In the case of MnO, etc., even the number of exchange invariants of sixth-order alone is extremely large.

*) See Phys. Rev. **B13**, 5065, 5078, 5086 (1976) (Transl. note).

1) The total free energy differs from (2) by a quantity $F_0(\tau)$, which gives the specific heat.

2) This situation must not be confused with that obtaining in the RG introduced by Wilson (cf., e.g.,[8]). There, the RG equations are written for other charges g. In our approximation, $g\sim\xi\Gamma$, and, in agreement with Wilson, g tends to constant values, proportional to ε, at the transition point.

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Size quantization and the surface states in semiconductors

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The boundary conditions that must be satisfied by the envelopes of the electron wave function on the three-dimensional-semiconductor surface, near which the potential sharply varies over atomic distances, are derived. These conditions are used to determine energy spectrum of a semiconducting film under some simplest cases. The dispersion equation thus obtained describes both size quantization levels and Tamm levels. A condition for existence of Tamm states is formulated and the behavior of the states with variation of film thickness is studied. A new length R is introduced which characterizes the surface properties and which may be large in narrow-band semiconductors. It is shown that the quasiclassical quantization law for the transverse quasimomentum component is not applicable to lower levels in thin films ($d\lesssim 2R$). The approach employed in the present investigation can be used to find the conditions of applicability of the zero boundary conditions for the envelopes, as well as to go beyond the scope of the effective-mass approximation and take the nonquadratic behavior of the real dispersion law into account.

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1. INTRODUCTION

It is known[1-4] that the limitation of the transverse motion of an electron in a film leads to quantization of the transverse component k_z of the quasimomentum and to a substantial change of the energy spectrum of the electrons as compared with the spectrum in bulky crystals. The rules for the quantization of k_z were first obtained within the framework of a quasi-classical approximation[1] and take in the isotropic case the form

$$k_z=\pi n/d, \tag{1}$$

where d is the film thickness and n is an integer.

To determine the lower levels of the size-effect quantization (SQ), an important factor in semimetallic and semiconducting films, it is necessary to solve the complete Schrödinger equation. It is convenient for this purpose to represent the wave function of the electron inside the film in the form[5]

$$\Psi(\mathbf{r})=\sum_{j'}\Phi_{j'}(\mathbf{r})u_{j'0}(\mathbf{r}). \qquad (2)$$

Here $u_{j0}(\mathbf{r})$ is the Bloch function corresponding to the extremum of the j-th band; $\Phi_j(\mathbf{r})$ are envelopes that vary slowly over the period of the lattice; the summation is over all the bands. The Schrödinger equation then reduces to a multiband system of linear differential equations

$$\sum_{j'}\left\{\left(\varepsilon_{j'0}+\frac{\hat{\mathbf{p}}^2}{2m_0}-E\right)\delta_{jj'}+\frac{\mathbf{p}_{jj'}}{m_0}\hat{\mathbf{p}}\right\}\Phi_{j'}(\mathbf{r})=0, \qquad (3)$$

in which ε_{j0} is the energy of the extremum of the j-th band, E is the electron energy, m_0 is the mass of the free electron, $\mathbf{p}_{jj'}$ is the interband matrix element of the momenta operator $\mathbf{p}$ constructed on the functions $u_{j0}(\mathbf{r})$, while the subscripts j and j' run over all the bands.

Equations (3) are valid everywhere inside the film with the exception of the surface regions, where the potential changes abruptly over atomic distances. To solve these equations, a modification of the effective-mass method, which is valid near the extremum of the j-th band, was developed in[2-4], while the film potential was usually simulated by an infinitely deep potential well. This amounted in effect to the use of zero boundary conditions for the j-th envelope on the film surfaces $z=z_0$ and $z=z_0+d$:

$$\Phi_j(z_0)=\Phi_j(z_0+d)=0. \qquad (4)$$

The resultant rules for the quantization of k_z coincides with the quasi-classical rules (1).

The boundary conditions (4) do not carry all the information on the surface, even in the effective-mass approximation, since their use does not make it possible to obtain the surface (Tamm) states. No account is taken in them of the abrupt variation of the potential in the region near the surface. In addition, they cannot be generalized to include nonparabolic bands, which are needed for a comparison with the existing experimental data. This raises the problem of deriving the boundary conditions that the envelopes must satisfy on the surface of a semiconductor. The derivation of these conditions is the main purpose of the present paper. It is natural to use for this purpose the method developed in the theory of Tamm states for a semi-infinite three-dimensional crystal.

2. BOUNDARY CONDITIONS FOR SEMI-INFINITE CRYSTAL

We consider a semi-infinite crystal occupying the region of space $z\geqslant z_0$. If we denote the potential energy of the electron in an ideal crystal by $V(\mathbf{r})$ and the vacuum level by $V_0=\text{const}$, then the potential energy $W(\mathbf{r})$ of an electron takes in this system the asymptotic form

$$W(\rho,z)=\begin{cases}V_0, & z\to-\infty\\ V(\mathbf{r}), & z\to+\infty\end{cases}, \qquad (5)$$

where $\mathbf{r}=(\rho,z)$ and $\rho=(x,y)$.

We assume that $W(\rho,z)$ retains a two-dimensional periodicity in any plane with constant z. Then the two-dimensional quasimomentum $\varkappa=(\varkappa_x,\varkappa_y)$, determined accurate to a two-dimensional reciprocal-lattice vector $\mathbf{G}$, is a good quantum number. The total wave function of an electron inside the crystal and far enough from the boundary should be a superposition of all the particular solutions of the Schrödinger equation, which we shall number by the index λ, with fixed values of E and $\varkappa$[6]:

$$\Psi_{\text{cr}}(\varkappa,E,\mathbf{r})=\sum_\lambda C_\lambda\Psi_\lambda(\varkappa,E,\mathbf{r}), \qquad (6)$$

where C_λ are arbitrary coefficients that must be determined from the boundary conditions. Since there is no detailed information on the properties of the surface region in (5), we propose for the problem a formulation in which the concrete form of $W(\mathbf{r})$ is of no importance.

Namely, assume that the perturbing action of the surface on the total wave function of the crystal $\Psi_{\text{cr}}(\mathbf{r})$ can be described by some real integro-differential boundary operator $\hat{\Gamma}$:

$$\hat{\Gamma}\Psi_{\text{cr}}[\varkappa,E,\rho]=0. \qquad (7)$$

The variables in the square brackets of (7) pertain to the results of the action of $\hat{\Gamma}$ on $\Psi_{\text{cr}}(\varkappa,E,\rho,z)$. The explicit form of $\hat{\Gamma}$ can in principle be obtained if one knows the behavior of $W(\mathbf{r})$ near the boundary. By way of example we derive in the Appendix an expression for $\hat{\Gamma}$ in the rectangular-jump model (A.1) on the boundary, which is usually employed in the theory of Tamm states.[7] We note that the expression for $\hat{\Gamma}$ depends on the choice of the positive direction on the z axis, but this should not affect the physically observable quantities. The approximation (A.1) has significant shortcomings[7] and will be used henceforth only for purposes of illustration.

We assume that the transition of $W(\mathbf{r})$ to its volume value $V(\mathbf{r})$ occurs over distances on the order of several lattice constants from the surface. The possible existence in the crystal of a potential that varies weakly over such distances (e.g., band bending at the surface of a semiconductor) can be subsequently taken into account by the usual modification of Eqs. (3).[5]

It can therefore be assumed that the kernel of the integral operator $\hat{\Gamma}$ [$\delta(z-z_0)$ in the model (A.1)] is concentrated at atomic distances near the surface $z=z_0$. We shall also assume that in the energy interval ΔE of interest to us the value of $\hat{\Gamma}$ depends little on E. In the model of (A.1) this is satisfied when

$$\Delta E/(V_0-E)\ll 1. \qquad (8)$$

It is well known that each of the infinite set of functions entering in (6) has formally a Bloch form, except that the quasimomentum component perpendicular to the surface can assume complex values q_λ[8-10]:

$$\Psi_\lambda(\varkappa,E,\mathbf{r})=\exp\{i\varkappa\rho+i(q_\lambda'+iq_\lambda'')z\}u_\lambda(\varkappa,E,\mathbf{r}). \qquad (9)$$

It is assumed that $\operatorname{Re}q_\lambda=q_\lambda'$ lies in the first Brillouin zone, $\operatorname{Im} q_\lambda = q_\lambda'' \geqslant 0$, and the factor u_λ is the solution of the equation

$$\left\{\frac{(\hat{\mathbf{p}}_\parallel+\hbar\varkappa)^2}{2m_0}+\frac{(\hat{p}_z+\hbar q_\lambda'+i\hbar q_\lambda'')^2}{2m_0}+V(\mathbf{r})\right\}u_\lambda=Eu_\lambda \tag{10}$$

with conditions that are periodic on the unit cell. Therefore $q_\lambda(\varkappa, E)$ is the root of the equation

$$\varepsilon(\varkappa, q_\lambda)=E, \tag{11}$$

the left-hand side of which contains the dispersion law of the crystal, continued analytically into the complex q plane.

The values that it takes on in bands that are allowed for an infinite crystal (i.e., at $q''=0$) are different branches of a single analytic function $(\varkappa, q)$.[11] Analytic continuation makes (10) non-Hermitian, and the dispersion law is no longer real, so that (11) should be equivalent to the following system of equations[12]:

$$\operatorname{Re}\varepsilon(\varkappa, q_\lambda'+iq_\lambda'')=E, \quad \operatorname{Im}\varepsilon(\varkappa, q_\lambda'+iq_\lambda'')=0.$$

The properties of the lines in the plane (q', q''), along which the function $\varepsilon(\varkappa, q)\equiv\varepsilon(\varkappa, q'+iq'')$ is real (they are called "real lines") have been investigated in detail,[13,8,9] so that we are able to analyze qualitatively the roots of Eq. (11).

Figure 1 shows qualitatively the behavior of $\varepsilon(q')$ and $\varepsilon(q'')$ along real lines—respectively the right and left halves of Fig. 1, and also the graphic of Eq. (11) for the case when E lies in a band that is forbidden for an infinite crystal; the value of $\varkappa$ is fixed. The number of roots q_λ is $2N^2$,[12] where N^2 is the number of two-dimensional unit cells spanned by the XY plane. This distinguishes a three-dimensional crystal in principle from a one-dimensional one, in which case there are only two roots.[13] In a semi-infinite crystal half of these roots, for which $q_\lambda''<0$, should be discarded, since the functions (9) corresponding to them diverge as $z\to\infty$.

We turn to the boundary condition (7) for the complete wave function. With allowance for (6), this condition takes the form

$$\sum_\lambda C_\lambda\hat{\Gamma}\Psi_\lambda=0 \tag{12}$$

at each point of the boundary plane. In view of the two-dimensional translational invariance of $\hat{\Gamma}$, each of the terms in (12) can be expanded in a Fourier series in the two-dimensional vectors $\mathbf{G}$ of the reciprocal lattice:

$$\hat{\Gamma}\Psi_\lambda=\sum_{\mathbf{G}}f_{\lambda\mathbf{G}}(\varkappa, E)\exp\{i(\varkappa+\mathbf{G})\rho\}. \tag{13}$$

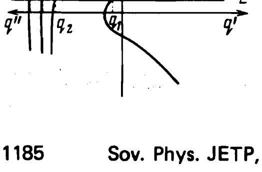

FIG. 1.

Substituting (13) in (12) and equating the coefficients of equal harmonics, we obtain a homogeneous system of linear equations

$$\sum_\lambda C_\lambda f_{\lambda\mathbf{G}}(\varkappa, E)=0. \tag{14}$$

When E lies in the forbidden band, it follows from the properties listed above for Eq. (11)[9,10,12] that the number of the unknowns in the system (14) is equal to the number of equations, so that the equation can be solved under the condition

$$\det\left(f_{\lambda\mathbf{G}}(\varkappa, E)\right)=0. \tag{15}$$

To find the Tamm states, Eq. (15) is solved with respect to E in various approximations, and as a rule in the model of (A.1).[6,10] In the proposed formulation of the problem, it is meaningful to transform (15) to the simplest possible form. To this end we assume that in the energy interval of interest to us only one root q_1, of (11) is essentially dependent on E (see Fig. 1). This root lies on a real line of the "loop" type,[9] which connects the extrema of the conduction band and the valence band, and exists also in the one-dimensional case.[13] We assume that all the remaining roots q_λ, $\lambda\geqslant 2$, which appear only in the three-dimensional case,[9] are large in comparison with q_1:

$$|q_1/q_\lambda|\ll 1, \quad \lambda\geqslant 2, \tag{16}$$

and the corresponding terms in (6) fall off at atomic distances from the boundary. These roots, in contrast to q_1, depend little on E in the energy interval ΔE of interest to us. Therefore the principal term in (6) (the one corresponding to q_1) can be written in the language of the envelopes (2), where in this case we put

$$\Phi_j(\mathbf{r})\equiv A_j\cdot\exp(i\varkappa\rho+iq_1z)\equiv\Phi_j(z)\exp(i\varkappa\rho), \tag{17}$$

with A_j a constant.

In the approximations (8) and (16), the envelopes introduced with the aid of (2) and (17) change little over the lattice constant, so that by virtue of the short-range character of $\hat{\Gamma}$ we can assume that

$$\hat{\Gamma}\Phi_j(\mathbf{r})u_{j0}(\mathbf{r})\approx\Phi_j(z_0)\hat{\Gamma}u_{j0}\exp(i\varkappa\rho)=\Phi_j(z_0)\sum_{\mathbf{G}}f_{j\mathbf{G}}^{(0)}\exp\{i(\varkappa+\mathbf{G})\rho\}, \tag{18}$$

where, in analogy with (13), we expand it in a Fourier series.

Taking (12) and (18) into account, Eq. (15) becomes

$$\sum_{j'}\Phi_{j'}(z_0)\Delta_{j'}(+)=0, \tag{19}$$

where $\Delta_j(+)$ is a determinant of infinite order, which differs from the determinant (15) in that the first line $f_{1\mathbf{G}}$ is replaced by the line $f_{j\mathbf{G}}^{(0)}$, and the summation is carried out over all the bands. The plus sign corresponds to the chosen positive direction on the z axis (15). The opposite choice of the direction means replacement of $\hat{\Gamma}(+)$ by $\hat{\Gamma}(-)$ in condition (7) (see, e.g., (A.6)), which corresponds in (19) to replacement of $\Delta_j(+)$ by $\Delta_j(-)$ for all j. We confine ourselves first to the case $\varkappa=0$, and assume the z axis to be a twofold axis. We also assume that the extremal Bloch factors in the expansion (2) correspond to the center of the Brillouin zone. All the roots q_λ of Eq. (11) are then pure imaginary,[9] and the corresponding wave functions (9) can be chosen to be real. It can therefore be assumed that all Δ_j are real constants that do not depend on the energy by virtue of the smallness of the parameters (8) and (16).

In the derivation of (19) we considered the simplest case, when only one root of (11) depends essentially on E. It is possible to consider analogously a more general case, when several roots q_λ depend essentially on E, and also $\varkappa \neq 0$. Each of the selected roots corresponds in this case to a separate set of envelopes, which the boundary conditions entangles with one another. We now illustrate the solution of the system (3) with boundary conditions (19) for particular cases.

3. TAMM PROBLEM IN THE EFFECTIVE-MASS APPROXIMATION

In the effective-mass approximation, which is valid near the extremum of the band, the system (3) reduces with the aid of the standard **kp** perturbation theory for the j-th band to an equation with effective mass m^* (we recall that $\varkappa=0$):

$$(p_z^2/2m^*)\Phi_j(z)=E\Phi_j(z). \qquad (20)$$

The boundary condition (19) then becomes

$$\left(1\mp R_j(+)\frac{\partial}{\partial z}\right)\Phi_j(z_0)=0, \qquad (21)$$

$$R_j(+)=\sum_{j'}{}' \frac{\hbar}{m_0}\frac{ip_{jj'}}{\varepsilon_{j0}-\varepsilon_{j'0}}\frac{\Delta_{j'}(+)}{\Delta_j(+)}. \qquad (22)$$

The quantity $R_j(+)$ is a real constant with the dimension of length. Equation (20) has as its solution (17), in which $\varkappa=0$ and

$$\Phi_j(z)=A\exp(ik_z z),$$

where we have introduced the symbol $k_z\equiv q_1$, and A is a normalization constant.

Substituting this solution in (21) we obtain

$$k_z=ik_z'', \quad k_z''=1/R_j(+)>0. \qquad (23)$$

The energy of a shallow Tamm state with $\varkappa=0$, reckoned from the extremum of the j-th band, is therefore

$$E_T=-\hbar^2/2m^*[R_j(+)]^2. \qquad (24)$$

The criterion for its existence, as seen from (23), is

$$R_j(+)>0, \qquad (25)$$

if the crystal occupies, in accordance with condition (5), the right-hand half-space.

Let now the crystal occupy the left-hand half-space and then

$$k''_{z,L}=1/R_j(-)<0. \qquad (26)$$

However, the Tamm-state energy (24) should not depend on the choice of the positive direction on the z axis, if the problem is symmetrical with respect to the substitution $z\to -z$. To this end, say in the model of (A.1), the boundary plane $z=z_0$ must be a symmetry plane of the crystal potential. From this and from Eqs. (23) and (26) it follows that in this symmetrical case

$$R_j(+)=-R_j(-). \qquad (27)$$

The characteristic length $R_j(+)$, as seen from (23), has the meaning of the span of the wave function of the shallow Tamm state.

4. ENERGY SPECTRUM OF FILM

The boundary condition (19) was derived under the condition that the energy is in the forbidden band. It is easy to show, however, that in the case when the energy is in the allowed band, the boundary condition for the envelopes retains the form (19). To this end it is necessary to take into account the fact that on going from the forbidden bands to the allowed band the root q_λ with $\lambda\geq 2$, by virtue of (16), remain practically unchanged (see Fig. 1), whereas the principal root q_1 changes from pure imaginary into a pair of real roots, which we designate k_z and $-k_z$ (we assume for simplicity, as before, an isotropic nondegenerate band). The pair of terms in the sum (6), corresponding to these roots, is represented in the form (2), where in this case one of the envelopes is equal to

$$\Phi_j(z)=A\exp(ik_z z)+B\exp(-ik_z z), \qquad (28)$$

and the remaining ones are expressed in its terms from the system (3). Then the constants A and B should be determined from the boundary condition (19) on the boundary $z=z_0$.

We consider now a film with boundaries $z=z_0$ and $z=z_0+d$. If the film thickness d essentially exceeds the lattice constant, or more accurately if

$$dq_\lambda\gg 1, \quad \lambda\geq 2,$$

then the terms in (6) corresponding to $\lambda\geq 2$ do not feel the second boundary of the film. The second boundary is therefore subject to the boundary condition

$$\sum_{j'}\Phi_{j'}(z_0+d)\Delta_{j'}(-)=0, \qquad (29)$$

which differs from (19) in that $\Delta_j(+)$ is replaced by $\Delta_j(-)$. Let us solve the system (3) with boundary conditions (19) and (29) in the effective-mass approximation, and then in the two-band approximation.

In the effective-mass approximation, the problem, in analogy with the preceding section, reduces for the j-th band to Eq. (20), which has at $\varkappa = 0$ the solution (28) with boundary conditions

$$\left(1+R_j(+)\frac{\partial}{\partial z}\right)\Phi_j(z_0)=0, \quad \left(1+R_j(-)\frac{\partial}{\partial z}\right)\Phi_j(z_0+d)=0.$$

By letting the solution satisfy these conditions, we obtain a system of two algebraic equations for the constants A and B. The condition for its solvability yields a dispersion equation for the determination of k_z:

$$\exp(2ik_zd)=\frac{[1+ik_zR_j(+)][1-ik_zR_j(-)]}{[1+ik_zR_j(-)][1-ik_zR_j(+)]}.$$

For a film whose potential is symmetrical with respect to the central plane, $z = z_0 + d/2$, $R_j(-)$ and $R_j(+)$ are connected by relation (27). To satisfy this relation in the model of (A.1), it suffices to require that the boundary planes be symmetry planes of the crystal potential.

We introduce the notation

$$R_j = R_j(+),$$

and then, taking (27) into account, the dispersion equation simplifies to

$$\exp(ik_zd)=\pm(1+ik_zR_j)/(1-ik_zR_j);$$

the minus and plus signs pertain here to the solutions of (28), which are even and odd, respectively, with respect to the plane $z = z_0 + d/2$. The last equation can be represented in a form more convenient for graphical investigation:

$$\operatorname{ctg} k_zd={}^1/_2[1/k_zR_j-k_zR_j]. \qquad (30)$$

The results of the investigation of (30) are shown in Fig. 2, the right half of which pertains to the case $R_j > 0$ and the left to $R_j < 0$. The upper part of Fig. 2 shows the dependence of the real roots of Eq. (30), which determine the size-effect quantization levels, on the reciprocal thickness. On the lower part of the figure is shown the behavior of the energy of the Tamm states, which correspond to pure imaginary roots of (30), with decreasing film thickness. The energy is reckoned from the extremum of the considered band into the interior of the forbidden band, which is shown shaded.

In thick films, when

$$\pi n|R_j|/d \ll 1, \quad n=1,\ 2,\ldots, \qquad (31)$$

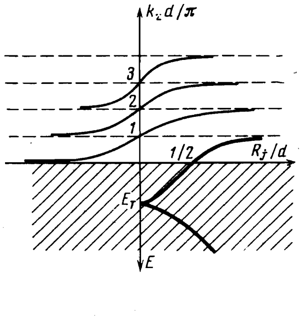

FIG. 2.

the quasiclassical quantization (1) takes place for the size-effect quantization levels, i.e., $k_zd/\pi = n = 1, 2, \ldots$. Here, as expected, the boundary condition (21) goes over into (4). With decreasing thickness, and hence with the violation of the condition (31), the n-th level of the size-effect quantization tends to occupy the place of the $(n+1)$-st quasiclassical level if $R_j > 0$, or the $(n-1)$-st quasiclassical level if $R_j < 0$. As to the Tamm states, there are none at $R_j < 0$.

At $R_j > 0$ in thick ($d \gg R_j$) films, there exists a practically doubly degenerate Tamm level with energy (24). When the thickness of the film begins to approach the localization length of the Tamm state R_j, the degeneracy is lifted. A pair of Tamm states is produced, one even and one odd relative to the center of the film. One of them moves into the interior of the forbidden band and the other "creeps" to its edge, crosses it at $d = 2R_j$, and behaves in thinner films in analogy with the remaining size-effect quantization levels. The slope of the n-th branch is determined in thick films by the expression

$$\frac{d(k_zd/\pi)}{d(R_j/d)} \to 2n \quad \text{as} \quad d\to\infty.$$

The problem is solved similarly in the two-band approximation. In the case of symmetrical film, for which (27) is valid, the dispersion equation with respect to k_z takes the form

$$\operatorname{ctg} k_zd=\frac{1}{2}\left[\frac{\varepsilon+{}^1/_2\varepsilon_g}{k_zR_c\varepsilon_g}-\frac{k_zR_c\varepsilon_g}{\varepsilon+{}^1/_2\varepsilon_g}\right], \qquad (32)$$

in which the dispersion law

$$\varepsilon(k_z)=\pm{}^1/_2\varepsilon_g[1+(k_zl)^2]^{1/2}$$

describes the conduction band (+) and the valence band (−), which are separated by the forbidden band ε_g. We have introduced here the two-band length

$$l=(2\hbar^2/m^*\varepsilon_g)^{1/2}$$

and have discarded terms of order $m^*/m_0 \ll 1$. For R_c, expression (22) is valid, in which, by virtue of the two-band behavior, we retain only one term corresponding to the contribution of the valence band.

The results of a graphic solution of (32) are shown in Fig. 3. It shows the dependence of the real roots of (32) on the reciprocal thickness in the conduction band and in the valence band (upper and lower parts of the figure, respectively), and also the energies of the Tamm states in the forbidden band (the central part of Fig. 3). In Fig. 3 we have introduced the notation

$$E_T=\frac{\varepsilon_g}{2}\left[\frac{1-(l/2R_c)^2}{1+(l/2R_c)^2}\right]$$

$$\Delta n_{c,v}=\frac{1}{\pi}\operatorname{arcctg}\frac{1}{2}\left(\frac{l}{2|R_{c,v}|}-\frac{2|R_{c,v}|}{l}\right),$$

with the lengths R_c and R_v (the latter is obtained from R_c by interchanging the subscripts c and v) are connected in the two-band approximation by the relation

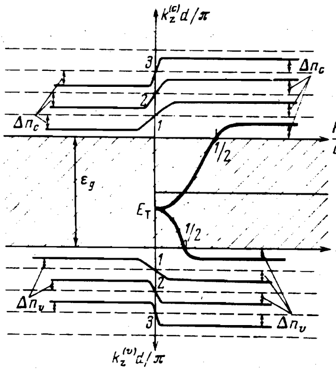

FIG. 3.

$$R_cR_v=(l/2)^2, \tag{33}$$

from which follows the connection between Δn_c and Δn_v:

$$\Delta n_c+\Delta n_v=1.$$

It is seen that if the deviations from the quasiclassical quantization rules (1) in thin films are small in the conduction band ($\Delta n_c \ll 1$), these deviations are large in the valence band ($\Delta n_v \approx 1$), and vice versa. This is essential for the lower levels of the size-effect quantization.

From comparison of Figs. 2 and 3 it is seen that they differ qualitatively only in their asymptotic behavior in the thin-film limit.

In concluding this Section, we note that Cottey[14] obtained by another method and in the one-dimensional case a dispersion equation that coincides formally with (30), apart from the notation. Cottey[14] investigated mainly the dependence of the roots of this equation on the form of the one-dimensional potential barrier at the film boundary.

5. CONCLUSIONS AND DISCUSSION OF RESULTS

It was shown that the behavior of the Tamm levels and the size-effect quantization levels is determined by the characteristic length R_j, which can greatly exceed the lattice constant in semiconductors. This quantity contains information on the complex band structure of the crystal and on the form of the surface potential. It depends also on the state of the surface and can be altered by surface treatment. For semiconductors with narrow forbidden bands, it can be roughly estimated from (33) by putting

$$|R_c|\sim|R_v|\sim l/2\sim 10^{-6}\text{ cm}$$

for $m^*\sim 10^{-2}m_0$ and $\varepsilon_g\sim 10^{-14}$ erg. The experimental determination of R_j from experiments on size-effect quantization in thin films would make it possible to obtain significant information on the microscopic properties of the surface.

In the effective-mass approximation, as seen from (21), R_j^{-1} is, apart from the sign, the logarithmic derivative of the envelope on the boundary of the film. This makes it possible to formulate, in the language of envelopes and in the effective-mass approximation, a model of the semiconductor boundary, by using the equivalence of the boundary condition (21) and the point interaction.[15] It can be formally assumed that the surface region of the crystal is a potential well of depth U_0 and width b, bounded on the vacuum side by an infinite wall. The introduction of this well is equivalent to the boundary condition (21) if $U_0\to\infty$ and $b\to 0$ such that the product b^2U_0 is constant.[15] Then the quantity R_j is formally the scattering length on this singular well, and the condition for the appearance in it of a level coincides with the criterion for the existence of a Tamm state (25). This interpretation is based on the approximation made in this paper, wherein the boundary operator $\hat{\Gamma}$, information on which is contained in R_j, is of the short-range type (in comparison with the characteristic lengths of variation of the envelopes).

The results are directly applicable, for example, to III-V semiconductors if we neglect the spin-orbit interaction and if the normal to the film is directed along the twofold axis C_2. This enables us to classify the states at $\varkappa=0$ in parity with respect to C_2. It is then easy to show that the states generated by heavy holes, i.e., lying on the real line made up of the band of heavy holes, can be regarded independently of the states generated by the conduction band and by the light-hole band, which are described by the two-band approximation.

As already noted in Sec. 2, the problem admits of a generalization to the case when the semiconductor contains an additional one-dimensional potential that varies slowly over the lattice constant. The boundary conditions then retain the form (19), and the envelopes should be determined from the modified system (3).

The states obtained in this paper pertain to $\varkappa=0$ and can serve as a basis for a $\varkappa\cdot\mathbf{p}$ perturbation theory when determining the forms of the two-dimensional Tamm and film subbands.

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APPENDIX

Let us find the explicit form of the boundary operator $\hat{\Gamma}$ in the investigated model:

$$W(\rho,z)=V_0,\ z\leqslant z_0;\ W(\rho,z)=V(\mathbf{r}),\ z\geqslant z_0. \tag{A.1}$$

On the boundary plane $z=z_0$ it is necessary in this case to satisfy the conditions for the continuity of the wave function and of its normal derivative:

$$\begin{gathered}\Psi_{\text{vac}}(\rho,z_0)=\Psi_{\text{cr}}(\rho,z_0),\\ \frac{\partial}{\partial z}\Psi_{\text{vac}}(\rho,z_0)=\frac{\partial}{\partial z}\Psi_{\text{cr}}(\rho,z_0),\end{gathered} \tag{A.2}$$

where the wave function for motion below the barrier in vacuum ($E<V_0$) takes the form[9]

$$\Psi_{\text{vac}}(\varkappa,E,\mathbf{r})=\sum_{\mathbf{G}}B_{\mathbf{G}}\exp\left\{z\left[\frac{2m_0}{\hbar^2}(V_0-E)+(\varkappa+\mathbf{G})^2\right]^{1/2}+i(\varkappa+\mathbf{G})\rho\right\}; \tag{A.3}$$

The summation is carried out over all the two-dimensional reciprocal-lattice vectors $\mathbf{G}=(G_x, G_y)$, while $B_\mathbf{G}$ are arbitrary coefficients. We introduce an arbitrary periodic function

$$v(\rho)=\sum_{\mathbf{G}} B_\mathbf{G} e^{i\mathbf{G}\rho}. \qquad (A.4)$$

Taking into account the notation of (A.4), we can rewrite (A.3) in more compact form[12]:

$$\Psi_{\text{vac}}(\varkappa, E, \mathbf{r})=\exp\left\{z\left[\frac{2m_0}{\hbar^2}\left(V_0-E+\frac{\hat{\mathbf{p}}_\parallel^2}{2m_0}\right)\right]^{1/2}\right\} e^{i\varkappa\rho}v(\rho). \qquad (A.5)$$

Substituting (A.5) in the matching equation (A.2) and eliminating $v(\rho)$ from them, we obtain the boundary condition in the form (7), where in the given particular case

$$\hat{\Gamma}(\pm)=\delta(z-z_0)\left\{\pm\left[\frac{2m_0}{\hbar^2}\left(V_0-E+\frac{\hat{\mathbf{p}}_\parallel^2}{2m_0}\right)\right]^{1/2}-\frac{\partial}{\partial z}\right\}. \qquad (A.6)$$

It is necessary to take the plus sign in (A.6) if the crystal occupies in accordance with (A.1) the right-hand half of the space. The opposite case corresponds to the choice of the minus sign in (A.6).

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Antiferromagnetism of the garnet $Mn_3Al_2Ge_3O_{12}$

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Possible types of magnetic ordering in dodecahedral sites of the garnet are analyzed within the framework of the generalized molecular field theory. The real magnetic structure of the garnet $Mn_3Al_2Ge_3O_{12}$, whose antiferromagnetic ordering at $T_N=6.65\pm0.05$°K is due to exchange interaction between the Mn^{2+} dodecahedral ions, is considered by taking into account the features of the exchange bonds. The magnetic properties (1.6–80°K) and heat capacity (2–20°K) of polycrystalline $Mn_3Al_2Ge_3O_{12}$ are measured. The exchange field is determined, $H_E(3°\mathrm{K})=210$ kOe, as well as the exchange interaction integrals $J_1=-0.57$°K, $J_2'=-0.12$°K. It is shown that the experimental data can be satisfactorily described by the molecular field theory.

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1. INTRODUCTION

The properties of cubic antiferromagnetic garnets in which the dodecahedral sites (c) are occupied by rare-earth ions have by now been investigated quite in detail. Most of these compounds—gallates ($R_3Ga_5O_{12}$) and aluminates ($R_3Al_5O_{12}$)—become antiferromagnetically ordered at $T_N<1$ °K. The singularities of the magnetic properties of rare-earth gallates and aluminates are due to the competition between the exchange, anisotropy, dipole, and hyperfine interactions, which are comparable in size. Capel[1] has demonstrated, using the molecular-field method with allowance for the dipole forces and the anisotropic exchange, that three types of magnetic order of rare-earth ions are possible, two antiferromagnetic and one ferrimagnetic. The realized type of order is determined mainly by the character of the one-ion anisotropy.

It is of interest to study the magnetic ordering of the S ions in the dodecahedral sublattice of the garnet, since we can expect here a great diversity of magnetic structures, owing to the isotropic exchange. This calculation, in the molecular-field approximation with allow-