tag{4}$$

with $\mathbf{k}$ as a 1D wave vector along the wire axix. The reality of $\xi(\mathbf{r})$ requires that the real and imaginary parts of its Fourier components, $\xi_{\mathbf{k}m}=\xi'_{\mathbf{k}m}+i\xi''_{\mathbf{k}m}$, have to satisfy the constraint

$$\xi'_{\mathbf{k}m}=\xi'_{-\mathbf{k},-m},\quad \xi''_{\mathbf{k}m}=-\xi''_{-\mathbf{k},-m}. \tag{5}$$

This implies that the independent Fourier components cover only one half-space, e.g., the $\mathbf{k}$, $m\geqslant 0$ half-space. Then, the Feynman measure is written as a product

$$\int \mathcal{D}\xi(\mathbf{r})=\prod_{\mathbf{k},m\geqslant 0}^{\infty}\left(\int_{-\infty}^{\infty}d\xi'_{\mathbf{k}m}\int_{-\infty}^{\infty}d\xi''_{\mathbf{k}m}\right). \tag{6}$$

As seen below, the effect of ionic correlation becomes important only when the impurity system is of small size. Accordingly, we will restrict the discussion to the case where the radius of the impurity tube is small compared with the Debye one. Then, for the screening factor entering Eq. (3) with $\rho=\rho'=a$, we may adopt the following approximation:

$$\exp(-|\mathbf{r}-\mathbf{r}'|/\lambda_{\mathrm{D}})\approx\exp(-|x-x'|/\lambda_{\mathrm{D}}), \tag{7}$$

with $a\ll\lambda_{\mathrm{D}}$. For further calculation, we employ an expansion of the inverse distance between two points $\mathbf{r}$ and $\mathbf{r}'$ (Coulomb potential) in cylindrical coordinates.[24] As a consequence, the screened Coulomb potential appearing in Eq. (3) is represented in terms of a series

$$\frac{\exp(-|\mathbf{r}-\mathbf{r}'|/\lambda_D)}{|\mathbf{r}-\mathbf{r}'|} = \frac{2}{L}\sum_{\mathbf{k},m=-\infty}^{\infty} e^{-|x-x'|/\lambda_D + i\mathbf{k}(x-x') + im(\varphi-\varphi')} \times I_m(k\rho_<)K_m(k\rho_>), \tag{8}$$

with L the length of the wire, $\mathbf{k}=|k|$, and $\rho_< = \min\{\rho,\rho'\}$, $\rho_> = \max\{\rho,\rho'\}$. Hereafter, $I_m(x)$ and $K_m(x)$ are the modified Bessel functions of the first and second kind.[25] By inserting Eqs. (4) and (8) into Eq. (3), we may rewrite the exponent of the probability functional as a sum

$$\Omega[\xi(\mathbf{r})] = \frac{2\pi L}{N_i}\sum_{\mathbf{k},m\geqslant 0}^{\infty} |\xi_{\mathbf{k}m}|^2 \left[1 + \frac{8\pi(Ze)^2 N_i}{\epsilon_L k_B T_0} \times \frac{1}{L}\sum_{k'=-\infty}^{\infty} \frac{\lambda_D}{1+\lambda_D^2(k+k')^2} I_m(k'a)K_m(k'a)\right]. \tag{9}$$

Next, we are dealing with a random field due to all the charged impurities present in the sample. This can be given in terms of fluctuations in the impurity density by the following equation:

$$U(x) = \int d\mathbf{r}'\,\xi(\mathbf{r}')\,v_{ei}(x-\mathbf{r}'), \tag{10}$$

where $v_{ei}(x-\mathbf{r}')$ means the Green's function of Poisson's equation and coincides with the potential energy of an electron at point x on the wire axis ($\rho=0$) created by an impurity at point $\mathbf{r}'$ on the tube ($\rho'=a$). The electron-impurity interaction is to be modified by a finite extension of the electron state in the transverse directions, i.e., weighted as

$$v_{ei}(x-\mathbf{r}') = 2\pi\int d\rho\rho|\psi(\rho)|^2 v(\mathbf{r}-\mathbf{r}'). \tag{11}$$

Here $\psi(\rho)$ denotes the electron wave function of the lowest 1D subband (of cylindrical symmetry), and $v(\mathbf{r}-\mathbf{r}') = -Ze^2/\epsilon_L|\mathbf{r}-\mathbf{r}'|$ is the Coulomb potential of an electron at point $\mathbf{r}$ by an impurity of charge Ze at point $\mathbf{r}'$. For simplicity, we ignore at this stage of the derivation the screening of the one-impurity field by 1D electrons in the wire (after the solidification), which will be included later via the dielectric function [see Eqs. (33) and (34)]. With the use of the expansion of the Coulomb potential in cylindrical coordinates, the electron-impurity interaction (11) is rewritten as

$$v_{ei}(x-\mathbf{r}') = -\frac{4\pi Ze^2}{\epsilon_L L}\sum_{\mathbf{k}=-\infty}^{\infty} e^{i\mathbf{k}(x-x')}A(kR,k\rho'), \tag{12}$$

where R is the radius of the wire, and

$$A(kR,k\rho') = \int d\rho\rho|\psi(\rho)|^2 I_0(k\rho_<)K_0(k\rho_>). \tag{13}$$

Upon putting Eq. (12) into Eq. (10), we obtain the Fourier series for the random field due to an impurity tube of radius a and zero thickness:

$$U(x) = -\frac{8\pi^2 Ze^2}{\epsilon_L}\sum_{\mathbf{k}=-\infty}^{\infty} e^{i\mathbf{k}x}\xi_{\mathbf{k}0}A(kR,ka). \tag{14}$$

We are now able to calculate the autocorrelation function in question. By replacing $U(x)$ figuring in Eq. (1) with Eq. (14), we get the Fourier series for this function:

$$W(x-x') = \left(\frac{8\pi^2 Ze^2}{\epsilon_L}\right)^2 \sum_{\mathbf{k}=-\infty}^{\infty} e^{i\mathbf{k}(x-x')}\langle|\xi_{\mathbf{k}0}|^2\rangle A^2(kR,ka). \tag{15}$$

Next, one has to do the configuration average entering Eq. (15). With the aid of Eqs. (6) and (9), the path integrals (2) with $O=\xi'^2_{\mathbf{k}0}$ and $\xi''^2_{\mathbf{k}0}$ are straightforward, yielding

$$\langle\xi'^2_{\mathbf{k}0}\rangle = \langle\xi''^2_{\mathbf{k}0}\rangle = \frac{N_i}{4\pi L}F_C(\mathbf{k}). \tag{16}$$

Here we have introduced a correlation factor $F_C(k)$, whose inverse is defined by

$$F_C^{-1}(\mathbf{k}) = 1 + \frac{2(Ze)^2 n_i}{\pi\epsilon_L k_B T_0}\int_0^\infty dt\, I_0(at)K_0(at) \times\left[\frac{\lambda_D}{1+\lambda_D^2(t+\mathbf{k})^2} + \frac{\lambda_D}{1+\lambda_D^2(t-\mathbf{k})^2}\right], \tag{17}$$

with $n_i = 2\pi N_i$ being the 1D impurity density and, as before, $I_0(x)$ and $K_0(x)$ the modified Bessel functions of zero order.

Finally, upon setting Eq. (16) into Eq. (15) and replacing the $\mathbf{k}$ sum with a $\mathbf{k}$ integral, we may factorize out the Fourier transform of the autocorrelation function for correlated impurities as follows:

$$W_C(\mathbf{k}) = W_R(\mathbf{k})F_C(\mathbf{k}), \tag{18}$$

where $W_R(\mathbf{k})$ is the one for independent impurities,

$$W_R(\mathbf{k}) = \left(\frac{4\pi Ze^2}{\epsilon_L}\right)^2 n_i A^2(kR,ka). \tag{19}$$

Thus, Eq. (18) indicates that for taking into account the ionic correlation we ought to introduce a relevant factor into the Fourier transform of the autocorrelation function. It is evidently seen from Eq. (17) that $F_C(\mathbf{k})<1$ and, hence, $W_C(\mathbf{k})<W_R(\mathbf{k})$; i.e., the correlation among impurities is, as expected, to weaken their random field. The correlation factor depends not only on doping conditions such as the impurity density and the freezing temperature for impurity diffusion as in the case of bulk semiconductors, but also on the size of the impurity system.

The size dependence is distinctive of quantum structures: with a reduction of the size a of the impurity system the correlation factor $F_C(\mathbf{k})$ becomes smaller, so that the ionic correlation is stronger and the impurity field is weaker. With the help of the limiting form of the modified Bessel functions of interest for small arguments[25]

$$I_0(x) \sim 1, \quad K_0(x) \sim -\ln x, \quad \text{for} \quad x \to 0, \tag{20}$$

the integral in Eq. (17) is readily estimated for small a. The inverse correlation factor for an impurity system of small size ($a \ll \lambda_D$) is then given by

$$F_C^{-1}(\mathbf{k}) = 1 - \frac{2(Ze)^2 n_i}{\epsilon_L k_B T_0} \ln(ka), \tag{21}$$

which implies $F_C(\mathbf{k}) \to 0$ for $a \to 0$. Thus, if the impurities are located on the wire axis, the correlation among them may completely suppress their random field at any finite doping level. This means that in the limiting case of 1D (sizeless) impurity systems, the ionic correlation is very strong, irrespective of the doping level being high or low. The situation is somewhat analogous to the case of electron correlation in one dimension, where due to any small electron-electron interaction the 1D electrons make up a singular Tomonaga-Luttinger liquid.[22] This is in sharp contrast to the 2D and 3D impurity systems, where the ionic correlation, even in the absence of the screening of it by charge carriers in the high-temperature plasma, is of some importance merely at a high doping level.[10–16,18–20] In particular, the electrons in a 1D impurity system move seemingly freely along the wire axis without impurity scattering even under a high density of charged impurities.

The inverse correlation factor (17) is reduced to a simple form when the screening of the impurity correlation in the sample preparation is neglected. By letting $\lambda_D \to \infty$ and with the aid of

$$\frac{1}{\pi} \frac{\eta}{\eta^2 + x^2} \to \delta(x), \quad \text{for} \quad \eta \to 0, \tag{22}$$

we easily arrive at

$$F_C^{-1}(\mathbf{k}) = 1 + \frac{2(Ze)^2 n_i}{\epsilon_L k_B T_0} I_0(ka) K_0(ka). \tag{23}$$

III. EFFECT OF THE IMPURITY CORRELATION

A. Electron mobility

In this section, we will apply the foregoing theory to estimate the effects of ionic correlation on the electronic properties of QWR's, e.g., the electron mobility and the energy spectrum. Recently, Das Sarma and co-workers[26–28] have proved, basing on a realistic model of disordered interacting 1DEG's in semiconductor QWR's (parabolic 1D subband, finite electron density, and actual Coulomb interaction) that these electron systems behave, for all practical purposes, essentially as delocalized Fermi liquids. The available experiments have seemed to justify this theoretical claim.[29–31] Therefore, we shall start from the standard Fermi-liquid model for disordered interacting 1DEG's in semiconductor QWR's.

It is well known[2,3] that at zero temperature impurity scattering is one of the main mechanisms for governing the electron mobility. The mobility is determined via the momentum-relaxation time for zero frequency by

$$\mu = e\tau/m^*, \tag{24}$$

with m^* the effective mass of the charge carriers A general expression for the relaxation time of a d-dimensional interacting electron gas in the presence of disorder was derived by Gold and Götze.[32] For the lowest subband, the inverse relaxation time for zero frequency and zero temperature is given in terms of the Fourier transform of the autocorrelation function by

$$\frac{1}{\tau} = \frac{1}{\hbar d m^* n_e} \sum_{\mathbf{k}} k^2 W(\mathbf{k}) \phi''(\mathbf{k}), \tag{25}$$

where $\phi''(\mathbf{k})$ means the density-density relaxation function of the noninteracting electron gas and n_e the 1D carrier density. Electron-electron interaction effects are, as quoted above, included in $W(\mathbf{k})$ via the dielectric function. For one dimension, we use the results due to Williams and Bloch[33] to get

$$\phi''(\mathbf{k}) = 2\pi \rho_F m^* k_F \delta(2k_F - k)/k^2, \tag{26}$$

where ρ_F is the DOS of the free-electron gas at the Fermi energy E_F: $\rho_F = 2m^*/\pi k_F$, with the Fermi wave vector $k_F = (\pi/2) n_e$.

By inserting Eqs. (25) and (26) into Eq. (24), we may express the electron mobility in terms of the Fourier transform of the autocorrelation function as follows:

$$\mu = \frac{e\hbar}{m^*} \frac{E_F}{k_F W(2k_F)}. \tag{27}$$

By means of Eq. (27), we immediately obtain a simple relationship between the mobilities limited by correlated and independent impurities:

$$\frac{\mu_C}{\mu_R} = F_C^{-1}(2k_F). \tag{28}$$

The ratio (28) is to be considered as a measure of the influence from ionic correlation on the electron mobility. This is fixed by the inverse correlation factor at the doubled Fermi wave vector and depends then on the electron density. It is clearly observed from Eqs. (17) and (28) that the mobility limited by correlated impurities is larger than that by independent ones. As indicated in the end of Sec. II, in the limiting case of 1D impurity systems, $F_C(2k_F) \to 0$ for $a \to 0$, so that the impurity-limited mobility μ_C may become very large. In this case a finite electron mobility is governed by other scattering mechanisms, e.g., interface roughness[34,35] and alloying.[36,37] In addition, when neglecting the screening of ionic correlation by charge carriers the ratio (28) depends, as seen from Eq. (23), on the electron density and the size of the impurity system via a combination of $n_e a$.

B. Density of states

It is well known that the DOS is the most adequate concept for describing the energy spectrum of disordered systems. Moreover, at a high enough doping level the impurity field is proved to be smooth in space on the average so that

a semiclassical approach is applicable. The DOS of disordered 1DEG's may then be derived by Quang and Tung[9,23] in the following form:

$$\rho(E)=\frac{1}{\pi}\left(\frac{2m^*}{\hbar^2}\right)^{1/2}\frac{1}{(2\gamma)^{1/2}}\exp\left(-\frac{E^2}{4\gamma^2}\right)\times\left[D_{-1/2}\left(-\frac{E}{\gamma}\right)-\frac{\hbar^2F^2}{24m^*\gamma^3}D_{5/2}\left(-\frac{E}{\gamma}\right)\right], \quad (29)$$

where γ and F denote the rms of the potential and force of the random field, and $D_\nu(x)$ is a parabolic cylinder function.[25] The random parameters are given in terms of the Fourier transform of the autocorrelation function by

$$\gamma^2=\int_{-\infty}^{\infty}\frac{d\mathbf{k}}{2\pi}W(\mathbf{k}) \quad (30)$$

and

$$F^2=\int_{-\infty}^{\infty}\frac{d\mathbf{k}}{2\pi}k^2W(\mathbf{k}). \quad (31)$$

Since $W_C(\mathbf{k})<W_R(\mathbf{k})$, we have $\gamma_C<\gamma_R$ and $F_C<F_R$; i.e., the strength of the field created by charged impurities is diminished when they are correlated distributed.

For simplicity, the electrons are usually assumed to be uniformly distributed in the wire section.[3,9] Accordingly, the wave function of the lowest 1D subband is taken in the form

$$\psi(\rho)=\begin{cases}1/\sqrt{\pi R^2}, & \rho<R,\\ 0, & \rho\geq R,\end{cases} \quad (32)$$

which enables the integral appearing in Eq. (13) to be analytically done. Consequently, the autocorrelation function for independent impurities depends on their position as follows:[3,9]

$$W_R(\mathbf{k})=\left(\frac{4Ze^2}{\epsilon_L}\right)^2\frac{n_i}{\epsilon^2(\mathbf{k})}\frac{1}{(kR)^4}[1-(kR)K_1(kR)I_0(ka)]^2 \quad (33)$$

for $a\leq R$ and

$$W_R(\mathbf{k})=\left(\frac{4Ze^2}{\epsilon_L}\right)^2\frac{n_i}{\epsilon^2(\mathbf{k})}\frac{1}{(kR)^2}I_1^2(kR)K_0^2(ka) \quad (34)$$

for $a\geq R$. Here $\epsilon(k)$ is the dielectric function, which allows for the screening of the impurity field by 1D electrons in the wire at low temperatures after the solidification. Within the random phase approximation, this is given at zero temperature by

$$\epsilon(k)=1+\frac{2m^*}{\pi\hbar^2}\frac{v_{ee}(k)}{k}\ln\left|\frac{k+2k_F}{k-2k_F}\right|, \quad (35)$$

where $v_{ee}(k)$ is the electron-electron interaction potential weighted with the wave function (32) as

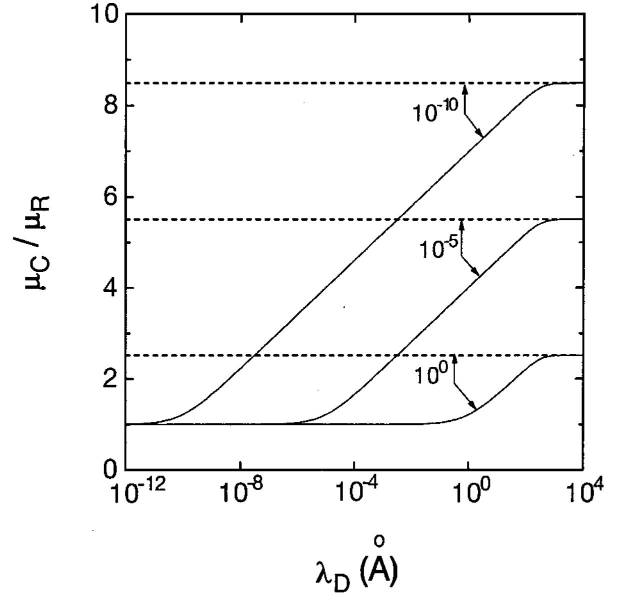

FIG. 1. Ratio μ_C/μ_R vs Debye screening radius λ_D under an impurity density $n_i=10^6$ cm^{-1} and different sizes of the impurity system a (denoted on lines in units of Å). Solid and dashed lines refer to the ionic correlation in the presence and absence of screening, respectively.

$$v_{ee}(k)=\frac{4e^2}{\epsilon_L}\frac{1}{(kR)^2}[1-2I_1(kR)K_1(kR)]. \quad (36)$$

The dielectric function (35) appearing in Eq. (27) at $k=2k_F$ is divergent and is to be replaced[2–4] with the one at a low temperature ($k_BT\ll E_F$):

$$\epsilon(2k_F)=1+\frac{2m^*}{\pi\hbar^2}\frac{v_{ee}(2k_F)}{2k_F}\ln\left(\frac{8e^{\mathcal{C}}}{\pi}\frac{E_F}{k_BT}\right), \quad (37)$$

with $\mathcal{C}=0.577\,215\ldots$ the Euler constant.

C. Numerical results and conclusions

We have carried out numerical calculations for a cylindrical QWR made from GaAs/$Al_xGa_{1-x}As$ ($x=0.30$). The material parameters are the effective mass $m^*=0.067m_e$, the dielectric constant $\epsilon_L=12.9$, and the freezing temperature for impurity diffusion, $T_0=1000$ K. The DOS is scaled in units of $\rho^*=1/\mathrm{Ry}^*a^*=1.79\times10^5$ meV^{-1} cm^{-1}, with $a^*=100$ Å the effective Bohr radius, and Ry$^*=5.6$ meV the effective Rydberg number (used as the energy unit). The modulation doping is such that the impurity density ranges from $n_i=10^5$ to 2×10^6 cm^{-1}, the corresponding Debye screening radius is larger than 10 Å.

Figures 1–3 display, according to Eq. (28), the ratio between the mobilities limited by correlated and independent impurities. To estimate the influence from the screening of the ionic correlation by charge carriers in the high-temperature plasma, Fig. 1 sketches the ratio μ_C/μ_R as a function of the Debye radius λ_D under an impurity density $n_i=10^6$ cm^{-1} and different sizes of the impurity system $a=10^{-10}$, 10^{-5}, and 1 Å. The solid and dashed lines corre-

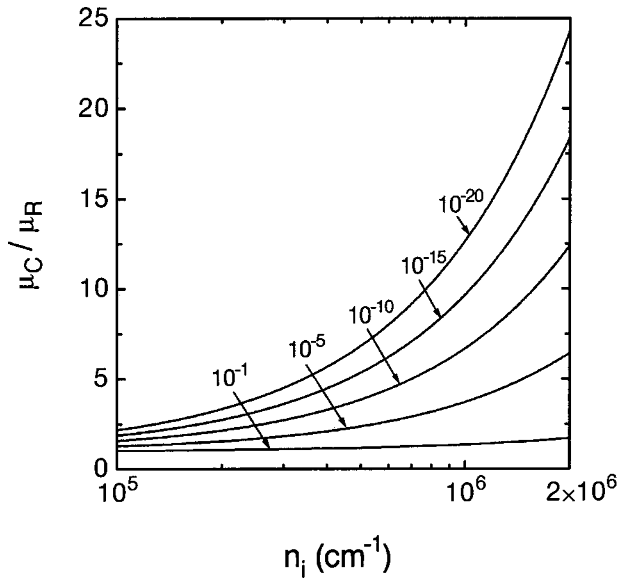

FIG. 2. Ratio μ_C/μ_R vs impurity density n_i under different radii of the impurity tube a (denoted on lines in units of Å).

spond to the ionic correlation in the presence and absence of the screening, respectively. In what follows, the mobilities are evaluated, taking account of the screening effect. In Fig. 2 the mobility ratio is plotted versus impurity density n_i under different radii of the impurity tube $a=10^{-20}$, 10^{-15}, 10^{-10}, 10^{-5}, 1, and 10^2 Å, whereas in Fig. 3 it is plotted versus impurity system size a under various impurity densities $n_i=10^5$, 5×10^5, 10^6, and 2×10^6 cm^{-1}. Figures 4 and 5 show, following Eq. (27), the dependence of μ_C and μ_R on the doping conditions for the wire of radius $R=100$ Å, temperature $T=1.3$ K, and electron density $n_e=10^5$ cm^{-1}. In Fig. 4 these are plotted versus impurity density n_i under different radii of the impurity tube $a=10^{-20}$, 10^{-10}, 10, and 10^2 Å, whereas in Fig. 5 they are plotted versus impurity system size a under various impurity densities $n_i=10^5$, 10^6, and 2×10^6 cm^{-1}. In addition, μ_C and μ_R are plotted in Fig. 6 versus electron density n_e under a doping level $n_i=10^6$ cm^{-1} and different radii of the impurity tube, $a=10^{-10}$, 10, and 10^2 Å. The electron density has been chosen to satisfy the condition $n_e<2/R$, so that the lowest subband approximation is valid.[4] In Fig. 7 the rms potential γ

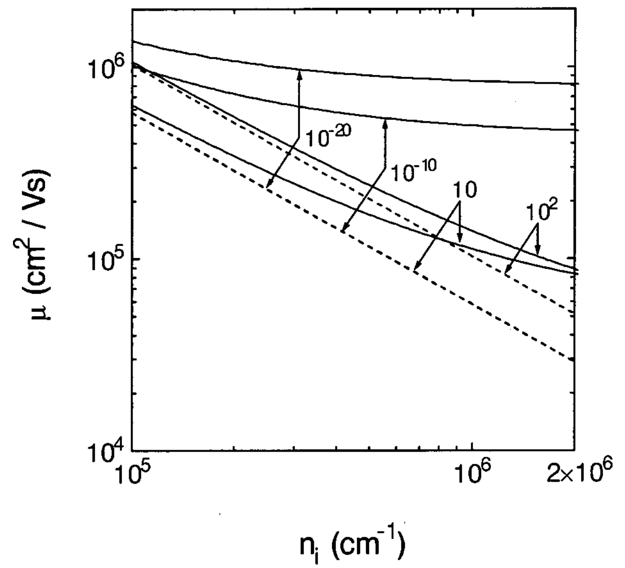

FIG. 4. Mobilities μ_C and μ_R for the wire of a radius $R=100$ Å, temperature $T=1.3$ K, and electron density $n_e=10^5$ cm^{-1} vs impurity density n_i under different radii of the impurity tube a (denoted on lines in units of Å). Solid and dashed lines refer to μ_C and μ_R, respectively.

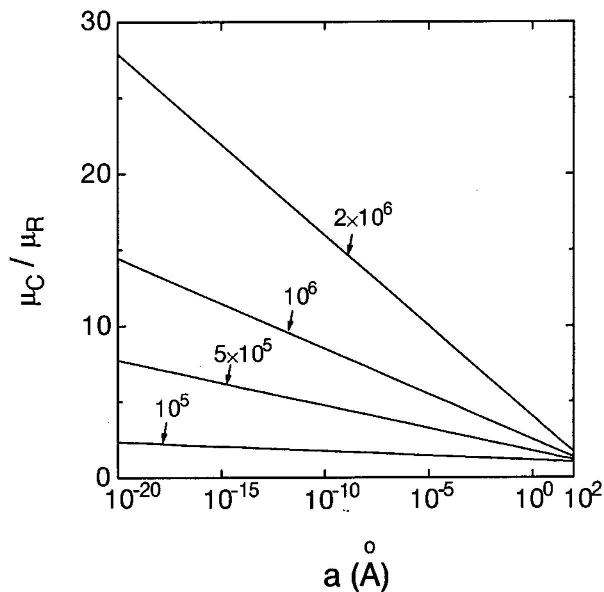

FIG. 3. Ratio μ_C/μ_R vs impurity system size a under various impurity densities n_i (denoted on lines in units of cm^{-1}).

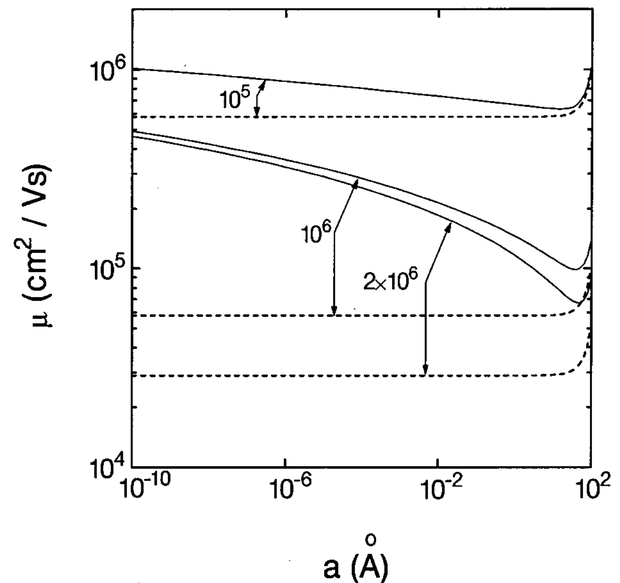

FIG. 5. Mobilities μ_C and μ_R for the wire in Fig. 4 vs impurity system size a under various impurity densities n_i (denoted on lines in units of cm^{-1}). Solid and dashed lines refer to μ_C and μ_R, respectively.

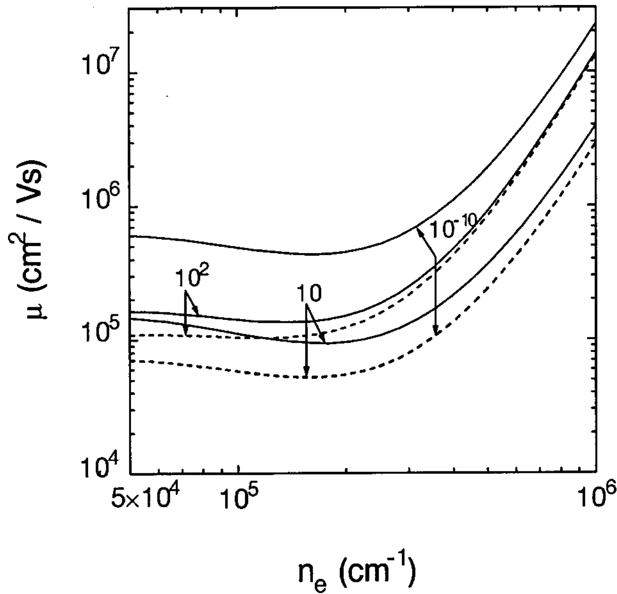

FIG. 6. Mobilities μ_C and μ_R for the wire in Fig. 4 vs electron density n_e under an impurity density $n_i = 10^6$ cm^{-1} and different radii of the impurity tube a (denoted on lines in units of Å). Solid and dashed lines refer to μ_C and μ_R, respectively.

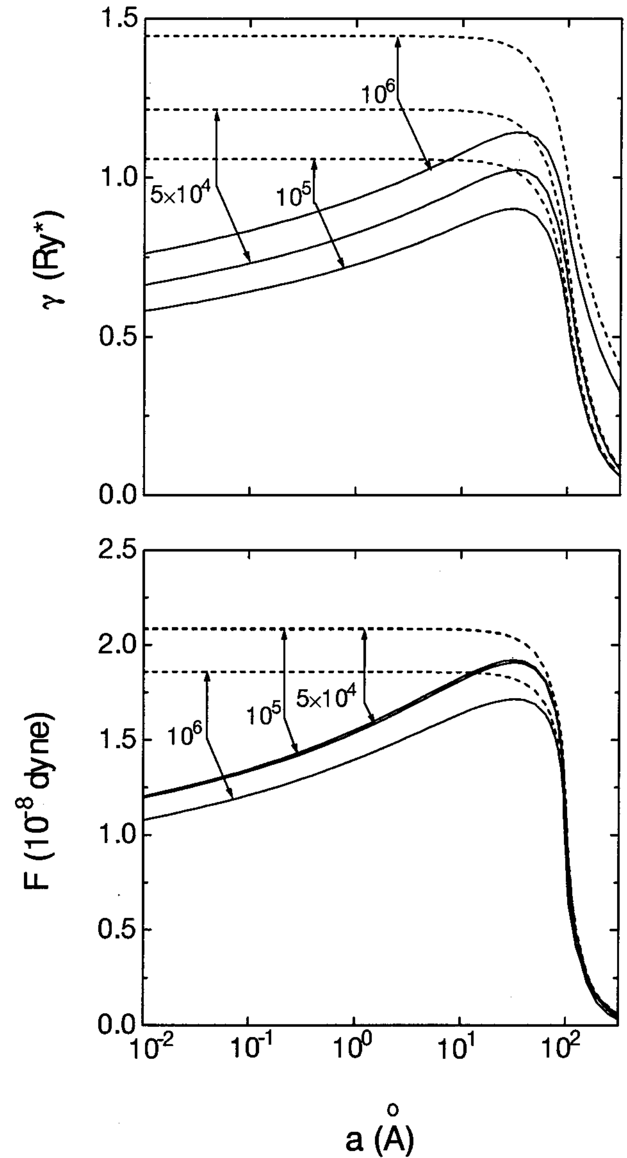

FIG. 7. rms of the (a) potential γ and (b) force F for the wire of a radius $R = 100$ Å doped with an impurity density $n_i = 10^6$ cm^{-1} vs impurity system size a under various electron densities n_e (denoted on lines in units of cm^{-1}). Solid and dashed lines refer to the correlated and random impurity distributions, respectively.

and force F for the wire of a radius $R = 100$ Å doped with an impurity density $n_i = 10^6$ cm^{-1} are plotted versus impurity system size a under various electron densities $n_e = 5\times10^4$, 10^5, and 10^6 cm^{-1}. Figure 8 sketches, according to Eq. (29), the DOS versus energy for the wire in question doped with $n_i = n_e = 10^6$ cm^{-1} under different radii of the impurity tube, $a = 10^{-10}$, 10, and 10^2 Å. The solid and dashed lines in Figs. 4–7 correspond to the correlated and random impurity distributions, respectively.

From the results thus obtained we may draw the following conclusions.

(i) Figure 1 reveals as in the case of 2D and 3D impurity systems,[11–14] the screening of impurity correlation in the growth is generally of minor importance for real samples. Indeed, the screening is negligibly small for the Debye radius $\lambda_D \gtrsim 10^2$ Å. The effect becomes more important with a reduction of λ_D. It is found that the ionic correlation is considerably suppressed by charge carriers merely with a very short Debye radius $\lambda_D \lesssim 1$ Å. This is not the case of the systems under consideration, where the screening radius ($\lambda_D > 10$ Å) exceeds the average interimpurity distance along the wire axis ($1/n_i < 1$ Å).

(ii) It follows from Fig. 2 that the ratio μ_C/μ_R is, as expected, increased when elevating the impurity density n_i, more quickly at a smaller radius of the impurity tube. For instance, with $a = 10^{-15}$ Å the electron mobility of a QWR may be raised by a factor of 22 at a doping level $n_i = 2\times10^6$ cm^{-1}, while the relevant factor of a δ-doped sheet GaAs:Be was estimated[17] to be about 3 at a very high 3D doping level of 3.2×10^{20} cm^{-3}. Further, with the used values of a the ionic correlation is of some importance at a doping level $n_i \gtrsim 10^5$ cm^{-1}.

(iii) It follows from Fig. 3 that the ratio μ_C/μ_R is increased nearly linearly (on a semilogarithmic scale) with a reduction of a. This exhibits a logarithmic dependence of the effect on the size of the impurity system. As clearly seen from Figs. 2 and 3, the ionic correlation is of some importance with $a \lesssim 1$ Å, so that Eq. (7) is a very good approximation for real systems.

(iv) Figure 4 indicates the mobility μ_R is linearly decreased with elevating the doping level n_i, irrespective of the impurity tube radius. This is because that the autocorrelation function for independent impurities is proportional to n_i, as seen from Eqs. (33) and (34). However, due to the ionic correlation, the mobility μ_C is found to exhibit an apparent deviation from linearity and to be a more slowly decreasing function of n_i, especially for impurity systems of a small size.

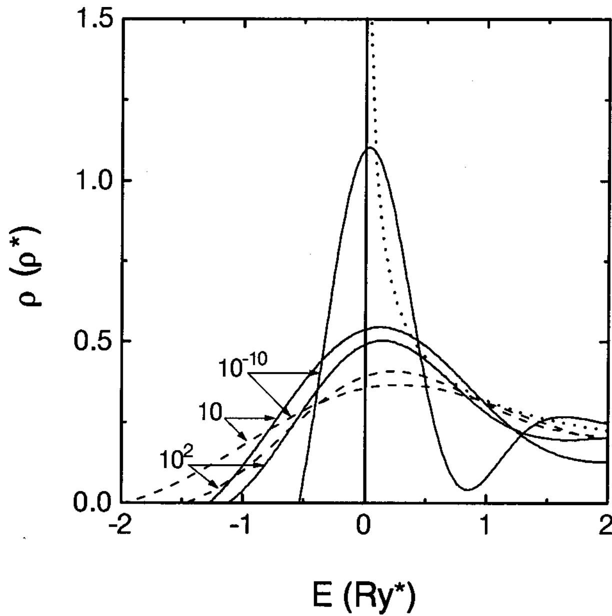

FIG. 8. Normalized DOS $\rho(E)$ vs energy for the wire of a radius $R=100$ Å doped with $n_i=n_e=10^6\ \mathrm{cm}^{-1}$, under different radii of the impurity tube a (denoted on lines in units of Å). Solid and dashed lines refer to the correlated and random impurity distributions, respectively. The dotted line represents the DOS of the ideal 1DEG.

(v) An examination of Fig. 5 shows the mobility μ_R is in general an increasing function of the impurity system size, and for a small tube, e.g., of $a\lesssim 10$ Å, μ_R is found to be almost independent of a. On the contrary, in such an impurity system the ionic correlation is strong, so that μ_C is remarkably decreased with increasing a.

(vi) It is observed from Fig. 6 that the ionic correlation is of more importance under a smaller electron density. For $n_e\lesssim 5\times 10^4\ \mathrm{cm}^{-1}$ the mobility may be raised by up one order of magnitude at $a=10^{-10}$ Å, but for $n_e=10^6\ \mathrm{cm}^{-1}$, μ_C almost coincides with μ_R at $a\gtrsim 10$ Å.

(vii) Figure 7 reveals that influence of ionic correlation on the strength of the random field is measured by the ordinate separation between the relevant solid and dashed lines. The effect is enhanced with a reduction of the size of the impurity system.

(viii) It is seen from Fig. 8 that the impurity-induced DOS tail below the subband edge becomes narrower and higher due to ionic correlation.

IV. SUMMARY

To summarize, in this paper we have pointed out that the correlation among impurities in QWR's weakens their field. The ionic correlation changes the electron mobility of QWR's as regards not only its magnitude but its dependence on the doping conditions as well. The effect exhibits a peculiar dependence on the size of the impurity system. For a thin system, the effect becomes larger than that in 2D and 3D ones. In a strictly 1D impurity system, the ionic correlation, no matter how to weak, totally suppresses the random field acting on the electrons in the wire. It is worth noting that the conclusions obtained for modulation-doped QWR's turn out to be qualitatively valid for background-doped QWR's, where the impurities are located not on a hollow tube, but in a solid cylinder.

It is well known that the electron system in a modulation-doped low-dimensional semiconductor structure has a high mobility since the effect of ionized impurities is minimized in this structure by their spatial separation from the active channel. In this paper we have proved that the quality of doped QWR's may, in another way, be improved if they undergo a thermal treatment and the impurity system size is reduced.

As mentioned in Ref. 38 and more recently in Ref. 39, so far there have been no available experimental results on electronic properties of QWR's such as the electron mobility and DOS. Therefore, a detailed comparison of our theory with experiment is presently impossible. However, we hope that our theoretical results evidently stimulate future experimental studies on impurity systems of small size, especially in one dimension.

ACKNOWLEDGMENTS

The authors would like to thank Professor M. Saitoh and Professor K. Slevin, Department of Physics, Osaka University, Japan for valuable discussions. Part of this work was done during the stay of one of the authors (D.N.Q.) at the Abdus Salam International Center for Theoretical Physics, Trieste, Italy.

[1] H. Sakaki, Jpn. J. Appl. Phys., Part 2 **19**, L735 (1980); J. Vac. Sci. Technol. **19**, 148 (1981).
[2] L. Lee and H. P. Spector, J. Appl. Phys. **57**, 366 (1985).
[3] G. Fishman, Phys. Rev. B **34**, 2394 (1986).
[4] A. Gold and A. Ghazali, Phys. Rev. B **41**, 7626 (1990).
[5] J. S. Thakur and D. Neilson, Phys. Rev. B **56**, 4679 (1997); **56**, 7485 (1997).
[6] M. Takeshima, Phys. Rev. B **33**, 7047 (1986).
[7] E. A. de Andrada e Silva, I. C. da Cunha Lima, and A. Ferreira da Silva, Phys. Rev. B **37**, 8537 (1988).
[8] A. Ghazali, A. Gold, and J. Serre, Semicond. Sci. Technol. **8**, 1912 (1993).
[9] D. N. Quang and N. H. Tung, Phys. Rev. B **60**, 13 648 (1999).
[10] R. L. Headrick, L. C. Feldman, and I. K. Robinson, Appl. Phys. Lett. **55**, 442 (1989).
[11] E. F. Schubert, J. M. Kuo, R. F. Kopf, H. S. Luftman, L. C. Hopkins, and N. J. Sauer, J. Appl. Phys. **67**, 1969 (1990).
[12] E. F. Schubert, in *Epitaxial Microstructures*, edited by A. C. Gossard, Vol. 40 of *Semiconductors and Semimetals*, edited by R. K. Willardson, A. C. Beer, and E. R. Weber (Academic, Boston, 1994), Chap. 1.
[13] B. I. Shklovskii and A. L. Efros, Zh. Éksp. Teor. Fiz. **58**, 657 (1970) [Sov. Phys. JETP **31**, 351 (1970)].
[14] Yu. S. Galpern and A. L. Efros, Fiz. Tekh. Poluprovodn. **6**, 1081

(1972) [Sov. Phys. Semicond. **6**, 941 (1972)].

[15] F. G. Pikus and A. L. Efros, Zh. Éksp. Teor. Fiz. **96**, 985 (1989) [Sov. Phys. JETP **69**, 558 (1989)].

[16] A. L. Efros, F. G. Pikus, and G. G. Samsonidze, Phys. Rev. B **41**, 8295 (1990).

[17] A. F. J. Levi, S. L. McCall, and P. M. Platzman, Appl. Phys. Lett. **54**, 940 (1989).

[18] D. N. Quang, N. N. Dat, and D. V. An, Phys. Lett. A **182**, 125 (1993).

[19] D. N. Quang, N. N. Dat, and D. V. An, J. Phys. Soc. Jpn. **66**, 140 (1997).

[20] D. N. Quang and N. H. Tung, Phys. Status Solidi B **207**, 111 (1998).

[21] P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).

[22] G. D. Mahan, *Many-Particle Physics*, 2nd ed. (Plenum, New York, 1990).

[23] D. N. Quang and N. H. Tung, Phys. Rev. B **62**, 15 337 (2000); J. Phys. Soc. Jpn. **70**, 449 (2001).

[24] J. D. Jackson, *Classical Electrodynamics*, 2nd ed. (Wiley, New York, 1975).

[25] F. W. J. Olver, in *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972), Chap. 9.

[26] B. Y.-K. Hu and S. Das Sarma, Phys. Rev. Lett. **68**, 1750 (1992); Phys. Rev. B **48**, 5469 (1993).

[27] Q. P. Li, S. Das Sarma, and R. Joynt, Phys. Rev. B **45**, 13 713 (1992).

[28] S. Das Sarma and E. H. Hwang, Phys. Rev. B **54**, 1936 (1996).

[29] A. S. Plaut, H. Lage, P. Grambow, D. Heitmann, K. von Klitzing, and K. Ploog, Phys. Rev. Lett. **67**, 1642 (1991).

[30] A. R. Gõni, A. Pinczuk, J. S. Weiner, J. M. Calleja, B. S. Dennis, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. **67**, 3298 (1991).

[31] A. Schmeller, A. R. Gõni, A. Pinczuk, J. S. Weiner, J. M. Calleja, B. S. Dennis, L. N. Pfeiffer, and K. W. West, Phys. Rev. B **49**, 14 778 (1994).

[32] A. Gold and W. Götze, Phys. Rev. B **33**, 2495 (1986).

[33] P. F. Williams and A. N. Bloch, Phys. Rev. B **10**, 1079 (1974).

[34] T. J. Thornton, M. L. Roukes, A. Scherer, and B. P. Van de Gaag, Phys. Rev. Lett. **63**, 2128 (1989).

[35] M. Notomi, M. Okamoto, and T. Tamamura, J. Appl. Phys. **75**, 4164 (1994); W. Heuring and D. Grützmacher, Appl. Phys. Lett. **57**, L4164 (1994).

[36] A. Menschig, A. Forchel, B. Roos, R. Germann, and K. Pressel, Appl. Phys. Lett. **57**, 1757 (1990).

[37] B. Tanatar and A. Gold, Phys. Rev. B **52**, 1996 (1995).

[38] F. Stern, in *Physics of Low-Dimensional Semiconductor Structures*, edited by P. Butcher, N. H. March, and M. P. Tosi (Plenum, New York, 1993), Chap. 4.

[39] B. R. Nag and S. Gangopadhyay, Semicond. Sci. Technol. **13**, 417 (1998).