

QUASICLASSICAL QUANTIZATION IN THE NEIGHBORHOOD OF SINGULAR CLASSICAL TRAJECTORIES

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It is shown that in general the only singular trajectories in phase space which are important in thermodynamics are trajectories which are self-intersecting. Such trajectories necessarily exist if the potential well has several minima. In the case of a metal in a magnetic field this corresponds to a non-convex bounding Fermi-surface. The system of equations for these cases is found and it is shown that near the point of self-intersection the separation between levels contains a part which oscillates with the magnetic field.

1. INTRODUCTION

It is known<sup>1</sup> that to determine the energy levels in the quasi-classical case it is sufficient to express the energy  $\epsilon$  as a function of the action variables  $I_i$  and to replace  $I_i$  in zeroth approximation by  $2\pi n_i \hbar$  ( $n_i$  is an integer,  $\hbar$  is Planck's constant) and in first approximation by  $2\pi(n_i + \gamma_i)\hbar$ ,  $0 < \gamma_i < 1$ .

For a one-dimensional motion (two-dimensional in phase space)

$$\epsilon = \epsilon(I), \quad I = \oint p dq = \Sigma(\epsilon),$$

where  $\Sigma(\epsilon)$  is the area bounding the classical orbit in phase space, and  $p$  and  $q$  are the generalized momentum and coordinate.

For the actual determination of the value of  $\gamma$  it is necessary to solve the Schroedinger equation; however, to find the separation  $\Delta\epsilon$  between levels in the zeroth approximation it is not necessary to know  $\gamma$ , since in any case it is a slowly varying function of  $n$  (compared with  $n$ ). Thus  $\gamma \approx \text{const}$ , and

$$\Sigma(\epsilon) = 2\pi(n + \gamma)\hbar, \tag{1.1}$$

$$\Delta\epsilon = \hbar\omega, \quad \omega = 2\pi(\partial\Sigma/\partial\epsilon)^{-1}. \tag{1.2}$$

I. M. Lifshitz and Kosevich<sup>2</sup> pointed out that the quantization rules (1.1) and (1.2) can be used directly to obtain the system of levels for an electron with an arbitrary dispersion law  $\epsilon = \epsilon(\mathbf{p})$  ( $\mathbf{p}$  is the quasimomentum) in a constant magnetic field  $\mathbf{H}(0, 0, H)$ . In momentum space the motion occurs in the plane  $(p_x, p_y)$ , and  $p_y$  and  $q_y = cp_x/eH$ , for which  $[\hat{p}_y, \hat{q}_y] = \hbar/i$ , can be regarded as the generalized coordinate and momentum. We therefore obtain immediately from (1.1) and (1.2) for this

case (cf. reference 2)

$$S(\epsilon, p_z) = \oint p_y dp_x = (n + \gamma)2\pi\alpha, \tag{1.3}$$

$$\alpha = \frac{|e|H\hbar}{c}, \quad \Delta\epsilon = \hbar\omega, \quad \omega = \frac{\alpha}{m^*\hbar}, \quad m^* = \frac{1}{2\pi} \frac{\partial S}{\partial \epsilon}. \tag{1.4}$$

Here  $m^*$  is the effective mass. Obviously (1.3) and (1.4) coincide with (1.1) and (1.2), if we replace  $S$  by  $\Sigma$  and  $\alpha$  by  $\hbar$ .

If the velocity  $\dot{\mathbf{p}}$  in momentum space [case (1.3) and (1.4)] or the velocity  $(\dot{p}, \dot{q})$  in phase space [the case of (1.1) and (1.2)] does not vanish, then it is known<sup>1</sup> that  $\gamma = 1/2$ . This fact was first established for an arbitrary dispersion law by Zil'berman.<sup>3</sup>

However, in both cases the presence of one free parameter (the energy  $\epsilon$  for the potential well and the momentum  $p_z$  for the case of fixed energy equal to the chemical potential  $\zeta$ , which alone is important for the electrons in a metal) has the result that in general there exists a quasi-classical trajectory on which, for the electrons in the metal, there is a point with  $\dot{\mathbf{p}} = 0$ :

$$\epsilon(\mathbf{p}) = \zeta, \quad v_x = v_y = 0. \tag{1.5}$$

Here we have used the relations

$$\dot{\mathbf{p}} = \frac{e}{c} [\mathbf{v} \times \mathbf{H}], \quad \mathbf{v} = \frac{\partial \epsilon}{\partial \mathbf{p}}, \quad \dot{p}_z = 0,$$

so that  $p_z$  is conserved.

For a one-dimensional potential well we have in this case  $\dot{p} = 0, \dot{q} = 0$ , so that

$$u'(q) = 0, \quad \epsilon = u(q), \tag{1.6}$$

where  $u(q)$  is the potential energy. In deriving (1.6) we have used the relation

$$\dot{p} = -\partial u/\partial q, \quad \dot{q} = p/m = \sqrt{2[\epsilon - u(q)]/m}.$$

It is easy to see that the equations (1.5) and (1.6) determine a trajectory which is self-intersecting (in momentum and phase space respectively). Such a trajectory is always present if the bounding Fermi surface is nonconvex or if the potential well has more than one minimum. In the neighborhood of this trajectory, naturally,  $\gamma \neq 1/2$ .

2. We shall, to be specific, consider throughout the following the more general case of an electron with an arbitrary dispersion law in a magnetic field; all the results are easily taken over to the case of a potential well with one or more "bumps."

It might seem that since the value of  $\gamma$  does not affect the distance between levels in zeroth approximation (as is to be expected since this separation is immediately obtained from the correspondence principle), the actual calculation of  $\gamma$  would be of no interest. However, this is not so. It turns out (cf. below) that the dependence of  $\gamma$  on  $n$  (and consequently on  $H$ ) in the neighborhood of the point of self-interaction appears, not in the next approximation in  $1/n$  as for the usual trajectories, but in the next approximation in  $1/\ln n$ :

$$\gamma = \gamma[(n - n_0)/\ln n] \quad (1.7)$$

( $n_0 \gg 1$  is the number labelling the level which is closest to the point of self-intersection), and if we carry out a computation correct to terms of order  $1/n$  the dependence of  $\gamma(n)$  must be taken into account.

This dependence is extremely important in computing the partition function, since the function (1.7) has, as a function of  $n$  in the complex plane, singularities at distances from  $n_0$  of the order of  $|n - n_0| \sim \ln n_0$ , which gives a quantum correction to the partition function of the order of some power of  $1/n_0$  (whereas the complex neighborhood of an ordinary point gives an exponentially small contribution, in accordance with the fact that the singularities are located at distances  $\sim n_0$  or  $\sim \sqrt{n_0}$  (cf. below).

This contribution can turn out to be especially large because of the fact that for real magnetic fields  $\ln n_0 \sim \ln(S/\alpha)$  is very small (for  $H \sim 10^4$  oe, for the anomalously small zones which mainly determine quantum effects,  $\ln n_0 \sim 1 - 4$ ; for the fundamental zones,  $\ln n_0 \sim 10$ ) and it can turn out, especially in sufficiently strong magnetic fields or in the case of strong anisotropy, that this contribution is comparable to, or even smaller than, the dimensionless characteristics of the orbit (which have a magnitude of the order of unity; how these enter we shall see later on). In this case, naturally, even the distance between

levels is not given correctly by formulas (1.2) and (1.4), since these refer to the case  $n_0 \rightarrow \infty$ ,  $\ln n_0 \rightarrow \infty$ .

In this sense it is important that the quantity  $\ln n_0$  be bounded for the section we are considering both from below and from above, since the magnetic field must be sufficiently large so that the magnitude of the quantum corrections to the thermodynamic quantities shall not be exponentially small:

$$\mu H \geq 2\pi^2 kT, \quad H \geq 2\pi^2 kT/\mu \quad (1.7')$$

( $\mu$  is the Bohr magneton for a conduction electron), and sufficiently small so that even one period of oscillation in the reversed magnetic fields is significant. These oscillations essentially alone permit us to distinguish the classical part of the given quantity from the quantum part:

$$H < 1/\Delta (H^{-1}) \sim cS/e\hbar. \quad (1.8)$$

Thus  $\ln n_0$  varies within a very limited range under ordinary experimental conditions.

In addition, as it turns out,  $\gamma H$  depends periodically on the magnetic field, which results in a new phenomenon: on top of the monotonic dependence of the distance between levels on magnetic fields there is superposed a periodic dependence which already makes itself manifest in the next approximation in  $1/\ln(S/\alpha)$ .

Thus the determination of the function  $\gamma(n, H)$  is very important for two reasons: first, only a knowledge of this function allows us correctly to compute the quantum part of the partition function (as well as, it is understood, the quantum part of the kinetic coefficients); and, secondly, finding  $\gamma$  enables us to clarify the interesting feature of the levels in the neighborhood of the trajectory which intersects itself: the presence of a part of the level separation which oscillates with the magnetic field.

3. We must explain why it is that in the present case the dependence of  $\gamma$  on  $n$  and  $H$  appears even in the next approximation in  $1/\ln n$ , and not in the approximation in some power of  $1/n$ . From what we have said above it is clear that the latter case is not of interest, and neither is the consideration of open trajectories, which give a much smaller contribution (except possibly for specially selected directions of the magnetic field) than the closed trajectories which are always present.

In order to answer this question, we note that the special feature of our case could make itself felt also in a somewhat different way. It is clear that formula (1.3) with  $\gamma = 1/2$  is always correct if in (1.4) the quantity  $m^* = (2\pi)^{-1} \partial S / \partial \epsilon$  is finite and

not equal to zero, so that  $\Delta\epsilon \neq 0$  and  $\Delta\epsilon \neq \infty$ . A priori this formula could break down for  $m^* = \infty$  or  $m^* = 0$ . The latter case is not at all possible:  $S(\epsilon)$  is always a monotonic function, since the intersection of orbits corresponding to different values of  $\epsilon$  for a given  $p_z$  and the same zone is impossible for a Hermitian energy operator. (This was pointed out by I. M. Lifshitz.) As for the case  $m^* = \infty$ , this just corresponds, as one easily sees from the definition of  $S$ , to the case we are considering of a trajectory which is self-intersecting.

It might seem that those cases should also be "suspect" where there are several areas corresponding to different zones. However, this is not so, since the probability of transitions between corresponding orbits is exponentially small if the orbits do not intersect, and in general is proportional to  $\hbar^{3/2}$ , if the orbits intersect (Zil'berman<sup>3</sup>), so that  $\gamma = \gamma(\sqrt{n})$ .

Contact of orbits with  $\epsilon = \zeta$  is an exceptional case, since it requires simultaneously satisfying the two relations

$$\begin{aligned} \epsilon_1(\mathbf{p}) = \zeta, \quad \epsilon_2(\mathbf{p}) = \zeta; \quad v_{1x} = v_{2x}, \quad v_{1y} = v_{2y}, \\ (v_1 = \partial\epsilon_1/\partial\mathbf{p}, \quad v_2 = \partial\epsilon_2/\partial\mathbf{p}). \end{aligned} \quad (1.9)$$

4. The only singular case of interest is thus the case of self-intersecting orbits. The form of the orbit near the point of self intersection is determined, for a given  $p_z$ , by the equations

$$v_x = v_y = 0, \quad (1.10)$$

$$\epsilon = \epsilon_0(p_z) \quad (1.11)$$

and can be found easily. Choosing the origin of coordinates at the point of self intersection and directing the coordinate axis so that at this point

$$\begin{aligned} \partial^2\epsilon/\partial p_x \partial p_y = 0, \quad \partial^2\epsilon/\partial p_x^2 = 1/m_1 > 0, \\ \partial^2\epsilon/\partial p_y^2 = -1/m_2 < 0, \end{aligned} \quad (1.12)$$

we have

$$\epsilon(\mathbf{p}) = \epsilon_0(p_z) + p_x^2/2m_1 - p_y^2/2m_2. \quad (1.13)$$

The closing of the curves in regions far from the origin can occur in two ways, as shown in Figs. 1 and 2 (we recall that, in accordance with the definition (1.12), all three axes have been chosen uniquely). The first case (Fig. 1) is realized for a Fermi surface with a "neck," (Fig. 3), and the second (Fig. 2) for a surface with an indentation (Fig. 4). In the following we shall, for brevity, call the case corresponding to Fig. 1 the case of a "neck" and that of Fig. 2 the case of an "indentation."

As we approach the trajectory which is self

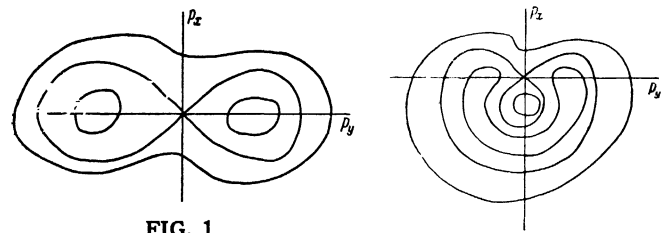


FIG. 1

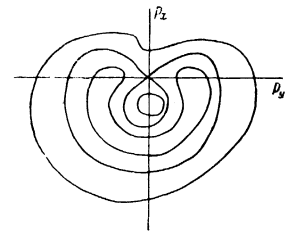


FIG. 2

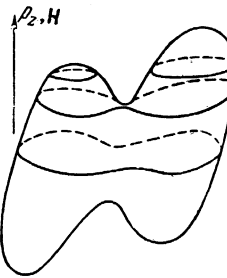


FIG. 3

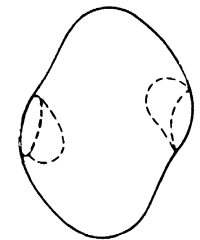


FIG. 4

intersecting, the velocity of the electron in the neighborhood of the point of self intersection tends to zero, while the time for passage of the segment in the neighborhood of the point of self intersection goes to infinity logarithmically<sup>4</sup> with  $\epsilon_0(p_z)(\epsilon - \epsilon_0(p_z))^{-1}$ . Almost the entire self-intersecting trajectory is traversed by the electron in a finite time, but then the electron takes an infinite time to approach the point of self-intersection; passage through this point does not occur classically.

In coordinate space in the  $(x, y)$  plane the motion differs from the motion in momentum space, aside from a proportionality factor, by a rotation through  $-\pi/2$ <sup>5</sup>

$$x = \int v_x dt = -cp_y/eH, \quad y = \int v_y dt = cp_x/eH. \quad (1.14)$$

Let us now proceed immediately to the determination of the function  $\gamma$ . For the singular case of orbits which are symmetric with respect to the two axes for arbitrary  $p_z$  (which, it is understood, is possible only for selected directions of the magnetic field), this was done by Zil'berman.<sup>6</sup> However, it is precisely in this (and only in this) case that there is no correction to the level separation which is an oscillating function of  $H$ . The thermodynamic quantities themselves have not even been found for this special case.

## 2. FORMULATION OF THE PROBLEM

Suppose that in the absence of a magnetic field the dispersion law has the form

$$\epsilon = \epsilon(p_x, p_y, p_z). \quad (2.1)$$

Then<sup>1,3</sup> the Hamiltonian operator in the magnetic field should be obtained by replacing  $P_x$  by  $P_x$

—  $(\hbar eH/ic) \partial/\partial p_y$ :

$$\hat{\varepsilon} = \varepsilon \left( P_x + \Delta \frac{\partial}{\partial p_y}, p_y, p_z \right), \quad \Delta = -i\Delta_0, \quad \Delta_0 = -\frac{eH\hbar}{c}. \quad (2.2)$$

It is understood that formula (2.2) still does not determine the energy operator so long as we are not given the rule for symmetrization of the non-commuting operators  $\Delta\partial/\partial p_y$  and  $p_y$ . The correct rules for symmetrization can be stated starting from very general considerations (cf. Zil'berman<sup>3</sup> and I. M. Lifshitz and Kaganov<sup>4</sup>).

However, the precise symmetrization is not necessary for the solution of the questions we are interested in (finding the levels in the neighborhood of points whose contributions to the thermodynamic quantities are not exponentially small), since it is sufficient to know the operator  $\hat{\varepsilon}$  written to terms including  $\Delta_0^2$ . To this accuracy,  $\varepsilon$  is already determined by the requirement of Hermiticity<sup>7</sup>.

As a matter of fact,<sup>7</sup> any two Hermitian operators which are obtained from (2.2) by different symmetrizations can obviously differ from one another only by an even number of commutations ( $\Delta$  is pure imaginary!), that is, by terms of no lower order than  $\Delta^2$ . Consequently, to find the energy levels, i.e., the eigenvalues, of the equation

$$\begin{aligned} \hat{\varepsilon}\psi &= \varepsilon(P_x + \Delta\partial/\partial p_y, p_y, p_z)\psi(P_x, p_y, p_z) \\ &= \varepsilon\psi(P_x, p_y, p_z), \end{aligned} \quad (2.3)$$

the operator  $\hat{\varepsilon}$  can, in accordance with what we have said above, be given for example as follows.

If

$$\varepsilon(P_x + \xi, p_y, p_z) = \sum_{j,k} \frac{1}{2} \alpha_{jk}(P_x, p_z) \xi^j p_y^k, \quad (2.4)$$

we may define  $\hat{\varepsilon}$  as

$$\hat{\varepsilon} = \sum \frac{1}{4} \alpha_{jk}(P_x, p_z) \left\{ \left( \Delta \frac{\partial}{\partial p_y} \right)^j p_y^k + p_y^k \left( \Delta \frac{\partial}{\partial p_y} \right)^j \right\}. \quad (2.5)$$

Equations (2.3) — (2.5) are already sufficient for solving the problem. Now we shall show that there is an infinite degeneracy with respect to  $P_x$  (in the quasiclassical approximation), so that even for the determination of  $\gamma(H)$  in our case we can set  $P_x = 0$  in (2.3) — (2.5).

We shall show for the general case how, to an accuracy of terms of order  $\Delta$ , this follows directly from (2.3). (Zil'berman<sup>3</sup> first proved by direct calculations that there was an infinite degeneracy with respect to  $P_x$ .) Setting

$$\psi = \exp \{ \tilde{S}/\Delta - P_x p_y/\Delta \}, \quad (2.6)$$

and introducing the notation

$$\pi_x = \frac{\partial \tilde{S}}{\partial p_y}, \quad \tilde{S} = \int \pi_x(p_y) dp_y, \quad v_x(p_y) = \frac{\partial \varepsilon}{\partial \pi_x}, \quad (2.7)$$

we find the equation for  $\pi_x(p_y, p_z)$  where  $p_z$  is a parameter:

$$\varepsilon(\pi_x, p_y, p_z) + \frac{1}{2} \Delta \partial v_x / \partial p_y = \varepsilon, \quad (2.8)$$

and this equation is just as general as (2.3) and (2.5).

Since (2.8) does not contain  $P_x$ , it is already evident that with the same accuracy as before (up to terms  $\Delta^2$ , inclusive) there is an infinite degeneracy with respect to  $P_x$ . Equation (2.8) also shows that, to this same accuracy, for the determination of the energy levels in equation (2.3) we can formally set  $P_x = 0$ , writing the equation in the form

$$\varepsilon(\Delta\partial/\partial p_y, p_y, p_z)\psi_1 = \varepsilon\psi_1, \quad \psi_1 = \psi \exp(P_x p_y/\Delta). \quad (2.9)$$

To find the levels when there is a self intersection, it is sufficient to solve (2.9) in the neighborhood of the point of self intersection and to join on to the wave function in other regions where one can use the usual solution\*.

Before we go on to determine the energy levels, let us make one further comment. The classical orbits  $\varepsilon(p_x, p_y, p_z) = \varepsilon$ ,  $p_z = \text{const}$ , in general are asymmetric with respect to the  $p_x$  axis (Figs. 1 and 2) [except for the region near the point of self intersection, where the symmetry follows from equations (1.5) and (1.6)], and the turning points do not lie on the  $p_x$  axis. However, since the quantization is determined only by the corresponding areas, it is natural to expect that a deformation of the curves far from the singular point, i.e., the point of self-intersection, will have no effect on the quantization if this deformation does not change the areas of the orbits  $S(\varepsilon)$  and  $\partial S/\partial \varepsilon$ . This theorem can be proven rigorously. Using it, we can simplify the problem by assuming that the turning points lie on the  $p_x$  axis.

If in addition we have the case shown in Fig. 1, a still further simplification is possible — replacement of all the curves by curves which are symmetric with respect to the  $p_x$  axis and have the same area as before and the same value of  $\partial S/\partial \varepsilon$ . We note that, as is clear from (1.13), symmetrization of the operator (2.9) in the neighborhood of singular points is not necessary in general.

### 3. DETERMINATION OF ENERGY LEVELS

As was shown in the preceding sections, the determination of the quasi-classical energy levels in the general case reduces to determining the

\*It is therefore more convenient in solving to use (2.9) instead of (2.8).

largest eigenvalues of Eq. (2.9), when the turning points of the corresponding orbits (2.9) lie on the  $p_x$  axis. To do this in the quasiclassical case, we must join the solution far from the point of self-intersection with the solution near this point. The joining is accomplished as usual in the region where the solution far from the point of self intersection is still valid, and where one can still use asymptotic formulas for the solution near the point of self intersection. (Such a region is known always to exist in the quasiclassical case.) In doing this it is sufficient to restrict oneself to considering orbits close to the point of self intersection, since the arguments given below are suitable for "distances"  $\Delta\epsilon$  in energy from the point of self-intersection such that  $\Delta\epsilon \ll \epsilon$ , while corrections to levels because of the presence of two orbits with possible transitions becomes exponentially small already for  $\Delta\epsilon \gg \mu H$  ( $\epsilon \gg \mu H$ !).

Comparing the coefficients for the linearly independent functions, we obtain a system of homogeneous equations whose determinant must be equal to zero. This gives the energy levels of the system.

4. INVESTIGATION OF THE LEVEL STRUCTURE

The level system when there is a self intersection has the form ( $n$  an integer)

$$\cos(S_1 \pm S_2 + \varphi(k)) = - \frac{e^{\mp k\pi}}{\sqrt{2 \cosh 2k\pi}} \cos(S_1 \mp S_2), \quad (4.1)$$

$$f_{\pm}^{(1)}(k) \equiv S_1 \pm S_2 + \varphi(k)$$

$$+ \cos^{-1} \left\{ \frac{e^{\mp k\pi}}{\sqrt{2 \cosh 2k\pi}} \cos(S_1 \mp S_2) \right\} = (2n + 1)\pi, \quad (4.2)$$

$$f_{\pm}^{(2)}(k) \equiv S_1 \pm S_2 + \varphi(k) - \cos^{-1} \left\{ \frac{e^{\mp k\pi} \cos(S_1 \mp S_2)}{\sqrt{2 \cosh 2k\pi}} \right\} = (2n + 1)\pi, \quad (4.3)$$

$$\varphi(k) = 2 \left\{ k \ln \frac{|k|}{e} - \frac{1}{2i} \ln \frac{\Gamma(1/4 + ik)}{\Gamma(1/4 - ik)} \right\} - \tan^{-1} \tanh k\pi,$$

$$S_{1,2} = \frac{S_{1,2}(p_z)}{2\Delta_0}, \quad k = \frac{\epsilon - \epsilon_0(p_z)}{2\hbar e H} c \sqrt{m_1 m_2}. \quad (4.4)$$

Here the upper sign refers to the case of "necking-in" (Figs. 1 and 3) and the lower sign to the "indentation" (Figs. 2, 4); the meaning of  $S_1(p_z)$  and  $S_2(p_z)$  is clear from Figs. 5 and 6.\* (It is understood that after determining the function  $\epsilon^{(1,2)}(n, p_z)$  from Eqs. (4.2) - (4.4) we should still take account of the presence of spin by adding both to  $\epsilon^{(1)}(n, p_z)$  and  $\epsilon^{(2)}(n, p_z)$  the term

\*In the case of a potential well with a "hump" (Fig. 7)

$$S(k) = S/2\hbar, \quad k = (e - \epsilon_0) \sqrt{m} [2\hbar \sqrt{|U''(x_0)|}]^{-1/2},$$

where  $S$  is the area of the orbit in phase space.

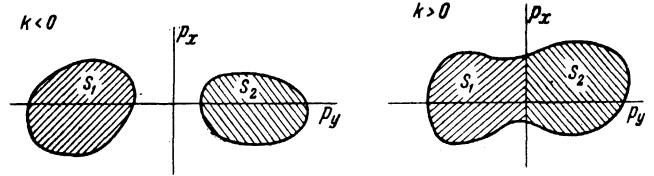


FIG. 5

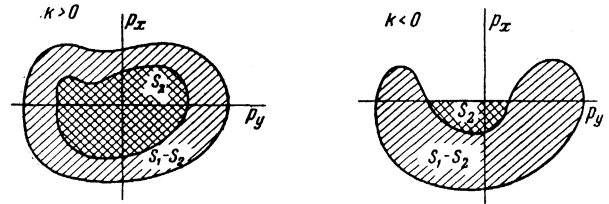


FIG. 6

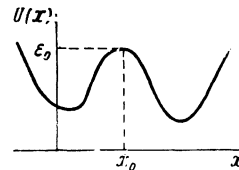


FIG. 7

$\pm e\hbar/2m_0c$ , where  $m_0$  is the mass of the free electron; for brevity we shall not write down this term which is of no interest to us.)

First let us consider the limiting cases when the orbits are still far from the point of self-intersection, i.e.,  $|k| \gg 1$  and  $\varphi(k) \rightarrow 0$ . If  $k \rightarrow +\infty$  in the case of the "neck", or  $k \rightarrow -\infty$  for the "indentation",

$$S_1 \pm S_2 = (n + \frac{1}{2})\pi, \quad (4.4a)$$

which corresponds to the usual quasiclassical quantization rules for a single orbit with area  $S_1 + S_2$  in the case of the "neck" (Fig. 5,  $k > 0$ ) and with an area  $S_1 - S_2$  in the case of an "indentation" (Fig. 6,  $k < 0$ ).

If  $k \rightarrow -\infty$  for the "neck" or  $k \rightarrow +\infty$  for the "indentation,"

$$S_{1,2} = (n_{1,2} + \frac{1}{2})\pi, \quad (4.4b)$$

which corresponds to the usual quantization rules for individual orbits (Figs. 5 and 6).

It may at first sight seem strange that formulas (4.4a) and (4.4b) for  $|k| \gg 1$  hold not with an accuracy which is exponential in  $|k|$ , but only with an accuracy  $1/|k|$ , whereas it is physically clear that the probability of transition between different orbits associated with the tunneling effect is exponentially small.

For  $\Delta p_z \sim p_0$  this is related to the fact that from the very beginning the accuracy of writing the equations and their solutions was not exponential, but of order  $1/n$  in formulas of the type (4.4a),

(4.4b), while in the formula for the energy the error was of the order of  $1/n^2$ . For  $\Delta p_z \ll p_0$ , the non-exponentially small terms give a correction to the usual quantization formulas for a single section, in the case of the geometry we are studying for the Fermi surface (the presence of a nearby saddle point).

Let us follow this transition directly from the two-level systems (4.2), (4.3). As an example we shall consider the case of a "neck." For  $k \rightarrow \infty$  it follows from (4.2) and (4.3) that

$$S_1 + S_2 = (2n + \frac{1}{2})\pi, (2n + 1 + \frac{1}{2})\pi,$$

i.e., these level systems have the same separation between levels and are shifted with respect to one another by half the level separation, so that altogether they lead to the usual equations:

$$S_1 + S_2 = (n + \frac{1}{2})\pi.$$

Now let  $k \rightarrow -\infty$ . Let us consider two cases:

- 1)  $\left[ \frac{S_1 - S_2}{\pi} \right] = 2m, S_1 = (n + m + \frac{1}{2})\pi,$   
 $S_2 = (n - m + \frac{1}{2})\pi;$
- 2)  $\left[ \frac{S_1 - S_2}{\pi} \right] = 2m - 1, S_1 = (n - m + \frac{1}{2})\pi,$   
 $S_2 = (n + m + \frac{1}{2})\pi$

( $m$  is an integer,  $[x]$  is the largest integer contained in  $x$ ).

Thus for  $k < 0$ , each of the branches "builds up" a level system corresponding in turn to one and then to the other of the individual areas, where each time we "build up" levels corresponding to the two areas.

Let us follow this process in more detail. Suppose that, in a certain energy interval  $[(S_1 - S_2)/\pi]$  is even. Then the first branch in this energy interval begins to form a level system corresponding to  $S_1$  and the second a branch corresponding to  $S_2$ . Later on, as the energy changes,  $[(S_1 - S_2)/\pi]$  becomes odd and the first branch begins to extend the "work" of the second branch, the construction of levels corresponding to  $S_2$ , while the second branch starts the building up of those corresponding to  $S_1$ . Later on the roles of the branches are alternated once again, etc. This process for larger and larger values of  $|k|$  is shown in Fig. 8 (where, since  $k$  is in the argument of the arc cos in the exponent, it is practically sufficient already to have  $|k| > 1$ ).

Obviously, in the case of an "indentation" one can repeat these same arguments with a replacement of  $k$  by  $-k$ .

2. Now let us explain how the distance between

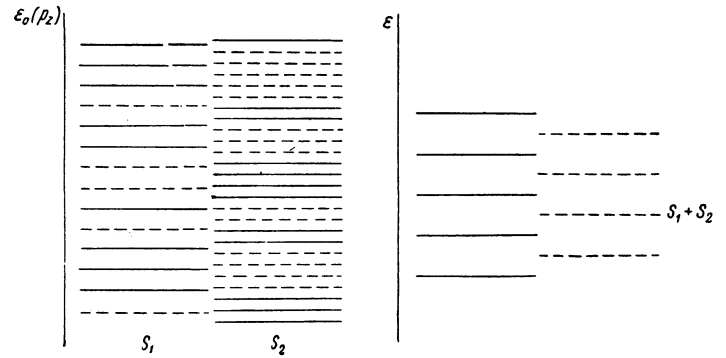


FIG. 8. Picture of levels for a self-intersecting trajectory. The solid lines show the first branch, the dotted lines the second; on the left  $\varepsilon < \varepsilon_0(p_z)$ , on the right  $\varepsilon > \varepsilon_0(p_z)$ .

levels changes [we are especially interested in this for levels near  $\varepsilon_0(p_z)$ ]. By using formula (1.13) for  $|k| \ll k_0$ , it is easy to show that the functions  $f_{\pm}^{(1,2)}(k)$  in (4.2) and (4.3) are always monotonic differentiable functions, so that the distance between levels in each of the branches corresponds to  $\Delta k \sim (\partial S / \partial k)^{-1}$  and never becomes zero or infinity. (For levels near the point of self intersection this was not obvious beforehand.) As for the dependence of the distance  $\Delta k$  between levels on magnetic field, as one easily shows, it has an oscillatory correction.

From formulas (4.1) - (4.3) and our remarks above, it is clear that the only case considered by Zil'berman,<sup>6</sup> the case of a "neck" for  $S_1 = S_2 = S$  is a case of degeneracy where

$$2S + \varphi(k) \pm \cos^{-1}(e^{-k\pi} / \sqrt{2 \cosh 2k\pi}) = (2n + 1)\pi,$$

and where both for  $k \gg 1$ , as well as for  $-k \gg 1$ , there is a single equation system

$$2S = (n + \frac{1}{2})\pi \quad (k \gg 1), \quad S = (n + \frac{1}{2})\pi \quad (-k \gg 1),$$

there is no "alternation" of levels as in Fig. 8, and there is no oscillation of levels with magnetic field in the neighborhood of  $\varepsilon_0(p_z)$ .

If we go over from closed sections of the Fermi surface to open sections, we should see a picture analogous to that described by us, but possibly complicated still more by broadenings of the levels (Zil'berman<sup>4</sup> considered only the special case of sections which are periodic throughout the lattice).

<sup>1</sup>L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Pergamon (1958).

<sup>2</sup>I. M. Lifshitz and A. M. Kosevich, JETP 29, 730 (1955), Soviet Phys. JETP 2, 636 (1956).

<sup>3</sup>G. E. Zil'berman, JETP 32, 296 (1957) and 33, 387 (1957), Soviet Phys. JETP 5, 208 (1957) and 6, 299 (1958).

<sup>4</sup>I. M. Lifshitz and M. I. Kaganov, Usp. Fiz. Nauk **69**, 419 (1959), Soviet Phys. Uspekhi **2**, 831 (1960).

<sup>5</sup>M. Ya. Azbel' and É. A. Kaner, JETP **32**, 896 (1957), Soviet Phys. JETP **5**, 730 (1957).

<sup>6</sup>G. E. Zil'berman, JETP **34**, 748 (1958), Soviet Phys. JETP **7**, 513 (1958).

<sup>7</sup>M. Ya. Azbel', JETP **34**, 969 (1958), Soviet Phys. JETP **7**, 669 (1958).

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239