

Complete Hamiltonian Description of Wave-Like Features in Classical and Quantum Physics

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Abstract The analysis of the Helmholtz equation is shown to lead to an exact Hamiltonian system describing in terms of ray trajectories, for a stationary refractive medium, a very wide family of wave-like phenomena (including diffraction and interference) going much beyond the limits of the geometrical optics (“eikonal”) approximation, which is contained as a simple limiting case. Due to the fact, moreover, that the time independent Schrödinger equation is itself a Helmholtz-like equation, the same mathematics holding for a classical optical beam turns out to apply to a quantum particle beam moving in a stationary force field, and leads to a system of Hamiltonian equations providing exact and deterministic particle trajectories and dynamical laws, and containing the laws of Classical Mechanics in the eikonal limit.

Keywords Geometrical optics · Hamilton equations · Quantum foundations · Indeterminism

1 Introduction

The present paper proposes a simple (but exact) Hamiltonian approach holding, in principle, for a wide family of wave-like phenomena in stationary media, including both classical and quantum features.

Its main elements of novelty are the following:

1.1 A Step beyond the Geometrical Optics Approximation

It is often believed that the “naïve” concept of optical *rays* applies only to a very limited set of physical cases which may be ascribed to the so-called *geometrical optics*

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approximation, while more general and complex phenomena (such as diffraction and interference) would necessarily require a fully wave-like treatment. In the *first* (classical) part of our work (Sects. 2 and 3) we show that this commonplace is not correct. Starting from the *Helmholtz* equation we obtain, *without any omission or approximation*, a Hamiltonian set of ray-tracing equations providing (in stationary media) the *exact* description in term of *rays* of a family of wave phenomena much wider than that allowed by the standard geometrical optics, which is contained as a simple limiting case. Such an exact description includes both the ray *geometry* and their *motion law*.

1.2 A Remarkable Property of Optical Beams

The rays of a classical electromagnetic wave beam are shown to be mutually coupled (in a kind of self-refractive behavior, strongly dependent on the space amplitude distribution of the beam) by a term acting *perpendicularly* to the rays themselves, and affecting therefore their geometry without altering the amplitude of their velocity. This property is shown to provide, moreover, a basic tool for the numerical solution of the Hamiltonian ray-tracing system. An important consequence of this mutual coupling is the necessity of taking simultaneously into account the propagation of all the rays of the beam.

1.3 Mathematical Coincidence between Classical Optical Rays and Quantum Particle Trajectories

And here begins the *second* (quantum) part (Sects. 4–8) of our paper. We recall in fact that the particle trajectories encountered in Classical Mechanics were often suggested to constitute the *geometrical optics approximation* of the wave-like quantum behavior of the particles themselves. This suggestion was aimed, of course, to enforce the necessity of abandoning, in general, the very concept of particle trajectories, just as the ray picture was supposed to collapse in standard optics. The basic consequence of this philosophy is *quantum uncertainty*, according to which no position *and* momentum can be exactly and simultaneously ascribed to a particle.

Since, however—thanks to our previous extension of the concept of “ray” much beyond the limits of the geometrical optics approximation—no collapse of the optical ray description does occur, and since, after all, the time-independent *Schrödinger* equation is itself a *Helmholtz*-like equation, it is quite natural to expect, now, that the same peculiar properties holding in Classical Optics may be extended to Quantum Mechanics. This expectation, indeed, is immediately satisfied, and the trajectories and dynamical laws of a quantum particle beam turn out to be provided by an *exact* Hamiltonian system mathematically *coinciding* (in suitable dimensionless variables) with the system found in the previous optical case, and involving therefore—in correspondence with the same boundary conditions—the same geometrical trajectories, with the same transverse correlation property discovered in the classical case, requiring therefore to take simultaneously into account the motion of all the particles of the beam.

1.4 Complete and Exact Hamiltonian Quantum Description

This Hamiltonian system provides a complete and exact description of the motion of a quantum particle beam, showing no trace of probabilistic features and containing the laws of *classical* Dynamics as a limiting case (just as the geometrical optics approximation turns out to be a particular case of our *exact* ray approach).

Although, of course, neither the *Helmholtz* equation nor the time-independent (*Helmholtz*-like) *Schrödinger* equation can directly describe any propagation phenomenon, they provide (for any assigned stationary medium, and for any set of boundary conditions) a *fixed frame of trajectories* (i.e. a fixed “weft” of “rails”), which are *determined at the very outset* (in a way somewhat reminding *Fermat’s* and *Maupertuis’* variational principles) by the boundary conditions, and along which each particle (or ray) moves according to well-defined motion laws, in agreement with the time-independent character of the underlying Hamiltonian. These trajectory patterns and motion laws, in their turn, are shown to strongly depend on the beam amplitude distribution, but not on the number of particles (or rays), which could even be reduced to a single particle at a time: a peculiar feature which has often induced to speak (in the quantum context) of single particle self-diffraction.

1.5 Wave-Like Origin of the So-Called “Quantum Potential”

Within the mathematical coincidence observed here between classical optical rays and quantum trajectories, an important feature is represented by the fact that the same mathematical term omitted in the standard geometrical optics approximation and taken into account in the present work under the name of “wave potential”, turns out to give rise, in the quantum case, to the so-called “quantum potential” of the *de Broglie* and *Bohm* theory [1–5]. Such a term is simply due, therefore, to the structure itself of *Helmholtz*-like equations, both in classical and in quantum waves.

2 Helmholtz Equation and Geometrical Optics

In order to establish our mathematical formalism, let us start from a *classical case* of wave-like behaviour.

Although many kinds of physical waves would lend themselves to the considerations we have in mind here, we shall refer, in order to fix ideas, to a monochromatic electromagnetic wave beam, with a time dependence $\div \exp(i\omega t)$, travelling through an isotropic and inhomogeneous dielectric medium. Its basic features are accounted for by the *Helmholtz* equation

$$\nabla^2\psi + (nk_0)^2\psi = 0, \quad (1)$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2};$$

ψ represents any component of the electric or magnetic field; $n(x, y, z)$ is the refractive index of the medium, and

$$k_0 \equiv \frac{2\pi}{\lambda_0} = \frac{\omega}{c}, \tag{2}$$

with obvious meaning of λ_0 and c . The phase velocity is given, in its turn, by

$$v_{ph}(x, y, z) = c/n(x, y, z). \tag{3}$$

Because of its time-independence, (1) cannot describe propagation phenomena in time-varying media: in stationary media, however, it determines both the *fixed* trajectory frame where propagation occurs and, as we shall see, the ray motion laws along such a frame. By performing the quite general replacement

$$\psi(x, y, z) = R(x, y, z)e^{i\varphi(x, y, z)}, \tag{4}$$

with real $R(x, y, z)$ and $\varphi(x, y, z)$, and separating the real from the imaginary part, (1) splits into the well known [6] and strictly equivalent system of coupled equations

$$\begin{cases} (\nabla\varphi)^2 - (nk_0)^2 = \frac{\nabla^2 R}{R}, \\ \nabla \cdot (R^2 \nabla\varphi) = 0, \end{cases} \tag{5}$$

where $\nabla \equiv \partial/\partial\mathbf{r} \equiv (\partial/\partial x, \partial/\partial y, \partial/\partial z)$, and the second of (5) expresses the constancy of the flux of the vector $R^2 \nabla\varphi$ along any tube formed by the lines of $\nabla\varphi$ itself.

When the space variation length, L , of the amplitude $R(x, y, z)$ may be assumed to satisfy the condition $k_0 L \gg 1$, the first of (5) is well approximated by the *eikonal equation*

$$(\nabla\varphi)^2 \cong (nk_0)^2, \tag{6}$$

decoupled from the second of (5) (whose presence is generally neglected) and allowing the so-called *geometrical optics approximation*, which describes the wave propagation in terms of “rays” travelling along the field lines of the *wave vector*

$$\mathbf{k} = \nabla\varphi \tag{7}$$

independently from the amplitude distribution $R(x, y, z)$ of the beam. To be sure, by multiplying (6), for convenience, by the constant factor $\frac{c}{2k_0}$, we obtain the relation

$$D(\mathbf{r}, \mathbf{k}) \equiv \frac{c}{2k_0}[k^2 - (nk_0)^2] \cong 0 \tag{8}$$

(where $\mathbf{r} \equiv (x, y, z)$), whose differentiation

$$\frac{\partial D}{\partial \mathbf{r}} \cdot d\mathbf{r} + \frac{\partial D}{\partial \mathbf{k}} \cdot d\mathbf{k} = 0 \tag{9}$$

directly provides, for any assigned refractive function $n(x, y, z)$, both the geometrical form of the rays and their motion law in the simple Hamiltonian form

$$\begin{cases} \frac{dr}{dt} = \frac{\partial D}{\partial \mathbf{k}} = \frac{c\mathbf{k}}{k_0}, \\ \frac{d\mathbf{k}}{dt} = -\frac{\partial D}{\partial \mathbf{r}} = \frac{c}{2k_0} \frac{\partial}{\partial \mathbf{r}} (nk_0)^2 \end{cases} \quad (10)$$

where a ray velocity $\mathbf{v}_{ray} = \frac{c\mathbf{k}}{k_0}$ is implicitly defined. We may observe that $v_{ray} \equiv |\mathbf{v}_{ray}| = c$ when $k = k_0$, and that $v_{ray}v_{ph} = c^2$. The rays of a wave beam are described, within the eikonal approximation (10), *independently* from one another, requiring only the knowledge of the (time-independent) refraction index $n(x, y, z)$ of the medium. The generalization of the eikonal approach of (10) to the classical anisotropic case of electromagnetic waves travelling through a magnetoactive plasma in steady state thermonuclear devices was treated, for instance, in [7, 8].

We conclude the present section by recalling *Fermat's* variational principle, according to which any optical ray travelling between two points A, B shall follow a trajectory satisfying the condition

$$\delta \int_A^B k ds = 0, \quad (11)$$

where $k = |\mathbf{k}|$ and ds is an element of a (virtual) line connecting A and B .

The relevance of this variational principle in the context of the present work is limited to the single *but fundamental* fact that it finds its quantum mechanical counterpart, as we shall see, in Maupertuis principle.

3 Beyond the Geometrical Optics Approximation

Let us consider now the *first* of (5) in its *complete* form, arriving therefore at the *exact* relation, generalizing the function $D(\mathbf{r}, \mathbf{k})$ of (8),

$$D(\mathbf{r}, \mathbf{k}) \equiv \frac{c}{2k_0} \left[k^2 - (nk_0)^2 - \frac{\nabla^2 R}{R} \right] = 0, \quad (12)$$

whose differentiation, formally coinciding with (9), leads to the *exact* Hamiltonian ray-tracing system

$$\begin{cases} \frac{dr}{dt} = \frac{\partial D}{\partial \mathbf{k}} = \frac{c\mathbf{k}}{k_0}, \\ \frac{d\mathbf{k}}{dt} = -\frac{\partial D}{\partial \mathbf{r}} = \frac{c}{2k_0} \frac{\partial}{\partial \mathbf{r}} [(nk_0)^2 + \frac{\nabla^2 R}{R}]. \end{cases} \quad (13)$$

The exact Hamiltonian system (13) lends itself to a practicable numerical solution even in physical cases where the standard geometrical optics approximation is completely inapplicable. Such a system completely avoids the approximations of the “eikonal” approach (10), although fully retaining the idea of optical “rays” travelling along the field lines of $\mathbf{k} \equiv \underline{\nabla}\varphi$. The r.h.s. of the second of (13) contains, with respect

to the eikonal case, an additional term which may be written in the form $-\frac{\partial W}{\partial r}$, thus defining a function

$$W(x, y, z) = -\frac{c}{2k_0} \frac{\nabla^2 R}{R}$$

which we shall call “wave potential”, coupling all the rays of the beam. Such a function (having the dimensions of a frequency) is an intrinsic, stationary property of the beam, entirely determined in the whole *space* by the launching conditions imposed to the beam amplitude $R(x, y, z)$, and therefore by the experimental set-up.

For any set of boundary conditions imposed to the function $R(x, y, z)$ on the launching surface of the beam, and for any assigned refractive stationary medium, the system (13) provides both a fixed “weft” of “rails” along which the rays are channelled and the motion laws along these “rails”.

In order to analyze the properties of the *wave potential* we make use of the *second* of (5), which may be written in the form

$$\underline{\nabla} \cdot (R^2 \underline{\nabla} \varphi) \equiv 2R \underline{\nabla} R \cdot \underline{\nabla} \varphi + R^2 \underline{\nabla} \cdot \underline{\nabla} \varphi = 0. \tag{14}$$

Since no new ray trajectory may suddenly arise in the space region spanned by the beam, we must have, of course, $\underline{\nabla} \cdot \underline{\nabla} \varphi = 0$, so that (14) splits into the system

$$\begin{cases} \underline{\nabla} \cdot \underline{\nabla} \varphi = 0, \\ \underline{\nabla} R \cdot \underline{\nabla} \varphi = 0, \end{cases} \tag{15}$$

where the second equation is automatically entailed by the first one. The values of the function $R(x, y, z)$ are therefore constant (i.e. “transported”) along the field lines of $\mathbf{k} \equiv \underline{\nabla} \varphi$, to which $\underline{\nabla} R$ turns out to be *perpendicular*, and this transverse character is shared by the gradient $\frac{\partial}{\partial r} \frac{\nabla^2 R}{R}$. The absolute value v_{ray} of the ray velocity remains, in vacuum, equal to c all along its trajectory, because such a gradient may only modify the *direction*, but not the *amplitude*, of the wave vector \mathbf{k} : the only possible changes of $k \equiv |\mathbf{k}|$ could be due, in a medium different from vacuum, to its refractive function $n(x, y, z)$.

Thanks to its constancy along each ray trajectory, the function $R(x, y, z)$, once assigned on the launching surface from which the ray beam is assumed to start, may be numerically built up step by step, together with its derivatives and therefore with the *wave potential* $W(x, y, z)$, in the whole region crossed by the beam.

The beam amplitude distribution $R(x, y, z)$ is entirely determined, in the whole space, by the form assumed on the launching surface in the experimental set-up. The relevant energy input of the beam, on the other hand, is quite arbitrary, and could even be reduced to a single ray at a time: a ray belonging, however, to a pattern which is fixed from the very start by the launching conditions, and couples all the rays of the beam. The virtual presence of the other trajectories of the beam must be kept into account step by step, in any numerical computation, in order to build up (wave-front after wave-front, since every front may be considered as the launching surface of the beam) the proper form of the wave potential.

4 The Time-Independent Schrödinger Equation

The *classical* motion of a mono-energetic beam of non-interacting particles of mass m through a force field deriving from a potential energy $V(x, y, z)$ not explicitly depending on time may be described for each particle of the beam, as is well known, by means of the so-called “reduced” (or “time-independent”) Hamilton-Jacobi equation [6]

$$(\underline{\nabla}S)^2 = 2m(E - V), \quad (16)$$

where E is the total energy, and one of the main properties of the function $S(x, y, z)$ is that the particle momentum is given by

$$\mathbf{p} = \underline{\nabla}S. \quad (17)$$

Recalling *Maupertuis’* variational principle

$$\delta \int_A^B p ds \equiv 0, \quad (18)$$

with $p = |\mathbf{p}|$, the formal analogy between (6, 7, 11) on one side, and (16–18) on the other side, suggests, as is well known, that the *classical* particle trajectories could constitute the *geometrical optics approximation* of an equation (analogous to the Helmholtz (1)), which is immediately obtained by means of the substitutions

$$\begin{cases} \varphi = \frac{S}{a} & \text{and therefore} \\ \mathbf{k} = \underline{\nabla}\varphi = \frac{\underline{\nabla}S}{a} = \frac{\mathbf{p}}{a} \\ k_0 \equiv \frac{2\pi}{\lambda_0} = \frac{\sqrt{2mE}}{a} \equiv \frac{p_0}{a} \\ n^2(x, y, z) = 1 - \frac{V(x, y, z)}{E}, \end{cases} \quad (19)$$

where the parameter a represents a constant *action* whose value is *a priori* arbitrary— as far as the relations (19) are concerned—but is imposed by the history itself of Quantum Mechanics:

$$a = \hbar \cong 1.0546 \times 10^{-27} \text{ erg} \cdot \text{s}. \quad (20)$$

The equation obtained from the Helmholtz equation (1) by means of the substitutions (19) and (20) takes up the form

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0, \quad (21)$$

which is the standard *time-independent* Schrödinger equation.

By applying now to (21) the same procedure leading from (1) to (5), and assuming therefore

$$\psi(x, y, z) = R(x, y, z) e^{iS(x, y, z)/\hbar}, \quad (22)$$

(21) splits [9] into the well-known coupled system

$$\begin{cases} (\nabla S)^2 - 2m(E - V) = \hbar^2 \frac{\nabla^2 R}{R}, \\ \nabla \cdot (R^2 \nabla S) = 0. \end{cases} \tag{23}$$

By taking the gradient of the first of (23) we get moreover

$$\left(\frac{\nabla S}{m} \cdot \nabla \right) \frac{\nabla S}{m} + \frac{\nabla V}{m} = \frac{\hbar^2}{2m^2} \nabla \left(\frac{\nabla^2 R}{R} \right). \tag{24}$$

Equation (24), together with the second of (23), is often interpreted as describing, in the “classical limit” $\hbar \rightarrow 0$ (whatever such a limit may mean), a “fluid” of particles with mass m and velocity $\frac{\nabla S}{m}$, moving in an external potential $V(x, y, z)$: an interpretation consistent with the probabilistic character usually ascribed to the Schrödinger equation.

5 Hamiltonian Description of Quantum Particle Motion

Let us now observe that, by simply maintaining (17), the first of (23) may be written in the form of a generalized, time-independent Hamiltonian

$$H(\mathbf{r}, \mathbf{p}) \equiv \frac{p^2}{2m} + V - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} = E, \tag{25}$$

including the crucial term $-\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}$, coinciding with the well known *quantum potential* of the *de Broglie-Bohm* theory [1–5].

By differentiating (25) we get the relation

$$\frac{\partial H}{\partial \mathbf{r}} \cdot d\mathbf{r} + \frac{\partial H}{\partial \mathbf{p}} \cdot d\mathbf{p} = 0 \tag{26}$$

leading to a Hamiltonian dynamical system of the form

$$\begin{cases} \frac{d\mathbf{r}}{dt} = \frac{\partial H}{\partial \mathbf{p}} = \frac{\mathbf{p}}{m}, \\ \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{r}} = -\frac{\partial}{\partial \mathbf{r}} \left[V(\mathbf{r}) - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \right] \end{cases} \tag{27}$$

strictly similar to the ray-tracing system (13).

The “quantum potential” $Q(x, y, z) = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}$ is strictly analogous to the “wave potential” $W(x, y, z)$ of Sect. 3, and is therefore due to the wave-like nature of quantum particles. Its presence causes the interconnection between the trajectories of the whole beam, and its absence would reduce the system (27) to the standard classical set of Hamiltonian dynamical equations, which are therefore its “eikonal approximation”.

If we envisage the Hamiltonian system (27) for what it appears to be, without superimposing any interpretative prejudice, it is quite evident that its mathematical treatment is the same employed in the classical ray-tracing case, including the fact

that the function $R(x, y, z)$ is “transported” along the field lines of $\mathbf{p} \equiv \nabla S$, to which ∇R turns out to be perpendicular. The gradient $\frac{\partial}{\partial r} \frac{\nabla^2 R}{R}$, in its turn, remains tangent to the wave-front, without acting on the *amplitude* of the particle velocity (but modifying, in general, its *direction*). The only possible amplitude changes could be due to the presence of an external potential $V(x, y, z)$.

Once more, thanks to its constancy along each trajectory, the function $R(x, y, z)$ may be assigned on the launching surface from where the beam is assumed to start, and numerically built up step by step (i.e. wave-front after wave-front) in the whole region spanned by the motion of the beam; and once more the numerical treatment of each trajectory requires the simultaneous treatment of all the (real or virtual) trajectories of the beam consistent with the experimental set-up.

6 The Unique Dimensionless Hamiltonian System

A quite expedient step is now the passage to the new, dimensionless variables $\underline{\xi}, \underline{\rho}, \tau$ defined as the ratio of \mathbf{r}, \mathbf{p} and t , respectively, with $\lambda_0 \equiv 2\pi \hbar/p_0$ for the space variables, $p_0 \equiv (2mE)^{1/2}$ for the momentum variables (so that $\rho_0 = 1$), and $\frac{\lambda_0}{p_0/m}$ for the time variable.

The equation system (27) takes up therefore the form

$$\begin{cases} \frac{d\underline{\xi}}{d\underline{t}} = \underline{\rho}, \\ \frac{d\underline{\rho}}{d\underline{t}} = -\frac{\partial}{\partial \underline{\xi}} \left[\frac{V(\underline{\xi})}{2E} - \frac{1}{8\pi^2} G(\underline{\xi}) \right] \end{cases} \tag{28}$$

with

$$\begin{aligned} G(\underline{\xi}) &= \frac{1}{R} \left(\frac{\partial^2 R}{\partial \xi^2} + \frac{\partial^2 R}{\partial \eta^2} + \frac{\partial^2 R}{\partial \zeta^2} \right); \\ \underline{\xi} &\equiv (\xi, \eta, \zeta) \equiv (x/\lambda_0, y/\lambda_0, z/\lambda_0). \end{aligned} \tag{29}$$

It may be observed that no direct reference is present, in the dimensionless form (28) assumed by the *quantum* dynamical system (27), to the mass of the moving particles, and not even to \hbar .

Let us also observe that *the same dimensionless form* (28) is taken up by the ray-tracing system (13)—relevant to the *classical* electromagnetic case—by simply assuming $\tau = \frac{ct}{\lambda_0}$ and replacing $\underline{\rho}$ with $\frac{\mathbf{k}}{k_o} \equiv \frac{\mathbf{v}_{ray}}{c}$ and $\frac{V(x,y,z)}{E}$ with $[1 - n^2(x, y, z)]$, in agreement with the relations (19).

The basic Hamiltonian equations underlying the classical as well as the quantum cases are, therefore, exactly the same.

Once assigned on the launching surface of the beam, the function $G(\underline{\xi})$ may be numerically determined step by step, in principle, together with its derivatives, along the full set of trajectories of the beam. This function (to which both the “wave potential” $W(x, y, z)$ and the “quantum potential” $Q(x, y, z)$ reduce in dimensionless form) determines, together with the external refractive index or force field, the trajectory geometry and the motion laws both of classical electromagnetic rays and of *quantum* particles. In its absence the system (28) would simply describe either the

electromagnetic behaviour of each ray of the beam in the eikonal approximation or the classical motion of each particle of the beam, and both rays and particles of the beam would move along trajectories independent from one another.

Due to the small coefficient $\frac{1}{8\pi^2}$, the transverse gradient $\frac{\partial G}{\partial \xi}$ acts along the ray (or particle) trajectories in a soft and cumulative way: a fact granting the main justification for omitting such a term, as is done both in classical dynamics and in the standard geometrical optics approximation.

The trajectory pattern, in its turn, is a stationary structure determined at the very outset in a way somewhat reminding the spirit of classical variational principles, such as the ones of Fermat and Maupertuis. For any set of boundary conditions imposed to the function $R(x, y, z)$ on the launching surface of the beam, and for any assigned refractive stationary medium (or force field), the system (28) provides both a fixed “weft” of “rails” and a motion law (in agreement with the underlying time-independent Hamiltonian) to which particles (or rays) are deterministically bound, *showing no trace of probabilistic features*. Each quantum particle (as well as each classical electromagnetic ray) turns out to be conceivable indeed, on the basis of the present analysis, as *starting and remaining* on a well-defined trajectory belonging to a pattern which is *a priori* fixed, as a whole, by the properties of the medium and by the beam amplitude distribution on the launching surface, and therefore by the experimental set-up.

The equation system (28), derived from a time-independent Hamiltonian, provides in conclusion a complete set of motion laws which replace (and contain as an approximation, when the wave—or quantum—potential may be neglected) both geometrical optics and classical dynamics in stationary media. In striking divergence from these approximated limits, however, the new set of equations does not represent an ensemble of mutually independent rays (or particles), but requires in general, for its solution, the full set of boundary conditions and the simultaneous treatment of all the rays (or particles) of the beam, which are mutually coupled by the wave (or quantum) potential.

7 Wave-Like Features in Hamiltonian Form

Although an accurate and general numerical treatment lies beyond the aims of the present paper, we propose here the application of the equation system (28) to the propagation of a collimated beam injected at $\zeta = 0$ parallel to the ζ -axis, and centred at $\xi = 0$, in order to simulate wave diffraction through a single slit.

The problem may be faced by taking into account for simplicity sake (but with no substantial loss of generality) either a (quantum) *particle beam* in the absence of external fields ($V = 0$), or a (classical) *electromagnetic beam* in vacuum ($n^2 = 1$), with a geometry allowing to limit the computation to the trajectories lying on the (ξ, ζ) -plane.

The Hamiltonian system (28) takes up therefore the form

$$\begin{cases} \frac{d\xi}{d\tau} = \rho_x, \\ \frac{d\zeta}{d\tau} = \rho_z, \\ \frac{d\rho_x}{d\tau} = \frac{1}{8\pi^2} \frac{\partial}{\partial \xi} G(\xi, \zeta), \\ \frac{d\rho_z}{d\tau} = \frac{1}{8\pi^2} \frac{\partial}{\partial \zeta} G(\xi, \zeta) \end{cases} \tag{30}$$

with

$$\begin{aligned} G(\xi, \zeta) &= \frac{1}{R} \left(\frac{\partial^2 R}{\partial \xi^2} + \frac{\partial^2 R}{\partial \zeta^2} \right); \\ \rho_x(\zeta = 0) &= 0; \quad \rho_z(\zeta = 0) = \rho_0 = 1 \end{aligned} \tag{31}$$

and a suitable amplitude distribution $R(\xi, \zeta = 0)$ (from whose normalization the function G is obviously independent) imposed at $\zeta = 0$.

Because of the transverse nature of the gradient of $G(\xi, \zeta)$, the *amplitude* of the vector $\underline{\rho}$ remains unchanged (in the absence of external fields and/or refractive effects) along each trajectory, leading therefore to the relation

$$\rho_z = \sqrt{\rho_o^2 - \rho_x^2} \equiv \sqrt{1 - \rho_x^2}, \tag{32}$$

which may advantageously replace the fourth equation of the Hamiltonian system (30). Two possible models of the amplitude distribution $R(\xi, \zeta = 0)$, and therefore of the beam launching conditions, are obtained by assuming either

- a Gaussian distribution centred at $\xi = 0$, in the form

$$R_0(\xi; \zeta = 0) \div e^{-\left(\frac{x}{w_0}\right)^2} \equiv e^{-\varepsilon^2 \xi^2} \tag{33}$$

(with constant w_0 and $\varepsilon = \frac{\lambda_0}{w_0} \leq 1$), a functional form suggested by its smooth analytical behaviour; or

- algebraic distributions, in the form

$$R_N(\xi; \zeta = 0) \div \frac{1}{1 + \left(\frac{x}{w_0}\right)^{2N}} \equiv \frac{1}{1 + (\varepsilon \xi)^{2N}} \tag{34}$$

(with integer $N \geq 1$), allowing the presence of flat central regions, widening with increasing N . We show in Fig. 1, for $\varepsilon = 0.25$, both the Gaussian launching distribution $R_0(\xi; \zeta = 0)$ and the (algebraic) distributions $R_{1,2}(\xi; \zeta = 0)$ (with $N = 1$ and $N = 2$, respectively).

Figures 2 and 3 represent, in their turn, the functions

$$G_{1,2}(\xi; \zeta = 0) = \frac{1}{R_{1,2}} \frac{d^2 R_{1,2}}{d\xi^2} \tag{35a}$$

respectively, each one compared with

$$G_0(\xi; \zeta = 0) = \frac{1}{R_0} \frac{d^2 R_0}{d\xi^2}. \tag{35b}$$

Fig. 1 Plot of the amplitude distributions $R_{0,1,2}$ assigned to the beam on the launching plane $\zeta = 0$, for $\varepsilon = \lambda_0/w_0 = 0.25$, in the Gaussian case of (33) (continuous heavy line) and in the algebraic cases of (34), with $N = 1$ (dotted line) and $N = 2$ (continuous light line), respectively

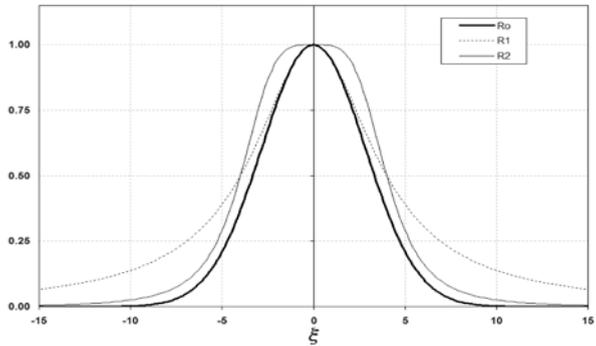


Fig. 2 Comparison between the initial “potential” functions G_0 and G_1 corresponding to the distributions R_0 and R_1 , respectively

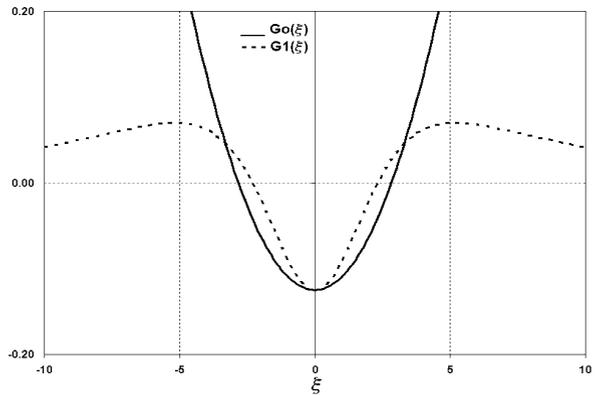
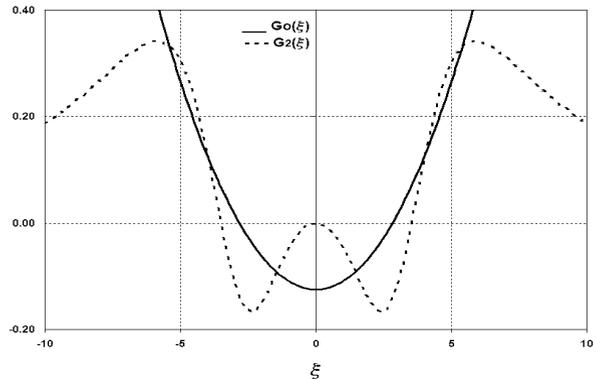


Fig. 3 Comparison between the initial functions G_0 and G_2 corresponding to the distributions R_0 and R_2 , respectively



Let us recall that the functions $G_{0,1,2}$ are the dimensionless forms (with the opposite sign) of the wave (and quantum) potential. Figure 3 shows, in particular, that apparently similar amplitude distributions, such as R_0 and R_1 , may give rise to quite different potential functions G_0 and G_1 .

The ray (or particle) trajectories were obtained, in our numerical computation, by means of a Runge-Kutta method, and the functions $G_{0,1,2}(\xi; \zeta > 0)$ were built

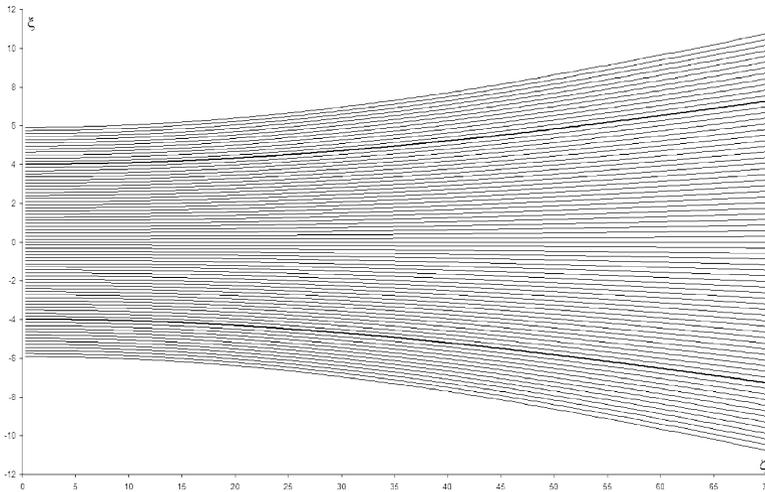


Fig. 4 Trajectory pattern on the (ξ, ζ) -plane, in the Gaussian case. The heavy lines are the “waist” rays of (36)

up step by step, together with their derivatives, by means of a Lagrange interpolation.

Figure 4 presents the trajectories corresponding to the Gaussian case (33). As predicted by the standard optical diffraction theory [10], no “fringe” is found in this case, due to the fact that the Fourier transform of the distribution R_0 consists of another Gaussian function.

An excellent agreement is observed with the well-known relation

$$\xi(\zeta) = \pm \sqrt{\frac{1}{\varepsilon^2} + \left(\frac{\varepsilon}{\pi}\right)^2 \zeta^2} \tag{36}$$

holding, *in vacuo*, for the rays starting (at $\zeta = 0$) from $\xi = \pm 1/\varepsilon$ (i.e. from the “waist” positions $x = \pm w_0$), which delimit the so-called “paraxial” part [11] of the Gaussian beam. In the figure (where $\varepsilon = 0.25$) these rays are evidenced by the heavy lines starting from $\xi = \pm 4$.

Figure 5 shows the trajectories starting with the algebraic amplitude distribution $R_1(\xi; \zeta = 0)$. It may be seen that trajectories somewhat similar to the ones of the Gaussian case are observed only in the central, “paraxial” part of the beam. The other trajectories are quite different from the Gaussian ones, and exhibit two diffraction “fringes” (in the form of gathering trajectories).

Figure 6 shows the evolution of the relevant transverse intensity of the beam at different sections along ζ , and Fig. 7 presents the corresponding evolution of the potential function G_1 .

Figures 8–10 present, finally, the ray trajectories and the evolution of the beam intensity and of the potential function corresponding to the algebraic launching distribution $R_2(\xi; \zeta = 0)$.

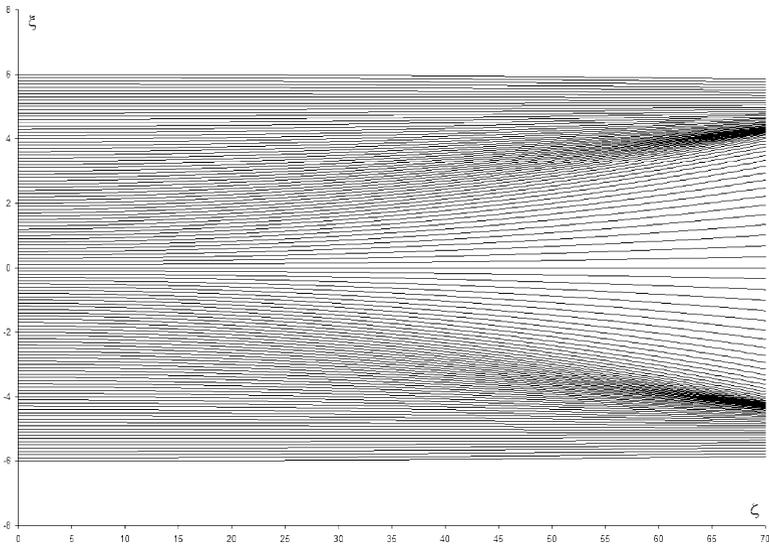


Fig. 5 Trajectory pattern on the (ξ, ζ) -plane, in the algebraic case $N = 1$

Fig. 6 (a)–(e): Transverse intensity distributions corresponding to Fig. 5, computed at different sections of the beam for increasing values of ζ

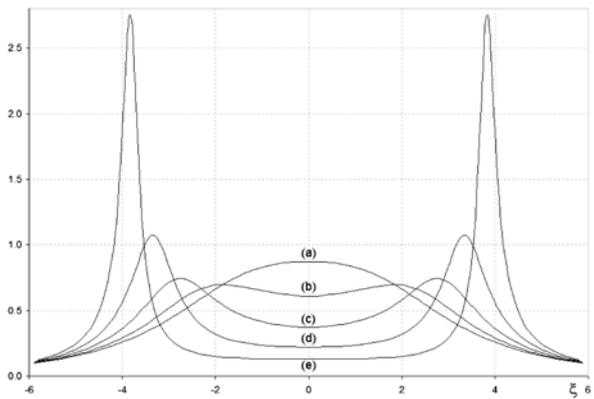
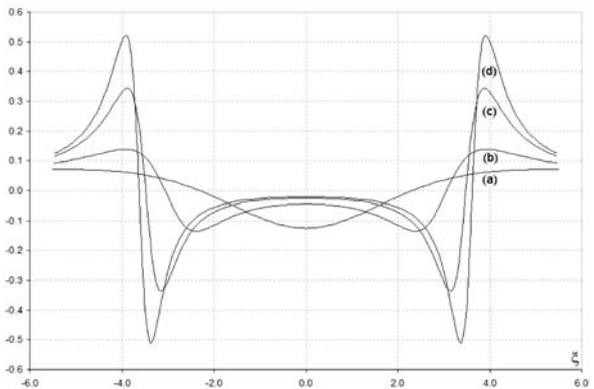


Fig. 7 (a)–(d): Plot of the function G_1 at different sections of the beam of Fig. 5 for increasing ζ



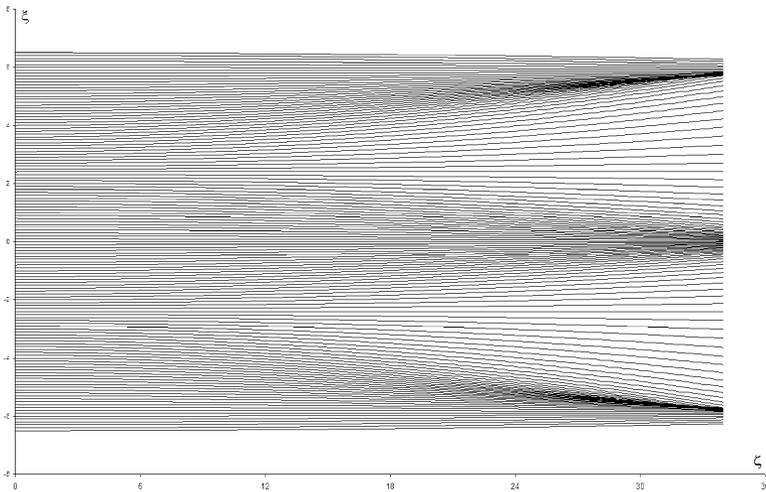


Fig. 8 Trajectory pattern on the (ξ, ζ) -plane, in the algebraic case $N = 2$

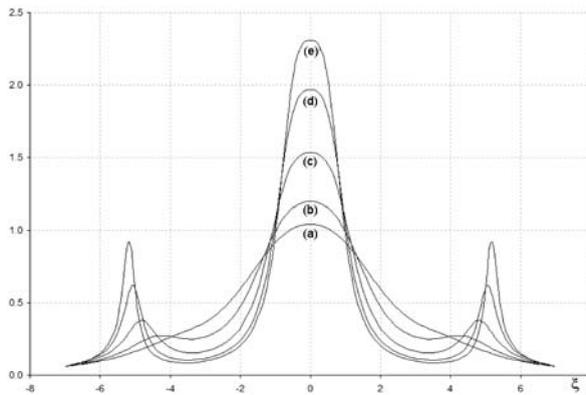


Fig. 9 (a)–(e): Transverse intensity distributions corresponding to Fig. 8, computed at different sections of the beam for increasing ζ

Both Figs. 7 and 10 show the progressive steepening of the functions $G_{1,2}$ in correspondence with the formation of the side-fringes.

An important general observation is the strong dependence of each trajectory on the wave (or quantum) potential of the whole beam, which is strongly dependent, in its turn, on the beam amplitude profile, and therefore on the experimental set-up.

8 Discussion and Conclusions

Let us repeat here that the first purpose of the present work was to present a unified Hamiltonian treatment of wave-like features holding both in classical and quantum stationary media.

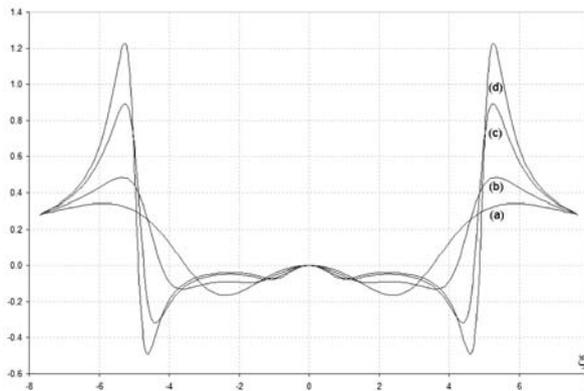


Fig. 10 (a)–(d): Plot of the function G_2 at different sections of the beam of Fig. 8 for increasing ζ

Referring, in particular, to the quantum case, we stress that, to our knowledge, most previous “deterministic” approaches (such as that of *de Broglie* and *Bohm* [1–5], together with their direct developments [12–15]) make use of the *time-dependent* Schrödinger equation. This generally leads to equations whose solution is a very hard task. The obstacle of a highly non-linear Hamilton-Jacobi set of equations (needing an often unattainable *generating function*) is usually avoided by an entangled solution method requiring the previous knowledge of the wave function, and hindering therefore the very concept of individual trajectories.

A line of thought which appears to minimize difficulties is developed in [16–18] by means of hydrodynamic considerations, where however individual trajectories are still a somewhat indirect concept.

A quite different point of view is adopted in [19, 20], where a time independent eikonal approximation is employed for the nuclear trajectories and coupled to quantum electron transitions in the treatment of molecular collisions. Here the role of individual trajectories is clearly recognized, but affected by the limit of representing a *classical* approximation, and not a general physical property.

Other mixed quantum-classical systems are considered, for instance, in [21, 22].

Finally, a *quasi-optical* approximation (involving a complex eikonal equation) is employed in classical and quantum contexts, respectively, in [23, 24] and [25].

Since, on the other hand, the present work aims to avoid any kind of approximation, and to arrive at an *exact* set of individual trajectories and motion laws, we based it on the general properties of *Helmholtz*-like equations, thus eluding the most complex and general *time-dependent* treatments, although still allowing to face wave-like steady state features going much beyond the reach of geometrical optics.

The next step of our research should concern a deeper analysis of the properties of the wave (or quantum) potential and an improvement of the trajectory computation method, including also interference cases.

We would like to conclude the present paper by mentioning one of its conceivable consequences. Let us remind that when, in a *quantum* diffraction experiment, the launching conditions are modified, the motion of each particle previously passed through the slit is usually assumed to be “non-locally” affected in an instantaneous

way (wherever it may be), because of the ubiquitous properties of *quantum potential* [26]. In the *classical* electromagnetic case, however, the interpretation of this fact would simply say that the information is carried along by the electromagnetic rays, with their characteristic velocity: every wave-front may be seen, in fact, as a new launching surface, where the transverse distribution of the *wave potential* provides the necessary and sufficient boundary conditions determining—in a quite “local” way—the subsequent ray trajectories. Recalling therefore that, as we have shown, the “wefts” of trajectories are the same in classical and quantum waves, we are induced to believe that the same interpretation should hold in the two cases, so that a non-local behavior should be either a property both of classical and quantum theories, or an avoidable concept.

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