Derivation of the Schrödinger equation from the Hamilton-Jacobi equation in Feynman's path integral formulation of quantum mechanics

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Abstract

It is shown how the time-dependent Schrödinger equation may be simply derived from the dynamical postulate of Feynman's path integral formulation of quantum mechanics and the Hamilton-Jacobi equation of classical mechanics. Schrödinger's own published derivations of quantum wave equations, the first of which was also based on the Hamilton-Jacobi equation, are also reviewed. The derivation of the time-dependent equation is based on an a priori assumption equivalent to Feynman's dynamical postulate. De Broglie's concepts of 'matter waves' and their phase and group velocities are also critically discussed.

PACS 03.30.+p

1 Introduction

In the years 1925-1926 modern quantum mechanics was discovered by two separate routes: the matrix mechanics of Heisenberg, Born and Jordan [1, 2, 3] and the wave mechanics of de Broglie and Schrödinger [4, 5, 6, 7]. The two formalisms were soon shown to be mathematically equivalent by Schrödinger [6], Dirac [8] and Eckart [9]. Because of the facility of its application to physical problems (both idealised and in relation to experiments) via solutions of the Schrödinger equation, text book teaching of quantum mechanics is largely based on the Schrödinger formulation in association with consideration of an abstract Hilbert space of quantum mechanical state vectors.

There exists however a third, independent, formulation of quantum mechanics the conceptual foundations of which were laid down in Dirac's 1933 paper 'The Lagrangian in Quantum Mechanics' [10] which was the basis for Feynman's later path-integral formulation [11]. This approach has two great advantages as compared to the earlier matrix mechanics and wave mechanics ones: (i) An axiomatic formulation comparable to that provided by Newton's Laws for classical mechanics (ii) Immediate introduction of the key physical concept —quantum-mechanical superposition—that differentiates quantum from classical mechanics. This is of particular importance for the teaching of the subject since, in the conventional approach, it is often difficult to distinguish physical principle from manipulation of the abstract mathematical formalism. For example, there is no conceptual difference between seeking solutions of the quantum Schrödinger equation, to seeking those of any partial differential equation of classical physics. The relation between projection operations in an abstract Hilbert space and measurements in an actual quantum experiment is far from clear.

It is interesting to note that Dirac's work was preceded by similar considerations in a paper written by de Broglie in 1923 [12] (cited by neither Dirac nor Feynman) in which the outline of a relativistic electrodynamic theory incorporating photons (termed light quanta) obeying the laws of relativistic kinematics was proposed ¹.

Unfortunately, knowledge of the path integral formulation has yet to penetrate in any significant way into text books on, and the teaching of, quantum mechanics. In one widely used book [13] the name 'Feynman' does not even appear in the index! In another, more recent, one [14] the postulates (I and II of Section 3 below) of Feynman's formulation are stated but no applications are described. Notable exceptions are the introductory text book of Lévy-Leblond and Balibar [15] which is entirely based on Feynman's approach, and contains many applications to experiment, as well as the work of Taylor [16, 17] that has particularly stressed the unified view of classical and quantum mechanics provided by the approach and its mathematical simplicity. In fact, as already pointed out by Dirac [10], the formalism provides a derivation of the Principle of Least Action (and hence all of classical mechanics, via the Lagrange Equations) as the $h \to 0$ limit of quantum mechanics. Good introductions to Feynman's axiomatic formulation are to be found in Sections 2-4 of

¹This paper, predating both matrix mechanics and wave mechanics, actually contains all the essential conceptual elements of Feynman's formulation of Ref. [11] —interfering amplitudes (called 'waves') that give the probability of observing a photon (or any other particle) around a given space-time point. Even the Lorentz-invariant phase of the path amplitude of a free particle (see Eq. (6.2) below) was correctly given, in an added note, together its connection to Hamilton's Principle, as later stated by Dirac.

Ref. [11], in Chapter 3 of Volume III of the 'Feynman Lectures in Physics' [18] as well as in the first chapter of the Feynman and Hibbs book [19].² A clear presentation of Hamilton-Jacobi theory can be found in Goldstein's 'Classical Mechanics' [21]. The interested reader who is unfamiliar with the path-integral formulation of quantum mechanics or Hamilton-Jacobi theory is advised to consult the above sources before reading the present paper.

Actually, the most detailed working-out of the concepts of the space-time approach to quantum mechanics are to be found, not in the research or pedagogical literature, but in the popular book 'QED the Strange Story of Light and Matter' [22], that Feynman completed shortly before his death. In this book many physical effects —rectilinear propagation, reflection, refraction and diffraction of light, which are considered in standard text books to be examples of applications of the 'classical wave theory of light' ³ are shown to be, in fact, pure applications of the space-time formulation of quantum mechanics. The detailed mathematical description of many of the examples presented, in a qualitative way, in Feynman's book can be found in a recent paper by the present author [25].

The motivation of the present paper is to improve the general knowledge of the path integral formulation of quantum mechanics, and illustrate its importance, by exploring the connections of this approach with the more conventional one based on the Schrödinger wavefunction. In particular, relations are pointed out, in the context of the path integral formalism, between the Hamiltonian description of a system in classical mechanics, and the quantum mechanical description of the same system by Schrödinger's equation.

The most evident application of Feynman's formulation is to experiments where path amplitudes of free particles enter essentially into the description of the experiment considered: for example, refraction, diffraction and interference experiments in physical optics as discussed in Feynman's popular book, or 'particle oscillations', involving, either neutral bound states containing heavy quarks, or neutrinos. Examples of such applications are given in Ref. [25] where it is also shown that the classical wave theory of light, based on solutions of the Helmholtz equation, is actually a necessary consequence of the path integral formulation of quantum mechanics, as it applies to photons interacting with matter.

The utility of the path integral formulation to the problem, the resolution of which gave birth to modern quantum mechanics —atomic structure— is less evident. Feynman derived, in Ref. [11], the time-dependent Schrödinger equation from the path integral postulates. However as will be demonstrated in the present paper, the latter were actually implicit in Schrödinger's own original derivation of this equation.

The action function, S, that appears in the fundamental dynamical postulate of the path integral formulation (Eq. (3.1) below) is actually Hamilton's principle function, which is the solution of the Hamilton-Jacobi partial differential equation for the system under consideration. The related Hamilton's characteristic function and the corresponding Hamilton-Jacobi equation are, as will be seen below, by a devious route, the basis for

²Feynman's original path-integral paper [11] is included in a recently published book [20] which also contains Feynman's PhD thesis on the same subject, as well as an introductory preface by L. M. Brown that sets the work in its historical context, as seen from a near-contemporary viewpoint.

³See, for example, Born and Wolf [23] and, particularly, Jenkins and White [24] in which the 'phase arrows' of Feynman's popular book [22] are analysed in full mathematical detail.

Schrödinger's first published derivation of the time-independent Schrödinger equation, from which the correct energy levels for the hydrogen atom are obtained

The main aims of the present paper are, firstly, to show how the time-dependent Schrödinger equation follows directly from the Hamilton-Jacobi equation and the dynamical postulate of the path integral formulation and, secondly, to review Schrödinger's own derivations of both the time-independent and time-dependent quantum wave equations. In order to do this in a comprehensible manner some related topics are briefly described in the preceding sections 5, 6 and 7.

The structure of the paper is as follows: In the following section, Hamilton's principle function and the Hamilton-Jacobi equation for a classical mechanical system are defined. In Section 3 the postulates of Feynman's path amplitude formulation of quantum mechanics are stated. Section 4 contains the derivation of the time-dependent Schrödinger equation. The Lorentz-invariant phase of the path amplitude for a free particle is derived from the transformation equations for Hamilton's principle function in Section 5. In Section 6 the de Broglie and Planck-Einstein relations are are obtained by mathematical substitution in the formula for the phase of the path amplitude of a free particle. Also discussed in this section are de Broglie's original derivation of the wavelength formula, Hamilton's 1834 analogy between classical mechanics and geometrical optics, particle velocity, group velocity, phase velocity and 'wave-particle duality'. In Section 7, dynamical operators associated with the path amplitude of a free particle are introduced together with their eigenvalues. The same operators are shown to respect canonical commutation relations and to enable derivation, from the appropriate Hamiltonian function, of the time-independent Schrödinger equation for the hydrogen atom. Dirac's original derivation of the commutation relations, by consideration of their relation to the Poisson brackets of classical mechanics, is also discussed. Section 8 describes Schrödinger's various derivations of the quantum wave equation published in 1926. The concluding Section 9 contains a summary of the previous sections and a brief discussion of connections to related work.

The material presented in the present paper is of particular interest to university teachers of advanced quantum mechanics courses, at both undergraduate and graduate level, and their students. Teachers of quantum mechanics, at all levels, may also benefit from a reading of the paper. Certain topics presented in Sections 6 and 7 as well as the whole of Section 8 may be of interest to teachers of, and researchers on, the history of science.

2 The Hamilton-Jacobi equation and Hamilton's principle function

A contact, or canonical, transformation applied to the spatial coordinates, q_i , and canonical momenta, p_i , (i = 1, 2, ..., n) of an n-dimensional classical mechanical system, is one which leaves invariant the form of the Hamilton equations:

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}.$$
 (2.1)

The canonically transformed coordinates, Q_i , and momenta, P_i , then satisfy the Hamilton equations:

$$\frac{dQ_i}{dt} = \frac{\partial K}{\partial P_i}, \qquad \frac{dP_i}{dt} = -\frac{\partial K}{\partial Q_i}$$
 (2.2)

where the transformed Hamiltonian, K, is related to the original one, H, by [21]:

$$K(Q_i, P_i, t) = H(q_i, p_i, t) + \frac{\partial F}{\partial t}$$
(2.3)

and, F, the generating function of the canonical transformation, may have any of the following functional dependences: $F(q_i, Q_i, t)$, $F(q_i, P_i, t)$, $F(p_i, Q_i, t)$ and $F(p_i, P_i, t)$. Hamilton's principle function: $S \equiv F(q_i, P_i, t)$, is the generating function for which the transformed Hamiltonian K vanishes, so that:

$$H(q_i, p_i, t) + \frac{\partial S}{\partial t} = 0. {(2.4)}$$

The transformation equations relating coordinates and momenta are, in this case [21]:

$$p_i = \frac{\partial S}{\partial q_i}, \qquad Q_i = \frac{\partial S}{\partial P_i}.$$
 (2.5)

Substituting the first of these equations in (2.4) gives the Hamilton-Jacobi (H-J) equation:

$$H(q_i, \frac{\partial S}{\partial q_i}, t) + \frac{\partial S}{\partial t} = 0.$$
 (2.6)

For a single non-relativistic particle of Newtonian mass, m, moving in a time-independent potential, V, the H-J equation is:

$$\frac{1}{2m} \left[\left(\frac{\partial S}{\partial x} \right)^2 + \left(\frac{\partial S}{\partial y} \right)^2 + \left(\frac{\partial S}{\partial z} \right)^2 \right] + V + \frac{\partial S}{\partial t} = 0. \tag{2.7}$$

This equation is the basis of the derivation of the time-dependent Schrödinger equation in Section 4 below. The H-J partial differential equation (2.6) may be solved for the function S. This solution gives immediately the equations of motion of the system described by H when Q_i and P_i are identified with initial values of the coordinates and momenta. The n equations:

$$Q_i = \frac{\partial S(q_i, P_i, t)}{\partial P_i} \tag{2.8}$$

are solved for the q_i to yield the solution of the dynamical problem:

$$q_i = q(Q_i, P_i, t). (2.9)$$

The solution for the p_i is then given by the first of Eqs. (2.5) as:

$$p_i = \left. \frac{\partial S(q_i, P_i, t)}{\partial q_i} \right|_{q_i = q(Q_i, P_i, t)}.$$
(2.10)

Since the P_i are constants, fixed by initial conditions, S is a function only of the q_i and t so that

$$dS = \sum_{i=1}^{n} \frac{\partial S}{\partial q_i} dq_i + \frac{\partial S}{\partial t} dt.$$
 (2.11)

Making use of (2.4) and the first of Eqs. (2.5):

$$\frac{dS}{dt} = \sum_{i=1}^{n} p_i \frac{dq_i}{dt} - H = L \tag{2.12}$$

where $L(q_i, dq_i/dt, t)$ is the Lagrangian function for the dynamical system. Integrating (2.12) identifies S as the indefinite time integral of the Lagrangian:

$$S = \int Ldt + \text{constant.}$$
 (2.13)

As will be discussed in the following section, in virtue of this equation, Hamilton's principle function S constitutes the mathematical basis of the Feynman path integral formulation of quantum mechanics.

3 Feynman's path integral formulation of quantum mechanics

Feynman's path integral formulation of quantum mechanics is based on the following two postulates [11]:

- I If an ideal measurement is performed to determine whether a particle has a path lying in a region of spacetime, the probability that the result will be affirmative is the absolute square of a sum of complex contributions, one from each path in the region.
- II The paths contribute equally in magnitude but the phase of their contribution is the classical action (in units of \hbar) i.e. the time integral of the Lagrangian taken along the path.

The postulate I is a statement of the superposition property of the amplitudes for different paths combined with Born's probabilistic interpretation [26] of them. Postulate II states that the amplitude for a given path is some real function, A, times $\exp\{(i/\hbar)S_{BA}([\vec{x}(t)])\}$ where

$$S_{BA}([\vec{x}(t)]) \equiv \int_{t_A}^{t_B} L([\vec{x}(t)], t) dt.$$
 (3.1)

Here L is the classical Lagrangian of the system considered and $[\vec{x}(t)]$ corresponds to a particular space time path between specific (fixed) times t_A and t_B . It can be seen from Eq. (2.13) that S is actually Hamilton's principle function for the system considered. The constant in (2.13) cancels in the definite integral on the right side of (3.1). As discussed by Feynman [11, 27] S_{BA} is a functional of the path $[\vec{x}(t)]$, since the value of S_{BA} given by (3.1) is different for different paths. A particular path $[\vec{x}(t)^{(j)}]$ can be specified, to any desired precision, by an array of space-time coordinates. Considering one spatial dimension:

$$[x(t)^{(j)}]: \quad x_A^{(j)}, t_A^{(j)}; \quad x_1^{(j)}, t_1^{(j)}; \quad x_2^{(j)}, t_2^{(j)}; \dots \quad x_n^{(j)}, t_n^{(j)}; \dots \quad x_B^{(j)}, t_B^{(j)}$$

$$t_A^{(j)} < t_1^{(j)} < t_2^{(j)} \dots < t_n^{(j)} \dots < t_B^{(j)}$$

Notice that the velocity argument, $\dot{x}(t) \equiv dx(t)/dt$, of the Lagrangian is implicit in the specification of the path $[x(t)^{(j)}]$:

$$\dot{x}^{(j)}(t) = \operatorname{Lim}(t_{n+1} \to t_{n-1}) \frac{x_{n+1}^{(j)} - x_{n-1}^{(j)}}{t_{n+1}^{(j)} - t_{n-1}^{(j)}}.$$
(3.2)

Postulate II defines the space-time propagator, Green function, or kernel which gives the amplitude that a particle system with initial space-time coordinate \vec{x}_A , t_A is found at later time t_B at \vec{x}_B , having followed a particular path $[\vec{x}^{(j)}(t)]$:

$$K_{BA}^{(j)} \equiv K^{(j)}(\vec{x}_B, t_B; \vec{x}_A, t_A) = A^{(j)}(\vec{x}_B, t_B; \vec{x}_A, t_A) \exp\left\{\frac{i}{\hbar} S_{BA}([\vec{x}^{(j)}])\right\}$$

$$\equiv A_{BA}^{(j)} \exp\left\{\frac{i}{\hbar} S_{BA}^{(j)}\right\}$$
(3.3)

where

$$S_{BA}([\vec{x}^{(j)}]) \equiv \int_{t_A}^{t_B} L([\vec{x}^{(j)}(t)], t) dt.$$
 (3.4)

The exponential dependence of the propagator on S_{BA} and the definition of the latter in (3.1) as the definite time integral of the Lagrangian implies that the propagator has a factorisation property:

$$K_{BC}K_{CA} = A_{BC}A_{CA}\exp\left\{\frac{i}{\hbar}(S_{BC} + S_{CA})\right\} = A_{BA}\exp\left\{\frac{i}{\hbar}S_{BA}\right\} = K_{BA}$$
(3.5)

where $A_{BA} \equiv A_{BC}A_{CA}$. This equation is a manifestation of the property of sequential factorisation of path amplitudes [11, 15, 25].

The total amplitude for finding a system, originally at \vec{x}_A, t_A , at \vec{x}_B at t_B is then, according to the postulate I, given by the sum over all allowed paths:

$$K_{BA} \equiv K(\vec{x}_B, t_B; \vec{x}_A, t_A) = \sum_j K_{BA}^{(j)} = \sum_j A_{BA}^{(j)} \exp\left\{\frac{i}{\hbar} S_{BA}^{(j)}\right\}.$$
 (3.6)

In the following section the propagator, K, of a particle moving in a time-independent potential, V, is related to the conventional quantum-mechanical wavefunction of such a particle. It is seen that the fact that the action functional S in (3.3) is just the Hamilton's principle function, which is a solution of the H-J equation (2.7), requires the wavefunction to satisfy the time-dependent Schrödinger equation.

4 Derivation from the H-J equation of the time-dependent Schrödinger equation

To make the connection between a quantum wavefunction, ψ , and a single path amplitude, the path labels j, A and B are dropped, the space-time point \vec{x}_B , t_B is denoted

simply as \vec{x} , t, and the functional dependence of K and A on these space-time coordinates is considered. The wavefunction is then defined as:

$$\psi(\vec{x},t) \equiv \frac{K}{A} = \exp\left[\frac{i}{\hbar}S(\vec{x},t)\right]. \tag{4.1}$$

It will be seen, in the following, that when the function ψ is defined in this manner it has all the properties of the well-known wavefunction of wave mechanics. In particular, it is a solution of the Schrödinger equation. As discussed in Section 8 below, Schrödinger used a very similar equation relating ψ and S when the former was introduced, for the first time, in Ref. [4]. Only the all-important factor $i = \sqrt{-1}$ was missing!

Inverting (4.1) gives

$$S = -i\hbar \ln \psi \tag{4.2}$$

and, with $\vec{x} \equiv (x, y, z)$:

$$\frac{\partial S}{\partial x} = -\frac{i\hbar}{\psi} \frac{\partial \psi}{\partial x}, \quad \frac{\partial S}{\partial y} = -\frac{i\hbar}{\psi} \frac{\partial \psi}{\partial y}, \quad \frac{\partial S}{\partial z} = -\frac{i\hbar}{\psi} \frac{\partial \psi}{\partial z}, \quad \frac{\partial S}{\partial t} = -\frac{i\hbar}{\psi} \frac{\partial \psi}{\partial t}. \tag{4.3}$$

Transposing the first of Eqs (4.3), differentiating w.r.t. x a second time:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{i}{\hbar} \frac{\partial \psi}{\partial x} \frac{\partial S}{\partial x} + \frac{i}{\hbar} \psi \frac{\partial^2 S}{\partial x^2}.$$
 (4.4)

Differentiating, w.r.t. x, the first of the transformation equations (2.5) gives:

$$\frac{\partial^2 S}{\partial x^2} = \frac{\partial p_x}{\partial x} = m \frac{d}{dt} \left(\frac{\partial x}{\partial x} \right) = 0 \tag{4.5}$$

so that substituting for $\partial \psi / \partial x$ in (4.4) from (4.3), using (4.5), and transposing:

$$\left(\frac{\partial S}{\partial x}\right)^2 = -\frac{\hbar^2}{\psi} \frac{\partial^2 \psi}{\partial x^2}.\tag{4.6}$$

Substituting (4.6) and the corresponding equations for the y and z coordinates as well as the time derivative equation in (4.3) in the H-J equation, (3.7), for a non-relativistic particle moving in a time-independent potential:

$$\frac{1}{2m} \left[\left(\frac{\partial S}{\partial x} \right)^2 + \left(\frac{\partial S}{\partial y} \right)^2 + \left(\frac{\partial S}{\partial z} \right)^2 \right] + V + \frac{\partial S}{\partial t} = 0 \tag{4.7}$$

then yields the time-dependent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi - i\hbar\frac{\partial\psi}{\partial t} = 0$$
 (4.8)

where

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

Such a brief and elegant derivation of the Schrödinger equation directly from the H-J equation was mentioned as a possibility by Feynman in his seminal path integral paper [28] but never actually given by him.

This derivation shows that a Schrödinger wavefunction, which is a solution of (4.8), is in fact a path amplitude. Consideration of (4.1) shows that ψ is dimensionless, but in view of the linear nature of (4.8) it remains valid when ψ is multiplied by the dimensional constant that is required for its physical interpretation when applied to any specific physical problem.

Specialising to the spatial wavefunctions of an electron in a hydrogen atom, corresponding to a time-independent potential function, and which are interpreted according to the Born rule, the normalisation constants have dimension $L^{-\frac{3}{2}}$. In his original paper on transformation functions in quantum mechanics [8] Dirac made the following comment on the physical meaning of such atomic wavefunctions (Dirac's italics):

The eigenfunctions of Schrödinger's wave equation are just the transformation functions (or the elements of the transformation matrix...) that enable one to transform from the (q) [i.e. spatial coordinate] scheme of matrix transformations to a scheme in which the Hamiltonian is a diagonal matrix.⁴

This was probably the key physical insight, concerning the physical interpretation of Dirac's mathematical formalism, that this paper contained. The derivation of the Schrödinger equation just presented shows that Dirac's assertion, stated in the language of Feynman's formulation of quantum mechanics, is:

The Schrödinger wavefunction of an atom is the probability amplitude that an electron is found at a certain position in the atom when the latter is in a stationary energy state.

The probability to find the electron at a certain position does not depend upon time as long as the atom remains in the same stationary state. As will be discussed in the following section, the situation is entirely different when path amplitudes are used to describe particles moving freely in space-time. It is shown there how the appropriate path amplitudes for such particles may be derived directly from the transformation equations (2.5) and (2.6) of Hamilton's principle function.

5 Derivation of the path amplitude for a free particle from Hamilton's principle function

The Hamilton's principle function for a free particle (denoted as S) with energy E and momentum p is obtained immediately by integration of the transformation equations for S in (2.4) and (2.5):

$$\frac{\partial \mathcal{S}}{\partial x} = p, \quad \frac{\partial \mathcal{S}}{\partial t} = -H = -E$$
 (5.1)

These equations have the evident solution:

$$S = px - Et \tag{5.2}$$

⁴Wavefunctions, ψ_i , for which the Hamiltonian is a diagonal matrix are eigenfunctions of the energy: $H\psi_i = E_i\psi_i$. Then $\int \psi_i^* H\psi_j d^3x \equiv H_{ij} = \delta_{ij}E_i$ as a consequence of the orthonormality of the eigenfunctions: $\int \psi_i^* \psi_j d^3x = \delta_{ij}$.

where p and E are constants, independent of spatial position and time. This equation can be used as the basis, not only for the quantum mechanical description of a freely moving particle, but also to develop its relativistic kinematics and space-time geometry. If the particle, of Newtonian mass m, is at rest then $E = mc^2$ and the path amplitude is, from (4.1) and (5.2):

$$\psi(\tau) = \exp\left\{-\frac{imc^2}{\hbar}\tau\right\} \tag{5.3}$$

where τ is the proper (rest frame) time. Since it was demonstrated, in the previous section, that in Feynman's formulation the conventional wavefunction is a path amplitude, the wavefunction symbol ψ is consistently employed for the path amplitude on the right side of (5.3). This formula, with the replacement $mc^2 \to mc^2 - i\hbar/(2T)$, where T is the mean lifetime of an unstable particle⁵, has been employed in the phenomenology of temporal flavour oscillations of neutral kaons since the middle 1950's [29].

The Lorentz invariant quantity S can be written in several equivalent ways. With a suitable choice of the origins of spatial and temporal coordinates (such that x = 0 when t = 0) the equation of motion of the particle may be written as x = vt. The latter may then be used to eliminate x from (5.2):

$$S = px - Et = (pv - E)t = -E\left(1 - \frac{p}{E}v\right)t. \tag{5.4}$$

In the non-relativistic limit where

$$E \simeq mc^2 + \frac{p^2}{2m}, \quad p \simeq mv$$
 (5.5)

(5.4) may be written as

$$S = -\left(mc^2 + \frac{p^2}{2m}\right) \left[1 - \frac{pv}{mc^2 + \frac{p^2}{2m}}\right] t + O(\beta^4)$$
 (5.6)

$$= -\left(mc^2 + \frac{p^2}{2m}\right) \left[1 - \frac{mv^2}{mc^2}\right] t + \mathcal{O}(\beta^4)$$
 (5.7)

$$= -\left(mc^2 + \frac{p^2}{2m}\right)(1 - \beta^2)t + \mathcal{O}(\beta^4)$$
 (5.8)

where $\beta \equiv v/c$. With the replacements $mc^2 + p^2/2m \rightarrow E$ in (5.8) and $p/E \rightarrow v/c^2$ in (5.4) the approximate equation (5.8) becomes identical to the exact one (5.4). Then

$$S = -E(1 - \beta^2)t = -\frac{E}{\gamma}\frac{t}{\gamma} = -mc^2\tau$$
 (5.9)

where

$$E \equiv \gamma mc^2, \qquad p \equiv \gamma mv, \qquad \tau \equiv \frac{t}{\gamma}$$
 (5.10)

and $\gamma \equiv 1/\sqrt{1-\beta^2}$. These, together with the equation of motion x=vt, are the fundamental equations of relativistic kinematics and space-time geometry. It also follows from (5.9) that

$$S = -mc^{2}(\sqrt{1-\beta^{2}})t = \int -mc^{2}(\sqrt{1-\beta^{2}})dt$$
 (5.11)

 $^{^5}$ See Section 7 below for the connection of the T-dependent term with the energy-time uncertainty relation.

which, making use of (2.13) identifies the non-covariant relativistic Lagrangian, \mathcal{L} , of a free particle as:

$$\mathcal{L} \equiv -mc^2 \sqrt{1 - \beta^2}.\tag{5.12}$$

For consistency with quantum mechanics there can be no arbitary additive constant on the right side of (5.12). Planck used the Lagrangian of (5.12) (including also an arbitary additive constant on the right side) in his original derivation [30] of the formulae in (5.10) for relativistic energy and momentum. This Lagrangian may also be written in a manifestly covariant manner as [31]

$$\mathcal{L} = -\frac{m}{2}(V^2 + c^2) \tag{5.13}$$

where V is the four-vector velocity: $V \equiv (\gamma c, \gamma \vec{v})$. Integrating the corresponding Lagrange equation for the temporal coordinate gives the time dilation relation, the last of Eqs. (5.10) [31].

The Lorentz-invariant form (5.2) for the phase of the path amplitude for a free particle as well as its interpretation according to Feynman's postulates were both implicit in work by de Broglie published in (1924) [12]. This paper also contains contains an interpretation of interference effects in electrodynamics in terms of probability amplitudes for detection of photons, as in quantum electrodynamics.

6 The de Broglie and Planck-Einstein relations. 'Wave particle duality' and 'wave packets' for free particles

The various related topics discussed in this section are either of intrinsic interest or introduce background material essential for the critical review of Schrödinger's derivations of quantum wave equations in Section 8 below. The topics are:

- (i) Derivation of the de Broglie wavelength and Planck-Einstein relations by mathematical substitution in the path amplitude formula for a free particle.
- (ii) A review of de Broglie's own derivation of the wavelength formula and his (independent) introduction of the concepts of the phase and group velocities of 'matter waves'.
- (iii) A review of Hamilton's analogy between the classical mechanics of particle motion and geometrical optics.
- (iv) A discussion of 'matter waves' in the presence of electromagnetic fields leading to a short path amplitude derivation of the magnetic Aharonov-Bohm effect.

Point (iii) is essential for the understanding of Schrödinger's second derivation of the quantum wave equation. (ii) is of historical interest in its own right, while (i) and (iv) give a modern perspective on 'wave-particle duality' within the path integral formulation.

All this means inevitably a certain amount of repetition. For example, different derivations of the 'phase velocity', v_{ϕ} , are found in (i), (ii) and (iii), and of the 'group velocity' u, in (i) and (ii). In fact, the same problem is addressed from two different historical perspectives (those of de Broglie and Hamilton) and one modern one —the path integral formulation. An attempt is made in the discussion to distingush between the useful phenomenological concept of the de Broglie wavelength and the empty mathematical abstractions which are the phase and group velocities of hypothetical 'matter waves'.

The path amplitude for a free particle in one dimensional motion may be written, using (5.2), as

$$\psi(x,t) \equiv \exp\left\{-\frac{i}{\hbar}\phi(x,t)\right\} \tag{6.1}$$

where

$$\phi(x,t) \equiv \frac{2\pi}{h}(Et - px) = 2\pi(\nu t - \frac{x}{\lambda}) = \frac{2\pi}{\lambda}(v_{\phi}t - x), \tag{6.2}$$

$$\nu \equiv \frac{E}{h},\tag{6.3}$$

$$\lambda \equiv \frac{h}{p},\tag{6.4}$$

$$v_{\phi} \equiv \nu \lambda = \frac{E}{p} = \frac{c^2}{v} \ge c. \tag{6.5}$$

Here (6.3) is a transposition of the Planck-Einstein relation $E = h\nu$ and (6.4) defines the de Broglie wavelength, λ , of the particle. The energy, E, and the momentum, p, are the relativistic quantities defined in (5.10). The last member of (6.2) suggests the association of a 'wave' with phase velocity v_{ϕ} with the path amplitude. According to the last member of (6.5) since the particle velocity $v \leq c$ then $v_{\phi} \geq c$. For photons or other massless particles with v = c, then $v_{\phi} = c$ so that the phase and particle velocities are the same. For massive particles the 'phase velocity' defined by the purely mathematical substitutions in (6.3)-(6.5) is superluminal and devoid of any operational physical meaning.⁶ However, following the original suggestion of de Broglie, the particle velocity, v, is commonly associated with the 'group velocity' of a hypothetical 'wave packet' that follows from the wavelength dependence of the frequency (actually, from Eqs. (6.3) and (6.4), the relativistic momentum dependence of relativistic energy) of the associated 'phase wave'. The definitions of E, p and γ in (5.10) and (6.3)-(6.5) give:

$$m^2 c^4 \equiv m^2 c^4 (\gamma^2 - \gamma^2 \beta^2) = E^2 - p^2 c^2 \equiv h^2 \nu_0^2 = h^2 \nu^2 - \frac{h^2 c^2}{\lambda^2}$$
 (6.6)

so that

$$k \equiv \frac{1}{\lambda} = \frac{\sqrt{\nu^2 - \nu_0^2}}{c}.\tag{6.7}$$

Differentiating (6.7) gives the 'group velocity' $u \equiv d\nu/dk$:

$$\frac{1}{u} = \frac{dk}{d\nu} = \frac{1}{c} \frac{\nu}{\sqrt{\nu^2 - \nu_0^2}} = \frac{\nu\lambda}{c^2} = \frac{v_\phi}{c^2}$$
 (6.8)

⁶This superluminal phase velocity of hypothetical 'matter waves' should not be conflated with the real physical effects that have apparently been observed in several recent experiments; for example in quantum tunneling [32, 33] on in the near-zone of electromagnetic waves [34, 35, 36].

or

$$u = \frac{c^2}{v_\phi} = v \tag{6.9}$$

where (6.5) has been used. Thus the hypothetical group velocity associated with the hypothetical phase wave suggested by the last member of (6.2) is indeed equal to the physical velocity of the particle, but this does not mean, as asserted by de Broglie, and subsequently in most text books on quantum mechanics, that a moving particle is a wave packet and so has a dual ontological nature. In this context, there is an important difference, discussed in some detail in Ref. [37], between massive particles and massless photons, for which 'phase', 'group' and particle velocities are all equal and for which 'electromagnetic waves' are manifestations of beams of real photons. There is no equivalent, for massive particles, of the macroscopic potentials and fields \vec{A} , \vec{E} and \vec{B} which constitute the fundamental physical concepts of classical electromagnetism.

It is interesting to compare de Broglie's derivation of the formula (6.4) in his 1927 Nobel Prize acceptance speech [38] with that presented above. This calculation used directly the definitions of relativistic energy and momentum given in (5.10). It is first assumed that the phase of a particle at rest is $\phi_0 = 2\pi\nu_0\tau$ where $\nu_0 \equiv mc^2$ and τ is the proper time of the particle. The Lorentz transformation is then used to transform the proper time into a frame in which the particle is in motion with velocity $v = \beta c$ to give:

$$\phi_0 = 2\pi \nu_0 \tau = 2\pi \nu_0 \gamma (t - \frac{\beta x}{c}). \tag{6.10}$$

The frequency transformation is given by the Planck-Einstein relation, $E = h\nu$, and the relativistic energy definition in (5.10), as:

$$\nu = \gamma \nu_0. \tag{6.11}$$

Inspection of (6.10) shows that the phase velocity of the associated wave is (compare with the last member of (6.2)):

$$v_{\phi} = \frac{c}{\beta} \tag{6.12}$$

The formula defining the 'de Broglie wavelength', λ , given by $\lambda = v_{\phi}/\nu$, follows directly from (6.12), the definitions of relativistic momentum and energy and the Planck-Einstein relation:

$$p \equiv \gamma m v = \frac{Ev}{c^2} = \frac{h\nu\beta}{c} = \frac{h\nu}{v_\phi} = \frac{h}{\lambda}.$$
 (6.13)

There is, therefore, no appeal to the concept of 'group velocity' in this calculation that introduces the measurable (and experimentally confirmed) de Broglie wavelength of a free particle. Nevertheless, de Broglie used (6.11), (6.12) and the 'refractive index': defined as $n \equiv v/v_{\phi}$ to derive the relation:

$$\beta = n = \sqrt{1 - (\nu_0/\nu)^2} \tag{6.14}$$

which together with a formula for the group velocity due to Lord Rayleigh:

$$\frac{1}{u} = \frac{1}{c} \frac{d(n\nu)}{d\nu} \tag{6.15}$$

is used to show that u = v, so that, from (6.12), the phase and group velocities are related according to:

$$uv_{\phi} = c^2. \tag{6.16}$$

This calculation of de Broglie is of particular interest because the formula (6.10) for the x, t dependence of the path amplitude phase, which is (up to a sign) identical to that of Eq. (6.2), is here derived not from the transformation equations of S, but from a relativistic time transformation that demonstrates the Lorentz invariance of the phase:

$$\phi_0 \equiv \frac{2\pi mc^2}{h} \tau = \frac{2\pi (Et - px)}{h} \equiv \phi = \frac{2\pi (E't' - p'x')}{h} \equiv \phi'.$$
 (6.17)

This suggests, as indicated by the discussion of Eqs. (5.6)-(5.9), that relativistic kinematics and space-time geometry are already somehow implicit in the formula S = px - Et for Hamilton's principle function for a free particle. In particular, the fundamentally important relative minus sign between spatial and temporal components in the Minkowski metric is predicted. De Broglie had earlier pointed out [12] this Lorentz scalar character of the path amplitude phase.

In his second 1926 paper on wave mechanics [5] Schrödinger gave an extended discussion of the analogy between the classical mechanics of particles and geometrical optics, as suggested by Hamilton in 1834. In view of the connection between this discussion and Schrödinger's second derivation in the same paper of the time-independent quantum wave equation, Hamilton's ideas are briefly reviewed here. In the case of a time-independent Hamiltonian: H = E, Hamilton's principle function may be written as [21]:

$$S(\vec{x}, t) = W(\vec{x}) - Et \tag{6.18}$$

where W, which is a function only of the spatial coordinates \vec{x} , is called Hamilton's characterstic function. A consequence of (6.18) is that surfaces of constant S correspond to a time evolution of W according to dW = Edt. The spatial evolution of W, analogous to that of a wave front in physical optics, is then:

$$dW = |\vec{\nabla}W|ds \tag{6.19}$$

where ds is the displacement of a spatial surface of constant W and

$$\vec{\nabla} \equiv \hat{\imath} \frac{\partial}{\partial x} + \hat{\jmath} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}$$
 (6.20)

where $\hat{\imath},\hat{\jmath},\hat{k}$ are unit vectors parallel to the x,y,z axes. A spatial surface of constant W therefore moves with speed:

$$v_W = \frac{ds}{dt} = \frac{1}{|\vec{\nabla}W|} \frac{dW}{dt} = \frac{E}{|\vec{\nabla}W|}.$$
 (6.21)

The generalisation of the first of Eqs. (2.5) gives

$$\vec{\nabla}S = \vec{\nabla}W = \vec{p} \tag{6.22}$$

so that

$$v_W = \frac{E}{|\vec{p}|}. (6.23)$$

For relativistic motion of a free particle comparison of (6.23) with (6.5) shows that

$$v_W = v_\phi = \frac{c^2}{v}. (6.24)$$

For non-relativistic motion in a time-independent potential, as considered by Schrödinger, use of the non relativistic (NR) Hamiltonian:

$$H_{NR} = E_{NR} = \frac{p^2}{2m} + V \equiv T_{NR} + V$$
 (6.25)

gives, according to (6.23),

$$v_W(NR) = \frac{E_{NR}}{p} = \frac{E_{NR}}{\sqrt{2m(E_{NR} - V)}} = \frac{E_{NR}}{\sqrt{2mT_{NR}}}.$$
 (6.26)

For a free particle where $E_{NR} = p^2/2m$:

$$v_W(NR) = \frac{p^2}{2mp} = \frac{p}{2m} = \frac{v}{2}.$$
 (6.27)

Since the relativistic formula (6.24) is valid for all values if v, including those for which the approximation $T \simeq T_{NR} = p^2/(2m)$ is a good one, the inconsistency between the value of v_W and $v_W(NR)$ is an indication of the lack of any operational physical meaning for the hypothetical 'phase velocities' v_{ϕ} , v_W and $v_W(NR)$ within classical mechanics. The relativistic Hamiltonian H differs from H_{NR} by the inclusion of the rest-mass contribution mc^2 . As is well-known, arbitary additive constants in Hamiltonians or Lagrangians leave unchanged all physical predictions in classical mechanics. As will be discussed Section 8 below, Schrödinger used (6.26) together with a classical wave equation in his second published derivation of the time-independent quantum-mechanical wave equation.

Within quantum mechanics, the formula (6.27) can be derived directly from the formula (6.2) for $\phi(x,t)$ without any consideration of Hamilton's analogy between classical mechanics and geometrical optics:

$$\phi = -\frac{2\pi}{h}(Et - px) = -\frac{2\pi}{h}(\gamma mc^2 t - \gamma mxv)$$

$$= -\frac{2\pi}{h}\left[\left(mc^2 + \frac{mv^2}{2}\right)t - mvx\right] + O(\beta^2)$$

$$= \phi_m + \phi_{NR} + O(\beta^2)$$
(6.28)

where

$$\phi_m \equiv -\frac{2\pi mc^2}{h}t, \quad \phi_{NR} \equiv -\frac{2\pi p}{h}\left(\frac{v}{2}t - x\right) = -\frac{2\pi}{\lambda}(v_W(NR)t - x). \tag{6.29}$$

The unphysical nature of the 'phase velocities' v_{ϕ} , v_{W} and $v_{W}(NR)$ is to be contrasted with that of the measurable de Broglie wavelength of a free particle for which, unlike, v_{W} and $v_{W}(NR)$, λ and λ_{NR} have consistent values:

$$\lambda = \frac{h}{p} = \frac{h}{\gamma m v} = \frac{h}{m v} + \mathcal{O}(\beta^2) \equiv \lambda_{NR} + \mathcal{O}(\beta^2)$$
 (6.30)

while

$$\frac{v_W(NR)}{v_W} = \frac{v/2}{c^2/v} = \frac{1}{2}\beta^2. \tag{6.31}$$

So that the ratio of v_W and $v_W(NR)$, not their difference, is of $O(\beta^2)$!

The unphysical nature of the 'phase velocity' of a massive particle and the associated 'phase wave' is further illustrated by considering the generalisation of de Broglie's 'refractive index' in Eq. (6.14) to the case of the motion of a charged particle in electric and magnetic fields [39]. It is found that not only the 'phase velocity' but also the 'wavefront' directions as well as the associated 'wavelength' all depend on the gauge function ξ used the specify the vector potential according to $\vec{A}(\xi) \equiv \vec{A}_0 + \vec{\nabla} \xi$. The phase of the path amplitude of a particle of electric charge q, moving from A to B along a path j in a region of non-vanishing vector potential is

$$\phi_{AB}^{(j)} = \int_{A}^{B} [L_{\text{kin}}^{(j)} + q\vec{v} \cdot \vec{A}^{(j)}(\xi)] dt
\equiv -S_{AB,\text{kin}}^{(j)} + q \int_{A}^{B} \hat{s} \cdot \vec{A}^{(j)}(\xi) ds
= -S_{AB,\text{kin}}^{(j)} + q \int_{A}^{B} \hat{s} \cdot \vec{A}_{0}^{(j)} ds + q \int_{A}^{B} \hat{s} \cdot \vec{\nabla} \xi^{(j)} ds
= -S_{AB,\text{kin}}^{(j)} + q \int_{A}^{B} \hat{s} \cdot \vec{A}_{0}^{(j)} ds + q(\xi_{B} - \xi_{A})$$
(6.32)

where \hat{s} is a unit vector along the path of the particle, and $L_{\rm kin}^{(j)}$ is the free-particle Lagrangian of Eq. (5.12). Thus the physically measureable *phase difference* between two paths with fixed start and end points, is, unlike the phase velocity, wavefront direction or wavelength, independent of ξ and therefore gauge invariant. Considering two paths with equal values of $S_{AB,\rm kin}$, (6.32) gives:

$$\Delta \phi_{AB} = \phi_{AB}^{(l)} - \phi_{AB}^{(j)} = q \left[\int_{A}^{B} \hat{s} \cdot \vec{A}^{(l)} ds - \int_{A}^{B} \hat{s} \cdot \vec{A}^{(j)} ds \right]
= q \int_{S} \hat{n} \cdot \vec{H} dS = q f_{H}$$
(6.33)

where in the last member Stoke's theorem has been used and f_H is total flux of the magnetic field \vec{H} threading the area between the paths l and j. The phase shift $\Delta \phi_{AB}$ in (6.33) is the magnetic Aharonov-Bohm effect [40], as actually first pointed out by Ehrenberg and Siday [39]

In conclusion, the 'waves' commonly associated with the path amplitudes, defined over macroscopic distances, of massive particles moving either freely or in fields of force, are a mathematical abstraction that unlike the electromagnetic waves associated with massless photons, or the path amplitudes themselves, are devoid of any operational physical significance. Also meaningless is the ontological concept of 'wave particle duality'. What exist in the physical world are the particles. Following de Broglie, the probability amplitudes of quantum mechanics, which are purely mathematical in nature, have been historically conflated with conjectured 'matter waves'. Indeed, as shown above, there is an exact correspondence between the space time functionality of quantum path amplitudes and that of the physically-existing, but completely independent, waves of classical physics. This

is a mathematical accident devoid of any physical significance. To summarise: only the particles exist physically, the purely mathematical probability amplitudes⁷ tell how they propagate in space-time. The only 'wave like' parameter of phenomenological significance is the de Broglie wavelength of a free particle, which, unambigously determined by the values of its momentum and Planck's constant, is a useful, but not fundamental, physical quantity. It was, of course, natural, historically, and before the advent of quantum mechanics, to associate 'waves' with light, in view of the simple and quantitatively correct explanations of the interference experiments of Young and Fresnel provided by the photon de Broglie wavelength concept, within the classical wave theory of light.

It is not generally known that the first quantitative quantum mechanical experiment was performed, not in the 19th or early 20th Century, but some two hundred years earlier, by Newton, in his analysis of the structure of interference patterns produced in the thin air film between a flat glass plate and a convex lens —Newton's Rings [41]. It is demonstrated in Ref. [25] that the classical wave theory of light, in which only the spatial component of the wave is considered, is a necessary consequence of the Feynman path integral description [22, 25] of the production of a photon by an excited atom and its subsequent detection.

7 Eigenvalues, eigenstates, canonical commutation relations and the time-independent Schrödinger equation

Considering the wavefunction or path amplitude for a free particle in one-dimensional motion, it follows from (6.1) and (6.2) that:

$$-i\hbar \frac{\partial \psi(x,t)}{\partial x} = p\psi(x,t) \tag{7.1}$$

which may be generalised to three spatial dimensions by making the making the replacement:

$$px \to \vec{p} \cdot \vec{x} = p_x x + p_y y + p_z z$$

in (6.2) to obtain:

$$-i\hbar \frac{\partial \psi}{\partial x} = p_x \psi, \quad -i\hbar \frac{\partial \psi}{\partial y} = p_y \psi, \quad -i\hbar \frac{\partial \psi}{\partial z} = p_z \psi.$$
 (7.2)

The function $\psi(\vec{x},t)$ is therefore an eigenfunction of the differential operator $-i\vec{\nabla}$ with eigenvalue \vec{p} . Similarly since

$$i\hbar \frac{\partial \psi(\vec{x}, t)}{\partial t} = E\psi(\vec{x}, t) \tag{7.3}$$

⁷They are mathematical constructs analogous to potentials in classical mechanics which clearly have an ontological status quite different to that of the physical objects, the motion of which, they encode.

 $\psi(\vec{x},t)$ is an eigenfunction of the differential operator $i\hbar\partial/\partial t$ with eigenvalue E. Introducing symbols for the differential operators:

$$\vec{\mathcal{P}} \equiv -i\hbar \vec{\nabla}, \quad \mathcal{E} \equiv i\hbar \frac{\partial}{\partial t}$$
 (7.4)

the eigenvalue equations (7.2) and (7.3) are:

$$\vec{\mathcal{P}}\psi(\vec{x},t;\vec{p},E) = \vec{p}\psi(\vec{x},t;\vec{p},E), \quad \mathcal{E}\psi(\vec{x},t;\vec{p},E) = E\psi(\vec{x},t;\vec{p},E)$$
(7.5)

where the eigenfunction ψ is labelled by its eigenvalues. These equations may be contrasted with the case of a particle moving under the influence of a non-vanishing potential V, for example the electron in a hydrogen atom. In this case, the electron wavefunctions are eigenstates of the energy of the *atom* while the electron itself is neither in an eigenstate of momentum nor of energy. See the detailed discussion around Eqs. (7.18)-(7.28) below.

It is important to notice here that, in order that ψ be an eigenfunction it is necessary that its space-time dependence is a complex exponential with phase as in (6.2). Replacing the complex exponential function by a real harmonic function such as $\cos[(\vec{p}\cdot\vec{x}-Et)/\hbar]$ will not give the eigenvalue equations (7.5). Here the appearance, in the equations of quantum mechanics, of $\sqrt{-1}$ is mandatory, if the concepts of eigenfunctions and eigenvalues are to introduced.

In view of the definitions of $\vec{\mathcal{P}}$ and \mathcal{E} , the following identities hold, where f and F are arbitrary functions of x and t, as a consequence of the product rule of differential calculus:

$$\left(\mathcal{P}_x f - f \mathcal{P}_x + i\hbar \frac{\partial f}{\partial x}\right) F \equiv 0, \tag{7.6}$$

$$\left(\mathcal{E}f - f\mathcal{E} - i\hbar \frac{\partial f}{\partial t}\right)F \equiv 0. \tag{7.7}$$

To verify (7.6) the definition: $\mathcal{P}_x \equiv -i\hbar \partial/\partial x$ is substituted on the left side to give:

$$\mathcal{P}_{x}fF - f\mathcal{P}_{x}F + i\hbar\frac{\partial f}{\partial x}F = -i\hbar\left(\frac{\partial(fF)}{\partial x} - f\frac{\partial F}{\partial x} - \frac{\partial f}{\partial x}F\right)$$
$$= -i\hbar\left(\frac{\partial f}{\partial x}F + f\frac{\partial F}{\partial x} - f\frac{\partial F}{\partial x} - \frac{\partial f}{\partial x}F\right)$$
$$= 0.$$

Setting f = x or f = y, (7.6) is conventionally written, in a symbolic manner, on cancelling the arbitrary factor F on both sides of the equation:

$$x\mathcal{P}_x - \mathcal{P}_x x = [x, \mathcal{P}_x] = i\hbar \tag{7.8}$$

$$y\mathcal{P}_x - \mathcal{P}_x y = [y, \mathcal{P}_x] = 0 (7.9)$$

where the commutator $[A, B] \equiv AB - BA$ is introduced. With the notation:

$$(x, y, z) \equiv (x_1, x_2, x_3), \quad (\mathcal{P}_x, \mathcal{P}_y, \mathcal{P}_z) \equiv (\mathcal{P}_1, \mathcal{P}_2, \mathcal{P}_3)$$

(7.8) and (7.9) generalise to

$$x_j \mathcal{P}_k - \mathcal{P}_k x_j = [x_j, \mathcal{P}_k] = i\hbar \delta_{jk} \quad j, k = 1, 2, 3$$

$$(7.10)$$

where δ_{jk} , the Kronecker δ -function is unity when j=k and zero otherwise. The relations (7.10) called canonical commutation relations or fundamental quantum conditions [42] played a key role in the conceptual development of the matrix mechanics version of quantum mechanics. However, it should not be forgotten that due to the presence of the term $x_j \mathcal{P}_k$, which is a differential operator, the relations are mathematically meaningless unless multiplied on the right by some function of x_1 , x_2 and x_3 . Also the meaning of the term $\mathcal{P}_k x_j$ depends also on the presence of the function F, because the differental operator \mathcal{P}_k in general acts not only on x_j i.e. to give $\mathcal{P}_k(x_j)$, corresponding to F=1, but implictly on the omitted arbitary function F to give instead $\mathcal{P}_k(x_jF)$. In all actual physical applications of (7.10), for example, derivations of the Heisenberg uncertainty relation [43], or the eigenvalues of the harmonic oscillator [44], or calculation of atomic transition matrix elements [45] the relation (7.10) is indeed multiplied on the right by spatial wavefunctions that do depend on x_1 , x_2 and x_3 .

Dirac [42, 46] introduced quantum commutation relations for arbitary canonically-conjugate variables, u, v by postulating a priori the following connection with a corresponding Poisson bracket, $\{u, v\}$, of classical mechanics:⁸

$$[u, v] \equiv i\hbar\{u, v\} \tag{7.11}$$

where, for a system with spatial coordinates q_r and momenta p_r [47]:

$$\{u, v\} \equiv \sum_{r} \left(\frac{\partial u}{\partial q_r} \frac{\partial v}{\partial p_r} - \frac{\partial u}{\partial p_r} \frac{\partial v}{\partial q_r} \right)$$
 (7.12)

The equation (7.11) is a fair copy of Dirac's one in [42], except that the latter wrote explicitly the commutator as uv - vu and used the notation [u, v] for the Poisson bracket. However it is clear from reading the accompanying text that the symbols u and v have different meanings on the left and right sides of the equation. On the left side they represent as-yet-unspecified quantum-mechanical operators, while on the right side they are the corresponding classical-mechanical quantities. Only later is the classical \leftrightarrow quantum correspondence: $\vec{p} \leftrightarrow \vec{\mathcal{P}} \equiv -i\hbar \vec{\nabla}$ suggested. If u and v are a Cartesian cordinate, x_j , and momentum component, p_k , respectively and $q_r = x_r$, then (7.12) gives:

$$\{x_j, p_k\} = \sum_r \left(\frac{\partial x_j}{\partial x_r} \frac{\partial p_k}{\partial p_r} - \frac{\partial x_j}{\partial p_r} \frac{\partial p_k}{\partial x_r}\right) = \sum_r \left(\frac{\partial x_j}{\partial x_r} \delta_{kr}\right) = \sum_r \delta_{jr} \delta_{kr} = \delta_{jk}$$
 (7.13)

The Poisson bracket on the right side of (7.11), in the interesting case when $u \equiv x_j$ and $v \equiv p_j$ and $q_r = x_r$, is then nothing more than a very complicated way to write the Kronecker δ -function δ_{jk} on the right side of (7.10) above! This means that Dirac's postulate (7.11) is equivalent to the relation (7.10) in this case. However (7.10) is not postulated in the present paper but *derived* from the path amplitude of a free particle, (6.1) and (6.2).

By inverting the mathematical manipulations leading from (7.1) to (7.10) above it is possible to start with (7.11) as initial premise and arrive at (7.1). Just this approach is the one followed in Chapter IV of Dirac's book [42]. The operator relation $\vec{\mathcal{P}} \equiv -i\hbar\vec{\nabla}$

⁸This is the place (on p84!) in Dirac's book on quantum mechanics [42] where Planck's constant makes its first appearence.

of Eq. (7.4) is derived as a consequence of (7.11). Similarly, in the following Chapter V of [42] the constant with dimensions of action, \hbar , is introduced for a second time in the equation:

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \tag{7.14}$$

where H is the Hamiltonian. As shown below, on making the substitution $\vec{p} \to \vec{P} \equiv -i\hbar\vec{\nabla}$ for the momentum argument of H, (7.14) becomes the time-dependent Schrödinger equation. This is how the latter is introduced in Ref. [42]. Feynman's postulate II: $\psi = \exp[iS/\hbar]$ finally appears on p121 of Ref. [42]. in a section with the title 'The motion of wave packets'. The presentation of the subject matter in Ref. [42] is an accurate representation of Dirac's own road to discovery but, from a modern perspective, has serious pedagogical shortcomings. Feynman's postulate II (actually first proposed for free particles by de Broglie [12], and later, in complete generality, by Dirac himself [10]) with its clearly specified physical meaning, immediate introduction of the fundamental constant \hbar and its direct connection, via Hamilton's principle, with classical mechanics [10, 11, 16, 17] is clearly an infinitely preferable initial postulate to Dirac's somewhat arcane premise (7.11).

Similarly, setting f = t in (7.7) the energy-time commutation relation:

$$\mathcal{E}t - t\mathcal{E} = i\hbar \tag{7.15}$$

is obtained by symbolically cancelling the arbitrary factor F on both sides. By the method of Ref. [43] this relation may be used to derive an energy-time uncertainty relation¹⁰:

$$\Delta t \Delta E \ge \hbar. \tag{7.16}$$

An application of this is to the phase of the path amplitude of an unstable particle, as discussed after Eq. (5.3) above, where Δt is identified with the mean lifetime, T, of the particle and ΔE with the Breit-Wigner decay width Γ , so that the equality in (7.16) gives:

$$mc^2 \to mc^2 - i\frac{\hbar}{2T} = mc^2 - i\frac{\Gamma}{2}.$$
 (7.17)

A particle moving in free space is in an eigenstate of both energy and momentum. This may be contrasted with the case for a bound particle, for example the electron or proton in a hydrogen atom. The *atom* is in an eigenstate of both energy and momentum (for example at rest) but the electron has a variable momentum and position. These distributions are connected by a Fourier transform that predicts that their widths are related by a Heisenberg uncertainty relation. The problem of determining the spatial wavefunctions (eigenfunctions describing the position of the electron relative to the proton, but with fixed atomic, not electron or proton, energies) first solved by Schrödinger, will now be considered from the viewpoint of Feynman's path integral formulation of quantum mechanics. This analysis is important for the comparison with Schrödinger's second derivation of the quantum wave equation that is critically reviewed in the following section.

⁹Dirac actually replaces ψ with ψ/A where A is an arbitary real function of the space-time coordinates, so that Dirac's ψ is actually the propagator K of Eq. (3.3) above.

¹⁰Although the mathematics of the derivation of this equation by the method of Ref. [43] is similar to that of the more familiar space-momentum uncertainty relation: $\Delta x \Delta p \geq \hbar$, its physical meaning is more controversial. See [48] and references therein.

Since the potential function, and hence the Hamiltonian, for the hydrogen atom in a bound state i is time-independent, Hamilton's principle function is given by (6.18):

$$S_{H,i} = W_{H,i}(\vec{x}) - E_{H,i}t \tag{7.18}$$

where $W_{\mathrm{H},i}(\vec{x})$ is the corresponding Hamilton's characteristic function. The wavefunction of the hydrogen atom in the *i*th bound state is then:

$$\psi_{\mathrm{e}}(\vec{x}, t; E_{\mathrm{H},i}) = \exp\left[\frac{iS_{\mathrm{H},i}}{\hbar}\right] = \exp\left[\frac{i}{\hbar}(W_{\mathrm{H},i}(\vec{x}) - E_{H,i}t)\right]$$
(7.19)

Writing explicitly the different contributions to $E_{H,i}$ gives:

$$H_{\mathrm{H},i} = E_{\mathrm{H},i} = E_{\mathrm{e},i} + E_{\mathrm{p},i} + V = m_{\mathrm{e}}c^2 + T_{\mathrm{e},i} + m_{\mathrm{p}}c^2 + T_{\mathrm{p},i} + V$$
 (7.20)

where $m_{\rm e}$, $m_{\rm p}$ are the Newtonian electron and proton masses and $T_{{\rm e},i}$, $T_{{\rm p},i}$ their kinetic energies in the *i*th bound state. Introducing the (negative) bound state energy, or binding energy, $E_{{\rm H},i}^{\rm BS}$, defined as:

$$E_{\mathrm{H},i}^{\mathrm{BS}} \equiv E_{\mathrm{H},i} - M_0 c^2 = T_{\mathrm{e},i} + T_{\mathrm{p},i} + V, \quad M_0 c^2 \equiv m_{\mathrm{e}} c^2 + m_{\mathrm{p}} c^2$$
 (7.21)

(7.19) can be written as:

$$\psi_{e}(\vec{x}, t; E_{H,i}) = \exp\left[\frac{iS_{H,i}}{\hbar}\right]$$

$$= \exp\left[\frac{-iM_{0}c^{2}t}{\hbar}\right] \exp\left\{\frac{i}{\hbar}(W_{H,i}(\vec{x}) - E_{H,i}^{BS}t)\right\}$$

$$\equiv \exp\left[\frac{-iM_{0}c^{2}t}{\hbar}\right] \psi_{e}(\vec{x}, t; E_{H,i}^{BS}).$$
(7.22)

Differentiating $\psi_{\rm e}(\vec{x}, t; E_{{\rm H},i}^{\rm BS})$ twice w.r.t. \vec{x} , using the first transformation equation in (2.5), gives

$$\vec{\nabla}^2 \psi_{\rm e}(\vec{x}, t; E_{\rm H,i}^{\rm BS}) = -\frac{p_{\rm e}^2}{\hbar^2} \psi_{\rm e}(\vec{x}, t; E_{\rm H,i}^{\rm BS})$$
 (7.23)

Since the spatial wavefunction $\psi_{\rm e}(\vec{x}; E_{{\rm H},i}^{\rm BS})$ is given by (7.22) as

$$\psi_{e}(\vec{x}; E_{H,i}^{BS}) \equiv \exp\left[\frac{i}{\hbar} W_{H,i}(\vec{x})\right] = \psi_{e}(\vec{x}, t; E_{H,i}^{BS}) \exp\left[i\frac{E_{H,i}^{BS}t}{\hbar}\right]$$
(7.24)

a factor $\exp[-iE_{\mathrm{H},i}^{\mathrm{BS}}t/\hbar]$ may be cancelled from both sides of (7.23) giving, on transposing the resulting equation:

$$p_{\rm e}^2 = -\hbar^2 \frac{\vec{\nabla}^2 \psi_{\rm e}(\vec{x}; E_{\rm H,i}^{\rm BS})}{\psi_{\rm e}(\vec{x}; E_{H,i}^{\rm BS})}.$$
 (7.25)

In the non-relativistic (NR) approximation, appropriate to the motion of the electron and proton in a hydrogen atom bound state, $T \simeq p^2/(2m)$ and, since the momenta and the electron and proton are equal and opposite in the rest frame of the atom:

$$\frac{T_{p,i}}{T_{e,i}} = \frac{m_e}{m_p} \ll 1.$$

The proton kinetic energy term in (7.21) may therefore be neglected, in first appreoximation, so that

$$H_{\mathrm{H},i}^{\mathrm{BS,NR}} = E_{\mathrm{H},i}^{\mathrm{BS,NR}} = \frac{p_{\mathrm{e}}^2}{2m_{\mathrm{e}}} + V.$$
 (7.26)

Setting $E_{\mathrm{H},i}^{\mathrm{BS}}$ equal to $E_{\mathrm{H},i}^{\mathrm{BS,NR}}$ in (7.25) and substituting for p_{e}^2 in (7.26) using the resulting equation, gives, on rearrangement, the *time-independent Schrödinger equation* for the spatial wavefunction of an electron in a bound state of the hydrogen atom:

$$\vec{\nabla}^2 \psi_{\rm e}(\vec{x}; E_{\rm H,i}^{\rm BS,NR}) + \frac{2m_{\rm e}}{\hbar^2} (E_{\rm H,i}^{\rm BS,NR} - V) \psi_{\rm e}(\vec{x}; E_{\rm H,i}^{\rm BS,NR}) = 0.$$
 (7.27)

Transposing (7.24) and differentiating w.r.t. t gives

$$\frac{\partial \psi_{\mathbf{e}}(\vec{x}, t; E_{\mathbf{H}, i}^{\mathrm{BS}})}{\partial t} = -\frac{i E_{\mathbf{H}, i}^{\mathrm{BS}}}{\hbar} \psi_{\mathbf{e}}(\vec{x}, t; E_{\mathbf{H}, i}^{\mathrm{BS}}). \tag{7.28}$$

Substituting $\psi_{\rm e}(\vec{x},t;E_{{\rm H},i}^{\rm BS})$, and its time derivative from (7.28), in the time dependent Schrödinger equation (4.8), cancelling out a common multiplicative factor $\exp[-iE_{{\rm H},i}^{\rm BS}t/\hbar]$, and setting $E_{{\rm H},i}^{\rm BS}$ equal to $E_{{\rm H},i}^{\rm BS,NR}$, the time-independent equation (7.27) is recovered. Notice that the NR approximation is implicit in the H-J equation (4.7) from which (4.8) is derived.

Eq.(7.27), containing the spatial electron wavefunction and the (negative) bound state energy $E_{\mathrm{H},i}^{\mathrm{BS}}$, is just the partial differential equation from which Schrödinger derived the bound state energies and wavefunctions of the hydrogen atom [4]. Schrödinger's own derivations of this equation and of the time-dependent equation (4.8) are discussed in the following section.

8 Schrödinger's derivations of quantum wave equations

Schrödinger's first published derivation of the time independent-quantum wave equation (7.27) [4] considers the H-J equation of a system with a time-independent Hamiltonian so that

$$\frac{\partial S}{\partial t} = -H = -E \tag{8.1}$$

where E is constant, so that the H-J equation (2.6) is written:

$$H(q_i, \frac{\partial S}{\partial q_i}) = E \tag{8.2}$$

Schrödinger then introduces the following ansatz relating the 'wavefunction' ψ (which is here introduced for the first time) to Hamilton's characteristic function, denoted here as S, rather than W, as is conventional, and done in Sections 6 and 7 above:

$$S = K \ln \psi \tag{8.3}$$

or

$$\psi = \exp\left[\frac{S}{K}\right] \tag{8.4}$$

where K is a real constant, which, like h, has the dimensions of action. This ansatz is the same as the fundamental postulate II of Feynman's formulation of quantum mechanics, for the spatially-dependent part of the path amplitude, on making the replacement $K \to -i\hbar$.

Using (8.2) and (8.3) and following the same chain of arguments from which the time-dependent Schrödinger equation (4.8) is derived from the H-J equation (4.7) and Feynman's postulate (4.2) instead of (8.3), yields the equation:

$$\vec{\nabla}^2 \psi - \frac{2m_e}{K^2} (E - V) \psi = 0 \tag{8.5}$$

which resembles the time-independent Schrödinger equation (7.27) except that \hbar is replaced by K and the second term on the left side has a minus sign instead of a plus sign. Now (8.5) is a necessary mathematical consequence of (8.2) and (8.3) when H has the form of the non-relativistic Hamiltonian of Eq. (4.7), but (8.5) is not the time-independent Schrödinger equation, and would not, if solved, give the correct bound state wavefunctions and energies of the hydrogen atom. In order to derive the correct equation (7.27) starting from (8.2), (8.3) and the Hamiltonian of Eq. (2.7) Schrödinger had to introduce a further ansatz concerning the wavefunction ψ . Differentiating (8.3) to obtain equations analogous to (4.3) and substituting for $\partial S/\partial x_i$ in (8.2) gives the equation

$$\left(\frac{\partial \psi}{\partial x}\right)^2 + \left(\frac{\partial \psi}{\partial y}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 - \frac{2m_e}{K^2}(E - V)\psi^2 = 0$$
(8.6)

The quantity:

$$J \equiv \int \int \int \left[\left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial \psi}{\partial y} \right)^2 + \left(\frac{\partial \psi}{\partial z} \right)^2 - \frac{2m_e}{K^2} (E - V) \psi^2 \right] dx dy dz \tag{8.7}$$

is now introduced and the condition is imposed that J should be stationary for arbitary variations of the wave function $\psi: \delta J = 0$. Now

$$\delta \left(\frac{\partial \psi}{\partial x} \right)^2 = 2 \frac{\partial \psi}{\partial x} \frac{\partial (\delta \psi)}{\partial x} \tag{8.8}$$

Integrating by parts:

$$\int_{x_L}^{x_U} \delta \left(\frac{\partial \psi}{\partial x} \right)^2 dx = 2 \left[\frac{\partial \psi}{\partial x} \delta \psi \right]_{x_L}^{x_U} - 2 \int_{x_L}^{x_U} \frac{\partial^2 \psi}{\partial x^2} \delta \psi dx \tag{8.9}$$

also

$$\delta(\psi)^2 = 2\psi\delta\psi\tag{8.10}$$

Substituting (8.9) and similar formulae for the y and z coordinates, and (8.10), into the expression for δJ and assuming that $\delta \psi$ vanishes at the limits of integration in the first term on the right side of (8.9) and the similar formulae for the other spatial coordinates, gives:

$$\frac{\delta J}{2} = -\int \int \int dx dy dz \left[\vec{\nabla}^2 \psi + \frac{2m_e}{K^2} (E - V) \psi \right] \delta \psi = 0$$
 (8.11)

Since this equation must hold for arbitary $\delta\psi$ then

$$\vec{\nabla}^2 \psi + \frac{2m_e}{K^2} (E - V) \psi = 0 \tag{8.12}$$

which is just the time-independent Schrödinger equation (7.27) on setting $K = \hbar$.

Schrödinger's notes [49] show that he was well aware that the solution of (8.12) gives correctly the bound state energies of the hydrogen atom before introducing in [4] the anstaz concerning the hypothetical quantity J. This artifice compensates for the physically incorrect ansatz (8.3). The constant K should actually be the pure imaginary quantity $-i\hbar$ in which case (8.5) becomes the correct equation (7.27). Repeating Schrödinger's stationarity algorithm starting with the correct relation $S = -i\hbar \ln \psi$ would then give the incorrect equation (8.5)! Indeed, since the H-J equation and the properties of the generating function S already follow from Hamilton's equations which in turn are a consequence of Hamilton's Principle — the condition that the action S should be stationary for arbitrary variations of space-time paths— it would seem that Schrödinger is attempting here to close a door that is already shut.

In fact the time dependent Schrödinger equation (4.7), and hence (8.12), can be derived from a stationarity requirement imposed on an action function derived from a certain Lagrangian under arbitary variations of the wavefunction ψ . The appropriate Lagrangian, given by Heisenberg, is [50]:

$$L = -\frac{\hbar^2}{2m_e} \nabla \psi^* \cdot \nabla \psi - \frac{\hbar}{2i} \left(\frac{\partial \psi}{\partial t} \psi^* - \frac{\partial \psi^*}{\partial t} \psi \right) + eV \psi \psi^* + \frac{1}{8\pi} \nabla V \cdot \nabla V. \tag{8.13}$$

Requiring that the corresponding action is stationary for variations of ψ or ψ^* derives the time-dependent Schrödinger equation (4.7), or its complex conjugate, respectively. Similarly varying V gives Poisson's equation:

$$\nabla^2 V = -4\pi(\rho + \rho_0) \tag{8.14}$$

where $\rho \equiv -e\psi\psi^*$ and ρ_0 represents electric charges other than that of the electron described by ψ .

As already mentioned, Schrödinger's second paper on wave mechanics [5] discusses Hamilton's analogy between classical mechanics and geometrical optics, via the H-J equation that Schrödinger calls the 'Huygens' Principle'. Essentially the same argument as that given above in Section 6 leads to the formula (6.26) for the phase velocity of the waves. In [5] the time-independent equation (8.12) is then rederived from the corresponding classical wave equation:

$$\nabla^2 \psi - \frac{1}{v_W(NR)^2} \frac{\partial^2 \psi}{\partial t^2} = 0. \tag{8.15}$$

On the assumption the ψ has harmonic time dependence with frequency ν then:

$$\frac{\partial^2 \psi}{\partial t^2} = -4\pi^2 \nu^2 \psi. \tag{8.16}$$

Assuming also the Planck-Einstein relation (6.3) then combining (6.26), (8.15) and (8.16) gives:

$$\nabla^2 \psi - \frac{1}{v_W(NR)^2} \frac{\partial^2 \psi}{\partial t^2} = \nabla^2 \psi - \frac{2m_e(E - V)}{h^2 \nu^2} \frac{\partial^2 \psi}{\partial t^2} = \nabla^2 \psi + \frac{2m_e(E - V)}{\hbar^2} \psi = 0 \quad (8.17)$$

so that (8.12) is recovered. The time dependence of ψ is given explicitly in [5] as $\exp(2\pi i\nu t)$, i.e. as a complex exponential, but this is not necessary for the above derivation since (8.16) holds also if ψ is a real harmonic function (sine or cosine) of t. It may be remarked that the quantity E in the Planck-Einstein relation is the relativistic energy of the electron whereas Eq. (6.26) contains the non-relativistic bound state energy (c.f. Eq.(7.21), E_{NR} , (denoted by Schrödinger as E) of Eq. (6.25). Use of the Planck-Einstein relation here then implies the introduction of an unphysical negative frequency. This, together, with the unphysical nature of the phase velocity, $v_W(NR)$, introduced in (8.15) implies that this second 'derivation' of the quantum wave equation should also be considered more as a heuristic exercise than a mathematically sound proof.

Neither of the above derivations of (7.27) requires the introduction into the equations of $\sqrt{-1}$. The spatial eigenfunctions that are solutions of (7.27) are real, not complex, functions of the spatial coordinates of the electron.

Schrödinger finally derived the time-dependent quantum wave equation (4.7), after considerable discussion, in the first section of his fifth and last paper written in 1926 on wave mechanics [7]. This was done by introducing the ansatz that the time dependence of ψ is given by a complex exponential:

$$\psi = u(x) \exp\left[\pm \frac{iEt}{\hbar}\right] \tag{8.18}$$

so that

$$i\hbar \frac{\partial \psi}{\partial t} = \mp E\psi \tag{8.19}$$

which when substituted in the last member of the last equation in (8.17) and transposing gives:

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi + V\psi \mp i\hbar\frac{\partial\psi}{\partial t} = 0.$$
 (8.20)

On choosing the minus sign in (8.18) and (8.20) the time-dependent equation (4.8) is obtained. Here $\sqrt{-1}$ makes an essential and necessary appearence. However, Schrödinger's ansatz (8.18) is just the fundamental second postulate of Feynman's formulation of quantum mechanics for the time dependence of a path amplitude. c.f. Postulate II, Eq. (3.3) and Eq. (6.18). It was therefore, in a sense, not necessary for Feynman to demonstrate that the Schrödinger equation (4.8) follows from his postulates, since, in fact, Schrödinger had made, a priori, essentially the same postulate, (8.18), in order to derive the equation!

9 Summary and discussion

The H-J equation (2.6) is a first order partial differential equation for Hamilton's principal function $S = F(q_i, P_i, t)$, the generating function that transforms canonical

coordinates and momenta, that respect Hamilton's equations, from q_i , p_i to Q_i , P_i , in such a way that the transformed Hamiltonian vanishes. The same function $S = \int L dt$, where L is the Lagrangian of the dynamical system considered, occurs in the fundamental formula (3.3) of Feynman's path integral formulation of quantum mechanics [11]: $K_{\rm BA}^{(j)} = A_{\rm BA}^{(j)} \exp[iS_{\rm BA}^{(j)}/\hbar]$ giving the amplitude $K_{\rm BA}^{(j)}$ to find a particle, originally at space-time point A, at the point B, having followed the space time path j. Writing $\psi \equiv K/A$ and substituting for S in the H-J equation (4.7) for a non-relativistic particle confined by a time-independent potential V gives immediately the time-dependent Schrödinger equation (4.8) on identifying ψ with the quantum mechanical wavefunction. Application of the Schrödinger equation to the hydrogen atom then shows that its spatial wavefunction, according to Feynman's first postulate, that combines quantum mechanical superposition with Born's probabilistic interpretation of quantum mechanics [26], is the probability amplitude to find the bound electron at a particular spatial position in a particular bound state of the atom. This is in accordance with Dirac's more formal interpretation of the wavefunction as a transformation matrix element between representations with different eigenstates [8].

For a free particle, with relativistic energy E and momentum p, the Hamilton's principal function takes the Lorentz-invariant form: S = px - Et, as follows by integrating the transformation equations in (2.4) and (2.5). The replacements $p/E \to v/c^2$ and $x \to vt$ in this formula for S gives the relativistic Lagrangian: $\mathcal{L} = -mc^2\sqrt{1-\beta^2}$ for a free particle as well as the fundamental formulae of relativistic kinematics and space-time geometry in (5.10). The Planck-Einstein relation $E = h\nu$, (6.3) and the de Broglie relation $\lambda = h/p$, (6.4) are derived by mathematical substitution in the formula, (6.2), for the phase of the path amplitude for a free particle.

The derivation by de Broglie of his wavelength relation by Lorentz transformation of the path amplitute phase and use of the Planck-Einstein relation is compared with that obtained from Eq. (6.2). Also de Broglie's derivation of a 'group velocity' equal to the particle velocity v, by introducing the concept of a refractive index for 'matter waves' in free space is compared with that obtained from the energy-momentum-mass relation (6.6) in conjunction with the Planck-Einstein and de Broglie relations.

Hamilton's discussion of the analogy between particle kinematics and geometrical optics, based on 'wave-fronts' associated with Hamilton's characteristic function, W, in Eq. (6.18) is used to derive an associated phase velocity: $v_W = E/|\vec{p}|$. For relativistic motion, where $E/|\vec{p}| = v/c^2$, v_W is equal to v_{ϕ} . However for non-relativistic motion it is found that $v_W = v/2$ whereas the relativistic formula $v_W = v_{\phi} = c^2/v$ must hold for all values of v. This inconsistency is indicative of the unphysical nature of the 'matter waves' in free space and their associated 'phase velocity'. This conclusion is reinforced by the gauge dependence of the wavefront direction, phase velocity and wavelength of the 'matter waves' associated with particle motion in magnetic fields [39], to be contrasted with the gauge independence, and hence physical uniqueness, of the phase difference between the amplitudes of different paths.

The path amplitude for a free particle is an eigenfunction of the differential operators $\mathcal{P} \equiv -i\hbar \vec{\nabla}$, $\mathcal{E} \equiv i\hbar \partial/\partial t$ with eigenvalues \vec{p} , E respectively. Consideration of the application of these operators to arbitrary functions of space-time allows derivation of the canon-

ical commutation relations (7.10) and (7.11), while their application to the wavefunction of an electron in a bound state of the hydrogen atom with the Hamiltonian of (7.26) enables derivation of the time-independent Schrödinger equation for this wavefunction. It is argued that these path integral derivations have important pedagogical advantages over the presentation of the same subjects in Dirac's book on quantum mechanics [42].

Schrödinger's first published derivation of the time-independent quantum wave equation [4] also took as its primary postulate the H-J equation (4.7) for a non-relativistic particle constrained by a time-independent potential V. The relation between the wavefunction ψ (introduced here for the first time) and Hamilton's principle function S, is given by the ansatz: $S = K \ln \psi$ where K is real constant with the dimensions of action, instead of the path-integral postulate $S = -i\hbar \psi$. The correct equation is obtained by the artifice of introducing the quantity J defined in Eq. (8.7) and requiring that it is stationary for arbitrary variations of ψ . In fact, as pointed out by Heisenberg [50], the quantum wave equation can be derived by requiring stationarity with respect to variations of ψ of the Lagrangian given in (8.13), i.e. by an application of Hamilton's principle, which is also the basis for Hamilton's equations and the H-J equation itself.

Schrödinger's second published derivation of the time-independent quantum wave equation [5] was based on Hamilton's mechanical/geometric optics analogy discussed in Section 6. The equation is given on substituting the non-relativistic phase velocity $v_W(NR)$ of Eq. (6.26) in the classical wave equation (8.15). Other postulates are a harmonic time dependence of ψ , and the Planck-Einstein relation $E = h\nu$. This derivation, unlike that presented in Section 7 leading to (7.27) requires the introduction, in an intermediate step, of the unphysical quantity $v_W(NR)$. Also the energy in the Planck-Einstein relation is the relativistic energy given in Eq. (5.10), whereas in the derivation it is equated with the non-relativistic energy E_{NR} of Eq. (6.26). Furthermore, the symbol E in the equation is interpreted by Schrödinger as the (negative) bound state energy ($E_{H,i}^{BS}$ of Eq. (7.21)) of the hydrogen atom in order to obtain the atomic wavefunctions. This second derivation is, therefore, also mathematically flawed.

To derive the time-dependent equation [7] Schrödinger makes the ansatz: $\psi = u(x)[\exp(\pm iEt/\hbar)]$, which, when used to eliminate E from the previously derived time-independent equation, yields (4.8) on choosing the minus sign in the complex exponential. The ansatz used (except that a sign ambigity devoid of any physical significance is retained) is exactly the time dependence of the path amplitude phase (c.f. Eq. (6.18)) specified by Feynman's postulate II, in the case of a time-independent Hamiltonian. It is then not surprising that Feynman was able to derive the Schrödinger equation from his postulates!

The work presented in the present paper is in some ways complementary to, and in others overlaps with, that presented in a previous paper by the present author [37] published in this journal. In the latter several of the results of Section 7 of the present paper are derived starting from different considerations—the 'inverse correspondence', low photon density, limit of classical electrodynamics— where quantum mechanical concepts become applicable. The basic premise of Ref. [37]—interpretation of the equations of classical electrodynamics as a description of photonic behaviour, is the same as that of the de Broglie paper [12] of which the present author was unaware at the time of writing

Ref. [37]. As previously mentioned, the essential concepts of Feynman's formulation of quantum mechanics are also to be found in Ref. [12].

In all applications of the Feynman path amplitude formulation of quantum mechanics to actual experiments care must be taken in the identification of all parameters relevant to the space time description. Some examples are described in Ref. [25], For example, in physical optics experiments where interference effects involving real photons are observed, then since in (6.2) x/t = c = E/p it follows that $\phi = (xp - Et)/\hbar = 0$, so, as pointed out by Feynman [51]¹¹, the phase of the propagator of the photon vanishes! Detailed calculation [25] shows that, in fact, the 'photon wavefunction' actually contains the phase of the decay amplitude of the photon's unstable source atom.

Acknowledgement I would like to thank an anonymous referee for a careful reading of an earlier version of this article and for many helpful suggestions that have improved both its content and clarity of presentation.

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¹¹ 'Once a photon has been emitted there is no further turning of the arrow as the photon goes from one place to another in space-time.' i.e. there is no change in the phase of the photon path amplitude.

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