MAGNETIC SURFACE LEVELS IN A SUPERCONDUCTOR

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It is shown that finite motion of the single-particle excitations in a magnetic field near the surface of a superconductor may lead to the existence of a comparatively large number of discrete quantum levels located below the energy gap. The quasiclassical problem of surface excitations is solved, and the spectrum of these excitations is found. The results are illustrated by calculations on an electronic computer.

In a normal metal the finite motion of the electrons in a magnetic field near the surface of the metal corresponds to the system of quantum levels investigated by Prange and Nee.[1] In particular, the spectrum of the surface electron states may be obtained quasiclassically from the well-known rule of quantization

$$\int_0^{x_0} p(x)\,dx = (n+\gamma)\pi\hbar,$$

where p and x denote the corresponding momentum and coordinate, and the motion is enclosed between the surface of the metal and the turning point of the electron in a magnetic field.

Somewhat earlier Pincus[2] pointed out the possibility of the existence of bound states of single-particle excitations near the surface of a superconductor and showed that the gap in the spectrum of the surface excitations decreases in comparison with the energy gap Δ, characteristic of a superconductor, by an amount of the order of the energy of the interaction of the excitations with the magnetic field, $e\mathbf{A}\cdot\mathbf{v}/c \sim \Omega\delta p_0$. Here $\mathbf{A}$ is the vector potential, v is the electron's velocity, Ω is the cyclotron frequency, δ is the penetration depth of the field, and p_0 is the Fermi momentum. Due to the large value of the momentum in the plane of the surface, the "shift" of the gap in the spectrum of the surface excitations is already comparable with Δ in fields of the order of a few oersteds. The existence of surface excitations leads to singularities in the density of the single-particle states at energies below Δ and appears, in particular, in the resonance absorption of the electromagnetic field at frequencies corresponding to the shifted energy gap.[3]

The results of article[2] are obtained by numerical solution of the equations for a superconductor[1)] and therefore are hard to interpret. Since the spectrum of the surface excitations is extremely sensitive to a small change of the parameters, in the scheme of the Pincus calculations it is difficult to also answer the question of the number of levels under the gap. In the present article we show that in a certain range of variation of the parameters the number of surface levels turns out to be sufficient so that the problem can be regarded as quasiclassical, analogous to what is done in a normal metal.

[1)]Numerical calculation of the surface levels is also carried out in article [4].

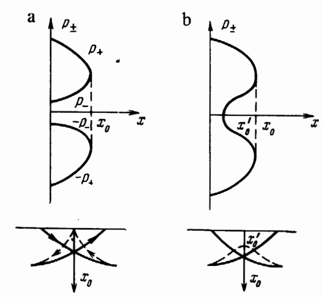

FIG. 1

From a quasiclassical point of view, in a superconductor a bound state near the surface is realized in the form of an electron-hole pair, each of the excitations of which is localized in a layer of the order of the penetration depth, or more exactly—in a layer of the order of the depth of the potential well near the surface, created by the magnetic field.[2)] The motion of such a pair along the surface of the superconductor corresponds to the quantization rule which, in a typical case, has the form

$$\int_0^{x_0} (p_+(x) - p_-(x))\,dx = (n+\alpha)\pi\hbar,$$

where $p_\pm$, respectively, are the quasiclassical momenta of the electron and hole. At the turning point a mutual transformation of the electron and hole takes place (see Fig. 1 below). This assertion was contained in article[6]; here we give a rigorous derivation of it with the aid of a quasiclassical solution of the problem of surface excitations.

We note that the surface levels in superconductors are not at all analogous to the levels in a normal metal, although caused by the same diamagnetic interaction mechanism. The spectrum of surface excitations in a superconductor consists of a finite number of levels, distributed in the range from $\Delta - \Omega\delta p_0$ to Δ. The discrete levels turn into states of the continuous spectrum for $\epsilon > \Delta$ (ϵ denotes the excitation energy). Above Δ the motion of only one of the quasi-particles

[2)]In the region of weaker fields than the magnetic fields under consideration here, the excitations near the surface of a superconductor are localized over distances larger than the penetration depths, as a result of which a quasi-local level appears. This case is considered in the article by Azbel'. [5]

may turn out to be bound (this corresponds to the Prange levels); the motion of the other will be infinite. Therefore, the Prange levels arising in a superconductor for $\epsilon > \Delta$ are smeared out. Only as ϵ increases, when the binding between the excitations becomes all the more weak, we arrive at the surface levels for a normal metal (taking account, of course, of the inhomogeneity of the magnetic field).

1. In order to investigate the problem in a superconductor we shall start from the homogeneous Gor'kov equations for the wave functions of the quasiparticles[7]

$$\hat{H}\psi = \begin{pmatrix} \varepsilon + \frac{\hbar^2}{2m}\left(\nabla - i\frac{e}{\hbar c}\mathbf{A}\right)^2 + \mu & \Delta \\ -\Delta & -\varepsilon + \frac{\hbar^2}{2m}\left(\nabla + i\frac{e}{\hbar c}\mathbf{A}\right)^2 + \mu \end{pmatrix}\begin{pmatrix} g \\ f^+ \end{pmatrix} = 0. \quad (1)$$

The superconductor occupies the half-space $x > 0$. The vector potential is given by

$$\mathbf{A} = \left(0, -\int_x^\infty H(x')\,dx', 0\right).$$

Being interested in excitations moving along the surface, for which the angles of collisions with the surface are small ($\varphi < \varphi_0 \sim (\delta/R)^{1/2}$, where R denotes the radius of the orbit), we shall assume that the conditions for specular reflection are satisfied on the boundary

$$g|_{x=0} = f^+|_{x=0} = 0. \quad (2)$$

Since the number of surface excitations is small ($\sim\varphi_0$), the energy gap Δ is determined as usual by the self-consistent interactions inside the volume of the metal. In the linear approximation with respect to the magnetic field, the gap is constant. In Eqs. (1) we also neglect those terms which are quadratic in the vector potential.

Since the momenta $\hat{p}_y$ and $\hat{p}_z$ commute with the Hamiltonian $\hat{H}$, one can seek the solution of the system (1) in the form

$$\psi(r) = \begin{pmatrix} A \\ B \end{pmatrix} \exp\left\{i\frac{p_y y}{\hbar} + i\frac{p_z z}{\hbar}\right\} \exp\left\{i\frac{S(x)}{\hbar}\right\}, \quad (3)$$

where in the quasiclassical approximation S(x) is a rapidly varying function of the coordinates. Substituting (3) into (1) and defining the generalized momentum of the system by $p = \partial S/\partial x$, we obtain the following result in the main approximation with respect to the quasiclassical parameters

$$p_\pm^2/2m = \mu - \varepsilon_\perp \pm \left[\left(\varepsilon + \frac{e}{mc}A_y p_y\right)^2 - \Delta^2\right]^{1/2}, \quad (4)$$

where $\epsilon_\perp = (p_y^2 + p_z^2)/2m$.

The condition for the validity of the quasiclassical treatment has the usual form:

$$\frac{\partial}{\partial x}\left(\frac{\hbar}{p_\pm}\right) < 1.$$

For quasiparticles whose angles of flight from the surface do not exceed $(\delta/R)^{1/2}$, $p_\pm \sim (m\Omega\delta p_0)^{1/2}$ as is evident from Eq. (4). Thus, the criteria for the quasiclassical treatment can be written in the form

$$\hbar / \delta(m\Omega\delta p_0)^{1/2} < 1 \quad (5)$$

or, expressing δ in terms of the critical field H_c, $\delta^{-1} \sim evH_c/c\Delta$, and introducing the correlation radius $\xi_0 = \hbar v/\Delta$,

$$H > \hbar\xi_0 H_c / \delta^2 p_0. \quad (5')$$

Assuming $\xi_0 \sim 10^{-4}$ cm, $\delta \sim 10^{-5}$ cm, and $H_c \sim 10^2$ Oe, one can see thta there is a rather broad range of fields in which a quasiclassical treatment is valid.

Condition (5) expresses the usual requirement for a quasiclassical treatment, that the number of levels should be sufficiently large, $n \gg 1$. We note that the condition for the quasiclassical nature of the problem, obtained in article[5], coincides with formula (5).

Let us determine the boundaries of the classically accessible regions from the conditions that the velocities of the quasiparticles vanish:

$$v = \frac{\partial\varepsilon}{\partial p_\pm} = \pm m^{-1} p_\pm \left[\left(\varepsilon + \frac{e}{mc}A_y p_y\right)^2 - \Delta^2\right]^{1/2} \left(\varepsilon + \frac{e}{mc}A_y p_y\right)^{-1}. \quad (6)$$

As is evident from expression (6) the particles may possess two turning points, determined by the conditions $p_\pm(x_0') = 0$ and $(\epsilon + eA_y(x_0)p_y/mc)^2 = \Delta^2$. Therefore the following situations may arise.

There are no turning points at all. This corresponds to a large value of $\mu - \epsilon_\perp$, and the motion of the particles is infinite.

There is one turning point determined by the first of the conditions. This corresponds to $\epsilon > \Delta$ and corresponds to finite motion of one of the particles and infinite motion of the other. As already indicated in the Introduction, this case is characteristic for Prange levels above the energy gap.

Finally, a turning point may exist which is common for electron and hole, determined by the second of the conditions. In this connection the turning point $p(x_0') = 0$ may exist simultaneously.

We note that the turning point x_0 in the case of an electron ($\epsilon > 0$) will occur for $p_y < 0$, and for a hole ($\epsilon < 0$) for $p_y > 0$, which is related to the sign of the effective potential well. It is not difficult to see that the turning point x_0 arises only in the case $\epsilon < \Delta$, i.e., the quantum levels are located below the gap Δ. In fact, for $\epsilon = \Delta$ the second of the conditions is satisfied only for $x \to \infty$. The dependence of $p_\pm(x)$ for the latter two cases is shown in Fig. 1 a and 1 b. The dependence $p_\pm(x)$ corresponds to the classical trajectories $v_\pm(x) = \dot{x}_\pm(x)$ shown on the same figure. It is obvious that discrete quantum levels correspond to periodic trajectories near the surface of the metal.

2. Let us consider the situation shown in Fig. 1 a in detail. In this case the only turning point x_0, common to the electron and hole, is a reflection point for the particles. An electron traveling from the surface arrives at the point x_0 with momentum p_+, is reflected at this point and is transformed into a hole with momentum p_- (to depart with a different momentum is "forbidden" by the presence of a momentum jump between the pairs of branches at $x = x_0$). Correspondingly, a hole $(-p_-)$ at the turning point turns into an electron with momentum $-p_+$ upon reflection.

Let us prove this result. In order to do this it is convenient, having eliminated the function f^+ from the system (1), to proceed to an equation of fourth order for the wave function g. Introducing the dimensionless coordinate $\xi = xp_0/\hbar$, let us write it in the form

$$\left[\frac{\partial^4}{\partial\xi^4}+2\alpha\frac{\partial^2}{\partial\xi^2}+2\frac{\partial^2 A}{\partial\xi^2}+4\frac{\partial A}{\partial\xi}\frac{\partial}{\partial\xi}+\alpha^2+\left(\frac{\Delta}{\mu}\right)^2-\left(\frac{\varepsilon}{\mu}+2A\right)^2\right]g=0, \tag{7}$$

where $A = eA_y p_y/cp_0^2$ and $\alpha = (\mu - \epsilon_\perp)/\mu$.

The term containing the second derivative of the vector potential is of the order of $\hbar\Omega a/\delta$ (a is the lattice constant) and is small in comparison with the term $(\Delta/\mu)^2$. In the quasiclassical approximation one should also neglect the term containing the first derivative of g. The final equation, which we shall use in the quasiclassical treatment, takes the form

$$\left\{\frac{\partial^4}{\partial\xi^4}+2\alpha\frac{\partial^2}{\partial\xi^2}+\alpha^2+\left(\frac{\Delta}{\mu}\right)^2-\left(\frac{\varepsilon}{\mu}+2A\right)^2\right\}g=0 \tag{8}$$

Let us construct quasiclassical solutions of Eq. (8). As usual, in the region to the left of the turning point $(\xi < \xi_0)$ we represent the wave function in the form of a sum of oscillating exponentials, but by damped exponentials to the right $(\xi > \xi_0)$

$$g_{\xi<\xi_0}=(\xi_0-\xi)^{-1/4}\{A_1p_+^{-1/2}e^{iS_+}+A_2p_-^{-1/2}e^{iS_-}+A_3p_+^{-1/2}e^{-iS_+}+A_4p_-^{-1/2}e^{-iS_-}\},$$

$$g_{\xi>\xi_0}=-\frac{1}{2}(\xi-\xi_0)^{-1/4}\{B_1|p_+|^{-1/2}e^{i(S_+-\vartheta/2)}+B_2|p_-|^{-1/2}e^{i(S_-+\vartheta/2)} \tag{9}$$

$$+B_3|p_+|^{-1/2}e^{-i(S_++\vartheta/2)}+B_4|p_-|^{-1/2}e^{-i(S_--\vartheta/2)}\}, \tag{10}$$

where

$$S_\pm=\int_{\xi_0}^{\xi}p_\pm(\xi)\,d\xi,\qquad p_\pm=|p_\pm|e^{\pm i\vartheta}. \tag{11}$$

We note that in the region $\xi > \xi_0$ the wave function is represented by a product of oscillating, damped, and increasing exponentials in contrast to the usual quasiclassical solution.

The amplitudes B_i and A_i are related to each other by the transition matrix $B = \hat{\beta}A$. The general form of the matrix $\hat{\beta}$, which follows from relations of the type of unitarity,[3] was indicated in article[6]:

$$\hat{\beta}=\begin{pmatrix}\begin{matrix}u & v\\ z & w\end{matrix} & 0\\ 0 & \begin{matrix}z^* & \omega^*\\ u^* & v^*\end{matrix}\end{pmatrix} \tag{12}$$

The explicit form of the matrix $\hat{\beta}$ may be obtained by matching the solutions (9) and (10) with the asymptotic exact solution of Eq. (8) in the neighborhood of a turning point.

Let us find a solution near a turning point. We expand the vector potential in a series and confine our attention to the linear term $A(\xi) = A(\xi_0) + A'(\xi_0)(\xi - \xi_0)$, $A'(\xi_0) < 0$. Equation (8) takes the form

$$\left(\frac{\partial^4}{\partial\xi^4}+2\alpha\frac{\partial^2}{\partial\xi^2}+a_0+\beta^2\xi\right)g=0, \tag{13}$$

where

$$a_0=\alpha^2-\beta^2\xi_0,\qquad \beta^2=4\frac{\Delta}{\mu}|A_0'|.$$

We shall solve it by the Laplace method (see, for example,[8])

$$g=\sum_{i=1}^{4}C_i\int_{\Gamma_i}\exp\left[\frac{1}{\beta^2}\left(\frac{t^5}{5}+\frac{2}{3}\alpha t^3+(a_0+\beta^2\xi)t\right)\right]dt, \tag{14}$$

where the contours of integration Γ_i, corresponding to the four linearly independent solutions, must lie in those regions of the complex t plane where Re $t^5 < 0$ (see Fig. 2). Asymptotic representations of the solution (14) to the right and left of the turning point can be obtained by the saddle-point method, in analogy to the way this is done for Airy functions. The saddle points are given by

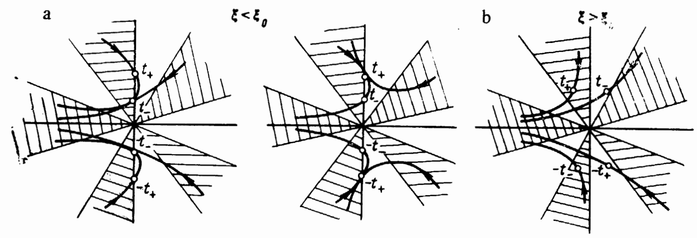

FIG. 2

$$t_{1,2}^2=-\alpha\mp\beta\sqrt{\xi_0-\xi}=-p_\pm^2(\xi). \tag{15}$$

For $\xi < \xi_0$ the saddle points are located on the imaginary axis, but the lines of descent pass through them, respectively, at angles $-\pi/4$, $-3\pi/4$ in the upper half-plane and $\pi/4$, $3\pi/4$ in the lower half-plane. The corresponding contours are shown in Fig. 2 a (the chosen directions of going around the contours are denoted by arrows). We note that the contours passing through the first and fourth quadrants (for $\xi > \xi_0$ they correspond to increasing solutions, as it is not difficult to see) can be continued in a nonunique manner. Both possibilities are shown in Fig. 2 a.

For $\xi > \xi_0$ the saddle points are displaced in the complex plane and the lines of descent go at angles of $3\pi/2 - \theta/2$ and $\pi + \theta/2$ respectively into the second and first quadrants, and at angles $\pi/2 + \theta/2$ and $\pi - \theta/2$ into the third and fourth quadrants. The contours of integration in this case are shown in Fig. 2 b.

For $\xi < \xi_0$ all solutions oscillate; for $\xi > \xi_0$ the solutions corresponding to contours passing through the points t_+ and $-t_-$ decrease exponentially, and the solutions which correspond to contours passing through t_- and $-t_+$ increase exponentially.

As a result the solutions (14) may be written in the form

$$\xi<\xi_0,\quad g=\begin{cases}C_1I_1+(C_1+C_2)I_2+C_4I_4+(C_3+C_4)I_3,\\ (C_1+C_2)I_1+C_1I_2+(C_3+C_4)I_4+C_4I_3,\end{cases} \tag{15}$$

$$\xi>\xi_0,\qquad g=\sum_i C_iI_i, \tag{16}$$

where I_i denote the values of the integrals (14) at the points t_+, t_-, $-t_-$, and $-t_+$, respectively, with the directions of circuit taken into account. Calculating the integrals by the method of steepest descent, for $\xi < \xi_0$ we obtain:

$$g=(\xi_0-\xi)^{-1/4}\{C_1p_+^{-1/2}e^{i(\Phi_+-\pi/4)}+(C_1+C_2)p_-^{-1/2}e^{i(\Phi_--3\pi/4)}$$

$$+(C_3+C_4)p_-^{-1/2}e^{-i(\Phi_--3\pi/4)}+C_4p_+^{-1/2}e^{i(\Phi_+-\pi/4)}\} \tag{17}$$

when the contours $\Gamma_{2,3}$ pass through the points $\pm t_-$ and

$$g=(\xi_0-\xi)^{-1/4}\{(C_1-C_2)p_+^{-1/2}e^{i(\Phi_+-\pi/4)}+C_1p_-^{-1/2}e^{i(\Phi_--3\pi/4)}$$

$$+(C_3-C_4)p_+^{-1/2}e^{-i(\Phi_++3\pi/4)}+C_4p_-^{-1/2}e^{-i(\Phi_--3\pi/4)}\}, \tag{18}$$

if the contours $\Gamma_{2,3}$ pass through the points $\pm t_+$.

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[3] We take this opportunity to correct an error in article [6]. Since in [6] the spectrum is determined correct to within a phase factor, only the fact of the diagonal nature of the matrix $\hat{\beta}$ is essential.

For $\xi > \xi_0$

$$g = (\xi - \xi_0)^{-1/4}\{C_1|p_+|^{-1/2}e^{i(\Phi_+ + 3\pi/2 - \vartheta/2)} + C_2|p_-|^{-1/2}e^{i(\Phi_- + \pi + \vartheta/2)} + C_3|p_+|^{-1/2}e^{-i(\Phi_+ - \pi + \vartheta/2)} + C_4|p_-|^{-1/2}e^{-i(\Phi_- - \pi/2 - \vartheta/2)}\}. \quad (19)$$

(All of the real factors not containing a dependence on ξ, which arise upon integration, entered into the definition of the constants C_i). Here

$$\Phi_\pm(\xi) = \frac{4}{\beta^2}\left(\frac{\alpha p_\pm^3}{3} - \frac{p_\pm^5}{5}\right), \quad (20)$$

where $p_\pm(\xi)$ are determined by formula (15). The functions $\Phi_\pm(\xi)$ are real for $\xi < \xi_0$ and complex for $\xi > \xi_0$.

At the same time, carrying out the integration in (11) near the turning point (here $S_\pm(\xi) = \Phi_\pm(\xi)$), we obtain the asymptotic behavior of the quasiclassical solutions (9) and (10). Joining them with the asymptotic exact solution (17)—(19), we find the transition matrix

$$\hat{\beta} = \begin{pmatrix} \hat{a} & 0 \\ 0 & \hat{a} \end{pmatrix}, \quad \hat{a} = \begin{pmatrix} e^{-\pi i/4} & e^{\pi i/4} \\ e^{\pi i/4} & e^{-\pi i/4} \end{pmatrix}. \quad (21)$$

In agreement with Eq. (12) the transition matrix is diagonal, where the eigen matrices $\hat{a}$ are transition matrices for the one-particle Schrödinger equation. Using the transition matrix (21), let us find the quantization rule for surface excitations. We write the wave function (9) in the region to the left of the turning point in the form

$$g = (\xi_0 - \xi)^{-1/4}\sum_i A_i p_\pm^{-1/2}\exp\left\{\pm i\int_{\xi_0}^{\xi} p_\pm d\xi\right\} = (\xi_0 - \xi)^{-1/4}\sum_i A_i' p_\pm^{-1/2}\exp\left\{\pm i\int_0^{\xi} p_\pm d\xi\right\},$$

where

$$A_i = A_i' \exp\{\pm i\int_0^{\xi_0} p_\pm d\xi\}.$$

From the boundary conditions (2) we find $A_1' = -A_3'$ and $A_2' = -A_4'$. Expressing the amplitudes B_2 and B_3 of the increasing solutions in the region to the right of the turning point in terms of the amplitudes A_i with the aid of Eq. (21), and letting $B_2 = B_3 = 0$, we obtain the corresponding condition

$$\begin{vmatrix} e^{i(S_+ + \pi/4)} & e^{i(S_- - \pi/4)} \\ e^{-i(S_+ + \pi/4)} & e^{-i(S_- - \pi/4)} \end{vmatrix} = 0,$$

from which the quantization rule

$$S_+ - S_- = \int_0^{x_0} (p_+ - p_-)\,dx = (n + 1/2)\pi\hbar. \quad (23)$$

follows.

In the situation shown in Fig. 1 b when there are two turning points x_0 and x_0', similar calculations lead to the result

$$\int_0^{x_0} p_+\,dx - \int_{x_0'}^{x_0} p_-\,dx = (n + 1/4)\pi\hbar \quad (24)$$

3. Let us consider formula (23) in more detail:

$$(2m)^{1/2}\int_0^{x_0}\left\{\left[\mu - \varepsilon_\perp + \left(\left(\varepsilon + \frac{e}{mc}A_y p_y\right)^2 - \Delta^2\right)^{1/2}\right]^{1/2} - \left[\mu - \varepsilon_\perp - \left(\left(\varepsilon + \frac{e}{mc}A_y p_y\right)^2 - \Delta^2\right)^{1/2}\right]^{1/2}\right\}dx = \left(n + \frac{1}{2}\right)\pi\hbar. \quad (25)$$

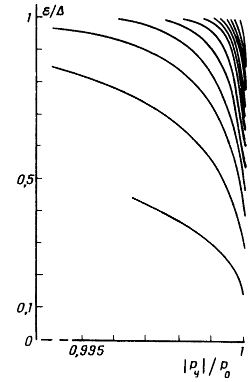

FIG. 3

The integral in (25) has a value $\sim\delta(m\Omega\delta p_0)^{1/2}$; therefore the number of levels $n \sim \delta(m\Omega\delta p_0)^{1/2}/\hbar$ with a relative distance between them given by $\Omega\delta p_0/n\Delta \sim (\Omega p_0/m\delta)^{1/2}\hbar/\Delta$. This rough estimate, as the results of machine calculations cited below show, nevertheless gives the correct order of magnitude of the number of levels. As is evident from this formula $n \sim \delta^{3/2}$. Such a substantial dependence of n on δ leads to an abrupt decrease in the number of levels for small penetration depths, and in particular explains the results of articles[2,4] ($n = 2$ for $\delta = 5 \times 10^{-6}$ cm). For $\delta \geq 10^{-5}$ cm one can expect on the order of ten or more levels. Unfortunately, even in the case of an exponential decrease of the vector potential the spectrum cannot be calculated in explicit form; however, the integrals in (25) reduce to elliptic integrals and can easily be calculated on a machine. The results of a calculation of the spectrum on an electronic computing machine are shown in Fig. 3, the calculations being carried out for the following values of the parameters: $A_y = -H\delta e^{-x/\delta}$, $H = 10$ Oe, $\delta = 6 \times 10^{-5}$ cm, and $\Delta = 6 \times 10^{-16}$ erg. As is evident from the figure, more than ten levels fit within the depth δ. The values of the parameters taken are somewhat arbitrary; however, they occur within experimentally attainable limits.

The spectrum presented in Fig. 3 agrees with the general picture of a transition from a local level to a quasiclassical situation, which was described by Azbel',[5] and corresponds to excitations, whose trajectories make angles of inclination to the surface which do not exceed $(\delta/R)^{1/2}$. For the indicated values of the parameters the characteristic angles of inclination are of the order of a few minutes:

$$\varphi \sim \frac{p_\pm}{p_y} \lesssim \frac{(m\Omega\delta p_0)^{1/2}}{p_0} \sim 10^{-3}.$$

In the present investigation we have neglected damping of the excitations. It is obvious that at low temperatures in a superconductor, just as in a normal metal, collisions with surface roughnesses are the basic mechanism of dissipation. Our investigation is based on the strict specular nature of the scattering; a small amount of diffuse scattering will lead to a washing out of the levels.[4)] The question of taking account of a small amount of diffuse scattering in the collisions of surface excitations with the boundaries in a super-

[4)] See the article by Fal'kovskiĭ [9] in which a calculation of the diffuse scattering of electrons in a normal metal is carried out.

conductor is of a rather fundamental nature and will be investigated separately.

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