Some Mathematical Material for Introductory Courses in Quantum Wave Mechanics *

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Abstract

This work is an exposition of basic wave mechanics, and of the connection between wave mechanics and classical mechanics.

A particular notational convention is shown to make the correct Schrödinger wave equation follow automatically from the standard axiom in all cases, without introducing arbitrary rules of manipulation. The standard axiom is an interpretation of the Hamiltonian $H$ in the statement

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

It will be further shown that the geometrical optics approximation procedure is the link which connects classical and wave mechanics: the Hamilton-Jacobi equation (an abstract description of families of classical trajectories) is the eikonal equation for the corresponding wave equation, and conversely the wave equation is the natural one to have that particular eikonal. Thus:

$$\text{Hamilton-Jacobi equation } \Rightarrow \text{ geometrical optics } \Rightarrow \text{ Schrödinger wave equation}$$

Key words

Classical mechanics; wave mechanics; geometrical optics; Schrödinger wave equation; Hamilton-Jacobi equation; eikonal equation.

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1 Introduction

The usual descriptions of the construction of the explicit equations of wave mechanics treat as axiomatic the statement in Cartesian coordinates

$$H\psi = i\hbar \frac{\partial \psi}{\partial t}$$  \hspace{1cm} (1.1)

in which $H$ is an adaptation of a classical Hamiltonian, now interpreted as the differential operator constructed by substituting a differential operator for the classical momentum $P$,

$$P \rightarrow -i\hbar \nabla,$$  \hspace{1cm} (1.2)

and $\hbar$ is the modified Planck constant. Equation (1.1) is a Schrödinger equation.

A revealed truth, as implied by equation (1.1) with the identification (1.2), is unusual in the light of mathematical physics’ tradition of deductive rather than inductive modelling. Matters are often made further opaque by the use of unsuitable notations: in particular it will be seen to be preferable in reducing (1.1) to use (with the superfix denoting transposition) the factorization

$$(P + A)^T(P + A)$$  \hspace{1cm} (1.3)

instead of such alternatives as

$$|P + A|^2 \text{ or } (P + A) \cdot (P + A).$$  \hspace{1cm} (1.4)

The first notation (1.3) will make automatic some of the steps in the evaluation of (1.1) which are obscure or ambiguous if the latter (1.4) are used, with particular improvement if the substitution rule (1.2) is replaced by the pair

$$P^T \rightarrow (-i\hbar) \times \text{div(ergence operator), } P \rightarrow (-i\hbar) \times \text{grad(ient operator)}$$  \hspace{1cm} (1.5)

The efficacy of the proposed approach is demonstrated in Section 3 below.

Equally as desirable as a clear notation is a rational mechanism leading to the rules (1.1), (1.5) themselves. Although hints of the existence of such a mechanism can be found in a number of sources, so far as the writer is aware no explicit description is available. Yet the demonstration of the nexus between classical mechanics and wave mechanics is a sufficiently simple undertaking that it is appropriate to introductory courses in the latter.

The key to this connection (Section 4) is the geometrical optics method of constructing high frequency approximations to the solutions of linear and weakly nonlinear wave equations. This approximation proceeds by introducing an ansatz for the wave function $\psi$ whose leading term is

$$\psi \sim W \exp(iS/\hbar)$$  \hspace{1cm} (1.6)

where $W$ and $S$ are real-valued functions of the independent variables. It turns out (Section 4) that the phase $S$ satisfies the Hamilton-Jacobi equation appropriate to the classical dynamic setting, and $S$ is thus the classical action. As the equation determining the phase function $(S)$ in geometrical optics is generically called an eikonal equation, so one can say that classical mechanics, as manifest in the appropriate Hamilton-Jacobi equation, is the eikonal of the corresponding wave mechanics.
The argument also works in reverse, although not as strongly: the Schrödinger equation is the dominant equation having the Hamilton-Jacobi equation as its eikonal, for all wave equations

\[ H \psi - i \hbar \frac{\partial \psi}{\partial t} + O(\hbar^2) = 0 \]  

(1.7)

share the same eikonal. (An implied assumption here that the high frequency parameter is in fact \( \hbar \), the modified Planck constant, can be justified by making the putative wave equation correct for de Broglie waves.)

In Section 5 the transport equation, which determines \( W \), is noted, while Section 6 indicates how a dynamical definition can replace the Hamilton-Jacobi equation in order to replicate the (wave-type) equation governing a transformation function. Section 7 contains an account of basic relativistic wave mechanics through the prism of geometrical optics.

2 Notation

The Cartesian position vector is

\[ \mathbf{r} = \left( \begin{array}{c} x \\ y \\ z \end{array} \right) \],

(2.1)

and the generalized coordinate position vector is

\[ \mathbf{\rho} = \left( \begin{array}{c} \xi \\ \eta \\ \zeta \end{array} \right) = \mathbf{\rho}(\mathbf{r}). \]

(2.2)

The Jacobian matrix is

\[ J = \left[ \begin{array}{ccc} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{array} \right] \]

(2.3)

(where the suffix denotes partial derivative), its inverse is

\[ J^{-1} = \left[ \begin{array}{ccc} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{array} \right] \]

(2.4)

and the Jacobian determinant is

\[ g = \det J = (\det J^{-1})^{-1}. \]

(2.5)

It is convenient to introduce a notation for the product

\[ J^{-1}(J^{-1})^T = J^{-1}(J^T)^{-1} = U \]

(2.6)

which is a symmetric matrix, as the superfix denotes transposition. The symbol \( \nabla \) will be interpreted in any particular context as the first order partial differential operator vector with respect to relevant independent variables

\[ \nabla = \left( \begin{array}{c} \partial/\partial \xi \\ \partial/\partial \eta \\ \partial/\partial \zeta \end{array} \right) ; \]

(2.7)
\( \nabla^T \) is the transposed operator.

Kinematic and dynamic quantities are represented as follows. The Cartesian components of velocity are
\[
v = \frac{dr}{dt} \quad (2.8)
\]
and the generalized velocity vector is
\[
\nu = \frac{d\rho}{dt} \quad (2.9)
\]
so that at any particular point in the same velocity field
\[
v = J \nu. \quad (2.10)
\]
For a particle of mass \( m \), the Cartesian components of its momentum vector are
\[
P = mv, \quad (2.11)
\]
its kinetic energy is
\[
K = \frac{m}{2} v^T v = \frac{1}{2m} P^T P,
\]
and so
\[
\frac{\partial K}{\partial \nu} = P. \quad (2.13)
\]
In generalised coordinates then, the kinetic energy is
\[
K = \frac{m}{2} \nu^T J^T J \nu \quad (2.14)
\]
and the generalized momentum vector, by definition
\[
P = \frac{\partial K}{\partial \nu},
\]
is evaluated as
\[
P = m J^T J \nu. \quad (2.15)
\]
After inversion, this last equation yields the expression
\[
\nu = \frac{1}{m} J^{-1} (J^T)^{-1} P \quad (2.16)
\]
for the generalised velocity in terms of the generalised momentum, and so the kinetic energy is, using the definition (2.6)
\[
K = \frac{1}{2m} P^T J^{-1} (J^{-1})^T P = \frac{1}{2m} P^T U P
\]
in its most general form.
3 Standard descriptions

It can be shown (see, for example Mott & Sneddon, 1963, p.39) that the classical Hamiltonian $H$ describing the motion of a charged particle of mass $m$ moving in an electromagnetic field having vector potential $A$ and scalar potential $\phi$ is in Cartesian coordinates

$$H = \frac{1}{2m} (P + c_1 A)^T (P + C_1 A) + c_2 \phi,$$

where $c_1$ and $c_2$ are constants, proportional to the particle’s charge. The Schrödinger wave equation associated with this system is obtained by replacing in $H$

P with $(-i\hbar) \times$ divergence operator ($= -i\hbar \nabla^T$)

$P_T$ with $(-i\hbar) \times$ gradient operator ($= -i\hbar \nabla$)  

and supplying the operand $\psi$ (the wave function), which also multiplies the scalar potential. The substituted expression is then equated to $i\hbar \partial \psi / \partial t$; in symbols

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

(Basdevant & Dalibard, 2002, p.103), and explicitly

$$\frac{1}{2m} \left( -i\hbar \text{ div} + c_1 A^T \right) \left( -i\hbar \text{ grad} + c_1 A \right) \psi + c_2 \phi \psi$$

$$= \frac{1}{2m} \left( -\hbar^2 \text{ div(grad } \psi) - i\hbar c_1 \text{ div}(A \psi) - i\hbar c_1 A^T \text{ grad } \psi + c_1^2 A^T A \psi \right) + c_2 \phi \psi$$

$$= i\hbar \frac{\partial \psi}{\partial t}.$$  

This is the general form of the Schrödinger wave equation.

In terms of generalized coordinates (2.2-2.7), and with

$$A = (J^{-1})^T Q,$$

equation (3.4) is explicitly

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m} \left( -\frac{\hbar^2}{g} \nabla^T (gU \nabla \psi) - i\frac{\hbar}{g} c_1 \nabla^T (gU Q \psi) - i\hbar c_1 Q^T U \nabla \psi + c_1^2 Q^T U Q \psi \right) + c_2 \phi \psi$$

$$= \frac{1}{2m} \left( -\frac{i\hbar}{g} \nabla^T g + c_1 Q^T \right) U \left( -i\hbar \nabla + c_1 Q \right) \psi + c_2 \phi \psi,$$

after factorizing the spatial operator. Since it is preferable to express all differential operators in Hermitian (and also more symmetric) form, both sides of equation (3.5) are multiplied by the Jacobean determinant $g$ (see (2.5)) to give

$$i\hbar g \frac{\partial \psi}{\partial t} = \frac{1}{2m} \left( -i\hbar \nabla^T + c_1 Q^T \right) g U (-i\hbar \nabla + c_1 Q) \psi + c_2 g \phi \psi.$$  

Because the classical Hamiltonian (3.1) transforms as

$$H = \frac{1}{2m} (P^T + c_1 Q^T) U (p + c_1 Q) + c_2 \phi \psi$$  

(3.7)
or
\[
(gH) = \frac{1}{2m} (p^T + c_1 Q^T) g U (P + c_1 Q) + c_2 g \phi \psi, \tag{3.8}
\]
the rules for obtaining the wave equation in generalized coordinates are thus: replace
\[
p^T \text{ with } -i\hbar \nabla^T g \quad \text{and} \quad p \text{ with } -i\hbar \nabla \tag{3.9}
\]
in the classical Hamiltonian, or more symmetrically from (3.8) and (3.6) replace
\[
p^T \text{ with } -i\hbar \nabla^T \quad \text{and} \quad p \text{ with } -i\hbar \nabla \tag{3.10}
\]
in \(g\) times the classical Hamiltonian; that is in (3.7) and (3.9) equate
\[
H \psi \text{ with } i\hbar \frac{\partial \psi}{\partial t}
\]
and in (3.8) and (3.10) equate
\[
(gH) \psi \text{ with } i\hbar g \frac{\partial \psi}{\partial t}.
\]
These rules are more general than (3.2). The foregoing procedure connecting the Hamiltonian and the Schrödinger wave equation is axiomatic and apparently arbitrary.

4 The Schrödinger wave equation, geometrical optics, and the Hamilton-Jacobi equation

In this section it is shown how classical mechanics and wave mechanics connect with one another through the geometrical optics approximation procedure. The demonstration starts by noting the calculation properties of the form
\[
G = M(P,t) \exp(i\theta(P,t)/\epsilon) \tag{4.1}
\]
of the geometrical optics approximation. Here (ideally) \(\theta\) is a real-valued, dimensionless function, and \(\epsilon > 0\) a dimensionless parameter small in comparison with 1 almost everywhere. The real coefficient \(M\) is neither large nor small almost everywhere.

Thus one has, for any vector valued \(B(P)\), the formal calculation
\[
(-i\epsilon \nabla + B)G = (\nabla \theta + B)G + 0(\epsilon). \tag{4.2}
\]
Similarly, if instead the form has a vector coefficient
\[
F = L(P,t) \exp(i\theta(P,t)/\epsilon), \tag{4.3}
\]
then
\[
(-i\epsilon \nabla^T + B^T)F = \left((\nabla \theta)^T L + B^T L\right) \exp(i\theta/\epsilon) + 0(\epsilon) = \exp(i\theta/\epsilon) L^T (\nabla \theta + B) + 0(\epsilon) = F^T (\nabla \theta + B) + 0(\epsilon) \tag{4.4}
\]
The results (4.3) and (4.4) are standard in geometrical optics. Now calculate the leading term in the geometrical optics approximation to

$$\psi \sim W \exp(iS/\hbar) + \sum_{n} \hbar^n W_n$$ (4.5)

by substituting this approximation in the Schrödinger equation (3.6). Start with the spatial differential operator’s ($D$ say) evaluation of the leading term in the representation (4.5) of $\psi$, using (as stated) the form (3.6) of the wave equation, and working inside out, as is natural:

$$D\psi = \frac{1}{2m} \left(-i\hbar \nabla^T + c_1 Q\right) gU \left(i\hbar \nabla + c_1 Q\right) \left(W \exp(iS/\hbar) + O(h^2)\right)$$

$$= \frac{1}{2m} \left(-i\hbar \nabla^T + c_1 Q\right) \{gWU(\nabla S + c_1 Q)\} \exp(iS/\hbar) + O(h)$$ (4.6)

as a consequence of result (4.2). In employing result (4.4) next, the vector $L$ in it is the {...} term in (4.6), so by (4.4)

$$D\psi = \frac{1}{2m} (\nabla S + c_1 Q)^T U^T gW(\nabla S + c_1 Q) \exp(iS/\hbar) + O(h)$$

$$= \frac{1}{2m} (\nabla S + c_1 Q)^T gU(\nabla S + c_1 Q) W \exp(iS/\hbar) + O(h)$$ (4.7)

since the matrix $U$ is symmetric, and the order in which the scales $g$ and $W$ occur in the product is unimportant. The temporal derivative in (3.6) is approximated as

$$i\hbar g \frac{\partial \psi}{\partial t} = i\hbar g \left(\frac{\partial}{\partial t} \left(W \exp(iS/\hbar) + O(h^2)\right)\right)$$

$$= -g \frac{\partial S}{\partial t} W \exp(iS/\hbar) + O(h).$$ (4.8)

Then the wave equation (3.6) is approximated, by combining the results (4.7) and (4.8), if the requirement

$$gW \exp(iS/\hbar) \left(\frac{1}{2m} (\nabla S + c_1 Q)^T U(\nabla S + c_1 Q) + c_2 \phi + \frac{\partial S}{\partial t}\right) + O(h) = 0$$ (4.9)

is met; and a necessary condition for it is

$$g \left(\frac{1}{2m} (\nabla S + c_1 Q)^T U(\nabla S + c_1 Q) + c_2 \phi + \frac{\partial S}{\partial t}\right) = 0$$

or where the generalized coordinate system is non-singular

$$\frac{1}{2m} (\nabla S + c_1 Q)^T U(\nabla S + c_1 Q) + c_2 \phi + \frac{\partial S}{\partial t} = 0.$$ (4.10)

This last equation can have two labels. It is, in the first place the “eikonal” equation arising from the construction of a geometrical optics approximation (4.5) to the solution of the wave equation (3.6). In the second, it is the Hamilton-Jacobi equation of classical mechanics appropriate to the same dynamical environment

$$H(\nabla S, P) + \frac{\partial S}{\partial t} = 0$$ (4.11)
where $\nabla S = p$ (Synge & Griffiths, 1959, p.468), whose solution provides an abstract
description of families of particle trajectories arising from families of initial data – at least in
principle.

The procedure used in obtaining equation (4.10) is, in a sense, reversible. For any suitably
smooth scalar-valued function $G(P)$ the equation

$$\frac{1}{2m}(\nabla S + c_1 Q)^TGU(\nabla S + c_1 Q) + c_2 G \phi + G \frac{\partial S}{\partial t} = 0$$

is $G$ times a physically possible Hamilton-Jacobi equation, and one can infer a coordinate
specific wave equation from it

$$\frac{1}{2m}(-i\epsilon \nabla + c_1 Q)GU(-i\epsilon \nabla + c_1 Q)\psi + c_2 G \phi \psi - \epsilon G \frac{\partial \psi}{\partial t} = 0,$$

whose geometrical optics approximate solution

$$\psi \sim W \exp(iS/\epsilon) + O(\hbar^2)$$
generates the eikonal equation (4.12) when $\epsilon$ is the small parameter. But, if and only if

$$G = g = (\det U)^{-1/2},$$

does this wave equation satisfy the rules of the transformation calculus. (Of course, one must
set $\epsilon = \hbar$ in order to ensure the reduced ($Q = \phi = 0$) equation in Cartesian coordinates is
satisfied by a de Broglie wave.)

5 The transport equation

While not strictly relevant to the present discussion, for completeness the “transport” equation,
which governs the evolution of the amplitude function $W$ introduced in Section 4, is now calculated. The argument is stripped to essentials if given in Cartesian coordinates, in
which case the wave equation is (3.4) and the corresponding eikonal equation ($g = 1, U = I$)
are given by

$$\frac{1}{2m}(\nabla S + c_1 A)^T(\nabla S + c_1 A) + c_2 \phi + \frac{\partial S}{\partial t} = 0 = \frac{1}{2m}(P + c_1 A)^T(P + c_1 A) + c_2 \phi + q.$$

In a solution of this equation by the method of characteristics (Courant & Hilbert 1962,
vol.2, p.103) the characteristic lines of the eikonal equation (5.1) are described by the ordinary
differential equations

$$\frac{dr}{dt} = \frac{1}{m}(P + c_1 A), \quad \frac{dq}{dt} = 1,$$

where $t$ is a parameter used to describe the characteristic strips. The other characteristic
equations, which give expressions for $dS/dt$ and $dP/dt$, are not needed for the present
discussion. They are, however, required to complete the characteristic solution description.

Then, after making the geometrical optics substitution (4.5) in equation (3.4), and collect-
ting terms multiplied by $(-i\hbar)$, one arrives at the transport equation

$$\frac{1}{2m} \left( 2(\nabla S + c_1 A)^T \nabla W + (c_1 \nabla^T A + \nabla^T \nabla S) W \right) + \frac{\partial W}{\partial t} = 0.$$
It is striking that the last equation shares the same characteristic lines (5.2) as the eikonal equation, and so it (5.3) can be expressed as follows: on lines described by (5.2), \( W \) evolves as

\[
\frac{dW}{dt} + \frac{1}{2m} \left( c_1 T A + \nabla^T \nabla S \right) W = 0. \tag{5.4}
\]

While the form of equation (5.4) is simple, and allows qualitative inferences to be drawn, detailed calculations are impractical in all but elementary cases – for example, basic diffraction problems.

It is emphasized at this point that geometrical optics has special applicability, but is unhelpful in the calculation of natural modes. An example arises in the calculation of eigenstates of the hydrogen atom, where an ansatz in spherical polar coordinates, effectively

\[
\psi(r, \theta, \phi, t) = R(r/\bar{\hbar}) T(\theta) F(\phi) e^{i\lambda t} \tag{5.5}
\]

is introduced into the \( Q = 0 \) Schrödinger wave equation. This assumed form selectively stretches the \( r \) coordinate, whilst geometrical optics treats all coordinates equally.

### 6 Angular momentum

Inferring the equation governing the transformation eigenstates for the square of the modulus of angular momentum (\( M^2 \)) of a particle provides a model for extensions to the method of Section 4. In Cartesian coordinates the required quantity is

\[
M^2 = (r \times \mathbf{P})^T (r \times \mathbf{P}) \tag{6.1}
\]

and the equation governing the transformation eigenstates is to be inferred. This is done most easily by effecting a change to spherical polar coordinates \((r, \theta, \phi)\)

\[
x = r \sin \theta \cos \phi \quad 0 \leq r
\]

\[
y = r \sin \theta \sin \phi \quad 0 \leq \phi < 2\pi
\]

\[
z = r \cos \theta \quad 0 \leq \theta \leq \pi, \tag{6.2}
\]

as generalized coordinates.

The kinetic energy of a particle of mass \( m \) is

\[
\mathcal{K} = \frac{m}{2} (\dot{r}^2 + r^2 \sin^2 \theta \, \dot{\phi}^2 + r^2 \dot{\theta}^2), \tag{6.3}
\]

where (\( \dot{\cdot} \)) denotes time derivative, so the generalized momenta components \( \partial \mathcal{K} / \partial \dot{\mathbf{p}} \) are

\[
p_r = m \dot{r}, \quad p_\theta = mr^2 \dot{\theta}, \quad p_\phi = mr^2 \sin^2 \theta \, \dot{\phi}, \tag{6.4}
\]

and consequently

\[
M^2 = m^2 \left( r^4 \sin^2 \theta \, \dot{\phi}^2 + r^4 \dot{\theta}^2 \right)
\]

\[
= \frac{p_\theta^2}{\sin^2 \theta} + \frac{p_\phi^2}{\sin^2 \theta}
\]

\[
= \mathbf{p}^T \mathcal{L} \mathbf{p} \tag{6.5}
\]
where the matrix
\[
\mathbf{L} = \begin{bmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1/\sin^2 \theta
\end{bmatrix}
\]
(6.6)
is defined. Hence the putative eikonal equation for some wave equation could be
\[
\mathbf{p}^T \mathbf{L} \mathbf{p} - M^2 = 0,
\]
but in the light of the previous discussion it will be taken as
\[
\mathbf{p}^T g \mathbf{L} \mathbf{p} - M^2 g = 0,
\]
(6.7)
where the Jacobian determinant evaluates as
\[
g = r \sin \theta.
\]
(6.8)
The inferred “wave” equation governing the transformation eigenstates \(\Omega(M)\) is therefore
\[
(-i\hbar \nabla^T)g \mathbf{L}(-i\hbar \nabla)\Omega - M^2 g \Omega = 0,
\]
(6.9)
or explicitly
\[
\hbar^2 \left\{ \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Omega}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2 \Omega}{\partial \phi^2} \right\} + M^2 \sin \theta \Omega = 0
\]
(6.10)
after the \(r\) factor is divided out. This result (6.10) is standard.

7 The Klein-Gordon and Dirac equations

The relativistic Hamiltonian describing the motion of a charged particle in an electromagnetic field whose vector and scalar potentials are \(\mathbf{A}\) and \(\phi\) is (in Cartesian coordinates, from Mott \& Sneddon, 1963, p. 293)
\[
H = c \sqrt{m^2 c^2 + (\mathbf{P} + c_1 \mathbf{A})^T (\mathbf{P} + c_1 \mathbf{A}) + c_2 \phi},
\]
(7.1)
so the corresponding Hamilton-Jacobi equation is
\[
\frac{1}{c} \left( \frac{\partial S}{\partial t} + c^2 \phi \right) + \sqrt{m^2 c^2 + (\nabla S + c_1 \mathbf{A})^T (\nabla S + c_1 \mathbf{A})} = 0
\]
(2.2)
where \(c\) is the speed of light.

There are two ways of coping with the fractional power – at least in wave mechanics. The first is to multiply equation (7.2) by
\[
- \frac{1}{c} \left( \frac{\partial S}{\partial t} + c_2 \phi \right) + \sqrt{m^2 c^2 + (\nabla S + c_1 \mathbf{A})^T (\nabla S + c_1 \mathbf{A})},
\]
to obtain the equation
\[
- \frac{1}{c^2} \left( \frac{\partial S}{\partial t} + c_2 \phi \right)^2 + m^2 c^2 + (\nabla S + c_1 \mathbf{A})^T (\nabla S + c_1 \mathbf{A}) = 0,
\]
(7.3)
one of whose roots, namely (7.2), is the eikonal equation for the Klein-Gordon model. On the other hand, the natural linear wave equation whose eikonal equation is (7.3) is constructed as follows. Define the 4-vector

$$\Pi = \begin{pmatrix} \mathbf{P} + c_1 \mathbf{A} \\ (q + c_2 \phi)/c \end{pmatrix}$$

(7.4)

and the (diagonal) 4 x 4 matrix

$$\Lambda = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

(7.5)

(with $P = \nabla S$ and $q = \partial S/\partial t$) and consider

$$\Pi^T \Lambda \Pi + m^2 c_2 = 0.\nonumber$$

(7.6)

A wave equation which has eikonal (7.6) is

$$\left[(-i\hbar \nabla + c_1 \mathbf{A})^T, \frac{1}{c} (-i\hbar \frac{\partial}{\partial t} + c_2 \phi) \right] \Lambda \left[(-i\hbar \nabla + c_1 \mathbf{A}), \frac{1}{c} (-i\hbar \frac{\partial}{\partial t} + c_2 \phi) \right]^T \psi + m^2 c_2 \psi = 0$$

(7.7)

and this is the Klein-Gordon model.

The concomitant transport equation is obtained as follows. Using a slightly modified parameter $\tau$ say, then along the characteristic lines of equation (7.2) are given by

$$\frac{d\mathbf{r}}{d\tau} = \mathbf{P} + c_1 \mathbf{A} \nonumber$$

(7.8a)

$$\frac{dt}{d\tau} = -\frac{1}{c} (q + c_2 \phi), \nonumber$$

(7.8b)

and the geometrical optic amplitude evolves as

$$2 \frac{dW}{dT} + \left(\nabla^T \nabla S - c^{-2} \frac{\partial^2 S}{\partial t^2} + c_1 \nabla^T \mathbf{A} - c_2 c^{-2} \frac{\partial \phi}{\partial t} \right) W = 0.\nonumber$$

(7.9)

The second way of treating the Hamiltonian (7.1) was suggested by Dirac; the following is essentially an account of Dirac’s work as given by Mott & Sneddon (1963, p.296). When taken to its ultimate conclusion, Dirac’s approach has proved to be more fruitful than the Klein-Gordon, supplying as it does an accurate measure of the magnetic moment of the electron (“spin”), and providing a suggestion of anti-matter (positron).

The core of Dirac’s approach is to introduce elements of a Clifford algebra of 4 x 4 matrices

$$\alpha_x, \alpha_y, \alpha_z, \alpha$$

with the properties

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \alpha^2 = I$$

where $I$ is the identity, and anti-commutivity

$$\alpha_x \alpha_y = -\alpha_y \alpha_x \text{ etc.}$$

$$\alpha \alpha_x = -\alpha_x \alpha \text{ etc.}$$

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so that the surd in equation (7.1) can be evaluated
\[
\sqrt{m^2c_2 + (\mathbf{P} + c_1 \mathbf{A})^T(\mathbf{P} + c_1 \mathbf{A})I} = [(\mathbf{P} + c_1 \mathbf{A})^T, m^2c^2] \mathcal{A},
\]
(7.12)
if \( \mathcal{A} \) represents the column “vector” of Clifford matrices
\[
\mathcal{A} = \begin{pmatrix} \alpha_x \\ \alpha_y \\ \alpha_z \\ \alpha \end{pmatrix}.
\]
(7.13)
The statement (7.12) is thus a linear combination of Clifford matrices. Thus Dirac’s Hamilton-Jacobi statement would be
\[
\frac{1}{c}(q + c_2 \phi)I + \left[ \left( (\mathbf{P} + c_1 \mathbf{A})^T, m^2c^2 \right) \mathcal{A} \right] = 0,
\]
(7.14)
which is the eikonal equation for his vector wave equation
\[
\frac{1}{c} \left( -i\hbar \frac{\partial}{\partial t} + c_2 \phi \right) \tilde{\psi} + \left[ \left( (-i\hbar \nabla + c_1 \mathbf{A})^T, m^2c^2 \right) \mathcal{A} \right] \tilde{\psi} = 0,
\]
(7.15)
where \( \tilde{\psi} \) is a 4-vector of unknowns, and the geometrical optics ansatz is
\[
\tilde{\psi} = W \exp(iS/\hbar)
\]
(7.16)
with \( W \) a 4-vector.

References and notes


Mott & Sneddon’s book is a curate’s egg. Unfortunate aspects include: different notations to mean the same operation; identical notations for different variables; errors in derivations. Good aspects include explanation of Pauli spin matrices, for example.

Basdevant & Dalibard’s book is uniformly to a high standard, although excessively formal and algebraic sometimes. Good examples are worked out.