Nonmonotonic screening of the field in semiconductor accumulation layers

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An investigation is made of the screening of an external electric field in an intrinsic semiconductor as a function of the field intensity. Various approximations are used. It is shown that in the Hartree approximation only one transverse quantization subband exists in weak fields and only this band is filled. A second localized band drops out smoothly from the continuous spectrum and becomes filled as the field on the semiconductor surface is increased. The problem is solved semiclassically in the case of high fields when the number of subbands is $N \gg 1$ and this gives the dependence of the number of subbands on the electric field $N \propto F^{1/5}$ as well as an expression for the critical fields in which new localized subbands appear. The critical field F_1 corresponding to the appearance of the second localized subband is obtained in the Hartree approximation and it agrees well with the results of semiclassical calculations. Allowance for the exchange energy increases considerably F_1 (by about an order of magnitude) and results in a small jump in the occupancy of the second subband at $F = F_1$. It is shown that the critical field F_1 can be deduced from an abrupt change in the 1f capacitance of a metal-insulator-semiconductor structure. The Hartree approximation is used to show that the spectral dependence of the matrix element for transitions from a localized subband to a continuous spectrum is in the form of an asymmetric curve with a maximum and a characteristic energy which is proportional to $F^{2/3}$ and represents the fall at high frequencies. A determination is made of the range of positions of the Fermi level (in the bulk of the semiconductor) in which "overscreening" of the field occurs, i.e., the range of fields in which more electrons reach the surface of the semiconductor than the number required to screen the external field.

1. INTRODUCTION

The most frequently cited and fundamental papers on the theory of screening of an external field in accumulation layers in semiconductors are those of Refs. 1–4. However, the screening behavior patterns deduced from these papers are contradictory. In particular, Appelbaum and Baraff[1,2] do not explain the dependence of the number of subbands on the field intensity F_0 at the surface of a semiconductor. Moreover, Ando[4] referring to Refs. 1 and 2 and to his own work states that the Hartree approximation predicts the existence of just one subband and only allowance for the exchange and correlation energies increases the number of subbands. Pals[3] follows the transition from one to two filled subbands as the field is increased. Formation of the second subband is deduced from the condition that the Fermi level μ on the surface merges with the continuous spectrum. A shared shortcoming of the cited papers is the absence of investigations of the thermodynamic potential of the system and replacement of the matching of the Fermi levels on the surface and in the bulk of a semiconductor with the relationship between the field on the semiconductor surface F_0 and the surface density of electrons n_s:

$$F_0 = 4\pi e n_s/\varepsilon, \tag{1}$$

where ε is the permittivity of the semiconductor. We shall show that a nonlinear self-consistent Schrödinger equation has a solution for an arbitrary number of filled levels and the selection between the various configurations is determined by a minimum of the thermodynamic potential. Strictly speaking, Eq. (1) is invalid. A deviation from this equation results in overscreening of the potential and the field inside the semiconductor reverses its sign, whereas the number N of the localized transverse quantization subbands increases monotonically with the field going over to a dependence $N \propto F_0^{1/5}$ in strong fields. Rogachev *et al.*[5] were the first to draw attention to the possibility of overscreening. They used the Hartree approximation and the variational method to solve the problem of the screening of a field by an accumulation layer in a semiconductor where the Fermi level coincides with the bottom of the conduction band. However, Rogachev *et al.*[5] did not investigate the conditions for the appearance of overscreening and particularly the dependence of this effect on the Fermi level position. Moreover, description of an accumulation layer by a single filled subband used in Ref. 5 is valid, as shown below, only in the case of fields less than a certain critical value.

We shall solve exactly the problem of the screening of the field in the case of one subband using the Hartree approximation. Moreover, we shall investigate the thermodynamic potential and find the critical field F_1 in which the second subband appears, and find the field dependences of the parameters in the case of two subbands using the variational solution. We shall adopt the semiclassical description valid in the case of strong fields when the number of subbands is $N \gg 1$ and the potential becomes a monotonic function of the coordinate. We shall discuss the influence of the exchange energy in a system of this kind on the screening. We shall also suggest potential optical and capacitance measurements that can reveal the characteristics of the field screening in accumulation layers. We shall obtain numerical values of the parameters for the (100) surface of Si.

2. THERMODYNAMIC POTENTIAL AND THE EQUATION OF STATE OF THE SYSTEM

We shall consider the problem of the screening of an external field of intensity F_0 applied along the z axis at right-angles to the surface of a semiconductor. We shall assume

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that the semiconductor is of length L and that it is intrinsic; we shall also assume that the semiconductor is at a sufficiently low temperature, so that the Debye radius is greater than L. The Fermi level in the semiconductor is then determined by the Fermi level in a metal electrode formed on one of the semiconductor surfaces ($z = L$). The action of the field on the semiconductor surface creates transverse quantization subbands along the z axis and the number of these subbands is N. The wave function of the ith subband (where $i = 1$–N) is $\Psi_i(z)$ and it is subject to zero boundary conditions at the ends of the semiconductor $\Psi_i(z=0) = \Psi_i(z=L) = 0$; it also satisfies the normalization condition. In a plane parallel to the surface the wave functions are proportional to $\exp(i\mathbf{k}\cdot\mathbf{r})$, where $\mathbf{k}$ and $\mathbf{r}$ are the quasimomentum and the radius vector in this plane.

We shall write down the thermodynamic potential of the system:

$$\Omega = \sum_{i=1}^{N} (E_{k\parallel}^{(i)} + E_{k\perp}^{(i)}) + \frac{\varepsilon}{8\pi}\int_0^L F^2(z)\,dz - \mu\sum_{i=1}^{N} n_i. \qquad (2)$$

Here, $E_{k\parallel}^{(i)}$ and $E_{k\perp}^{(i)}$ are the kinetic energies of electrons in the ith subband in the plane of the semiconductor surface and along the z direction, respectively;

$$E_{k\perp}^{(i)} = \frac{\hbar^2 n_i}{2m_\perp}\int_0^L \left(\frac{d\Psi_i}{dz}\right)^2 dz, \quad E_{k\parallel} = \frac{n_i^2}{2N_0},$$

n_i is the surface density of electrons in the ith subband; $N_0 = g_v m_\parallel/\pi\hbar^2$ is the two-dimensional density of states; $m_{\perp,\parallel}$ is the effective mass of an electron along the z axis and in a plane perpendicular to the semiconductor surface; g_v is the valley degeneracy. The electric field in the semiconductor can be found by integrating the Poisson equation:

$$F(z) = F_0 - \frac{4\pi e}{\varepsilon}\sum_{i=1}^{N} n_i \int_0^z \Psi_i^2(z')\,dz'. \qquad (3)$$

We shall introduce the following notation:

$$\eta_i = \frac{4\pi e n_i}{\varepsilon F_0}, \quad \sum_{i=1}^{N}\eta_i = \eta, \quad \sigma = \frac{\varepsilon F_0 a_B^2}{4e},$$

$$a_B = \frac{\varepsilon\hbar^2}{e^2 m_\perp}, \quad E_B = \frac{e^2}{\varepsilon a_B},$$

and adopt the dimensionless variables

$$z \to z\left(\frac{a_B}{2\sigma^{1/3}}\right)^{-1}, \quad \Psi \to \Psi\left(\frac{2\sigma^{1/3}}{a_B}\right)^{-1/2},$$

$$E \to \frac{E}{2E_B\sigma^{2/3}}, \quad \mu \to \frac{\mu}{2E_B}, \quad \Omega \to \Omega\left(\frac{2E_B}{\pi a_B^2}\right)^{-1}\sigma^{-5/3}.$$

We note that η_i is the normalized density of electrons in the ith subband and that $\eta = 1$ corresponds to complete screening of the external field by the surface electrons.

Substituting the field intensity of Eq. (3) into the thermodynamic potential, we obtain

$$\Omega = \frac{M}{4}\sigma^{1/3}\sum_{i=1}^{N}\eta_i^2 + \sum_{i=1}^{N}\eta_i K_i + \frac{1}{2}(1-\eta)^2 L$$

$$+ (1-\eta)\sum_{i=1}^{N}\eta_i l_i + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\eta_i\eta_j l_{ij} - \frac{\mu\eta}{\sigma^{2/3}}, \qquad (4)$$

where the following notation is used:

$$M = \frac{m_\perp}{g_v m_\parallel}, \quad K_i = \int_0^L \left(\frac{d\Psi_i}{dz}\right)^2 dz,$$

$$l_i = \int_0^L dz \int_z^L \Psi_i^2(z')\,dz', \quad l_{ij} = \int_0^L dz \int_z^L \Psi_i^2(z')\,dz' \int_z^L \Psi_j^2(z')\,dz'.$$

We now have an expression for the thermodynamic potential which contains $2N$ variables η_i and Ψ_i. The equations of state of the system can be found by minimalization of Ω relative to these variables:

$$\partial\Omega/\partial\eta_i = 0, \quad \delta\Omega/\delta\Psi_i = 0. \qquad (5)$$

Using Eq. (4) for Ω, we obtain the following system of $2N$ equations:

$$\frac{M}{2}\sigma^{1/3}\eta_i + K_i - (1-\eta)(L-l_i) - \sum_{j=1}^{N}\eta_j(l_j - l_{ij}) - \frac{\mu}{\sigma^{2/3}} = 0, \qquad (6)$$

$$-\Psi_i''(z) - \varphi(z)\Psi_i = E_i\Psi_i. \qquad (7)$$

Here the potential is described by the expression

$$\varphi(z) = (1-\eta)(L-z) + \sum_{j=1}^{N}\eta_j\int_z^L dz'\int_{z'}^L \Psi_j^2(z'')\,dz'', \qquad (8)$$

where $\varphi(z = L) = 0$.

An important feature is that the nonlinear Schrödinger equations of the type described by Eq. (7), together with the potential (8) do not contain an external field parameter, i.e., the system of equations (7)–(8) has solutions for an arbitrary number of filled surface bands N with an arbitrary density of electrons in each subband η_i. The selection between the various occupancies and the numbers of subbands is made on the basis of the system of equations (6), which requires that the Fermi level in each surface subband should coincide with the Fermi level in the bulk of the semiconductor. This corresponds to a minimum of the thermodynamic potential of Eq. (4). The additional condition that governs the number of the filled subbands N is the obvious requirement $\eta_i > 0$.

Multiplying Eq. (7) by Ψ_i and integrating with respect to z, we can find the energies of the transverse quantization subbands:

$$E_i = K_i - \sum_{j=1}^{N}\eta_j(l_j - l_{ij}) - (1-\eta)(L-l_i). \qquad (9)$$

The last term in the above expression represents the shift of the localized subbands because of partial penetration of the external field into the bulk of the semiconductor beyond the accumulation layer. This shift is found from the system of equations (6), according to which the field in the bulk of the semiconductor is characterized by $(1-\eta) \propto 1/L$ if $L \gg l_i$ and tends to zero in the limit $L \to \infty$. However, the displacement of the potential remains finite and it appears as a single energy shift of the levels (Fig. 1).

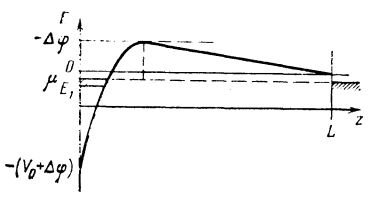

FIG. 1. Qualitative distribution of the potential along the length of a sample; here, Δ is the overscreening potential.

3. CASE OF ONE FILLED SUBBAND

We shall consider the situation when the screening is due to one transverse quantization subband so that $N = 1$. We shall show that this is true of fields less than a certain critical value σ_1 ($\sigma < \sigma_1$). The potential drop in the bulk of the semiconductor $\Delta\varphi$ deduced from Eq. (6) is described by the expression

$$\Delta\varphi = (1-\eta)L = M\sigma^{1/3}/2 + K_1 + l_{11} - l_1 - \mu/\sigma^{2/3}. \tag{10}$$

We shall rewrite the Schrödinger equation of Eq. (7) by introducing $E = E_1 + \Delta\varphi$ and assuming that $L \to \infty$:

$$-\Psi'' - \Psi \int_z^\infty dz_1 \int_{z_1}^\infty \Psi^2(z')\,dz' = E\Psi. \tag{11}$$

An analysis of this equation shows that its solution can be represented by an exponential series:

$$\Psi = a\sum_{n=1}^{\infty} a_n \exp[-(2n-1)\lambda z], \tag{12}$$

where $a_1 = 1$. Substituting Eq. (12) into Eq. (11), we find that $E = -\lambda^2$ and for a_n we obtain a recurrence relationship valid when $n > 1$:

$$a_n = -\frac{A}{(n-1)n}\sum_{m=1}^{n-1}\frac{a_{n-m}B_m}{m^2}. \tag{13}$$

Here, $A = a^2/16\lambda^4$ and $B_m = \Sigma_{n=1}^{m} a_n a_{m-n+1}$. It follows from this relationship that $a_n = a_n^* A^{n-1}$, where a_n^* is found from Eq. (13) by substituting $A = 1$. The convergence radius of this power series is given by the expansion

$$R = \lim_{n\to\infty}\frac{a_n^*}{a_{n+1}^*}.$$

Figure 2 shows the dependence of $R_n = Aa_n/a_{n+1}$ on n. It is clear from this figure that the convergence radius is of the order of 7.

The boundary condition for the wave function on the semiconductor surface ($z = 0$)

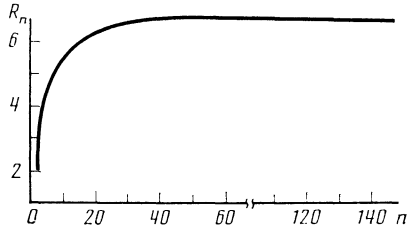

FIG. 2. Dependence of $R_n = Aa_n/a_{n+1}$ on n.

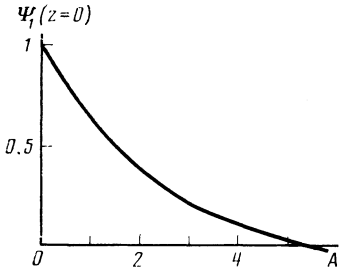

FIG. 3. Wave function of the ground state on the surface of a semiconductor $\Psi_1(z=0)$ plotted as a function of the parameter $A = a^2/16\lambda^4$.

$$\Psi_1(z=0) = \sum_{n=1}^{\infty} a_n^* A^{n-1} = 0 \tag{14}$$

allows us to find A. The condition of normalization of Ψ yields λ:

$$\lambda = (8AC)^{-1/3}, \quad C = \sum_{m=1}^{\infty}(B_m/m). \tag{15}$$

Figure 3 shows the results of a calculation of $\Psi_1(z=0)$ on A. It is clear from this figure that there is a root at $A_1 = 5.074$ which corresponds to the ground state with an energy $E = -\lambda_1^2 = -(0.5087)^2 = 0.2588$ and the value $a = 2.332$. The number of terms in the expansion of Eq. (12) is limited to 100, which ensures that the calculations of Ψ are accurate to within 10^{-5}.

This solution makes it possible to calculate the coordinate dependence of the potential $V(z) = \varphi(z) - \Delta\varphi$:

$$V(z) = \left(\frac{A_1}{C^2}\right)^{1/3}\sum_{m=1}^{\infty}\frac{B_m}{m^2}\exp(-2\lambda_1 mz), \tag{16}$$

and also the quantities occurring in the thermodynamic potential:

$$l_1 = V(z=0) = V_0, \tag{17}$$

$$l_{11} = \left(\frac{A_1}{C^5}\right)^{1/3}\sum_{n=2}^{\infty}\frac{1}{n}\sum_{m=1}^{n-1}\frac{B_m B_{n-m}}{m(n-m)}, \tag{18}$$

$$K_1 = 8\lambda_1^5 A_1\sum_{n=1}^{\infty}\frac{1}{n}\left[\sum_{m=1}^{n}(2m-1)(2n-2m+1)a_m a_{n-m+1}\right]. \tag{19}$$

This gives $l_1 = 2.2535$, $l_{11} = 1.5982$, and $K_1 = 0.39658$. We shall compare these values with the results of variational

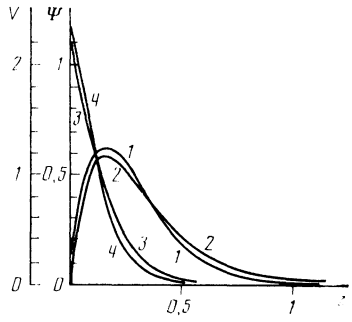

FIG. 4. Coordinate dependences of the wave function and of the potential obtained by exact (curves 1 and 3) and variational (curves 2 and 4) calculations.

calculations for a wave function of the form $\Psi = (b^3/2)^{1/2} z \exp(-bz/2)$: $b = (33/16)^{1/3} \approx 1.273$, $l_1 = 2.357$, $l_{11} = 1.620$, $K_1 = 0.405$. We can see that the precision of the variational calculation is within the range 1.4–4.6%. Figure 4 shows the dependences $V(z)$ and $\Psi(z)$ obtained as a result of the exact and variational calculations. The errors in V_0 and E obtained by the variational calculations are 4.6 and 28.2%, respectively.

Turning back to Eq. (10), we find that, depending on the position of the Fermi level in the semiconductor, we can expect both overscreening ($\eta > 1$) and underscreening of the field on the semiconductor surface ($\eta < 1$). The overscreening condition can be rewritten in the form

$$M\sigma^{1/3}/2 - \mu/\sigma^{2/3} < l_1 - l_{11} - K_1 = 0.259. \tag{20}$$

Having determined the maximum value of the left-hand side of the inequality with respect to σ we can substitute this value into the inequality and thus find the overscreening condition:

$$\mu > -16(l_1 - l_{11} - K_1)^2/27M^2 = -0.010/M^2. \tag{21}$$

In the most commonly discussed case when $\mu = 0$ (Refs. 3 and 5), we find that Eq. (20) yields a relationship for the critical field σ_1 in which the overscreening of the system with one filled subband disappears:

$$\sigma_1 = [2(l_1 - l_{11} - K_1)/M]^3 = 0.139/M^3. \tag{22}$$

Knowing the potential $V(z)$ governed by Eq. (16) we can find whether there are additional localized subbands in this potential. We used the Runge-Kutta method to calculate numerically the Schrödinger equation (7) with a potential described by Eq. (16) and we found that there were no additional localized subbands.

We shall now obtain the wave functions Ψ_k in a continuous spectrum characterized by energies $E = k^2 > 0$. It follows from the Schrödinger equation (11) with $V(z)$ described by Eq. (16) and from conditions of normalization of Ψ_k and the absence of charge transfer that

$$\Psi_k = \frac{1}{(2L)^{1/2}} \left\{ e^{i(kz+\alpha)} \sum_{n=1}^{\infty} D_n^{+} e^{-2(n-1)\lambda_1 z} + e^{-i(kz+\alpha)} \sum_{n=1}^{\infty} D_n^{-} e^{-2(n-1)\lambda_1 z} \right\}. \tag{23}$$

Here, $D_1^{\pm} = 1$, $\alpha_1 = 0$. The relationship $(D_n^{+})^* = D_n^{-}$ is obeyed also when $n \geqslant 2$:

$$D_n^{\pm} = -A_1\lambda_1 \exp(\pm i\alpha_n) \times \sum_{m=1}^{n-1} \frac{B_m D_{n-m}^{\pm}}{m^2} \{(n-1)[\lambda_1^2(n-1)^2 + k^2]^{1/2}\}^{-1}, \tag{24}$$

where $\alpha_n = \tan^{-1}[k/\lambda_1(n-1)]$. The condition $\Psi_k(z=0) = 0$, written in the form

$$\sum_{n=1} (e^{i\alpha} D_n^{+} + e^{-i\alpha} D_n^{-}) = 0, \tag{25}$$

allows us to find $\alpha(k^2)$. The results of the calculations are given in Fig. 5.

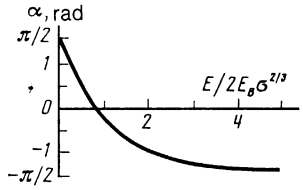

FIG. 5. Dependence of the phase of a wave function in the continuous spectrum on the normalized energy.

4. SCREENING BY TWO FILLED SUBBANDS

We shall assume that screening of the external field in an accumulation layer creates two transverse quantization subbands ($N = 2$). We shall also assume that $L \to \infty$ and, consequently, $\eta_1 + \eta_2 = 1$. From this last relationship and the two equations in the system (6), we find the occupancy of the second subband:

$$\eta_2 = \frac{M\sigma^{1/3}/2 + K_1 - K_2 + l_{11} - l_{12}}{M\sigma^{1/3} + l_{11} - 2l_{12} + l_{22}}. \tag{26}$$

We can easily see that if the denominator of the above fraction is positive, whereas the numerator may be negative if the field σ is sufficiently weak and, consequently, the second subband does not appear. Substituting Eq. (26) into Eqs. (4) and (6), we can rewrite the thermodynamic potential and the overscreening potential in the form

$$\Omega = \frac{M}{4}\sigma^{1/3} + K_1 + \frac{1}{2} l_{11} - \frac{1}{2} \frac{(M\sigma^{1/3}/2 + K_1 - K_2 + l_{11} - l_{12})^2}{M\sigma^{1/3} + l_{11} - 2l_{12} + l_{22}} - \frac{\mu}{\sigma^{2/3}}, \tag{27}$$

$$\Delta\varphi = \frac{M}{2}\sigma^{1/3} + K_1 + l_{11} - l_1 - \eta_2 \left(\frac{M}{2}\sigma^{1/3} - l_1 + l_{11} + l_2 - l_{12} \right) - \frac{\mu}{\sigma^{2/3}}. \tag{28}$$

It is clear from Eq. (27) that the appearance of the second band is favored, provided the condition $\eta_2 > 0$ is satisfied.

The Schrödinger equation (7) can also be solved as in the preceding section, using an exponential expansion

$$\Psi_{1,2} = \sum_n \sum_m A_{nm}^{(1,2)} \exp[-(n\lambda_1 + m\lambda_2)z].$$

However, this increases greatly the volume of the calculations, so that we shall obtain a variational solution. The orthonormalized wave functions will be described by

$$\Psi_1(z) = (b_1/2)^{1/2} z \exp(-b_1 z/2), \tag{29}$$

$$\Psi_2(z) = \left[\frac{3b_2^5}{2(b_1^2 - b_1 b_2 + b_2^2)} \right]^{1/2} \left[z - \frac{(b_1 + b_2)z^2}{6} \right] \exp\left(-\frac{b_2 z}{2} \right), \tag{30}$$

where b_1 and b_2 are the variational parameters. Using these functions, we can calculate the quantities occurring in the thermodynamic potential:

$$K_1 = \frac{b_1^2}{4}, \quad l_1 = \frac{3}{b_1}, \quad l_{11} = \frac{33}{16 b_1},$$

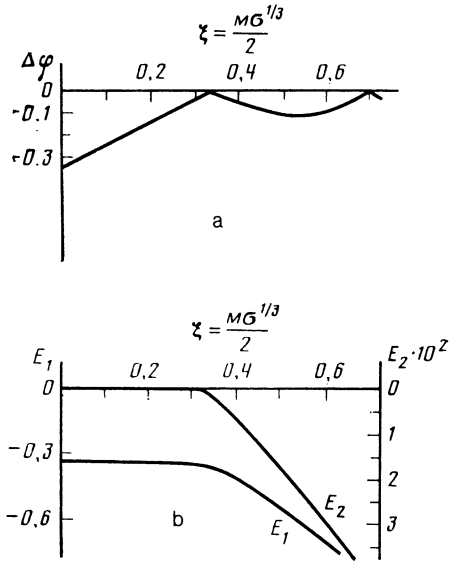

FIG. 6. Changes in the overscreening potential (a) and in the subband energy (b) with the field on the surface. Here, ξ_1 and ξ_2 are separated by $10\Delta\varphi$.

$$K_2=\frac{b_2^2(b_1^2-b_1b_2+7b_2^2)}{12(b_1^2-b_1b_2+b_2^2)},\quad l_2=\frac{5b_1^2-2b_1b_2+2b_2^2}{b_2(b_1^2-b_1b_2+b_2^2)},$$

$$l_{12}=\frac{3b_1^6+12b_1^5b_2+18b_1^4b_2^2+15b_1^3b_2^3+15b_1^2b_2^4+8b_1b_2^5+2b_2^6}{(b_1+b_2)^4(b_1^3+b_2^3)},$$

$$l_{22}=\frac{965b_1^4-1162b_1^3b_2+1464b_1^2b_2^2-814b_1b_2^3+347b_2^4}{256b_2(b_1^2-b_1b_2+b_2^2)^2}.$$

Substituting these values in Eq. (27), we shall minimize the thermodynamic potential with respect to b_1 and b_2. This gives the results presented in Fig. 6. At the moment of appearance of the second subband we can obtain the following analytic results if we utilize the fact that the population of this subband is low ($\eta_2 \ll 1$):

$$b_1^3=\frac{33}{16}+\frac{8064}{4825}\left(\frac{3}{5}\right)^{1/2}(\xi-\xi_1)^{3/2}, \tag{31}$$

$$b_2^2=\frac{12}{5}(\xi-\xi_1), \tag{32}$$

$$\eta_2=\frac{2048}{4825}\left(\frac{3}{5}\right)^{1/2}(\xi-\xi_1)^{3/2}, \tag{33}$$

where $\xi = M\sigma^{1/3}/2$ and $\xi = M\sigma_1^{1/3}/2$. We recall that σ_1 is the critical field in which the overscreening disappears ($\xi_1 = l_1 - l_{11} - K_1$) in the one-level solution when $\mu = 0$. Substituting Eqs. (31)–(33) into Eqs. (17), (28), and (9), we obtain the potential on the surface and the overscreening as well as the subband energies:

$$V_0=l_1(\xi_1)+\frac{1024}{965}(\xi-\xi_1), \tag{34}$$

$$\Delta\varphi=E_2=-\frac{59}{965}(\xi-\xi_1), \tag{35}$$

$$E_1=-\xi_1-\frac{1024}{965}(\xi-\xi_1). \tag{36}$$

Therefore, when the overscreening potential vanishes a second localized subband of Eq. (35) separates smoothly from the continuous spectrum as the field is increased. This is accompanied by the appearance of the overscreening potential of Eq. (35). Second vanishing of $\Delta\varphi$ on increase in the field corresponds to the appearance of the third subband, and so on.

It should be pointed out that an analytic solution of b_1, b_2, and η_2 given by Eqs. (31)–(33) agrees, to within a few percent, with the results of numerical minimization of the thermodynamic potential in the region of existence of two subbands.

5. SEMICLASSICAL SCREENING

We shall now consider screening in the case of a large number of subbands when $N \gg 1$. We can then use the semiclassical description in which the wave functions are given by[6]

$$\Psi_E=\frac{C_E}{p^{1/2}}\sin\left[\int_0^z p\,dz\right], \tag{37}$$

where

$$p=(\varphi+E)^{1/2},\quad C_E^2=2\left(\int_0^{z_E}\frac{dz}{p(z)}\right)^{-1},$$

the turning point z_E is defined by $\varphi(z_E) = -E$, and the momentum p is normalized to $2\sigma^{1/3}(m_\perp E_B)^{1/2}$. The subband energies are deduced using the Bohr-Sommerfeld condition

$$\int_0^{z_E} p\,dz=\pi\left(n+\frac{3}{4}\right), \tag{38}$$

which yields also the separation between the levels[6]:

$$\Delta E=\pi\left(\int_0^{z_E}\frac{dz}{p(z)}\right)^{-1}. \tag{39}$$

Using Eq. (39) and going over in the coordinate dependence of the charge

$$\rho(z)=-e\sum_E N_0 E\Psi_E^2(z)$$

from summation with respect to the energy to integration, we obtain the Poisson equation in the form

$$d^2\varphi/dz^2=2\varphi^{3/2}/3\pi\xi \tag{40}$$

subject to the boundary conditions

$$\left.\frac{d\varphi}{dz}\right|_{z=0}=-1,\quad \varphi(z\to\infty)=0.$$

Solving this equation in the case when $\mu = 0$, we obtain

$$\varphi=\varphi_0(1+z/4\varphi_0)^{-4}, \tag{41}$$

where the potential on the surface is $\varphi_0 = (60\pi\xi)^{2/5}/4 \approx 2.03\xi^{2/5}$. Therefore, in the semiclassical approximation the potential $\varphi(z)$ varies monotonically with the coordinate and there is no overscreening. The solution $\varphi(z)$ and Eq. (39) allow us to calculate the number of transverse quantization subbands:

$$N=\int_0^{\varphi_0}\frac{dE}{\Delta E}=\frac{1}{\pi}\int_0^{\varphi_0}dE\int_0^{z_E}\frac{dz}{p(z)}. \tag{42}$$

Integration with respect to the coordinate gives

$$N=\frac{4\varphi_0^{5/4}}{\pi}\int_0^{\varphi_0}\frac{dE}{E^{3/4}}\left\{\sqrt{2}E'\left(\zeta,\frac{\sqrt{2}}{2}\right)-\frac{\sqrt{2}}{2}F\left(\zeta,\frac{\sqrt{2}}{2}\right)\right\}, \quad (43)$$

where $\zeta=\arccos(E/4\varphi_0)$; $E(\zeta,\sqrt{2}/2)$ and $F(\zeta,\sqrt{2}/2)$ are incomplete elliptical integrals of the first and second kinds, respectively. Estimating the expression in the braces at the maximum of the integrand function $(\sqrt{2}E(\pi/2,\sqrt{2}/2)-(\sqrt{2}/2)F(\pi/2,\sqrt{2}/2)\approx 0.29)$, we find that the number of subbands is given by

$$N=4.29\xi^{3/5}=2.83M^{3/5}\sigma^{1/5}. \quad (44)$$

Therefore, the number of subbands increases monotonically on increase of the field. If we assume that $N=2$, we find that Eq. (44) yields a critical field in which the second localized subband appears in the semiclassical approximation: $\xi_1=0.28$. This value is practically identical with the exact value $\xi_1=0.259$, whereas the variational calculations indicate that $\xi_1=0.331$. The third band appears when $\xi_2=0.55$ according to the semiclassical calculations and when $\xi_2=0.70$ in the case of the variational calculation.

Comparing the solutions for $N=1$ and 2 and also for $N\gg 1$, we can say that in the Hartree approximation the number of subbands in an accumulation layer is a monotonic function of the field with the asymptote $N\propto F_0^{1/5}$.

6. OPTICAL AND CAPACITANCE MEASUREMENTS

We shall now discuss the characteristics of optical and capacitance measurements of the properties of accumulation layers. We shall consider the spectral dependence of the absorption coefficient $\alpha(\omega)$ in the case of relatively weak fields when $N=1$. The absorption by direct transitions occurs when the vector potential of an electromagnetic wave is parallel to the z axis. The dependence $\alpha(\omega)$ is proportional to the square of the dipole transition between a localized subband and the continuous spectrum[7]:

$$\alpha\propto d_{1k}=\left|\int_0^\infty \Psi_k\frac{d\Psi_1}{dz}dz\right|^2. \quad (45)$$

The right-hand side of this relationship can be rewritten with the aid of Eqs. (12) and (23):

$$d_{1k}=\frac{2\lambda_1^2a^2}{L}\left\{\sum_{n=2}^{\infty}\left[4\left(n-\frac{3}{2}\right)^2\lambda_1^2+k^2\right]^{-1/2}\times\sum_{m=1}^{n-1}(2m-1)a_m|D_{n-m}^{+}|\right\}^2. \quad (46)$$

The results of our calculations are presented in Fig. 7. It is important to note that $\alpha(\omega)$ has a sharp asymmetric maximum in the absorption due to transitions in the continuous spectrum, which can be interpreted as transitions to the second localized subband.[8] The distinguishing feature is the asymmetry. The characteristic energy of the fall on the side of high values of $\hbar\omega$ is $2E_B\sigma^{2/3}$, whereas in the direction of smaller values of $\hbar\omega$ it is governed by the lifetime in the continuous spectrum.

In this range of fields we can expect illumination to create a second localized subband so that there should be an additional maximum in the absorption spectrum and the position of this maximum should vary with the illumination intensity.

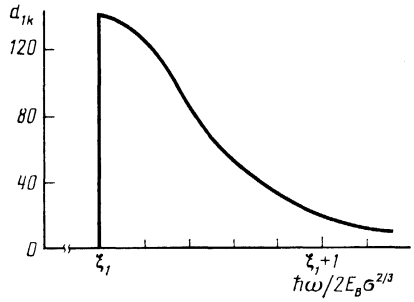

FIG. 7. Frequency dependence of the probability of direct optical transitions between a local subband and the continuous spectrum.

We shall show that oscillations of the potential $\Delta\varphi$ as a function of the field result in abrupt changes of the capacitance of a metal-insulator-semiconductor (MIS) structure at points corresponding to the onset of filling of new subbands on the surface of the semiconductor. The voltage applied to an MIS structure is V_g and it can be expressed readily in terms of the field on the semiconductor surface:

$$eV_g=2E_B\sigma^{2/3}\left[\frac{2\varepsilon\sigma^{1/3}d}{\varepsilon_i a_B}+V_0+\Delta\varphi\right], \quad (47)$$

where ε_i and d are the permittivity and the thickness of the insulator, respectively. Bearing in mind that the charge Q on an MIS structure is $e\sigma\eta/\pi a_B^2$, we find that the 1f capacitance C of such a structure is

$$C=\frac{dQ}{dV_g}=C_i\left(\eta+\sigma\frac{d\eta}{d\sigma}\right)\left\{1+\gamma\left[\frac{2}{3}(V_0+\Delta\varphi)+\sigma\frac{d(V_0+\Delta\varphi)}{d\sigma}\right]\right\}^{-1}, \quad (48)$$

where $\varepsilon_i/4\pi d=C_i$ and $\gamma=\varepsilon_i a_B/2\sigma^{1/3}\varepsilon d$. Substituting Eqs. (10), (17), (34), (35) into Eq. (48), we obtain the following expression for the capacitance in the case of one filled subband C_1 and the onset of filling in the case of the second subband C_2:

$$C_1=C_i\left[1+\frac{\mu}{3\sigma^{2/3}L}-\frac{1}{L}\left(\frac{4}{3}\xi-\xi_1\right)\right]\left[1+\gamma+\frac{2\gamma}{3\xi}(l_1-\xi_1)\right]^{-1}, \quad (49)$$

$$C_2=C_i\left[1+\frac{\mu}{3\sigma^{2/3}L}+\frac{59}{965L}\left(\frac{4}{3}\xi-\xi_1\right)\right]\times\left[1+\gamma+\frac{2\gamma}{3\xi}(l_1-\xi_1)\right]^{-1}. \quad (50)$$

Comparing these expressions, we can see that at the onset of filling of the second subband the capacitance changes abruptly by a value of the order of $C_i a_B/\sigma_1^{1/3}L$.

7. EXCHANGE INTERACTION

We shall now allow for the influence of the exchange interaction on the screening of a field in accumulation layers. We can do this by including in the thermodynamic potential (2) the exchange energy of the system Ω_{ex}:

$$\Omega_{ex}=\frac{-e^2}{\varepsilon S}\sum_{i,j=1}^{N}\iiint\frac{d\mathbf{r}\,d\mathbf{r}'\,dz\,dz'}{(|\mathbf{r}-\mathbf{r}'|^2+|z-z'|^2)^{1/2}}\Psi_{i\mathbf{k}}^{*}(\mathbf{r}',z')\times\Psi_{j\mathbf{k}'}^{*}(\mathbf{r},z)\Psi_{j\mathbf{k}'}(\mathbf{r}',z')\Psi_{i\mathbf{k}}(\mathbf{r},z). \quad (51)$$

Here, $\Psi_{ik}(\mathbf{r},z)=S^{-1/2}\exp(i\mathbf{kr})\Psi_i(z)$; S is the surface area of the semiconductor; the summation is carried out over all the filled states with parallel spins. Adopting the dimensionless variables introduced earlier, replacing summation with respect to $\mathbf{k}$ and $\mathbf{k}'$ by integration, and integrating with respect to $\mathbf{r}$ and $\mathbf{r}'$ and partly with respect to $\mathbf{k}$, we obtain

$$\Omega_{o6}=-\frac{g_v\sigma^{-1/2}}{\pi}\sum_{i=1}^{N}\sum_{j=1}^{i}c_{ij}\eta_j\iint_0^\infty\frac{dz\,dz'}{|z-z'|}\Psi_i(z)\Psi_j(z)\Psi_i(z')\times\Psi_j(z')\int_0^{(\eta_i/\eta_j)^{1/2}}x\,dx\int_0^{\pi}d\theta\{1-\exp[\sigma^{1/6}|z-z'|x_1(\eta_j/2g_v)^{1/2}]\}, \quad (52)$$

where $x_1=-x\cos\theta+(1-x^2\sin^2\theta)^{1/2}$; $(\eta_j/2g_v)^{1/2}=k_{Fj}$ is the quasi-Fermi momentum of the jth subband; k is normalized to $2\sqrt{\sigma}/a_B$ and $c_{ij}=2-\delta_{ij}$; δ_{ij} is the Kronecker delta. Bearing in mind that the kernel of the integral expression has a maximum in the range of small values of $|z-z'|$, and expanding the exponential function in Eq. (52), we obtain

$$\Omega_{ex}=-\frac{\sigma^{-1/6}}{\pi}\left(\frac{g_v}{2}\right)^{1/2}\sum_{i=1}^{N}\sum_{j=1}^{i}c_{ij}\eta_j^{3/2}\iint_0^\infty dz\,dz'\,\Psi_i(z)\Psi_i(z')\times\Psi_j(z)\Psi_j(z')\times\left\{\frac{2}{3}\left[\left(1+\frac{\eta_i}{\eta_j}\right)E\left(\left(\frac{\eta_i}{\eta_j}\right)^{1/2}\right)-\left(1-\frac{\eta_i}{\eta_j}\right)K\left(\left(\frac{\eta_i}{\eta_j}\right)^{1/2}\right)\right]-\frac{\pi\sigma^{1/6}|z-z'|}{4(2g_v\eta_j)^{1/2}}\right\}. \quad (53)$$

Here, $K(x)$ and $E(x)$ are complete elliptic integrals of the first and second kinds.

It follows from the normalization of Ω_{ex} that the exchange interaction is significant in weak fields ($\sigma\ll1$), so that we shall limit our analysis to a transition to one of the two filled subbands.

Using the variational wave functions of Eqs. (29) and (30), we can describe the exchange energy by

$$\Omega_{ex}=-\frac{2}{3}\frac{\beta}{\sigma^{1/6}}\eta_1^{3/2}+\frac{\beta_1\eta_1^2}{2b_1}-\beta_2\frac{\eta_1\eta_2}{b_1}\left(\frac{b_2}{b_1}\right)^5-\frac{2}{3}\frac{\beta}{\sigma^{1/6}}\eta_2^{3/2}+\frac{\beta_3\eta_2^2}{2b_2}, \quad (54)$$

where

$$\beta=(2g_v)^{1/2}/\pi,\quad \beta_1=15/32,\quad \beta_2=30,\quad \beta_3=315/64[1-1/9(b_2/b_1)^2].$$

Minimization of the thermodynamic potential Ω with respect to η_1 and η_2, inclusion of μ, and the assumption that $L\to\infty$, i.e., that $\eta_1+\eta_2=1$, yields

$$\frac{M}{2}\sigma^{1/3}+K_1-l_{12}+l_{11}+\frac{\beta_1}{b_1}-\frac{\beta}{\sigma^{1/6}}(1-\eta_2)^{1/2}=-\frac{\beta}{\sigma^{1/6}}\eta_2^{1/2}+K_2+\eta_2\left[M\sigma^{1/3}+l_{11}-2l_{12}+l_{22}+\frac{\beta_3}{b_2}+\frac{\beta_1}{b_1}+\frac{\beta_2}{b_1}\left(\frac{b_2}{b_1}\right)^5\right]. \quad (55)$$

Minimization of Ω with respect to b_1 and b_2 subject to the condition $\eta\ll1$ gives

$$b_1^3=\frac{81}{32}\left[1+\frac{37}{21}\eta_2\right], \quad (56)$$

$$b_2^3=\frac{6675}{256}\eta_2. \quad (57)$$

Using these relationships, the smallness of η_2, and the values of K_i and l_{ij} calculated earlier, we can now simplify Eq. (55) to

$$\frac{M}{2}\sigma^{1/3}+\frac{b_1^2}{4}-\frac{15}{32b_1}-\frac{(2g_v)^{1/2}}{\pi\sigma^{1/6}}=-\frac{(2g_v)^{1/2}}{\pi\sigma^{1/6}}\eta_2^{1/2}+\frac{25}{64}\left[\left(\frac{5}{3}\right)^{1/2}\frac{89}{2}\eta_2\right]^{1/2}. \quad (58)$$

The right-hand side of this equation $F(\eta_2)$ has a minimum at η_{2m} defined by

$$\eta_{2m}=3.83\cdot10^{-8}g_v^3/\sigma, \quad (59)$$

where $F(\eta_{2m})=-8.5\cdot10^{-5}g_v^2/\sigma^{2/3}$. Therefore, it follows from Eq. (58) that inclusion of the exchange interaction gives rise to an abrupt appearance of the second subband. The field σ_1 in which this happens is given by Eq. (58) and it is approximately an order of magnitude higher than the value of σ_1 obtained in the Hartree approximation [Eq. (22)]. Using Eq. (58) and assuming that $g_v=2$, we find that $M\sigma_1^{1/3}/2=0.71$. Further expansion of Eq. (55) in terms of η_2 shows that after an abrupt change second subband rises linearly on increase in the field.

8. CONCLUSIONS

We shall now consider the main results of our investigation. The Hartree approximation provides a universally valid description of the screening in an accumulation layer. At low field intensities there is only one localized transverse quantization subband on the surface of a semiconductor and only this band becomes filled. In a field higher than a certain critical value ($\sigma\geqslant\sigma_1$) the second localized subband splits off and begins to fill smoothly as the field increases.

The critical field σ_1 can be deduced from an abrupt change in the lf capacitance of an MIS structure. It is shown that the spectral dependence of the matrix elements for transitions from a localized subband to the continuous spectrum is an asymmetric curve with a maximum and the characteristic energy of the fall at high frequencies is proportional to $E_B\sigma^{2/3}$.

A determination is reported of the range of positions of the Fermi level (in the bulk of the semiconductor) corresponding to overscreening of the field, i.e., to a situation when the number of electrons that reach the semiconductor surface is greater than that needed to screen the external field and the field in the bulk of the semiconductor changes its sign. Overscreening is due to the fact that the screening of the field requires the charge flowing through the surface to be proportional to σ, whereas the characteristic energies due to band bending are proportional to $\sigma^{2/3}$. Therefore, at low values of σ a well contains more electrons than those needed for the screening.

An allowance for the exchange energy does not alter qualitatively the nature of the screening process, but gives

rise to the following special features. The range μ where the overscreening effect is observed becomes greater compared with that given by Eq. (21). This range is readily found if we assume that the left-hand side of Eq. (58) is less than $\mu/\sigma^{2/3}$. The second subband is filled abruptly and this corresponds to an abrupt change in the capacitance of an MIS structure in the course of filling. The field σ_1 corresponding to the filling of the second subband increases by an order of magnitude see [Eqs. (22) and (58)].

We shall consider the (100) surface of Si and find the numerical values of the field F_1 and of the surface density n_{s1} corresponding to the filling of the second subband. If we assume that $m_\perp = 0.916m_0$ and $m_\parallel = 0.19m_0$, $g_v = 2$, and $\varepsilon = 11.5$, we find that Eq. (22) yields $F_1 = 1.13\times 10^5$ V/cm and $n_{s1} = 7.16\times 10^{11}$ cm^{-2}.

We shall now make some comments about the influence of doping. To be specific, we shall consider a lightly doped compensated n-type semiconductor with donor and acceptor concentrations N_d and N_a, respectively. Overscreening occurs if the Fermi level, which in such a semiconductor coincides with the donor level, satisfies the inequality of Eq. (21). The presence of the potential $\Delta\varphi$ increases the number of the surface electrons in an accumulation layer by Δn_s, where $\Delta n_s \approx [\Delta\varphi(N_d - N_a)/2\pi e^2]^{1/2}$. The length of the sample is then defined as the total localization length of surface electrons $a_B/\sigma^{1/3}$ and of the positive charge at donors $L_1 = \Delta n_s/(N_d - N_a)$, whereas the singularities of the behavior of $\Delta\varphi(\sigma)$ become singularities of $\Delta n_s(\sigma)$. The self-consistent potential $\Delta\varphi$ found allowing for the impurity charge decreases or disappears completely, depending on the relationship between the density of surface electrons $\sigma^{4/3}\pi a_B^3$ and the concentration of charged impurities $N_d - N_a$. The case of reduction in $\Delta\varphi$ corresponds to the inequality

$$N_d - N_a < \sigma^{4/3}/\pi a_B^3, \tag{60}$$

whereas $\Delta\varphi$ vahishes when the opposite inequality is obeyed. In particular, in the range of transition from one to two filled subbands on the (100) surface of Si we have $\sigma_1^{4/3}/\pi a_B^3 \approx 10^{18}$ cm^{-3}, i.e., if $N_d - N_a \approx 10^{18}$ cm^{-3}, we can ignore the influence of doping in the region of the transition from one to two filled subbands.

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