# Band-bending effects on the electronic properties of square quantum wells

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We present a theory of the band-bending effects on two-dimensional (2D) carriers confined in a modulation-doped square quantum well. We develop a tractable variational evaluation of several physical quantities that are important in the theory of 2D systems. Analytic expressions of the envelope wave function and the 2D screening form factor allow us to compute various electronic properties such as electrical mobility, density of states in the presence or in the absence of magnetic fields, and Landau level broadening. We prove that in the case of the interface roughness scattering, the band-bending effects lead to a peak in the channel-width dependence of the mobility and a minimum in the Landau level broadening. Our modeling explains recent measurements for a 2D hole gas.

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## I. INTRODUCTION

As well known,[1] the autocorrelation function (ACF) of two-dimensional (2D) systems captures most of their features, since this allows us to compute many electronic properties, e.g., electrical mobility and broadening of Landau levels. The density of states of disordered systems is also given in terms of the ACF within the path-integral approach based on a cumulant or a semiclassical expansion.[2,3] The ACF is determined by important functions such as the envelope wave function and the 2D screening function. Thus, the ACF is specified by characteristics of the system under study, in particular, by the shape of the potential well, i.e., the band edge profile. In the flat-band model, the confining potential is fixed merely by the potential barriers (band edge offsets), while in the bent-band model by the barriers and, moreover, by some band-bending sources.

The band-bending effects on the electronic properties of doped 2D systems were explored theoretically and experimentally by a number of authors. It is well known[1,4] that the band bending is of vital importance for the formation of a quantum well (QW) in heterojunctions. The existing theories of the band-bending effects adopted, as usual, a variational approach based on the Fang-Howard envelope wave function,[5] which enables a simple mathematics concerning the quantum confinement. However, this function was used successfully merely for the triangular QW in (bilayer) heterojunctions. When applied to the square (trilayer) QW, this was used as an approximation only for describing the temperature and carrier-density dependences, but to any degree, inapplicable for describing the channel-width one.

It was believed[4] that the variational approach to the band-bending effects on quantum transport in square QWs is very tedious to work with, so they were ignored, and the flat-band model has been used so far.[4,6,7] Hence, one could not explain some experimental findings. The most striking is the existence of a sharp maximum in the channel-width dependence of the hole mobility.[8–13] Recently, we have shown[14,15] that scatterings related to interface roughness are very sensitive to the band bending.

Therefore, our goal is to provide a theory of the band-bending effects on the carriers confined in a modulation-doped square QWs. In contrast to the previous belief, we try to formulate the variational approach in an analytically tractable framework.

## II. SINGLE-SIDE MODULATION-DOPED SQUARE QUANTUM WELL

### A. Variational wave function

The ACF for an unscreened disorder interaction is defined as a configuration average of the 2D Fourier transform of its potential $U(\mathbf{q},z)$, which is weighted with an envelop wave function $\zeta=\zeta(z)$ as follows: $\langle|U(\mathbf{q})|^2\rangle=\langle|(\zeta|U(\mathbf{q},z)|\zeta)|^2\rangle$, with $\mathbf{q}$ as a 2D momentum in the in-plane. Thus, the band-bending effects are included via the wave function, i.e., the distribution of carriers.

We examine the effect from doping-induced band bending on the carrier distribution in a square QW. A single-side modulation doping gives rise to some band bending, so the asymmetric modifications of this distribution are as follows: an increase near the top (doping-side) interface ($z<0$) and a decrease near the bottom one ($z>0$). Thus, within a variational approach to the lowest subband of the square QW with high enough potential barriers, we may take an asymmetric wave function such that

$$\zeta(z)=\begin{cases} B\sqrt{\pi/L}\cos(\pi z/L)e^{-cz/L} & \text{for} \quad |z|<L/2 \\ 0 & \text{for} \quad |z|>L/2, \end{cases} \tag{1}$$

with $L$ as the well width. Here, $B$ and $c$ are variational parameters to be determined. The normalization requires that

$$\frac{\pi}{2}B^2\gamma_1(c)=1, \tag{2}$$

where $\gamma_1(c)$ is a simple function defined by Eq. (A3) in Appendix. Thus, there is a single independent parameter, say, $c$. As clearly seen from Eq. (1), this parameter is a measure

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of the doping-induced band-bending effect on the carrier distribution.

### B. Hartree potential

The envelop wave function of the ground-state subband given by Eq. (1) is to minimize the total energy per particle.[1] In the bent-band model, the Hamiltonian is determined by

$$H = T + V_b(z) + V_H(z), \tag{3}$$

where $T$ is the kinetic energy, $V_b(z)$ and $V_H(z)$ are the barrier and the Hartree potentials, respectively. The Hartree potential is specified by the distribution of ionized impurities $N_I(z)$ and that of charge carriers $p(z)$. The doping profile $N_I(z)$ is with a bulk density $N_I$ in the top barrier from a doping position $-z_d$ to $-z_s$, where $z_d = L_d + L_s + L/2$ and $z_s = L_s + L/2$, with $L_d$ and $L_s$ as thicknesses of the doping and spacer layers, respectively. The carrier profile is $p(z) = p_s|\zeta(z)|^2$, with a sheet density $p_s$ and the wave function from Eq. (1). The charge neutrality claims that $p_s = N_I L_d$.

We solve the Poisson equation for the Hartree potential in combination with the boundary conditions at $z = -\infty$: $\partial V_H(-\infty)/\partial z = 0$, and $V_H(-\infty) = E_I$ with $E_I$ as the binding energy of an ionized impurity in the top barrier.[16] As a result, the Hartree potential is given by

$$V_H(z) = E_I + \frac{4\pi e^2}{\varepsilon_L}\begin{cases} 0 & \text{for} \quad z < -z_d \\ (N_I/2)(z+z_d)^2 & \text{for} \quad -z_d < z < -z_s \\ (N_I/2)(z_d - z_s)(2z + z_d + z_s) & \text{for} \quad -z_s < -L/2 \\ (N_I/2)(z_d^2 - z_s^2) - p_s[g(z) - z g'_+ - h_-] & \text{for} \quad -L/2 < z < L/2 \\ (N_I/2)(z_d^2 - z_s^2) - p_s(h_+ - h_-) & \text{for} \quad z > L/2, \end{cases} \tag{4}$$

where $\varepsilon_L$ is the dielectric constant of the QW, and by definition,

$$g(z) = \frac{\pi B^2 L}{8} e^{-2cz/L}\left\{ \frac{1}{c^2} + \frac{1}{(c^2+\pi^2)^2} \times \left[ (c^2 - \pi^2)\cos\frac{2\pi z}{L} - 2\pi c \sin\frac{2\pi z}{L} \right] \right\} \tag{5}$$

and

$$h(z) = g(z) - z g'(z). \tag{6}$$

Here, the prime stands for the differention with respect to $z$ and the subindices $\pm$ for the values at $z = \pm L/2$; for instance, $g'_+ = \partial g/\partial z|_{z=+L/2}$.

### C. Total energy per particle

We are dealing with the total energy per particle in the lowest subband determined by the Hamiltonian given by Eqs. (3) and (4). As clearly seen from Eq. (4), the Hartree potential may be represented as a sum of two terms: $V_H(z) = V_I(z) + V_s(z)$. The first term is to be regarded as the impurity potential fixed by the doping profile, viz., their bulk density $N_I$ and doping positions $z_d, z_s$, while the second one as the carrier potential fixed by their sheet density $p_s$ and their distribution, i.e., the variational parameters. As a result, for very high-barrier QWs, the expectation value of the Hamiltonian is defined as a function of the band-bending parameter such that

$$E(c) = \langle T \rangle + \langle V_I \rangle + \langle V_s \rangle. \tag{7}$$

The total energy per particle is given by a modification of Eq. (7), in which the average potential due to the carrier distribution $\langle V_s \rangle$ is to be replaced with its half.[1,4]

The individual energies appearing in the total energy are supplied in the following. The average kinetic energy is

$$\langle T \rangle = -\frac{\pi \hbar^2 B^2}{4 m_z L^2}[(c^2 - \pi^2)\gamma_1(c) + 2\pi c \omega_1(c)], \tag{8}$$

where $m_z$ is the out-of-plane carrier effective mass of the well layer and $\gamma_n$ and $\omega_n$ with $n$ as an integer are functions of a variable defined simply by Eqs. (A3) and (A4).

The average impurity potential is

$$\langle V_I \rangle = E_I + \frac{2\pi e^2 N_I}{\varepsilon_L}(z_d^2 - z_s^2). \tag{9}$$

The average carrier potential is

$$\langle V_s \rangle = -\frac{\pi^3 e^2 B^4 p_s L}{4\varepsilon_L (c^2+\pi^2)}\left\{ \frac{\pi^2}{c}\left[ e^c \gamma_1(c) \frac{c^3 - 6c^2 + \pi^2(c-2)}{c(c^2+\pi^2)} - e^{-c}\frac{\partial \gamma_1(c)}{\partial c} \right] + \frac{1}{c^2+\pi^2}\left[ \left( 2c^2 + \pi^2 + \frac{\pi^4}{c^2} \right)\gamma_1(2c) + \frac{c^2 - \pi^2}{2}[\gamma_2(2c) - \gamma_0(2c)] - \pi c[\omega_2(2c) + 2\omega_1(2c)] \right] \right\}. \tag{10}$$

It is observed from Eqs. (7)–(10) that the band bending parameter $c$ is fixed not only by the carrier density, i.e., the doping level, but also by the channel width.

## III. LOW-TEMPERATURE TRANSPORT AND QUANTUM LIFETIMES

### A. Basic equations

Within the linear transport theory, which ignores the multiple scattering effects, the transport ($\tau_t$) and quantum ($\tau_q$) lifetimes at very low (zero) temperature are represented in terms of the ACF for each disorder,[6,17]

$$\frac{1}{\tau_t} = \frac{1}{(2\pi)^2 \hbar E_F} \int_0^{2k_F} dq \int_0^{2\pi} d\varphi \frac{q^2}{(4k_F^2 - q^2)^{1/2}} \frac{\langle |U(\mathbf{q})|^2 \rangle}{\varepsilon^2(q)} \tag{11}$$

and

$$\frac{1}{\tau_q} = \frac{1}{(2\pi)^2 \hbar E_F} \int_0^{2k_F} dq \int_0^{2\pi} d\varphi \frac{2k_F^2}{(4k_F^2 - q^2)^{1/2}} \frac{\langle |U(\mathbf{q})|^2 \rangle}{\varepsilon^2(q)}. \tag{12}$$

Here, $\mathbf{q}=(q,\varphi)$ is the 2D momentum transfer by a scattering event in the $x$-$y$ plane (in polar coordinates): $q=|\mathbf{q}| =2k_F \sin(\vartheta/2)$, with $\vartheta$ as a scattering angle. The Fermi energy is given by $E_F=\hbar^2 k_F^2/2m^*$, with $k_F=\sqrt{2\pi p_s}$ as the Fermi wave number and $m^*$ as the in-plane hole effective mass of the well.

The dielectric function $\varepsilon(q)$ in Eqs. (11) and (12) takes account of the screening of scattering potentials by the 2D carriers. As usual, this is evaluated within the random phase approximation,[1]

$$\varepsilon(q) = 1 + \frac{q_s}{q} F_S(q)[1 - G(q)] \quad \text{for } q \leqslant 2k_F, \tag{13}$$

with $q_s=2m^* e^2/\varepsilon_L \hbar^2$ as the inverse 2D Thomas-Fermi screening length. The local field corrections arising from a many-body exchange effect in the in plane are included by the function[18] $G(q)=q/2\sqrt{q^2+k_F^2}$.

The screening form factor $F_S(q)$ takes account of the extension of the particle state along the growth direction, given by

$$F_S(q) = \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' \, \zeta^2(z) \zeta^2(z') e^{-q|z-z'|}. \tag{14}$$

The previous theories[19,20] believed that it is too tedious to calculate the screening function with a wave function such as that in Eq. (1), so an empirical formula has been used so far, which is simpler than Eq. (14), but still nonanalytic. With the aid of our mathematical functions $\gamma_n$ and $\omega_n$, the calculation is lengthy, however, straightforward. As a result, one may achieve an exact analytic expression,

$$F_S(t) = (\pi^2 B^4/8)[F_U(t) + F_L(t)], \tag{15}$$

with $t=qL$ as the dimensionless in-plane wave number. The functions appearing here are defined as follows:

$$\begin{aligned} F_{U/L}(t) = {} & \pm \frac{1}{c \mp t/2} [e^{\pm(c \mp t/2)} \gamma_1(c \pm t/2) - \gamma_1(2c)] \\ & \mp \frac{c \mp t/2}{2[\pi^2 + (c \mp t/2)^2]} [2e^{\pm(c \mp t/2)} \gamma_1(c \pm t/2) + \gamma_2(2c) \\ & + 2\gamma_1(2c) - \gamma_0(2c)] \pm \frac{\pi}{2[\pi^2 + (c \mp t/2)^2]} [\omega_2(2c) \\ & + 2\omega_1(2c)], \end{aligned} \tag{16}$$

where the upper (lower) signs refer to the subindex $U$ ($L$). It is interesting to note that in the absence of doping ($c=0$), the screening function given by Eqs. (15) and (16) is simplified to the one for the flat-band model.[6,7]

### B. Autocorrelation function for surface roughness scattering

To illustrate the band-bending effects on the electronic properties, we calculate the transport and quantum lifetimes limited by surface roughness scattering. As indicated,[1] the weighted potentials in wave vector space for scattering from the rough interfaces are given in terms of the local values of the wave function $\zeta_\mp=\zeta(z=\mp L/2)$ by

$$U_\mp(\mathbf{q}) = V_0 |\zeta_\mp|^2 \Delta_{\mathbf{q}}, \tag{17}$$

with $\Delta_{\mathbf{q}}$ as a Fourier transform of the interface profile. For high enough barriers $V_0$, one may replace the wave function in Eq. (17) by its derivative,

$$V_0 |\zeta_\mp|^2 = \frac{\hbar^2}{2m_z} |\zeta'_\mp|^2. \tag{18}$$

As dramatically warned,[1,21] the use of the values of an approximate (variational) wave function and its derivative at an interface plane can cause serious errors in the calculation of surface roughness scattering. Indeed, these local values can lead to a wrong dependence, e.g., on carrier density, and to surface roughness scattering too big by a factor of about 1 order of magnitude. The drawback is more severe in the case when surface roughness scattering is dominant and, with some recent attempts at structural optimization, the mobility has been raised by merely a few times.[22,23] For getting rid thereof, we need a formula, in which the weighted scattering potentials are given in terms of quantities that are insensitive to the trial wave function, such as the maximum of a wave function and some integrals of it on the $z$ axis. The peak of the wave function from Eq. (1) is located at the point $z_0 =\delta L$, with $\delta=-(1/\pi)\arctan(c/\pi)$.

For the above-mentioned purpose, we integrate the one-dimensional Schrödinger equation for a bound-state wave function $\zeta(z)$ from $z=\mp\infty$ to $z=z_0$. As a result, we obtain

$$V_0 |\zeta_\mp|^2 = [E(c) - V_H(z_0)]\zeta^2(z_0) + \int_{\mp\infty}^{z_0} dz \zeta^2(z) \frac{\partial V_H(z)}{\partial z}. \tag{19}$$

With the use of the wave function from Eq. (1), we may express the weighted scattering potentials of interest in an analytic form,

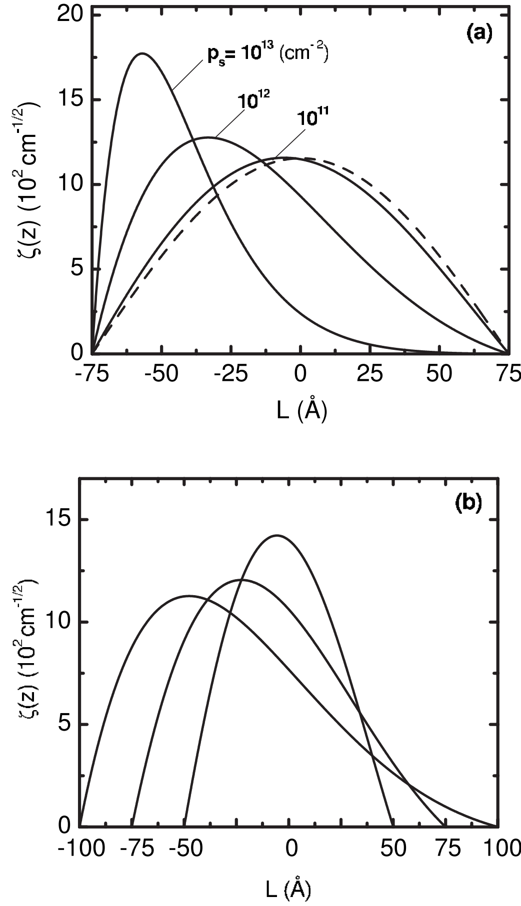


FIG. 1. Ground-state wave function $\zeta(z)$ for a hole in the GaAs square QW in the bent-band (solid) and flat-band (dashed line) models for (a) a channel width $L=150$ Å and sheet carrier densities $p_s=10^{11}$, $10^{12}$, and $10^{13}$ cm$^{-2}$ and (b) a sheet carrier density $p_s=5\times10^{11}$ cm$^{-2}$ and channel widths $L=100$, 150, and 200 Å.

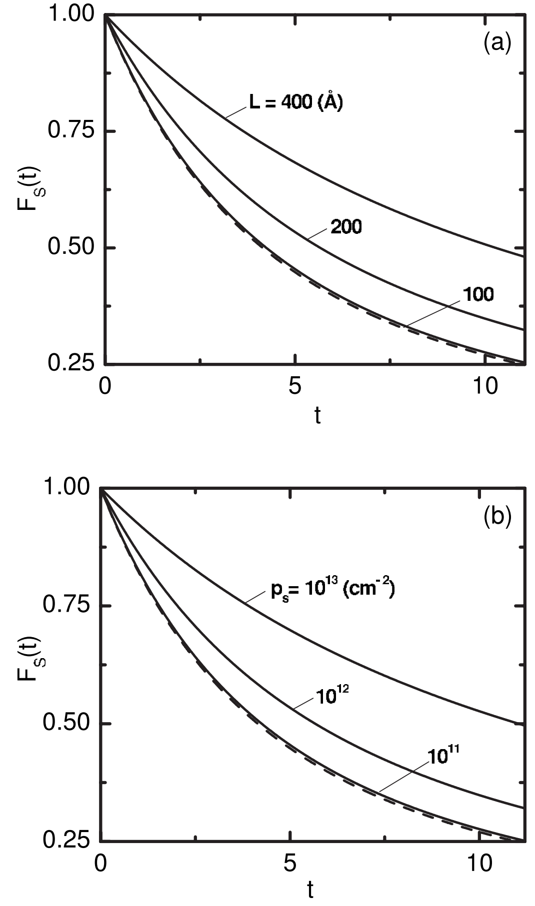


FIG. 2. Screening form factor $F_S(t)$ vs the dimensionless momentum $t$ for 2DHG in the GaAs square QW in the bent-band and flat-band models. The interpretation is the same as in Fig. 1 with diverse parameters.

$$
\begin{aligned}
V_0|\zeta_{\mp}|^2 = {} & [E(c) - V_H(z_0)]\zeta^2(z_0) \\
& \mp \frac{\pi^3 e^2 B^4 p_s}{2\varepsilon_L(c^2+\pi^2)} \Bigg\{ \pi^2 \frac{e^{-c}}{c} \Gamma_1(\pm c, \pm \delta) \\
& - \left(2c + \frac{\pi^2}{c}\right)\Gamma_1(\pm 2c, \pm \delta) - \frac{c}{2}[\Gamma_2(\pm 2c, \pm \delta) \\
& - \Gamma_0(\pm 2c, \pm \delta)] \pm \frac{\pi}{2}[\Omega_2(\pm 2c, \pm \delta) \\
& + 2\Omega_1(\pm 2c, \pm \delta)] \Bigg\}.
\end{aligned}
\tag{20}
$$

Here, as in Eq. (19), the upper (lower) signs refer to the top (bottom) interface.

It is worth mentioning the merits of Eqs. (19) and (20). First, these are exact and applicable to any bound state in any QW, i.e., a two-interface (trilayer) structure of any depth $V_0$. Second, they enable a reduction of the errors associated with the use of an approximate wave function. Third, they are convenient for use in the case of infinite QWs since their right-hand side remains definite, whereas the left-hand one becomes indefinite at this limit ($V_0 \to \infty$ and $\zeta_{\mp} \to 0$).

## IV. RESULTS AND CONCLUSIONS

We have carried out numerical calculations to evaluate the band-bending effects from single-side modulation doping on the carrier distribution (Fig. 1), the 2D screening (Fig. 2), and their quantum transport (Figs. 3 and 4) in square QWs. The quantum transport is limited by interface roughness with a Gaussian profile. From the results obtained, we may draw the following conclusions.

(i) As shown in Fig. 1, due to band bending, the hole distribution is strongly modified, increased near the top interface and decreased near the bottom one. The modification is found increased with a rise of the sheet hole density, i.e., the doping level and of the channel width.

(ii) As seen from Fig. 2, the flat-band model can remarkably underestimate the 2D screening. The bent-band screening is raised with a rise of the channel width and of the doping level.

(iii) In accordance with the above conclusions, in the bent-band theory, the surface roughness scattering of holes from the top interface is, as seen from Fig. 3, remarkably enhanced, so dominating over that from the bottom one. The total two-dimensional hole gas (2DHG) mobility is, following the Matthiessen rule, much lower than the flat-band one (up to more than 1 order of magnitude).

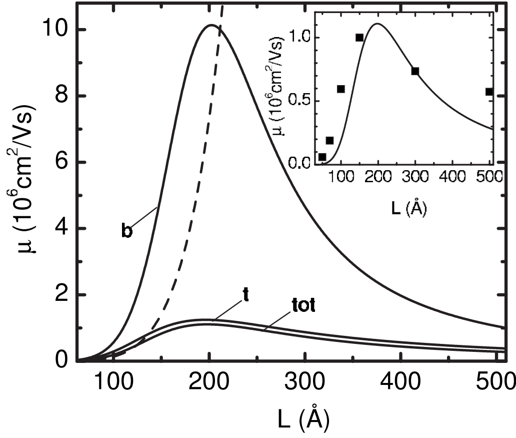


FIG. 3. Mobilities limited by surface roughness scattering with a roughness amplitude $\Delta=5$ Å and a correlation length $\Lambda=44$ Å for 2DHG in a GaAs QW ($m^*=0.112m_e$) vs channel width $L$ at a hole density $p_s=1.1\times10^{11}$ cm$^{-2}$ in the bent-band (solid) and flat-band (dashed line) models. The mobility limited by scattering from the top (bottom) interface is labeled $t$ ($b$). The 0.3 K measured data (Ref. 12) are marked by squares.

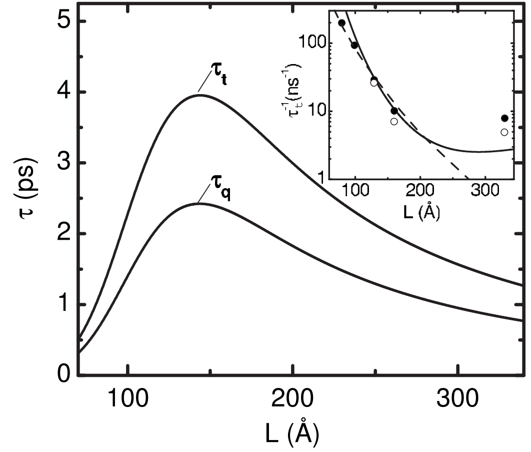


FIG. 4. Bent-band transport $\tau_t$ and quantum $\tau_q$ lifetimes limited by a interface profile with $\Delta=4.5$ Å and $\Lambda=40$ Å for 2DEG in a GaAs QW ($m^*=0.067m_e$) vs channel width $L$ at an electron density $n_s=5\times10^{11}$ cm$^{-2}$. The inset shows $\tau_t^{-1}$ at $n_s=5.8\times10^{10}$ cm$^{-2}$ in the bent-band (solid) and the finite-barrier flat-band (dashed line) models, and the 0.3 K measured data (Ref. 25).

(iv) The band bending in square QWs causes not only a reduction in the magnitude of the 2DHG mobility as stated above but also an alteration of its functional dependence on the channel width, viz., a nonmonotonic evolution with a sharp peak instead of a monotonic increase in the flat-band case. Our theory provides a satisfactory description of the recently measured[12] dependence of the 2DHG mobility of a GaAs channel on its width (inset of Fig. 3).

Following Ref. 13, the peak in Fig. 2 is located at a larger well width ($L_{\max}\sim300$ Å). However, this seems to be implausible, since this was inferred with the use of a hole mass $m^*$ measured by cyclotron resonance. The mass thus obtained may be a spintronic effective one, so differs from the zero-field mass.[24]

It should be mentioned that the peak of the 2DHG mobility in modulation-doped square QWs of diverse channels was experimentally found in 1993 by Xie *et al.*[8] and then by a number of authors.[9–13] However, up to date, no satisfactory explanation has been available, so its nature still remains as a challenge in the transport theory for square QWs.

(v) In difference from the previous belief,[11–13] in the bent-band theory, the transport and quantum lifetimes of two-dimensional electron gas (2DEG) in Fig. 4 also exhibit a sharp peak for a high enough electron density ($n_s \gtrsim 10^{11}$ cm$^{-2}$). Thus, the broadening of Landau levels, given by $\Gamma\sim\hbar/\tau_q$, shows a corresponding minimum. As seen from the inset, the bent-band inverse transport lifetime $\tau_t^{-1}$ at $L>160$ Å is in agreement with the recent data better than that in the flat-band model even with finite barriers.[25,26]

(vi) It is found that the peak shape, viz., its height and position, in the channel-width dependence of both lifetimes is fixed by some parameters, especially the doping level. With its increase, the peak becomes sharper and located at a smaller width, while with its decrease, the peak becomes smeared out or even disappears, the band-bending effect being negligibly weak.

## V. SUMMARY

To summarize, within a variational approach, we obtain analytic expressions for the envelop wave function and the 2D screening function for bent-band square QWs. These form a basis for calculating their properties such as electrical transport, density of states, and broadening of Landau levels.

The band-bending effects are of more importance with an increase of the doping level and of the channel width. The bent-band system exhibits some features.

We prove that the band bending leads to a peak in the channel-width dependence of both transport and quantum lifetimes, whose existence has not been explained so far. The peak is reproduced for 2DHG as detected experimentally and, further, predicted for 2DEG.

We derive a special formula allowing to exactly calculate surface roughness scattering with the use of an approximate wave function. Our theory is clearly applicable to other band-bending sources, e.g., external normal electric field.

## APPENDIX: AUXILIARY FUNCTIONS

In this Appendix, we introduce some mathematical functions, which make up a tool helpful to the description of the modulation-doping effects in an infinite square QW. These are defined as algebraic combinations of elementary functions, given by

$$\Gamma_n(\eta;\nu)=\frac{2}{L}\int_{-L/2}^{\nu L}dz\,\cos^2(n\pi z/L)e^{-2\eta z/L}$$
$$=\frac{e^{\eta}-e^{-2\nu\eta}}{2\eta}+\frac{1}{2(\eta^2+n^2\pi^2)}[(-1)^n\eta e^{\eta}+e^{-2\nu\eta}(n\pi\sin2\nu n\pi-\eta\cos2\nu n\pi)] \quad (A1)$$

and

$$\Omega_n(\eta;\nu) = \frac{1}{L}\int_{-L/2}^{\nu L} dz \sin(2n\pi z/L)e^{-2\eta z/L} = \frac{1}{2(\eta^2+n^2\pi^2)}[(-1)^n n\pi e^{\eta} - e^{-2\nu\eta}(n\pi\cos 2\nu n\pi + \eta\sin 2\nu n\pi)], \quad (A2)$$

with $n=0,1,2,\ldots.$ as an integer.

For $\nu=1/2$, the functions are rewritten as follows: $\gamma_n(\eta)=\Gamma_n(\eta;1/2)$ and $\omega_n(\eta)=\Omega_n(\eta;1/2)$, such that

$$\gamma_n(\eta) = \left[\frac{1}{\eta} + \frac{(-1)^n\eta}{\eta^2+n^2\pi^2}\right]\sinh\eta \quad (A3)$$

and

$$\omega_n(\eta) = (-1)^n n\pi\frac{\sinh\eta}{\eta^2+n^2\pi^2}. \quad (A4)$$

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