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# *LOCALIZED ELECTRON STATES IN THIN LAYERS DUE TO GEOMETRIC DEFECTS OF THE SURFACE*

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It is shown that isolated geometric surface defects result in the appearance of localized electron states in quantizing layers. The conditions of existence of local levels are found and their energies are calculated.

WE consider here thin layers of a semiconductor or a semimetal, where the motion of the electrons is quantized in a direction perpendicular to the layer. This may pertain to quantum films, inversion layers on a semiconductor surface, or magnetic surface levels. In all these situations, the geometrical irregularity of the surface exerts a strong influence on the spectrum and on kinetics of the carriers.

Scattering of electrons by a rough surface was investigated in a large number of papers[1-4]. We are interested in the interaction of electrons with isolated geometrical surface defects from the point of view of the possible occurrence of bound states. Examples of such defects are planar or spherical nucleations, emergence of a screw dislocation to the surface, etc.

The idea of carrier capture by geometrical surface defects was advanced in[5,6] as applied to the conditions of the field effect in semiconductors. The occurrence of localized states of this type can be easily understood from qualitative considerations. If there is a sufficiently gently sloping projection on the surface of the film, then the bottom of the first subband of transverse quantization $E_1(\rho)$ drops in this location ($E_1(\rho) \propto a^{-2}(\rho)$, where $a(\rho)$ is the local thickness of the film and $\rho$ is a planar vector). Consequently a two-dimensional potential well, in which bound states can exist, is produced for the electron. Quasistationary levels located near the edges of higher subbands can also be produced.

Let us consider bound states in a quantum film. The shape of the surface is described by the equation $z = u(\rho)$, $\rho = (x, y)$, $u(\rho)$ vanishes as $\rho \to \infty$. In the effective-mass approximation, the wave function of the electron $\psi(\rho, z)$ vanishes at $z = u(\rho)$. The boundary condition on the opposite surface of the layer of thickness a is $\psi(\rho, z = a) = 0$. We represent the new function of the electron in the form

$$\psi = \sum_n v_n(\rho)\varphi_n(z;\rho),$$

where the function $\varphi_n(z;\rho)$ is normalized by the condition $\int|\varphi_n(z;\rho)|^2 dz = 1$ and satisfies the equation ($\hbar = m = 1$)

$$\frac{d^2}{dz^2}\varphi_n(z;\rho) + 2(E_n(\rho) - V(z))\varphi_n(z;\rho) = 0 \tag{1}$$

under the boundary conditions indicated above. In Eq. (1), $\rho$ is regarded as a parameter and $V(z)$ is the potential energy of the electron in a film with an ideally even surface.

For the quantity $V_n(\rho)$ we obtain a system of equation analogous to the Born-Fock equations in adiabatic perturbation theory (see, e.g.,[7]

$$\begin{gathered}[-{}^1\!/_2\Delta_\rho + E_n(\rho)]\,v_n(\rho) - \sum_m \nabla_\rho v_m \int \varphi_n^*(z;\rho)\cdot\nabla_\rho\varphi_m(z;\rho)\,dz \\ -{}^1\!/_2\sum_m v_m(\rho)\int\varphi_n^*(z;\rho)\cdot\Delta_\rho\varphi_m(z;\rho)\,dz = Ev_n(\rho).\end{gathered} \tag{2}$$

The quantities $E_n(\rho)$ in (1) and (2) play the role of "instantaneous" terms of transverse motion. If we use for the film the model of a square potential well, then $E_n(\rho) = \pi^2n^2/2a^2(\rho)$, $\varphi_n(z,\rho) = \sqrt{2/a(\rho)}\sin(\pi nz/a(\rho))$; $a(\rho) = a - u(\rho)$.

Separating the terms diagonal in m and n, we obtain

$$\Delta_\rho v_n(\rho) + [2E - \pi^2n^2/a^2(\rho) - ({}^1\!/_8 + \pi^2n^2/6)(\nabla_\rho a/a)^2]\,v_n(\rho) = \sum_{n\neq m}\hat{K}_{mn}v_m(\rho)\cdot \tag{3}$$

The structure of the operator $\hat{K}_{mn}$ is clear from (2); its order of magnitude is determined by the derivatives of $a(\rho)$ with respect to $\rho$. We are interested in the ground state of the system, i.e., the lowest possible value of E in Eqs. (2) and (3). We use a variational principle, choosing as the trial function $\psi = v_1(\rho)\varphi_1(z;\rho)$, where $v_1(\rho)$ is the solution of Eq. (3) with zero right-hand side for n = 1 (first subband). Calculating the mean value of the operator $\hat{K}$ with the indicated trial function, we obtain $\Sigma\delta_{n1}\langle\tilde{v}_1\hat{K}_{nm}\tilde{v}_1\rangle\delta_{m1} = 0$, so that $\hat{K}_{nm}$ does not have any diagonal elements by definition. Consequently, if it turns out that the equation

$$\Delta_\rho\tilde{v}_1(\rho) + \left[2E - \frac{\pi^2}{a^2(\rho)} - \left(\frac{1}{8} + \frac{\pi^2}{6}\right)\left[\left(\frac{\nabla_\rho a}{a}\right)^2\right]\right]\tilde{v}_1(\rho) = 0 \tag{4}$$

admits of the existence of an energy level $E_0$ located below $E_1 = \pi^2/2a^2$, then the true ground level of the electron certainly lies below the bottom of the first subband. In this case the asymptotic form of the wave function is proportional to $\exp[-\sqrt{2(E_1 - E_0)}]$, as $\rho \to \infty$, i.e., there exists a state localized on the surface defect.

The role of the effective potential energy in (4) is played by the quantity

$$U_{eff}(\rho) = \frac{\pi^2}{2a^2(\rho)} - \frac{\pi^2}{2a^2} + \left(\frac{1}{16} + \frac{\pi^2}{12}\right)\left(\frac{\nabla_\rho a}{a(\rho)}\right)^2, \tag{5}$$

$U_{eff}$ vanishes as $\rho \to \infty$. It is necessary to ascertain the conditions for the existence of a negative energy level in the potential (5). Let us consider several examples.

a) Rectangular step; $u(\rho) = -H$ inside a rectangle with sides $L_1$ and $L_2$; $u(\rho) = 0$ everywhere outside the rectangle. We see first that the level can occur only of $H > 0$, i.e., if there is a projection rather than a depression on the surface of the film. In the opposite case $U_{\text{eff}}$ is everywhere positive. The term with $\nabla a$ in (5) is proportional to the square of a $\delta$-function on the contour of the rectangle and vanishes inside the rectangle. Thus, we have the problem of a two-dimensional square well with inpenetrable walls, the bottom of which corresponds to the energy $\pi^2/2((a + H)^{-2} - a^{-2})$. The lowest level will be negative if $1/L_1^2 + 1/L_2^2 + 1/(a + H)^2 < 1/a^2$. We emphasize this criterion is too strong, since the true level lies below the one obtained by the variational principle. The criterion acquires a particularly lucid form for a quadratic step of small height, $L_1 = L_2 = L$, $H \ll a$. In this case we obtain $HL^2 > a^3$.

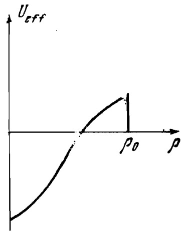
b) Circular cone (emergence of screw dislocation); $u(\boldsymbol{\rho}) = -H(1 - \rho/\rho_0)$ for $\rho \leq \rho_0$ and $u(\boldsymbol{\rho}) = 0$ for $\rho > \rho_0$. Then

$$U_{eff} = \left[\frac{\pi^2}{2} + \frac{1}{2}\left(\frac{1}{8} + \frac{\pi^2}{6}\right)\frac{H^2}{\rho_0^2}\right]\left[a + H\left(1 - \frac{\rho}{\rho_0}\right)\right]^{-2} - \frac{\pi^2}{2a^2}, \quad \rho < \rho_0;$$
$$U_{eff} = 0, \quad \rho \geqslant \rho_0. \tag{6}$$

The potential (6) describes a well surrounded by a barrier (see the figure). It is interesting that a negative-energy level can exist even in a shallow well ($|U_{\text{eff}}|\rho_0^2 \ll 1$). In this case we can use the method described in[8]: The logarithmic derivative of the wave function at the point $\rho_0$ is equal to $\int_0^{\rho_0} U_{\text{eff}}\rho d\rho$ and should be negative. The condition $|U_{\text{eff}}|\rho_0^2 \ll 1$ is equivalent to the requirements $H, \rho_0 \ll a$. As a result we obtain the sought criterion in the form $\rho_0^2 > (3/16 + \pi^2/4)aH$. The binding energy itself is proportional here to the factor $\exp[-6a^3/H(\rho_0^2 - \gamma aH)]$, where $\gamma = 3/16 + \pi^2/4$.

So far we did not use any approximations. The system (2) is fully equivalent to the exact Schrödinger equation. Therefore the conclusion that local levels exist (when the criteria indicated above are satisfied) is also exact. We now consider the adiabatic situation. If we neglect the terms with derivatives of $u(\rho)$ in the system (3), then we arrive at a two-dimensional Schrodinger equation with potential $\frac{1}{2}\pi^2 n^2(a^{-2}(\rho) - a^{-2})$. Obviously, if $u(\rho) = u(\rho)$ and is negative everywhere, negative groups of levels, i.e., levels that lie under the bottom of the corresponding subbands, always exist in such a potential. All the levels lying above the bottom of the first subband of the transverse quantization turn out to be quasistationary. Their lifetimes are determined by the probability of transition to a state of free motion under the influence of the off-diagonal terms in the Hamiltonian.

The considered local bulge of the film plays the role of an adiabatic trap for the electrons. It is assumed here that the electron mean free path in the film greatly exceeds the period of motion in the trap. Let us estimate the number $N_{\text{capt}}$ of the captured particles in the quasiclassical approximation, which can be realized, e.g., for a metal film. The sought quantity is determined by the phase-space volume bounded by the condition $p^2/2 + \pi^2 n^2/2a^2(\rho) < \min(E_F, \pi^2/2a^2)$ for each subband. Here $p$ is the longitudinal momentum and $E_F$ is the Fermi energy. The presented condition means that the particle can not go off to infinity. Summing over the subband with allowance for this inequality, we get



$$N_{\text{capt}} = \frac{2^{3/2}}{3\pi^2} E_F^{3/2} \int d^2\rho\, |u(\rho)|,$$

which coincides with the electron concentration multiplied by the volume of the projection.

Thus, the additional electrons that appear in the film as a result of the increase of its volume by an amount equal to the volume of the projection turn out to be captured. Their contribution to the conductivity is proportional to the collision frequency $1/\tau$, since it is precisely the collisions that cause the particle to be knocked out from the trap. At the same time, the uncaptured electrons give a conductivity inversely proportional to the collision frequency. The ratio of these contributions is of the order of $(T/\tau)^2 N_{\text{capt}}/N_{\text{uncapt}} \ll 1$, where $T$ is the period of the longitudinal motion in the trap.

In addition to the obvious case $n = 1$, stationary states can arise also when $n > 1$, if $n^2 \cdot \min a^{-2}(\boldsymbol{\rho}) < a^{-2}$. In the case of a small roughness $|u(\boldsymbol{\rho})| \ll a$, the stationary states belong to the first subband. The effective potential takes the form $\pi^2 u(\boldsymbol{\rho})a^{-3}$, and if $\frac{1}{2}\pi a^{-3}\int d^2\boldsymbol{\rho}\,|u(\boldsymbol{\rho})| \gg 1$, then several levels can exist. In the opposite limiting case there exists a single energy level, whose value $E_0$ can be obtained from[8]

$$E_0 - \pi^2/2a^2 \sim -L^{-2}\exp(-2a^3/\pi V_0), \tag{7}$$

where $L$ is the characteristic longitudinal dimension and $V_0 = \int d^2\boldsymbol{\rho}\,|u(\boldsymbol{\rho})|$ is the volume of the projection.

Formula (7) was obtained neglecting the interaction with the higher subbands. If $L \lesssim a$, then the Fourier spectrum of the perturbation contains the momenta $p \sim 1/L \gtrsim 1/a$, and consequently the influence of the other subbands becomes appreciable. Naturally, the adiabatic approximation is not applicable in this case.

We use for the effective Green's function of the electron $\nu(\mathbf{p}, \mathbf{p}')$ an equation derived in[2] and valid of $u(\rho)$ is smaller than the transverse wavelength of the particle (for $p \sim 1/L$ this means that $u/L \ll 1$):

$$R^{-1}(\mathbf{p})\,\mathrm{tg}(R(\mathbf{p})a)\,\nu(\mathbf{p},\mathbf{p}') + \int u(\mathbf{p}-\mathbf{q})\,\nu(\mathbf{q},\mathbf{p}')\frac{d^2q}{(2\pi)^2} = \delta(\mathbf{p}-\mathbf{p}'),$$

where $R(p) = \sqrt{2E - \mathbf{p}^2}$, and $u(\mathbf{p})$ is the Fourier transform of $u(\rho)$. The quantity $R(p)\cot(R(p)a)$ plays the role of the bare Green's function. The energy levels coincide with the poles of the vertex part that satisfies the equation

$$\Gamma_E(\mathbf{p},\mathbf{p}') = u(\mathbf{p}-\mathbf{p}') + (2\pi)^{-2}\int u(\mathbf{p}-\mathbf{p}_1)R(p_1)\,\mathrm{ctg}(R(p_1)a)\,\Gamma_E(\mathbf{p}_1,\mathbf{p}')\,d^2p_1. \tag{8}$$

It is obvious beforehand that the characteristic dimension of the bound state in the plane of the film is much larger than the diameter $L$ of the roughness. It is therefore necessary to know the value of $\Gamma_E(p, p')$ for momenta $p, p' \ll 1/L$. In this region, accurate to terms of small order in the parameters $L/a$ and $u/L$, Eq. (8) has a solution $\Gamma_E(0, 0) = Mu(0)$, where we have in the vicinity of the pole $\Gamma_E$

$$M = \left[1 + \frac{\pi V_0}{2a^3}\ln\left(\frac{\pi^2}{2a^2} - E\right)a^2\right]^{-1}.$$

From this we obtain the level energy $E_0 \sim \pi^2/2a^2 \sim -a^2\exp\{-2a^3/\pi V_0\}$. The difference between this result and (7) lies only in the pre-exponential factor.

Thus, in the case under consideration the binding energy depends only on the volume of the projection. Under real conditions, there is always a scatter in the dimensions of the local bulges, and this leads to a smearing of the edge of the ideal-film band. For sufficiently infrequent roughnesses, when the wave functions of the particles localized on the neighboring projections do not overlap, the density of states near the edge of the band is determined by the distribution $P(V_0)$ of the projections over the values. The density of states $\nu(\epsilon)$ is equal to $P(V_0(\epsilon))dV_0/d\epsilon$, where $\epsilon(V_0) = \pi^2/2a^2 - E_0$. Generally speaking, the statistics of the local projections depend strongly on the method of obtaining the film. In the simplest case one can assume that the probability of the fluctuations of the volumes $V_0$ is determined by the factor $\exp(-\Delta E/T)$, where $\Delta E$ is proportional to $V_0$ and T is the crystalization temperature. Thus, $P(V) = (\overline{V})^{-1}e^{-V/\overline{V}}$ and the density of state is equal to

$$\nu(\varepsilon) = \frac{2a^3}{\pi\overline{V}}\frac{1}{\varepsilon\ln^2(\varepsilon a^2)}\exp\left[\frac{2a^3}{\pi\overline{V}\ln(\varepsilon a^2)}\right], \quad \varepsilon a^2 < 1.$$

In the case when the wave functions of the bound electrons overlap and the longitudinal dimension of the projections is small, the problem reduces to finding the density of states of a particle in a field of randomly located short-range centers (the effective potential of the center is $\pi^2 u(\rho)/a^3$). The problem can be solved in full analogy with[9,10].

Finally, if the roughnesses themselves overlap, then it is natural to assume that the random function $u(\rho)$ has a Gaussian distribution. In this case one can use the results of Zittartz and Langer[11], in which the correlation function of the potential should be replaced by the quantity $\pi^4 W(\rho)/a^6$, where $W(\rho) = \langle u(\rho)u(0)\rangle$ is the correlator of the surface roughnesses.

The considered electron levels on the local bulges of the film may turn out to be not exponentially shallow in terms of the parameter $a^3/V_0$. This takes place in the case of strong anisotropy of the effective masses, $m_x \ll m_y$ (e.g., a cylindrical section of an equal-energy surface). If the cylinder axis is parallel to the film, then the motion of the electron becomes effectively one-dimensional. The binding energy is equal to $(1/2m_x)[\int \pi^2 u a^{-3} dx]^2$, where the integral is taken over an arbitrary projection cross section perpendicular to the large-mass axis. In this case each projection gives a continuous spectrum of states.

The energy level density can be calculated in the following manner. Since one of the effective masses $m_y$ is large, the motion of the electron along the y axis is quasiclassical, and we can use the formula for the state density of a one-dimensional quasiclassical particle

$$\nu(\varepsilon) = \frac{\sqrt{m_y}}{2\sqrt{2}\pi}\int\frac{dy}{(\varepsilon(y) - \varepsilon)^{1/2}}, \quad \varepsilon(y) = \frac{\pi^4 S^2(y)}{2a^6 m_x}, \tag{9}$$

where $S(y) = \int u(x; y)dx$ is the area of the cross section of the projection at the point y, and the integral in $\nu(\epsilon)$ is taken over the region in which $\epsilon < \epsilon(y)$. We note that $\nu(\epsilon)$ vanishes jumpwise when $\epsilon > \epsilon_{max} = \max\epsilon(y)\nu(\epsilon)$ if $u(\rho)$ is a smooth function. Indeed, $S^2(y)$ near the extremum can be represented in the form $S^2(y) \approx S^2_{max} - ay^2$, where $\alpha > 0$. We then see from (9) that $\nu(\epsilon) = \text{const}$ at $\epsilon < \epsilon_{max}$ and $\nu(\epsilon) = 0$ at $\epsilon > \epsilon_{max}$. It is easy to verify that in the case of a rectangular step the singularity of $\nu(\epsilon)$ near $\epsilon_{max}$ takes the form $(\epsilon_{max} - \epsilon)^{-1/2}$, and in the case of a conical projection we have

$$\nu(\varepsilon \to \varepsilon_{max}) \sim \left[\ln\left(\frac{1}{\varepsilon_{max} - \varepsilon}\right)\right]^{-1/2}.$$

Near the edge of the ideal-film band (i.e., as $\epsilon \to 0$), the density of states behaves in the same manner as the period of motion of a classical particle with zero total energy in a potential well $V(y) = -\pi^2 S^2(y)/2a^6 m_x$. If the projection $u(\rho)$ is extended formally to infinity, then $\nu(\epsilon)$, can also tend to infinity as $\epsilon \to 0$. It is reasonable to assume, however, that the longitudinal dimensions of the projection are finite, and then $S(y) \equiv 0$ at $|y| > y_{max}$, and consequently $\nu(\epsilon \to 0)$ remains finite.

We have thus shown in thin layers of solids the electrons can form localized states of a special type. For such states to occur, there is no need for the presence of any centers producing an attractive potential. Instead it suffices to have local bulges, which always exist in real films. Such bulges lead to capture of mobile carriers, which is important for the interpretation of experiments on the measurement of the voltage-capacitance characteristics, the conductivity, the Hall effect, etc. If we assume that the characteristic diameter of the projection is of the order of $10^{-6}$ cm, then the numbers $10^{10}$–$10^{11}$ cm$^{-2}$, which are perfectly reasonable for estimates of the number of projections per unit roughness, and consequently the density of the captured charge is of the same order. This value ($10^{10}$–$10^{11}$ cm$^{-2}$) is close to that observed in experiments on the capture of carriers by a crystal surface[12]. Consequently the capture mechanism indicated in the present paper is capable of competing with such traditional mechanisms as, e.g., the adsorption of impurity atoms. If the effective thickness of the layer is also of the order of $10^{-6}$ cm, then the parameter is $V_0/a^3 \sim 1$, i.e., the binding energy is comparable with the distance between the transverse energy levels of the electron. At temperatures in which the size quantization is significant ($T \lesssim 300$°K for $m^* \sim 0.1$ m), a noticeable fraction of the electrons will then turn out to be captured by geometrical surface defects and will make no contribution to the transport processes.

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[1] F. G. Bass, V. D. Freĭlikher, and I. M. Fuks, ZhETF Pis. Red. 7, 485 (1968) [JETP Lett. 7, 373 (1968)].

[2] A. V. Chaplik and M. V. Éntin, Zh. Eksp. Teor. Fiz. 55, 990 (1968) [Sov. Phys.-JETP 28, 514 (1969)].

[3] E. M. Baskin and M. V. Éntin, Zh. Eksp. Teor. Fiz. **57**, 460 (1969) [Sov. Phys.-JETP 30, 252 (1970)].

[4] L. A Fal'kovskiĭ, Zh. Eksp. Teor. Fiz. **58**, 1830 (1970) [Sov. Phys.-JETP **31**, 981 (1970)].

[5] A. V. Sachenko and V. A. Tyagaĭ, Ukr. Fiz. Zh. 11, 258 (1966).

[6] O. S. Frolov and O. V. Snitko, Fiz. Tekh. Poluprov. **2**, 1144 (1968) [Sov. Phys.-Semicond. **2**, 956 (1969)].

[7] L. Schiff, Quantum Mechanics (Russian translation), IIL, 1969, p. 247 [McGraw Hill].

[8] L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, 1963, p. 193 [Addison-Wesley, 1965].

[9] I. M. Lifshitz, Usp. Fiz. Nauk **83**, 617 (1964) [Sov. Phys.-Usp. **7**, 549 (1965)].

[10] B. V. Petukhov, V. L. Pokrovskiĭ, and A. V. Chaplik, Zh. Eksp. Teor. Fiz. **53**, 1150 (1967) [Sov. Phys.-JETP **26**, 678 (1968)].

[11] G. Zittartz and G. S. Langer, Phys. Rev., **148**, 741 (1966).

[12] A. V. Rzhanov, Élektronnye protsessy na poverkhnosti poluprovodnikov (Electronic Processes on Semiconductor Surfaces), Nauka, 1971.

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