[1]W. M. Walsh and N. Bloembergen, Phys. Rev. **107**, 904 (1957).
[2]S. N. Lukin and G. A. Tsintsadze, Zh. Eksp. Teor. Fiz. **69**, 250 (1975) [Sov. Phys. JETP **42**, 128 (1975)].
[3]A. Yu. Kozhkhar', S. N. Lukin, and G. A. Tsintsadze, Fiz. Tverd. Tela (Leningrad) **17**, 1870 (1975) [Sov. Phys. Solid State **17**, 1231 (1975)].
[4]A. G. Taylor, L. C. Olsen, D. K. Brise, and J. W. Culwahouse, Phys. Rev. **152**, 403 (1966).
[5]G. N. Neĭlo, V. P. Petrenko, and G. A. Tsintsadze, Prib. Tekh. Eksp. No. 5, 210 (1972) [Instrum. Exp. Tech. **15**, 1538 (1972)].
[6]I. P. Kaminow and R. V. Jones, Phys. Rev. **123**, 1122 (1961).
[7]E. S. Itskevich, Prib. Tekh. Eksp. No. 4, 148 (1963) [Instrum. Exp. Tech. No. 4, 740 (1964)].
[8]B. Bleaney and D. J. E. Ingram, Proc. Roy. Soc. **A208**, 143 (1951).

Translated by V. Zilberstein

Electron dispersion law in a bounded crystal

V. A. Volkov and T. N. Pinsker

Institute of Radio Engineering and Electronics, USSR Academy of Sciences
(Submitted July 22, 1976)
Zh. Eksp. Teor. Fiz. **72**, 1087–1096 (March 1977)

The problem of calculating the dispersion law in a semi-infinite crystal (the Tamm problem) and in a film is formulated in the terms of envelopes and is solved analytically as applied to cubic semiconductors with narrow forbidden bands. The solution of the Tamm problem points to the existence of one two-dimensional Tamm subband. Depending on the surface properties, the extremum of this subband lies either in the forbidden band or coincides with the top of the valence band. In the latter case, the states in the Tamm subband are quasistationary. The dispersion curve in the Tamm subband is double-humped. The energy spectrum of the carriers in the film is analyzed and the existence of two-dimensional subbands of a new type (besides the usual Tamm and size-quantized ones) is predicted: 1) hybrid subbands to which states localized near the film boundaries as well as delocalized states correspond; 2) a pair of subbands with anomalously small masses, which realize the two-dimensional analog of the zero-gap state in a definite film-thickness interval. It is shown the effective masses at the bottom of the lower size-quantized subbands can differ substantially in thin films from their quasiclassical values. The most important of the foregoing results cannot be obtained within the framework of one-dimensional models of a bounded crystal or models that can be reduced to one-dimensional.

PACS numbers: 71.25.Cx, 71.25.Jd

1. INTRODUCTION

It is known[1–4] that size quantization leads to a splitting of each energy band in the conduction-electron spectrum into two-dimensional size-quantized subbands. In the classical approximation,[1] the dispersion law in the n-th subband ($n \gg 1$) can be obtained in the isotropic case from the condition

$$E=\varepsilon(\varkappa,\ \pi n/d), \tag{1}$$

where E is the electron energy, $\varkappa(\varkappa_x, \varkappa_y, 0)$ is the two-dimensional quasimomentum in the plane of the film, $k_z=\pi n/d$ is the quantized value of the transverse component of the quasimomentum, n is a positive integer, and d is the thickness of the film, the z axis coincides with the normal to the film, and $\varepsilon(\mathbf{k})$ is the electron dispersion in a perfect crystal.

The problem of calculating the spectrum of the electrons in a film at $n \sim 1$ is usually formulated in the language of envelopes, i.e., of functions that vary slowly over the lattice periods and are the effective wave functions of the electron in the crystal.

The boundary conditions that the envelopes must satisfy on the crystal surface have already been derived earlier.[5] In contrast to the null conditions,[3,4] these boundary conditions take into account the abruptness of the variation of the electron potential energy near the surface; this, as is well known,[6] is the cause of the appearance of surface (Tamm) states. The case $\varkappa=0$ was considered and it was shown that the quasiclassical quantization rules $k_z=\pi n/d$ are valid only in sufficiently thick films. The deviation of $\varkappa$ from zero not only changes the system of equations for the envelopes,[7] but also renormalizes appreciably the boundary conditions. The latter is due to the face that the $\varkappa\hat{\mathbf{p}}$ interaction jointly with the potential of the boundary entangle the electron motions transverse and longitudinal relative to the surface. The result is that k_z becomes dependent on $\varkappa$.

The purpose of the present paper is to consider the case $\varkappa \neq 0$ and to determine the electron dispersion law in each subband—both the size-quantized band and the Tamm band. The work is based on a derivation of the boundary conditions for the envelopes (Sec. 2). The problem of determining the electron spectrum in a semi-infinite crystal (the Tamm problem, Sec. 3) or in a film (Sec. 4) then reduces to a solution of relatively simple equations for the envelopes with the obtained boundary conditions. The problem was solved for cubic semicon-

 0038-5646/77/4503-0568$02.40

ductors with inversion centers in the four-band approximation (a conduction band and three valence bands), and also in the effective-mass approximation. The results can be nevertheless used, at least qualitatively, also for a much larger class of substances.

2. BOUNDARY CONDITIONS FOR THE ENVELOPES

We consider a semi-infinite crystal occupying the region of space $z \geq z_0$ and bordering on a vacuum ($z < z_0$). We assume that the Hamiltonian preserves the two-dimensional translational invariance, i.e., the boundary is an atomic plane. The two-dimensional quasimomentum $\varkappa$ is then a good quantum number.

The complete wave function of the electron in the crystal assumes, far enough from the boundary, the form[8]

$$\Psi_{cr}(\varkappa, E, \mathbf{r}) = \sum_{\lambda=1}^{\infty} C_\lambda \Psi_\lambda(\varkappa, E, \mathbf{r}), \tag{2}$$

where C_λ are indeterminate coefficients and

$$\Psi_\lambda(\varkappa, E, \mathbf{r}) = \exp\{i\varkappa\rho + iq_\lambda z\} u_\lambda(\varkappa, E, \mathbf{r}) \tag{3}$$

are Bloch functions analytically continued into the plane of complex $q = q' + iq''$; $\boldsymbol{\rho} = (x, y, 0)$; the summation in (2) is over all possible roots (including the complex ones) of the equation

$$E = \varepsilon(\varkappa_x, \varkappa_y, q_\lambda), \tag{4}$$

which is solved for q. In accordance with the boundary conditions, as $z \to +\infty$ the roots of Eq. (4) are subject to the constraint

$$q_\lambda'' > 0. \tag{5}$$

Just as before,[5] we assume that the perturbing action of the boundary $z = z_0$ on Ψ_{cr} is described as follows:

$$\hat{\Gamma}\Psi_{cr} = 0, \tag{6}$$

where $\hat{\Gamma}$ is a certain integro-differential operator having a kernel localized at atomic distances near the plane $z = z_0$. The actual form of $\hat{\Gamma}$ is immaterial in what follows. (Expressions for $\hat{\Gamma}$ are given in[5].)

Substituting (2) and (6) and then expanding each of the terms in a Fourier series in the two-dimensional reciprocal-lattice vector $\mathbf{G}$, and equating the coefficients of like harmonics to zero, we obtain a homogeneous system of linear equations for the coefficients C_λ:

$$\begin{Vmatrix} f_{G\lambda_1}(\varkappa, E) & g_{G\lambda_2}(\varkappa, E) \\ h_{G'\lambda_1}(\varkappa, E) & f_{G'\lambda_2}(\varkappa, E) \end{Vmatrix} \begin{Vmatrix} C_{\lambda_1} \\ C_{\lambda_2} \end{Vmatrix} = 0, \tag{7}$$

where

$$\hat{\Gamma}\Psi_{\lambda_1} = \left[\sum_{G} f_{G\lambda_1}(\varkappa, E)\cos G\rho + \sum_{G'} h_{G'\lambda_1}(\varkappa, E)\sin G'\rho\right] e^{i\varkappa\rho},$$

$$\hat{\Gamma}\Psi_{\lambda_2} = \left[\sum_{G'} f_{G'\lambda_2}(\varkappa, E)\sin G\rho + \sum_{G} g_{G\lambda_2}(\varkappa, E)\cos G\rho\right] e^{i\varkappa\rho}.$$

In the derivation of (7) it was assumed that the z axis coincides with a twofold (or in general an even-fold) symmetry axis C_2. In the case $\varkappa = 0$, which was considered earlier,[5] the operator $\hat{\Gamma}$ commutes with the operation $\hat{C}_2$, and the functions $\Psi_\lambda(0, E, \mathbf{r})$ are either even or odd relative to $\hat{C}_2$. The even functions, the roots of (4) corresponding to them, and the coefficients C_λ are labeled by the index λ_1, while the odd ones are labeled λ_2. The infinite matrix in the double brackets in (7) consists of four matrix blocks. The off-diagonal blocks $g_{G\lambda_2}(\varkappa, E)$ and $h_{G'\lambda_1}(\varkappa, E)$ are linear in $\varkappa$ and vanish at $\varkappa = 0$. They are the result of the $\varkappa\hat{\mathbf{p}}$ interaction, which entangles the roots of (4) which are even and odd relative to $\hat{C}_2$. Since we are interested in values of $|\varkappa|$ that are small compared with the reciprocal-lattice vector, we shall neglect the dependence of $\hat{\Gamma}$ on $\varkappa$.

To analyze the system (7), we separate those roots of (4) which depend essentially on E and $\varkappa$ in the energy interval of interest to us, and label them by the index i. We assume that E lies in the forbidden band. The separation is with respect to the parameter

$$|q_i/q_\lambda| \ll 1, \quad \lambda \neq i. \tag{8}$$

These roots make the principal contribution to the wave function (2) at distances from the boundary much larger than atomic distances. In semiconductors with diamond or zincblende structure (the spin-orbit interaction is disregarded), three roots q_i ($i = 1, 2, 3$) are separated and correspond to "real lines" (see[8]) from four bands: a conduction band of S type and valence bands of type X, Y, and Z (Fig. 1).[9] The root q_1 is even at $\varkappa = 0$, since it lies on the real line that joins S- and Z-type bands that are even relative to $\hat{C}_2$. The Z-band is in this case the band of the light holes. The roots q_2 and q_3 are odd at $\varkappa = 0$.

When $|\varkappa| \lesssim |q_i|$ is turned on, the far roots $q_\lambda (\lambda \neq i)$ remain practically unchanged in the approximation (8), so that their contribution to the off-diagonal blocks of the system (7) can be neglected. The matrix $\|h_{G'\lambda_1}(\varkappa, E)\|$ has then only one nonzero column corresponding to $\lambda_1 = 1$, while the matrix $\|g_{G\lambda_2}(\varkappa, E)\|$ has two nonzero columns corresponding to $\lambda_2 = 2$ and 3. The contributions of the singled-out roots $q_i (i = 1, 2, 3)$ will be taken into account exactly.

Those terms of (2) which correspond to the singled-out roots q_i can be expressed in terms of envelopes Φ_j that vary slowly over the lattice period:

$$\Psi_i = e^{i\varkappa\rho}\left\{\sum_j \Phi_j^{(i)}(z) u_{j0} + \sum_{j'} \Phi_{j'}^{(i)}(z) u_{j'0}\right\}. \tag{9}$$

Here $u_{j0}(\mathbf{r})$ is a Bloch factor corresponding to the extremum of the band j. It is assumed that the extrema of the bands lie in the center of the Brillouin zone. The summation in (9) and henceforth is over all the bands that are even (j) or odd (j') relative to $\hat{C}_2$.

If (9) is taken into account, then the condition that the determinant of the system (7) vanish yields for the envelopes boundary conditions in the form

$$\sum_j \Delta_j(+)\left[\Phi_j^{(1)}(z_0) + \varphi_j(z_0)\right] = 0. \tag{10}$$

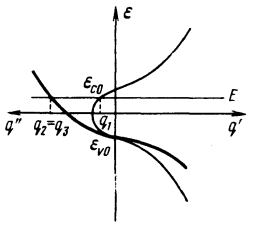

FIG. 1. Graphical solution of Eq. (4) at $\varkappa = 0$ for a four-band semiconductors. The "far" roots q_λ ($\lambda > 3$) are not shown; ε_{c0} and ε_{v0} are the extrema of the conduction and valence bands, respectively. The thick line separates the doubly degenerate band of heavy holes.

Each of the real constants $\Delta_j(+)$ in (10) is a determinant of infinite order and contains information on the microscopic properties of the surface. Expressions for $\Delta_j(+)$ are given in[5]. The + sign corresponds to the chosen positive direction of the z axis. If the choice is the opposite, then $\Delta_j(+)$ is replaced by $\Delta_j(-)$. The general expression for φ_j is complicated in form. At $\varkappa_y = 0$, when one of the singled-out odd roots q_3, which is not connected with the even roots, since there is no $\varkappa_y \hat{p}_y$ interaction, the expression for φ_j becomes much simpler:

$$\varphi_j(z_0) = -\Phi_j^{(2)}(z_0) \sum_{j'} \Phi_{j'}^{(1)}(z_0)\Delta_{j'}(+) \Big/ \sum_{j'} \Phi_{j'}^{(2)}(z_0)\Delta_{j'}(+). \quad (11)$$

3. DISPERSION LAW IN THE SURFACE SUBBAND OF A SEMI-INFINITE CRYSTAL

Let us solve the Tamm problem for a semiconductor with a narrow forbidden band, in which the four-band approximation is well satisfied, for the case $\varkappa_y = 0$. We seek the envelopes in the form

$$\Phi^{(i)} \sim \exp(iq_i z), \quad (12)$$

where $q_i(\varkappa, E)$ $(i = 1, 2)$ are the roots of Eq. (4) (see also Fig. 1).

From (10) and (11), with allowance for (12) and for the connection that ensues between the $\Phi_j(z)$ from the $\mathbf{k}\hat{\mathbf{p}}$ system of equations,[7] we obtain a dispersion equation relative to E for the Tamm problem:

$$1 + iR_c(+)\frac{E_g q_1(\varkappa_x, E)}{E_g/2 + E}\left[1 + \frac{\varkappa_x^2}{q_1(\varkappa_x, E) q_2(\varkappa_x, E)}\right] = 0; \quad (13)$$

where

$$R_c(+) = -P\Delta_z(+)/E_g\Delta_c(+) \quad (14)$$

is the length characterizing the microscopic properties of the surface.[5] We denote by l the quantity

$$l = \frac{2|P|}{E_g} \equiv \left(\frac{2\hbar^2}{m_0^* E_g}\right)^{1/2},$$

then

$$\varepsilon_1 = \pm\frac{E_g}{2}(1 + l^2 q_1^2 + l^2 \varkappa_x^2)^{1/2} \quad (15)$$

is the dispersion law that describes the conduction band (+) and the light-hole band (–); E_g is the width of the forbidden band; P is the intrband matrix elements of the velocity[9]; m_0^* is the effective mass at the extremum of the conduction band. In the derivation of (13) and (15), m_0^* was assumed to be small relative to the mass of the free electron, and the energy was reckoned from the center of the forbidden band.

It is known that the four-band approximation is too crude for a description of the dispersion of the heavy holes, whose contribution to (13) becomes appreciable at energies close to the top of the valence band. When the dispersion equation is derived under these conditions it is necessary to use a more exact expression for the dispersion law[10]:

$$\varepsilon_{1,2} = -\tfrac{1}{2}E_g + \tfrac{1}{2}(L+M)(\varkappa_x^2 + q_i^2) \pm [\tfrac{1}{4}(L-M)^2(\varkappa_x^2 - q_i^2)^2 + N^2\varkappa_x^2 q_i^2]^{1/2},$$

where the + sign corresponds to $i = 1$ and the – sign corresponds to $i = 2$. L, M, and N are negative constants.

It is easy to show that the dispersion equation for a Tamm subsystem located close to the top of the valence band is of the form

$$1 + iq_1 R_v(+) - (1 + iq_2 R_v(+))\frac{q_1(L\varkappa_x^2 + Mq_2^2 - E + E_g/2)}{q_2(L\varkappa_x^2 + Mq_1^2 - E - E_g/2)} = 0, \quad (16)$$

and in the approximation of a narrow forbidden band $R_c(+)$ and $R_v(+)$ are connected by the relation[5]

$$R_c(+)R_v(+) = l^2/4. \quad (17)$$

In the isotropic case, when $|N| = |L - M|$, the dispersion law goes over into the expressions

$$\varepsilon_1 = -\tfrac{1}{2}E_g + L(\varkappa_x^2 + q_1^2), \quad \varepsilon_2 = -\tfrac{1}{2}E_g + M(\varkappa_x^2 + q_2^2) \quad (18)$$

for the light- and heavy-hole bands, respectively. Equation (16), with (18) taken into account, simplifies and takes the form

$$1 + iq_1(\varkappa_x, E)R_v(+) + iR_v(+)\frac{\varkappa_x^2}{q_1(\varkappa_x, E)} + \frac{\varkappa_x^2}{q_1(\varkappa_x, E)q_2(\varkappa_x, E)} = 0. \quad (19)$$

It is easy to verify, using (17), that (13) goes over into (19) when E approaches the top of the valence band.

An analysis of (13) shows that regardless of the sign of $R_c(+)$ there exists one Tamm subband. At small $|\varkappa_x|$, when

$$|\varkappa_x^2/q_1 q_2| \ll 1, \quad (20)$$

the dispersion law in this subband can be obtained in analytic form

$$E_T^{(1,2)}(\varkappa_x) = -\frac{E_g l^2}{2(l^2 + 4R_c^2(+))} \times \left[1 - \operatorname{sign} R_c(+)\frac{4R_c^2(+)}{l^2}\left(1 + \varkappa_x^2 l^2\left(1 + \frac{l^2}{4R_c^2(+)}\right)\right)^{1/2}\right], \quad (21)$$

with $E_T^{(1)}(\varkappa_x)$ corresponding to $R_c(+) > 0$ and $E_T^{(2)}$ to $R_c(+) < 0$. The position $E_T^{(1)}(0)$ of the bottom of the first subband was calculated in[5] in the two-band approximation, while the effective mass on the bottom of this subband

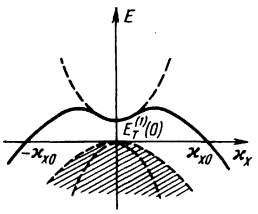

FIG. 2. Tamm subband $E_T^1(\varkappa_x)$ existing at $R_v>0$. The volume states of the light and heavy holes are shaded.

coincides with m_0^*. In all other respects, however, it differs in shape from the conduction band, and the difference is larger the closer $E_T^{(1)}(0)$ is to the top of the valence band.

To analyze the contribution of the heavy holes to the formation of the Tamm subband $E_T^{(1)}(\varkappa_x)$ we shall use the dispersion equation (19). Allowance for the corrections in terms of the parameter (20) leads to the following results: First, a renormalization of the effective mass

$$m_T(0)\equiv\hbar^2\left[\frac{\partial^2 E_T^{(1)}}{\partial\varkappa_x^2}(0)\right]^{-1}=-\frac{\hbar^2}{2L}\left[1-2\left(\frac{M}{L}\right)^{1/2}\right]^{-1}$$

on the bottom of this subband, the position of the bottom being determined in this case by the expression

$$E_T^{(1)}(0)=-{}^1/_2E_g-L/R_v^2(+).$$

Second, as $|\varkappa_x|$ increases and the condition (20) is violated, the dispersion law in the Tamm subband deviates more and more from formula (21) and reaches a maximum at an energy (see Fig. 2)

$$E_{max}^{(1)}=-\frac{E_g}{2}-\frac{L}{R_v^2(+)}\frac{L}{M}f\left(\frac{4M}{L}\right),$$

where $f(4M/L)\sim10^{-1}$ at $4M/L\ll1$, a condition well satisfied in semiconductors with narrow forbidden bands. The effective mass at the maximum is of the order of the mass of the heavy holes, $\hbar^2/2M$. At

$$|\varkappa_x|\geqslant|\varkappa_{x0}|\equiv(L+M)/M2|R_v(+)|$$

$E_T^{(1)}$ begins to overlap the volume spectrum. The asymptotic form of $E_T^{(1)}(\varkappa_x)$ at $|\varkappa_x/\varkappa_{x0}|\gg1$ is also determined by the mass of the heavy holes:

$$E_T^{(1)}(\varkappa_x)\approx-E_g/2-L^2/MR_v^2(+)+M\varkappa_x^2.$$

We note that a Tamm subband of similar shape was calculated for Ge by the LCAO method in the nearest-neighbor approximation.[11]

The appearance of the Tamm subband $E_T^{(2)}(\varkappa_x)$ at $R_c(+)<0$ is due to degeneracy of the valence band. Its top $E_T^{(2)}(0)$ coincides with the top of the valence band, and the effective mass near the extremum is equal to the light-hole mass $\hbar^2/2L$. Since this subband intersects with the heavy-hole band, the states in it are quasistationary:

$$E_T^{(2)}(\varkappa_x)\approx-{}^1/_2E_g+(L+M)\varkappa_x^2+iR_v(+)(LM)^{1/2}|\varkappa_x|^3$$

under the condition

$$|(M/L)^{1/2}\varkappa_xR_v(+)|\ll1,$$

and the behavior of the wave function (the damping length and the period of the oscillations) is determined by the expressions

$$q_1''=-R_v(+)\varkappa_x^2,\quad q_1'=(M/L)^{1/2}|\varkappa_x|.$$

4. DISPERSION LAW FOR ELECTRONS IN A FILM

We consider a film occupying the region of space

$$0\leqslant z\leqslant d.$$

It follows from the preceding section that if $|\varkappa_x|$ is not too large, and the inequality (20) is satisfied, we can disregard in the boundary conditions for the envelopes the entanglement of the roots of Eq. (4) that are even and odd relative to $\hat{C}_2$. This means that we can neglect the off-diagonal blocks in (7), as well as the increment φ_j in (10). Following now Sec. 4 of[5], we can easily show that for films whose thickness satisfies the condition

$$|dq_\lambda|\gg1\quad(\lambda\geqslant2),$$

the boundary conditions for the envelopes take the form

$$\left(1+R_c(+)\frac{E_g}{E+E_g/2}\frac{\partial}{\partial z}\right)\Phi_c(0)=0,$$
$$\left(1+R_c(-)\frac{E_g}{E+E_g/2}\frac{\partial}{\partial z}\right)\Phi_c(d)=0,\qquad(22)$$

where

$$\Phi_c(z)=A\exp(ik_zz)+B\exp(-ik_zz),\qquad(23)$$

and A and B are coefficients that must be determined from (22).

We have omitted in (22) and (23) the envelope superscript corresponding to the number of the root of Eq. (4), since we are considering only one root. In the Tamm problem it was designated q_1 (see Fig. 1). The requirement (5) is waived for a film, and corresponds therefore to a pair of roots of Eq. (4), which we designate k_z and $-k_z$, and the right-hand side of this equation should contain a dispersion law determined from (15).

Substituting (23) in the boundary conditions (22) and using the relation (see[5])

$$R_c(+)=-R_c(-)\equiv R_c$$

for a film whose potential is symmetrical relative to the central plane $z=d/2$, we obtain a dispersion equation with respect to E

$$-\frac{d}{E_gR_c}\left(E+\frac{E_g}{2}\right)=\pm k_z(\varkappa,E)d\left[\operatorname{tg}\frac{k_z(\varkappa,E)d}{2}\right]^{\pm1}.\qquad(24)$$

The signs + and − pertain to envelopes (23) that are re-

spectively even and odd relative to the central plane of the film.

The results of a graphical solution of Eq. (24) are shown in Figs. 3 and 4. It is seen from these figures that size quantization leads to formation of size-quantized subbands corresponding to real k_z, and to splitting of the Tamm subband. The interaction between the size-quantized and Tamm subbands can result in hybrid subbands. In the case $R_c<0$ (Fig. 3), the hybrid subband is the one with $n_v=1$; at small $|\varkappa_x|$,

$$|\varkappa_x|\leqslant\varkappa_1\equiv\frac{1}{d}\left[\frac{2(2R_c-d)}{R_v}\right]^{1/2},$$

this subband can be regarded as size quantized, and at $|\varkappa_x|>\varkappa_1$ it can be regarded as a Tamm subband. The structure of the electron wave function in this subband changes radically at $|\varkappa_x|=\varkappa_1$: if $|\varkappa_x|\leqslant\varkappa_1$, then the envelopes take the form of standing waves, but if $|\varkappa_x|>\varkappa_1$ then they are sums of exponentials localized near the film boundaries, and the localization is stronger the larger $|\varkappa_x/\varkappa_1|$.

A distinguishing feature of the spectrum in the valence band is that it contains a size-effect subband whose extremum coincides at $\varkappa=0$ with the top of the valence band ($n_v=0$ on Figs. 3 and 4a). This distinguishes in principle the degenerate valence band from the conduction band.

It is also seen from Fig. 4 that if $R_c>0$ one of the Tamm subbands approaches the top of the valence band with decreasing film thickness, and crosses the top at $d=2R_v$. The $\varkappa\hat{p}$ interaction between this subband and the $n_v=0$ subband causes the effective mass in each of these subbands to reverse sign and to pass through zero at $d=2R_v$ (the two-dimensional analog of the zero-gap state[12]).

It follows from (24) that, in contrast to the quasiclassical approximation (1), k_z depends on $\varkappa_x$, and this leads to renormalization of the effective mass at the bottom of each subband. If $|\varkappa_x|$ is small we can seek k_z in the form

$$k_z(\varkappa_x)\approx k_z(0)+a\varkappa_x^2, \tag{25}$$

$$|a\varkappa_x^2/k_z(0)|\ll 1. \tag{26}$$

Substituting (25) and (24) and expanding in powers of the parameter (26), we obtain for the sought effective mass the expression

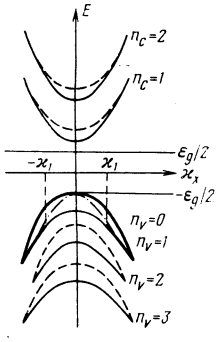

FIG. 3. Size-quantized and Tamm subbands in a film at $R_c<0$ and $R_v<0$. The thick lines separate the states with imaginary k_z, the dash-dot line—the Tamm subband in a semi-infinite crystal, and the dashed line—the quasiclassical size-quantized subbands.

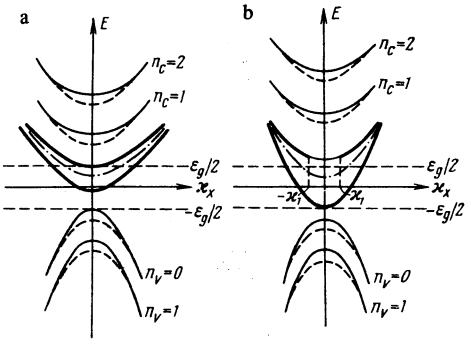

FIG. 4. The same as Fig. 3, but for $R_c>0$ and $R_v>0$. a) Thick films ($d>2R_c$, $d>2R_v$), b) thin films ($d<2R_c$, $d<2R_v$).

$$\frac{m_{кв}^*}{m^*}=1-\left(1-\frac{m_0^*}{m_{кв}^*}\right)\left[\frac{d}{4R_c}\left(1+\frac{R_c}{R_v}\right)\left(\frac{m_{кв}^*}{m_0^*}+\frac{R_v-R_c}{R_v+R_c}\right)-\frac{m_0^*}{m_{кв}^*}\right]^{-1}$$

where

$$m_{кв}^*=\pm m_0^*[1+l^2k_z^2(0)]^{1/2}.$$

In sufficiently thick films ($l^2k_z^2(0)\ll 1$) there is no mass renormalization. The variation of $m_z(0)$ with thickness, which is known from[5], makes it possible to determine the mass renormalization in the thin-film limit, when the nonparabolicity of the dispersion law (15) is essential:

$$\frac{m_{кв}^*}{m^*}\approx 1\mp\frac{2}{\pi}\left[(n_j+\Delta n_j\operatorname{sign}R_j)\left(\frac{l}{2R_j}+\frac{2R_j}{l}\right)\right]^{-1}, \tag{27}$$

where

$$l^2k_z^2(0)\sim l^2\pi^2n_j^2/d^2\gg 1,$$

$$\Delta n_j=\frac{1}{\pi}\operatorname{arcctg}\frac{1}{2}\left(\frac{l}{2|R_j|}-\frac{2|R_j|}{l}\right)\quad(j=c,v).$$

The upper sign in (27) pertains to the conduction band and the lower to the valence band. As expected, for high-lying size-quantized subbands ($n_j\gg 1$) one can use the quasiclassical approximation, and the mass renormalization is inessential. For the subband with $n_j=1$ we have

$$m_{кв}^*/m^*\approx 1\pm 2/\pi,$$

if $R_c<0$ and $|R_c|\approx|R_v|\approx l/2$.

A more radical change of the effective mass with decreasing d takes place in the Tamm and hybrid subbands. For example, for the upper subband in the valence band, in which $k_z(0)=0$ and (26) cannot be used, m^* is given by the expression

$$-m^*/m_0^*=1-2R_v/d,$$

which can even reverse sign at $d=2R_v$, a fact already noted in the qualitative discussion of Eq. (24).

In the considered isotropic case, a renormalization of m^* takes place only if the dispersion is nonparabolic. Allowance for the anisotropy, even in the case of a quadratic dispersion, can lead to an analogous effect if the

crystal has no symmetry plane parallel to the film surfaces.

We did not mention in this section the heavy holes, for which the quasiclassical quantization (1) is valid. If condition (20) is satisfied, they can be treated independently of the light holes. Allowance for the corrections relative to the parameter (20) leads to spectrum correction proportional to $M/L \ll 1$ and to an increase in the distance between the size-quantized subbands corresponding to the heavy and light holes at the points of their intersection.

Size quantization in the vicinity of the top of a degenerate valence band was considered earlier[4] with null boundary conditions used for the envelopes. This approach cannot yield Tamm states which, as shown in the present paper, alter significantly the spectrum of the size-quantized subbands in the valence band at $n_v \lesssim 1$. None the less, the positions of the extrema of the size-quantized subbands corresponding to $n_v > 1$ agree with Nedorezov's results[4] in the limit of thick films ($d \gg \pi n_v |R_v|$). A more detailed comparison of his and our results is difficult, since Nedorezov considers the opposite limiting case, where the spin-orbit interaction is assumed large and the mass of the heavy holes is assumed finite.

We note in conclusion that the boundary condition (10) retains the same form in those cases when additional fields that can be described in the language of envelopes are present in the system.

The authors are deeply grateful to V. B. Sandomirskiĭ for constant interest in the work and to M. I. Kaganov for valuable remarks.

[1]I. M. Lifshitz and A. M. Kosevich, Izv. Akad. Nauk SSSR Ser. Fiz. **19**, 395 (1955); I. M. Lifshitz, M. Ya. Azbel', and M. I. Kaganov, Élektronnaya teoriya metallov (Electron Theory of Metals), Nauka, 1971, §7.
[2]V. B. Sandomirskiĭ, Zh. Eksp. Teor. Fiz. **52**, 158 (1967) [Sov. Phys. JETP **25**, 101 (1967)].
[3]B. A. Tavger and V. Ya. Demikhovskiĭ, Usp. Fiz. Nauk **96**, 61 (1968) [Sov. Phys. Usp. **11**, 644 (1969)]; V. N. Lutskiĭ, Phys. Status Solidi A **1**, 199 (1970).
[4]S. S. Nedorezov, Fiz. Tverd. Tela (Leningrad) **12**, 2269 (1970) [Sov. Phys. Solid State **12**, 1814 (1971)].
[5]V. A. Volkov and T. N. Pinsker, Zh. Eksp. Teor. Fiz. **70**, 2268 (1976) [Sov. Phys. JETP **43**, 1183 (1976)].
[6]S. G. Davison and J. Levine, Surface (Tamm) States [Russ. transl.], Mir, 1973.
[7]J. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955); L. V. Keldysh, Zh. Eksp. Teor. Fiz. **45**, 364 (1963) [Sov. Phys. JETP **18**, 253 (1964)].
[8]V. Heine, Proc. Phys. Soc. London **81**, 300 (1963).
[9]E. O. Kane, Semicond. and Semimet., Vol. 1, New York, 1966, p. 75.
[10]I. M. Tsidil'kovskiĭ, Élektrony i dyrki v poluprovodnikakh (Electrons and Holes in Semiconductors), Nauka, 1972, p. 210
[11]K. Hirabayashi, Phys. Soc. Jpn. **27**, 1475 (1969).
[12]A. A. Abrikosov and S. D. Beneslavskiĭ, Zh. Eksp. Teor. Fiz. **59**, 1280 (1970) [Sov. Phys. JETP **32**, 699 (1971)].

J. G. Adashko

Level crossing and instability of magnetic structure in rare-earth iron garnets

A. K. Zvezdin, A. A. Mukhin, and A. I. Popov

(Submitted July 28, 1976)
Zh. Eksp. Teor. Fiz. **72**, 1097–1110 (March 1977)

When the ground-state levels of a rare-earth ion cross (or approach one another) in a rare-earth iron garnet, the magnetic structure of the garnet becomes unstable. This phenomenon is very close to the well known Jahn-Teller effect. If the rare-earth ions have a strong magnetic-moment anisotropy, this instability involves some distinctive anomalies of the magnetic behavior of the crystal. We have investigated a theoretical model in which the rare-earth ions are treated in an extreme anisotropic (Ising) approximation. It is shown that at different orientations of the external magnetic field the instability produced by the level crossing has a fine structure that reflects the detailed character of the magnetization reversal of rare-earth ions situated in differnt non-equivalent positions. The magnetization curves of such a system are investigated and a comparison is made with the experimental data on holmium-yttrium ion garnets.

PACS numbers: 75.10.Hk, 75.30.Gw

1. INTRODUCTION

Demidov, Levitin, and Popov[1,2] have observed an interesting phenomenon: in some mixed rare-earth iron garnets (REIG), the magnetization curves $M(H)$ exhibit magnetization jumps in strong fields at low temperatures. These jumps arise at different orientations of the external field relative to the crystal axes and are accompanied by hysteresis phenomena. The probable cause of these anomalies, in their opinion, is the crossing (or approach) of the low-lying levels of the rare-earth ions (REI) when the external magnetic field H is

 0038-5646/77/4503-0573$02.40