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PSEUDOVARIATIONAL CALCULATION OF ENERGY LEVELS AND WAVEFUNCTIONS IN GaAs QUANTUM WELLS

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ABSTRACT

It is by now widely accepted that the role played by quantum effects cannot be ignored if one wishes to gain insight in the transport properties of submicron structures such as MOSFETS or heterojunctions. For example, tunneling currents and/or mobilities in these devices cannot be adequately predicted without taking into account the existence of discrete energy levels and spatially confined wavefunctions (Ando,1982;Zöllner,1986).

We have developed a pseudovariational algorithm, details of which are given elsewhere (Magnus,1988), capable of simultaneously solving Schrödinger's and Poisson's equations in an accurate way. Moreover, if compared with purely numerical solution schemes, its low computational cost makes it

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more suitable for implementation in a device simulator.

In this paper we report on improvements of this method to account for a more complete description of the depletion layer potential in Si inversion layers, as well as to calculate characteristic quantities (Fig.1) for AlGaAs/GaAs heterojunctions as a function of temperature, spacer layer thickness and doping.

1. DESCRIPTION OF THE METHOD

Details of the method employed in SCALPEL to calculate subband energies and wavefunctions have already been published (Magnus,1988). In short, SCALPEL starts from an ad hoc form for the Hartree inversion layer potential and a suitably scaled orthonormal basis of wavefunctions, both of which can be modified at discretion. At each iteration, the diagonalization of the Hamiltonian yields the energy levels and the mixing coefficients of the subband wavefunctions, while the Fermi level of the system is determined by fixing the total (mean) number of electrons.

Subsequently, the parameters making up the Hartree potential are extracted by matching the first few moments of the charge distributions n_1 and n_2, obtained from Schrödinger's and Poisson's equations respectively , and the new Hamiltonian is calculated. Thus, convergence yields the Hartree parameters as a function of the wavefunction scaling factor, which is in turn iteratively determined by requiring the free energy function of the system,

$$F(b) = - 1/\beta \ln \mathrm{Tr}\, e^{-\beta H^*}, \quad \beta = 1/kT \qquad (1.1)$$

where H^* is the exact Hamiltonian of the many-electron system, to be a minimum.

An exact calculation of the free energy is impossible, as this would require the complete diagonalization of H^*, which is not known. However, a perturbation expansion for F in the basis of the unperturbed initial wavefunctions can be used (Feynman,1972) to obtain a rigorous upper bound for F, F':

$$F \leq F' \text{ where } F' = F_o + \langle H^* - H_o \rangle_o \qquad (1.2)$$

Here, F_o is the free energy of the system in the initial wavefunction basis, and the second term is the unperturbed ensemble average of the difference between the inversion layer potential (i.e. the sum of the depletion and the Hartree potentials) and the potential from which the initial set is derived.

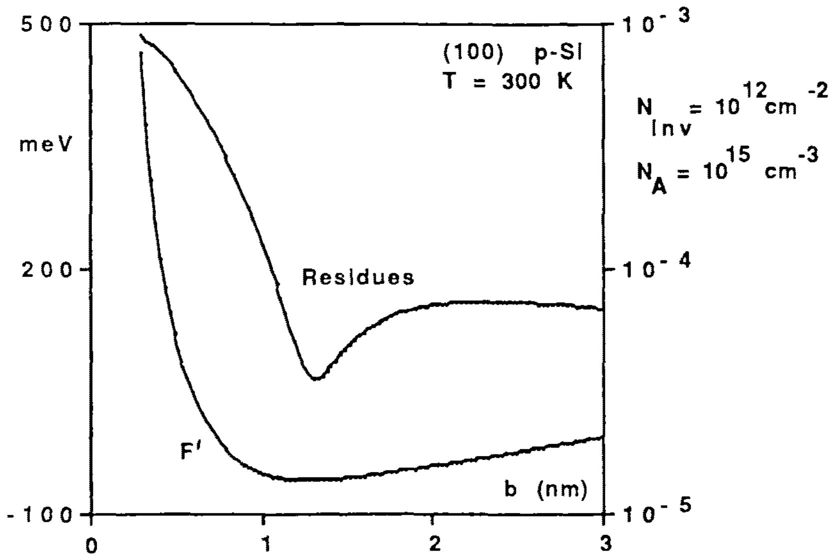

Fig 1.1: Free energy of the 2DEG and rms residue of the charge densities vs b.

Fig 1.1 shows a plot of F' versus wavefunction

scaling factor b for typical inversion and depletion layer densities: notice that the curve is smooth and has a unique minimum. In this figure, the mean square residue of the charge densities n_1 and n_2 for the same values of b is also plotted. This quantity too, which can be interpreted as a figure of merit for the selfconsistency of the iteration, has a sharp, single minimum at a value of b which is approximately the same as that for F'. The coincidence of the minima, though no proof in itself, nonetheless seems to suggest that this approximation for F can be used to find the thermodynamical equilibrium state of the two dimensional electron gas (2DEG).

The initial wavefunction basis employed in this paper is the same as the one previously used (Magnus,1988), namely Laguerre-type functions which are solutions of a one-dimensional inverse distance potential.

The choice of the Hartree potential is in principle independent of the specific basis adopted; however, since these two quantities are related to one another through Poisson's equation, better convergence is obtained in practice if the potential is engineered so that its second derivative has a functional dependence approximately resembling that of the wavefunctions. In any case, we have observed that modifying the Hartree potential has limited repercussions on typical macroscopic properties of the 2DEG, such as the average spatial extent of the charge density, or the subband populations.

2. FULL DESCRIPTION OF THE DEPLETION LAYER POTENTIAL IN A Si-INVERSION LAYER

A number of attempts at solving the inversion layer problem (Pals, 1972; Khondker, 1987) in Si and GaAs

have approximated the form of the depletion layer potential by retaining only the linear term, thus giving

$$V_{dep}(z) = -qN_{dep}z/\varepsilon_s \qquad (2.1)$$

where $N_{dep} = N_A z_d$, N_A is the dopant concentration in the bulk and ε_s is the permittivity. The thickness of the depletion layer z_d is obtained by requiring the potential at the edge of the depletion layer to be continuous with the bulk values:

$$-qV_{dep}(z_d) = E_{Fp} + W_b \qquad (2.2)$$

where W_b, the distance between the conduction band edge and the quasi-Fermi level for majority carriers E_{Fp}, is a function of N_A.

In any case z_d, being a function of N_A and E_F, must be included in the selfconsistent calculation if the problem is stated in terms of N_A rather than N_{dep}. This is done by solving (2.2) (Pals,1972) for

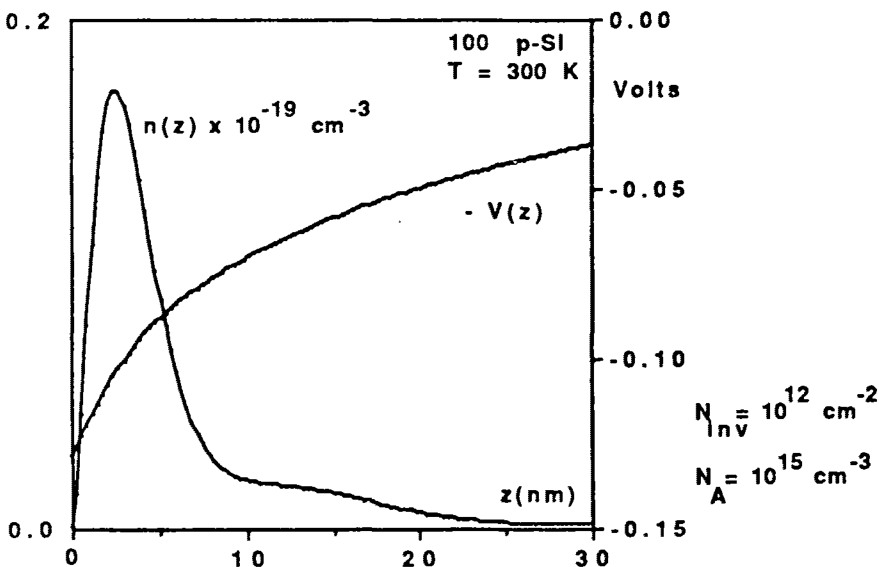

Fig. 2.1 : Electronic charge density and potential versus inversion layer distance.

z_d at each iteration until convergence is attained; an Aitken acceleration scheme (Gerald, 1984) is employed to reduce the number of iterations necessary.

Fig 2.1 shows the charge density n(z) as a function of distance z in the inversion layer superimposed on a plot of the total potential V(z). The potential remains linear even for distances at which the charge density is practically zero, demonstrating that the assumption that the squared term can be neglected is indeed justified. Notice also that n(z) shows a bump in the tail; this suggests that the initial wavefunction basis, although yielding relatively accurate results as far as macroscopic parameters are concerned, does not mirror the spatial behaviour of the true wavefunctions to their full extent. Indeed, a least-squares fit of fully numerical solutions of the selfconsistent problem show that the charge density varies as the product of a polynomial and $\exp[-(z/b)^{3/2}]$, whereas the exponential dependence of the Laguerre-type functions is linear. This result agrees with the findings of Takada (1977), and efforts are now underway to look for a potential whose solutions display the correct spatial behaviour.

3. AlGaAs/GaAs HETEROJUNCTIONS

It is well-known that the channel current in a HEMT is determined directly by N_s, the areal density of the quasi-two-dimensional electron gas (2DEG) near the heterointerface. Consequently, any reliable model for a HEMT should enable one to calculate N_s as a function of extrinsic quantities like spacer layer thickness (d_1), donor concentration (N_d) and Al-mole

fraction (x).

However, all previous calculations of this type (Park and Kwack, 1986 and references therein) are just based on empirical expressions for the subband energies. On the other hand SCALPEL could be adapted in a straightforward way to the heterojunction case to yield an expression for the Fermi energy as a function of N_s without having to fit experimental data.

As an application, we have modified Park and Kwack's (1986) two-step calculation of the density N_s at the AlGaAs/GaAs heterointerface as follows.

First, we calculated the relative position of the Fermi level E_F with respect to the AlGaAs conduction band edge, using Fermi-Dirac statistics.

Subsequently, we inserted the explicit dependence of E_F on N_s in the equation, which was derived by Park and Kwack (1986) to obtain N_s in terms of d_1, N_d and x.

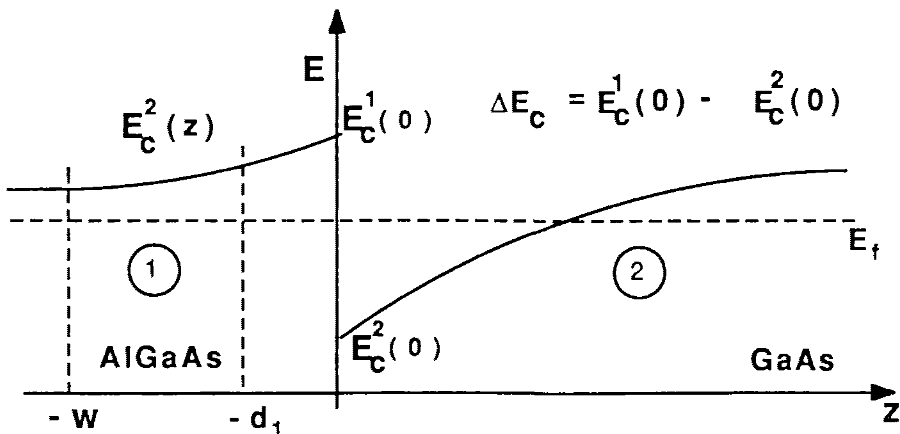

Fig 3.1: Energy band diagram at the heterointerface

In practice, we considered the heterojunction of a AlGaAs/GaAs HEMT, the interface of which is taken to be at z=0 as shown in fig. 3.1.

The AlGaAs part (region 1) consists of a

heavily doped Al_xGaAs_{1-x} layer ($-W \leq z \leq -d_1$) and an undoped spacer layer ($-d_1 \leq z \leq 0$). Since the GaAs part (region 2, $z \geq 0$) is assumed to be unintentionally doped, the formation of a quantum well is caused solely by ΔE_c, the energy-band discontinuity at the heterointerface.

In the local density approach, the free electron concentration in the AlGaAs region may be expressed in terms of the local conduction band edge $E_{c1}(z)$ as follows :

$$n(z) = N_c F_{1/2}\left(\frac{E_F - E_{c1}(z)}{kT}\right) \qquad (3.1)$$

where N_c is the effective density of states in the conduction band and $F_{1/2}(x)$ represents the Fermi-Dirac integral. If $x \leq 2$, the latter may be approximated with a maximum error of less than 1% by

$$F_{1/2}(x) \approx \frac{\sqrt{\pi}}{2} . \ln(1+e^x)\left[1+0.7357*\left(x+\sqrt{x^2+1.980851}\right)\right] \qquad (3.2)$$

In the same way the ionized donor concentration reads

$$N_d^+(z) = \frac{N_d}{1+2e^{\beta[E_d+E_F-E_{c1}(z)]}}, \quad \beta = 1/kT, \qquad (3.3)$$

where E_d is the donor ionization energy.

The charge neutrality at $z=-W$ requires $n_1(-W)=N_d^+(-W)$ and leads to an equation for $\lambda=\beta[E_F-E_{c1}(-W)]$, which is first solved :

$$\frac{1}{1+e^{\beta E_d+\lambda}} = \frac{N_c}{N_d} \ln(1+e^{\lambda})\left[1+0.7357*\left(\lambda+\sqrt{\lambda^2+1.980851}\right)\right]$$

(3.4)

On the other hand, the equation which is satisfied by N_s may be derived (Park and Kwack, 1986) by integrating the one-dimensional Poisson equation between z=-W and the heterointerface z=0 and using the continuity of the electric displacement vector at z=0, yielding

$$\frac{q^2N_s^2}{\varepsilon_1 N_d} - \frac{2q^2 d_1 N_s}{\varepsilon_1} - \Delta E_c + E_F - E_{c2}(0) - 2kT\lambda$$
$$- 2kT\ln\left\{1 + e^{\beta[E_d - \Delta E_c + E_F - E_{c2}(0) + q^2 N_s d_1/\varepsilon_1]}\right\}$$
$$+ 2kT\ln\left\{1 + e^{\beta E_d + \lambda}\right\} = 0 \qquad (3.5)$$

where ε_1 is the permittivity of $Al_xGa_{1-x}As$. The Fermi energy is calculated with the help of SCALPEL (two-subband calculation) and may be approximated accurately by the following analytical expression :

$$y = \frac{1}{2a}\left[-b + \sqrt{b^2 + 4a(n_s^\rho - c)}\right], \qquad (3.6)$$

where

$$E_F - E_{c2}(0) = y \text{ meV}, \ N_s = n_s \times 10^{+12} \text{cm}^{-2}, \qquad (3.7)$$

and a = -3.03075×10^{-7}, b = 3.36549×10^{-3}, c = 0.63301, ρ = 0.29631 are room-temperature values.

The comparison between our results and those of Park and Kwack (1986) is shown in figures 3.2 and 3.3. It is clear that the densities reported by Park and Kwack (1986) are systematically lower than our results. This may be explained by considering their analytical approximation for the Fermi-Dirac

integral, which overestimates the contribution of the free electrons in the AlGaAs part and therefore underestimates the channel density N_s.

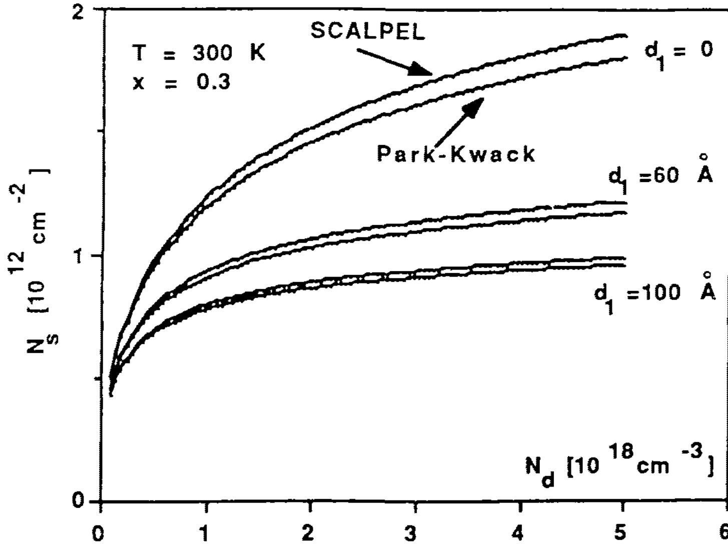

Fig 3.2 : Areal electron density versus donor concentration.

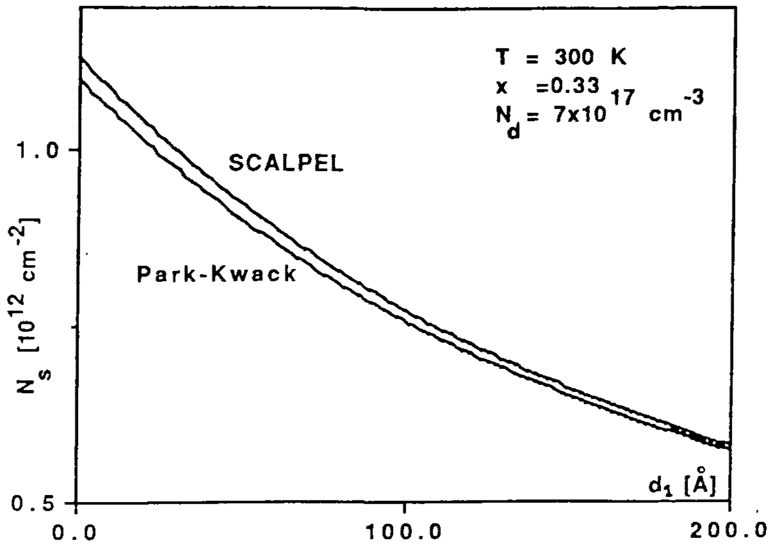

Fig. 3.3: Areal electron density vs spacer layer thickness

However, the fact that in both cases the calculated density is higher than the experimental one, may be a consequence of the uncertainty in the value of α appearing in

$$\Delta E_c = \alpha x \text{ meV} \tag{3.9}$$

as becomes clear by inspection of equations (3.5). Incidentally, recent papers (Park,1986;L.Eaves,1986) report values of α ranging from 800 to 1100, which may give rise to appreciable differences in N_s.

4. CONCLUSION

In this paper, we have reported on some applications of SCALPEL, a robust and flexible algorithm designed to calculate subband energies and wavefunctions in quasi-two-dimensional electron gases.

We have derived an unequivocal upper bound for the free energy of the system, whose minimization allows us to extract the spatial scaling factor of the quantummechanical charge density.

Moreover, we applied SCALPEL to the calculation of channel densities in HEMT'S as a function of typical design parameters, obtaining results in good agreement with previously published work.

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