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Ground-state variational wave function for the quasi-one-dimensional semiconductor quantum wire

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An analytic variational wave function is proposed for the ground state of a quasi-one-dimensional electron system as occurring in narrow inversion layers in metal-oxide-semiconductor field-effect-transistor structures. The ground-state energy and the charge density are evaluated as functions of the average channel-electron density and the width of the metal gate by solving Poisson's equation and Schrödinger's equation in the variational self-consistent Hartree approximation.

Recent advances in technology[1-5] have made possible the fabrication of quasi-one-dimensional electron systems confined on the semiconductor side of metal-oxide-semiconductor field-effect-transistor (MOSFET) structures. One of the techniques used in producing these one-dimensional structures is to use very narrow metal gates (deposited lithographically) which confine the electron gas in the x-y plane with z being the direction normal to the interface. In a normal MOSFET structure the electronic motion along the z direction is quantized[6] in the space-charge layer due to the strong confining electric field at the interface produced by the gate electrode, but the motion in the x-y plane is free in the effective-mass sense. Quantum aspects of such two-dimensional confinement in systems like Si inversion layers and the electronic structure of the confined electron states have been extensively studied[6] in the last fifteen years. On the other hand, one-dimensional systems associated with narrow inversion layers have only been studied[7-9] within simple particle-in-a-box-type quantization models where the confinement in the x-y plane is assumed to be caused by well-defined model potentials like the infinite-square-well or harmonic oscillator potential. In this Rapid Communication we go beyond these simple models and provide a variational approximation for the ground state of a narrow-channel inversion layer in the MOSFET structure assuming an extreme quantum limit with only the lowest level occupied.

We make the usual[6,10] effective-mass approximation and consider electrons moving under the influence of the self-consistent confining field in the conduction band of the semiconductor. The confining potential V obeys a two-dimensional Poisson's equation given by

$$\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)V(y,z)=-\frac{4\pi}{\varkappa_s}\rho(y,z) \quad , \tag{1}$$

where ρ is the charge density and $\varkappa$ is the background lattice dielectric constant. We are assuming the electrons to be completely free in the x direction so that the electronic wave function is given by

$$\psi(x,y,z)=L_x^{-1/2}e^{ik_x x}\phi(y,z) \quad . \tag{2}$$

The wave function $\phi(y,z)$ obeys a two-dimensional Schrödinger equation given by

$$-\left(\frac{\hbar^2}{2m_y}\frac{\partial^2}{\partial y^2}+\frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2}\right)\phi(y,z)+V(y,z)\phi(y,z)=E\phi(y,z) \quad . \tag{3}$$

The total charge density ρ in Eq. (1) consists of the fixed depletion charge and the inversion-layer electronic charge density itself so that

$$\rho(y,z)=\rho_d(y,z)+\rho_s(y,z) \quad , \tag{4}$$

where

$$\rho_s(y,z)=\sum_i N_i|\phi_i(y,z)|^2 \tag{5}$$

is the electronic charge density with i as the quantum index for the confined states defined by Eq. (3). N_i is the density occupancy of the ith level. There is an additional image-potential (V_I) contribution[6] to V which arises from the mismatch in background dielectric constants at the interface. We employ the following model for the depletion charge density to mimic the narrow-gate systems:

$$\rho_d(y,z)=-e(N_A-N_D) \text{ for } -a\leq y\leq a \text{ and } 0<z<d$$
$$=0 \text{ otherwise} \quad , \tag{6}$$

where d is the thickness (in the z direction) of the depletion layer whereas $2a$ is the width (in the y direction) of the depletion layer. In Eq. (6), N_A and N_D are the bulk accepter and donor concentrations, respectively. Our boundary conditions are $V=0$ for $z=0,d$ and $V=0$ for $y=0$, $\pm a$. The width $2a$ is in general much larger than the width w of the strip in which the electrons are confined.

A numerical self-consistent treatment of the above set of equations [(1)–(6)] is feasible, but perhaps somewhat involved computationally. Instead we concentrate on an analytic approach which gives one some insight into the nature of the confined electronic states. We start by introducing the classical Green's function $G(y,z;y',z')$ which formally solves Poisson's equation:

$$V(y,z)=\int G(y,z;y',z')\rho(y',z')dy'dz' \quad . \tag{7}$$

One can solve for the Green's function G using standard[11] techniques to obtain

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$$G(y,z;y',z')=\left(\frac{2}{\pi}\right)\sum_{m=1}^{\infty}\frac{\sin[(m\pi/a)y]\sin[(m\pi/a)y']}{m\sinh[(m\pi/a)d]}\times\begin{cases}\sinh\left(\frac{m\pi}{a}(d-z')\right)\sinh\left(\frac{m\pi}{a}z\right) & \text{for } z<z' ,\\ \sinh\left(\frac{m\pi}{a}z'\right)\sinh\left(\frac{m\pi}{a}(d-z)\right) & \text{for } z>z' .\end{cases}\quad(8)$$

The main advantage of this formula is that the arguments y and z have been separated into a highly convergent series. In fact, for our case it turns out that it is sufficient to keep only the first term in the series defined by Eq. (8) since the second term is more than an order of magnitude smaller than the first term. Keeping only the leading term in the series, Poisson's equation is now directly solved to give

$$V_d(y,z)=-\frac{4\pi e(N_A-N_D)}{\varkappa_s}\left(\frac{2}{\pi}\right)a^2\frac{\sin[(\pi/a)|y|]}{\sinh[(\pi/a)d]}\left[\sinh\left(\frac{\pi}{a}d\right)-\sinh\left(\frac{\pi}{a}z\right)-\sinh\left(\frac{\pi}{a}(d-z)\right)\right]\quad(9)$$

and

$$V_s(y,z)=-\frac{4\pi e}{\varkappa_s}\left(\frac{2}{\pi}\right)N_0\int_{-a}^{a}dy'\frac{\sin[(\pi/a)|y|]}{\sinh[(\pi/a)d]}\sin\left(\frac{\pi}{a}y'\right)\left[\int_0^z dz'\sinh\left(\frac{\pi}{a}z'\right)\sinh\left(\frac{\pi}{a}(d-z)\right)|\phi(y',z')|^2+\int_z^d dz'\sinh\left(\frac{\pi}{a}(d-z')\right)\sinh\left(\frac{\pi}{a}z\right)|\phi(y',z')|^2\right] .\quad(10)$$

In Eq. (9), N_0 is the electronic charge density *per unit length* and $N_0|\phi(y,z)|^2$ is the strip electronic charge density (per unit volume) at the spatial point (y,z). It is easy to see that in the limit $a>>d$ Eqs. (9) and (10) reduce to the well-known[6] two-dimensional forms. The total self-consistent potential entering Eq. (3) is now given by $V=V_d+V_s+V_I$ where V_d, V_s are, respectively, the potentials due to the fixed depletion charge and the self-consistent Hartree potential due to the confined electrons themselves.

We solve the above set of equations self-consistently by using the following analytic variational wave function:

$$\phi(y,z)=Aze^{-b_0z/2}(e^{-b_0b_1|y|z/2})F(y) ,\quad(11)$$

where A is a normalization constant and the function $F(y)$ is given by

$$F(y)=\begin{cases}\cos\left(\frac{\pi y}{w}\right)+\frac{\pi}{w\gamma}, & |y|\leqslant w/2 ,\\ \frac{\pi}{w\gamma}e^{-\gamma(|y|-w/2)}, & |y|\geqslant\frac{w}{2} .\end{cases}\quad(12)$$

The variational parameters are b_0, b_1, and γ whereas w is the width of the strip (for simplicity we choose $a=2w$ which gives good accuracy and convergence in our numerical results). The geometry is such that the semiconductor occupies the $z\geqslant 0$ half-space and the narrow rectangular strip (of infinite length along the x axis) is centered around $y=0$.

Our variational wave function defined by Eq. (12) has the character of a particle-in-a-box-type wave function in the y direction except that it has tails outside the strip because the confining potential is not infinite. The wave function in the z direction has the Fang-Howard-Stern variational form[6] which has been quite successful for regular (i.e., *non-narrow*) two-dimensional silicon inversion layers. A new feature of the wave function defined by Eq. (11) is the mixing between the y and z terms (i.e., the wave function is nonseparable) which has been parametrized by the term in parentheses. The physics behind this mixing is that as one makes the inversion layer narrow by squeezing down the infinite two-dimensional structure along the y direction, there is an intermixing between the ground and the excited states of the simple Fang-Howard-Stern wave function as one can see by expanding the parentheses in Eq. (11):

$$\exp(-b_0b_1|y|z/2)\approx 1-b_0b_1|y|z/2+(b_0b_1|y|/2)^2z^2/2!+\cdots .$$

The variational parameter b_1 defines the extent of this mixing by making the maxima of the electron density distribution in the z direction an explicit function of y.

Using the variational wave function it is now straightforward (and, quite tedious) to obtain the ground-state expectation value of the Hamiltonian (Eq. 3) given by

$$H=T+V=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}-\frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2}+V(y,z)\right) ,$$

and to minimize the ground-state energy

$$E(b_0,b_1,\gamma)=\langle T\rangle+\langle V_d\rangle+\tfrac{1}{2}\langle V_s\rangle+\langle V_I\rangle$$

with respect to the variational parameters b_0, b_1, and γ for given values of the inversion and depletion charge densities. Details are tedious and will not be shown here. We will present our numerical results for the wave function and ground-state energy appropriate for *narrow* inversion layers on $Si(100)$-SiO_2 system.[6]

In Fig. 1 we show three-dimensional plots of the ground-state probability density $|\phi(y,z)|^2$ as a function of y and z for $w=600$ Å, $N_s=1.4\times10^{12}$ cm^{-2}, $N_{depl}=1.01\times10^{11}$ cm^{-2}, and for $w=100$ Å, $N_s=5\times10^{12}$ cm^{-2}, $N_{depl}=1.01\times10^{11}$ cm^{-2}. In Fig. 2 we show the wave function as a function of z for various fixed values of y to explicitly bring out the mixing of y and z parts of the wave function which gives rise to the "bending" effect apparent in Figs. 1 and 2. The ground-state energy has been shown as a function of $N=N_s+N_{depl}$ in Fig. 3 for two different situations. We also show $z_{00}=\langle z\rangle$ in Fig. 3 to give some idea about the width of the wave function. For one set of curves in

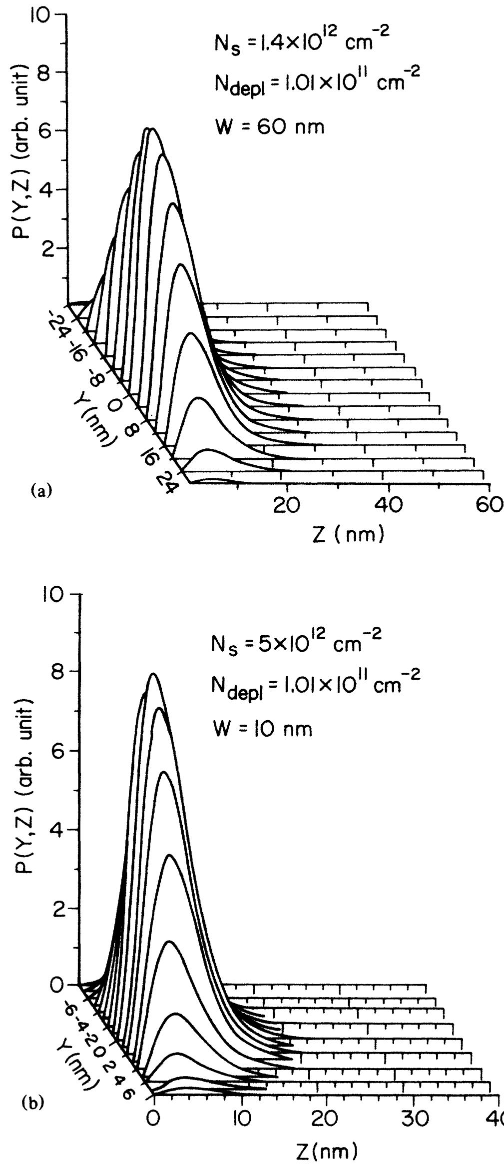

FIG. 1. Ground-state envelope wave function as a function of y and z for two different situations.

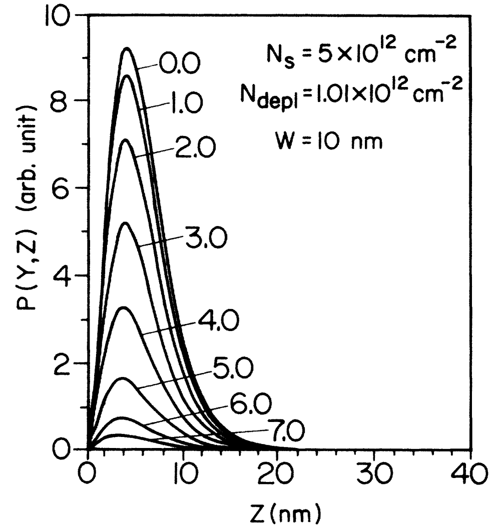

FIG. 2. Ground-state envelope wave function as a function of z for various fixed values of y (in nm) as marked on the curves.

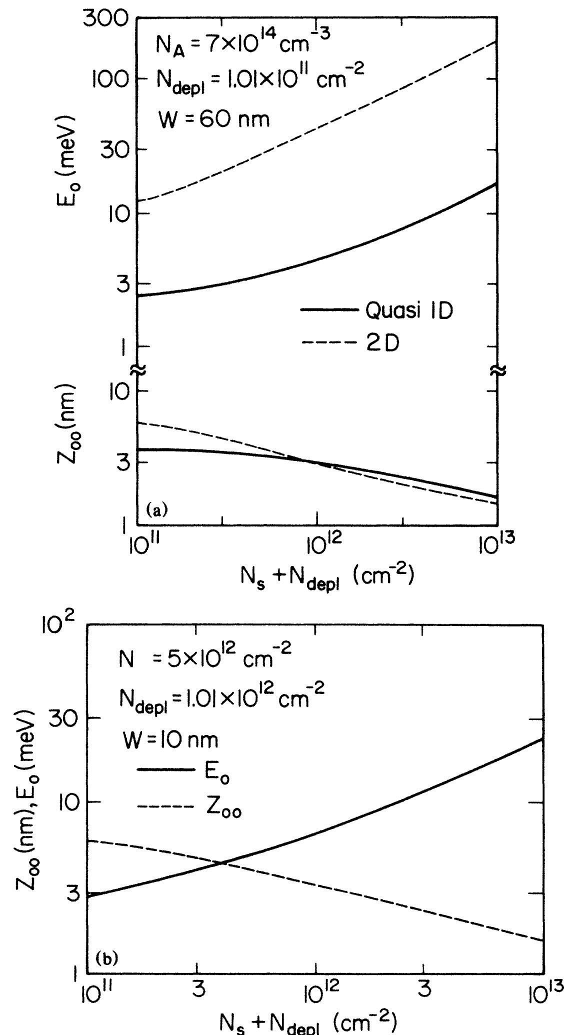

FIG. 3. Ground-state energy (E_0) and the z-spatial extent (z_{00}) of the ground-state wave function for two different situations. (a) Dashed lines are the corresponding results for the two-dimensional limit ($w = \infty$).

Fig. 3 we show, for the sake of comparison, our results for E_0 and z_{00} in the two-dimensional situation where $w = \infty$, and there is no lateral confinement.

The main conclusions which we derive from our numerical results is that the bending effect (i.e., the intermixing of the y and z parts) is important for narrow inversion layers and that the tailing effect is important for narrower strips. Our calculation being the very first one for quantum wire structures involves a number of simplifying approximations like the neglect of exchange-correlation effects[12] and the electric quantum-limit approximation (i.e., the neglect of excited levels). But the advantage is that the work is mostly analytic (except for the variational minimization in the end) which enables one to develop a good physical feel for the quantum-confinement effects. One can, in principle, attempt to solve the set of equations [(1)–(8)] self-consistently by direct numerical integration. However, such

calculations are bound to be numerically quite complex in view of the two-dimensional nature of the basic Schrödinger's and Poisson's equations.

In conclusion, we have developed a variational theory for the ground-state one-electron wave function of a quasi-one-dimensional quantum wire as occurring in narrow inversion layer in metal-insulator-semiconductor structure. We solve the two-dimensional Poisson's equation by using a classical Green's function expansion, and then the Schrödinger's equation is solved variationally in the Hartree approximation. Our numerical results for narrow channel silicon (100) inversion layers are most appropriate for one-dimensional structures produced in narrow gate devices.[2,3,5]

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