# LOCAL STATES OF AN ELECTRON, IN A POTENTIAL WELL, CAUSED BY A STRONG MAGNETIC FIELD

L. S. KUKUSHKIN

Physicotechnical Institute of Low Temperatures, Academy of Sciences, Ukrainian SSR

Submitted November 11, 1967

Zh. Eksp. Teor. Fiz. 54, 1213–1219 (April, 1968)

The problem studied is the spectrum of an electron in a shallow potential well, of arbitrary radius, in the presence of a constant magnetic field. The treatment is carried out exactly for potentials of special form, but qualitatively the results are sufficiently general. A brief discussion is given of certain low-temperature effects to which these local states can lead in homopolar semiconductors.

## 1. INTRODUCTION

IT was first shown by Bychkov[1] that a potential well in the presence of a constant magnetic field always leads to the appearance of a bound electron state. The shape of the well was considered to be of $\delta$ form; this can be justified in the case of good metals, where, in consequence of the strong shielding of the impurity potential, its radius $\alpha$ is considerably smaller than the other important dimensions of the problem, in particular the characteristic magnetic length $\rho_0 = \sqrt{c\hbar/eH}$. Scattering of an electron by a $\delta$-form potential well was also treated by Skobov[2] and by Demkov and Drukarev[3]; scattering by a linear dislocation of small radius was treated by Kosevich and Tanatarov[4].

In semiconductors, where the local states may manifest themselves in an important way in galvanomagnetic phenomena, even at not very large magnetic fields the value of $\rho_0$ may be found to be of the order of or even smaller than $\alpha$. Potential wells of large radius, for electrons in homopolar crystals, can also be produced by strain fluctuations of the lattice. The case $\alpha \gg \rho_0$ and the $\delta$-form potential were studied in detail in the fundamental work of Kubo, Miyake, and Hashitsume[5]. Although local states were not considered in this work, the method presented there presumably makes it possible to obtain them for both limiting cases.

Local levels can lead to an independent effect in a strong magnetic field only in a case in which there are no local states in the well without the magnetic field; that is, when

$$\varkappa \equiv -2m^*V_0\alpha^2/\hbar^2 < \varkappa_{cr}, \tag{1}$$

where $V_0 < 0$ is a characteristic value of the potential in the well and where $m^*$ is the effective mass of the electron, which for simplicity will henceforth be considered isotropic. The dimensionless parameter $\kappa$ determines the "strength" of the well with respect to the formation in it of localized states in the absence of a magnetic field (for potential wells of simple form, $\kappa \approx 2$).

The present paper investigates the intermediate case $\alpha = 0(\rho_0)$ when $\kappa < \kappa_{cr}$. Although in this case it is feasible to treat only potentials of special form, the results obtained are qualitatively correct under sufficiently general suppositions about the form of the well, so that the local levels are determined by integral properties of the potential.

## 2. THE CASE $\alpha = O(\rho_0)$

The Hamiltonian of the system under consideration has the form

$$H = \frac{1}{2m^*}\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + V(\mathbf{r}) = H_0 + V(\mathbf{r}). \tag{2}$$

We shall be interested in the density of the electronic spectrum corresponding to (2),

$$\rho(E) = \operatorname{Im}\operatorname{Sp} G(E)/\pi, \tag{3}$$

where $G(E) = (E - i0 - H)^{-1}$. For the resolvent G we can write the integral equation

$$G = G^0 + G^0VG, \tag{4}$$

where $G^0 = (E - i0 - H_0)^{-1}$, and for (4) the Neumann series

$$G = G^0 + G^0VG^0 + G^0VG^0VG^0 + \ldots \tag{5}$$

In the calculation of $\rho(E)$ for $E^* \equiv E - \mu H < 0$ (local levels) or close to the bottom of the continuous spectrum, $0 < E^* \ll \mu H$ ($\mu$ is the Bohr magneton), in the case of strong magnetic fields and of potential wells $V(\mathbf{r})$ with $\kappa < \kappa_{cr}$, we can choose as a basis for Sp G states belonging to the first Landau band; that is, the functions

$$\psi_{k_x, k_z, 0} = \frac{\exp\{i(k_xx + k_zz)\}}{\pi^{1/4}\rho_0^{1/2}V^{1/3}}\exp\left\{-\frac{1}{2}\left(\frac{y - y_0}{\rho_0}\right)^2\right\}, \tag{6}$$

where $y_0 = \rho_0^2 k_x$; V is the volume of the crystal. An estimate of the error that results from neglect of the states with $n \neq 0$ is made in the next section.

Let

$$V(\mathbf{r}) = V_0W(z)\exp\{-(x^2 + y^2)/\alpha^2\}. \tag{7}$$

Since for $n = 0$ the matrix elements of $G^0$ depend only on $k_z$ and are

$$(E^* - i0 - \hbar^2k_z^2/2m^*)^{-1}\delta_{k_zk_z'} \equiv G^0_{k_z}\delta_{k_zk_z'}, \tag{8}$$

it follows that

$$\rho(E) = \rho_0(E) + \frac{1}{\pi}\operatorname{Im}\left\{\sum_{k_x}(e^{-(x^2+y^2)/\alpha^2})_{k_xk_x}\sum_{k_z}G^0_{k_z}W_{k_zk_z}G^0_{k_z}\right. \tag{9}$$
$$\left. + \sum_{k_xk_x'}(e^{-(x^2+y^2)/\alpha^2})_{k_xk_x'}(e^{-(x^2+y^2)/\alpha^2})_{k_x'k_x}\sum_{k_z,k_z'}G^0_{k_z}W_{k_zk_z'}G^0_{k_z'}W_{k_z'k_z}G^0_{k_z} + \ldots\right\};$$

$\rho_0(E)$ is the density of the spectrum in the absence of the potential well;

$$W_{k_x k_x'} = \frac{1}{V^{1/3}} \int_{-\infty}^{\infty} W(z) e^{i(k_z - k_z')z}\, dz, \tag{10}$$

$$\left[\exp\left(-\frac{x^2+y^2}{\alpha^2}\right)\right]_{k_x k_x'} = \frac{\sqrt{\pi}}{V^{1/3}} \frac{\alpha}{\sqrt{1+\gamma}}$$

$$\times \exp\left\{\frac{\alpha^2}{4}\frac{1+2\gamma}{1+\gamma}\left[-\left(1+\frac{2\gamma^2}{1+2\gamma}\right)(k_x^2+k_x'^2)+2k_x k_x'\right]\right\}; \tag{11}$$

$$\gamma = (\rho_0/\alpha)^2. \tag{12}$$

We shall calculate the sums that occur in (9),

$$A_n = \sum_{k_1, k_2, \ldots, k_n} \left[\exp\left(-\frac{x^2+y^2}{\alpha^2}\right)\right]_{k_1 k_2} \ldots$$

$$\ldots \left[\exp\left(-\frac{x^2+y^2}{\alpha^2}\right)\right]_{k_{n-1} k_n} \left[\exp\left(-\frac{x^2+y^2}{\alpha^2}\right)\right]_{k_n k_1}. \tag{13}$$

On going over to an integration with respect to $k_i$,

$$\sum_{k_i} \ldots \to \frac{V^{1/3}}{2\pi} \int_{-\infty}^{\infty} dk_i \ldots$$

and on making the substitution $\frac{1}{2}\alpha[(1+2\gamma)/(1+\gamma)]^{1/2} k_i = \tilde{k}_i$, we get

$$A_n = \frac{1}{[2\pi(1+2\gamma)]^{n/2}} \tag{14}$$

$$\times \int d\mathbf{k}_n \exp\left\{-\left(1+\frac{2\gamma^2}{1+2\gamma}\right)\sum_{i=1}^{n} k_i^2 + (k_1 k_2 + \ldots + k_{n-1}k_n + k_n k_1)\right\},$$

where $k_n$ is the n-dimensional vector $(k_1, k_2, \ldots, k_n)$; the integration is carried out over the whole n-dimensional space.

We shall reduce the positive definite quadratic form in the exponent of the exponential function in the integrand to canonical form. The reduction is conveniently carried out by means of an orthogonal transformation, since then the Jacobian of the transformation is unity. The desired characteristic values are the roots of the equation

$$\det \| a_{im} - \lambda \delta_{im} \| = 0, \tag{15}$$

where $\| a_{im} \|$ is the matrix of the quadratic form. As a result of some transformations we get

$$\lambda_l = -\left(1+\frac{2\gamma^2}{1+2\gamma} - \cos\frac{2\pi l}{n}\right), \quad l = 0, 1, \ldots n-1, \tag{16}$$

that is,

$$A_n = \left[\prod_{l=0}^{n-1}\left\{1 - 2(1+2\gamma)\cos\frac{2\pi l}{n} + (1+2\gamma)^2\right\}\right]^{-1/2}. \tag{17}$$

It is easy to show that for arbitrary n

$$A_n = \frac{1}{(1+2\gamma)^n - 1} = \left[\frac{1}{1+2\gamma}\right]^n + \left[\frac{1}{(1+2\gamma)^2}\right]^n + \ldots. \tag{18}$$

Substitution of (18) into (9) allows us to state the final result: the desired spectral density $\rho(E)$ for $E^* < 0$ and for $0 < E^* \ll \mu H$ is written as the sum of the spectral densities $\rho_l(E^*)$ of the one-dimensional problems obtained in the absence of the magnetic field for potentials $V_0 W(z) \cdot (1+2\gamma)^{-l}$; that is,

$$\rho(E) = \sum_{l=1}^{N} \rho_l(E^*). \tag{19}$$

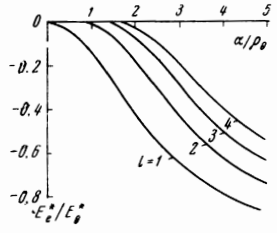
It is not difficult to reason that N is equal to the multiplicity of the degeneracy with respect to $k_x$ of the spectrum of $H_0$ for given $k_x$ and given number of the Landau band; that is, $N = V^{2/3}/2\pi\rho_0^2$. For $E^* < 0$,

$$\rho(E) = \sum_{l=1}^{N} \delta(E^* - E_l^*), \tag{20}$$

where $E_l^*$ is the local level in the one-dimensional potential well $V_0 W(z)(1+2\gamma)^{-l}$. The condition $\kappa < \kappa_{cr}$ guarantees the uniqueness of such a level for each well $l$, if the radius of $W(z)$ is also of order $\alpha$. The same condition permits use, for finding $E_l^*$, of the well-known formula (see [6])

$$E_l^* = -\frac{2m^* V_0^2}{\hbar^2 (1+2\gamma)^{2l}} \left(\int_{-\infty}^{\infty} W(z)\, dz\right)^2. \tag{21}$$

For $\alpha < \rho_0$ and even for $\alpha = 0(\rho_0)$, the level $E_1^*$ is important, but the rest are squeezed to the bottom of the continuous spectrum, and for even a small broadening (see Sec. 4) they fuse with the continuous spectrum; this leads only to a small shift of its edge. For $\alpha \gg \rho_0$, the local levels fill the $E^*$ interval $(E_0^*, 0)$ densely; but in the limit $\alpha \to \infty$, all N local levels "creep" on to the level $E_0^*$. This was to be expected, since in this limit $V(r) = V_0 W(z)$, and the Schrödinger equation permits separation of variables. This picture is illustrated in the figure, which shows the change of the depth of the local levels as a function of $\alpha/\rho_0$ for a given potential.




The results obtained become graphic if, instead of (6), we consider wave packets, localized in a plane perpendicular to the magnetic field, along both axes, and constituting stationary states of $H_0$ in consequence of the degeneracy with respect to $k_x$. It is possible to construct packets of such form that their centers are at sites of a square lattice with distance $\sqrt{2\pi}\,\rho_0$, and their radii are equal to $2\rho_0$:

$$\psi_{l'm} = \frac{e^{ik_z z}}{V^{1/6}\sqrt{2\pi}\,\rho_0} \exp\left\{\frac{i(y+y_l)(x-x_m)}{2\rho_0^2}\right\}$$

$$\times \exp\left\{-\frac{(y-y_l)^2 + (x-x_m)^2}{4\rho_0^2}\right\}. \tag{22}$$

where

$$x_l = y_l = \sqrt{2\pi}\rho_0 l; \quad l = 0, \pm 1, \ldots, \pm \tfrac{1}{2} V^{1/3} / \sqrt{2\pi}\rho_0.$$

If $\alpha \ll \rho_0$, a single state (22) is significantly perturbed by the potential, and practically a single localized level is split off from the continuous spectrum; the others are shallow in accordance with the smallness of the overlapping of the wave functions of the other states with the potential. For $\alpha \gg \rho_0$, on the contrary, there are a multitude of $\psi_{l,m}$'s within the range of the potential; therefore many levels split off from the continuous spectrum, filling the interval $(E_0^*, 0)$ densely. In this case the one-dimensional character of the problem is obvious.

To investigate formula (21), we shall suppose that $V(r)$ is spherically symmetric; that is, $W(z) = \exp\{-z^2/\alpha^2\}$. Then

$$E_l^* = -\frac{\pi}{4}\varkappa^2\frac{\hbar^2}{2m^*\rho_0^2}\frac{\gamma}{(1+2\gamma)^{2l}}. \quad (23)$$

For $\alpha \gg \rho_0$, the ground level ($l = 1$) is

$$E_1^* \approx E_0^* = -\frac{\pi}{8}\frac{\hbar^2}{m^*\alpha^2}\varkappa^2, \quad (24)$$

that is, for given strength $\kappa$ of the well the value of $|E_1^*|$ decreases with increase of $\alpha$. For $\alpha \ll \rho_0$,

$$E_1^* = -\frac{\pi}{8}(\mu H)^2\frac{m^*\alpha^2}{\hbar^2}\varkappa^2, \quad (25)$$

that is, the value of $|E_1^*|$ increases with increase of $\alpha$. Formula (25) agrees with the results of [1] and [3], if we introduce the concept of scattering length for a $\delta$-form potential. Thus for constant H and for constant $\kappa < \kappa_{cr}$, the depth of the ground level is greatest for $\alpha = 0(\rho_0)$. (If $V(r) = V_0\exp(-r^2/\alpha^2)$, then the optimum value of $\alpha$ is $\sqrt{2}\rho_0$.) This is a very important property of potentials with $\alpha = 0(\rho_0)$, since the manifestation of a localized level depends to an appreciable degree on its depth.

## 3. THE CASE $\alpha \ll \rho_0$. DISCUSSION OF THE APPROXIMATIONS CHOSEN

In order to estimate the error that arises in the calculation of local levels if we take account only of the first Landau band, we consider the case $\alpha \ll \rho_0$, which permits exact solution. The potential $V_0\exp(-r^2/\alpha^2)$ can in this case be replaced by an operator of first rank, introduced by Lifshits [7]:

$$\hat{\Lambda}\psi = \frac{V_0}{\sqrt{8}}(\varphi,\psi)\varphi, \qquad \varphi = \left(\frac{2}{\pi\alpha^2}\right)^{3/4}\exp\left(-\frac{r^2}{\alpha^2}\right) \quad (26)$$

(the brackets in (26) denote the scalar product), since when $\alpha$ is much smaller than the characteristic length over which $\psi$ changes, $\hat{\Lambda}\psi \approx V_0\exp(-r^2/\alpha^2)\psi$. It is not difficult to show that (3) in this case has the form

$$\rho(E) = \rho_0(E) + \frac{V_0}{\sqrt{8}}\mathrm{Im}\Big\{\sum_\lambda (G_{\lambda\lambda}{}^0)^2|(\psi_\lambda,\varphi)|^2 \times\Big[1-\frac{V_0}{\sqrt{8}}\sum_\lambda G_{\lambda\lambda}{}^0|(\psi_\lambda,\varphi)|^2\Big]^{-1}\Big\}, \quad (27)$$

$\lambda$ designates the combination $(n, k_x, k_y)$. For $E_0^* < 0$ the spectral density in the absence of the perturbation is $\rho_0(E) = 0$, and the $G_{\lambda\lambda}{}^0$'s are real; therefore the local level $E_{loc}{}^*$, which in this case is unique, is determined by the equation

$$1-\frac{V_0}{\sqrt{8}}\sum_\lambda G_{\lambda\lambda}{}^0|(\psi_\lambda,\varphi)|^2 = 0. \quad (28)$$

By means of quite cumbersome calculations, (28) can be transformed to the form

$$1-\frac{\sqrt{\pi}}{4\sqrt{2}}\frac{\varkappa}{\gamma}\exp\left\{-\frac{E_{loc}}{2\gamma\mu H}\right\}\sum_{n=0}\left[1-\Phi\left(\sqrt{-\frac{E_{loc}}{2\gamma\mu H}}+\frac{n}{\gamma}\right)\right] \times\exp\left\{n\frac{c_n}{\gamma^3}\right\}\left(-\frac{E_{loc}}{2\gamma\mu H}+\frac{n}{\gamma}\right)^{-1/2} = 0. \quad (29)$$

For $n \ll \gamma$, $c_n \approx 1/24$; it thereafter increases slowly to $1/6$; $\Phi(x)$ is the probability integral. If in the sum (29) we keep only the first term and if we suppose that $E_{loc}{}^* \ll \mu H$, then we get $E_{loc}{}^*$ an expression that agrees with (25).

The exact value of $|E_{loc}{}^*|$ exceeds $|E_1^*|$, since all terms of the sum (29) have the same sign; $E_{loc}{}^*$ can be determined from (29) by the method of successive approximations. Even the first approximation, obtained by substitution in the terms with $n \geq 1$ of the value of $E_1^*$ instead of $E_{loc}{}^*$, insures good accuracy when $\kappa < \kappa_{cr}$ (in the case considered, $\kappa_{cr} = 2$). If $\kappa \ll \kappa_{cr}$, then $E_{loc}{}^*$ practically coincides with $E_1^*$. If we extrapolate equation (29) to the case $\alpha = 0(\rho_0)$, then for $\alpha = \rho_0$ and $\kappa = 1$ the value of $|E_{loc}{}^*|$ is found to be about 30% greater than $|E_1^*|$. When $\kappa \approx \kappa_{cr}$, taking account of the first Landau band becomes insufficient; this is clear from the fact that when $\kappa > \kappa_{cr}$, when the local level appears in the absence of a magnetic field, $E_{loc}{}^*$ depends only slightly on $\alpha$ and does not approach zero when $\alpha \to 0$.

## 4. LOCAL STATES IN SEMICONDUCTORS

In concluding this paper, we shall discuss briefly certain effects to which these local states can lead in semiconductors. For the appearance of such a local state it is necessary, first of all, that its width shall be smaller than the binding energy; that is, the distance of the local level from the continuous spectrum. If the local levels are due to impurities, then the chief cause of broadening of them is overlapping of the wave functions of different centers (similar concentration broadening leads to the occurrence of an impurity band in semiconductors). When $r_0c^{1/3} \ll 1$, where $r_0$ is the radius of the local state and c is the concentration of the impurity, the concentration broadening is much less than $|E_{loc}{}^*|$. In homopolar crystals, where the electrons interact appreciably only with long-wave acoustic vibrations, as long as this interaction is not too strong the phonon broadening of the local levels at low temperatures is also small.

The most interesting manifestation of local levels in homopolar crystals is connected, it seems to us, with the case in which the potential well occurs in consequence of strain fluctuations of the lattice. In this case there is a possibility of the appearance of coupled electron-phonon states, which at large radii of the states may turn out to be energetically favorable (in contrast to the condenson states without a magnetic field, considered by Deĭgen and Pekar [8]).

We indicate also an obvious low-temperature effect, consisting in the rapid increase of the longitudinal magnetoresistance at a value of the magnetic field at which the broadening of the local levels becomes less than their depth.

I take this occasion to express my thanks to I. M. Lifshitz, A. M. Kosevich, and I. O. Kulik for discussion of the results of the research.

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Translated by W. F. Brown, Jr.
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