Thomas-Fermi theory of δ-doped semiconductor structures: Exact analytical results in the high-density limit

L. Ioriatti
Departamento de Física e Ciência dos Materiais, Instituto de Física e Química de São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560 São Carlos, São Paulo, Brazil
(Received 5 September 1989; revised manuscript received 31 October 1989)

The nonlinear Thomas-Fermi formulation of δ doping is proven to represent an exactly solvable model which is equivalent to the Hartree model in a wide range of doping densities. Analytical solutions to the eigenvalue problem of Schrödinger's equation in the Thomas-Fermi field are proven to exist and to represent the exact solutions to the many-body inhomogeneous electron system in the limit of high densities.

I. INTRODUCTION

Spatial localization of impurities in a single monolayer of semiconductor crystals obtained by epitaxial-growth techniques, such as molecular-beam epitaxy (MBE), represents the ultimate physical limit of dopant distributions in semiconductors. δ doping is one of the several names, others include planar doping, pulse doping, or atomic layer doping, for a particular epitaxial method whereby dopant atoms are introduced into a semiconductor while epitaxial growth is interrupted.[1] Currently, δ doping has been successfully used to produce Si layers in GaAs and $Al_xGa_{1-x}As$,[2] Sb layers in Si,[3] and S layers in InP.[4]

In the δ-doping concept of GaAs, shallow Si donor impurities are located in an atomic monolayer of the (100)-oriented GaAs host material.[5] The fractional coverage of the impurities can reach several donors per unit effective Bohr area of an impurity and provides a nearly continuous distribution of charge that can be mathematically described by a Dirac delta function. Due to electrostatic attraction, electrons remain close to their parent ionized donors and form a high-density quasi-two-dimensional (quasi-2D) electron gas in the field created by the ionized sheet of positive charge. In the narrow effective-field potential well electronic levels are quantized into two-dimensional subbands.

One of the characteristic features of δ doping is the occupation of many subbands, and there have been various theoretical investigations on the electronic levels of these systems. The WKB approximation[6] and empirical potentials[7] have been employed in the determination of subband energies and relative subband concentrations of δ-doped GaAs. Zrenner *et al.*[8] and Gillman *et al.*[9] have performed self-consistent calculations for the determination of the subband structure of δ-doped GaAs by solving Poisson's equation and the one-dimensional Schrödinger equation for motion perpendicular to the δ-doped surface. Direct evidence for the formation of 2D subbands in δ-doped GaAs came from Shubnikov–de Haas oscillations observed during magnetotransport measurements[8] and, more recently, from experiments on far-infrared absorption of radiation by subband resonant modes.[10] The self-consistent calculations for the subband structure turn out to be in very good agreement with the result of these experiments.

The difficulty of the problem of δ-doping lies in the necessity of self-consistent determination of the effective potential since electrons already populate several excited subbands even at modest areal doping densities. The effective field depends strongly on subbands, and there has been no *a priori* way to determine this field. In contrast to other two-dimensional electron systems,[11] however, the fact that electrons occupy many excited subbands suggests that a semiclassical approach may be a valid description of such systems.

In this paper the Thomas-Fermi (TF) model for δ-doped semiconductor structures is proposed and demonstrated to be equivalent to the self-consistent approximation in a wide range of doping densities. It is also shown that the effective-mass formulation of the TF theory of δ doping presents a completely soluble model. Not only explicit algebraic solutions of the nonlinear TF equation for the effective field are determined, but also explicit power-series solutions for the eigenstates of Schrödinger's equation in the TF field are presented.

The nonlinear TF theory, which is the topic of this paper, has an enormous physics literature[12,13] and few exact results. As is expected from the inherent statistical nature of the method, best results are expected in high-density regimes where the Pauli exclusion principle for electrons is likely to play a major role.

Rigorous proof that under a suitable large nuclear-charge limit the many-body quantum-mechanical energy is asymptotic to the TF energy for atoms, molecules, and solids was given by Lieb and Simon.[14,15] For the system under consideration, a similar proof can be given, provided the large nuclear-charge limit is translated into the limit of a large number n_D of ionized donors per unit effective Bohr area. The proof follows the same scaling and Dirichlet-Neumann bracketing arguments of Ref. 15 and will not be given here.

The TF model for δ-doping and the solutions of the nonlinear TF equation are described in Sec. II of this pa-

per. The analytical solutions of the TF Schrödinger eigenvalue problem are presented in Sec. III where calculated TF results for the subband structure are presented and compared with those of the more elaborate self-consistent calculation. Discussion and conclusion will be given in Sec. IV.

II. THE NONLINEAR THOMAS-FERMI EQUATION

The Thomas-Fermi theory of δ doping developed in this paper is based on a density-functional formulation[16] where one adopts a local view for the kinetic-energy term and seeks a mean-field description in terms of the local electron density $n(x)$. The many-body exchange and correlation effect are known to be unimportant in the present system and will be neglected completely.[17] In what follows, x is a coordinate that runs perpendicular to the doping plane, and the validity of the effective-mass approximation and the representation of the doping layer by a continuous positive sheet of charge of vanishing thickness are explicitly assumed.

If the effective Bohr radius and the effective Rydberg are taken as the natural units of distance and energy, which for GaAs parameters are 98.7 Å and 5.83 meV, respectively, the TF energy-density functional is written as

$$E_{\mathrm{TF}}[n(x)]=\tfrac{3}{5}\int(3\pi^2 n)^{2/3}n\,dx+4\pi n_D\int|x|n(x)dx -2\pi\int\int n(x)n(x')|x-x'|\,dx\,dx' . \quad (2.1)$$

Notice that in the chosen system of units, the impurity areal density n_D is given as the number of donors per unit Bohr area (0.97×10^{-12} cm^2 for GaAs).

The Euler-Lagrange equation for minimizing Eq. (2.1), in conjunction with Poisson's equation and the subsidiary condition for a fixed number n_S of electrons per unit Bohr area, yields the following equation for the effective field

$$\frac{d^2V}{dx^2}=-\frac{8}{3\pi}(\mu-V)^{3/2}+8\pi n_D\delta(x) . \quad (2.2)$$

Notice that the Fermi energy μ appears in Eq. (2.2) as the Lagrange multiplier for the subsidiary condition on the total number of electrons. Equation (2.2) is recognized as the Thomas-Fermi equation for the problem; it is a nonlinear second-order differential equation that can be solved by quadrature. Physically it holds only for negative $V-\mu$; for positive $V-\mu$ the electron density vanishes because there are no populated states with energy larger than the Fermi energy μ in a degenerated δ layer. The correct differential equation for positive $V-\mu$ is therefore $d^2(\mu-V)/dx^2=0$.

A simple mechanical picture of a particle climbing an energy barrier, with $V-\mu$ playing the role of position and $x\geq0$ of time, is useful in clarifying the nature of the solutions of Eq. (2.2). If $V(0)-\mu<0$ is taken as the initial "position" of such a "particle" and $4\pi n_D$ as its initial "velocity," as implied by the presence of the δ-function term on the right-hand side of Eq. (2.2), energy conservation demands three different classes of solutions.

If, for instance, $V(0)-\mu$ is small, a small energy barrier is to be surpassed, and after a short elapsed "time" x_c the "particle" starts to run freely to $+\infty$, i.e., $V(x)-\mu=4\pi(n_D-n_S)(x-x_c)$; $x\geq x_c$. This situation clearly corresponds to a nonneutral situation where $n_D>n_S$. Further decrease in $V(0)-\mu$ implies in a larger energy barrier, and this situation continues until we reach a critical situation where the initial "kinetic energy" is just enough to put the "particle" on top of the energy barrier [$V(\infty)=\mu$] after an infinite elapsed time ($x_c=\infty$). This refers to the neutral case ($n_S=n_D$). Further decrease in $V(0)-\mu$, implies that there will not be sufficient energy to climb the energy barrier, and the "particle" should return back past the point it had started. This third class of solutions are clearly impossible since there is no way for Eq. (2.2) to be satisfied for any finite number of electrons. It implies that negatively charged structures do not exist in the TF theory. In the atomic case where the same is known to occur,[13] the situation represents a failure of the TF theory since negatively charged atoms do exist. Whether or not this is true for the structures under consideration for finite n_D, may be a largely irrelevant question in view of the small number and very weak binding of the extra electrons.

The second class of solutions is the most interesting since it refers to neutral structures. The following expression for $V(x)$, i.e.,

$$V(x)-\mu=-\frac{\alpha^2}{(\alpha|x|+x_0)^4} , \quad (2.3)$$

where $\alpha=2/15\pi$ is a numerical constant and x_0 a parameter, is easily verified as a solution of Eq. (2.2) satisfying the boundary condition of local charge neutrality at $|x|\to\infty$. A unique solution is obtained through $dV/dx|_{0+}=4\pi n_D$ as implied by the presence of the δ function in the right-hand side of Eq. (2.2). In this way one finds

$$x_0=(\alpha^3/\pi n_D)^{1/5} . \quad (2.4)$$

As one can see from Eq. (2.3), the parameter x_0 in Eq. (2.4) represents a fundamental length scale for the problem. It tells us, for instance, that the system shrinks in size for increasing n_D as $n_D^{-1/5}$.

As it was stated earlier in this paper, the local TF description expressed by Eq. (2.1) is exact in the high-density limit. If small departures from this limit are considered, corrections to the local TF picture for neutral structures can be obtained by considering the first few terms of a gradient expansion in the exact effective-mass kinetic-energy density functional.[16] To leading terms in this expansion, evaluated at the TF extremum $n(x)$, one finds

$$E_g=\frac{5}{9}\frac{\alpha^2}{x_0^4}n_D(1+\tfrac{9}{7}x_0^2) . \quad (2.5)$$

In this expression, the multiplicative factor in front of the parentheses is the TF ground-state energy per unit Bohr area, while the correction $O(n_D^{7/5})$ inside represents the leading gradient correction to the system's kinetic ener-

gy. Since a term $O(n_D^{7/5})$ also represents the leading nonvanishing exchange contribution to the ground-state energy, one is led to conclude that the TF and the self-consistent theories for δ doping are equivalent to the extent that the leading many-body (exchange) correction is ignored in both models. This is surprising and contrasts with the analogous situation encountered in the atomic case where the kinetic first-gradient correction (innercore correction) is known to dominate over the leading exchange contribution in the large nuclear limit.[15]

A final remark about the TF potential for neutral structures, as given in Eq. (2.3), is that it implies that $\mu=0$ when this quantity is measured from the bottom of the conduction band in the bulk ($|x|\to\infty$). Besides, it has power-law decay for large distances in contrast to an expected exponential decay for finite n_D. The fact is that as n_D increases, an increasing number of subbands with vanishing small populations and large kinetic energies starts to appear. Since these states are very much delocalized, the combination of an infinite number of them, which is the case when $n_D\to\infty$, gives rise to the power-law decay observed in Eq. (2.3).

III. THE TF SCHRÖDINGER EIGENVALUE PROBLEM

In the TF model, neutral δ-doped structures are described by a universal one-parameter potential energy function. Since it is even in x and has translational invariance along directions that are perpendicular to x, solutions of the Schrödinger equation in this field are described by parity and transverse (parallel if referred to the doping plane) linear momentum. The energy spectrum is quantized for motion along x while it is continuous for directions that are perpendicular to x. The electronic system is quantized into 2D subbands whose number density, in electrons per unit Bohr area, is given by

$$n_j=\frac{1}{2\pi}(\mu-\varepsilon_j)\ , \tag{3.1}$$

where $n_D=\sum_j n_j$. In Eq. (3.1), ε_j is the jth bound-state (subband bottom) eigenvalue of the TF Schrödinger equation

$$-\psi''+V\psi=\varepsilon\psi\ , \tag{3.2}$$

where V is the TF field of Eq. (2.3).

As it was advanced earlier in this paper, Eq. (3.2) admits exact analytical solutions. From Eq. (2.3) and by the definition of a new independent variable z as

$$z=\sqrt{\kappa}(\alpha x+x_0)\ , \tag{3.3}$$

where $\kappa=\sqrt{-\varepsilon}/\alpha$, Eq. (3.2) can be rewritten as

$$z^2\psi''+\kappa\left[\frac{1}{z^2}-z^2\right]\psi=0\ . \tag{3.4}$$

The differential equation in Eq. (3.4) is peculiar in the sense that it has two irregular singular points ($z=0$ and $z=\infty$). Therefore, it cannot be solved by usual methods.[18] It can be mapped into Mathieu's equation by suitable redefinitions of the dependent and independent variables. In the course of this, however, the independent variable becomes complex and, as it is known from the theory of Mathieu's functions, the determination of the spectra becomes extremely complex.[19] For this reason, an entirely different route was adopted.

First, a WKB ansatz for ψ is proposed, i.e.,

$$\psi(z)=\sqrt{\lambda(z)}\sin\left[J\int_z^\infty\frac{dz'}{\lambda(z')}\right]\ , \tag{3.5}$$

where the constant J and $\lambda(z)$, such that $\lambda(z)\sim e^{2\sqrt{\kappa}z}$ as $z\to\infty$, are as yet unknown. The Wronskian of any two linearly independent solutions of Eq. (3.4), is independent of z, and simple inspection of the Wronskian equation reveals another solution of Eq. (3.4). For this new solution the sine function in Eq. (3.5) is simply replaced by the cosine with J being the Wronskian of the two solutions. Notice that, from the required asymptotic behavior of λ, only $\psi(z)$ as given in Eq. (3.5) is acceptable in the description of bound states. Substitution of either solution into Eq. (3.4) yields

$$4J^2=2\lambda''\lambda-\lambda'^2+4\kappa\lambda^2\left[\frac{1}{z^4}-1\right]\ . \tag{3.6}$$

Equation (3.6) is rather discouraging since it is a nonlinear second-order differential equation. If a first derivative is taken on both sides of the equation, however, a linear third-order equation is obtained; that is,

$$z\lambda'''+4\kappa\left[\frac{1}{z^2}-z^2\right]z\lambda'-\frac{8\kappa}{z^2}\lambda=0 \tag{3.7}$$

The structure of singularities and the invariance of Eq. (3.4) upon the changes $z\to 1/z$, $\psi(z)\to z\psi(1/z)$, suggests

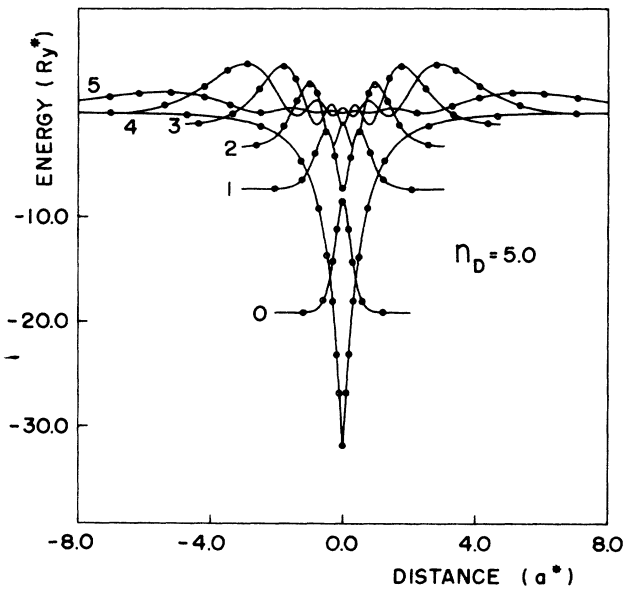

FIG. 1. The TF effective field and the eigenstates of the TF Schrödinger equation for a neutral δ-doped structure with $n_D=5$. The circles indicate the corresponding Hartree results. Energy and distance scales are given in reduced units.

TABLE I. A comparison between the TF and the Hartree theory for a neutral δ-doped structure for $n_D=5$, for various quantities. Subband bottoms, Fermi energies, and the values of effective fields at the position of the doping plane have been measured with respect to the bottom of the conduction band in the bulk. Ground-state energies are measured with respect to the bottom of the conduction band at the doping plane. All energies are in reduced units.

	Hartree		Thomas-Fermi	
Subband	Occupation n	Energy ε	Occupation n	Energy ε
0	3.07	−19.30	3.06	−19.20
1	1.18	−7.40	1.18	−7.44
2	0.52	−3.31	0.54	−3.37
3	0.18	−1.12	0.19	−1.18
4	0.05	−0.32	0.06	−0.36
5	0.004	−0.039	0.008	−0.054
μ	−0.013		0	
$V(0)$	−32.29		−32.05	
E_g	89.86		89.02	

the following Laurent series expansion for $\lambda(z)$:

$$\lambda(z)=z\sum_{n=0}^{\infty}a_n\left[z^{2n}+\frac{(-1)^n}{z^{2n}}\right] \tag{3.8}$$

with $a_0=1$.

Further substitution of these series into Eq. (3.7) yields a three-term recursion formula for the unknown coefficients that can be solved in terms of continued fractions.[18] The subsequent analysis of the thus emerging series reveals that Eq. (3.8) has, indeed, the required asymptotic behavior following Eq. (3.5).

The solution of the bound-state eigenvalue problem is completed first by calculating J as given in Eq. (3.6), for instance, from the values of λ and λ' at $z=1$, and second, by requiring definite parity for the solutions. In this way one arrives to an exact Bohr-Sommerfeld quantization rule for the spectrum of the TF Schrödinger equation of Eq. (3.2); that is,

$$J\int_{\sqrt{\kappa}x_0}^{\infty}dz\frac{1}{\lambda(z)}=n\pi\quad(n=1,2,\ldots) \tag{3.9a}$$

for odd-parity states and

$$J\int_{\sqrt{\kappa}x_0}^{\infty}dz\frac{1}{\lambda(z)}=\tan^{-1}[2J/\lambda'(\sqrt{\kappa}x_0)]+n\pi \qquad (n=0,1,2,\ldots) \tag{3.9b}$$

for even-parity states.

A summary of the analytical results obtained from the TF approach to neutral structures is presented in Fig. 1, where the TF field as well as the eigenstates of the TF Schrödinger equation were plotted for $n_D=5$ (5.13×10^{12} donors/cm^2 in GaAs). The corresponding results obtained from the numerical solutions of Hartree's equations for the same density are indicated by solid circles. As it is seen, the TF and the Hartree field are indistinguishable in the scale of the graph. Remarkable coincidence is also found for the eigenstates.

Table I summarizes the results obtained from the TF theory and those from the self-consistent field for various quantities such as subband energy bottoms, concentrations of electrons in different subbands, Fermi energies, ground-state energies, and bottoms of the potential well, for the same doping density as indicated in Fig. 1. As can be seen from Table I, the TF predictions are in remarkable overall agreement with those of the self-consistent field. Larger relative errors in subband bottoms and electronic concentrations are observed for the highly excited subbands, but these discrepancies are expected in view of the previous remarks concerning the tail of the effective field at large distances. As it is seen from Table I, the electron concentration in these subbands are so small that their presence may be largely irrelevant to the overall properties of the structures under consideration.

IV. DISCUSSION AND CONCLUSION

A clear indication that the TF theory of this paper remains valid in the entire experimental range of doping densities, while the 2D subband concept is meaningful for δ-doped GaAs (10^{12}–10^{13} cm^{-2}), is provided by Eq. (2.5) which predicts a very weak dependence with n_D for relative corrections in the system's ground-state energy as one departs from the exact high-density limit. If Eq. (2.5) is used to predict the system's ground-state energy at $n_D=5$, for instance, one finds 89.87 Ry as compared with the Hartree value of 89.86 Ry of Table I. For small doping densities, on the other hand, the description in terms of 2D subbands is certainly not valid, and it is necessary to treat the δ layer as a system of randomly distributed impurities in a plane. Presumably, when the number of donors per unit Bohr area is less than unity, a metal-insulator transition takes place as one may infer from the recently observed thermally activated hopping transport in δ-doped GaAs in the low doping regime.[20]

In conclusion, a very simple model approximation has been proposed for the calculation of the subband structure of δ-doped semiconductors. The approximation consisted in the use of the semiclassical Thomas-Fermi po-

tential suggested by occupation of many subbands. It was demonstrated that this simple procedure yields results that are equivalent to those obtained from the much more elaborated, and purely numerical, self-consistent approximation. In addition, the Thomas-Fermi model for δ doping of this paper was proven to represent the exact solutions to a nontrivial inhomogeneous many-body system in the limit of high densities. Possible extensions of the present model would include the study of the positively charged structures produced by electron recombination with holes in a uniform *p*-type doped semiconducting background, the diffusion of donors along the growth direction, small nonparabolicities in conduction band, and many-body effects within the local-density approximation (LDA).

ACKNOWLEDGMENTS

The author wants to thank P. Basmaji for fruitful discussions on various problems related to δ doping. This work was supported by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Brazil, and by Financiadora de Estudos e Projetos (FINEP), Brazil.

[1]C. E. Wood, G. Metze, J. Berry, and L. F. Eastman, J. Appl. Phys. **51**, 383 (1980).

[2]K. Ploog, J. Cryst. Growth **81**, 304 (1987).

[3]H. P. Zeindl, T. Wegehaupt, I. Eisele, H. Oppolzer, H. Reisinger, G. Tempel, and F. Koch, Appl. Phys. Lett. **50**, 1164 (1987).

[4]Wenchao Cheng, A. Zrenner, Qiu-Yi Ye, F. Koch, D. Grützmacher, and P. Balk, Semicond. Sci. Technol. **4**, 16 (1989).

[5]T. H. Chiu, J. E. Cunningham, B. Tell, and E. F. Schubert, J. Appl. Phys. **64**, 1578 (1988); E. F. Schubert, J. B. Stark, B. Ulrich, and J. E. Cunningham, Appl. Phys. Lett. **52**, 1508 (1988).

[6]E. F. Schubert, A. Fischer, and K. Ploog, IEEE Trans. Electron Dev. **ED-33**, 625 (1986).

[7]D. Lavielle, J. C. Portal, M. Stöhr, S. P. Najda, A. Briggs, G. Gillmann, P. Bois, E. Barbier, and B. Vinter, Rev. Phys. Appl. **24**, 539 (1989).

[8]A. Zrenner, F. Koch, and K. Ploog, Surf. Sci. **196**, 641 (1988).

[9]G. Gillmann, B. Vinter, E. Barbier, and A. Tardella, Appl. Phys. Lett. **52**, 972 (1988).

[10]N. Schwarz, F. Müller, G. Temple, F. Koch, and G. Weimann, Semicond. Sci. Technol. **4**, 571 (1989).

[11]T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 457 (1982).

[12]N. H. March, Adv. Phys. **6**, 1 (1957).

[13]H. A. Bethe and R. Jackiw, *Intermediate Quantum Mechanics* (Benjamin, New York, 1968), Chap. 5.

[14]E. Lieb and B. Simon, Phys. Rev. Lett. **31**, 681 (1973).

[15]E. Lieb and B. Simon, Adv. Math. **23**, 22 (1977).

[16]W. Kohn and P. Vashishta, in *Theory of the Inhomogeneous Electron Gas*, edited by S. Lundquist and N. H. March (Plenum, New York, 1983), pp. 79.

[17]Recent LDA density-functional calculations for δ-doped GaAs [P. Koenraad *et al.* (unpublished)] have shown that exchange effects gives negligible contributions to subband energies in the 10^{12}–10^{13} range of doping densities.

[18]P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. 1, Chap. 5.

[19]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1970), Chap. 20.

[20]Qui Yi-Ye, A. Zrenner, F. Koch, and K. Ploog, Semicond. Sci. Technol. **4**, 500 (1989).