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Existence of a quasi-continuous distribution oj bound state level sub-bands at an accumulation or inversion layer of semiconductor-insulator interfaces

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Fisica matematica. — *Existence of a quasi-continuous distribution of bound state level sub-bands at an accumulation or inversion layer of semiconductor-insulator interfaces.* Nota di ERCOLE DE CASTRO e PIERO OLIVO (*), presentata (**) dal Corrisp. E. DE CASTRO.

RIASSUNTO. — Con riferimento alla quantizzazione nella direzione ortogonale all'interfaccia, viene sviluppato un semplice procedimento approssimato per stabilire se esiste un intervallo di livelli quasi continui corrispondenti a stati legati allo strato di accumulazione di una giunzione isolante-semiconduttore opportunamente polarizzata.

Il procedimento, in quanto determina la distanza fra tali livelli, ne dà anche la densità, quindi la distribuzione delle sottobande di stati legati nel problema tridimensionale.

Il procedimento è utile in una varietà di problemi connessi ai suddetti strati di accumulazione, ad esempio nello studio dell'iniezione di elettroni attraverso l'ossido di gate di un dispositivo MOS per effetto Fowler-Nordheim. Lo stesso procedimento può essere utilizzato anche per gli strati di inversione.

INTRODUCTION

Accumulation and inversion layers at semiconductor-insulator interfaces are of great theoretical and practical interest. In the first case because of the physical phenomena that can be investigated [1-10], in the second because they are basic in the performance of such important electronic devices like the MOS in very large scale integrated circuits.

Thus it is easily understood why, in recent years, thanks to the impulse of Microelectronics, a great deal of research has been devoted to thorough investigation of the Si—SiO_2 interface of MOS structures.

One of the most interesting phenomena in which accumulation or inversion layers are involved is related to Fowler-Nordheim. i.e. high-field tunnel injection of electrons from the Silicon substrate to the metal gate of an MOS device through a SiO_2 film less than 100 Å thick [11-16].

Experiments on such phenomena are generally made on MOS capacitors, where injection takes place from a Silicon accumulation layer to a metal gate or a heavily doped polycrystalline Silicon film.

Thus, any theory aiming at interpretation of the transport phenomena through the thin dielectric SiO_2 film has to start from accurate knowledge of

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the injection level distribution from the Silicon accumulation layer. To such a layer we shall refer from now on, though the method is equally valid for an inversion layer.

It is well known that accumulation layers at Si—SiO_2 interfaces can be very thin and this can strongly influence distribution of the levels of their bound states, while leaving those of bulk states almost unperturbed.

Referring to quantization in the x direction orthogonal to the interface, one says the energy eigenvalues E_x are "quasi-continuous" when their spacing $\Delta E_x \ll kT$, while they are in the "quantum limit" when $\Delta E_x \gg kT$.

The so-called "quantum effects" refer to the latter case. It is also well known that a uniform sub-band of bound state levels of the three-dimensional problem [1] is associated to each eigenvalue $E_x < E_C$ (E_C being the lower edge of the unperturbed conduction band of the semiconductor).

Exact evaluation of the distribution of the levels $E_x < E_C$ is however very difficult, as we shall soon show.

A number of Authors have computed them with simplifying assumptions as to the nature of the semiconductor or its working conditions (e.g. low temperatures), they being interested in the broad features of the inherent physical phenomena [1-10]. Others, in the course of investigations on the aforementioned transport problems in MOS devices, have made "a priori" simplifying assumptions on the distribution of the levels. The quasi-continuous case, which is customary in the theory of semiconductor devices and is plausible when the layer is not very thin, is often assumed. On the contrary, being interested in the case of thin layers, a single sub-band of bound state levels (i.e. the $E_x < E_C$ only) to roughly evaluate quantum effects in Silicon at any temperature [11] has been recently assumed.

However, as far as the Authors know, no one has given criteria to ascertain the case for any given semiconductor and potential $\phi = \phi(x)$, nor methods to compute the density of the eigenvalues $E_x < E_C$ when their spacing is so small (e.g. 10^{-10} eV as compared with the 1.12 eV energy gap in Silicon) that direct numerical evaluations, for instance by Sommerfeld-like conditions in the WKB effective-mass approximation, fail to be manageable. The present work is devoted to this problem.

Outline of the method

Let us consider the electrons of the conduction band of an n-type semiconductor and suppose $x = 0$ to be the plane interface between the semiconductor and the insulator of a metal-insulator-semiconductor structure. The x axis will be oriented as in fig. 1, where E_C is the edge of the unperturbed semiconductor conduction band, while $\phi = \phi(x)$ is the electrostatic potential in the one electron effective mass approximation. Then, denoting q the absolute value of the electron charge and assuming $E_C = 0$, $V(x) = -q\,\phi(x)$ is the potential energy of an electron.

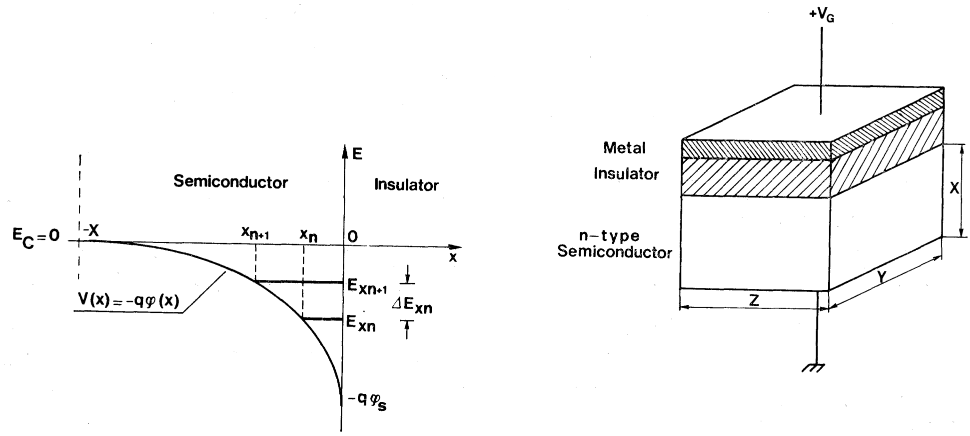

Fig. 1.

Let us now suppose that a voltage V_G be applied (see fig. 1) such that $\phi_s = \phi(0) > 0$. In the semiconductor, at the interface with the insulator, an accumulation layer will then be formed. Therefore, the potential energy $V(x)$, which is "a priori" unknown, can be assumed as a monotonically decreasing function inside the semiconductor.

Neglecting spin-orbit interaction, a stationary one-electron state is described by the normalized orbital

$$\psi(x, y, z) = \frac{1}{\sqrt{YZ}} f(x, E_x) \exp\left[i\left(l \frac{2\pi}{Y} y + r \frac{2\pi}{Z} z\right)\right] \tag{1}$$

and by the spin orientation. Periodic boundary conditions are assumed in the y and z directions, along which the lengths of the semiconductor slab are Y and Z respectively. The normalized factor $f = f(x, E_x)$ satisfies the Schrödinger equation

$$\frac{d^2 f}{d x^2} + \frac{2 m_x^*}{\hbar^2} [E_x - V(x)] f = 0 \tag{2}$$

with the boundary conditions

$$f(0, E_x) = f(-X, E_x) = 0 \tag{3}$$

which are justified because the injection of electrons into the dielectric is considered a small perturbation and the tails of the wavefunctions beyond the plane $x = 0$ and behind the plane $x = -X$, are neglected. Obviously X is the length of the semiconductor in the x direction, while l, r in (1) are positive or negative integers and m_x^*, m_y^*, m_z^* the effective masses of the electrons for states near a given minimum of the energy function in the conduction band.

The energy corresponding to the orbital (1) is given by

$$E = E_x + \frac{\hbar^2}{2}\left[\frac{1}{m_y^*}\left(\frac{2\pi}{Y}\right)^2 l^2 + \frac{1}{m_z^*}\left(\frac{2\pi}{Z}\right)^2 r^2\right]. \tag{4}$$

Varying l and r, for a given $E_x < 0$, a sub-band of bound states is described, the density of which turns out to be a constant.

Evaluation of the eigenfunctions and eigenvalues of (1) is a very difficult task because $V(x)$ is unknown, being determined by the unknown occupied electronic states themselves.

Therefore, the system of Schrödinger equations (2) and the so called Poisson equation have to be solved by the self-consistent Hartree method, as Stern did for the simpler case of inversion layers where the population of bulk states can be neglected [6], or in some other way.

The Authors did it in the WKB approximation [17], which is always feasible in the broad class of problems concerning practical applications of accumulation layers. Within this approximation the expression of $f(x, E_x)$ is known as a function of $\phi(x)$. Hence, one has to solve only the Poisson equation, which takes a rather complicated integro-differential form easily reduced to a pure integral equation. Approximate solutions of the last equation can be found by the Ritz method, i.e. by conveniently chosen parametrized expressions of $\phi(x)$, minimizing the mean square error between the two sides of the integral equation. Therefore $\phi(x)$ becomes specified by a certain number of numerical parameters (generally two). The search for $\phi(x)$ is then reduced to determination of these parameters, numerically effected by oriented trials, $\phi(x)$ being considered a known function at each trial.

Therefore, within the WKB-Ritz approximation, the problem of recognizing whether a quasi-continuous band of levels $E_x < 0$ exists can be faced for a given $V(x) = -q\,\phi(x)$ at each iteration. Such a problem, which can obviously be of interest in much more general contexts, will now be easily solved, subject only to very understandable approximations. At the same time the density of the levels will be immediately computed even when their direct numerical evaluation by the appropriate Sommerfeld-like condition

$$2\int_{x_n}^{0} \sqrt{2\, m_x^* \left[E_{xn} - V(x)\right]}\, dx = \left(n + \frac{3}{4}\right) h\,, \tag{5}$$

becomes impractical because of their extremely narrow spacing. In equation (5) x_n represents the turning point corresponding to the negative eigenvalue E_{xn} (see figure 1), given by

$$V(x_n) = E_{xn}\,, \tag{6}$$

while h is obviously the Plank constant.

Letting

$$\Delta E_{xn} = E_{x\,n+1} - E_{xn} \tag{7}$$
$$\Delta x_n = x_{n+1} - x_n ,$$

one can derive from (5) that

$$(n + 1 + \frac{3}{4})\, h = 2 \int_{x_{n+1}}^{0} \sqrt{2\, m_x^* \left[E_{x\,n+1} - V(x) \right]}\, dx =$$

$$\begin{aligned} &= 2 \Bigg\{ \int_{x_{n+1}}^{x_n} \sqrt{2\, m_x^* \left[\Delta E_{xn} + E_{xn} - V(x) \right]}\, dx + \\ &+ \int_{x_n}^{0} \left(\sqrt{2\, m_x^* \left[\Delta E_{xn} + E_{xn} - V(x) \right]} - \sqrt{2\, m_x^* \left[E_{xn} - V(x) \right]} \right) dx + \\ &+ \int_{x_n}^{0} \sqrt{2\, m_x^* \left[E_{xn} - V(x) \right]}\, dx \Bigg\} . \end{aligned} \tag{8}$$

If ΔE_{xn} is small enough to allow the assumption (see figure 1)

$$V(x) = V(x_n) + \left(\frac{dV}{dx} \right)_{x = x_n} (x - x_n) \simeq E_{xn} + \frac{\Delta E_{xn}}{\Delta x_n} (x - x_n) \tag{9}$$

in the interval $[x_{n+1} , x_n]$, it turns out that

$$\begin{aligned} &\int_{x_{n+1}}^{x_n} \sqrt{2\, m_x^* \left[\Delta E_{xn} + E_{xn} - V(x) \right]}\, dx \cong \\ &\cong \int_{x_{n+1}}^{x_n} \sqrt{2\, m_x^* \left[\Delta E_{xn} - \frac{\Delta E_{xn}}{\Delta x_n} (x - x_n) \right]}\, dx = \\ &= \sqrt{2 m_x^*\, \Delta E_{xn}} \int_{x_{n+1}}^{x_n} \sqrt{1 - \frac{x - x_n}{\Delta x_n}}\, dx = - \frac{2}{3}\, \Delta x_n \sqrt{2\, m_x^*\, \Delta E_{xn}} . \end{aligned} \tag{10}$$

Similarly, by letting

$$F(E_{xn}) = \int_{x_n}^{0} \sqrt{2\, m_x^* \left[E_{xn} - V(x) \right]}\, dx \tag{11}$$

one can derive

$$\left(\int_{x_n}^{0}\sqrt{2\,m_x^*\left[\Delta E_{xn}+E_{xn}-V(x)\right]}-\sqrt{2\,m_x^*\left[E_{xn}-V(x)\right]}\right)dx=$$

$$(12)\qquad =F(E_{xn}+\Delta E_{xn})-F(E_{xn})\simeq\frac{dF}{dE_{xn}}\Delta E_{xn}=$$

$$=\Delta E_{xn}\sqrt{\frac{m_x^*}{2}}\int_{x_n}^{0}\frac{dx}{\sqrt{E_{xn}-V(x)}}\,.$$

The last integral converges in spite of the singularity for $x=x_n$ [see equation (6)], because $V(x)$ is a monotonically decreasing function, hence $(dV/dx)_{x=x_n}\neq 0$.

Subtracting (5) from (8) and taking (10) and (12) into account, the equation

$$(13)\qquad -\frac{4}{3}\Delta x_n\sqrt{\Delta E_{xn}}+\Delta E_{xn}\int_{x_n}^{0}\frac{dx}{\sqrt{E_{xn}-V(x)}}=\frac{h}{\sqrt{2m_x^*}}$$

is finally obtained. With the other two equations

$$(14)\qquad V(x_n)=E_{xn}\,,\ \Delta E_{xn}=\left(\frac{dV}{dx}\right)_{x=x_n}\Delta x_n$$

(13) gives a system of three equations which can be solved for x_n, Δx_n and ΔE_{xn} (hence E_{xn+1}), once E_{xn} is known.

In practice, application of the above procedure is very simple. Having chosen the interval $[E'_x, E''_x]$ in which one suspects the eigenvalues $E_x<0$ to be quasi-continuous, any point of it can be approximately identified with the nearest eigenvalues E_{xn} from which to start. Then one finds the corresponding turning point x from $V(x)=E_x$, evaluates dV/dx and

$$\int_{x}^{0}\frac{dt}{\sqrt{E_x-V(t)}}$$

hence ΔE_x. If $\Delta E_x \ll kT$ the suspicion is proven for the given $V(x)$, and $1/\Delta E_x$ gives the density of the levels $E_x<0$, i.e. the density of bound state level sub-bands. If we let $\xi=\sqrt{\Delta E_{xn}}$

$$(15)\qquad \begin{aligned} a&=-\frac{3}{4}\left(\frac{dV}{dx}\right)_{x=x_n}\int_{x_n}^{0}\frac{dx}{\sqrt{E_{xn}-V(x)}}\\ b&=-\frac{3}{4}\left(\frac{dV}{dx}\right)_{x=x_n}\frac{h}{\sqrt{2\,m_x^*}}\end{aligned}$$

the coefficients a and b turn out to be positive and the preceding system can be easily reduced to the algebraic equation

$$\xi^3 + a\,\xi^2 - b = 0 . \tag{16}$$

It is easily seen that the above equation has a single positive real root which can be straightforwardly computed.

AN EXAMPLE

To illustrate the procedure with an exactly solvable example, let

$$\mathrm{V}(x) = -\frac{q\,\phi_s}{\cosh^2\left(\dfrac{x}{\sigma}\right)} , \tag{17}$$

σ being a constant. The asymptotic behaviour of $\mathrm{V}(x)$ for $x \to -\infty$ is obviously an exponential, the slope of which goes to zero. The assumption on decreasing $\mathrm{V}(x)$ is always satisfied, the only uninfluencing exception being $x = 0$. The test will be severe because of the exponential behaviour of $\mathrm{V}(x)$.

It is well known that the negative eigenvalues of (2) corresponding to the boundary and asymptotic conditions

$$\mathrm{f}(0) = 0 , \quad \lim_{\mathrm{X}\to\infty} f(-\mathrm{X}) = 0 \tag{18}$$

in the open interval $(-\infty , 0]$, are given by

$$\mathrm{E}_{xn} = -\mathrm{E}_0 \left(\theta - n - \frac{3}{4}\right)^2 \tag{19}$$

with $n = 0 , 1 , \ldots , \mathrm{N}$, N being the largest non-negative integer satisfying the inequality

$$\mathrm{N} < \theta - \frac{3}{4}, \tag{20}$$

and

$$\mathrm{E}_0 = \frac{2\,\hbar^2}{m_x^*\,\sigma^2} \quad , \quad \theta = \frac{1}{4}\sqrt{\frac{16\,q\,\phi_s}{\mathrm{E}_0} + 1} . \tag{21}$$

Hence

$$\Delta\mathrm{E}_{xn} = \mathrm{E}_0 \left(2\,\theta - 2\,n - \frac{5}{2}\right) . \tag{22}$$

The number of $E_{xn} < 0$ levels is therefore $N + 1$ and the condition for the existence of at least one of them is obviously expressed by $N \geqq 0$, i.e. by $\theta > 3/4$.

It makes sense to speak of a "band" of quasi-continuous eigenvalues $E_{xn} < 0$ if there is a large number of non-negative integers n satisfying the inequalities

$$n \leqq N \qquad (23)$$
$$\Delta E_{xn} < \eta\, k\, T$$

with a given $\eta \ll 1$. Therefore, if we let

$$F_1(\theta) = \begin{cases} \theta - \dfrac{\eta\, k\, T}{2\, E_0} - \dfrac{5}{4} & , \text{ if } \theta > \dfrac{\eta\, k\, T}{2\, E_0} + \dfrac{5}{4} \\ 0 & , \text{ if } \theta < \dfrac{\eta\, k\, T}{2\, E_0} + \dfrac{5}{4} \end{cases} \qquad (24)$$

$$F_2(\theta) = \begin{cases} \theta - \dfrac{3}{4} & , \text{ if } \theta > \dfrac{3}{4} \\ 0 & , \text{ if } \theta < \dfrac{3}{4} \end{cases} \qquad (25)$$

a large number $\mathcal{N}$ of non negative integers n has to satisfy the inequalities

$$F_1(\theta) < n < F_2(\theta) \qquad (26)$$

for the value of θ corresponding to the given ϕ_s.

Assuming $m_x^* = 10^{-30}$ Kg, $T = 300\ ^\circ K$, $\eta = 0.01$, $\phi_s = 0.4$ Volt, $\mathcal{N} = 500$, the following results are easily obtained

$\sigma =$ 100 Å, $15.6 \leqq n \leqq 16.2$: no band of quasi-continuous eigenvalues

$\sigma =$ 1000 Å, $158.9 \leqq n \leqq 168.8$: no band of quasi-continuous eigenvalues

$\sigma =$ 10000 Å, $764.5 \leqq n \leqq 1694.5$: both discrete and quasi-continuous eigenvalues, respectively for $n < 764$ and $764 \leqq n < 1695$.

To compare exact and approximate results, we have first of all to estimate the accuracy of the WKB approximation itself, i.e. the Sommerfeld-like expression (5) of the eigenvalues. It can be shown that from (5) it follows that

$$E_{xn} = -E_0 \left(\theta_{\mathrm{WKB}} - n - \frac{3}{4}\right)^2 \qquad (27)$$

where

$$\theta_{WKB} = \frac{1}{4}\sqrt{\frac{16\, q\, \phi_s}{E_0}} \tag{28}$$

$n = 0, 1, 2, \ldots, N_{WKB}$. Therefore the WKB expression of E_{xn} differs from the exact one only in the substitution of θ by θ_{WKB}, hence of N by N_{WKB}. It is immediately seen that θ and θ_{WKB} can be identified when $16\, q\, \phi_s / E_0 \geqslant 1$, i.e. when σ is sufficiently high and ϕ_s not too low. As to the applications involved, the above condition can always be considered verified.

Finally, we can test the accuracy of the proposed method by computing the approximate value of ΔE_{xn} and comparing this value with the exact one. To understand the reason for the error which affects the approximate value of ΔE_{xn}, we also computed:

1) the maximum variation of dV/dx in the interval $[x_{n+1}, x_n]$, measured by

$$\varepsilon_1 = \left| \frac{\left(\frac{dV}{dx}\right)_{x=x_{n+1}} - \left(\frac{dV}{dx}\right)_{x=x_n}}{\left(\frac{dV}{dx}\right)_{x=x_n}} \right| \tag{29}$$

2) the error involved in evaluation of the difference (12), measured by

$$\varepsilon_2 = \left| \frac{\left[F(E_{xn} + \Delta E_{xn}) - F(E_{xn})\right] - \frac{dF}{dE_{xn}} \Delta E_{xn}}{F(E_{xn} + \Delta E_{xn}) - F(E_{xn})} \right| . \tag{30}$$

The results (referred to the preceding case with $\sigma = 10000$ Å) are reported in figure 2, where

$$\varepsilon = \left| \frac{(\Delta E_{xn})_{\text{exact}} - (\Delta E_{xn})_{\text{approx.}}}{(\Delta E_{xn})_{\text{exact}}} \right| . \tag{31}$$

The agreement is good for all values of n except the very low and very large ones, the error always being essentially related to ε_2.

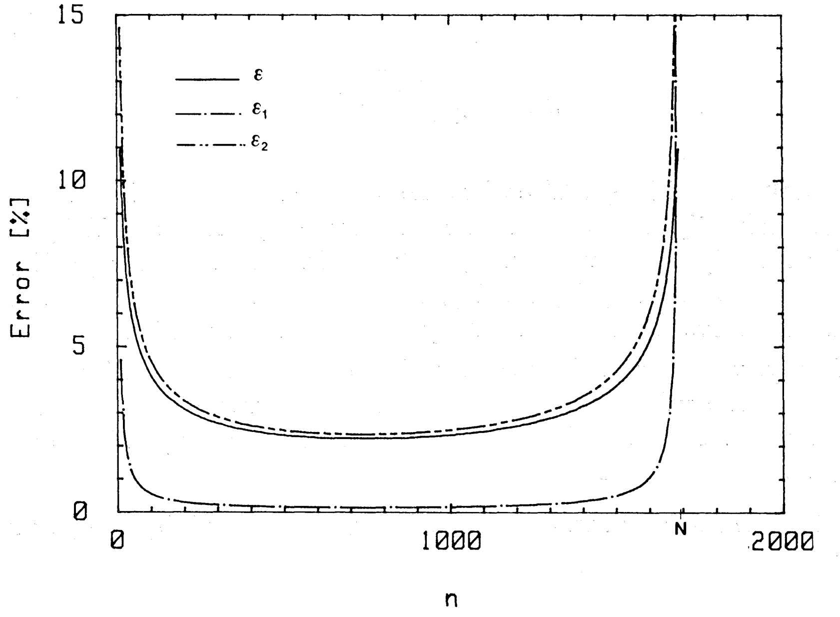

Fig. 2.

Conclusions

Referring to quantization in the x direction orthogonal to the interface, a simple procedure is given to establish whether or not a quasi-continuous band of bound state levels E_{xn} exists at an accumulation layer of a semiconductor-insulator junction. The procedure, giving the spacing ΔE_{xn} of such levels, obviously gives their density too, hence the distribution of the sub-bands of bound state levels of the tridimensional problem. The following assumptions are made: *i*) effective mass and WKB approximation are acceptable; ii) $V(x)$ is a known monotonically decreasing function along the accumulation layer; iii) if a quasi-continuous band of levels $E_{xn} < 0$ exists in any interval between two consecutive turning points of such a band the curve $V(x)$ can be approached by a straight line; iv)the Sommerfeld integral (11) can be linearized with respect to E_{xn} in $[E_{xn}, E_{xn+1}]$.

The procedure is useful in a variety of problems concerning accumulation layers, for instance in investigations on the Fowler-Nordheim injection of electrons from a Silicon accumulation layer through the gate oxide of an MOS device in VLSI microcircuits. The same procedure can also be made use of with inversion layers.

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