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V.S. Buslaev

II. Institut f. Theoretische Physik, Universität Hamburg

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On a quasiclassical approach on the theory of Bloch electrons in crystals

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Abstract

We propose a new approach to the asymptotic investigation of solutions of the equation

$$\mathcal{L}(\varepsilon x, x, -i\partial_x)\psi = 0, \quad x \in \mathbb{R}^d,$$

when $\varepsilon \to 0$. It is supposed that $\mathcal{L}$ depends on x periodically. Our approach is close to the standard quasiclassical approximation. Using this approach we suggest simple methods to solve a series of traditional problems in the theory of motion of Bloch electrons in external fields.

* Permanent address: Department of Mathematical Physics, Physical Faculty, Leningrad State University, 1 Maya 100, Petrodvoretz Leningrad 198904

Introduction

Our work is motivated by problems of the theory of motion of Bloch electrons in external electro-magnetic fields. This theory has a long history but we cannot describe it in this short text. A seires of principal publications will be indicated at the end of the preprint. Our aim is to propose a new approach to the problem which has from our point of view some advantages. These advantages give us the possibility to consider the main questions consistently in quite an elementary way. The indicated features of the approach can be explained by its similarity with the standard quasiclassical approximation. This similarity includes not only the essence of the subjects but also the system of main formulas.

We shall consider the differential equation

$$\mathcal{L}(\xi, x, -i\partial_x, \nu)\psi = 0, \tag{1.1}$$

where $\xi = \varepsilon x$, $x \in \mathbb{R}^d$, $\nu = -i\varepsilon$, $\varepsilon > 0$. The symbol $\mathcal{L}(\xi, x, p, \nu)$ denotes a smooth function. periodically depending on x on a periodic lattice T. Let us agree that $-i\partial_x$ acts before x. In solid state physics the following special equation of the type (1.1) is usually considered

$$\left[(-i\partial_x - A(\xi))^2 + \varphi(\xi) + v(x) - E\right]\psi = 0, \tag{1.2}$$

where v is the periodic potential of a crystal lattice and (φ, A) is the potential of an external field. If $\mathcal{L}$ does not depend on x then (1.1) reduces to the standard equation of the quasiclassical approach

$$\mathcal{L}(\xi, -i\varepsilon\partial_\xi, -i\varepsilon)\psi = 0. \tag{1.3}$$

Below we shall describe some special classes of local formal solutions of (1.1) which have the importance as the analogous more simple solutions in the case of equation (1.3). Using the Maslov construction, see /1/, we could describe with the help of these solutions the total asymptotic behaviour of the kernels of functions of the operator $\mathcal{L}$. However, we shall not discuss there the Maslov construction and restrict ourselves to the consideration of more elementary aspects of the problem, connected with the notion of turning point.

Part 2 of this preprint contains the description of the elementary solutions mentioned above in the many dimensional case. In part 3 we shall discuss questions connected with the notion of turning point in one dimensional case. Part 4 will be devoted to the problem of quantization of classical orbits in the subject under consideration. Finally in part 5 we shall give some short comments on the literature.

2. Quasiclassical approach

1. The initial point is quite elementary and well known in some different circles of problems. Instead of equation (1.1) we can consider the other equation

$$\mathcal{L}\left(\xi, x, -i\partial_x - i\varepsilon\partial_\xi, \nu\right)\psi = 0, \tag{2.1}$$

where $\psi = \psi(\xi, x, \varepsilon)$. The function $\psi(\xi, x, \varepsilon)$ will be a solution of equation (1.1), if $\xi = \varepsilon x$. But now we shall ignore the connection $\xi = \varepsilon x$ and remember it only in the final formulas. Equation (2.1) can be considered as the usual quasiclassical equation (1.3) for the vector-function $\xi \longmapsto \psi(\xi, \cdot, \varepsilon)$ which coordinates are labelled by the index x . From the mathematical point of view we have to restrict the character of dependence $\psi(\xi, x, \varepsilon)$ on x , more precisely in our case we shall consider only periodic dependence on x . After

this remark we can write down, not redeating the known computations, the solutions of equation (2.1) using the natural analogy between equation (2.1) an proper vector equations of the type (1.3), see for example /1/.

Let us introduce the operator

$$\hat{\mathcal{L}}(\xi, k) = \mathcal{L}(\xi, x, -i\partial_x + k, 0), \tag{2.2}$$

acting on the periodic functions on x . Here ξ and k are considered as parameters. Let $\hat{\mathcal{L}}(\xi, k)$ be a selfadjoint operator and $\mathcal{E}(\xi, k)$ its nondegenerate eigenvalue:

$$\hat{\mathcal{L}}(\xi, k)u(\xi, k, x) = \mathcal{E}(\xi, k)u(\xi, k, x). \tag{2.3}$$

Under some common additional conditions equation (2.1) has the following local solution:

$$\psi(\xi, x, \varepsilon) = \exp\left[\frac{i}{\varepsilon}\Theta(\xi)\right]\sum_{h\geq 0}(-i\varepsilon)^h\psi_h(\xi, x). \tag{2.4}$$

Here Θ is an arbitrary solution of the Hamilton-Jacobi equation

$$\mathcal{E}(\xi, \Theta_\xi) \doteq 0 \tag{2.5}$$

and the functions ψ_h are obeyed some transport equations. In particular

$$\psi_0(\xi, x) = M(\xi)u(\xi, k, x), \tag{2.6}$$

where

$$k = \Theta_\xi(\xi) \tag{2.7}$$

and M obeys the equation

$$\langle \mathcal{E}_\kappa, \partial/\partial\xi \rangle M + \tfrac{1}{2}\,\mathrm{tr}[\Theta_{\xi\xi}\,\mathcal{E}_{\kappa\kappa}]M + \{(\langle \mathcal{E}_\kappa, \partial/\partial\xi\, u\rangle, u) + \mathrm{tr}\,(\hat{\mathcal{L}} u_\xi, u_\kappa) + (\hat{\mathcal{L}}_\nu u, u)\}M = 0. \tag{2.8}$$

In this equation

$$\partial/\partial\xi = \partial_\xi + \Theta_{\xi\xi}\,\partial_\kappa, \tag{2.9}$$

$\langle\ ,\ \rangle$ is the scalar product on $\mathbb{C}^d$, $(\cdot\,,\cdot)$ –scalar product in $L_2(F)$, where F is an elementary cell of the lattice T, and the function u is supposed to be normalized in $L_2(F)$.

2. It is well known, equation (2.5) has some close connections with the Hamiltonian system

$$\xi_s = \mathcal{E}_\kappa, \quad \kappa_s = -\mathcal{E}_\xi \tag{2.10}$$

The arbitrary (local) solutions of equation (2.5) can be described in the following way. Let us consider a set of solutions of the system (2.10)

$$\xi = \xi(s,\alpha),\ \kappa = \kappa(s,\alpha),\ s \in \mathbb{R},\ \alpha \in \mathbb{R}^{d-1},$$
$$(s,\alpha) \in \mathcal{D} \subset \mathbb{R}^d. \tag{2.11}$$

If the correspondence $\xi \longleftrightarrow (s,\alpha)$ is a (local) diffeomorphism, then the function

$$\Theta(\xi) = \Theta_0(\alpha) + \int_{s_0}^{s} \langle \kappa, \xi_s\rangle\, ds \tag{2.12}$$

is a solution of equation (2.5). Here the function Θ_0 is arbitrary and the path

of integration in (2.12) is a trajectory of system (2.10). In terms of the set of solutions of system (2.10) the solution M of equation (2.8) is given by the formula

$$M(\xi) = M_0(\alpha)\left|\det \frac{\partial\xi}{\partial(s,\alpha)}\right|^{-1/2} \times \exp\int_{s_0}^{s}\left\{\tfrac{1}{2}\,\mathrm{tr}\,\mathcal{E}_{\kappa\xi} + \sigma\right\} ds, \tag{2.13}$$

$$\sigma = -(u_s, u) - \tfrac{1}{2}\,\mathrm{tr}\,(\hat{\mathcal{L}} u_\xi, u_\kappa) - (\hat{\mathcal{L}}_\nu u, u), \tag{2.14}$$

where M_0 is again an arbitrary function.

3. Let us now renormalize the eigenfunction u:

$$u(\xi,\kappa,x) \longrightarrow \Phi(\xi,\kappa)\,u(\xi,\kappa,x),\ \Phi(\xi,\kappa) \in \mathcal{U}(1). \tag{2.15}$$

Then

$$(\hat{\mathcal{L}}_\nu u, u) \longrightarrow (\hat{\mathcal{L}}_\nu u, u),$$
$$(\hat{\mathcal{L}} u_\xi, u_\kappa) \longrightarrow (\hat{\mathcal{L}} u_\xi, u_\kappa) + \mathcal{E}[\bar{\Phi}\Phi_\xi(u, u_\kappa) + \Phi\bar{\Phi}_\kappa(u_\xi, u) + \Phi_\xi\bar{\Phi}_\kappa(u,u)] = (\hat{\mathcal{L}} u_\xi, u_\kappa),$$
$$(u_s, u) \longrightarrow \Phi^{-1}\Phi_s + (u_s, u). \tag{2.16}$$

As a result

$$M(\xi) \longrightarrow \Phi_0(\alpha)\,\Phi^{-1}(\xi,\kappa)\,M(\xi), \tag{2.17}$$

where

$$\phi_0(\alpha) = \Phi\left(\xi(s_0,\alpha), \kappa(s_0,\alpha)\right). \tag{2.18}$$

This means that the renormalization of u after all is absorbed essentially by the renormalization of M:

$$\psi_0(\xi, x) \longrightarrow \phi_0(\alpha)\psi_0(\xi, x). \tag{2.19}$$

The factor

$$\exp(-1)\int_{s_0}^{s}(d_s u, u) \tag{2.20}$$

leading to this result, is known now owing to the supplements which have been done by M. Berry /2/ to the quantum adiabatic theorem. It is timely to mension that some effects connected with this factor have been studied by specialists in solid state physics still in the 50-s. We shall be concerned with this point once more in part 4.

4. The Hamilton-Jacobi equation (2.5) and the Hamiltonian system (2.10) appear also in cource of the investigation of the standard scalar equation of the quasiclassical approach:

$$\mathcal{E}(\xi, -i\varepsilon\partial_\xi)\chi = 0, \tag{2.21}$$

$$\chi = \exp\left[\frac{i}{\varepsilon}\Theta(\xi)\right]\sum_{h\geq 0}(-i\varepsilon)^h \chi_h(\xi). \tag{2.22}$$

The transport equation for χ_0 has the form

$$\langle \mathcal{E}_\kappa, \partial/\partial\xi \rangle \chi_0 + \frac{1}{2}\mathrm{tr}\left[\Theta_{\xi\xi}\,\mathcal{E}_{\kappa\kappa}\right]\chi_0 = 0. \tag{2.23}$$

Therefore in the leading order the following identity between the solutions ψ and χ is fulfilled:

$$\psi(\xi, x, \varepsilon) \approx \chi(\xi,\varepsilon)\,u(\xi,\kappa,x)\exp\int_{s_0}^{s}\sigma\, ds, \tag{2.24}$$

where $\kappa = \Theta_\xi(\xi)$. This formula can be considered as the exact expression of a connection between equations (1.1) and (2.21). The fact of the existence of some connection between these equations is not only well known but was widely used in problems of solid physics. It seems it had not so explicit elementary reflection yet in the general case.

In the special case of equation (1.2):

$$\mathcal{L}(\xi, x, p, \nu) = (p - A(\xi))^2 + \varphi(\xi) + v(x) - \nu\,\mathrm{div}A(\xi) - E \tag{2.25}$$

and

$$\hat{\mathcal{L}}(\xi, \kappa) = (-i\partial_x - A(\xi) + \kappa)^2 + \varphi(\xi) + v(x) - E, \tag{2.26}$$

The eigenvalues $\mathcal{E}(\xi,\kappa)$ and the eigenfunctions $u(\xi,\kappa,x)$ of the operator $\hat{\mathcal{L}}(\xi,\kappa)$ can be expressed in terms of the eigenvalues $\varepsilon(\kappa)$ and the eigenfunction $u(\kappa,x)$ of the operator

$$\hat{\mathcal{L}}(\kappa) = (-i\partial_x + \kappa)^2 + v(x): \tag{2.27}$$

$$\mathcal{E}(\xi,\kappa) = \varepsilon(\kappa - A(\xi)) + \varphi(\xi) - E, \tag{2.28}$$

$$u(\xi,\kappa,x) = u(\kappa,x). \tag{2.29}$$

Owing to (2.28) equation (2.21) has the form

$$\left[\mathcal{E}\left(-i\varepsilon\partial_{\xi} - A(\xi)\right) + \varphi(\xi) - E\right]\chi = 0 . \qquad (2.30)$$

This equation in the case $\varphi = 0$ appeared in solid state physics already in 1934 /3/ as a bright guess.

5. For completeness of the radiative let us shortly consider the nonstationary equation

$$\mathcal{L}\left(\xi, x, -i\partial_x, -i\varepsilon\right) \longrightarrow -i\partial_t + \mathcal{H}(\tau, \xi, x, -i\partial_x, -i\varepsilon), \qquad (2.31)$$

$\tau = \varepsilon t \in R$, $\xi = \varepsilon x \in R^d$, $\mathcal{H}$ depends periodically on x.

Equation (2.1) has the form

$$\left[-i\varepsilon\partial_\tau + \mathcal{H}(\tau, \xi, x, -i\partial_x - i\varepsilon\partial_\xi, -i\varepsilon)\right]\psi(\tau, \xi, x, \varepsilon) = 0 . \qquad (2.32)$$

In analogy with the operator $\hat{\mathcal{L}}(\xi, k)$ let us introduce the operator

$$\hat{\mathcal{H}}(\tau, \xi, k) = \mathcal{H}(\tau, \xi, x, -i\partial_x + k, 0) . \qquad (2.33)$$

We shall suppose that it possesses the same properties as $\hat{\mathcal{L}}(\xi, k)$ and consider its eigenfunction $u(\tau, \xi, k, x)$ and its eigenvalue $\mathcal{E}(\tau, \xi, k)$. In this case equation (2.32) has the following formal solution

$$\psi(\tau, \xi, x, \varepsilon) = \exp\left[\frac{i}{\varepsilon} S(\tau, \xi)\right] \sum_{h \geq 0} (-i\varepsilon)^h \psi_h(\tau, \xi, x) . \qquad (2.34)$$

The function S has to obey the equation

$$S_\tau + \mathcal{E}(\tau, \xi, S_\xi) = 0 . \qquad (2.35)$$

It is known that the solution of Hamilton-Jacobi equation (2.35) can be expressed equivalently in terms of some d-parametric set of solutions

$$\xi = \xi(\tau, \alpha), \; k = k(\tau, \alpha), \; \tau \in \mathbb{R}, \; \alpha \in \mathbb{R}^d, \; (\tau, \alpha) \in \mathfrak{D} \subset \mathbb{R}^{d+1}, \qquad (2.36)$$

of the Hamiltonian system

$$\xi_\tau = \mathcal{E}_k, \quad k_\tau = -\mathcal{E}_\xi . \qquad (2.37)$$

If the correspondence $(\tau, \xi) \longleftrightarrow (\tau, \alpha)$ is a local diffeomorphism, then there exists the following connection between the function S and the indicated set

$$S(\tau, \xi) = S_0(\xi) + \int_{\tau_0}^{\tau} \langle k, \xi_\tau \rangle \, d\tau , \qquad (2.38)$$

S_0 is an arbitrary function.

Using the solutions of system (2.37) let us describe the main term of series (2.34):

$$\psi_0(\tau, \xi, x) = M(\tau, \xi) u(\tau, \xi, k, x) , \qquad (2.39)$$

where

$$k = S_\xi(\xi) \qquad (2.40)$$

and M is given by the formula

$$M(\tau, \xi) = M_0(\xi) \left| \det \frac{\partial \xi}{\partial(\tau, \alpha)} \right|^{-1/2} \times$$

$$\times \exp \int_{\tau_0}^{\tau} \left(\frac{1}{2} \operatorname{tr} \mathcal{E}_{k\xi} + \hat{\sigma}\right) d\tau , \qquad (2.41)$$

$$\hat{\sigma} = -(u_\tau, u) - \frac{1}{2} \operatorname{tr}\left([\hat{\mathcal{H}} - \mathcal{E}] u_\xi, u_k\right) - (\hat{\mathcal{H}}_\nu u, u) . \qquad (2.42)$$

Hamilton-Jacobi equation (2.35) and Hamiltonian system (2.37) also appear when the scalar quasiclassical equation

$$\left[-i\varepsilon\partial_\tau + \mathcal{E}(\tau,\xi,-i\varepsilon\partial_\xi)\right]\chi(\tau,\xi,\varepsilon)=0, \tag{2.43}$$

$$\chi(\tau,\xi,\varepsilon)=\exp\left[\frac{i}{\varepsilon}S(\tau,\xi)\right]\sum_{h\geq 0}(-i\varepsilon)^h\chi_h(\tau,\xi), \tag{2.44}$$

is considered. In the leading order the function ψ and χ are connected by the following identity

$$\psi(\tau,\xi,x,\varepsilon)\approx\chi(\tau,\xi,\varepsilon)u(\tau,\xi,k,x)\exp\int_{\tau_0}^{\tau}\hat{\omega}\,d\tau, \tag{2.45}$$

where $\quad k=S_\xi(\tau,\xi)$

For the nonstationary equation

$$\left[-i\partial_t+(-i\partial_x-A(\xi))^2+\varphi(\xi)+v(x)\right]\psi=0 \tag{2.46}$$

the operator $\hat{\mathcal{H}}$ coincides with operator (2.26), therefore $u(\tau,\xi,k,x)=$ $=u(k,x)$, $\mathcal{E}(\tau,\xi,k)=\mathcal{E}(k-A(\xi))+\varphi(\xi)$.

As a result equations (2.35) and (2.43) have the form

$$S_\tau+\mathcal{E}(\mathcal{E}_\xi-A(\xi))+\varphi(\xi)=0, \tag{2.47}$$

$$\left[-i\varepsilon\partial_\tau+\mathcal{E}(-i\varepsilon\partial_\xi-A(\xi))+\varphi(\xi)\right]\chi=0. \tag{2.48}$$

3. Turning points

1. When we want to investigate the asymptotic behavior of the exact solutions of equation (1.1), the formal solutions of the being considered above can be unsufficient. First of all as in the standard case the solutions of the Hamilton-Jacobi equation can acquire singularities. This difficulty has a well known geometrical interpretation and can be overcome, for example, with the help of Maslov's approach /1/. In the case of the original equation (1.1) this means that one has to go a rather unexpected way: it is necessary to separate in equation (1.1) the dependence on the variables x and ξ, that is to pass from the equation (1.1) to equation (2.1), and then to carry out the Fourier transformation on some part of the variables ξ.

In the scalar case an other difficulty is also possible. It can happen that besides ε the original equation contains some other parameter δ and different branches of a solution of the Hamilton-Jacobi equation coincide on some set, for example on a finite set of points, when $\delta=0$. To overcome this difficulty it is necessary to use new special functions.

In the vector case additional difficulties can arise. They can be connected with a reconstruction of the multiplicity of eigenvalues and in our case also with their infinite number.

Here we shall discuss the first two difficulties and shall illustrate methods of their overcoming with the help of the elementary example of the one-dimensional equation, d = 1:

$$\left[(-i\partial_x)^2+v(x)+\varphi(\xi)-E\right]\psi=0, \tag{3.1}$$

v is a periodic function on x with some period a, a > 0. Discussing the first problem we shall come to a natural generalization of the classical notion of turning points. Concerning the second one we shall have to consider the question of two close turning points.

At the very beginning we would like to emphasize that the same line of reasoning which we have developed in part 2 to pass to the vector problem will allow us to investigate the questions indicated above.

2. The main results of this and the following subsection have been considered by the author earlier /4/ from a different point of view.

The constructions of part 2 in the case of equation (3.1) can be improved and made more explicit. The main peculiarity is that the supposition d = 1 allows us to continue the solutions to the region of complex momenta.

Let $\mathcal{E}_m(k)$, m = 1, 2, ..., be the system of eigenvalues of the equation

$$\left[(-i\partial_x + k)^2 + v(x) \right] \psi = E\psi \tag{3.2}$$

Let us furthermore introduce the function $\mathcal{E}(k) = \mathcal{E}_m(k)$, $\bar{k}_{m-1} \leq k \leq \bar{k}_m$, on the semiaxis $k \geq 0$ outside the points $\bar{k}_m = m\pi/a$, m = 0, 1, 2, ... It can be continued analytically as an even function on the complex plane with some cuts indicated in fig. 1. The hights of these cuts depend on the function v.

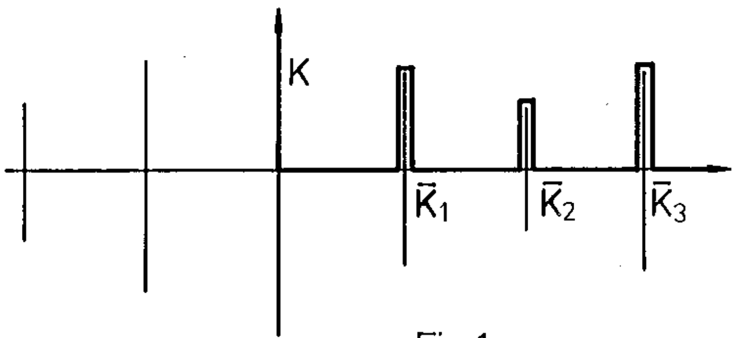

Fig.1

The function $\mathcal{E}$ maps the curve K, shown in fig. 1, into the whole of $\mathbb{R}$. The set of points

$$k_0 = 0,\ k_1 = \bar{k}_1 - 0,\ k_2 = \bar{k}_1 + 0,\ k_3 = \bar{k}_2 - 0,\ k_4 = \bar{k}_2 + 0,\ \dots$$

turns into the set of points

$$E_0 < E_1 \leq E_2 < E_3 \leq E_4 < \dots$$

The intervals $[E_0, E_1], [E_2, E_3]$, consist of the spectrum of the equation

$$\left[(-i\partial_x)^2 + v(x) \right] \psi = E\psi \tag{3.3}$$

on the axis $\mathbb{R}$. They are therefore named the admitted zones. The additional intervals $(-\infty, E_0), (E_1, E_2)$ are called the forbidden zones. The eigenfunction $k \mapsto \mathcal{E}(k) \mapsto u(k, x)$ of equation (3.2) are determined everywhere with the exception at the points $\pm \bar{k}_m$ uniquely up to a factor depending on K.

Let us introduce the function

$$\mathcal{E}(\xi, k) = \mathcal{E}(k) + \varphi(\xi). \tag{3.4}$$

Isoenergy curve (2.5) is described by the identity

$$\mathcal{E}(\xi, k) = E \tag{3.5}$$

For the simplicity of the representation we shall suppose that $\varphi' \leq -\varkappa < 0$. Then φ is a diffeomorphism $\mathbb{R} \to \mathbb{R}$. The isoenergy curve in this case is given by the solid lines of the curve shown in fig. 2. Their extensions are described by the equations $\mathcal{E}_m(\xi, k) = \mathcal{E}_m(k) + \varphi(\xi) = E$. The points ξ_ℓ, $\ell = 0, 1, \dots$ are determined by the relations

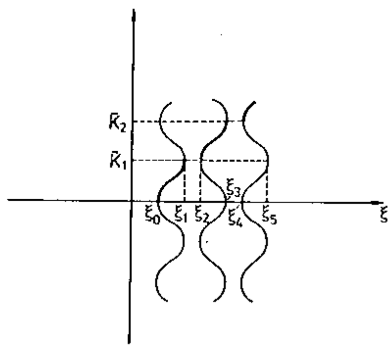

Fig. 2

$$E_\ell + \varphi(\xi_\ell) = E . \tag{3.6}$$

They are the turning points. On each interval $[\xi_0, \xi_1]$, $[\xi_2, \xi_3]$, the solution of the Hamilton-Jacobi equation (2.5) can be described by the formula

$$\Theta(\xi) = \int^{\xi} k(\xi)\, d\xi . \tag{3.7}$$

In the points $\xi_0, \xi_1, \ldots$ it loses its smoothness.

The solutions which were considered in part 2 exist on the indicated intervals and have asymptotic character when $\varepsilon \to 0$ outside the $\varepsilon^{2/3-\gamma}$ $(\gamma < 1/2)$ neighbourhoods of the points ξ_m. One of them $f(\xi, x, \varepsilon)$ in leading order has the following form

$$f(\xi, x, \varepsilon) = \mathcal{E}_k^{-1/2}(k)\, u(k, x) \exp\Big[\frac{i}{\varepsilon}\int^{\xi} k(\xi)\, d\xi - \int^{k} (d k\, u, u)\Big], \tag{3.8}$$

where k and ξ are connected by relation (3.5). The second, linearly independent, solution f can be obtained from f by complex conjugation, $f \to \bar{f}$ or (equivalently) by means of the transformation $k \to -k$.

The solution which is analogous to f also exists in the intervals (ξ_{2m-1}, ξ_{2m}) where k has an imaginary part. Let us denote it by g_1. The solution g_2 linearly independent of it cannot be obtained in this case by complex conjugation but as before it can be constructed by means of the transformation $k \to -k$.

3. The solutions f, f, g_1, g_2 have not asymptotical character in some small $(\varepsilon^{7/12+\gamma}, \gamma > 0$ -) neighbourhoods of the turning points ξ_m. The structure of isoenergy curve, see fig. 2, in this case locally and qualitatively has the form

$$k^2 + (\xi - \xi_\ell) = 0 . \tag{3.9}$$

Such a type of isoenergy curve arises in connection with the equation

$$-\varepsilon^2 A_{\xi\xi} + (\xi - \xi_\ell) A = 0 . \tag{3.10}$$

For this equation the natural variable is

$$\zeta = \varepsilon^{-2/3}(\xi - \xi_\ell) . \tag{3.11}$$

Using this fact let us introduce the two variables x and ζ in equation (3.1):

$$\Big[(-i\partial_x - i\varepsilon^{1/3}\partial_\zeta)^2 + v(x) + \varphi(\xi_\ell + \varepsilon^{2/3}\zeta) - E\Big]\cdot\psi(\zeta, x, \varepsilon) . \tag{3.12}$$

As in the case of equation (2.1) we shall ignore connection (3.11) until reading the final formulas. The function $\psi(\zeta, x, \varepsilon)$ will be supposed to be periodic or anti-periodic one with the period a in accordance with the spectral type of the point E_ℓ : periodicity, if $\ell = 4m-1, 4m$, anti-periodicity, if $\ell = 4m+1, 4m+2$. The dependence of the function ψ on ε can be fixed by the representation

$$\psi(\zeta, x, \varepsilon) = \sum_{n \geq 0} \varepsilon^{n/3} \psi_n(\zeta, x) . \tag{3.13}$$

If we substitute this formula into the equation (3.12) then after some easy calculations /4/ the following expression can be received for the leading term of :

$$\psi_0(\zeta, x) = M(\zeta)\, \psi_\ell(x) \tag{3.14}$$

Here

$$\psi_\ell(x) = \exp(i k_\ell x)\, u(k_\ell, x) . \tag{3.15}$$

and M satisfies the equation

$$-\frac{1}{2\varkappa_\ell} M'' + \alpha_\ell \xi M = 0, \qquad (3.16)$$

where $\alpha_\ell = \varphi'(\xi_\ell)$ and $\varkappa_\ell = [\varepsilon''(\kappa_\ell)]^{-1}$ is the so called effective mass at the point κ_ℓ.

The formulas of this subsection and the formulas of the previous part can be matched in the region of their common validity. We can show this using the known asymptotic formulas for the solutions of the Airy equation (3.16).

4. This and the next subsections will be based on unpublished point work with L. Dmitrieva.

The case of two close turning points is a subject of special interest for applications. Let two turning points $\xi_\ell, \xi_{\ell+1}$, corresponding to the forbidden zone $(E_\ell, E_{\ell+1})$ be close. The structure of the isoenergy curve near the turning points (on each K -period) is given by the relation

$$K^2 - (\xi - \bar{\xi}_m)^2 + \delta^2 = 0, \qquad (3.17)$$

where $2\delta, \delta > 0$ is the distance between the two turning points, see fig. 2. A curve of this type results from the standard quasiclassical equation

$$\left[(-i\varepsilon\partial_\xi)^2 + (\xi - \bar{\xi}_m)^2 - \delta^2\right]\psi = 0, \qquad (3.18)$$

It contains the noneliminated parameter δ. For this equation the natural variable η and the natural parameter μ are

$$\eta = \varepsilon^{-1/2}(\xi - \bar{\xi}_m), \quad \mu = \varepsilon^{-1}\delta^2. \qquad (3.19)$$

This remark dictates the choice of the natural variables and parameters in the

initial equation if two turning points are close. The width of the forbidden zone depends on the potential and we have to introduce in it a parameter which can characterize this width. Let us suppose

$$v = v_0 + \delta \cdot v_1. \qquad (3.20)$$

Here v_0 is a periodic potential for which the considered zone degenerates in the points $E_{2m-1} = E_{2m} = \bar{E}_m$, and $\delta \geqslant 0$ is a small parameter. In general the width of the zone $\Delta E_m = E_{2m} - E_{2m-1}$ is of the order δ. If an initial zone is narrow we always can choose the potential v_0 with the degenerate zone and δ will be small.

Let $\bar{\xi}_m$ be the solution of the equation $\bar{E}_m + \varphi(\bar{\xi}_m) = E$. Using variables (3.19) let us pass to the equation

$$\left[(-i\partial_x - i\varepsilon^{1/2}\partial_\eta)^2 + v_0(x) + \varepsilon^{1/2}\mu^{\frac{1}{2}} v_1(x) + \right.$$
$$\left. + \varphi(\bar{\xi}_m + \varepsilon^{1/2}\eta)\right]\psi(\eta, x, \mu, \varepsilon) = 0. \qquad (3.21)$$

As in the previous subsection the function ψ has to be periodic or anti-periodic. The dependence on ε has to be fixed by the representation

$$\psi(\eta, x, \mu, \varepsilon) = \sum_{n \geqslant 0} \varepsilon^{n/2} \psi_n(\eta, x, \mu). \qquad (3.22)$$

Equation (3.21) and representation (3.22) lead to the following result

$$\psi_0 = M(\eta, \mu)\chi_m(x) + N(\eta, \mu)\overline{\chi_m(x)}, \qquad (3.23)$$

where

$$\chi_m(x) = \exp(i\bar{\kappa}_m x)u(\bar{\kappa}_m, x) \qquad (3.24)$$

is a solution of the equation

$$\left[-(i\partial_x)^2 + v_0(x) - \bar{E}_m\right]\psi = 0, \tag{3.25}$$

obeying the (anti-) periodicity condition. We shall suppose that

$$\int_0^a |\chi_m|^2 dx = 1. \tag{3.26}$$

The coefficients M u N have to be solutions of the system

$$\begin{aligned} &i M_{\eta_1} + \sigma \tfrac{1}{2}\eta_1 M + \tau\sqrt{\mu_1}\, N = 0, \\ &-i N_{\eta_1} + \sigma \tfrac{1}{2}\eta_1 N - \tau\sqrt{\mu_1}\, M = 0. \end{aligned} \tag{3.27}$$

In this system

$$\begin{aligned} &\eta_1 = |\bar{\alpha}_m \varkappa^{-1}|^{1/2}\left(\eta + \mu^{1/2}\lambda/\bar{\alpha}_m\right), \quad \lambda = \int_0^a v_1|\chi_m|^2 dx, \\ &\mu_1 = \beta^2\mu / 4|\bar{\alpha}_m \varkappa|, \quad \bar{\alpha}_m = \varphi'(\bar{\xi}_m), \quad \tau = \operatorname{sgn}\beta\varkappa, \\ &\varkappa = -i\int_0^a \bar{\chi}_m' \cdot \chi_m dx, \quad \sigma = -\operatorname{sgn}\varkappa, \quad \beta = \int_0^a v_1 \chi_m^2 dx. \end{aligned} \tag{3.28}$$

Removing M or N from the system we receive the equations

$$\begin{aligned} &M_{\eta_1\eta_1} + \left(\tfrac{1}{4}\eta_1^2 - \mu_1 - \tfrac{i}{2}\sigma\right)M = 0, \\ &N_{\eta_1\eta_1} + \left(\tfrac{1}{4}\eta_1^2 - \mu_1 + \tfrac{i}{2}\sigma\right)N = 0. \end{aligned} \tag{3.29}$$

Therefore system (3.27) has the following pair (M_+, N_+) and (M_-, N_-) of linearly independent solutions:

$$\begin{aligned} &M_\pm = \mathcal{D}_{-i\sigma\mu_1}\left(\pm\sigma e^{-i\sigma\pi/4}\eta_1\right), \\ &N_\pm = \pm\tau\sqrt{\mu_1}\, e^{-i\sigma\pi/4}\mathcal{D}_{-i\sigma\mu_1 - 1}\left(\pm\sigma e^{-i\sigma\pi/4}\eta_1\right) \end{aligned} \tag{3.30}$$

Here $D_\mu(z)$ is the standard notion for the known special function.

The domain of validity of such solutions together with the domains of validity of the solutions considered earlier cover the real axis. Of course, on their common domains of validity they all agree with each other.

5. Let a narrow forbidden zone (E_{2m}, E_{2m+1}) separate two large admitted zones. In both of these admitted zones there exist the solutions of the type f, let us call them f_1 and f_2 respectively. In some neighbourhood of the interval $[\xi_{2m}, \xi_{2m+1}]$ we can consider the solutions (3.23) and with their help continue f_1 through the interval $[\xi_{2m}, \xi_{2m+1}]$:

$$f_1 \longrightarrow a f_2 + b \bar{f}_2 \tag{3.31}$$

It is convenient to renormalize the solutions f_1, f_2:

$$\tilde{f}_1 = \exp\left(\tfrac{i}{\varepsilon}\bar{K}_m \xi_{2m-1}\right) f_1, \quad \tilde{f}_2 = \exp\left(\tfrac{i}{\varepsilon}\bar{K}_m \xi_{2m}\right) f_2. \tag{3.32}$$

For the coefficients $\tilde{a}$ and $\tilde{b}$, determined by the relation

$$\tilde{f}_1 \longrightarrow \tilde{a}\tilde{f}_2 + \tilde{b}\bar{\tilde{f}}_2, \tag{3.33}$$

the following expressions can be obtained

$$\tilde{a} = \exp\left(\pi\mu_1 - i\delta\,\pi/2\right),$$

$$\tilde{b} = \frac{\sqrt{2\pi\mu_1}\,\exp\left(\pi\mu_1/2 + i\delta\mu_1 \ln \mu_1/e + i\delta\,\pi/4\right)}{\Gamma\left(i\delta\mu_1 + 1\right)} \qquad (3.34)$$

where Γ is the Euler gamma-function. If $\mu_1 = 0$ (the forbidden zone is degenerate) then

$$\tilde{a} = -i\delta, \quad \tilde{b} = 0. \qquad (3.35)$$

The energy transmission coefficient is equal to

$$P = |a|^{-2} = e^{-2\pi\mu_1}. \qquad (3.36)$$

Of course, the last formulae is known. It has been received earlier on the base of some analogies or approximate approaches. Another consistent deduction of this formula is unknown to us.

4. Quantization of orbits

1. Let us continue the analysis of equation (3.1). One of the main questions usually discussed in connection with the standard quasiclassical formulas is the description of the quantization conditions. If they are fulfilled there exists a solution exponentially decreasing outside the interval limited by the two turning points. The quantization conditions are formulated in terms of some closed iso-energy curve in phase space which we can connect with the admitted zone. Let us deduce the quantization conditions in our problem. We shall consider the asymptotical solutions f on the interval $(\xi_\ell, \xi_{\ell+1})$, $\ell = 2m$, corresponding to the spectral interval. We shall now obtain the conditions under which the linear combination exists which after the continuation through the neighbourhoods of the

points ξ_ℓ, $\xi_{\ell+1}$ will transform into decreasing solutions. Let us fix the solution f in the leading order by the formula

$$f \sim \mathcal{E}_k^{-1/2}\, u(k,x) \exp\left[\frac{i}{\varepsilon}\int_{\xi_\ell}^{\xi} k\,d\xi - \int_{k_\ell}^{k} (d_k u, u)\right], \qquad (4.1)$$

where $\mathcal{E}(k) + \varphi(\xi) = E$. When $\xi \to \xi_\ell$

$$\mathcal{E}(k) \approx E_\ell + \frac{1}{2\varkappa_\ell}(k - k_\ell)^2, \quad \varphi(\xi) \approx E - E_\ell + d_\ell(\xi - \xi_\ell). \qquad (4.2)$$

Therefore

$$k - k_\ell \approx |2\varkappa_\ell d_\ell|^{1/2} (\xi - \xi_\ell)^{1/2}. \qquad (4.3)$$

As a result, when $\xi \to \xi_\ell$

$$f \sim \mathcal{E}_k^{-1/2}\, u(k_\ell, x) \exp\left[\frac{i}{\varepsilon}\int_{\xi_\ell}^{\xi} k\,d\xi\right] \sim$$

$$\sim C_\ell(\mathcal{E}) \exp\left[-\frac{i}{\varepsilon}\xi_\ell k_\ell\right] \psi_\ell(x) |\zeta_\ell|^{-1/4} \exp\left[i\frac{2}{3}|2\varkappa_\ell d_\ell|^{1/2} |\zeta_\ell|^{3/2}\right], \qquad (4.4)$$

where

$$\zeta_\ell = \varepsilon^{-2/3}(\xi - \xi_\ell), \quad \psi_\ell(x) = \exp(i k_\ell x)\, u(k_\ell, x). \qquad (4.5)$$

Let us continue the solution f in the neighbourhood of the point $\xi_{\ell+1}$:

$$f \sim \exp i\Omega \times \mathcal{E}_k^{-1/2}\, u(k_{\ell+1}, x) \exp\left[\frac{i}{\varepsilon}\int_{\xi_{\ell+1}}^{\xi} k\,d\xi\right], \qquad (4.6)$$

$$\Omega = \frac{1}{\varepsilon}\int_{\xi_\ell}^{\xi_{\ell+1}} k\,d\xi + i\int_{k_\ell}^{k_{\ell+1}} (d_k u, u). \qquad (4.7)$$

Owing to the analogy with formula (4.4)

$$f \sim \exp i\Omega \times C_{\ell+1}(\varepsilon)\exp\left(-\frac{i}{\varepsilon}\xi_{\ell+1}k_{\ell+1}\right)\times$$

$$\times\psi_{\ell+1}(x)|\xi_{\ell+1}|^{-1/4}\exp\left[i\frac{2}{3}|2\varkappa_{\ell+1}\alpha_{\ell+1}|^{1/2}|\xi_{\ell+1}|^{3/2}\right]. \tag{4.8}$$

In (4.4) and (4.8) C_ℓ and $C_{\ell+1}$ are positive. The solutions ψ_ℓ and $\psi_{\ell+1}$ are supposed to be real.

Let

$$F = f - e^{-i\pi/4}\exp\left(-2\frac{i}{\varepsilon}\xi_\ell k_\ell\right)\bar{f}. \tag{4.9}$$

In this case when $\xi \longrightarrow \xi_\ell$

$$F \sim 2e^{i\pi/4}C_\ell\exp\left(-\frac{i}{\varepsilon}k_\ell\xi_\ell\right)\psi_\ell(x)|\xi_\ell|^{-1/4}\times$$

$$\times\sin\left(\frac{2}{3}|2\varkappa_\ell\alpha_\ell|^{1/2}|\xi_\ell|^{3/2}+\pi/4\right)\sim 2e^{i\pi/4}C_\ell\exp\left(-\frac{i}{\varepsilon}k_\ell\xi_\ell\right)w_\ell, \tag{4.10}$$

where

$$w_\ell = Ai\left(-2|\varkappa_\ell\alpha_\ell|^{1/3}\xi_\ell\right)\psi_\ell(x) \tag{4.11}$$

In formula (4.11) $A_i(z)$ is the known solution of the Airy equation

$$W'' = zW$$

$$Ai(z)\sim z^{-1/4}\exp\left(-\frac{2}{3}z^{3/2}\right),\quad z\to+\infty \tag{4.12}$$

$$Ai(z)\sim|z|^{-1/4}\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right),\quad z\to-\infty .$$

So the solution F decreases after continuation through the point ξ_ℓ .

In the neighbourhood of $\xi_{\ell+1}$

$$F\sim 2e^{i\pi/4}C_{\ell+1}\exp\left(-\frac{i}{\varepsilon}\xi_\ell\right)\psi_{\ell+1}|\xi_{\ell+1}|^{-1/4}\times$$

$$\times\sin\left[\frac{2}{3}|2\varkappa_{\ell+1}\alpha_{\ell+1}|^{1/2}|\xi_{\ell+1}|^{3/2}+\pi/4+\Omega-\right. \tag{4.13}$$

$$\left.-\frac{1}{\varepsilon}\left(\xi_{\ell+1}k_{\ell+1}-\xi_\ell k_\ell\right)\right].$$

If

$$-\Omega+\varepsilon^{-1}\left(\xi_{\ell+1}k_{\ell+1}-\xi_\ell k_\ell\right)=n\pi \tag{4.14}$$

n-integer, then

$$F\sim 2e^{i\pi/4}C_{\ell+1}\exp\left(-\frac{i}{\varepsilon}k_\ell\xi_\ell\right)w_{\ell+1}. \tag{4.15}$$

This means that the solution F decreases after continuation through the point $\xi_{\ell+1}$ if the condition (4.14) is valid.

2. In fact conditions (4.14) is the quantization condition. It can be written down in the following more simple form

$$\frac{1}{\varepsilon}\int_{k_\ell}^{k_{\ell+1}}\xi\,dk = i\int_{k_\ell}^{k_{\ell+1}}(du,u)+n\pi. \tag{4.16}$$

It should be noted that the first term on the right-hand side is real. The renormalization of u (if we take into account the restriction on   ) includes the choice of the ambiguous integer n.

Let us consider the curve in phase space which has two branches: $(\xi, \pm k(\xi))$, $\xi\in[\xi_\ell, \xi_{\ell+1}]$. If the points (ξ_ℓ, k_ℓ) $(\xi_\ell, -k_\ell)$ and $(\xi_{\ell+1}, k_{\ell+1})$, $(\xi_{\ell+1}, -k_{\ell+1})$

are identified, then some smooth closed curve γ arises. Let $u(-k,x)=\overline{u(k,x)}$ (this is a restriction on the normalization). In this case relation (4.16) is equivalent to the relation

$$\frac{1}{\varepsilon}\int_{\gamma}\xi\,dk = i\int_{\gamma}(du,u)+2\pi n \qquad (4.17)$$

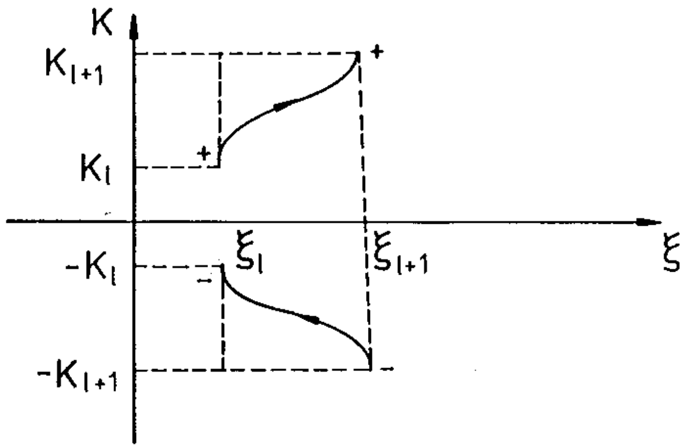

Fig 3

The signs "+" and "–" in fig. 3 characterize the signature of the intersection of and the set of its singular points, concerning the projection of the phase space onto the axis . It is clear that ind $\gamma = 0$ (ind γ -Maslov index, see /1/). This explains the absence of the famous additional term π in (4.17).

On the other hand the integral

$$\Gamma = \int_{\gamma}(du,u) \qquad (4.18)$$

is the so called Berry phase. In contrast to the usual point of view /5/ it can appear in problems connected with real operators. Our case has also the second peculiarity: the phase Γ can not be represented in terms of an integral on some two-dimensional surface, stretched on γ .

Apparently the phase factor (2.20) in the solution f which gives the origin to the additional term Γ in the explicit form appeared in /4/. In the case of the homogenious external electric field such a term has been known earlier /6/. Some different effects connected with so type additional terms in non-explicit form were discussed intensively already in the 50-s, see for example /7/. With particular care these effects were investigated in the case of Bloch electrons in an external magnetic field /8/. However, in this situation the explicit form of Γ has apparently not been received.

3. We have to wait that in more complex geometrical circumstances when ind $\gamma \neq 0$ the quantization conditions will transform into the form

$$\frac{1}{\varepsilon}\int_{\gamma}\xi\,dk + \frac{\pi}{2}\,\mathrm{ind}\,\gamma = i\int_{\gamma}(du,u)+2\pi n \qquad (4.19)$$

This situation can arise if the potential φ is not monotonous.

It can be expected that in the case of the general equation (1.1) the quantization conditions might have the following form

$$\frac{1}{\varepsilon}\int_{\gamma}\xi\,dk + \frac{\pi}{2}\,\mathrm{ind}\,\gamma = i\int_{\gamma}\Big[(du,u)+\mathrm{tr}\big(\hat{\mathcal{L}}u_{\xi},u_{k}\big) + \big(\hat{\mathcal{L}}_{\nu}u,u\big)\Big]ds+2\pi n . \qquad (4.20)$$

The curve γ is to be considered on the "cylindre", which arises after the factorization of the K -component of the phase space regarding the adjoint lattice T^*. Naturally the question arises about the normalization conditions on u in the singular points of γ . We have no possibilities to consider this question here.

The spectral meaning of quantization conditions (4.20) as in the standard quasiclassical approach cannot be universal. It is clear that these conditions are responsible for some singularities of operator $\mathcal{L}^{-1}$, but their spectral meaning depends on the global behavior of the coefficients of $\mathcal{L}$, and can be different, see for example /9/.

5. Short comments

Equation (1.2) was the subject of very intensive investigations from the beginning of 50-s. It is true, however, that it has not been written down in form (1.2) with the explicit division the dependence of the coefficients on x and $\xi = \varepsilon x$ We have mentioned the first work by R. Peierls /3/ containing the bright guess that equation (2.30) must have the connections with the initial equation (2.1). Let us indicate a very short list of reviews which give an impression of the main contributors and results: /6, 7, 9 - 17/. The approach developed here was proposed in /4/. About the turning points and the transition through the forbidden zone see, for example /7, 9, 11 - 13, 15, 17/. The quantization of orbits was discussed in /7, 8, 15, 17/.

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