Bound states of electron and optical phonon in a quantum well

S. M. Badalyan[1)] and I. B. Levinson

Institute for Problems of Technology, Microelectronics, and Specially Pure Materials, USSR Academy of Sciences

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The spectrum of a polaron in a magnetic field perpendicular to the walls of a quantum well is investigated. It is shown that a bound state of an electron with an optical phonon exists.

1. INTRODUCTION

It was shown in Refs. 1–3 (see also the reviews[4,5]) that bound itinerant electron + longitudinal optical (LO) phonon states exist in a quantizing field. The energy of these states lies near the threshold of LO-phonon emission by an electron in a lower Landau band. After emitting the LO phonon, the electron is located on the bottom of the Landau band, where the density of states is high. Therefore the effective interaction in the near-threshold region is strong even in the case of weak electron-phonon coupling. If the cyclotron frequency $\omega_H = eH/mc$ is of the order of the LO-phonon frequency ω_0, the binding energy is $W \sim \alpha^2 \hbar\omega_0$, where α is the Frölich coupling constant. In most III-V semiconductors $\alpha \lesssim 0.1$, so that the binding energy is quite small, $W \lesssim 0.3$ MeV. This may be one of the reasons why no bound states were observed in the absorption spectra.

If the electron motion along **H** is bounded by the walls of a quantum well, the density of the states on the bottom of the Landau band changes from a square-root singularity to the stronger delta function. The binding energy for such a $2D$ electron should therefore be higher than for a $3D$ electron.

We obtain in the present paper the bound states of an electron with an LO phonon in a quantum well with walls are perpendicular to **H**. The well walls are assumed for simplicitly to be infinitely high, so that the wave functions and energy of an electron moving along $z \| \mathbf{H}$ are

$$\psi_k(z) = \left(\frac{2}{d}\right)^{1/2} \sin\frac{\pi k}{d} z, \quad k = 1, 2, \ldots,$$

$$E_k = k^2 \hbar\omega_d, \quad \hbar\omega_d = \pi^2\hbar^2/2md^2, \tag{1}$$

where d is the width of the well. It is assumed also that the well is narrow enough, i.e., $E_2 - E_1 \gg \hbar\omega_0, \hbar\omega_H$.

In contrast to an electron, an LO phonon is not always localized in a quantum well. We consider therefore two limiting cases; of a nonlocalized $3D/LO$ phonon, when its wave function for motion along z is

$$\varphi_{q_\|}(z) = \frac{1}{L^{1/2}} \exp(iq_\| z), \quad q_\| = \frac{2\pi}{L} n, \quad n = 0, \pm 1, \pm 2, \ldots, \tag{2}$$

and of a localized $2D/LO$ phonon, when

$$\varphi_{q_\|}(z) = (2/d)^{1/2} \sin q_\| z, \quad q_\| = \pi n/d, \quad n = 1, 2, \ldots. \tag{3}$$

Here L^3 is the normalized volume. The dispersion of the LO phonon is neglected: $\omega(\mathbf{q}) = \omega_0$.

The energy levels are shown in Fig. 1. The lower thick line is the bottom of the conduction band. The energy is reckoned from the lower electron level, whose height above the bottom is $E_1 + \hbar\omega_H/2$. The dashed line shows the threshold $E_c = \hbar\omega_0$ near which the bound states of interest to us are located.

2. BOUND STATES

Bound states are sought by the same method as in Ref. 3 for the $3D$ case, viz., as the poles of the scattering amplitude Σ. The equation for Σ is illustrated in Fig. 2. In this equation ϵ is the total energy of the electron and phonon (we put $\hbar = 1$ for brevity). The equation is written in the gauge-invariant technique,[6] therefore only the number s of the Landau band is used for the electron (solid lines) and the gauge-noninvariant quantum number k_y is absent. The electron Green's function G is diagonal in s (Ref. 6) but is not diagonal in k. The assumption $E_2 - E_1 \gg \omega_H, \omega_0$, however, permits neglect of the off-diagonal elements $G_{kk'}$. In the dangerous cross section contained in the second term of the right-hand side of the equation in Fig. 2, the function G can be taken without allowance for the interaction with the phonons, and only the term $\bar{k} = 1$ is to be retained in the summation over $\bar{k}$. All the foregoing allows us to put everywhere $k = 1$ (and omit this subscript hereafter), so that

$$G_s(\varepsilon) = (\varepsilon - s\omega_H + i0)^{-1}. \tag{4}$$

Integration was carried out over the energy parameter of the phonon, so that the phonon propagator—the dashed line—corresponds to the matrix element

$$B(\mathbf{q}) = B_0 \Phi(\mathbf{q}),$$
$$B_0 = \pi\alpha (p_0/m)^2, \quad p_0^2 = 2m\omega_0,$$
$$\Phi(\mathbf{q}) = \frac{p_0}{\mathbf{q}_\perp^2 + q_\|^2} \left| \int_0^d dz\, |\psi(z)|^2 \varphi_{q_\|}(z) \right|^2 \equiv \Phi_n(\mathbf{q}_\perp). \tag{5}$$

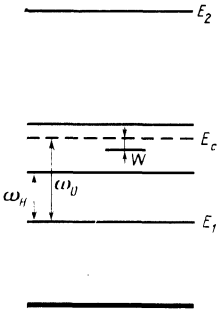

FIG. 1. Energy levels.

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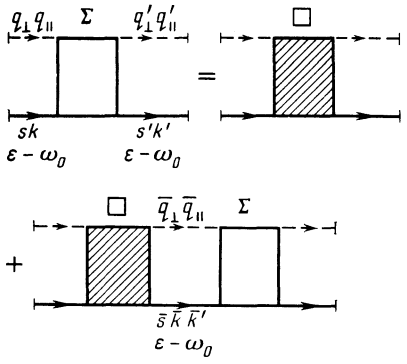

FIG. 2. Equation for the scattering amplitude.

The diagrams that contribute to the irreducible amplitude □ are shown in Fig. 3. The point corresponds to a gauge-invariant part of the electron-phonon interaction vertex:

$$\Lambda_{ss'}(\mathbf{q}_\perp)=e^{-i\varphi(s-s')}Q_{ss'}(t),$$
$$t=q_\perp{}^2a^2/2,\quad a^2=c/eH,$$
$$Q_{ss'}(t)=(s!/s'!)^{1/2}t^{(s-s')/2}e^{-t/2}L_s^{s-s'}(t)=(-1)^{s-s'}Q_{s's}(t), \tag{6}$$

where L are Laguerre polynomials and φ is the polar angle of the vector $\mathbf{q}_\perp$.

To find the spectrum of the bound states near the threshold $\varepsilon\approx E_c$ it suffices to consider the amplitude Σ for $s=s'=0$. By analogy with Ref. 3, we introduce the Fourier components

$$\Sigma^l_{nn'}(\varepsilon;tt')=\int_0^{2\pi}\frac{d\varphi}{2\pi}e^{-il(\varphi-\varphi')}\Sigma^l_{nn'}(\varepsilon;\mathbf{q}_\perp\mathbf{q}_\perp{}')$$
$$\times\exp\left\{\frac{ia^2}{2}[\mathbf{q}_\perp\mathbf{q}_\perp{}']\right\}, \tag{7}$$

where $l=0,\ \pm1,\ \pm2,\ldots$. Fourier components with different l satisfy the independent equations

$$\Sigma^l_{nn'}(\varepsilon;tt')$$
$$=\Box^l(tt')+\tilde{M}(\varepsilon)\sum_{\bar{n}}\int_0^\infty d\bar{t}\,\Box^l(t\bar{t})\Phi_{\bar{n}}(\bar{t})\Sigma^l_{\bar{n}n'}(\varepsilon;\bar{t}t'), \tag{8}$$

where $\Box^l$ is defined by analogy with Σ^l and

$$\tilde{M}(\varepsilon)=\alpha\omega_H\omega_0(\varepsilon-\omega_0+i0)^{-1}. \tag{9}$$

The equation for the amplitude Σ^l is simplified by symmetrizing it and averaging over n. We introduce for this purpose the averaged form factor

$$\bar{\Phi}(t)=\sum_n\Phi_n(t) \tag{10}$$

and new amplitudes

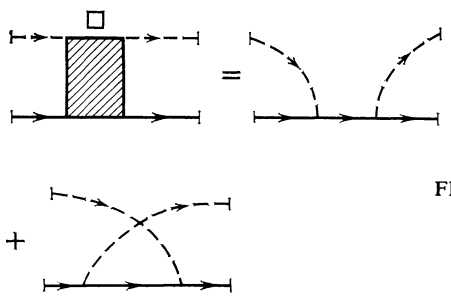

FIG. 3. Bare amplitude.

$$\hat{\Sigma}^l(\varepsilon;tt')=[\bar{\Phi}(t)\bar{\Phi}(t')]^{-1/2}\sum_{nn'}\Phi_n(t)\Phi_{n'}(t')\Sigma^l_{nn'}(\varepsilon;tt'),$$
$$\hat{\Box}^l(tt')=[\bar{\Phi}(t)\bar{\Phi}(t')]^{1/2}\Box(tt'). \tag{11}$$

Transforming to the dimensionless quantities

$$R^l(tt')=-\omega_0\hat{\Sigma}^l(\varepsilon;tt'),\quad K^l(tt')=-\omega_0\hat{\Box}^l(tt'),$$
$$\lambda(\varepsilon)=-\omega_0{}^{-1}\tilde{M}(\varepsilon), \tag{12}$$

we obtain the final equation

$$R^l(tt')=K^l(tt')+\lambda\int_0^\infty d\bar{t}\,K^l(t\bar{t})R^l(\bar{t}t'). \tag{13}$$

Thus, R is the Fredholm resolvent of the kernel K, which we now write out in explicit form

$$K^l(tt)=[\bar{\Phi}(t)\bar{\Phi}(t')]^{1/2}e^{-1/2(t+t')}$$
$$\times\sum_{s=0}^\infty\frac{1}{s!}(tt')^{s/2}\left[J_{l+s}(2(tt')^{1/2})\frac{\sigma}{s+\sigma}+\delta_{ls}\frac{\sigma}{s-\sigma}\right]. \tag{14}$$

Here $\sigma=\omega_0/\omega_H$, and the two terms in the square brackets are connected with the two terms of Fig. 3.

We see now that the amplitude Σ^l has a pole in ε if $\lambda(\varepsilon)$ coincides with an eigenvalue of the kernel K^l. In other words, the equation for the energies of the bound states of the electron and phonon is

$$\lambda(\varepsilon)=\lambda_r{}^l, \tag{15}$$

where the subscript r numbers different eigenvalues of the kernel K^l. It follows from (15) that the energies of the bound states are

$$E_r{}^l=E_c-\alpha\omega_H/\lambda_r{}^l\equiv E_c-W_r{}^l. \tag{16}$$

In the case of a $3D$ electron the bound states appeared only below the threshold, for in this case a continuum of two-particle electron + phonon states is located above the threshold. There is no such continuum for the $2D$ electron, so that bound states are present both below the threshold ($W>0$) and above it ($W<0$). This means that the energies

of the bound states are determined, according to (16), by eigenvalues of both signs.

3. INTRABAND ABSORPTION

Bound states should appear in the absorption spectrum of light at a frequency $\omega \approx \omega_0$. On absorbing a photon of this frequency, the electron remains on the initial energy level, and a phonon that is bound to the electron is created. If it is assumed, as in Ref. 7, that the temperature and density of the carrier are low enough, so that $T \ll W$ or $\varepsilon_F \ll W$, the absorption coefficient can be expressed in terms of the scattering amplitude Σ. It is assumed that the light propagates along z, has circular polarization, all the electron are on the level $k = 1$, and $s = 0$. Proceeding as in Ref. 8, we can show that the light-energy fraction absorbed in the quantum well is

$$w^{\pm}(\omega) = -\frac{4\pi c}{\omega(\varkappa(\omega))^{1/2}} \operatorname{Im} \Pi^{\pm}(\omega). \tag{17}$$

The plus and minus signs pertain here to right-hand and left-hand polarization of the light, and $\varkappa(\omega)$ is the dielectric constant of the well walls. Next,

$$\Pi^{\pm}(\omega) = \int\int dz_1\, dz_2\, \Pi^{\pm}(\omega; z_1 z_2)\, |\psi(z_1)|^2 |\psi(z_2)|^2, \tag{18}$$

where $\Pi^{\pm}(\omega; z_1, z_2)$ is the photon polarization operator in the coordinate representation. Proceeding as in Ref. 7, we can find an expression in terms of the scattering amplitude Σ^l with $l = \pm 1$:

$$\Pi^{\pm}(\omega) = \frac{1}{2} \mathcal{N} \frac{e^2}{mc^2} \frac{\omega_H \omega_0}{(\omega_0 \mp \omega_H)^2} [\lambda \bar{\Phi} + \lambda^2 \bar{R}^{\pm}]_{\varepsilon=\omega}. \tag{19}$$

Here $\mathcal{N}$ is the carrier density per cm^2 of quantum-well wall area, and

$$\bar{\Phi} = \int_0^\infty dt\, e^{-t} t \tilde{\Phi}(t),$$

$$\bar{R}^{\pm} = \int_0^\infty\int dt\, dt'\, e^{-1/2(t+t')} (tt')^{1/2} [\tilde{\Phi}(t)\tilde{\Phi}(t')]^{1/2} R^{\pm 1}(tt'). \tag{20}$$

Expanding the resolvent R as a sum over the poles, we obtain ultimately

$$w^{\pm}(\omega) = 2\pi \mathcal{N} \frac{e^2}{mc^2} \frac{c}{(\varkappa(\omega))^{1/2}} \sum_r f_r^{\pm} \pi \delta(\omega - E_r^{\pm 1}). \tag{21}$$

The oscillator strength for a transition to a bound state r with $l = \pm 1$ is here

$$f_r^{\pm} = \alpha \left(\frac{\omega_H}{\omega_0 \mp \omega_H}\right)^2 \left| \int_0^\infty dt\, e^{-t/2} t^{1/2} \tilde{\Phi}(t)^{1/2} \chi_r^{\pm 1}(r) \right|^2, \tag{22}$$

where $\chi_r(t)$ is an eigenfunction of the kernel (14). Using the completeness of the system of functions χ_r, it is easily shown that

$$\sum_r f_r^{\pm} = \left(\frac{\omega_H}{\omega_0 \mp \omega_H}\right)^2 \bar{\Phi}. \tag{23}$$

Note that the first term in the square brackets in (19) corresponds to a perturbation-theory calculation of the absorption and yields a delta-like absorption peak at the threshold for $\omega = \omega_0$. Actually, however there is no such peak in absorption, since it is cancelled out when the second term is taken into account. Recall that in the $3D$ case this corresponded to transformation of the singularity $(\omega - \omega_0)^{-1/2}$, which becomes infinite at the threshold, into the singularity $(\omega - \omega_0)^{1/2}$, which goes to zero.[7]

4. BINDING ENERGIES AND OSCILLATOR STRENGTHS

The actual calculation of the binding energy and of the oscillator strengths can be carried out by considering the limiting situations—strong and weak fields H (i.e., $\omega_H \gg \omega_0$ and $\omega_H \ll \omega_0$). Using the condition that the well be narrow, which is equivalent to $d \ll a, p_0^{-1}$, we find first the averaged form factors (10) and (20). For nonlocalized $3D/LO$ phonons we have

$$\tilde{\Phi}(t) = 2(\sigma/t)^{1/2}, \quad \bar{\Phi} = (\pi\sigma)^{1/2}. \tag{24}$$

For localized $2D/LO$ phonons,

$$\tilde{\Phi}(t) = \bar{\Phi} = b\delta^{1/2}, \tag{25}$$

where

$$b = \left(\frac{2}{\pi}\right)^3 \sum_{n=1}^{\infty} \frac{1}{n^2} \left| \int_0^\pi d\zeta \sin^2\zeta \sin n\zeta \right|^2 \approx 0.46,$$

$$\delta = \omega_0/\omega_d = (p_0 d/\pi)^2. \tag{26}$$

In the $3D/LO$ case the well width d does not enter in the kernel (14). The binding energies and the oscillator strengths are therefore independent of d (so long as $d \ll a$, p_0^{-1}). In the $2D/LO$ case the well width d enters in the kernel only as a factor d. Therefore the eigenvalues $\lambda_r \propto d$, and the eigenfunctions χ_r are independent of d. From this, using (16) and (22), we easily find the dependences of the binding energies and of the oscillator strengths on d:

$$W_r \sim d, \quad f_r \sim d. \tag{27}$$

Moreover, comparing the form factors (24) and (25) in the kernel (14), we see that

$$\frac{W_{2D/LO}}{W_{3D/LO}} \approx \frac{f_{2D/LO}}{f_{3D/LO}} \approx \left(\frac{\omega_H}{\omega_d}\right)^{1/2} \ll 1, \tag{28}$$

i.e., the binding energies and the oscillator strengths decrease as the phonon becomes localized. The reason is that for $3D/LO$ the actual phonon momentum in the matrix element (5) is $q_\parallel \approx a^{-1}$, as against $q_\parallel \approx d^{-1}$ for $2D/LO$. In the calculation of W and f below we confine ourselves to the branches $l = \pm 1$, for only they enter in the intraband absorption coefficient in the region $\omega \approx \omega_0$.

Strong fields ($\sigma \ll 1$). In strong fields only the term $s = 0$ is to be retained in the sum (14), so that

$$K^{\pm 1}(tt') = \pm [\tilde{\Phi}(t)\tilde{\Phi}(t')]^{1/2} e^{-1/2(t+t')} J_1(2(tt')^{1/2}). \tag{29}$$

We see hence that the spectra and oscillator strengths of the branches $l = 1$ and $l = -1$ are obtained from each other by mirror reflection about the threshold. All the physical parameters, particularly d and H, enter in the kernel $K^{\pm 1}$ only in the form of multipliers (via the from factors). The binding energies and the oscillator strengths of all the states depend

on d and H in like manner. All these conclusions are independent of the degree of localization of the phonon.

For $2D/LO$, the kernel K^l (14) differs only by a factor from the kernel investigated in Ref. 3. Therefore, borrowing the eigenvalues and eigenfunctions from this reference, we get

$$W_r^{\pm}=\pm(-1)^r b\alpha\omega_0\sigma^{-1}\delta^{1/2}\rho^{2(r+1)},$$
$$f_r^{\pm}=b\alpha\delta^{1/2}5(r+1)\rho^{4(r+1)}, \qquad (30)$$

where $\rho=(5^{1/2}-1)/2=0.618...$, $r=0,1,2,...$.

No resolvent could be found for $3D/LO$. It is easily seen, however, that

$$W_r^{\pm}=\pm(-1)^r b\alpha\omega_0\sigma^{-1}\delta^{1/2}\rho^{2(r+1)},$$
$$f_r^{\pm}=2\alpha\sigma^{1/2}\left|\int_0^{\infty}dt\, e^{-t/2}t^{1/4}\tilde{\chi}_r(t)\right|^2, \qquad (31)$$

where $\tilde{\lambda}_r$ and $\tilde{\chi}_r$ are the eigenvalues and eigenfunctions of the kernel

$$2e^{-1/2(t+t')}(tt')^{-1/4}J_1(2(tt')^{1/2}). \qquad (32)$$

Since this kernel contains no parameter, it follows that $\tilde{\lambda}_r$ and the integral in (31) are of order unity. Using, as in Ref. 3, the Sylvester determinants of the kernel (32), we can show that eigenvalues of either sign exist, and their number is infinite.

Weak fields ($\sigma\gg 1$). In this case the kernel K^l (14) can be approximated by a sequence of degenerate kernels.[3] Omitting the calculations, we present only the results.

In the lowest order in H we get three bound states above the threshold: two with $l=+1$ and one with $l=-1$. For $2D/LO$ we have

$$W^{+}=-\alpha\omega_0 b(2\pm 3^{1/2})\sigma^{-2}\delta^{1/2}, \quad f^{+}=\alpha b\frac{3^{1/2}\pm 1}{2\cdot 3^{1/2}}\sigma^{-2}\delta^{1/2},$$
$$W^{-1}=-\alpha\omega_0 b\sigma^{-2}\delta^{1/2}, \quad f^{-}=\alpha b\sigma^{-2}\delta^{1/2}. \qquad (33)$$

For $3D/LO$ we have

$$W^{+}=-\alpha\omega_0\pi^{1/2}\frac{23\pm(337)^{1/2}}{16}\sigma^{-1/2}, \quad f^{+}=\alpha\pi^{1/2}\frac{(337)^{1/2}\pm 11}{2(337)^{1/2}}\sigma^{-1/2},$$
$$W^{-}=-\alpha\omega_0\pi^{1/2}\sigma^{-1/2}, \quad f^{-}=\alpha\pi^{1/2}\sigma^{-1/2}. \qquad (34)$$

It is seen from these equations that the state with $l=-1$ is located between the two states with $l=+1$ and the oscillator strength of the state with $l=-1$ is the sum of the oscillator strengths of the two states with $l=+1$.

In higher orders in H, bound states appear with binding energies and oscillator strengths proportional to higher powers of H.

It is clear from the results of the calculations for W_r and f_r that the absorption spectrum in both right and left polarization should constitute an "asymmetric doublet" (Fig. 4). In a strong field H this is asymmetry with respect to a numerical parameter of type ρ, and in a weak field—with respect to the large parameter σ.

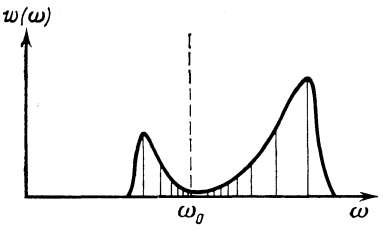

FIG. 4. Spectrum of absorption of bound states.

5. NUMERICAL ESTIMATES

It is clear from the results of Sec. 4 that the most favorable object for the observation of bound states in an absorption spectrum is a quantum well in which the LO phonon is not localized. This situation obtains in $Ga_{1-x}Al_xAs|GaAs|Ga_{1-x}Al_xAs$ structures with small x. For example, at $x=0.3$ the frequency of the LO oscillations of GaAs changes little on going from pure GaAs to the alloy $Ga_{1-x}Al_xAs$, viz., from 292 to 281 cm^{-1} (Ref. 9). The degree of localization of the LO phonon should therefore be small.

We choose for the estimates a GaAs quantum well with $d=100$ Å, where $\hbar\omega_D=57$ meV and $E_2-E_1=170$ meV, approximately five times larger than $\hbar\omega_0=36$ meV. Since $\hbar\omega_0=17$ meV even in a strong field $H=100$ kOe, the assumption that the well is narrow is well justified.

In a field $H=100$ kOe we have $\sigma=2.1$ and we can use Eqs. (34) for the estimates. This yields

$$|W^{+}|=\begin{cases}4 & \text{meV}\\ 0.4 & \text{meV}\end{cases}, \quad f^{+}=\begin{cases}0.03\\ 0.01\end{cases},$$
$$|W^{-}|=1.5 \text{ meV} \quad f^{-}=0.04.$$

Since these bound states lie above the threshold, their observation should not be hindered by strong lattice reflection, as was the case for $3D$ electrons, when all the bound states were below the threshold.

To estimate the absorbed energy fraction (21) we replace the delta function by a Lorentzian having a width corresponding to the lifetime τ. At the absorption maximum we have then $\pi\delta(\omega)\to\tau$, so that

$$w=2\pi\mathcal{N}\frac{e^2}{mc^2}\frac{c}{(\varkappa(\omega_0))^{1/2}}f\tau.$$

We assume for the estimate $\mathcal{N}=5\cdot 10^{11}$ cm^{-2} and $\tau=10$ ps (corresponding to a mobility $\mu=2.5\cdot 10^5$ $V\cdot cm^2/s^2$. We obtain then $w\approx 0.1$ for $f=0.04$. Recalculation to the bulk absorption coefficient $\chi=w/d$ yields $\chi\approx 10^5$ cm^{-1} (at a bulk density $\mathcal{N}/d=5\cdot 10^{17}$ cm^{-3}).

[1)] Physics Research Institute, Armenian Academy of Sciences.

[1]I. B. Levinson, Pis'ma Zh. Eksp. Teor. Fiz. **12**, 496 (1970) [JETP Lett **12**, 347 (1970)].
[2]I. B. Levinson, A. Yu. Matulis, and L. M. Shcherbakov, Zh. Eksp. Teor. Fiz. **61**, 843 (1971) [Sov. Phys. JETP **34**, 449 (1972)].
[3]B. I. Kaplan and I. B. Levinson, Fiz. Tverd. Tela (Leningrad) **14**, 1412 (1972) [Sov. Phys. Solid State **14**, 1212 (1972)].
[4]Y. B. Levinson and E. I. Rashba, Rep. Progr. Phys. **36**, 1499 (1973).

[5]I. B. Levinson and É. I. Rashba, Usp. Fiz. Nauk **111**, 683 (1973) [Sov. Phys. Usp. **16**, 892 (1974)].
[6]I. B. Levinson, A. Yu. Matulis, and L. M. Shcherbakov, Zh. Eksp. Teor. Fiz. **60**, 859 (1971) [Sov. Phys. JETP **33**, 464 (1971)].
[7]B. I. Kaplan and I. B. Levinson, Fiz. Tverd. Tela (Leningrad) **14**, 1663 (1972) [Sov. Phys. Solid State **14**, 1434 (1972)].
[8]L. I. Korovin and B. É. Éshpulatov, *ibid.* **21**, 3703 (1979) [**21**, 2137 (1979)].
[9]P. Parayanthal and F. H. Pollak, Phys. Rev. Lett. **52**, 1822 (1984).

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