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COMPLEXIFIED QUANTUM RULES

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ABSTRACT. Here is a short account of papers published earlier in Russian. We formulate a generalisation of well-known quantization rules by Bohr-Sommerfeld-Einstein-Keller-Maslov by adding terms which describe the tunneling of energy. This enables us to obtain imaginary radiational corrections to eigenvalues in the case of open systems as well as an exponentially small splittings of eigenvalues in systems with symmetry

§1. INTRODUCTION

We will consider semiclassical approximations to the eigenstates of the Schrödinger equation

$$(1.1) \qquad -\frac{\hbar^2}{2}\Delta\psi + V(x)\psi = E\psi$$

where Δ is the Laplacian operator in $\mathbb{R}^n$, $V(x)$ is a real valued function which is supposed to be semibounded from below, the variable x ranging over a domain $Q \subset \mathbb{R}^n$ with piecewise smooth boundary. For definiteness we pose the Dirichlet boundary conditions $\psi|_{\partial Q} = 0$.

The semiclassical theory of eigenstates is based on the study of motions in a corresponding classical dynamical system which is governed by the Hamiltonian function

$$(1.2) \qquad H(x,p) = \frac{1}{2}p^2 + V(x)$$

completed by a reflection condition at points which are projected to the boundary. At least a part of eigenstates can be found from quantization rules applied to KAM tori [L1]. In such a way one obtains a good approximation to eigenvalues, but instead of approximating the genuin eigenfunctions, we get so called "quasimodes"[A] which approximate a linear combination of eigenfunctions with very close eigenvalues.

As a one dimensional example of two symmetric wells (see Fig.1) shows, the splitting of the eigenstates can be exponentially small and has the tunnelling effect as the mechanism of the phenomena in question.
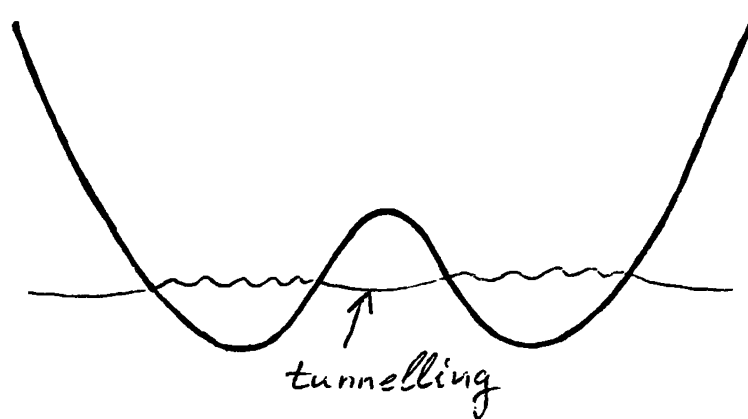
Fig.1 Two wells potential.

In more general case one can imagine an equation (1.1) with a symmetric potential which produces identical quasimodes shifted in space one from another by equal distance and interacting through the "forbidden" regions, the latters giving rise to an exponentially small splitting of eigenvalues.

Another kind of spectral problems, also connected with the tunnelling, is the shift of eigenvalues to the complex plane due to the radiation losses. Let the domain Q be unbounded (say $Q = \mathbb{R}^n$), and let $V(x)$ do not increase if x tends to infinity. Consider as the simpliest example again the one-dimensional problem with the potential like on Fig.2.
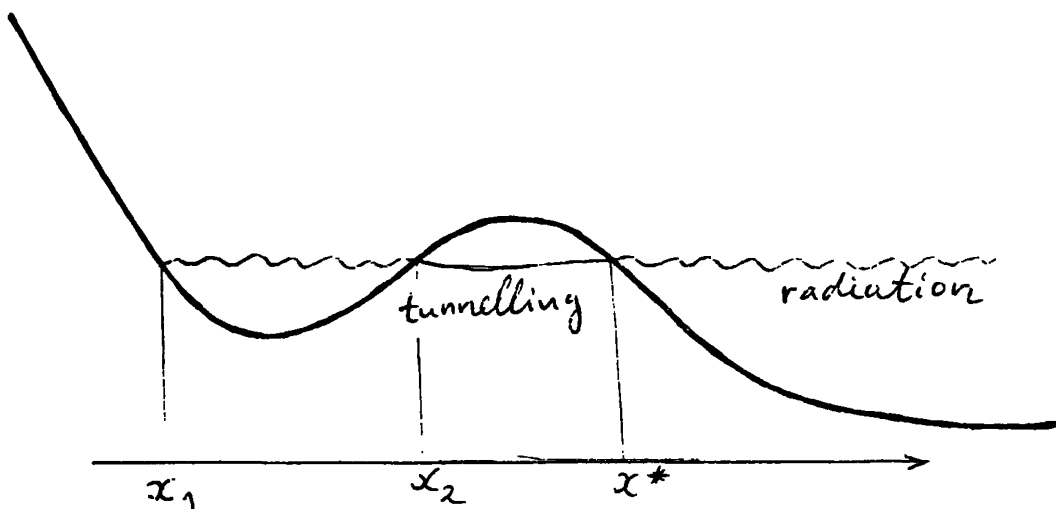

Fig.2 A well with tunnelling.

There is a neighbourhood of the minimum of the potential where an eigenfunction oscillates between x_1 and x_2, exponentially decreases a forbidden region between x_2 and x^*, and then, starting with x^*, again oscillates with very small amplitude due to the loss of energy via the tunneling throug the barrier. This results in an imaginary correction to an eigenvalue, so that the eigenfunction has a weak exponential growth in the region $(x^*, +\infty)$ (with the rate $\exp\left(x \cdot \exp(-C/\hbar)\right)$, $C > 0$.)

In mathematical setting one has to continue the Green function of the Scrödinger operator through the continuous spectrum. The complex "eigenvalues" in question are nothing more than the poles of the Green function on the second sheet of the energy complex plane.

The described phenomena, in spite of their exponentially small magnitude, play a significant role in nature. The goal of this paper is to formulate simple quantisation rules which generalize the well known rules of Bohr, Zommerfeld-Einstein-Keller-Maslov rules, [E],[KR],[M], and take into account the tunnelling effect. These rules enable us in some cases to calculate either the splitting of eigenvalues due to the symmetry or the imaginary correction to an eigenvalue due to radiation losses.

The contens of this article is based on papers earlier published in Russian: [L2],[L3],[T1], [T2] (see also [Ta],[LT1],[LT2]).

§2. COMPLEXIFICATION

A natural idea is to complexify everything, that is to consider an analytic continuation of everything to a complex domain, and to apply the known quantisation rules to the complexified objects.

Assume for a moment that the potential V is analytic, say a polynomial, $Q = \mathbb{R}^n$, and such a continuation makes sense. Consider a KAM torus, $\mathcal{T}$, in $\mathbb{R}^n \times \mathbb{R}^n$, and let $\mathcal{L}$ be its analytic continuation in $\mathbb{C}^n \times \mathbb{C}^n$. $\mathcal{L}$ is a Lagrangian sumbanifold of the complex phase space $\mathbb{R}^n \times \mathbb{R}^n$ endowed with a complex symplectic form $dx \wedge dp$, it has a complex dimension n, the real one being $2n$. In fact we have to consider a family of Lagrangian submanifolds $\mathcal{L}(E) \subset H^{-1}(E)$ depending on the energy E and maybe on some other parameters, and lying in the manifold of constant energy $H^{-1}(E)$. Applying the quantum rules to such a family selects the values of the energy E_m, $m = (m_1, m_2, \dots)$ being a collection of quantum numbers. In the real case $\mathcal{L}$ is always an $n-$dimensional torus, and the quantum rules can be expressed as the equaling of some integrals of a 1-form over the basic cycles of the torus to integers (quantum numbers). In the complex case we may try to do the same. Finally we want to obtaine an eigenfunction defined in the real domain $Q = \mathbb{R}^n$. So we have to return to the real coordinate space keeping the momenta complex: $\mathbb{R}^n \times \mathbb{C}^n \subset \mathbb{C}^n \times \mathbb{C}^n$. Only the intersection

$$(2.1) \qquad \mathcal{L}' = \mathcal{L} \cap (\mathbb{R}^n \times \mathbb{C}^n) \,.$$

plays the role in the construction of the eigenfunctions defined in Q. Simple calculation shows that the real dimension of $\mathcal{L}'$ is equal to n.

A new fact is that the $\mathcal{L}'$ does not coincide with the initial KAM torus $\mathcal{T}$, but contains something else:

$$(2.2) \qquad \mathcal{L}' = \bigcup_\rho \mathcal{L}_\rho \,.$$

It consists of several "components" $\mathcal{L}_\rho$, each being an n—dimensional Lagrangian submanifold, and the components are glued along an $(n-1)$—dimensional submanifold, the latter being the singularity with respect to the projection to the n—dimensional configuration space:

$$(2.3) \qquad\qquad \pi: \mathbb{R}^n \times \mathbb{C}^n \longrightarrow \mathbb{R}^n .$$

Only one of the components of (2.2) coincides with the initial torus $\mathcal{T}$. Others are either real KAM tori or nonreal Lagrangian submanifolds which are symmetric with respect to the operation of complex conjugating.

A generic point of the singularity manifold with respect to the projection (2.3) is a fold, two components meet at a point of the fold, one of them being real (KAM torus), another one being nonreal. In appropriate local coordinates $(\xi_1, \xi_2, \ldots, \xi_n, \eta_1, \eta_2, \ldots, \eta_n)$, $\xi_k \in \mathbb{R}$, $\eta_k \in \mathbb{C}$, the projection (3.3) and the equation of $\mathcal{L}'$ read:

$$(2.4) \qquad \begin{aligned} \pi: &\quad (\xi_1, \xi_2, \ldots, \xi_n, \eta_1, \eta_2, \ldots, \eta_n) \longmapsto (\xi_1, \xi_2, \ldots, \xi_n), \\ \mathcal{L}': &\quad \eta_1^2 = \xi_1, \quad \eta_k = 0, \quad k = 2, 3, \ldots, n. \end{aligned}$$

If we separate the real and the complex parts of $\eta_k = \eta_k' + i\eta_k''$, the equations of $\mathcal{L}'$ acquire the form:

$$(2.5) \qquad \begin{cases} \left(\eta_1'\right)^2 - \left(\eta_1''\right)^2 = \xi_1, \\ 2\eta_1'\eta_1'' = 0, \\ \eta_k' = \eta_k'' = 0, \quad k = 2, 3, \ldots, n. \end{cases}$$

The equations (2.5) define two pieces of $\mathcal{L}'$: the real one which corresponds to the region $\xi_1 \geq 0$

$$(2.6) \qquad \begin{cases} \eta_k' = 0, \quad k = 2, 3, \ldots, n, \\ \eta_k'' = 0, \quad k = 1, 2, \ldots, n, \\ \eta_1' = \pm\sqrt{\xi_1}, \end{cases}$$

which is a part of a KAM torus, say $\mathcal{L}_{\rho_1}$. and the nonreal one which corresponds to the region $\xi_1 \leq 0$

$$(2.7) \qquad \begin{cases} \eta_k' = 0, \quad k = 1, 2, \ldots, n, \\ \eta_k'' = 0, \quad k = 2, 3, \ldots, n, \\ \eta_1'' = \pm\sqrt{-\xi_1}, \end{cases}$$

which is a part of a nonreal component, say $\mathcal{L}_{\rho_2}$. The fold divides both the components into two sheets. The real component (2.6) is divided into *incoming sheet*, and *outcoming sheet*, according to the direction of the vector field of the Hamiltonian (1.2) at points of the fold. The nonreal component (2.7) is divided into *increasing sheet*, and *decreasing*
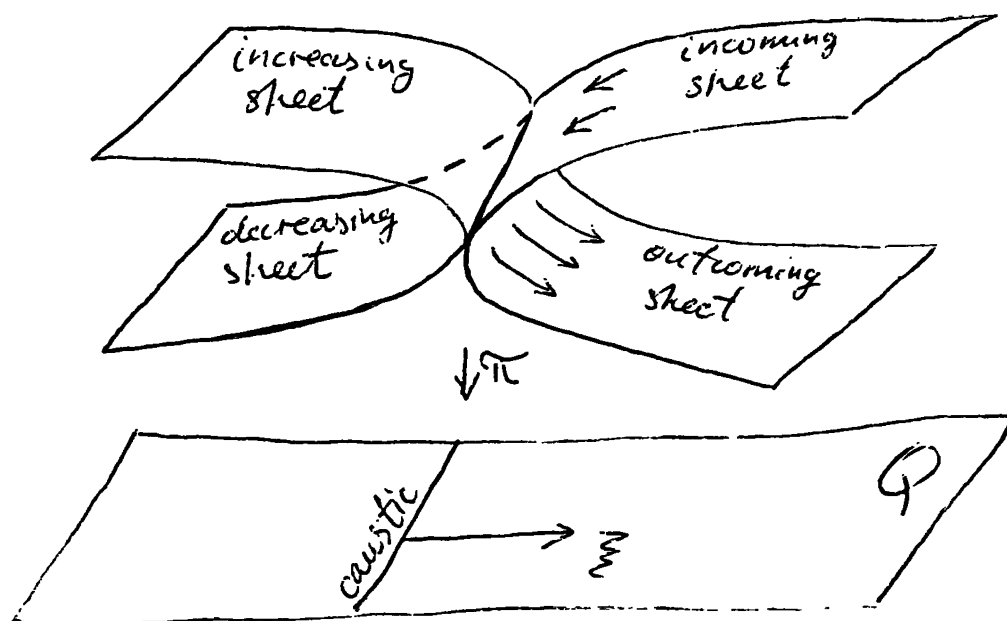
Fig.3 A MEETING OF THE FOUR SHEETS AT A FOLD

sheet, according to the sign of the function $\int_{z_0}^{z} p'' dx$ where z_0 belongs to the fold, z belongs to $\mathcal{L}_{p_2}$, the integration goes over a path on $\mathcal{L}_{p_2}$, the positive value corresponds to the increasing sheet.

Up to now we considered a hypothetical situation when everything can be prolonged analytically in the whole complex phase space. But really we do not need it: we need only to consider a part of the whole comlex object, namely (2.1). On the other hand the potentials and the domains which we meet in applications are not necessarily analytic, and do not admit an analytic continuation.

We assume only the existence of a collection of Lagrangian submanifolds in $Q \times \mathbb{C}^n$ of the form (2.2), some of them being real KAM tori, others bein nonreal, glued along the common singularity with respect to the projection (2.3), the typical behaviour in a neighbourhood of singularity point being described by equations (2.4)–(2.7). The Lagrangianness means that the form

$$(2.8) \qquad \Omega = dx \wedge dp = \sum_{k=1}^{n} dx^k \wedge dp'_k + i \sum_{k=1}^{n} dx^k \wedge dp''_k$$

vanishes at vectors belonging to the tangent space to $\mathcal{L}_p$. The latter has to be considered as a complex n–dimensional vector space, *i.e.* it is the complexificaton of the real n–dimensional vector space tangent to $\mathcal{L}_p$. after the inclusion of the latter in the comlex phase space via the inclusion map $Q \times \mathbb{C}^n \hookrightarrow \mathbb{C}^n \times \mathbb{C}^n$.

§3. QUANTUM RULES

Here we formulate a generalisation of the quantum rules which arises from a representation of the asymptotics of the wave function ψ in a neighbourhood of the projection of the fold (caustic) which uses the Airy functions, that is solutions of the ordinary linear differential equation

$$(3.1) \qquad W''(z) = zW(z).$$

We select two independent solutions of (3.1), $W_{\pm}$, by the rule: in the sector $|\arg(-z)| \leq \frac{\pi}{4}$

$$(3.2) \qquad W_{\pm}(z) \sim (-z)^{-1/4} \exp\left(\pm i\frac{\pi}{4} \pm \frac{2}{3}i(-z)^{3/2}\right).$$

In the opposite sector $|\arg z| \leq \frac{\pi}{4}$ we will use the following asymptotics (note that an exponentially decreasing term is retained!):

$$(3.3) \qquad W_{\pm}(z) \sim z^{-1/4}\left[\exp\left(\frac{2}{3}z^{3/2}\right) \pm \frac{i}{2}\exp\left(-\frac{2}{3}z^{3/2}\right)\right].$$

Not going into the details (see [L3]), we formulate the quantum rules which arise from (3.2),(3.3) as follows.

(1) We suppose that the folds are $(n-1)$−dimensional submanifolds, and acquire to each component, l_j, of the fold a number $\varkappa_j$, the *percolation coefficient* trough l_j.

(2) Given an oriented loop γ on a nonreal component $\mathcal{L}_\rho$, which crosses the folds transversally and avoids higher singularities,

$$(3.4) \qquad \frac{1}{\hbar}\oint_\gamma pdx + \nu^{\partial Q}[\gamma]\cdot\pi + \nu^M[\gamma]\cdot\frac{\pi}{2} + i\sum_j \pm\varkappa_j \equiv 0(\mod 2\pi).$$

The sum in (3.4) spreads on all intersections of γ with the fold. The $\nu^{\partial Q}[\gamma]$ is the intersection index mod 2 of γ with the preimage of ∂Q, $\nu^M[\gamma]$, Maslov index, is the intersection index mod 4 of γ with the fold, the latter being oriented so that the crossing from the decreasing sheet to the increasing one gives a contribution $+1$. The signum at $\varkappa_j$ is $+$ if the loop goes from the decreasing sheet to the increasing one, and $-$ otherwise.

(3) Given an oriented loop γ on a real component $\mathcal{L}_\rho$, which crosses the folds transversally and avoids higher singularities,

$$(3.5) \qquad \frac{1}{\hbar}\oint_\gamma pdx - \nu^{\partial Q}[\gamma]\cdot\pi - \nu^M[\gamma]\cdot\frac{\pi}{2} + i\sum_j \pm\ln\coth\frac{\varkappa_j + \ln 2}{2} \equiv 0(\mod 2\pi).$$

The sum in (3.5) spreads on all crossings of γ with the fold, the signum $+$ corresponding to the passings from the incoming sheet to the outcominig one, $-$ otherwise.

(4) If $\mathcal{L}_\rho$ is a noncompact real component, we set $\varkappa_j = i\pi - \ln 2$ for all components l_j of the fold adjacent to $\mathcal{L}_\rho$. If $\mathcal{L}_\rho$ is a noncompact nonreal component, we set $\varkappa_j = +\infty$ for all components l_j of the fold adjacent to $\mathcal{L}_\rho$.

(5) We suppose that there is a family of Lagrangian submanifolds $\mathcal{L}' \subset H^{-1}(E)$ of the form (2.2) depending on the energy E as a parameter and probably on other parameters. To find an exponentially small splitting of eigenvalues in case of symmetry (or an imaginary correction to an eigenvalue in case of an open system), we linearize the system (3.4), (3.5) with respect to the exponentially small splitting ΔE (or the correction $\Im E$) around *real* value of E.

(6) Finally, taking a finite colection of basic cycles $\gamma_1, \gamma_2, \ldots, \gamma_N$ on the components $\mathcal{L}_\rho$ of (2.2), we have to resolve the corresponding equations (3.4),(3.5) with respect to the unknown quantities E, ΔE (or $\Im E$), other parameters, and the unknown $\varkappa_j$ corresponding to the components of the folds not adjacent to noncompact $\mathcal{L}_\rho$.

Note. Such a strange entering of $\varkappa_j$ into (3.5) is due to the sewing condition between exponential asymptotics and asymptotics containing the Airy functions.

In the next two sections we illustrate the formulated rules by considering two simple 2-dimensional examples.

§4. Radiation through a hole

Here and in the next section we consider the wave equation

$$(4.1) \qquad \Delta u + k^2 u = 0$$

instead of (1.1). To get the quantum rules for calculating the eigenvalues k^2 one has to replace $\hbar^{-1}$ in (3.4) and (3.5) by k.

Concider a domain $Q \subset \mathbb{R}^2$ which is the complement to the curve which consists of the lower half of the ellipce

$$(4.2) \qquad \frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} = 1, \quad x_2 \leq 0,$$

and two rectilinear segments joining the foci with the ends of the lagre axis of the ellipce (see Fig.4).

It is convenient to pass to the elliptic coordinates by the formulae:

$$(4.3) \qquad \begin{aligned} x_1 &= h \cosh\mu \cos\varphi, & 0 \leq \mu < \infty, \\ x_2 &= h \sinh\mu \sin\varphi, & 0 \leq \varphi \leq 2\pi, \\ a &= h \cosh\mu_0, & b = h \sinh\mu_0. \end{aligned}$$

The equation of the Lagrangian manifold (2.2) can be found explicitely in the form $p = \mathrm{grad}S(x)$ where S is a generating function. The eiconal equation which arises for S, admits a separation of variables in the coordinates (4.3), and S can be found in the form:

$$(4.4) \qquad S_\theta = \pm F_\theta(\mu) \pm \Phi_\theta(\varphi),$$

$$(4.5) \qquad F_\theta(\mu) = h \int_0^\mu \sqrt{\cosh^2\tau - \cosh^2\theta}\, d\tau,$$

$$(4.6) \qquad \Phi_\theta(\varphi) = h \int_0^\varphi \sqrt{\cosh^2\theta - \cos^2\alpha}\, d\alpha,$$
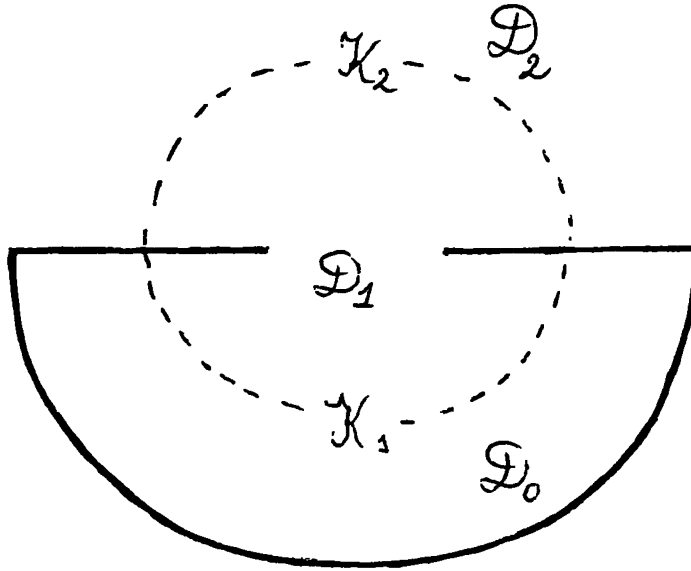
Fig.4 RADIATION FROM THE OPEN HALF OF AN ELLIPCE

θ being a parameter. For each $\theta \in [0, \mu_0]$ the function is a generating function for a Lagrangian manifold in the sense of §2. The surface $\mathcal{L}(\theta)$, the half of it is drâwn on Fig.5, has three components $\mathcal{L}_\rho$, $\rho = 0, 1, 2$, the latters being projected onto the domains D_ρ (see Fig.4) and glued along the folds l_1 and l_2.

Let us introduce the notations

$$J_1(\theta) = h \int_0^{2\pi} \sqrt{\cosh^2 \theta - \cos^2 \phi} d\phi,$$

(4.7)
$$J_2(\theta) = 2h \int_\theta^{\mu_0} \sqrt{\cosh^2 \mu - \cosh^2 \theta} d\mu,$$

$$R(\theta) = 2h \int_{-\theta}^\theta \sqrt{\cosh^2 \theta - \cosh^2 \mu} d\mu,$$

and write down the quantum conditions,which correspond to the basic cycles γ_s, $s = 1, 2, 3$, drawn on Fig.5, in the form:

(4.8)
$$\begin{cases} k J_1 = 2\pi m, \\ k J_2 = 2\pi \left(n + \dfrac{3}{4}\right) - i \ln \coth \dfrac{\varkappa + \ln 2}{2}, \\ i k R = \pi + i(\varkappa + i\pi - \ln 2) \quad m, n \in \mathbb{Z}, \ m, n \gg 1, \end{cases}$$
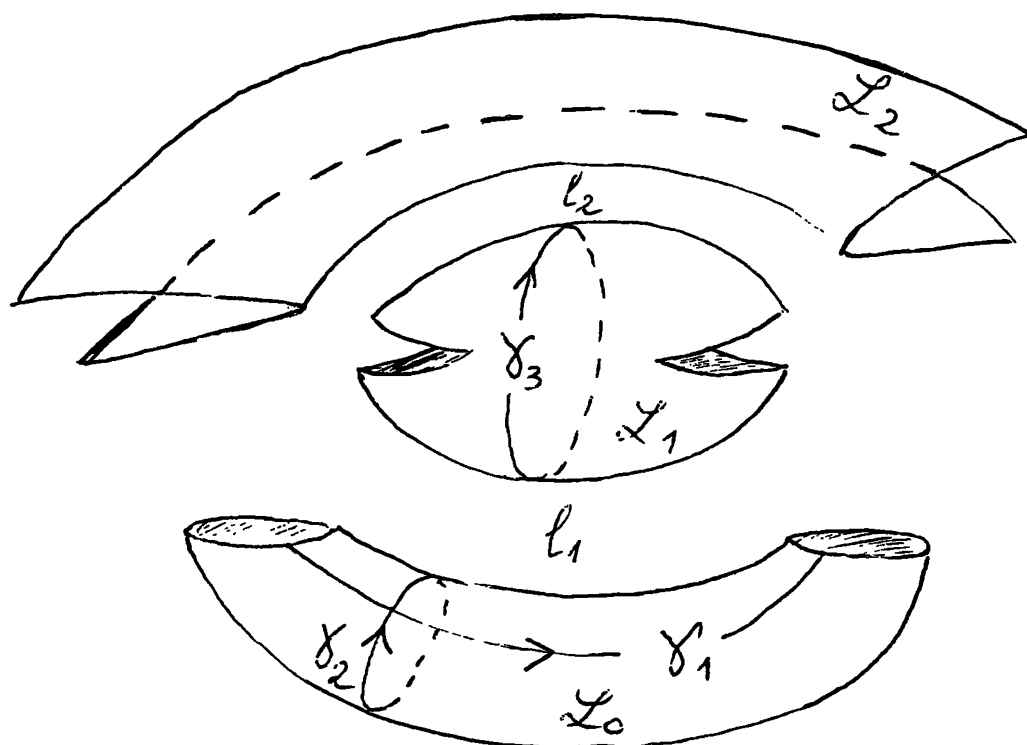
from which it follows, after the linearization with respect the imaginary part of $k = k' + i k''$

that

$$(4.9) \qquad k'_{mn} = 2\pi m J_1(\theta_{mn})^{-1} = 2\pi \left(n + \frac{3}{4}\right) J_2(\theta_{mn})^{-1},$$

$$(4.10) \qquad k''_{mn} = -\frac{1}{2} \cdot \frac{\exp\left(-k'_{mn}R(\theta_{mn})\right)}{J_2(\theta_{mn}) - J_1(\theta_{mn})J'_2(\theta_{mn})/J'_1(\theta_{mn})}.$$

The number θ_{mn} has to be defined from the equaling of two expressins for k'_{mn} in (4.9).

Fig.5 LAGRANGIAN SURFACES FOR THE HALF OF AN ELLIPSE WITH RADIATION

§5. SPLITTING OF SYMETRIC EIGENSTATES

In this section we consider the Dirichlet problem for the equation (4.1) in the whole ellipce with attached two cuts, the same ones as in the previous section (see Fig.6).

Using the same notations , one can write down the quantum conditions for the cycles γ_s, $s = 1,2,3,4,5$, drawn on Fig.7 which represents the Lagrangian surfaces for this
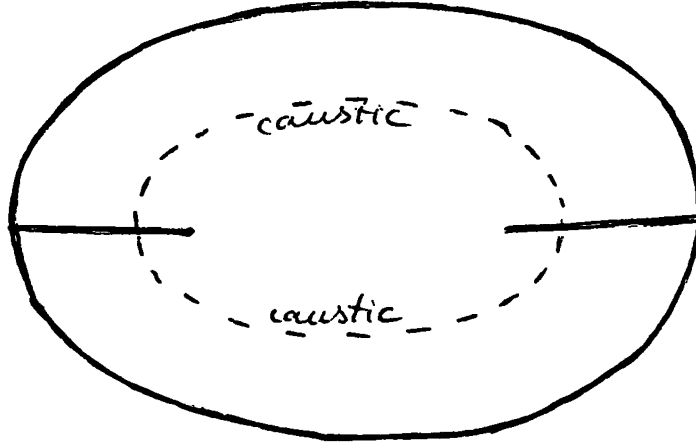
Fig.6 Ellipce with cuts. Two symmetric quasimodes

problem:

$$\gamma_1: \ kJ_1 = 2\pi m_1 \,,$$

$$\gamma_2: \ kJ_2 = 2\pi\left(n_1 + \frac{3}{4}\right) - i\ln\coth\frac{\varkappa_1 + \ln 2}{2}\,,$$

$$\gamma_3: \ ikR = -\pi - i(\varkappa_1 + \varkappa_2) = 2\pi r \,,$$

$$\gamma_4: \ kJ_1 = 2\pi m_2 \,,$$

$$\gamma_5: \ kJ_2 = 2\pi\left(n_2 + \frac{3}{4}\right) - i\ln\coth\frac{\varkappa_2 + \ln 2}{2}\,.$$

$$m_j, n_j, r \in \mathbb{Z}, j = 1, 2 \,.$$

It follows due to symmetry that

$$(5.1) \qquad \varkappa_1 = \varkappa_2 = \varkappa = i\pi r - i\frac{\pi}{2} + \frac{1}{2}kR, \quad m_1, m_2 = m \,.$$

We have

$$(5.2) \qquad \ln\coth\frac{1}{2}(\varkappa + \ln 2) \approx e^{-\varkappa} = \pm i\exp\left(-\frac{1}{2}kR\right) \,.$$

Note that the sign $\pm$ in (5.2) is the result of the choice of different values of the integer r in (5.1). Our quantum rules acqure the form:

$$(5.3) \qquad \begin{cases} kJ_1 = 2\pi m \,, \\[2mm] kJ_2 = 2\pi\left(n + \frac{3}{4}\right) \pm \exp\left(-\frac{1}{2}kR\right) \,. \end{cases}$$
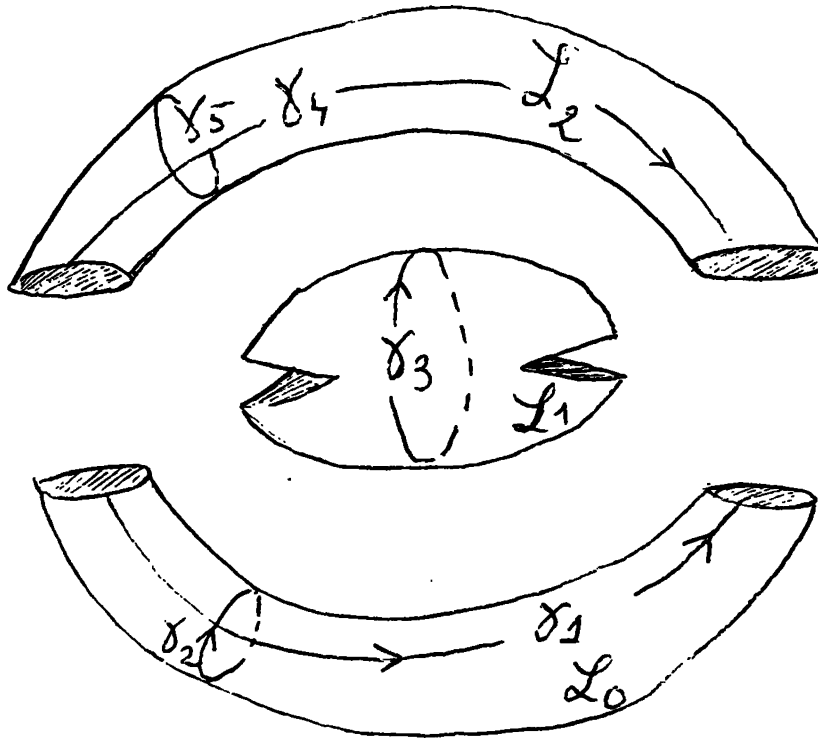
Fig.7 LAGRANGIAN SURFACES FOR THE ELLIPCE WITH CUTS

After the linearization procedure (5.3) gives the following value for the egenvalue splitting:

$$(5.4) \qquad \Delta k_{mn} = \frac{2J_1'(\theta_{mn})}{J_1'(\theta_{mn})J_2(\theta_{mn}) - J_1(\theta_{mn})J_2'(\theta_{mn})} \cdot \exp\left(-\frac{1}{2}kR\right).$$

where θ_{mn} is to be found as a solution of the equation

$$(5.5) \qquad \frac{J_1(\theta)}{J_2(\theta)} = \frac{m}{n + 3/4}.$$

This formula was confirmed in [T2] by direct computation of the eigenvalue asymptotics via the separation of variables in the equation (4.1).

§6. Variational principle for the complex phase

The problem of finding the Lagrangian manifolds with desired properties seems to be difficult. It contains as a part the computation of KAM tori, which is difficult itself. The equations for nonreal components are nonlinear and elliptic at least in the case $n = 2$. It is worthwile to mention here a variational principle for the case of equation (4.1) formulated in [T1].

To solve the equation

$$(6.1) \qquad (\nabla S)^2 = 1$$

let us separate S into real and imaginary part:

$$(6.2) \qquad S = \Phi + i\Psi.$$

Introducing a new function c by the equalities:

$$\frac{\partial \Psi}{\partial x} = c\frac{\partial \Phi}{\partial y}, \qquad \frac{\partial \Psi}{\partial y} = -c\frac{\partial \Phi}{\partial x},$$

one finds

$$c = \sqrt{1 - (\nabla\Phi)^{-2}},$$

and the function Φ satisfies the elliptic equation:

$$\frac{\partial}{\partial x}\left(c\frac{\partial \Phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(c\frac{\partial \Phi}{\partial y}\right) = 0.$$

The latter coincides with the Euler equation for the functional

$$(6.3) \qquad F(\Phi) = \int f((\nabla\Phi)^2)dxdy,$$

where

$$f(w) = \sqrt{w(w-1)} - \ln(\sqrt{w} + \sqrt{w-1}).$$

Thus, the problem of finding a nonreal Lagrangian surface is reduced to finding a minimum to (6.3) in a domain with partially unknown (free) boundary.

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