

A QUANTUM ROUTE TO HAMILTON–JACOBI EQUATION: COMMENTS AND REMARKS

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Abstract. We consider the short-wave limit of evolutionary wave equations to derive the Hamilton–Jacobi equation. In particular we consider how to get wave mechanics from the abstract picture on Hilbert spaces. This ‘realisation’ contains an additional ingredient which resembles the classical configuration space. We comment on the fact that Hamilton–Jacobi theory only considers one of the two equations obtained in the appropriate limit. We also comment on the fact that the superposition rule for the linear equation is no longer available for the approximate equation.

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1. Introduction. According to our present understanding, the description of physical reality should be a quantum description. Classical description should be obtained as an appropriate limit of the quantum one. A natural parameter to be used in this process limit should be Planck's constant \hbar [D2]. The belief, based on physical intuition, is that when the magnitude of actions involved in the physical system we are analysing is very large compared with \hbar , the classical description should be recovered. However the existence of alternative pictures to describe quantum phenomena does not help in making the 'process limit' well defined and unique.

In this paper we choose to consider the process of limit within the Schrödinger picture, what is known as *wave mechanics* [EMS]. In this picture, the analogue of the 'short-wave' limit of D'Alembert wave equation, gives us the Hamilton–Jacobi equation as the eikonal equation. This coincides with the equations of the characteristics of the evolutionary 'hyperbolic partial differential equation'; the Hamiltonian function entering the Hamilton–Jacobi equation defines Hamilton equations whose solutions on the phase-space, when projected onto the configuration space, give what are known as the bicharacteristics. In this manner we go from the evolutionary partial differential equation on the 'configuration space' to the Hamilton ordinary differential equation on the cotangent bundle of the configuration space. For a modern geometric approach to Hamilton–Jacobi equation see [CGMMMR1, CGMMMR2].

We shall briefly recall how we go from the Schrödinger–Dirac equations on some Hilbert space to the Schrödinger wave equations on the square integrable functions on the configuration space. We hope to make clear the basic steps and assumptions we use to recover the classical description. We also comment on the role played by the obtained classical equations when we try to reconstruct the equations we started with.

Some comments on the lessons we may learn from this process limit are made in the final section.

2. Quantum mechanics on Hilbert spaces and wave functions. In the Hilbert space picture, with every physical system we associate a Hilbert space \mathcal{H} . Due to the probabilistic interpretation of quantum mechanics, pure states are not vectors but rather rays in \mathcal{H} , observables are represented by (essentially) self-adjoint linear operators acting on rays of the Hilbert space \mathcal{H} . The time-evolution is ruled by the Dirac–Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle, \quad (1)$$

where the self-adjoint operator H is the generator of the dynamics. Here we find convenient to use the bra-ket notation of Dirac [D1] for vectors in the Hilbert space.

A very convenient way to parametrise the 'Hilbert manifold' of rays, the complex projective space associated to \mathcal{H} , is by means of rank-one projectors

$$\rho_{|\psi\rangle} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \quad (2)$$

This representation makes immediately clear that these rank-one projectors are invariant under multiplication of $|\psi\rangle$ by a non-zero complex number λ , i.e. $\rho_{\lambda|\psi\rangle} = \rho_{|\psi\rangle}$.

The evolution equation on this space is given by the Landau–von Neumann equation

$$i\hbar \frac{d}{dt} \rho_\psi = [H, \rho_\psi]. \quad (3)$$

Due to linearity of this equation, we can easily extend it from pure states to convex combinations

$$\rho = \sum_j c_j \rho_{\psi_j}, \quad c_j \geq 0, \quad \sum_j c_j = 1.$$

As $c_j \geq 0$ and $\sum_j c_j = 1$, this set of coefficients may be interpreted as a ‘probability vector’, finite or infinite. The combination represents an ensemble of pure states. The equation of evolution will be written on the full space of states as

$$i\hbar \frac{d}{dt} \rho = \sum_j c_j \left(i\hbar \frac{d}{dt} \rho_{\psi_j} \right) = \sum_j c_j [H, \rho_{\psi_j}] = [H, \rho].$$

The usual description of pure states in terms of wave-type equations requires that we identify a ‘configuration manifold’ M which is immersed in the Hilbert space \mathcal{H} with the help of a maximal set of pairwise commuting operators whose joint spectrum is the differentiable manifold M . Moreover, we need to choose an appropriate measure μ_M to define the Hilbert space $\mathcal{H} = \mathcal{L}^2(M, \mu_M)$. In this manner with every point $m \in M$ we can associate a unique non-zero vector $|m\rangle \in \mathcal{H}$. We also require that

$$\int |m\rangle \langle m| d\mu_M = 1,$$

i.e. the family of vectors associated with M provides a resolution of the identity. This completeness requirement ensures that states associated with M are sufficient to answer any possible physical question we may wish to ask on the physical system we are describing.

This family of vectors $\{|m\rangle | m \in M\}$, satisfying the resolution of the identity, may be used to define a ‘coordinate system’ on the Hilbert space, we set $\psi(m) = \langle m|\psi\rangle$ or, what is the same,

$$|\psi\rangle = \int_M \psi(m) |m\rangle d\mu_M.$$

Once such ingredients have been chosen, pure states will be described by normalised wave functions $\psi(m)$, and $\psi^*(m)\psi(m)$ represents a probability density on M . Operators, and observables, will now be represented by differential operators on M . These operators turn out to be, in general, unbounded operators and we will encounter ‘domain problems’. A special class of operators is provided by pairwise commuting operators (a maximal set of commuting operators) which act as multiplication operators

$$(\widehat{f}\psi)(m) = f(m)\psi(m);$$

they represent the subalgebra of order zero differential operators and coincide with smooth functions on M .

Therefore, differential operators play a crucial role in Quantum Mechanics and as far as the configuration space is not \mathbb{R}^n anymore, we should look more carefully at the definition of the concept of differential operator trying to extend such concept from \mathbb{R}^n

to arbitrary differentiable manifolds and we can follow the Weyl approach to differential operators. The elements of the linear space $\mathfrak{X}(M)$ of vector fields on M , say, are homogeneous first order differential operators which act as derivations on the algebra of multiplicative operators associated with $\mathcal{F}(M)$.

By considering the linear space $\widehat{\mathcal{F}}(M) = \{\widehat{f} \mid f \in \mathcal{F}(M)\}$ as a Lie algebra with trivial Lie product, together with the Lie algebra of derivations we can define the Holomorph Lie algebra

$$\text{Hol}(\widehat{\mathcal{F}}) : [(\widehat{f}_1, X_1), (\widehat{f}_2, X_2)] = (\mathcal{L}_{X_1} f_2 - \mathcal{L}_{X_2} f_1, [X_1, X_2]),$$

where \mathcal{L}_X denotes the Lie derivative with respect to X .

The enveloping algebra of the Holomorph Lie algebra on M provides the algebra of differential operators on M .

By using the Hermitean structure

$$\langle \psi_1 | \psi_2 \rangle = \int_M \psi_1^*(m) \psi_2(m) d\mu_M,$$

we can consider observable operators as those differential operators which are (essentially) self-adjoint with respect to the Hermitean product we have defined.

Different choices of the maximal set of pairwise commuting operators with joint spectrum being a differential manifold may be selected, for instance we might use position operators, momentum operators, or holomorphic or antiholomorphic operators.

By using the space of differential operators the Dirac–Schrödinger equation will acquire the symbolic form

$$i\hbar \frac{d}{dt} \psi = (a_0 \widehat{f}_0 + a_1 D_1 + a_2 D_2 + \dots + a_n D_n) \psi,$$

where \widehat{f}_0 stays for an operator of order zero, while D_k stays for a differential operator of order k , and a_0, a_1, \dots, a_n are functions on M .

In non-relativistic quantum mechanics, usually, in the position representation the operator describing the evolution is no more than second order. We may write symbolically

$$H = cD_2 + bD_1 + a\widehat{V}.$$

REMARK. Very often M itself may carry a Lie group structure, then the immersion of M in \mathcal{H} passes through a unitary irreducible representation of M along with a fiducial analytical vector $|\psi_0\rangle$, we would have

$$U(m)|\psi_0\rangle = |m\rangle.$$

For instance this is the case of coherent states or generalised coherent states [P].

We shall provide now a specific example of a manifold M which is a Lie group and show what is meant by the immersion of M into the Hilbert space. We may consider the well known case of a symplectic vector space $M = (V, \omega)$. An immersion of M into a Hilbert space \mathcal{H} may be built up in the following way. First we consider a Weyl system on V , say an up to a factor unitary representation of the Abelian vector group V , say for any $v \in V$,

$$v \mapsto W(v) \in \mathcal{U}(\mathcal{H}),$$

with the property

$$W(v_1)W(v_2)W^\dagger(v_1)W^\dagger(v_2) = e^{i\omega(v_1, v_2)}I.$$

If $|0\rangle$ is any fiducial vector in \mathcal{H} we immerse V into \mathcal{H} by setting $|v\rangle = W(v)|0\rangle$. By selecting a Darboux chart (atlas) for ω , say $\omega = dx \wedge d\alpha$, we may define $W(v)$ to be

$$W(v) = e^{i(x\widehat{P} - \alpha\widehat{Q})},$$

where \widehat{P} and \widehat{Q} act on the Hilbert space \mathcal{H} with an action provided by Stone–von Neumann construction:

$$\begin{cases} \lim_{s \rightarrow 0} \frac{W(sx, \alpha)|\psi\rangle - |\psi\rangle}{s} = x\widehat{P}|\psi\rangle \\ \lim_{s \rightarrow 0} \frac{W(x, s\alpha)|\psi\rangle - |\psi\rangle}{s} = \alpha\widehat{Q}|\psi\rangle \end{cases}$$

which defines both the action of \widehat{P} and the action of \widehat{Q} along with their domain when the limit exists.

It is possible to consider \mathcal{H} as the space of square integrable functions on any Lagrangian subspace of V . This Lagrangian subspace may be thought of as the joint spectrum of a maximal set of pairwise commuting operators, those operators that eventually will act as multiplication operators. Let us select one such subspace and denote it by \mathbb{R}^n , $\dim V = 2n$. We may use coordinates (y_1, \dots, y_n) on \mathbb{R}^n and we consider $\{(\mathbf{x}, \boldsymbol{\alpha})\}$ coordinates for $T^*\mathbb{R}^n$. Then

$$W(\mathbf{x}, \boldsymbol{\alpha}) = e^{i(\mathbf{x}\cdot\widehat{\mathbf{P}} - \boldsymbol{\alpha}\cdot\widehat{\mathbf{Q}})}$$

will act on square integrable functions on \mathbb{R}^n with respect to the Lebesgue measure

$$\begin{cases} W(\mathbf{x}, 0)\psi(\mathbf{y}) = \psi(\mathbf{x} + \mathbf{y}), \\ W(0, \boldsymbol{\alpha})\psi(\mathbf{y}) = e^{i\boldsymbol{\alpha}(\mathbf{y})}\psi(\mathbf{y}). \end{cases}$$

These operators are clearly unitary and the infinitesimal operators \widehat{P} and \widehat{Q} will be represented by $i\partial/\partial\mathbf{y}$ and multiplication by the components of \mathbf{y} , respectively.

Here we consider functions $f(\mathbf{y})$ as an Abelian Lie algebra and the algebra of derivations generated by $\{\partial/\partial y^1, \dots, \partial/\partial y^n\}$.

Then the holomorph will be described by differential operators $\sum_{J=0}^N a_J \frac{\partial^{1J}}{\partial \mathbf{y}^J}$, with J a multi-index.

A specific example would be provided by the harmonic oscillator in one dimension. We would use $\phi(p)$, $x = i\hbar\partial/\partial p$, $\widehat{p} = p \cdot$. The following operators will behave like annihilation and creation operators which by iteration will build up the full Hilbert space acting on the fiducial state identified by the annihilation operator:

$$\begin{aligned} \left(p + \frac{\partial}{\partial p}\right)e^{-p^2/2} &= (p - p)e^{-p^2/2} = 0, \\ \left(p - \frac{\partial}{\partial p}\right)e^{-p^2/2} &= (p + p)e^{-p^2/2} = 2pe^{-p^2/2}. \end{aligned}$$

In a coming example we shall consider also the case where we select holomorphic coordinates.

By properly normalising the functions that we generate with iterated use of the creation operator we obtain a basis of square-integrable functions on the real line parametrised by the momentum coordinate.

It is also possible to immerse a generic manifold M with a volume form Ω . The volume form defines a measure on M , say μ_Ω , and we can consider the Hilbert space of square integrable functions on M , $\mathcal{L}^2(M, \mu_\Omega)$. We choose an orthonormal set of functions $\{\phi_n(m) \mid n \in \mathbb{N}\}$ satisfying the finiteness and positiveness condition

$$0 < k(m) = \sum_{n \in \mathbb{N}} |\phi_n(m)|^2 < \infty,$$

almost everywhere. We select a Hilbert space \mathcal{H} in which we would like to immerse M and select an orthonormal basis $\{|n\rangle \mid n \in \mathbb{N}\}$. We define now

$$|m\rangle = \frac{1}{k(m)} \sum_{n \in \mathbb{N}} \phi_n^*(m) |n\rangle$$

and we find that

$$\langle m|m\rangle = 1, \quad \int_M k(m) |m\rangle \langle m| d\mu_\Omega(m) = I_{\mathcal{H}},$$

which represents a generalisation of the construction of coherent states.

In this immersion of M in the Hilbert space \mathcal{H} we can represent also operators as functions on the manifold and viceversa associate operators with functions on M . We obtain a non-local product on the space of functions which is provided by the image of the product of operators on the Hilbert space and vice versa.

We have a (quantiser) map

$$f \mapsto A_f = \int_M k(m) f(m) |m\rangle \langle m| d\mu_\Omega(m),$$

and a (dequantiser) map

$$A \mapsto f_A(m) = \langle m|A|m\rangle.$$

As an example of a different choice of Lagrangian subspace we recall now the usual construction of coherent states.

In our previous Weyl system, we can set

$$M = \mathbb{R}^2 \equiv \mathbb{C} = \left\{ z = \frac{\alpha + ix}{\sqrt{2}} \right\},$$

with the Lebesgue measure

$$d\mu_\Omega = \frac{d^2z}{\pi} = \frac{d\alpha dx}{2\pi}.$$

An appropriate orthonormal set would be

$$\left\{ \phi_n(z) = e^{-|z|^2/2} \frac{\bar{z}^n}{\sqrt{n!}}, \quad n = 0, \dots \right\}.$$

If we now consider the Hilbert space in which we want to immerse our manifold space say with basis $|0\rangle, |1\rangle, \dots, |n\rangle, \dots$, the standard Fock space we get the immersion in \mathcal{H}

$$|m\rangle \equiv |z\rangle = \sum_{n=0}^{\infty} \frac{e^{-|z|^2/2}}{\sqrt{n!}} |n\rangle.$$

They satisfy

$$\int_{\mathbb{C}} |z\rangle\langle z| \frac{d^2z}{\pi} = I_{\mathcal{H}},$$

with the scalar product

$$\langle z|z'\rangle = e^{-|z-z'|^2/2} e^{i\omega(z,z')}.$$

Again it is possible to define a quantiser and dequantiser map

$$A_f = \int_{\mathbb{C}} f(z, \bar{z}) |z\rangle\langle z| \frac{d^2z}{\pi}.$$

The operator A_f is symmetric if $f(z, \bar{z})$ is real valued, bounded if $f(z, \bar{z})$ is bounded, and selfadjoint if real-semibounded (through Friedrichs extension).

We have also

$$A_f \mapsto f(z, \bar{z}) = \langle z|A_f|z\rangle = \int_{\mathbb{C}} f(z', \bar{z}') |z\rangle\langle z'|^2 \frac{d^2z'}{\pi}.$$

If we use C^∞ functions $f(z, \bar{z}) = z$ or $f(z, \bar{z}) = \bar{z}$ we get

$$\begin{aligned} A_z &= a & a|n\rangle &= \sqrt{n}|n-1\rangle, \quad n \geq 1, \quad \text{and } a|0\rangle = 0 \\ A_{\bar{z}} &= a^\dagger & a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \end{aligned}$$

and

$$[a, a^\dagger] = I.$$

3. Wave mechanics on \mathbb{R}^n . The way it was formulated by Schrödinger required to set $M = \mathbb{R}^n$. By introducing Cartesian coordinates, say (x_1, x_2, \dots, x_n) , the algebra of pairwise maximally commuting operators is ‘generated’ by $\hat{x}_1, \hat{x}_2, \dots, \hat{x}_n$, while the algebra of derivations will be generated by $\partial/\partial x_1, \partial/\partial x_2, \dots, \partial/\partial x_n$. The algebra of differential operators is the enveloping algebra of the Holomorph Lie algebra of $\mathcal{F}(\mathbb{R}^n)$.

A generic differential operator will be written as

$$D = \sum_{|\sigma| \leq r} g_\sigma \frac{\partial^{|\sigma|}}{\partial x_\sigma}, \quad g_\sigma \in \mathcal{F}(\mathbb{R}^n),$$

and $\sigma = (i_1, \dots, i_n)$, $|\sigma| = \sum_k i_k$, while

$$\frac{\partial^{|\sigma|}}{\partial x_\sigma} = \frac{\partial^{|\sigma|}}{\partial x_1^{i_1} \dots \partial x_n^{i_n}}.$$

Here \mathbb{R}^n may be thought of as the translation Lie group and then the set of derivations $\{\partial/\partial x_j \mid j = 1, \dots, n\}$ will be a basis of infinitesimal generators. Further details on differential operators from this point of view may be found in a paper by Grabowski and Poncin [GP] (see also [GKP]).

When the manifold is not \mathbb{R}^n but a differentiable manifold we may define a differential operator D_k of degree k as an \mathbb{R} -linear map on $\mathcal{F}(M)$ satisfying the condition

$$[\dots [D_k, \hat{f}_0], \hat{f}_1] \dots, \hat{f}_k] = 0,$$

and such that

$$[\dots [D_k, \hat{f}_0], \hat{f}_1] \dots, \hat{f}_{k-2}]$$

is a vector field, where $[\cdot, \cdot]$ is the usual commutator for linear operators. For further details on these aspects we refer to [CIMM]. From the last property, it follows that the multiplication operator-function $[\dots [D_k, \widehat{f}_1] \dots, \widehat{f}_k]$ does not depend on possible translations $\widehat{f}_j \mapsto \widehat{f}_j + \widehat{c}_j$, c_j being a real or complex number. Therefore we may define what is called a principal symbol for the operator D_k of degree k to be the symmetric k -multilinear map

$$\sigma(D_k)(df_1, \dots, df_k) = [\dots [D_k, \widehat{f}_1], \dots, \widehat{f}_k].$$

The fact that $\sigma(D_k)$ is symmetric follows from the Lie algebra structure of the algebra of differential operators, indeed we have

$$[\widehat{f}_2, [D, \widehat{f}_1]] = [[\widehat{f}_2, D], \widehat{f}_1] + [D, [\widehat{f}_1, \widehat{f}_2]].$$

We deduce that

$$[[D, \widehat{f}_1], \widehat{f}_2] = [[D, \widehat{f}_2], \widehat{f}_1].$$

As an example

$$D = g_{jk} \frac{\partial^2}{\partial x_j \partial x_k}$$

has principal symbol $\sigma(D)$ given by

$$\sigma(D)(df_1, df_2) = g_{jk} \frac{\partial f_1}{\partial x_j} \frac{\partial f_2}{\partial x_k}.$$

We may consider $\sigma(D) = g_{jk} \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k}$.

If, with abuse of notation, we replace df with $\theta_0 = p^j dx_j$ we find also

$$\sigma(D)(\theta_0, \theta_0) = g_{jk} p^j p^k.$$

When $f_1 = S = f_2$ we get

$$\sigma(D)(dS, dS) = g_{jk} \frac{\partial S}{\partial x_j} \frac{\partial S}{\partial x_k}.$$

We recognise the important role that the principal symbol, the contravariant symmetric tensor

$$G = g_{jk} \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k},$$

plays. When each derivation $\partial/\partial x_j$ is thought of as a linear function on the fiber of the cotangent bundle, it can be replaced by the ‘momentum’ p^j and the symmetric tensor G by the polynomial function $g_{jk} p^j p^k$.

When the contravariant tensor field is thought of as a differential operator we have

$$D_G(f) = g_{jk} \frac{\partial^2 f}{\partial x_j \partial x_k}.$$

The transition from the contravariant tensor field to the second order differential operator is however ambiguous, indeed we could decide that the associated second order differential operator would be

$$\tilde{D}_G(f) = \frac{\partial}{\partial x_j} \left(g_{jk} \frac{\partial f}{\partial x_k} \right),$$

or also

$$\tilde{D}_G(f) = \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_k} (g_{jk}f).$$

The informed reader will recognise in this ambiguity the typical ambiguity we face in the so called quantisation procedure with ‘ordering problems’. Let us indulge a little more on the association of a differential operator with a contravariant tensor field. Actually, to go from the principal symbol

$$G = g_{jk} \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k}$$

to a second order differential operator we need to fix a rule on the order in which the differential operators g_{jk} (of order zero), $\partial/\partial x_j$ and $\partial/\partial x_k$ (of first order) should act on a given function; clearly this order is arbitrary and the various final differential operators we would get depend on the chosen order, and they will differ by lower order differential operators. For instance, we may use a non-holonomic basis which would diagonalise the symmetric contravariant tensor, say

$$G = X_j \otimes X_k \delta^{jk},$$

then $\mathcal{L}_{X_j} \mathcal{L}_{X_k} f$ and $\mathcal{L}_{X_k} \mathcal{L}_{X_j} f$ would differ by $[X_j, X_k]f$.

As an interesting example, let us consider the d’Alembert equation we have on $M = \mathbb{R}^4$ with adapted Minkowski coordinates

$$\left(\frac{\partial^2}{\partial x_0^2} - \frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} \right) u = 0. \tag{4}$$

The principal symbol gives rise to the contravariant symmetric tensor field

$$\frac{\partial}{\partial x_0} \otimes \frac{\partial}{\partial x_0} - \frac{\partial}{\partial x_1} \otimes \frac{\partial}{\partial x_1} - \frac{\partial}{\partial x_2} \otimes \frac{\partial}{\partial x_2} - \frac{\partial}{\partial x_3} \otimes \frac{\partial}{\partial x_3},$$

which on phase space defines the quadratic function

$$p_0^2 - p_1^2 - p_2^2 - p_3^2.$$

The equation $\square u = 0$ gives rise to the zero mass-shell relation $p_0^2 - p_1^2 - p_2^2 - p_3^2 = 0$.

The Hamilton–Jacobi equation emerges as

$$\sigma(\square)(dS, dS) = 0, \quad \text{or} \quad \left(\frac{\partial S}{\partial x_0} \right)^2 - \left(\frac{\partial S}{\partial x_1} \right)^2 - \left(\frac{\partial S}{\partial x_2} \right)^2 - \left(\frac{\partial S}{\partial x_3} \right)^2 = 0.$$

Thus with a differential operator D_k we can associate the PDE for S in the form

$$\underbrace{[\dots [D_k, \hat{S}], \hat{S}], \dots, \hat{S}}_{k \text{ times}} = 0,$$

or the Hamiltonian

$$\sigma(D_k)(\theta_0, \theta_0, \dots, \theta_0),$$

with the ‘mass-shell’ relation

$$\sigma(D_k)(\theta_0, \theta_0, \dots, \theta_0)S = 0.$$

As the d'Alembert equation may also be obtained by means of the Hodge codifferential, say $\delta = *d*$, with $*$ the Hodge operator, we have the intrinsic form of the wave equation

$$\delta du = 0.$$

It is now possible to consider the principal symbol

$$[[\delta d, \widehat{f}_1], \widehat{f}_2] = \sigma(\delta d)(df_1, df_2).$$

By spelling out the computations we have

$$\begin{aligned} [[\delta d, \widehat{f}_1], \widehat{f}_2]u &= [\delta d, \widehat{f}_1](\widehat{f}_2 u) - \widehat{f}_2([\delta d, \widehat{f}_1](u)) \\ &= \delta d(\widehat{f}_1(\widehat{f}_2 u)) - \widehat{f}_1(\delta d)(\widehat{f}_2 u) - \widehat{f}_2(\delta d(\widehat{f}_1 u) - \widehat{f}_1(\delta du)) \\ &= \delta d(f_1 f_2 u) - f_1 \delta d(f_2 u) - f_2(\delta d(f_1 u) - f_1(\delta du)), \end{aligned}$$

and after several cancellations we obtain

$$[[\delta d, \widehat{f}_1], \widehat{f}_2]u = \langle df_1, df_2 \rangle u.$$

The scalar product is the one defined by the metric tensor used to define δ .

3.1. The short-wave limit for the wave equation. If we consider the factorisation $u = Ae^{ik_0 S}$, as $du = e^{ik_0 S} dA + iuk_0 dS$, the d'Alembert equation may be written as

$$\begin{aligned} 0 &= \delta du = \delta(e^{ik_0 S} dA + iuk_0 dS) = *d*(e^{ik_0 S} dA + iuk_0 dS) \\ &= *d(e^{ik_0 S} *dA) + *d(ik_0 u *dS) = *(e^{ik_0 S} ik_0 dS \wedge *dA) \\ &\quad + e^{ik_0 S} *d*dA + ik_0 *(du \wedge *dS) + ik_0 u *d*dS. \end{aligned}$$

We may collect real and imaginary parts separately and we obtain the equations:

$$\begin{aligned} e^{ik_0 S} ik_0 *(dS \wedge *dA) + ik_0 u *d*dS + ik_0 *(e^{ik_0 S} dA \wedge *dS) &= 0, \\ (ik_0)^2 u *(dS \wedge *dS) + e^{ik_0 S} *d*dA &= u \left(-k_0^2 \langle dS | dS \rangle + \frac{\delta dA}{A} \right) = 0. \end{aligned}$$

The first equation reduces to

$$ik_0 *2(dS \wedge *dA) + ik_0 A *d*dS = 0,$$

which can be rewritten as

$$k_0 2A \langle dS, dA \rangle + k_0 A^2 \delta dS = 0,$$

or more simply,

$$\langle dS, dA^2 \rangle + A^2 \delta dS = 0,$$

which gives rise to the continuity equation

$$\delta(A^2 dS) = 0.$$

By introducing the metric tensor G , the 'principal symbol', we find

$$G(dS, dS) = \frac{1}{k_0^2} \frac{\delta dA}{A},$$

which reduces to the Hamilton–Jacobi equation when $\lambda = 1/k_0$ is very small and $\lambda^2 \frac{\delta dA}{A} \simeq 0$. The imaginary part is always a divergence-free vector field $A^2 \text{grad } S$ or a closed 3-form $*A^2 dS$.

The usual representations by means of a fiberwise quadratic function on the cotangent bundle will be in terms of the Liouville 1-form θ_0 , $G(\theta_0, \theta_0)$. The associated Hamiltonian vector field Γ is defined by

$$i_\Gamma d\theta_0 = -\frac{1}{2} dG(\theta_0, \theta_0),$$

where i_Γ denotes the contraction with the vector field Γ .

Projection of integral curves of Γ , the bi-characteristics, will be solutions of the ordinary differential equation on the configuration space

$$\frac{dx_\mu}{dt} = G(dS, dx_\mu).$$

3.2. Principal symbol, Klein–Gordon and Schrödinger equations. From our definition of principal symbol it is quite clear that when the operator is second order the double commutator will not take into account possible first order terms and order zero terms.

To remedy this situation it was proposed [LMSV] to enlarge the carrier space so as to turn the given operator into a homogeneous second order operator. In this enlarged space the principal symbol will also contain information on the lower order terms.

Let us illustrate the procedure for the Klein–Gordon equation and the Schrödinger equation.

a) The Klein–Gordon equation on \mathbb{R}^4 has the form

$$\left(\frac{\partial^2}{\partial x_0^2} - \frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - m_0^2 c^2 \right) u = 0.$$

We can put all terms as homogeneous of the same degree by adding a new degree of freedom s and replacing the function u by the new one $\tilde{u}(x, s) = e^{-is}u(x)$, and then the equation becomes

$$\left(\frac{\partial^2}{\partial x_0^2} - \Delta - m_0^2 c^2 \frac{\partial^2}{\partial s^2} \right) \tilde{u} = 0.$$

The associated Hamilton–Jacobi equation will be

$$\left(\frac{\partial F}{\partial x_0} \right)^2 - \sum_j \left(\frac{\partial F}{\partial x_j} \right)^2 - m_0^2 c^2 \left(\frac{\partial F}{\partial s} \right)^2 = 0.$$

b) We can proceed in a similar way for the *Schrödinger equation*:

$$i\hbar \frac{\partial u}{\partial t} + \frac{\hbar^2}{2m} \Delta u - \hat{V}u = 0.$$

As before we have to add an additional degree of freedom s and a vector field $i\partial/\partial s$ to get

$$-i\hbar \frac{\partial^2 \tilde{u}}{\partial s \partial t} + \frac{\hbar^2}{2m} \Delta \tilde{u} + V \frac{\partial^2 \tilde{u}}{\partial s^2} = 0,$$

with $\tilde{u} = e^{-is}u$. Then, the associated Hamilton–Jacobi equation will be

$$-i\hbar \frac{\partial F}{\partial s} \frac{\partial F}{\partial t} + \frac{\hbar^2}{2m} \left[\left(\frac{\partial F}{\partial x} \right)^2 + \left(\frac{\partial F}{\partial y} \right)^2 + \left(\frac{\partial F}{\partial z} \right)^2 \right] + V \left(\frac{\partial F}{\partial s} \right)^2 = 0.$$

A similar equation was arrived at by Grabowska, Grabowski and Urbański [GGU] but with different motivations.

From here we proceed in the usual manner and to recover results on \mathbb{R}^4 we have to consider the projection from $\mathbb{R}^4 \times S^1$ to \mathbb{R}^4 .

Thus with the presented trick the principal symbol, a (0,2) contravariant tensor, will contain also information on the potential or the mass term. With this requirement, we are naturally brought to consider Kaluza–Klein type of extensions of the Abelian type. For non-Abelian extensions we should start from matrix-valued differential operators where particles would also carry inner degrees of freedom.

4. Comments and remarks. We should notice two main aspects of our derivation:

1. From the wave-type equation, we have obtained a non-linear PDE, composed of two terms: one is the usual Hamilton–Jacobi equation and the other is a continuity equation.

In the standard approach to the Hamilton–Jacobi theory we consider only one of these equations, what happens to the other one?

2. The starting equation is a linear equation, thus it admits of a linear superposition rule for the solutions, what happens with the superposition rule in the short-wave limit?

Having made these remarks, we may reinterpret the quantisation procedure as a way to get a linear PDE from a non-linear one represented by the Hamilton–Jacobi equation.

Notice that the usual quantisation procedure appears to be a way to go from a non-linear PDE, the Hamilton–Jacobi equation, to a linear PDE represented by a wave-type equation. Thus, the more fundamental theory, the quantum description, appears to be simpler than the ‘approximated’ one!

4.1. Comments on the continuity equation. We have seen that the imaginary part of the short-wave limit of the wave-equation gives a continuity equation. Here we would like to consider what happens with it in the classical setting. It is also known that the Hamilton–Jacobi equation

$$H\left(q, \frac{\partial W}{\partial q}\right) = E$$

arises from

$$H\left(q, \frac{\partial S}{\partial q}, t\right) + \frac{\partial S}{\partial t} = 0$$

when, in the time-independent case, we set $S = W - Et$. We recall again that Hamilton–Jacobi equation arises from the search for a canonical transformation from $(q, p; t)$ to $(Q, P; t)$ on the extended phase space by requiring that there exists a function S such that

$$(p_j dq^j - H dt) - (P_k dQ^k - K dt) = dS(q, Q, t),$$

and imposing the additional condition $K \equiv 0$. In the sought for new coordinates, we would have

$$\frac{d}{dt}P_k = 0 = \frac{d}{dt}Q_k,$$

or more generally

$$\frac{d}{dt}f(P, Q, t) = \frac{\partial f}{\partial t}.$$

From the geometrical point of view, a complete solution of the Hamilton–Jacobi equation would define a map

$$dS : \mathcal{Q} \times \mathcal{Q} \rightarrow T^*\mathcal{Q},$$

where \mathcal{Q} is the configuration manifold.

This map allows us to replace the Cauchy data (initial position and initial momentum) with initial position and another position at some later time.

In general there will be open dense submanifolds on which dS will be a diffeomorphism. Moreover

$$\omega_S =: (dS)^*(\omega_0) = d(dS^*\theta_0) = \frac{\partial^2 S}{\partial q_j \partial Q_k} dq^j \wedge dQ^k$$

will be symplectic on the appropriate open dense submanifold. In particular this means that we can define a Hamiltonian vector field on $\mathcal{Q} \times \mathcal{Q}$ associated with the pull back $(dS)^*H$. As $\dot{Q} = 0$ and $\dot{P} = 0$, the vector field will have components only along one of the two factors, we shall get

$$\frac{d}{dt}q_j = \left(\frac{\partial H}{\partial p^j} \right)_{p^j = \partial S / \partial q_j},$$

with an implicit dependence on the variables of the second manifold. For a generalisation of this equation to general bundles see [CGMMMR2].

When $H = p^2/(2m)$, we get $\frac{d}{dt}q = \frac{\partial S}{\partial q}$. As this vector field on $\mathcal{Q} \times \mathcal{Q}$ is Hamiltonian, it will preserve the Liouville volume $\omega_S^{\wedge n}$. Before proceeding, we need the following result:

THEOREM. *If Γ preserves the volume form $f\Omega$, then $f\Gamma$ preserves the volume form Ω .*

This follows easily from Cartan’s identity,

$$0 = -\mathcal{L}_\Gamma(f\Omega) = d(i_\Gamma(f\Omega)) = d(i_{f\Gamma}\Omega) = -\mathcal{L}_{f\Gamma}\Omega.$$

In particular, $d(i_{f\Gamma}\Omega) = 0$.

In our case, Ω will be the symplectic volume on $\mathcal{Q} \times \mathcal{Q}$ and f will be the determinant $\det(\frac{\partial^2 S}{\partial q_j \partial Q_k})$, therefore the formula of page 7 becomes

$$d\left(*\det\left(\frac{\partial^2 S}{\partial q_j \partial Q_k}\right)dS\right) = 0,$$

and it reproduces the imaginary part we have got in the short-wave-limit if we set $A^2 = \det(\frac{\partial^2 S}{\partial q_j \partial Q_k})$. For an alternative proof of this result one may look at [F, EMS, MMM].

Thus, solving the real part of the limit equation we have got in the short-wave limit by means of a complete integral, we also solve the continuity equation, i.e. the imaginary part of the equation that we got in the limit.

EXAMPLE. Let us give a simple example to illustrate the situation. We consider the one-dimensional harmonic oscillator, a corresponding solution for the associated Hamilton–Jacobi equation is

$$W = \frac{m}{2} \omega q^2 \cot Q, \quad p = m\omega q \cot Q, \quad P = \frac{m\omega q^2}{2 \sin^2 Q}.$$

By solving for q and p ,

$$q = \sqrt{\frac{2P}{m\omega}} \sin Q, \quad p = \sqrt{2m\omega P} \cos Q.$$

On the symplectic manifold of boundary data, the pull backs ω_W of the natural symplectic structure on $T^*\mathcal{Q}$ and the Hamiltonian under the map $dW : \mathcal{Q} \times \mathcal{Q} \rightarrow T^*\mathcal{Q}$ will be, respectively, given by

$$\begin{aligned} \omega_W &= d(m\omega q \cot Q \, dq), \\ H_W &= \frac{(m\omega q \cot Q)^2}{2m} + \frac{m\omega^2}{2} q^2, \end{aligned} \tag{5}$$

and the dynamics $dq/dt = \omega q \cot Q$ is a one-parameter family of dynamics depending on the ‘parameter’ Q . From here it is possible to build an approximate solution of the Schrödinger equation associated with the harmonic oscillator as explained in [EMS].

4.2. Comments on the nonlinear real short-wave limit of the wave equations.

Very often, the linearity of the Schrödinger equation is advocated because of interference phenomena. Indeed, Dirac comments that “the superposition that occur in quantum mechanics is of an essentially different nature from any occurring in classical theory, as is shown by the fact that the quantum superposition principle demands indeterminacy in the results of observations in order to be capable of a sensible physical interpretation”.

In the quantum-to-classical transition, the linear Schrödinger equation is replaced first by two coupled nonlinear equations in the amplitude and phase of the wave function. From here, disregarding the term in λ^2 (or \hbar^2) we get the nonlinear partial differential equation represented by the Hamilton–Jacobi equation.

Going back, one may consider a modification of the Hamilton–Jacobi equation, i.e. searching for a correction term to be added to it so as to recover linearity. In other terms one may conceive of the ‘quantisation procedure’ or the ‘wavisation procedure’ as a way to linearise a nonlinear equation.

The way we derive the Hamilton–Jacobi equation from the Schrödinger equation says that we get a non-linear equation out of a linear one.

Once we have written the Hamilton–Jacobi equation in the form

$$H\left(x, \frac{\partial S}{\partial x}\right) = E,$$

we would look for a way to ‘linearise’ this equation.

It appears that any ‘quantisation’ procedure of $H(q, p)$, say by means of the operator $H(q, i\hbar \partial/\partial p)$, would provide a (non-unique) Schrödinger linear equation whose solutions may be superposed and the superposition would be a solution of the non-linear Hamilton–Jacobi equation and may be thought of as an ‘approximate’ superposition of the solutions associated with the two wave-functions we have superposed.

5. Final comments and general considerations. We would like to conclude this paper with some general considerations.

We have derived a nonlinear equation (the Hamilton–Jacobi equation) starting with a linear one. This is rather surprising. Indeed, in physics linear structures usually arise

as approximations to the more accurate nonlinear ones. Here the more accurate one is linear while the approximate one is nonlinear, and we can learn that more fundamental theories may be simpler, even though more abstract, than less fundamental theories.

The classical limit was obtained via a separation of the amplitude from the phase in the wave function, we went from an equation involving two fields (amplitude and phase) to an approximated one which involved only one field. The opposite route would require that we go from one field (the phase) to another one (the wave function) which puts together amplitude and phase. It seems therefore that a unification procedure, versus a reduction or separation procedure, is able to make descriptions much simpler than the separate descriptions. In this respect, the unification of electric field and magnetic field into electromagnetic field has made the theory of electrodynamics much simpler and powerful than the separate theories. Similarly, the unification of wave aspects and corpuscular aspects into the wave mechanics description, has created a more fundamental and simpler theory like quantum mechanics.

We believe that procedures which would make general relativity into a linear theory, perhaps better unifying ‘matter’ and ‘geometry’ into a theory with additional fields, may pave the way for a better theory which would unify the theory of gravitation with quantum mechanics. In this respect one may look at recent papers by M. Taronna and coauthors on Higher spin Interactions in four dimensions [BKST, NT].

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References

- [BKST] N. Boulanger, P. Kessel, E. D. Skvortsov, M. Taronna, *Higher spin interactions in four dimensions: Vasiliev vs. Fronsdal*, J. Phys. A 49 (2016), 095402, 52 pp.
- [CGMMMR1] J. F. Cariñena, X. Gràcia, G. Marmo, E. Martínez, M. C. Muñoz-Lecanda, N. Román-Roy, *Geometric Hamilton–Jacobi theory*, Int. J. Geom. Methods Mod. Phys. 3 (2006), 1417–1458.
- [CGMMMR2] J. F. Cariñena, X. Gràcia, G. Marmo, E. Martínez, M. C. Muñoz-Lecanda, N. Román-Roy, *Structural aspects of Hamilton–Jacobi theory*, Int. J. Geom. Methods Mod. Phys. 13 (2016), 1650017, 29 pp.
- [CIMM] J. F. Cariñena, A. Ibort, G. Marmo, G. Morandi, *Geometry from Dynamics, Classical and Quantum*, Springer, Dordrecht, 2015.
- [D1] P. A. M. Dirac, *A new notation for quantum mechanics*, Proc. Cambridge Philos. Soc. 35 (1939), 416–418.
- [D2] P. A. M. Dirac, *Principles of Quantum Mechanics*, 5th Ed., Oxford Univ. Press, 1982.
- [EMS] G. Esposito, G. Marmo, G. Sudarshan, *From Classical to Quantum Mechanics*, Cambridge Univ. Press, Cambridge, 2004.
- [F] V. A. Fock, *Fundamentals of Quantum Physics*, Mir Publishers, Moscow, 1978.

- [GGU] K. Grabowska, J. Grabowski, P. Urbański, *The Schrödinger operator as a generalized Laplacian*, J. Phys. A 41 (2008), 145204.
- [GKP] J. Grabowski, A. Kotov, N. Poncin, *Lie superalgebras of differential operators*, J. Lie Theory 23 (2013), 35–54.
- [GP] J. Grabowski, N. Poncin, *Derivations of the Lie algebras of differential operators*, Indag. Math. (N.S.) 16 (2005), 181–200.
- [LMSV] F. Lizzi, G. Marmo, G. Sparano, A. M. Vinogradov, *Eikonal type equations for geometrical singularities of solutions in field theory*, J. Geom. Phys. 14 (1994), 211–235.
- [MMM] G. Marmo, G. Morandi, N. Mukunda, *The Hamilton–Jacobi theory and the analogy between classical and quantum mechanics*, J. Geom. Mech. 1 (2009), 317–355.
- [NT] T. Nutma, M. Taronna, *On conformal higher spin wave operators*, J. High Energy Phys. 2014, no. 6, 066.
- [P] A. Perelomov, *Generalized Coherent States and their Applications*, Texts Monogr. Phys., Springer, Berlin 1986.