GEOMETRICAL THEORY OF DIFFRACED RAYS, ORBITING AND COMPLEX RAYS

ENRICO DE MICHELI
IBF – Consiglio Nazionale delle Ricerche
Via De Marini, 6 - 16149 Genova, Italy
E-mail: enrico.demicheli@cnr.it

GIOVANNI ALBERTO VIANO
Dipartimento di Fisica – Università di Genova,
Istituto Nazionale di Fisica Nucleare – Sezione di Genova,
Via Dodecaneso, 33 - 16146 Genova, Italy
E-mail: viano@ge.infn.it

Abstract. In this article, the ray tracing method is studied beyond the classical geometrical theory. The trajectories are here regarded as geodesics in a Riemannian manifold, whose metric and topological properties are those induced by the refractive index (or, equivalently, by the potential). First, we derive the geometrical quantization rule, which is relevant to describe the orbiting bound–states observed in molecular physics. Next, we derive properties of the diffractive rays, regarded here as geodesics in a Riemannian manifold with boundary. A particular attention is devoted to the following problems: (i) modification of the classical stationary phase method suited to a neighborhood of a caustic; (ii) derivation of the connection formulae which enable one to obtain the uniformization of the classical eikonal approximation by patching up geodesic segments crossing the axial caustic; (iii) extension of the eikonal equation to mixed hyperbolic–elliptic systems, and generation of complex–valued rays in the shadow of the caustic. By these methods, we can study the creeping waves in diffractive scattering, describe the orbiting resonances present in molecular scattering beside the orbiting bound–states, and, finally, describe the generation of the evanescent waves, which are relevant in the nuclear rainbow.

“Lumen propagatur seu diffunditur non solum directe, refracte ac reflexe, sed etiam alio quodam quarto modo, diffracte.”

Francesco Maria Grimaldi
(Physico–Mathesis de lumine, coloribus, et iride, alisque adnexis libri duo; Bononiae 1665)

1. Introduction

In the decade 1950–1960, J. B. Keller [1, 2, 3] wrote several papers in which he introduced the so–called Geometrical Theory of Diffraction (GTD). This theory can
be regarded as an extension of geometrical optics, which accounts for diffraction by introducing the diffracted rays in addition to the usual rays of geometrical optics. Nowadays, GTD includes features which were not present in Keller’s first derivation such as, for instance, uniform solutions at a caustic. It was, in fact, Ludwig [4] who obtained a uniform asymptotic expansion of the wavefield at the caustic, which is the locus where the rays of geometrical optics have an envelope and the amplitude presents a singularity. Ludwig derived a formal asymptotic series, which is uniformly valid. After these seminal works, there has been a steady flow of papers addressing various aspects of the theory. On one hand, papers oriented to pure and applied electromagnetic theory, like radiation and scattering of waves, antenna design, waveguide theory, and so on [3]; on the other hand, a highly theoretical and mathematically sophisticated theory of propagation of singularities, and diffraction of waves on manifolds [5]. Moreover, in theoretical physics, GTD is closely related to the Feynman integral approach. It is worth mentioning the recent paper by Schaden and Spruch [6], where a link between diffraction in the semiclassical approximation and Feynman’s path integral representation of the Green function can be found. These authors note that the evaluation of the Casimir effects needs the consideration of diffraction, at least semiclassically. Along with Casimir effects, the calculation of the exchange second virial coefficient of a hard–sphere gas evaluated by E. H. Lieb by means of the path integral should be recalled [7]. This problem is indeed similar to the classical problem of diffraction of waves (of short wavelength) around a sphere into the dark zone [7]. Last but not least, GTD also suggested the introduction of the complex angular momenta (CAM) in wave mechanics [8], which is not surprising since the most precise diffraction measurements can be performed in nuclear and particle physics.

A particularly useful mathematical tool in diffraction theory is the Watson re-summation of the partial wave expansion. Unfortunately, working with this transform leads quite frequently to technical convergence difficulties; this is the case, for instance, in the computation of the virial coefficient [7], and in the CAM theory of potential scattering if one considers potentials far beyond the Yukawian class. In this situation, one is naturally led to leave out the Watson transform and to push further the path integral approach. However, also in this case, a price has to be paid since one is forced to introduce various conjectures based on physical intuition. As a typical example, we can mention the splitting of grazing rays at the boundary of the obstacle and, accordingly, the generation of the diffracted rays. At this point a question emerges:

**Problem:** Is it possible to prove the conjectures of GTD by using the methods supplied by the differential geometry?

We believe that, at the moment, it is very hard to give a general and definitive positive answer. Nevertheless, an answer in some specific physical problem can be found. The purpose of this paper is precisely that of providing a geometrical theory of the following physical phenomena:

(a) orbiting resonances and bound states, which are observed in molecular scattering [9, 10];

(b) diffractive scattering at high–energy in nuclear and particle physics [11, 12, 13];
(c) the generation of evanescent waves in the shadow of the caustic, which are relevant for the nuclear rainbow [14, 15].

In a previous paper [16] we have obtained very preliminary results concerning problem (b); i.e., the diffractive scattering at high energy by a compact, convex and opaque object. Nevertheless, in spite of these efforts, many relevant problems remained. It is precisely the main purpose of the present article to fill this gap and, more specifically, to study in detail the following problems:

1) A method of geometric quantization based on a procedure of analytic continuation, appropriate for describing the spectrum of bound states in molecular physics. This problem will be addressed in Section 2.

2) The geometrical structure of the caustic in diffractive scattering, considering separately the axial caustic from the caustic generated by the border of the diffracting obstacle. This question will be treated in Section 3.

3) Still in Section 3 we derive eikonal equations of Ludwig–type, by using the Chester-Friedman-Ursell [17] approximation, which is a modification of the stationary phase method, suitable in the neighborhood of a caustic. In the same section, the mixed (hyperbolic–elliptic) character of the Ludwig system is proved and analyzed.

4) Section 4 is divided in three parts. In the first one, we derive the scattering amplitude at high energy of the creeping waves in diffractive theory by making use of an appropriate semi–phenomenological transport equation. In particular, we obtain an expression of the damping factor of the creeping waves, which depends upon the curvature of the obstacle, and it is related to the breaking of quantization. The second part is devoted to the analysis of the orbiting resonances, which are present in molecular physics, and some explicit expressions of the phase–shifts are obtained. In the third part of Section 4 we prove the existence of the evanescent waves in the shadow of the caustic, which follows from the elliptic character of the Ludwig eikonal system.

5) Finally, some conclusions are drawn in Section 5.

2. Geometrical theory of orbiting bound states

2.1. Geometric preliminaries. Let $\mathbb{M}^n$ denote a Riemannian manifold, let $\mathcal{C}$ be a chart of $\mathbb{M}^n$, let $x = (x_1, \ldots, x_n)$ be the local coordinates in $\mathcal{C}$, and let $g_{ij}$ be the metric tensor. As usual $g = |\det(g_{ij})|$, and $g^{ij} = (g_{ij})^{-1}$. Consider the Helmholtz equation

\[
(2.1) \quad \Delta \psi + k^2 \psi = 0,
\]

where $k$ is the wavenumber and $\Delta$ is the Laplace–Beltrami operator which, when applied to a function $\psi \in C^\infty(\mathbb{M}^n)$, reads as

\[
(2.2) \quad \Delta \psi = \frac{1}{\sqrt{g}} \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \left( \sum_{j=1}^{n} g^{ij} \sqrt{g} \frac{\partial}{\partial x_j} \right) \psi.
\]

We now introduce the infinite–dimensional space $\Omega(\mathbb{M}^n; p, q)$ of the piecewise differentiable paths $c$ connecting the point $p$ with the point $q$ on $\mathbb{M}^n$: i.e., if $p$ and $q$ are two fixed points on $\mathbb{M}^n$, then $c : [0, 1] \to \mathbb{M}^n$ is a piecewise differentiable path such that $c(0) = p$ and $c(1) = q$. To any element $c \in \Omega(\mathbb{M}^n; p, q)$ we associate an infinite–dimensional vector space $T_c \Omega$, which can be identified with the space tangent to $\Omega$ at the point $c$. More precisely, $T_c \Omega$ is the vector space formed by all
fields of piecewise differentiable vectors $V$ along the path $c$ such that $V(0) = 0$ and $V(1) = 0$. Next, we consider the action $S$ as a functional on the paths $\{c\}$ \cite{18}:

$$
S(c) = \int_0^1 \left| \frac{dc}{dt} \right|^2 dt = \int_0^1 g_{ij} \dot{x}_i \dot{x}_j dt.
$$

From the first variation of the functional $S$ we can derive that the extremals of the functional $S(c)$ are represented by geodesics $c(t) = \gamma(t)$ parametrized by $t$. Let us now consider the second variation $S_{\gamma}$ of the functional $S$ along the geodesic $\gamma$; it is referred to as the Hessian of $S$. For a given geodesic $\gamma = \gamma(t)$, $0 \leq t \leq 1$, a geodesic variation of $\gamma$ is a one–parameter family of geodesics $\gamma_s = \gamma_s(t)$ ($-\epsilon \leq s \leq \epsilon$) such that $\gamma_0 = \gamma$. For each fixed $s$, $\gamma_s(t)$ describes a geodesic as $t$ varies from 0 to 1. Each variation gives rise to an infinitesimal variation, which is a vector field defined along $\gamma$. The points $\gamma(0)$ and $\gamma(1)$ of $\gamma$ are said to be conjugate if there is a variation $\gamma_s$ inducing an infinitesimal variation vanishing at $t = 0$ and $t = 1$. We then denote by $\mu$ the index of the Hessian, i.e., the largest dimension of the subspace $T_\gamma \Omega$ on which $S_{\gamma}$ is negative definite. Then the following classical theorem due to Morse \cite{19} can be stated.

**Proposition 1.** (Morse Index Theorem \cite{19}) The index $\mu$ of the hessian $S_{\gamma}$ is equal to the number of points belonging to $\gamma(t)$ which are conjugate to the initial point $p = \gamma(0)$, counted according to their multiplicity.

In the theory of the orbiting bound states, the manifold $M^n$ under consideration is $M^2 = S^2$. The unit sphere can be described by the angular coordinates $\theta$ and $\varphi$; accordingly, the matrix elements $g_{ij}$ have the values: $g_{11} = 1$, $g_{22} = \sin^2 \theta$, $g_{12} = g_{21} = 0$. Now, choose a point $p_0 \in S^2$; all points of $S^2$, except for the antipodal one (say $q_0$), are connected to $p_0$ by only one geodesic of minimal length, whereas the antipodal point $q_0$ is connected to $p_0$ by a continuum of geodesics of minimal length, which can be obtained as the intersections of $S^2$ with the planes passing through the diameter of $S^2$ connecting $p_0$ to $q_0$. By rotating these planes, and keeping $p_0$ and $q_0$ fixed, we obtain a variation vector field which is a Jacobi field \cite{19} vanishing at $p_0$ and $q_0$. Thus, we can conclude that $p_0$ and $q_0$ are conjugate with multiplicity one because the possible rotations are along one direction only. Then, in view of the Morse Index Theorem, we can claim that the index $\mu$ of $S_{\gamma}$ jumps by one when the geodesic $\gamma(t)$, whose initial point is $\gamma(0) = p_0$, crosses $q_0$.

Now, we introduce the momenta associated with the coordinates $\theta$, $\varphi$ through the Legendre transformation,

$$
(2.4a) \quad p_{\theta} = \frac{\partial S}{\partial \dot{\theta}},
$$

$$
(2.4b) \quad p_{\varphi} = \frac{\partial S}{\partial \dot{\varphi}},
$$

whenever these equations yield a diffeomorphism of some sufficiently small neighborhoods $U_0$, $V_0$ of the points $(\theta^0, \varphi^0)$, $(p_{\theta}^0, p_{\varphi}^0)$, respectively. We are thus led to the phase space described by coordinates and momenta $(\theta, \varphi; p_{\theta}, p_{\varphi})$. In the phase space, one generates a family of trajectories, which forms a manifold $\Lambda$ smoothly embedded in the phase space. All the trajectories in this family have the same energy; this condition can be stated by setting the total Hamiltonian $q_{ij} p_i p_j = H = \text{Const.}$ (without loss of generality, the constant can be set equal to 1). Next, the first integrals $h$ of the Hamiltonian system described by $H$ can be determined by equating
the Poisson brackets to zero, i.e., \( \{ h, H \} = 0 \). We can thus obtain \([20]\)
\[
(p^2_\psi = c_1^2 = \text{Const.}, \tag{2.5a}
\]
\[
p_\theta^2 + \frac{c_1^2}{\sin^2 \theta} = 1, \tag{2.5b}
\]
Equation (2.5b) defines a smooth curve \( \gamma \) in the domain \( 0 < \theta < \pi, p_\theta \in \mathbb{R} \), which is diffeomorphic to the circle. Equations (2.5) determine a family of invariant Lagrangian manifold \( \Lambda \) diffeomorphic to the torus \( T \) and smoothly depending on \( c_1 \).

2.2. Oscillating integrals and eikonal approximation. We now look for a solution to (2.1) of the following form:
\[
\psi(x; k) = \int A(x; s) e^{ik\Phi(x; s)} \, ds, \tag{2.6}
\]
where \( \Phi(x; s) \) is the Hamilton characteristic function \([21]\), and \( s \) is a coordinate on the path connecting the source located at \( p_0 \) with the point of coordinate \( x \). The r.h.s. of (2.6) is an integral of oscillating type. The principal contribution to \( \psi(x, k) \), as \( k \to \infty \), corresponds to the stationary point of \( \Phi \), in the neighborhood of which the exponential ceases to oscillate rapidly. These stationary points can be obtained from the equation \( \frac{\partial \Phi}{\partial s} = 0 \) (provided that \( \frac{\partial^2 \Phi}{\partial s^2} \neq 0 \)): here for \( s \) we take the arc length coordinate of the paths. If condition \( \frac{\partial \Phi}{\partial s} = 0 \) is satisfied by a unique value \( s_0 \) of \( s \), which corresponds to a unique ray trajectory passing across the point of coordinate \( x \), we say that \( \Phi \) has a critical nondegenerate point at \( s = s_0 \). The surfaces \( \Phi = \text{Const.} \) represent the constant phase surfaces. Next, recalling the Morse Lemma, which refers to the representation of functions all of whose critical points are nondegenerate, we can obtain an asymptotic evaluation, for large \( k \), of integral (2.6) in the following form \([22]\):
\[
\psi(x; k) \simeq e^{ik\Phi(x; s_0)} \sum_{m=0}^{\infty} \frac{A_m(x)}{(ik)^m}. \tag{2.7}
\]
The leading term of expansion (2.7) reads
\[
\psi(x; k) \simeq A_0(x) e^{ik\Phi(x; s_0)}, \tag{2.8}
\]
where
\[
A_0(x) = A(x; s_0) \left( \left| \frac{\partial^2 \Phi}{\partial s^2} \right|_{s=s_0}^{-1/2} \right) \exp \left[ i \frac{\pi}{4} \text{sgn} \left( \frac{\partial^2 \Phi}{\partial s^2} \right)_{s=s_0} \right]. \tag{2.9}
\]
By substituting the leading term (which, for simplicity, will be written as \( A \exp(ik\Phi) \)) into equation (2.1), collecting the powers of \( (ik) \), and, finally, equating to zero their coefficients, two equations are obtained: the eikonal (or Hamilton–Jacobi) equation
\[
g^{ij} \frac{\partial \Phi}{\partial x_i} \frac{\partial \Phi}{\partial x_j} \equiv g^{ij} p_ip_j = 1, \tag{2.10}
\]
and the transport equation
\[
\frac{1}{\sqrt{g}} \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \left[ \sqrt{g} \left( A^2 \sum_{j=1}^{n} g^{ij} \frac{\partial \Phi}{\partial x_j} \right) \right] = 0, \tag{2.11}
\]
whose physical meaning is the conservation of the current density. Recalling that in the case of orbiting bound states the manifold \( M^n \) is the unit sphere \( S^2 \), and assuming that the phase \( \Phi \) and the amplitude \( A \) do not depend on the angle \( \varphi \), from (2.10) and (2.11) we obtain

\[
\left( \frac{d\Phi}{d\theta} \right)^2 = 1, \tag{2.12}
\]

\[
\frac{1}{|\sin\theta|} \left[ \frac{d}{d\theta} \left( |\sin\theta| A^2 \frac{d\Phi}{d\theta} \right) \right] = 0 \quad (\theta \neq m\pi, m \in \mathbb{Z}). \tag{2.13}
\]

It follows from (2.12) that \( \Phi = \pm \theta + \text{Const.} \), whereas (2.13) implies \( A(\theta) = \text{Const.} \cdot |\sin\theta|^{-1/2}, \theta \neq n\pi \ (n \in \mathbb{Z}) \). Therefore, the approximation (2.8) becomes

\[
\psi(\theta; k) = C \sqrt{|\sin\theta|} e^{\pm ik\theta} \quad (\theta \neq n\pi, n \in \mathbb{Z}, C = \text{constant}), \tag{2.14}
\]

where the terms \( \exp(\pm ik\theta) \) represent waves travelling in counterclockwise (\( \exp(ik\theta) \)) or clockwise (\( \exp(-ik\theta) \)) sense around the unit sphere. Since approximation (2.14) fails at \( \theta = n\pi \ (n \in \mathbb{Z}) \), we must consider the problem of patching these approximations when the surface rays cross the antipodal points \( \theta = 0, \pi \); these are conjugate points, and the Morse Index Theorem can be applied. Accordingly, the uniformization of approximation (2.14) consists precisely in finding the phase-shift associated with the crossing of rays through the antipodal conjugate points \( \theta = 0 \) and \( \theta = \pi \).

2.3. Uniformization of the eikonal approximation and geometric quantization. It follows from Maslov theory [20] that in any domain in which the configuration space representation of a Lagrangian manifold fails, one has the possibility of working out the problem in a momentum space representation. While the intensity of the ray tube, which is proportional to \( (\sin\theta)^{-1} \), is infinite in the neighborhood of the conjugate points, the intensity is instead finite in the \( p_\theta \)-representation [20]. Therefore, a semiclassical approximation to the wavefunction in almost any singular region can be obtained by means of a transformation to a suitably chosen momentum space, or mixed space representation. Once the local asymptotic solution in terms of the mixed \((p_\theta, \varphi)\) representation has been computed, it is possible to return to the configuration space \((\theta, \varphi)\) by transforming \( p_\theta \rightarrow \theta \) through the inverse Fourier transformation \( F_{k,p_\theta \rightarrow \theta}^{-1} \). In this way one determines the so-called Maslov indices, which allow us to obtain the uniformization of approximation (2.14) across the conjugate points.

Here we shall follow another approach based on the analytic continuation. With this in mind, we prove the following proposition.

**Proposition 2.** (i) The geometrical approximation (2.14) (eikonal approximation) can be extended to include the crossing of the conjugate points by adding a phase-shift \( (-\frac{\pi}{2}) \) \((\frac{\pi}{2}, \text{respectively})\) at each counterclockwise (clockwise) crossing of each antipodal conjugate point, i.e.,

(a) at each counterclockwise crossing, one has the shift

\[
e^{ik\theta} \rightarrow e^{i(k\theta - \pi/2)}; \tag{2.15}\]

(b) at each clockwise crossing, one has the shift

\[
e^{-ik\theta} \rightarrow e^{-i(k\theta - \pi/2)}. \tag{2.16}\]
(ii) The orbital angular momentum $L$ can assume only half-integer values according to the rule

$$L = \ell + \frac{1}{2} \quad (\ell = 0, 1, 2, \ldots; \hbar = 1).$$

(iii) The asymptotic representation of the angular orbiting bound state wavefunction $\psi_\ell(\theta, k)$ where $\ell = 0, 1, 2, \ldots$, is given by

$$\psi_\ell(\theta, k) \simeq \frac{C}{\sqrt{\sin \theta}} \sin \left( \left( \ell + \frac{1}{2} \right) \theta + \frac{\pi}{4} \right) \quad (\theta \neq n\pi, n \in \mathbb{Z}).$$

**Proof:** (i) Let us consider the function $(\sin \theta)^{-1/2}$, i.e., the amplitude of the eikonal approximation (2.14) up to a constant. This function presents branch singularities at $\theta = n\pi$ ($n \in \mathbb{Z}$). The continuation can be simply realized by overpassing these singularities by semicircular arcs, which are oriented counterclockwise for $\theta \in [0, +\infty)$, and oriented clockwise for $\theta \in (0, -\infty)$. Now, rewrite approximation (2.14) in the following form: $\psi(\theta, k) = C \exp(\log A \pm i k \theta)$ ($A = (\sin \theta)^{-1/2}$, $C = \text{Const.}$). When the wavefunction $\psi$ is varied across a branch point in the counterclockwise direction, the term $\log A$ acquires a factor $-i\pi$; analogously, when $\psi$ is varied across a branch point moving in clockwise direction, the term $\log A$ acquires a factor $i\pi$. Thus, the uniformization of the wavefunction approximation (2.14) can be achieved by patching the rays travelling along the circle $S^1$ as follows: add a phase-shift of $-\frac{\pi}{2}$ to the phase of the wave travelling in counterclockwise direction as the ray passes through each antipodal conjugate point whose relative distance on the unit sphere is $\pi$. Thus, the rule (2.15) is obtained. Analogously, add a phase-shift of $\frac{\pi}{2}$ to the phase of the wave travelling in clockwise direction as the ray passes through each antipodal conjugate point, thus obtaining the rule (2.16).

(ii) We now evaluate the variation of the phase of the wavefunction $\psi(\theta, k)$ associated with a circular orbit $\gamma^{(+)}$ $(0 \leq \theta \leq 2\pi)$ oriented counterclockwise. In order to guarantee the single-value-ness of the wavefunction $\psi$, we impose the following condition (see also (2.23)):

$$\Delta_{\gamma^{(+)}(0,2\pi)}(\log A) + i \Delta_{\gamma^{(+)}(0,2\pi)}(k \theta) = i2\pi\ell \quad (\ell = 0, 1, 2, \ldots).$$

Since $\Delta_{\gamma^{(+)}(0,2\pi)}(\log A) = -i\pi$, and $\theta = 2\pi$ when the circular orbit $\gamma^{(+)}$ is completed, it follows from formula (2.19) that

$$- \frac{1}{2} + \Delta_{\gamma^{(+)}(0,2\pi)}(k) = \ell \quad (\ell = 0, 1, 2, \ldots).$$

Recalling that we are considering, for simplicity, the orbiting around a unit sphere, it follows, from formula (2.20) that the values of the angular momentum compatible with the single-value-ness of the wavefunction $\psi$ are given by: $L = \ell + \frac{1}{2} \quad (\ell = 0, 1, 2, \ldots; \hbar = 1)$, i.e., by formula (2.17).

**Remark:** Let us note that the universal covering $p(t) : \mathbb{R}^1 \rightarrow S^1$, $p(t) = e^{2\pi i t}$, is generated by a properly discontinuous transformation group by the translations $t \rightarrow t + n \quad (n \in \mathbb{Z})$ of the axis $\mathbb{R}^3$, namely, the exponential map wraps the line $\mathbb{R}^1$ around the unit circle in $\mathbb{R}^2$. We can thus relate the semiclassical quantization of the orbital angular momentum $L$ (formula (2.17)) to the topological properties of the fundamental group $\pi_1(S^1) \simeq \mathbb{Z}$. 
(iii) Let $\psi^{(+)}_\ell$ and $\psi^{(-)}_\ell$ denote the contribution to the angular wavefunction $\psi_\ell$ given by the counterclockwise and clockwise travelling waves, respectively. The total wavefunction $\psi_\ell$ is the sum $\psi^{(+)}_\ell + \psi^{(-)}_\ell$. Taking the statements (i) and (ii) into account, at a chosen $\ell$, we have (see formula (2.17)):

$$
\psi_\ell(\theta, k) = \psi^{(+)}_\ell(\theta, k) + \psi^{(-)}_\ell(\theta, k) = C(k) A(\theta) \left[ e^{ik\theta} + i e^{ik(2\pi - \theta)} \right]
$$

$$
= 2C(k) A(\theta) e^{ik\pi} e^{i\pi/4} \left[ \frac{e^{i[k(\theta - \pi) - \pi/4]} + e^{-i[k(\theta - \pi) - \pi/4]}}{2} \right]
$$

(2.21)

$$
= 2 (-1)^\ell e^{i3\pi/4} C(k) A(\theta) \cos \left[ k(\theta - \pi) - \pi/4 \right].
$$

Since $k = \ell + \frac{1}{2}$, we obtain

$$
\psi_\ell(\theta, k) = \psi^{(+)}_\ell(\theta, k) + \psi^{(-)}_\ell(\theta, k)
$$

(2.22)

$$
= \frac{C_4(k)}{\sqrt{|\sin(\theta - \pi)|}} \cos \left[ \left( \ell + \frac{1}{2} \right) (\theta - \pi) - \frac{\pi}{4} \right] \quad (\theta \neq n\pi, n \in \mathbb{Z}),
$$

which is proportional to the well–known asymptotic behavior of the Legendre polynomials for large values of $\ell$. $\square$

Typical examples of phenomena which can be theoretically described in terms of semiclassical orbiting are the rotational resonances present in molecular scattering. These quasi–bound states have been observed with particularly clear evidence in the H–Kr collision. In [9], a phase–shift analysis of these experimental scattering data is presented. The energy values corresponding to the upward crossing through $\frac{\pi}{2}$ of these phase–shifts give the energy locations of the resonance peaks. In [10], these values of the center of mass energy are reported in correspondence with the integer values of $\ell$ ($\ell = 4, 5, 6$). Then, these points are interpolated with the line $\ell(\ell + 1)$ as a function of the center of mass energy $E$. The good agreement between the energy locations ($E > 0$) of the resonance peaks and the line $\ell(\ell + 1)$ strongly supports the correctness of the linear parametrization

$$
\ell(\ell + 1) = 2IE + c_0,
$$

(2.23)

where $I = \mu R^2$ is the moment of inertia of the two–particle system, $\mu$ is the reduced mass, $R$ is the interparticle distance, $E$ is the center of mass energy, and $c_0$ is a constant. Formula (2.23) proves that these resonances are generated by the rotational dynamics. Since the intercept $c_0$ turns out to be larger than zero (see Fig. 2 of [10]), the straight trajectory interpolating the resonances for $E > 0$ can be extrapolated to $E < 0$, and then the energy values of the bound states corresponding to $\ell = 0, 1, 2, 3$ can be determined (see once again Fig. 2 of [10]). Formula (2.17) gives the semiclassical approximation of the quantum–mechanical angular momentum $\sqrt{\ell(\ell + 1)}$ ($h = 1$). Let us finally note that the theoretical results obtained in this section refer strictly to the bound states phenomena ($E < 0$). The resonances ($E > 0$) will be reconsidered in Subsection 3.2 taking into account, in particular, the lifetime of these states, which is closely related to the tunnelling across the centrifugal barrier.

3. RIEMANNIAN OBSTACLE PROBLEM AND THE LUDWIG SYSTEM

3.1. EXISTENCE OF DIFRACTED RAYS AND NONUNIQUENESS OF THE CAUCHY PROBLEM FOR A RIEMANNIAN MANIFOLD WITH BOUNDARY. Let us now consider the so–called Riemannian obstacle problem [24]. A boundary component is viewed as
an obstacle around which a geodesic can bend, or at which a geodesic can end. Let \( K \) denote a convex obstacle which is embedded in a complete \( n \)-dimensional manifold \( M^n \) \((n \geq 3)\) equipped with a Riemannian metric, where \( g_{ij} \) stands for the metric tensor. Let us introduce the space \( M^n \setminus \overline{K} \equiv M^n_0 \), where the obstacle \( K \) is an open connected subset of \( M^n \), with regular boundary \( \partial K \) and compact closure \( \overline{K} = K \cup \partial K \). In the following, we shall denote the space \( M^n_0 \) simply by \( M \). We are thus led to consider the space \( M^* = M \cup \partial K \), which has the structure of a manifold with boundary. In order to remedy the lack of geodesic completeness, i.e., the possibility of extending every geodesic infinitely and in a unique way, one can introduce the notion of geodesic terminal \[[25]\] to represent a point where a geodesic stops. Indeed, following Plaut \[25\], it can be proved that \( M^* \) is the completion of \( M \) by observing that the set \( J \) of the geodesic terminals is nowhere dense, and \( \partial M^* = \partial K = J \).

It is convenient to model the manifold with boundary on the half-space \( \mathbb{R}^n_+ = \{(x_1, \ldots, x_n) \in \mathbb{R}^n | x_n \geq 0\} \subset \mathbb{R}^n \), where \( \mathbb{R}^{n-1}_+ \) stands for the boundary \( x_n = 0 \) of \( \mathbb{R}^n_+ \). Thus, for a manifold with boundary, there exists an atlas \( \{U^a\} \), with local coordinates \( (x_1^a, \ldots, x_n^a) \), such that, in any chart, we have the strict inequality \( x_n^a > 0 \) at the interior points, and \( x_n^a = 0 \) at the boundary points \[26\]. The set \( \partial M^* \) of the boundary points is a smooth manifold of dimension \((n-1)\). In particular, it is convenient to introduce suitable coordinates \( x_i^b \) \((i = 1, \ldots, n)\) adapted to the boundary, the so-called geodesic boundary coordinates \[23\], with \( x_i^b \) defined as the distance from the boundary \( \partial M^* \); note that \( x_i^b \) satisfies necessarily a positivity condition, i.e., \( x_i^b \geq 0 \). Then, starting with arbitrary coordinates \( x_i^b \), \( i < n \) on \( \partial M^* \), one extends them to be constant on ordinary geodesics normal to \( \partial M^* \). These coordinates have been used indeed by Alexander, Berg and Bishop (ABB) in order to write the equation of a geodesic \( \gamma \) of \( M^* \)[24]. Let us in fact note that the geodesics in a Riemannian manifold without boundary are the solutions of a system of differential equations with suitable Cauchy conditions, and the main result is the theorem which guarantees existence, uniqueness and smoothness of the solution of the Cauchy problem of this system. Conversely, the case of a Riemannian manifold with boundary is different from the classical one concerning uniqueness and smoothness of the solution. In [16], the following proposition, which is essentially due to (ABB), has been proved.

Proposition 3. (i) In a Riemannian manifold with boundary (the normal curvature of the boundary being different from zero) the determination of the geodesics by their initial tangents (Cauchy problem) is not unique.

(ii) In any point of the boundary \( \partial K \) (\( \partial K \) convex) we have

(a) a geodesics of class \( C^\infty \) bending around the boundary;

(b) a geodesics which leaves tangentially the boundary and which is of class \( C^1 \) at the point of contact with the boundary.

The diffracted rays are precisely the geodesics of \( M^* \) obtained by gluing together a geodesic segment belonging to the boundary (whose normal curvature is supposed to be different from zero) with a geodesic segment belonging to the interior of \( M^* \). They are of class \( C^1 \) at the transition point. If we assume that the space \( M^n_0 \) in which the obstacle is embedded is \( \mathbb{R}^3 \) (equipped with an Euclidean metric) then, before and beyond the obstacle, the diffracted rays consist of straight lines tangent to the obstacle. Therefore, as a consequence of the nonuniqueness of the Cauchy
problem at the boundary of the manifold, we can conclude by stating that at each point of the boundary we have a bifurcation; the ray splits in two parts, where one part continues as an ordinary straight line ray (diffracted ray of class $C^1$ at the splitting point) and the other part travels along the surface as a geodesic of the boundary.

3.2. Morse Index Theorem for Riemannian manifolds with boundary and homotopic classes of diffracted rays. From now on, as a typical example of obstacle, we regard the spherical ball of unit radius embedded in $\mathbb{R}^3$: $\partial K = S^2$, equipped with the standard metric. However, in view of the homotopic invariance, the results which we derive hold for any convex and compact obstacle represented by Besse–type manifolds (all of whose geodesics are closed) having a symmetry axis. Let us denote by $A$ the extended–axis of symmetry of the obstacle, passing through the point $p_0 \in M^*$, at which the source of light is located. Let $A_-$ denote the portion of this axis lying in the illuminated region (i.e., the same side of the light source), and $A_+$ the portion of the axis lying in the shadow. The axis $A$ equals $A_- \cup D \cup A_+$, where $D$ is the diameter of the sphere. Let us note that all the points of $M^*$ that do not belong to $A_+ \cup A_-$ are connected to $p_0$ by only one geodesic of minimal length, whereas the points $q \in A_+$ are connected to $p_0$ by a continuum of geodesics of minimal length that can be obtained as the intersections of $M^*$ with planes passing through the axis $A$. By rotating these planes, and keeping $p_0$ and $q$ fixed, we obtain a variation vector field which is a Jacobi field vanishing at $p_0$ and $q$. Thus, we can conclude that $p_0$ and $q$ are conjugate with multiplicity one, because the possible rotations are along one direction only. We are then led to pose the question whether the Morse Index Theorem can be extended to include Riemannian manifolds with boundary. To this end, we introduce the so–called regular geodesics in the sense of Alexander [27]. Following [27], a geodesic $\gamma$ is regular if

(a) all boundary contact intervals of $\gamma(t)$ have positive measure;
(b) the points of arrival of $\gamma(t)$ at $\partial M^*$ are not conjugate to the initial point $\gamma(0)$.

It is easy to show that the diffracted rays are regular geodesics. It is then possible to define a Hessian form which is simply given by the sum of the classical formulae for $\partial M^*$ on contact intervals and of the formulae for the interior of $M^*$ (i.e., $M^*$) on interior intervals. We can thus formulate the extended Morse Index Theorem as follows.

**Proposition 4.** (Morse Index Theorem for Riemannian Manifolds with Boundary [27]) Let $\gamma$ be a regular geodesic; then the index $\mu$ of $S_{\gamma(t)}$ is finite and equal to the number of points in $\gamma(t)$ conjugate to the initial point $\gamma(0)$ ($0 \leq t \leq 1$) and counted according to their multiplicities.

Next we focus on the points $q \in M^* \setminus (A_+ \cup A_-)$ (i.e., the points belonging to the interior of $M^*$ that do not lie on the axis of the obstacle). Consider the space $X_{p_0q} = (E^2_q) \cap M^*$, where $(E^2_q)$ is the Euclidean plane uniquely determined by the axis of the obstacle through $p_0$ and the point $q$. The space $X_{p_0q}$ (which will be denoted hereafter simply by $X$) is arcwise connected, and its boundary in $(E^2_q)$ is a circle $S^1$, which is a deformation retract of $X$. In view of these facts, the fundamental group $\pi_1(X; p_0)$ does not depend on the base point $p_0$ and is isomorphic to $\pi_1(S^1; 1)$, where 1, which is described in a convenient system by
the coordinates (0, 1) (see Fig. 1), represents the contact point of $A_+$ with $S^2$, $\pi_1(X; p_0) \sim \pi_1(S^1; 1) \simeq \mathbb{Z}$. Let us consider, within the fundamental grupoid $\Pi_1(X)$ of $X$, the set $\Pi_1(X; p_0, q)$ of the paths in $X$ connecting $p_0$ with $q$, modulo homotopy with fixed endpoints. Let us clarify our choices.

(i) We introduce in $(E^2_q)$ (q fixed in $X \setminus (A_+ \cup A_-)$) an orthogonal reference system, whose origin coincides with the centre of the spherical ball representing the obstacle, and the extended axis of symmetry $A$ coincides with the horizontal axis. Recall that the source is located in the point $p_0 \in A_-$, while the point q, exterior to $A$, lies in the upper half–plane of this reference system, i.e., in the first or in the second quadrant;

(ii) $\gamma_0$ is the geodesic from $p_0$ to $q$ of minimal length;

(iii) $\alpha_0$ is a loop in $X$ at $p_0$ such that:

- $[\alpha_0]$ is a generator of $\pi_1(X; p_0)$ (establishing an isomorphism $\pi_1(X; p_0) \simeq \mathbb{Z}$);
- $\alpha_0$ turns in counterclockwise sense around the obstacle (see Fig. 1).

We can now state the following proposition.

**Proposition 5.** (i) Each element of $\pi_1(X; p_0)$ is a homotopy class $[\alpha]$, with fixed endpoints, of a certain loop $\alpha$ in the space $X$, starting and ending at the point $p_0$.

(ii) Each path $c_0$ from $p_0$ to $q \in M^*(A_+ \cup A_-)$ determines a one–to–one correspondence $W$ between $\pi_1(X; p_0)$ and the set $\Pi_1(X; p_0, q)$. Such a correspondence can be constructed as: $\forall [c] \in \Pi_1(X; p_0, q) : [c \ast c_0^{-1}] \in \pi_1(X; p_0)$, where the symbol ‘$\ast$’ denotes the concatenation of paths, and $c_0^{-1}$ denotes the reverse path of $c_0$.

(iii) In each homotopy class of $\pi_1(X; p_0)$, there is precisely one element of minimal
length. In each homotopy class of $\Pi_1(X; p_0, q)$ ($q \in \mathbb{M}^* \setminus (A_+ \cup A_-)$) there is precisely one geodesic $\gamma$.

(iv) The correspondence $W$ assigns to each geodesics $\gamma$ the number $w(\gamma)$ defined by $[\gamma * \gamma_0^{-1}] = w(\gamma)[\alpha_0]$; $w(\gamma)$ is the winding number of the loop $[\gamma * \gamma_0^{-1}]$ determined by $\gamma$ (with respect to the chosen generator $[\alpha_0]$).

(v) A bijective correspondence can be established between the winding number $w(\gamma)$ of the loop $[\gamma * \gamma_0^{-1}]$ ($\gamma_0$ being the geodesics of minimal length connecting $p_0$ and $q$), and the crossing number $n(\gamma)$ which counts the intersections of the geodesics $\gamma$ with the horizontal axis (i.e., the extended symmetry axis). The winding number determines the crossing number through the following bijective correspondence:

$$
\begin{align*}
Z & \rightarrow \mathbb{N} \\
n & \rightarrow (2n + 1) \text{ if } n \geq 0, \\
n & \rightarrow -2n \text{ if } n < 0.
\end{align*}
$$

It follows from this proposition that the subset $A_+ \cup A_-$ of the extended symmetry axis of the obstacle $K$ (including the antipodal points of the spherical ball belonging respectively to $A_-$ and $A_+$) forms the set of conjugate points, which we can properly refer to as the axial caustic. Accordingly, in view of the extended Morse Index Theorem, the index $\mu$ of the Hessian jumps by one when the geodesic (i.e., the ray trajectory) crosses the caustic.

3.3. Geometric structure of the caustics. We can prove the following proposition.

**Proposition 6.** If the obstacle is a spherical ball of radius $R$ and the extended symmetry axis of the ball is given by $A = A_- \cup D \cup A_+$, then the caustics are as follows:

(a) the surface of the spherical ball, which is the envelope of the diffracted rays;
(b) the semiaxes $A_+$ and $A_-$, which form the axial caustic.

**Proof:** Let us introduce an orthogonal system of axes $(X, Y, Z)$ in $\mathbb{R}^3$ whose origin coincides with the center of the obstacle and such that the $Z$-axis (whose corresponding coordinate is denoted by $z$), chosen parallel to the incoming beam of rays, is positively oriented in the direction of the outgoing rays (see Fig. 2). Indeed, we assume that the point $p_0$, where the source is located, is pushed to $-\infty$. Then we introduce, in addition, the following coordinates on the sphere: $r_0$ is the radial vector, $\varphi_0$ is the azimuthal angle, $\theta_0$ is the angle measured along the meridian circle from the point of incidence of the ray trajectory on the sphere. We start by considering the rays that leave the surface of the sphere after diffraction. Let us recall that the interior of the space $M^*$ (i.e., $\mathbb{M}^*$), exterior to the obstacle, can be regarded as an Euclidean space without boundary. Next, we switch from the wave to the ray description, writing the eikonal equation

$$g^{ij} \frac{\partial \Phi}{\partial x_i} \frac{\partial \Phi}{\partial x_j} = 1$$

in Hamiltonian form, where $\Phi$ stands for the phase function, $x_i$ (for $i = 1, 2, 3$) are the Cartesian coordinates which refer to the axes $(X, Y, Z)$: $x_1 = x$, $x_2 = y$, $x_3 = z$. We then set $p_i = \frac{\partial \Phi}{\partial x_i}$ and introduce the function $F = \frac{1}{2} (g^{ij} p_i p_j - 1)$. The Hamilton characteristic system reads:

$$\begin{align*}
\frac{dx_i}{d\tau} &= g^{ij} p_j, \\
\frac{dp_i}{d\tau} &= -\frac{\partial F}{\partial x_i} = -\frac{1}{2} p_i p_j \frac{\partial g^{ij}}{\partial x_i},
\end{align*}$$

where $\tau$ is a running parameter along the ray emerging from the surface $\Phi = \text{Const}$. By (3.1a), we have

$$d\Phi = \sum_{i=1}^{3} \frac{\partial \Phi}{\partial x_i} dx_i = \sum_{i=1}^{3} p_i dx_i = g^{ij} p_i p_j d\tau = d\tau,$$

where the last equality follows from $g^{ij} p_i p_j = 1$. By Eqs. (3.1) and recalling that $\mathbb{M}^*$ is Euclidean, we obtain

$$\begin{align*}
\frac{dr}{d\tau} &= \mathbf{p}, \\
\frac{d\Phi}{d\tau} &= 0,
\end{align*}$$

where $\mathbf{r} = (x_1, x_2, x_3)$, and $\mathbf{p} = \nabla \Phi$. Then it follows from (3.3) that

$$\mathbf{r}(\theta_0, \varphi_0, \tau) = \mathbf{r}_0(\theta_0, \varphi_0) + \tau \mathbf{p}_0(\theta_0, \varphi_0),$$

where $\mathbf{p}_0$ is the unit vector tangent to the obstacle where the ray leaves the sphere.

Consider now the ray hitting the sphere at the point of coordinates $(-R, 0, 0)$ and then travelling in the counterclockwise direction. The components of the vectors $\mathbf{r}_0$ and $\mathbf{p}_0$ are (see Fig. 2):

$$\mathbf{r}_0 = (-R \cos \theta_0 \cos \varphi_0, R \cos \theta_0 \sin \varphi_0, R \sin \theta_0),$$

and

$$\mathbf{p}_0 = (\sin \theta_0 \cos \varphi_0, -\sin \theta_0 \sin \varphi_0, \cos \theta_0).$$
Substituting these expressions in (3.4) gives
\[ r(\theta_0, \varphi_0, \tau) = (-R \cos \theta_0 \cos \varphi_0 + \tau \sin \theta_0 \cos \varphi_0, R \cos \theta_0 \sin \varphi_0 - \tau \sin \theta_0 \sin \varphi_0, R \sin \theta_0 + \tau \cos \theta_0). \] (3.7)

Then the Jacobian determinant \( \left| \frac{\partial(x,y,z)}{\partial(\theta_0, \varphi_0, \tau)} \right| \) of the transformation \( (x,y,z) \leftrightarrow (\theta_0, \varphi_0, \tau) \) is
\[ |J| = \tau(R \cos \theta_0 - \tau \sin \theta_0). \]
It vanishes for \( \tau = 0 \) and for \( \tau = \tau \equiv R \cot \theta_0 \). Analogous calculations can be performed for the rays oriented clockwise. Finally, in order to distinguish the two orientations of the rays, we add the superscript (+) to everything referring to the counterclockwise oriented rays, and the superscript (−) when referring to the clockwise oriented rays. In conclusion, we see that the domain on which the Jacobian determinant vanishes is formed by

(i) the surface of the spherical ball corresponding to \( \tau^\pm = 0 \);
(ii) the semiaxes represented by
\[ \tau^\pm = \tau^\pm \equiv R \cot \theta^\pm_0 : \left\{ \begin{array}{ll}
\text{the semiaxis } A_+ & \text{if } 0 \leq \theta^+_0 \leq \pi, \\
\text{the semiaxis } A_- & \text{if } \pi \leq \theta^-_0 \leq 2\pi.
\end{array} \right. \] (3.9)

3.4. Chester, Friedmann and Ursell approximation and the Ludwig system. Let us now consider the caustic generated by the boundary. As we have seen in Proposition 3, at any point of the boundary, the ray splits into two parts: one part leaves the boundary along the tangent; the other one travels along the surface and bends around the obstacle. Therefore, in the domain at the exterior of the boundary but close to it, the Lagrangian manifold is composed of all the trajectories tangent to the boundary \( \partial K \) that have \( \partial K \) as an envelope. Each point \( P \) in this domain lies in the intersection of two diffracted rays which are tangent to the border of the diffracting body and cross two surfaces of constant phase orthogonally. When the point \( P \) is pushed on the boundary, the curves of constant phase meet, forming a cusp and the locus of such cusps is the caustic. In such a situation, the standard stationary phase method fails, and one must choose an appropriate phase function \( \Phi \) that parametrizes the Lagrangian manifold locally.

Now, let us return to the reference frame \( O(X,Y,Z) \) introduced above in connection with the proof of Proposition 3 and introduce ordinary spherical coordinates \( (r, \theta, \varphi) \). Moreover, we introduce geodesic boundary coordinates as well (defined in a general setting in Subsection 3.1), and now referred to the border of the obstacle. With this in mind, we fix a point \( b \) belonging to the boundary \( B \) and denote by \( v(r, \theta) \) the distance from the boundary along the normal to the boundary at \( b \) lying in the plane \( XZ \). Recall that the normal coordinate must satisfy a positivity condition and vanishes on the border. The border of the obstacle is represented by \( u(r, \theta) = 0 \). Beside these geodesic boundary coordinates, we also introduce an axis perpendicular to the normal at \( b \) (i.e., tangent to the border at \( b \)) and lying in the plane \( XZ \) and denote by \( \xi \) the corresponding coordinate. The mapping of the Lagrangian manifold composed by the ray trajectories generated by the border of the obstacle in the neighborhood of the point \( b \), is of the following form: \( \Lambda(\xi, \cdot) \rightarrow M^* (\xi^2, \cdot) \). In fact, expressing \( v \) as a smooth function of \( \xi \) and taking the
positivity of $v$ into account, we are led locally to the equality $v = \xi^2$; moreover, the convexity of the obstacle (e.g., of a spherical ball) imposes that $u$ depends on $\xi^2$ in a neighborhood of $b$. The following question arises: Is it possible to determine regular functions $u$ and $v$ depending on $\xi^2$ only and a phase function $\Phi(u, v; \xi)$ which realizes the mapping $\Lambda(\xi, \cdot) \to M^*(\xi^2, \cdot)$? We answer the previous question with the following proposition.

**Proposition 7.** The following phase function

\[
\Phi(u, v; \xi) = u(r, \theta) + v(r, \theta)\xi - \frac{1}{3}\xi^3
\]

gives a local map $\Lambda(\xi, \cdot) \to M^*(\xi^2, \cdot)$ of the Lagrangian manifold composed by the ray trajectories generated by the border of the obstacle in a neighborhood of the point $b$.

**Proof:** For $\Phi$ of the form (3.10), the critical set $C$, where $\partial \Phi / \partial \xi = 0$, is given by $v - \xi^2 = 0$; the positivity condition of the normal geodesic boundary coordinate is thus satisfied, i.e., $v = \xi^2$. The equality $\xi = \pm \sqrt{v}$ leads us to separate the two domains: $C^+$ corresponding to $\xi > 0$ and $C^-$ corresponding to $\xi < 0$. We have

\[
\Phi^+ \equiv \Phi(\xi \in C^+) = u + \frac{2}{3}v^{3/2},
\]
\[
\Phi^- \equiv \Phi(\xi \in C^-) = u - \frac{2}{3}v^{3/2}.
\]

These equalities imply

\[
(3.12a) \quad u = (\Phi^+ + \Phi^-),
\]
\[
(3.12b) \quad v^3 = \frac{9}{16}(\Phi^+ - \Phi^-)^2.
\]

Let us note that both $(\Phi^+ + \Phi^-)$ and $(\Phi^+ - \Phi^-)^2$ are even functions of the variable $\xi$. Then we make use of the following auxiliary Lemma due to Whitney.

**Lemma 8.** (Whitney [28]) Let $f$ be a smooth even function on the real line. Then there exists a smooth function $g$ on the real line such that $f(x) = g(x^2)$. If $f$ depends smoothly on a set of parameters, then $g$ can be chosen in such a way that it depends smoothly on the same parameter\(^1\).

It follows from this auxiliary lemma, since the functions $(\Phi^+ + \Phi^-)$ and $(\Phi^+ - \Phi^-)^2$ are even, that $u$ and $v^3$ exist as smooth functions of $\xi$\(^3\). Further we note that, since $(\partial \Phi / \partial \xi)_{(\xi=0)} = (\partial^2 \Phi / \partial \xi^2)_{(\xi=0)} = 0$, while $(\partial^3 \Phi / \partial \xi^3)_{(\xi=0)} \neq 0$, the Taylor series for $(\Phi^+ - \Phi^-)^2$ begins with a nonzero term of order 6. Thus, $v$ exists, and it is of order 2 with respect to $\xi$\(^2\), in agreement with the positivity condition of the normal geodesic boundary coordinate.

\[\square\]

The extension of the stationary phase method suggested by Proposition\(^7\) makes us to look for a solution of the wave equation of the following form:

\[
(3.13) \quad \psi(u, v; k) = \int A(u, v; \xi) e^{ik(u+v\xi - \frac{1}{3}\xi^3)} \, d\xi.
\]

\(^{1}\)Editors’ note: Certainly, the function $x \to |x|^p, p > 1, x \in \mathbb{R}$, cannot be represented as a smooth function of $x^2$ for $p < 2$. Therefore, the function $g$ can be nonsmooth at the origin.

\(^{2}\)Editors’ note: In the above sense.
By the Weierstrass–Malgrange preparation theorem \cite{[29]}, we can find functions $a_0(u, v), a_1(u, v), h(u, v; \xi)$ such that:

\begin{equation}
A(u, v; \xi) = a_0(u, v) + a_1(u, v)\xi + h(u, v; \xi)(v - \xi^2),
\end{equation}

where $v - \xi^2 = \partial \Phi / \partial \xi$. Thus integral \eqref{3.13} can be written in the following way:

\begin{equation}
a_0(u, v) \int e^{i\Phi(u,v;\xi)} d\xi + a_1(u, v) \int e^{i\Phi(u,v;\xi)} \partial \Phi / \partial \xi e^{i\Phi(u,v;\xi)} d\xi.
\end{equation}

The last term in \eqref{3.13} is $h(u, v; \xi) \frac{1}{i k} \frac{\partial}{\partial \xi} e^{i\Phi(u,v;\xi)} d\xi$, which is of the order of $1/k$.

One can then prove that there exist a formal asymptotic series in $k$, whose first terms are respectively denoted by $A_0$ and $A_1$, such that

\begin{equation}
\psi(u, v; k) \simeq e^{iku} \left[ \frac{A_0}{k^{1/3}} \int \xi e^{i(k^2/3v + 1/3\xi^2)} d\xi + \frac{A_1}{ik^{2/3}} \int \xi e^{i(k^2/3v + 1/3\xi^2)} d\xi \right],
\end{equation}

as $k \to \infty$. Next, recalling the integral representations of the Airy function and of its derivative, i.e.,

\begin{equation}
\text{Ai}(t) = \int e^{i(t + \xi^2/3)} d\xi,
\end{equation}

\begin{equation}
\text{Ai}'(t) = \int \xi e^{i(t + \xi^2/3)} d\xi,
\end{equation}

one can finally prove the following proposition (see \cite{[4]}).

**Proposition 9.** (i) In a neighborhood of a fold point of the Lagrangian manifold $\Lambda$ generated at the boundary $\partial K$ of a convex obstacle $K$, the wavefunction $\psi(u, v; k)$ can be represented for high values of the wavenumber $k$ ($k \to +\infty$) as follows:

\begin{equation}
\psi(u, v; k) \simeq e^{iku} \left[ \frac{A_0}{k^{1/3}} \text{Ai}(-k^{2/3}v) + \frac{A_1}{ik^{2/3}} \text{Ai}'(-k^{2/3}v) \right],
\end{equation}

where $A_0$ and $A_1$ are the first terms of the formal series asymptotic in $k$.

(ii) The functions $u$ and $v$ satisfy the following system (Ludwig system) \cite{[4]}:

\begin{equation}
|\nabla u|^2 + v|\nabla v|^2 = 1,
\end{equation}

\begin{equation}
\nabla u \cdot \nabla v = 0.
\end{equation}

**Proof:** (i) The asymptotic representation of $\psi(u, v; k)$ given by formula \eqref{3.18} follows from formulae \eqref{3.13} – \eqref{3.17}.

(ii) The Ludwig system \eqref{3.19} is obtained by inserting the r.h.s. of formula \eqref{3.18} into the Helmholtz equation \eqref{2.1}, and collecting the coefficients suitably. \hfill $\square$

So far we have treated only those physical problems characterized by the condition $v(r, \theta) = \xi^2 \geq 0$. However, there is some interest in studying phenomena which present the penetration of light beyond the caustic, i.e., the shadow of the caustic. This physical situation can be characterized mathematically by setting $v = (iv)^2 = -\eta^2$ (i.e., $\xi = i\eta$, $\eta \in \mathbb{R}$) in the Ludwig system. Then the mixed hyperbolic–elliptic character of the Ludwig system emerges. We study this peculiar feature using polar coordinates $(r, \theta)$. We prove the following proposition (see also \cite{[30]}).
Proposition 10. (i) The equation of the characteristics for the Ludwig system \((3.19)\) reads

\[
\frac{1}{r^2} \left( u_0^2 - vv_0^2 \right) \left( \frac{dr}{d\theta} \right)^2 - 2 \left( u_r v_0 - vv_r v_0 \right) \left( \frac{dr}{d\theta} \right) + r^2 \left( u_r^2 - vv_r^2 \right) = 0.
\]

The discriminant \(\Delta\) of \((3.20)\) is

\[
\Delta = v \left( u_r v_0 - u_0 v_r \right)^2 = v |J|^2,
\]

where \(J\) is the Jacobian determinant \(\left| \frac{\partial (u,v)}{\partial (r,\theta)} \right|\).

(ii) The characteristic curves are given by

\[
\left( \frac{dr}{r d\theta} \right) = \frac{u_r \pm \sqrt{v v_r}}{\frac{1}{r} u_\theta \pm \sqrt{v v_\theta}} = \frac{(\nabla \Phi^\pm)_r}{(\nabla \Phi^\pm)_\theta},
\]

where \(\nabla \Phi = (u_r, \sqrt{v v_r}, \frac{1}{r} u_\theta, \sqrt{v v_\theta})\). Then

\[
\Phi^\pm = u \pm \frac{2}{3} v^{3/2},
\]

\[
|\nabla \Phi^\pm|^2 = 1.
\]

(iii) According to the sign of \(\Delta\) (see \((3.21)\)), provided that \(|J| \neq 0\), we can distinguish among the following cases:

(a) For \(v > 0\), \(\Delta > 0\), we are in the hyperbolic case (the characteristics are real and distinct);

(b) For \(v = 0\), \(\Delta = 0\), we are in the parabolic case (the characteristics are real and coincident);

(c) For \(v < 0\), \(\Delta < 0\), we are in the elliptic case.

Proof: (i) We rewrite system \((3.19)\) in terms of the coordinates \((r,\theta)\), and obtain

\[
\begin{align*}
&u_r^2 + \frac{1}{r^2} u_\theta^2 + v \left( v_r^2 + \frac{1}{r^2} v_\theta^2 \right) = 1, \\
&u_r v_r + \frac{1}{r^2} u_\theta v_\theta = 0.
\end{align*}
\]

The characteristic determinant associated with system \((3.22)\) reads as follows

\[
\begin{vmatrix}
2u_r & \frac{2}{r} u_\theta & 2 v v_r & \frac{2}{r} v v_\theta \\
\frac{2}{r} u_r & 1 & 0 & 0 \\
\frac{1}{r} v_r & \frac{1}{r} u_\theta & u_r & \frac{1}{r} u_\theta \\
0 & 0 & \frac{1}{r^2} v_r & \frac{1}{r^2} u_\theta
\end{vmatrix},
\]

which is equal to

\[
\frac{2}{r^2} \left( u_0^2 - vv_0^2 \right) dr^2 - 4 \left( u_r u_\theta - vv_r v_\theta \right) dr d\theta + 2r^2 \left( u_r^2 - vv_r^2 \right) d\theta^2.
\]

Then the equation of the characteristics for the Ludwig system is given by \((3.20)\).

The discriminant \(\Delta\) of \((3.20)\) is

\[
\Delta = v (u_r v_0 - u_0 v_r)^2 = v |J|^2.
\]

(ii) From \((3.20)\) and \((3.27)\) it follows that

\[
\frac{dr}{d\theta} = r^2 \left( u_r u_\theta - v v_r v_\theta \right) \pm \sqrt{v (u_r v_0 - u_0 v_r)} \left( u_0^2 - vv_0^2 \right).
\]
The characteristic curves are then given by

\[
\frac{dr}{rd\theta} = \frac{u_r \pm \sqrt{v v_r}}{\frac{2}{3} u_\theta \pm \sqrt{v_\theta v_\theta}} \quad (v > 0).
\]

Therefore, the constant phase curves are

\[
\Phi^\pm = u \pm \frac{2}{3} v^{3/2} \quad (v > 0),
\]

which represent branches of cubic curves with negative ($\Phi^+$) and positive ($\Phi^-$) slopes. Let us note that at $v = 0$, these curves have cusps with vertical tangents. Furthermore, $\nabla \Phi^\pm = \left( u_r \pm \sqrt{v v_r}, \frac{1}{3} u_\theta \pm \sqrt{v_\theta v_\theta} \right)$ satisfies the equation:

\[
|\nabla \Phi^\pm|^2 = 1.
\]

(iii) It follows from (3.21).

**Remark:** In formula (3.18) the term involving the derivative of the Airy function is relatively small near the caustic, but significant away from the caustic \[4\]. This behavior follows from the asymptotic expansion of the functions $Ai$ and $Ai'$: the first one is proportional to $|v|^{-1/4}$, whereas the second one to $|v|^{1/4}$. We shall return to the use of formula (3.18) below, in connection with the specific physical problems in question.

### 4. Diffraeted rays, orbiting resonances and complex rays

#### 4.1. Diffraeted rays, singular eigenfunctions, and breaking of quantiza-

**4.1.1. Transport equation and damping of the amplitude.** The diffraction problem can be formulated by adding suitable boundary conditions to the Helmholtz equation (2.1): one condition at the border of the obstacle, and another one at infinity. The first one is an ordinary boundary condition (e.g., of Dirichlet type); the other is the Sommerfeld radiation condition. If the symmetry of the diffracting body enables one to apply the method of separation of the variables, then one can treat the angular problem separately from the radial one. Furthermore, if the obstacle is a spherical ball, then the radial problem leads to the first–kind Hankel functions $H_{n+1/2}^{(1)}(kr)$ (where $n$ is integer, $k$ is the wavenumber, and $r$ is the distance from the center of the sphere). The radiation condition is satisfied by the Hankel functions, but we are obliged to impose, in addition, a boundary condition at the border of the obstacle. If the latter is of Dirichlet type, then we arrive at the equation

\[
H_{n+1/2}^{(1)}(kR) = 0,
\]

(4.1)

(where $R$ stands for the radius of the spherical ball). The roots of (4.1) belong to the positive imaginary $n$–half–plane, and are infinite in number \[31\]. In order to stress that the index of these functions takes complex values, we replace $n + \frac{1}{2}$ by $\nu_n$. Accordingly, Eq. (4.1) will be rewritten as $H_{\nu_n}^{(1)}(kR) = 0$. 

Remarks: (i) The roots of the equation $H_{\nu_n{-1/2}}(kR) = 0$ are given by the rule

$$\nu_n = kR + \frac{1}{2} (kR)^{1/2} \left[ \frac{3}{4} \pi (4m - 1) \right]^{2/3} e^{i\pi/3},$$

$(m = 1, 2, 3, \ldots)$, and at any fixed value of $kR$, $\nu_n$ varies by varying $m$. They are located close to a curve which tends to become parallel to the imaginary axis of the $\nu$–plane.

(ii) It has been pointed out by Sommerfeld [31] that the functions $H_{\nu_n}(kr)$ form an orthogonal system. If we replace $kr$ by a real variable $x$, and assume that $k = 1$, we have:

$$\int_{-\infty}^{+\infty} H_{\nu_n}^{(1)}(x) H_{\nu_m}^{(1)}(x) \frac{dx}{x} = 0 \quad (m \neq n).$$

This orthogonality relation is of an unconventional kind since the Hankel functions $H_{\nu_n}(x)$ are complex–valued, but no conjugation occurs in (4.3). One could be tempted to reconsider the problem of the waves propagating along the spherical surface regarding the Hankel functions $H_{\nu_n}$ as eigenfunctions of a non–selfadjoint boundary value problem for Bessel’s differential operators. But, unfortunately, the Hankel functions $H_{\nu_n}^{(1)}(x)$ do not form a complete set of functions [31, 32].

A solution of the diffraction problem can be written as a formal series. In this expansion, the angular dependence is represented by Legendre polynomials (in the case of spherical diffracting bodies), the radial dependence by Hankel functions of the first kind, and the coefficients present at the denominator the terms $H_{\nu_n}^{(1)}(kR)$. However, these series converge very slowly and are, in fact, useless for numerical computation. Following Sommerfeld [31], one can perform a Watson–type resummation of these expansions, transforming a sum over $n$ ($n$ is an integer) into an integral along a suitable path in the complex $\nu$–plane [31]. Then the poles of the integrand under consideration are the roots of the equation $H_{\nu_n}^{(1)}(kR) = 0$. The sum over the residues at the poles located in the first quadrant of the $\nu$–plane is rapidly convergent for values of the angle sufficiently large (i.e., backwards). In particular, the term corresponding to the pole closest to the real axis is the dominant one, and, in general, it is sufficient for describing the diffraction in the backward angular region.

Coming back to the geometrical approximation, and specifically to the CFUL approximation formula (3.18), we note, first of all, that the term $v(r, \theta)$ is zero at $\xi = 0$ (i.e., on the border of the obstacle). It follows that formula (3.18) cannot satisfy the boundary condition (e.g., the Dirichlet condition) at the surface of the obstacle. Lewis, Bleinstein and Ludwig [33] proposed a new ansatz, which is a slight modification of formula (3.18), in order to obtain an approximation suitable for imposing appropriate boundary conditions. We follow a simpler approach based on some assumptions which can be controlled from the physical viewpoint. First of all, we choose Ludwig’s system (see (3.19)), which describes the geometry of rays in a neighborhood of the caustic generated by the border of the obstacle. Next, we note that the poles (in the $\nu$–plane) generated by the roots of the equation $H_{\nu_n}^{(1)}(kR) = 0$ (which follow by imposing the Dirichlet boundary conditions) describe the damping of the density of the flux of the trajectories bending around the obstacle. It follows
that it is precisely the transport equation that should be appropriately modified. With this in mind, we assume that the leakage of rays from the tube of trajectories running along the boundary of the obstacle is proportional to the flux. If we suppose that the diffracting body is a spherical ball, then the transport equation on the border of the obstacle reads as follows (see also [2]):

\begin{equation}
\frac{1}{|J_0|} \frac{d}{dr} (A_0^2 |J_0|) = -2\gamma_0 A_0^2,
\end{equation}

where \( J_0 \) is the Jacobian

\begin{equation}
J_0 = \left[ \frac{\partial (x, y, z)}{\partial (r, \varphi, \tau)} \right]_{r=R, \tau=\tau_0 \pm},
\end{equation}

and \( \gamma_0 \) depends upon the curvature of the obstacle and is constant in the case of a diffracting spherical ball. It follows from (4.4) and (4.5) for \( \theta_0 \neq (n + \frac{1}{2})\pi \) that

\begin{equation}
A_0 (\theta_0^\pm) = \frac{C}{|\cos \theta_0^\pm|} e^{-\gamma_0 R\theta_0^\pm} \quad (C = \text{Const.}).
\end{equation}

The meaning of \( \gamma_0 \) can be illustrated by returning to Proposition 3. It follows from statement (b) of Proposition 3 that, at any point of the boundary, the ray splits into two rays: one part travels along the surface as a geodesic bending around the obstacle whereas the other leaves the diffracting body tangentially. Then \( \gamma_0 \), at any chosen value of the wavenumber \( k \), depends on the curvature of the boundary, and this is true not only when the obstacle is a spherical ball but also for any compact and convex diffracting object. Finally, the zero subscript in the notation of \( \gamma_0 \) is for recalling that this damping factor corresponds to the mode associated with the pole closest to the real axis in the Sommerfeld–type summation illustrated above in the particular case of obstacles represented by spherical balls embedded in \( \mathbb{R}^3 \) (recall that only this type of diffracting bodies will be considered in the following).

4.1.2. Solution of the Ludwig system at \( v > 0 \). First, let us consider the counterclockwise oriented rays. We come back to the Ludwig system written in terms of coordinates \((r^+, \theta_0^+)\), appropriate to the counterclockwise trajectories. Notice that the orientation of \( r^+ \) coincides with that of the standard radial coordinate, and \( \theta_0^+ \) was introduced in Subsection 3.3. We now write \( u(r^+, \theta_0^+) = \theta_0^+ \) (assuming \( R = 1 \), for simplicity); accordingly, \( u_{r^+} = 0, u_{\theta_0^+} = 1 \). It follows from (3.24a) that \( v_{\theta_0^+} = 0 \). Moreover, from (3.24a) we get, for large values of \( r^+ \):

\begin{equation}
\sqrt{v} dv = \sqrt{1 - \left( \frac{1}{r^+} \right)^2} dr^+ \sim_{r^+ \to +\infty} dr^+.
\end{equation}

Integrating, we obtain

\begin{equation}
\frac{2}{3} v^{3/2} \sim_{r^+ \to +\infty} r^+.
\end{equation}

Next, we return to the expression of \( \Phi^+ \), and see that

\begin{equation}
\Phi^+ = u + \frac{2}{3} v^{3/2} = \theta_0^+ + r^+.
\end{equation}
Analogous calculations can be repeated for the clockwise rays. Taking \( u(r^-, \theta_0^-) = \theta_0^- \), we have

\[
\Phi^- = u - \frac{2}{3} \alpha^{3/2} = \theta_0^- - r^-.
\]

Now, we relate the coordinates \((r^\pm, \theta_0^\pm)\) to the coordinates appropriate for describing the outgoing rays at large distance from the obstacle, i.e., the scattering coordinates: \( r_s \equiv r \) and \( \theta_s \) \((0 < \theta_s < \pi)\). We have: \( \theta_0^+ = \theta_s \), \( r^+ = r_s \equiv r \); \( \theta_0^- = 2\pi - \theta_s \), \( r^- = -r_s = -r \). Therefore, in conclusion we have:

\[
\begin{align*}
\Phi^+ &= \theta_s + r, \\
\Phi^- &= 2\pi - \theta_s + r.
\end{align*}
\]

So far we have considered trajectories which have not completed a single turn. However the ray trajectories can perform several turns around the obstacle before emerging, and accordingly, the flux density along the border of the obstacle is not conserved, as we have shown above. It follows that the wavefunction does not return to the original value after one turn, and it is not single-valued. We are thus obliged to sum the contributions of both the counterclockwise and clockwise trajectories turning around the obstacle several times, and then emerging and contributing to the scattering amplitude.

4.1.3. Eikonal approximation and its uniformization. We now have to come back to formula (3.8) and to the analogous one for the clockwise rays. First we note that

\[
\tau^\pm = \sqrt{(r^\pm)^2 - R^2} \to r,
\]
and then

\[
\sqrt{|J|} \to r \sqrt{\sin \theta_s^\pm} = r \sqrt{\sin \theta_s}.
\]

We are thus led to consider the branch-cut singularities associated with the crossing of the trajectories through the axial caustic once again. As we have already noted, \( \theta_0^+ = \theta_s \) for the counterclockwise rays which have not completed one turn, and more generally, \( \theta_0^+ - 2\pi n = \theta_s \) \((n = 0, 1, 2, \ldots)\) for the rays which have performed \( n \) turns around the sphere before emerging. But the axial caustic corresponds to \( \theta_s = 0 \) or \( \pi \); accordingly, \( \theta_0^+ - 2\pi n = 2\pi n \) or \((2n + 1)\pi\). Analogous considerations hold for the clockwise rays. Therefore, proceeding as in the proof of Proposition 2 (see also Proposition 5), we can associate a phase-shift to each crossing of the ray trajectories through the axial caustic (including the antipodal points of the spherical ball). More precisely:

(i) at each counterclockwise crossing of the axial caustic we have a phase-shift of \( e^{-i\pi/2} \),

(ii) at each clockwise crossing of the axial caustic we have a phase-shift of \( e^{+i\pi/2} \).

Therefore, the bijective correspondence between the winding number \( w(\gamma) \) and the crossing number \( n(\gamma) \) (see statement (v) of Proposition 5) can be extended to the phase-shift associated with the crossing number. Therefore we have:

\[
\begin{array}{ccc}
Z & \to & \mathbb{N} \\
\quad & \to & \text{Crossing phase-shift} \\
(n) & (2n + 1) & \mapsto \mp \frac{\pi}{2}(2n + 1) \quad (n \geq 0) \\
(n) & -2n & \mapsto \mp \frac{\pi}{2}(-2n) \quad (n < 0)
\end{array}
\]
In view of these formulae and of the analysis performed above, we may work out a uniformized eikonal approximation. More precisely, the wavefunction $\psi^{(+)(0)}(r, \theta_s; k)$ associated with a counterclockwise ray which has not completed one turn presents the following asymptotic behavior for large values of $r$ and $k$:

$$\psi^{(+)(0)}(r, \theta_s; k) \xrightarrow{r \to \infty} \frac{e^{-i\pi/2} e^{i k (R \theta_s + r)} e^{-\gamma_0 R \theta_s}}{r \sqrt{\sin \theta_s}} \quad (0 < \theta_s < \pi),$$

where $C(k)$ is a diffraction coefficient depending only on $k$, the term $e^{-i\pi/2}$ corresponds to a single crossing of the ray across the axial caustic, $e^{-\gamma_0 R \theta_s}$ is the damping due to the leakage of the tube of trajectories along the border of the obstacle which is supposed to be a spherical ball of radius $R$ (i.e., we then write $R \theta_s$ instead of $\theta_s$). The scattering amplitude turns out to be given by:

$$f^{(+)(0)}(\theta_s; k) = C(k) \frac{e^{-i\pi/2} e^{i \nu_0 \theta_s}}{\sqrt{\sin \theta_s}}$$

$$(0 < \theta_s < \pi, \nu_0 = R(k + i \gamma_0)).$$

Note that the subscript zero in $\psi^{(+)(0)}$ and in $f^{(+)(0)}$ indicates that we are referring to the ray which has not completed one turn, while the subscript in $\nu_0$ is for recalling that $R(k + i \gamma_0)$ is a geometrical approximation to the first root of $H_{\nu_0}(k R) = 0$: i.e., the root closest to the real axis.

We can similarly evaluate the contribution to the scattering amplitude of the diffracted ray which travelling along the sphere, in clockwise direction, without completing one turn around the obstacle. We obtain

$$f^{(-)(0)}(\theta_s; k) = (-1) C(k) \frac{e^{i \nu_0 (2\pi - \theta_s)}}{\sqrt{\sin \theta_s}}$$

$$(0 < \theta_s < \pi),$$

where the factor $(-1)$ is precisely given by the product of two phase-shifts, where each of them is expressed by the exponential $e^{i\pi/2}$ since this grazing ray crosses the axial caustic twice.

**Remark:** In the derivation of formulae (4.15) and (4.16), instead of using formula (3.18) (i.e., the CFUL approximation), we have used the eikonal approximation implemented by the uniformization procedures derived in Section 3. We have followed this method since the Dirichlet boundary condition cannot be applied to formula (3.18), as we have already observed before. Further, the ray–tracing procedure, which we have implemented, is more satisfactory from the physical viewpoint and very close to Feynman’s path method. We recall, finally, that formula (3.18) implies again the eikonal approximation by using the asymptotic behavior of $\text{Ai}$ and $\text{Ai}'$ for large $v$ and $k \to \infty \ [4]$.

4.1.4. **Construction of singular eigenfunctions and breaking of quantization.** Adding $f^{(+)(0)}_0$ and $f^{(-)(0)}_0$, we obtain the scattering amplitude $f_0$ due to the rays not completing one turn around the obstacle:

$$f_0(\theta_s; k) = f^{(+)(0)}_0 + f^{(-)(0)}_0 = -i C(k) \frac{e^{i \nu_0 \theta_s} - i e^{i \nu_0 (2\pi - \theta_s)}}{\sqrt{\sin \theta_s}},$$

$$(0 < \theta_s < \pi).$$

Now, we are ready to take into account the contributions of all those rays that are orbiting around the sphere several times: consider rays performing $n$ $(n \in \mathbb{N})$ turns around the obstacle. Since the surface angles $\theta^{(\pm)}_{0,n}$ are related to the
scattering angle $\theta_s$ by the rule $\theta_{0,n}^{(\pm)} = \theta_s + 2\pi n, \theta_{0,n}^{(-)} = 2\pi - \theta_s + 2\pi n \ (n = 0, 1, 2, \ldots)$, we have, for $0 < \theta_s < \pi$:

\begin{equation}
\tag{4.18}
 f(\theta_s; k) = -iC(k) \sum_{n=0}^{\infty} (-1)^n e^{i2\pi n\nu_0} e^{in\theta_{0,n}^{(-)}} / \sqrt{\sin \theta_s}.
\end{equation}

We note that the factor $(-1)$, for any $n > 0$, is due to the product of two phase-shifts represented by the exponential factor $(e^{-i\pi/2})^2$ for the counterclockwise oriented rays, and by $(e^{i\pi/2})^2$ for the clockwise trajectories. In fact, both the counterclockwise and the clockwise oriented rays cross the axial caustic twice for each turn (see Fig. [2]).

Now, by exploiting the following expansion:

\begin{equation}
\tag{4.19}
\frac{1}{2 \cos \pi \nu_0} = e^{i\pi \nu_0} \sum_{n=0}^{\infty} (-1)^n e^{i2\pi n\nu_0} \quad (\text{Im} \nu_0 > 0),
\end{equation}

one can rewrite the amplitude (4.18) as

\begin{equation}
\tag{4.20}
f(\theta_s; k) = -C(k) e^{i\pi/4} \frac{e^{-i[\nu_0(\pi - \theta_s)-\pi/4]} + e^{i[\nu_0(\pi - \theta_s)-\pi/4]}}{2 \cos \pi \nu_0 \sqrt{\sin \theta_s}},
\end{equation}

$(0 < \theta_s < \pi)$. The r.h.s. of (4.20) gives the asymptotic behavior of the Legendre function $P_{\nu_0-1/2}(-\cos \theta_s)$ times $\sqrt{2\pi \nu_0}$ for $|\nu_0| \to \infty$ and $|\nu_0(\pi - \theta_s) | \gg 1$ [34]. Then, writing $P_{\nu_0-1/2}(-\cos \theta_s)$ instead of its asymptotic behavior, we have

\begin{equation}
\tag{4.21}
f(\theta_s; k) \approx G(k) P_{\lambda}(-\cos \theta_s) / \sin \pi \lambda,
\end{equation}

as $|\nu_0| \to \infty$ and for $0 < \theta_s < \pi$, where $G(k) = C(k) e^{i\pi/4} \sqrt{2\lambda + 1}, \lambda = \nu_0 - \frac{1}{2}$. We have thus obtained the expression of the scattering amplitude in terms of Legendre functions, which represent the angular part of the so-called singular eigenfunctions [31]. Let us in fact note that $P_{\lambda}(-\cos \theta_s)$ presents a logarithmic singularity at $\theta_s = 0$ [31], which indicates that the representation (4.21) of the scattering amplitude fails in the forward direction. Indeed, at small angles, the surface waves associated with the diffracted rays describe a very small arc of the circumference, and the damping factors $\exp(-\gamma_0 R_{\nu_0}^{(\pm)})$ (see (4.9)) are very close to one. We are then forced to consider the entire set of modes corresponding to the countable set of the roots of the equation $H_{\nu_0}^{(1)}(kR) = 0$. Conversely, at large angles, the root closest to the real axis gives the main contribution, and this is in agreement with the fact that the factor $\gamma_0 R_{\nu_0}^{(\pm)}$ is large backwards. Accordingly, $P_{\lambda}(-\cos \theta_s) = 1$ at $\theta_s = \pi$. Let us then note that $\text{Re} \nu_0 = kR = \text{Re} \lambda + \frac{1}{2} = \ell + \frac{1}{2}$ ($\ell$ integer), in agreement with the semiclassical formula for the angular momentum. Therefore the function $\text{Re} \lambda(k)$ ($k$ being the wavenumber) gives the trajectory in the complex $\lambda$-plane of the scattering amplitude singularity closest to the real axis. Coming back to formula (4.21), let us however note that if the term $R_{\nu_0}$ is large, then this pole does not produce sharp peaks in the observable quantity (i.e., in the scattering cross-section $\sigma(\theta_s; k) = |f(\theta_s; k)|^2$), in view of the factor $|\sin \pi \lambda|^{-1} \approx \exp(-\pi \gamma_0 R)$.

As we have seen before (see formula (2.20)), the geometrical quantization implies that the angular momentum is given by $\ell + \frac{1}{2}$ ($\ell = 0, 1, 2, \ldots$). Now, the leakage of rays from the tube of trajectories running along the boundary of the obstacle gives rise to a damping factor, which breaks the quantization rule. The angular
wavefunction is, in diffractive processes, represented by the Legendre function $P_\lambda$ ($\lambda \in \mathbb{C}$) rather than by the Legendre polynomials $P_\ell$ ($\ell = 0, 1, 2, \ldots$), and the angular symmetry is broken. For a detailed phenomenological analysis of the creeping waves in the $\pi^+ - p$ elastic scattering, see [13].

4.2. Orbiting resonances and bound states. The orbiting resonances observed in molecular scattering are produced by the trapping of the incoming colliding particles in the region delimited by the centrifugal barrier on one side and by the hard-core on the other side. The process can be depicted as follows: the trajectories of the incoming particles hit the impenetrable sphere which composes the hard-core and describe geodesic orbits around it. This part of the process is quite similar to diffraction by a totally opaque sphere outlined in the previous subsection, and it can be described by using the same geometrical tools. We can thus speak of a tube composed by those trajectories that describe circular orbits bending the spherical ball that represents the hard-core. However, now the leakage of rays from the tube composed by orbiting trajectories is attenuated by the centrifugal barrier. Therefore we shall find asymptotically (i.e., at large $r$) only the particles crossing the centrifugal barrier by tunnelling. At this point, the following problem emerges: in the tunnelling the energy $E$ of the particle is less than the height $V$ of the potential barrier; accordingly, $n^2 = 1 - \frac{E}{V}$ is negative, and therefore it cannot be identified with a Riemannian metric tensor. We loose the identification of a trajectory with a Riemannian real-valued geodesic. We can, however, extend the concept of ray by admitting complex-valued and/or imaginary phases, and speak of complex trajectories in the sense of Landau [35]. Coming back to the standard eikonal equation, an imaginary refractive index produces an imaginary phase. Therefore, the flux of particles beyond the centrifugal barrier is attenuated by a damping factor which is proportional to the ratio between the height of the barrier and the energy of the particles. The lifetime of the resonances is linked to the leakage of the tube of orbiting trajectories, and is controlled by the tunnelling across the centrifugal barrier. Coming back to the calculations of the previous subsection, we simply replace the factor $R_\gamma_0$ a factor denoted by $\beta$ (the subscript zero is now omitted for simplicity), which is related to the lifetime of the resonance: the longer is the life of the resonance the smaller is the value of $\beta$. At $\beta = 0$, the lifetime is infinite, the state is stable: we have orbiting bound states.

Let us then return to formula (4.21), with the notation $\lambda = \alpha + i \beta$. If $\alpha = \ell$ ($\ell$ is an integer) and $0 < \beta \ll 1$, then the factor $1/\sin \pi \lambda$ produces a sharp peak in the cross-section: we have a resonance in the $\ell$-th partial wave. By the formula (4.22)

$$\frac{1}{2} \int_{-1}^{+1} P_\lambda(-z)P_\ell(z)\,dz = \frac{\sin \pi \lambda}{\pi(\lambda - \ell)(\lambda + \ell + 1)} \quad (\ell = 0, 1, 2, \ldots; \lambda \in \mathbb{C}),$$

we can project the amplitude given by the r.h.s. of (4.21) on the $\ell$-th partial wave and (by using the standard notation) obtain the following expression (see [10]):

$$a_\ell = \frac{e^{2i\delta_\ell} - 1}{2ik} = \frac{C(E)}{\pi} \frac{1}{(\alpha + i\beta - \ell)(\alpha + i\beta + \ell + 1)},$$

($\lambda = \alpha + i\beta$, $E$ = center of mass energy, $k^2 = E$ in suitable units). Next, when the elastic unitarity condition can be used, we obtain [10]

$$C(E) = -\frac{\pi}{k^2} \beta(2\alpha + 1),$$

$$\frac{1}{2} \int_{-1}^{+1} P_\lambda(-z)P_\ell(z)\,dz = \frac{\sin \pi \lambda}{\pi(\lambda - \ell)(\lambda + \ell + 1)} \quad (\ell = 0, 1, 2, \ldots; \lambda \in \mathbb{C}),$$
and then

\[ \delta_\ell = \sin^{-1} \frac{\beta(2\alpha + 1)}{\{(\ell - \alpha)^2 + \beta^2\}(\ell + \alpha + 1)^2 + \beta^2} \]  

which represents a sequence of orbiting resonances, i.e., an ordered set of phase-shifts \( \delta_\ell \) that cross \( \frac{\pi}{2} \) with positive derivative. In the present analysis, we do not consider the downward crossing of the phase-shifts through \( \frac{\pi}{2} \), i.e., the echoes of the resonances (or antiresonances); the interested reader is referred to [10]. Now, the l.h.s. of (2.23) (see Section 2) can be extended to continuous values of the angular momentum \( \ell \) by writing

\[ \alpha(\alpha + 1) = 2IE + c_0. \]

As we already remarked in Section 2, it is precisely the extrapolation of this straight line from \( E > 0 \) to \( E < 0 \) that allows us to interpolate the orbiting bound states at \( E < 0 \).

4.3. Complex rays. Evanescent waves in the shadow of the caustic: The rainbow.

4.3.1. Generalized Cauchy–Riemann equations. We now consider the case \( v < 0 \), i.e., statement (iii) of Proposition 10. The Ludwig system is elliptic. Equations (3.19) inform us that the gradients of \( u \) and \( v \) are orthogonal; then, where \( |J| \neq 0 \), this amounts to writing

\[ \frac{u_r}{\sqrt{g}} = -v_r \]

from which the equalities

\[ u_r = \rho \frac{1}{r} v_\theta, \]
\[ u_\theta = -\rho r v_r, \]

follow, with \( \rho = |\nabla u|/|\nabla v| = (\frac{1}{\sqrt{1 - r^2}} - v)^{-1/2} > 0 \), since \( v < 0 \). Equations (4.28) are a generalization of the Cauchy–Riemann equations written in polar coordinates.

Coming back to the expression of the phase \( \Phi^\pm \), we have: \( \Phi^\pm = u \mp \frac{1}{2} i \sqrt{2(-v)^{3/2}} \), namely, a complex–valued phase naturally emerges as a consequence of the elliptic character of the eikonal system (Ludwig system) for \( v < 0 \).

4.3.2. Solution of the Ludwig equations at \( v < 0 \), and the evanescent waves. Writing again \( u(r^\pm, \theta^\pm_0) = \theta^\pm_0 \) in (3.19) and (3.24) and supposing once again that \( R = 1 \), we obtain: \( u_{r^\pm} = 0, u_{\theta^\pm} = 1, v_{\theta^\pm} = 0 \). Specifically, from (3.24a) we have

\[ \frac{1}{r^2} - 1 = (-v)u_r^2 \quad (v < 0). \]

Since we want to describe the shadow of the circular caustic, we integrate (4.29) over the domain inside the unit circle, i.e., over the interval \((r, 1)\), \( 0 < r < 1 \). We thus obtain, for \( 0 < r < 1 \):

\[ -\frac{2}{3} (-v)^{3/2} = \int_1^r \sqrt{\frac{1}{r^2} - 1} dr = \sqrt{1 - r^2} - \frac{1}{2} \ln \frac{1 + \sqrt{1 - r^2}}{1 - \sqrt{1 - r^2}}. \]
Since the approximation of the Airy function $\text{Ai}(-k^{2/3}v)$ (see formula (3.18)) is given, in the domain $v < 0$, by the following asymptotic formula

$$
\text{Ai}(-k^{2/3}v) \simeq \frac{1}{2\sqrt{\pi}k^{1/6}} \frac{e^{-\frac{2}{3}k(-v)^{3/2}}}{(-v)^{1/4}},
$$

we have from formulae (4.30) and (4.31) that

$$
\text{Ai}(-k^{2/3}v) \simeq \frac{g(r)}{2\sqrt{\pi}k^{1/6}} e^{-\frac{2}{3}k(-v)^{3/2}} \exp \left( k \sqrt{1 - r^2} - \frac{k}{2} \ln \frac{1 + \sqrt{1 - r^2}}{1 - \sqrt{1 - r^2}} \right).
$$

Now, let us note that, in the approximation (3.18) (i.e., the CFUL approximation), we can retain the first term only if we are in a region close to the caustic. The second term, proportional to $\text{Ai}'$, is relevant only far from the caustic. But, in any case, it can be neglected in view of its exponentially decreasing behavior. We thus obtain

$$
\psi_S(r, \theta_0^\pm; k) \simeq \frac{G_S(r, \theta_0^\pm)}{\sqrt{k}} e^{ik\theta_0^\pm} e^{ky} e^{-\frac{k}{2} \ln \frac{1 - y}{1 + y}} \exp \left( k \sqrt{1 - r^2} - \frac{k}{2} \ln \frac{1 + \sqrt{1 - r^2}}{1 - \sqrt{1 - r^2}} \right),
$$

where the subscript $S$ is to indicate that we treat the shadow region. When setting $y^2 = 1 - r^2$, formula (4.33) can be rewritten as follows:

$$
\psi_S(y, \theta_0^\pm; k) \simeq \frac{G_S(y, \theta_0^\pm)}{\sqrt{k}} e^{ik\theta_0^\pm} e^{ky} e^{-\frac{k}{2} \ln \frac{1 - y}{1 + y}} \left( \frac{1 - y}{1 + y} \right)^{k/2} e^{ky} \quad (y^2 = 1 - r^2, 0 \leq r \leq 1).
$$

On the circular caustic, i.e., $r = 1$, we have $y = 0$ and $\left( \frac{1 - y}{1 + y} \right)^{k/2} e^{ky} = 1$; then from (4.34), we remain with only counterclockwise $e^{ik\theta_0^+}$ or clockwise $e^{ik\theta_0^-}$ waves propagating on the unit circle. For $r \to 0$, we have $y^2 \to 1$, and the only physical admissible solution is for $y = +1$. Then, $\left( \frac{1 - y}{1 + y} \right)^{k/2} e^{ky} \to 0$, which describes the damping of the evanescent wave in the shadow of the caustic.

In order to study the shadow of the rainbow, it is convenient to map the interior of the unit disk into the outside part, by setting $r' = 1/r$, and accordingly, $y'^2 = 1 - 1/r'^2$. Therefore, formula (4.34) reads (for simplicity, we omit the prime):

$$
\psi_S(y, \theta_0^\pm; k) \simeq \frac{G_S(y, \theta_0^\pm)}{\sqrt{k}} e^{ik\theta_0^\pm} e^{ky} \left( \frac{1 - y}{1 + y} \right)^{k/2} e^{ky} \quad (y'^2 = 1 - 1/r^2; 1 \leq r < +\infty).
$$

Then for $r = 1$ we have $y = 0$ and $\left( \frac{1 - y}{1 + y} \right)^{k/2} e^{ky} = 1$; for $r \to +\infty$, $y \to 1$, and then $\left( \frac{1 - y}{1 + y} \right)^{k/2} e^{ky} \to 0$, which gives the damping of the evanescent waves in the shadow of the caustic.

The rainbow exemplifies the simplest caustic where two rays, deflected by refraction and reflection in a raindrop, coalesce. The two rays coalesce at the rainbow angle, and on the dark side there are no real rays. As examples of rainbow, we can consider the nuclear (on which we focus particularly our attention) and the Coulomb rainbows, which can be found in the scattering phenomenology, e.g., in $\alpha^{40}\text{Ca}$ elastic scattering [14]. The rainbow scattering is a case where the classical
cross–section has a shadow region. For scattering angle $\theta_s$ less than the critical angle $\theta_r$ (the rainbow angle), two classical trajectories contribute to the cross–section. On the other hand, no classical real–valued orbit has a scattering angle $\theta_s > \theta_r$, and there is a shadow. In a neighborhood of the rainbow angle $\theta_s \simeq \theta_r$, there is a bump in the cross–section; beyond $\theta_r$, the cross–section decreases almost exponentially, and this behavior is in agreement with formula (4.35) for sufficiently high values of $k$. Finally, it is worth mentioning the spectacular example of rainbow dip in the differential cross–section of $\alpha^{40}$Ca, i.e., the dip at the energy of 48.0 MeV (in the laboratory system), which can be associated with the nuclear rainbow generated by the refracted rays which penetrate the interaction region, without being absorbed, and then at the rainbow angle $\theta_r \simeq 120^\circ$ (deg. c.m.) coalesce (see Ref. [14]). Let us note that this phenomenon of rainbow is closely connected with a remarkable aspect of the $\alpha$–nucleus scattering, i.e., the reduced absorption of the particles penetrating the target nucleus. This is caused by the large binding energy of the nucleons in $^4\text{He}$ and the saturation of the nucleon–nucleon forces in cases (like the $\alpha^{40}$Ca) of projectiles and target nuclei with closed shells [36].

5. Conclusions

As is well–known, the solution of the wave equation obtained by the method of the geometrical optics is related, in a sense, to the asymptotic form of the integral representation of the field (if it exists), which is an exact solution of the wave problem. Suppose, for example, that the field, in a uniform medium, can be written in the form of an expansion in plane waves; the evaluation of this integral by the stationary phase method yields an asymptotic series. One then extracts the leading term of this asymptotic expansion, which is composed by an amplitude and a phase. The ray trajectories are the lines orthogonal to the constant phase surface, and are described by the eikonal equation; the amplitude satisfies the transport equation, whose physical meaning is the conservation of the flux density. In the simplest case of uniform medium, whose refractive index $n$ is a real constant, the rays are straight lines which can be characterized by the following properties:

(i) They are geodesics of the Euclidean space.
(ii) Phase and amplitude are real–valued functions.
(iii) They can be derived by the Fermat’s variational principle.

Constrained by these types of properties the methods of geometrical optics are rather limited and fail to explain several phenomena like, for instance, the diffraction by a compact and opaque obstacle, that is, the existence of non–null field in the geometrical shadow which, for this reason, is usually referred to as the classically (or geometrically) forbidden region.

In the present paper we have tried, following the ideas and methods proper of GTD, to widen the area of application of geometrical optics. We adopt, first of all, the Jacobi form of the principle of least action (instead of the Fermat’s), which is concerned with the path of the system point rather than with its time evolution [21]. More precisely, Jacobi’s principle (generally applied in mechanics) can be formulated as follows: If there are no forces acting on the body, then the system point travels along the shortest path length in the configuration space. Here we assume a wide extension of Jacobi’s principle, which can be formulated as follows: The geodesics associated with the Riemannian metric (written in standard notation)

\[
n(x, y)\sqrt{dx^2 + dy^2},
\]

(5.1)
i.e., the paths making

\[
\int n(x, y) \sqrt{\left(\frac{dx}{ds}\right)^2 + \left(\frac{dy}{ds}\right)^2} \, ds
\]

stationary, are nicknamed *rays*. The simplest realization of this Jacobi principle consists in identifying \(n^2\) with the Riemann metric tensor \(g_{ij}\), *whenever this identification is admissible* (see below). This identification is obviously possible in the case of a uniform non–absorbing medium: in this case we simply obtain a physical realization of Euclidean geometry. However, this is also certainly possible in the case of a refractive index of the form \(n(x, y) = 1/y (y > 0)\), where \(y\) denotes the coordinate of the vertical axis in an appropriate reference frame. In this case we are led to the Lobacevskian metric \(ds = \sqrt{dx^2 + dy^2}/y\), and the rays are the geodesics in a hyperbolic half–plane (Poincaré half–plane), i.e., Euclidean half–circles with centers on the \(x\)–axis (horizontal axis) and Euclidean straight lines normal to the \(x\)–axis lying in the strip \(0 < y \leq 1\) of the Poincaré half–plane [20]. Furthermore, in this case, the flow of geodesics (i.e., of ray trajectories), as well as in the Euclidean case, can be described in a rather simple and direct form, since in all spaces where the curvature is negative or null, there are no conjugate points at which two or more geodesics meet. But this is not the case if we consider the geodesics on the surface of a spherical ball. In this manifold the geodesics start spreading apart from one point, but then they begin crowding closer together and meet, and the antipodal points of the unit sphere are conjugate. We are then forced to past segments of geodesics together if we want to obtain a uniform eikonal approximation. This is precisely what we have done in Subsection 2.3 (Proposition 2) and in Subsection 4.3.

A wide extension of the GTD approach could be regarded as a sort of “*Equivalence Principle*”, which puts on equal footing the following procedures: either the trajectories can be seen as straight or curved lines in a Euclidean space or the trajectories can be regarded as geodesics in a space whose metric and topological properties are those induced by the refractive index (or, equivalently, by the potential). However, this *Equivalence Principle* must be interpreted with great caution. In fact, as we mentioned above, the identification of \(n^2\) with the Riemann metric tensor is not always admissible. In fact, the form \(g_{ij}dx^i dx^j\) must be symmetric and positive definite, and this poses a strict restriction. Consider, for instance, a refractive index (or a potential) of the following form: \(n^2 = 1 - V/E\) \((E < V)\), where \(E\) is the energy of the incoming particle, and \(V\) is the height of the potential, as in the case of the tunnel effect (see Subsection 4.2). In this case the geometric interpretation of the trajectory as a real–valued geodesic in a Riemannian manifold is lost. The only possibility remains to extend the admissible values of the phase to imaginary and/or complex values (giving up condition (ii) indicated at the beginning of this section) and to speak of complex rays in the sense of Landau [35] (see Subsection 4.3). However, it is of interest to note that evanescent waves and, accordingly, complex phases are generated in the shadow of the caustic as well; this is precisely the phenomenon studied in Subsection 4.3 and, in particular, in Subsection 4.3.2 in connection with the rainbow phenomenon.
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