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Probability and Quantum Symmetries. II. The Theorem of Nœther in quantum mechanics

S. Albeverio
Institut für Angewandte Mathematics, Abt. für Wahrsch. und Mathematische Statistik 53115 Bonn, Wegelerstasse 6, Germany

J. Rezende and J.-C. Zambrini
Grupo de Física-Matemática (GFMUL), Universidade de Lisboa, Av. Prof. Gama Pinto 2, P-1649-003 Lisboa, Portugal

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For the largest class of physical systems having a classical analog, a new rigorous, but not probabilistic, Lagrangian version of nonrelativistic quantum mechanics is given, in terms of a notion of regularized action function. As a consequence of the study of the symmetries of this action, an associated Nœther theorem is obtained. All the quantum symmetries resulting from the canonical quantization procedure follow in this way, as well as a number of symmetries which are new even for the case of the simplest systems. The method is based on the study of a corresponding Lie algebra and an analytical continuation in the time parameter of the probabilistic construction given in paper I of this work. Generically, the associated quantum first integrals are time dependent and the probabilistic model provides a natural interpretation of the new symmetries. Various examples illustrate the physical relevance of our results. [DOI: 10.1063/1.2199087]

I. INTRODUCTION

This paper is the continuation of the one, referred hereafter simply as paper I, whose subtitle was the "Theorem of Nœther in Schrödinger's Euclidean quantum mechanics."[1] There, a probabilistic (i.e., "Euclidean") generalization of Nœther's theorem of classical mechanics was presented, for a class of Lagrangians quadratic in the velocities, and involving a special family of time-symmetric $\mathbb{R}^3$-valued diffusion processes. At the end of paper I, our physical motivation was indicated: after an appropriate analytic continuation in the time parameters, the main conclusion of the construction was preserved as a theorem on quantum symmetries, in the Heisenberg picture. In other words, although the probabilistic content of the theorem of Nœther was destroyed by this continuation in time, its geometrical one survived.

The purpose of this second paper is to describe in a detailed way the reason of this apparently surprising conclusion. This will provide us with a new Lagrangian version of the quantum theory of such a class of systems. The symmetries of the associated new concept of regularized action functional will be expressed as a quantum version of the theorem of Nœther. All the unusual regularizations introduced on the quantum side will correspond to the ones given for free with the underlying diffusion process, whose probability measures make sense only in the Euclidean setting. In point of fact, it will be shown that the corresponding symbolic "quantum diffusions" in real time have all the properties of the heuristic ones manipulated by Feynman in his famous path integral method.[2] In this sense, our indirect method is very much along the line of Feynman's space–time approach. It will be shown that we obtain many more quantum symmetries in this way than using the usual theorems on quantum symmetries, even for the simplest class of elementary integrable systems. Those "new" quantum symmetries are the keys of basic relations with stochastic analysis. A general argument of Lie group theory assures us, in fact, that all quantum symmetries arise in this way.

The organization of this work is as follows.

Section II introduces the notions (implicit in Feyman's approach) of (complex-valued) space–time observables associated with a family of regular quantum observables and of quantum derivatives along a state. Although these quantum derivatives are not observables in the sense of Von Neumann, they constitute a key tool of our construction. Under the quantum expectation, such differential operators behave like derivations.

Then, we define the concept of quantum conditional expectation in a state, given a space–time point. In spite of the fact that this concept shares a number of properties with its counterpart in probability theory, we show why it is not a conditional expectation in the probabilistic sense. The associated "quantum diffusions" are precisely the ones introduced by Feynman in time discretized manner.

Section III is devoted to the definition of the regularized action function for this class of systems and its relations with quantum dynamics.

The study of the symmetries of this quantum action is the subject of Sec. IV. In particular, the definition of the invariance of the action corresponds to a natural regularization of the classical notion. The symmetry group of the underlying Schrödinger equation is used in an essential way here, and the regular concept of constant observable of the motion is adapted to our calculus on space–time observable (or *quantum calculus*, for short).

In Sec. V the construction is specialized to the case of Hamiltonians which are polynomials of degrees ≤ 2 in the position and momentum observables. This is the case where all the calculations are explicit. Although this class is supposed to be completely known, our method provides, even for the most elementary systems, more symmetries than the traditional approach. For general Hamiltonians the main results hold true; but no explicit basis of the symmetry algebra can be found, in general and, therefore, the method is more indirect.

Section VI is devoted to the analysis of the content of our Nœther theorem in a Riemannian manifold.

In Sec. VII we come back to the relation of what we did with the ideas of Feynman and show in what sense the content of the present paper is a natural counterpart of paper I, where stochastic analysis is involved in an essential way.

Finally, the last section is devoted to a short collection of explicit examples of quantum symmetries with some emphasis on those not directly accessible to regular methods. Of course, as soon as we know it, the theorem of Nœther in quantum mechanics can be verified without any use of our detour via probability theory and stochastic analysis. However, it is argued in favor of this detour for the intuition it provides, in the same sense as Feynman's path integral approach has proved to be very useful for the discovery of many new aspects of quantum theory. A short Errata for paper I will conclude the present work.

II. THE CONCEPT OF QUANTUM MECHANICAL CONDITIONAL EXPECTATION

Let H be a self-adjoint, lower bounded Hamiltonian operator in the Hilbert space $\mathcal{H}=L^2(\mathbb{R}^n,\mathrm{d}x)$ of square integrable complex-valued function over $\mathbb{R}^n$. Consider the one-parameter, strongly continuous groups of unitary operators $U_t:\mathcal{H}\to\mathcal{H}, t\in\mathbb{R}$,

$$U_t = e^{-(i/\hbar)tH},$$

with the reduced Planck constant $\hbar$. Then for any ψ in the definition domain $\mathcal{D}_H\subset\mathcal{H}$ of H,

$$\psi_t = U_t\psi, \tag{2.1}$$

solves the Schrödinger equation with the initial condition ψ:

$$\begin{aligned} i\hbar\frac{\partial\psi_t}{\partial t} &= H\psi_t, \\ \psi_0 &= \psi. \end{aligned} \tag{2.2}$$

Let consider a one-parameter family $A(t), t \in \mathbb{R}$, of self-adjoint operators in $\mathcal{H}$. Assume that $\mathcal{D}_{A(t)} \supset H\mathcal{D}_H$ and $A(t)\mathcal{D}_H \subset \mathcal{D}_H$, so that the commutators $[A(t),H]=A(t)H-HA(t)$ are well defined on $\mathcal{D}_H$. Let $0<T\leq\infty$ and define $\mathcal{D}_T^{\dot{A}}(t)\equiv\mathcal{D}^{\dot{A}}(t)$ by $\mathcal{D}^{\dot{A}}(t)=\cap_{T\geq\Delta t\geq 0}\mathcal{D}_{A(t+\Delta t)}$. In particular we have $\mathcal{D}^{\dot{A}}(t)\subset\mathcal{D}_{A(t)}$. If $A(t)$ is weakly differentiable on $\mathcal{D}^{\dot{A}}(t)$ with respect to the time parameter $t \in [0,T)$,then we can compute

$$\lim_{\Delta t\downarrow 0}\left(\psi,\frac{A(t+\Delta t)-A(t)}{\Delta t}\varphi\right)\equiv\varepsilon_t^{\dot{A}}(\psi,\varphi).$$

It exists for any $\psi\in\mathcal{H},\varphi\in\mathcal{D}^{\dot{A}}(t)$, where $(\cdot,\cdot)$ denotes the scalar product in $\mathcal{H}$, and is linear in the second vector. Provided that $\mathcal{D}^{\dot{A}}(t)$ is dense in $\mathcal{H}, \varepsilon_t^{\dot{A}}:\mathcal{H}\times\mathcal{D}^{\dot{A}}(t)\to\mathbb{C}$ is a densely defined sesquilinear form.

Now let us define, for $\psi_t\in\mathcal{H}$ and $\varphi_t\in\mathcal{D}_{A(t)}, I_{\psi,\varphi}(t)=(\psi_t,A(t)\varphi_t)$.

When $\varphi_t\in\mathcal{D}^{\dot{A}}(t)$ and ψ_t is the solution of (2.2) with $\psi_t\in D_{A(t)}, T>t\geq 0$ and $\Delta t>0$, we can compute the relative time increment of $I_{\psi,\varphi}(t)$ as follows:

$$\begin{aligned}I_{\psi,\varphi}(t,\Delta t) &\equiv \frac{I_{\psi,\varphi}(t+\Delta t)-I_{\psi,\varphi}(t)}{\Delta t}\\ &=\frac{1}{\Delta t}[(\psi_{t+\Delta t},A(t+\Delta t)\varphi_{t+\Delta t})-(\psi_t,A(t+\Delta t)\varphi_{t+\Delta t})\\ &\quad+(\psi_t,A(t+\Delta t)\varphi_{t+\Delta t})-(\psi_t,A(t)\varphi_{t+\Delta t})\\ &\quad+(\psi_t,A(t)\varphi_{t+\Delta t})-(\psi_t,A(t)\varphi_t)].\end{aligned}$$

If, in addition, $\varphi_t=U_t\varphi$ with $\varphi_0\equiv\varphi\in\mathcal{D}(H)$ then the strong derivative $\dot{\varphi}_t$ of φ_t with respect to t exists and $\dot{\varphi}_t=(1/i\hbar)H\varphi_t$. But, by assumption, $H\varphi_t\in D_{A(t)}$. This, inserted in the above relative increment of $I_{\psi,\varphi}(t)$ gives, when $\Delta t\downarrow 0$, using the strong differentiability of ψ_t,φ_t, the strong continuity of $A(t)\varphi_t$ on $\mathcal{D}^{\dot{A}}(t)$, the fact that $\varphi_{t+\Delta t}\in\mathcal{D}^{\dot{A}}(t)$ and that $A(t)$ is weakly differentiable on $\mathcal{D}^{\dot{A}}(t)$,

$$\lim_{\Delta t\downarrow 0}I_{\psi,\varphi}(t,\Delta t)=(\dot{\psi}_t,A(t)\varphi_t)+\varepsilon_t^{\dot{A}}(\psi_t,\varphi_t)+(\psi_t,A(t)\dot{\varphi}_t).$$

By (2.2), the corresponding equation for φ_t and the further assumption $\mathcal{D}^{\dot{A}}(t)\supset H\mathcal{D}_H$, we see that the latter relation can be rewritten as

$$\lim_{\Delta t\downarrow 0}I_{\psi,\varphi}(t,\Delta t)=\left(\frac{1}{i\hbar}H\psi_t,A(t)\varphi_t\right)+\varepsilon_t^{\dot{A}}(\psi_t,\varphi_t)+\left(\psi_t,\frac{1}{i\hbar}A(t)H\varphi_t\right).$$

Since $A(t)\mathcal{D}_H\subset\mathcal{D}_H$ by assumption, and so $A(t)\varphi_t\in\mathcal{D}_H$, this reduces, by the self-adjointness of H, to

$$\frac{1}{i\hbar}(\psi_t,[A(t),H]\varphi_t)+\epsilon_t^{\dot{A}}(\psi_t,\varphi t)=\frac{d}{\mathrm{d}t}(\psi_t,A(t)\varphi_t), \tag{2.3}$$

where we used the definitions of $I_{\psi,\varphi}(t,\Delta t)$, $I_{\psi,\varphi}(t)$, and $\epsilon_t^{\dot{A}}(\psi_t,\varphi_t)$.

We shall denote by $\varepsilon_D(\psi_t,\varphi_t)$ the sesquilinear form on left-hand side (lhs) of (2.3). So

$$\varepsilon_D(\psi_t,\varphi_t)=\frac{d}{\mathrm{d}t}(\psi_t,A(t)\varphi_t). \tag{2.4}$$

We recall that for $T>t\geq 0$, $\varepsilon_D(\psi_t,\ \varphi_t)$ is well defined if $\varphi_t\in\mathcal{D}^{\dot{A}}(t)$ and $A(t)\mathcal{D}_H\subset\mathcal{D}_H$.

Definition II.1: Let φ be in $\mathcal{H}$ and such that $\varphi_t\in\mathcal{D}_{A(t)}$. The complex-valued space–time observable $a_{\varphi_t}^A(x,t)$ associated with the family of quantum observable $A(t)$ in the state φ_t is defined *for all* $x \in \mathbb{R}^n, t \in \mathbb{R}, s.t.\, \varphi_t(x) \neq 0$, *by*

$$a^A_{\varphi_t}(x,t) \equiv \frac{(A(t)\varphi_t)(x)}{\varphi_t(x)}. \tag{2.5}$$

We shall consider, for any x,t, versions of $\varphi_t(x)$ jointly measurable in $t \in \mathbb{R}$, $x \in \mathbb{R}^n$, and denote them again by $\varphi_t(x)$. For x,t such that $\varphi_t(x)=0$ we set $a^A_{\varphi_t}(x,t) \equiv 0$. Therefore, for any ψ_t in $\mathcal{H}$ and φ_t in $\mathcal{D}_{A(t)}$ we have

$$(\psi_t, A(t)\varphi_t) = \int_{(N_t^\varphi)^c} \bar{\psi}_t A(t)\varphi_t \,\mathrm{d}x + \int_{N_t^\varphi} \bar{\psi}_t A(t)\varphi_t \,\mathrm{d}x = \int_{(N_t^\varphi)^c} \bar{\psi}_t A(t)\varphi_t \,\mathrm{d}x,$$

where $\mathcal{N}_t^\varphi = \{x \in \mathbb{R}^n \,|\, \varphi_t(x)=0\}, (N_t^\varphi)^c = \mathbb{R}^n - N_t^\varphi$.

Using (2.5), it is clear that, by construction,

$$(\psi_t, A(t)\varphi_t) = \int \bar{\psi}_t \varphi_t a^A_{\varphi_t} \,\mathrm{d}x. \tag{2.6}$$

Assumption on the zeroes of the wave function

We shall need that $\mathcal{N}_t^\varphi$ has zero Lebesgue measure. Sufficient conditions for this are known in terms of assumption on H. See Sec. V.

Using (2.3) and (2.4) and our assumption that $\mathcal{N}_t^\varphi$ has zero Lebesgue measure, we get

$$\varepsilon_D(\psi_t,\varphi_t) = \frac{1}{i\hbar}(\psi_t,[A(t),H]\varphi_t) + \varepsilon_t^{\dot{A}}(\psi_t,\varphi_t) = \frac{1}{i\hbar}\int_{(N_t^\varphi)^c} \bar{\psi}_t\varphi_t \frac{1}{\varphi_t}[A(t),H]\varphi_t \,\mathrm{d}x + \varepsilon_t^{\dot{A}/\varphi_t}(\psi_t\bar{\varphi}_t,\varphi_t), \tag{2.7}$$

where we have defined $\varepsilon_t^{\dot{A}/\varphi_t}$, for $f/\bar{\varphi}_t \in \mathcal{H}$ and $g \in \mathcal{D}^A(t)$, by

$$\varepsilon_t^{\dot{A}/\varphi_t}(f,g) \equiv \lim_{\Delta t \downarrow 0}\left(f, \frac{1}{\varphi_t}\left[\frac{A(t+\Delta t)-A(t)}{\Delta t}\right]g\right).$$

Now suppose that, in the strong sense on $\mathcal{D}^A(t)$, there exist a linear operator $\partial A(t)/\partial t$ such that

$$\lim_{\Delta t \downarrow 0}\frac{A(t+\Delta t)-A(t)}{\Delta t}\varphi_t = \frac{\partial A}{\partial t}(t)\varphi_t, \quad 0 \le t < T.$$

Then, for $\psi \in \mathcal{H}, \varphi_t \in \mathcal{D}^A(t)$, using the definition of $\varepsilon_t^{\dot{A}}(\psi_t,\varphi_t)$,

$$\left(\psi_t, \frac{\partial A}{\partial t}(t)\varphi_t\right) = \varepsilon_t^{\dot{A}}(\psi_t,\varphi_t).$$

Also, for any $\varphi_t \in \mathcal{D}^A(t)$,

$$\left(\frac{\partial A}{\partial t}(t) + \frac{1}{i\hbar}[A(t),H]\right)\varphi_t$$

is well defined [recall that we have assumed $H\mathcal{D}_H \subset \mathcal{D}_{A(t)}$ and $A(t)\mathcal{D}_H \subset \mathcal{D}_H$]. According to the definition (2.5), $a^A_{\varphi_t}\cdot\varphi_t = A(t)\varphi_t$ is also well defined. Therefore in the sense of the identification of the corresponding Bochner integrals,

$$\frac{\partial}{\partial t}(a^A_{\varphi t}\cdot\varphi_t)=\frac{\partial A}{\partial t}(t)\varphi_t+\frac{1}{i\hbar}A(t)H\varphi_t,$$

for any $\varphi_t\in\mathcal{D}^A(t)$ and Lebesgue a.e. $t\in[0,T)$ [recalling our assumption that $\mathcal{D}^A(t)\supset H\mathcal{D}_H$]. From this it follows that

$$\left(\frac{\partial}{\partial t}-\frac{1}{i\hbar}H\right)(a^A_{\varphi_t}\cdot\varphi_t)$$

is well defined and coincides, for Lebesgue a.e. t, with

$$\left(\frac{\partial A}{\partial t}+\frac{1}{i\hbar}[A(t),H]\right)\varphi_t.$$

Now for any $x\in(\mathcal{N}^{\varphi}_t)^c$ we defined $D_t a^A_{\varphi_t}$ by

$$(D_t a^A_{\varphi_t})(x)=\frac{1}{\varphi_t}\left(\frac{\partial}{\partial t}-\frac{1}{i\hbar}H\right)(a^A_{\varphi_t}\cdot\varphi_t)(x). \tag{2.8}$$

Using the relation above, we get first on $(N^{\varphi}_t)^c$ but then in the $L^2(\mathbb{R}^n)$-sense

$$D_t a^A_{\varphi_t}=\frac{1}{\varphi_t}\left(\frac{\partial A}{\partial t}+\frac{1}{i\hbar}[A(t),H]\right)\varphi_t. \tag{2.9}$$

From this, for all $\psi_0=\psi\in D_H$ we obtain

$$(\psi_t,(D_t a^A_{\varphi_t})\varphi_t)=\left(\psi_t,\left(\frac{\partial A}{\partial t}+\frac{1}{i\hbar}[A(t),H]\right)\varphi_t\right)=\frac{d}{\mathrm{d}t}(\psi_t,A(t)\varphi_t),$$

where (2.7) and (2.9) have been used. All equalities hold first for Lebesgue a.e. t but can be extended to all t if both sides of the equalities are continuous in t.

In summary, we have proved the following:

Proposition II.2:

Let H be a self-adjoint operator in $\mathcal{H}=L^2(\mathbb{R}^n,\mathrm{d}x)$ and $A(t)$ a one-parameter family of self-adjoint operators in $\mathcal{H}$ with $A(t)\mathcal{D}_H\subset\mathcal{D}_H$ and $\mathcal{D}^A(t)\supset H\mathcal{D}_H$. For $\varphi\in\mathcal{D}_H$, consider $\varphi_t=e^{-(i/\hbar)tH}\varphi$ and assume that $\mathcal{N}^{\varphi}_t$ has a zero Lebesgue measure. Suppose that $\partial A(t)/\partial t$ exists in the strong sense on $\mathcal{D}^A(t)$. Define $\mathcal{D}_t a^A_{\varphi_t}$ by equations (2.8) and (2.9). *Then, for any $\varphi\in\mathcal{D}_H$ and $\psi_t\in\mathcal{D}_{A(t)}$, with ψ_t satisfying* (2.2), *we have*

$$\frac{d}{\mathrm{d}t}(\psi_t,A(t)\varphi_t)=(\psi_t,(D_t a^A_{\varphi_t})\varphi_t), \tag{2.10}$$

for Lebesgue a.e. $t\in\mathbb{R}$. If both sides of (2.10) *are continuous in t, then* (2.10) *holds for all $t\in\mathbb{R}$.*

Corollary II.3:

If $A(t)$ is a quantum constant of motion *of the system with Hamiltonian H, defined on a dense domain $\mathcal{D}\subset\mathcal{H}$, in the sense that*

$$\left(\frac{\partial A}{\partial t}(t)+\frac{1}{i\hbar}[A(t),H]\right)\mathcal{X}=0\quad\text{for any }\mathcal{X}\in\mathcal{D},$$

then the space–time observable associated with $A(t)$ satisfies

$$D_t a^A_{\varphi_t}=0,$$

for all $\varphi_t\in\mathcal{D}^A(t)$.

Proof: By (2.9) we have $D_t a^A_{\varphi_t} = (1/\varphi_t)\dot{A}(t)\varphi_t = 0$, for

$$\dot{A}(t) \equiv \frac{\partial A}{\partial t}(t) + \frac{1}{i\hbar}[A(t),H].$$

$\dot{A}(t)$ is a closable operator since $A(t)$, $(\partial A/\partial t)(t)$ and H are all symmetric, defined on a common domain.

By approximation of $\varphi_t \in \mathcal{D}^A(t)$ through vectors in $\mathcal{D}$, and since $A(t)$ is a quantum constant of motion, we see that $\bar{\dot{A}}(t)\varphi_t = 0$, where the overbar denotes the closure. Since φ_t is in the domain of $\dot{A}(t)$, the conclusion follows. □

Remarks:

(1) If we call *quantum space–time observable* any operator-valued map $(x,t) \to g(x,t)$ measurable in the sense that $(x,t) \to (\phi, g(x,t)\varphi)$ is measurable for $\phi \in \mathcal{H}, \varphi \in \mathcal{D}$ a dense domain and $g(x,t)$ self-adjoint in $\mathcal{H}$, we can define D_t, $t \in \mathbb{R}$, on the set of such observables g by

$$D_t g \equiv \frac{1}{\varphi_t}\left(\frac{\partial}{\partial t} - \frac{1}{i\hbar}H\right)(g\varphi_t), \tag{2.11}$$

whenever the right-hand side (rhs) makes sense [with $(g\varphi_t)(x) \equiv (g(x,t)\varphi_t)(x)$]. Then, for $g = a^A_{\varphi_t}$, $D_t a^A_{\varphi_t}$ coincides with (2.9). If $g\varphi_t \in \mathcal{D}_H$, $\partial g/\partial t$ exists in the strong sense on $\mathcal{D}_H$ and $\mathcal{D}_{\partial g/\partial t} \supset \mathcal{D}_H$, then the rhs of (2.11) is well defined (for $\varphi_t \in \mathcal{D}_H$). However, we are going to show that there is a more natural definition of D_t regarded as differential operator densely defined in an associated Hilbert space.

(2) D_t, acting on space–time functions $a^A_{\varphi_t}$, for example, should not be confused with the familiar Heisenberg derivative D acting on the family of self-adjoint operators $A(t)$ and defined heuristically by

$$DA(t) = \frac{\partial A}{\partial t}(t) + \frac{1}{i\hbar}[A(t),H].$$

Indeed, according to (2.9), the relation between these two derivatives is $D_t a^A_{\varphi_t} = (1/\varphi_t)(DA(t)\varphi_t)$. In particular, Heisenberg's derivative D does not depend on the state φ_t. In order to avoid any confusion, from now on we shall call D_t the *quantum derivative* along φ_t.

(3) Consider two arbitrary observables A and H, time independent and with $\mathcal{D}_A = \mathcal{D}_H = \mathcal{D}$, a common dense domain in $\mathcal{H}$, invariant under A and H. We say that A and H commute, and write $[A,H]=0$ whenever for any f, g bounded and Borel measurable one has $f(A)g(H) - g(H)f(A) = 0$.

A necessary and sufficient condition for this property is, for example, that

$$[e^{i(\alpha/\hbar)A}, e^{i(t/\hbar)H}] = 0 \quad \forall\, \alpha,\ t \in \mathbb{R}.$$

(cf., for example, Ref. 3). If A is essentially self-adjoint on a domain $\mathcal{D}$, invariant under $e^{i(t/\hbar)H}$, $\forall t \in \mathbb{R}$, then A and H commute if

$$A(t)\chi \equiv e^{i(t/\hbar)H}Ae^{-i(t/\hbar)H}\chi = A\chi, \quad \forall\, \chi \in \mathcal{D} \text{ and } t \in \mathbb{R}.$$

So it suffices indeed to show that

$$\frac{d}{\mathrm{d}t}(\phi, e^{i(t/\hbar)H}Ae^{-i(t/\hbar)H}\chi) = \frac{d}{\mathrm{d}t}(\phi_t, A\chi_t) = \left(\phi_t, \frac{1}{i\hbar}[A(t), H]\chi_t\right) = 0$$

with

$$\phi_t \equiv e^{-i(t/\hbar)H}\phi, \quad \mathcal{X}_t \equiv e^{-i(t/\hbar)H}\chi, \quad \text{and } \forall\ \chi, \phi \text{ in } \mathcal{D} = \mathcal{D}_H \cap \mathcal{D}_A,$$

in order to prove that A and H commute (in the sense of the above-mentioned sufficient condition) and therefore that $A(t)$ is a constant of motion. According to the Corollary II.3, when this holds, we have $D_t a^A_{\varphi_t} = 0$.

Lemma II.4:

Let φ_t be the solution of the Schrödinger equation (2.2) *with initial condition φ in $L^2(\mathbb{R}^n)$ and let $\mathcal{N}^{\varphi}_t$ be a zero Lebesgue measure set. Then the quantum derivative D_t along the solution φ_t of the Schrödinger equation* (2.2) *with initial condition φ is a densely defined differential operator in* $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\,\mathrm{d}x)$.

Proof: Let φ_t be the solution of the Schrödinger equation (2.2) with the initial condition $\varphi \in L^2(\mathbb{R}^n, \mathrm{d}x) \equiv \mathcal{H}$ and consider the weighted Hilbert space $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\,\mathrm{d}x)$. Since, by assumption, $\mathcal{N}^{\varphi}_t$ has zero Lebesgue measure, the two Hilbert spaces are unitarily equivalent through the transformation

$$U_{\varphi_t}: \quad L^2(\mathbb{R}^n, |\varphi_t(x)|^2\,\mathrm{d}x) \to L^2(\mathbb{R}^n, \mathrm{d}x), \qquad g \mapsto g\varphi_t.$$

Let $\mathcal{K}$ be the space of $\mathbb{R}$-indexed families of functions $f = (f^{(t)})_{t\in\mathbb{R}}$ with each $f^{(t)}$ strongly continuously differentiable from $\mathbb{R}$ into $\mathcal{H}$, such that

$$\frac{\partial}{\partial t} f^{(t)} \equiv \lim_{\Delta t \downarrow 0} \frac{f^{(t+\Delta t)} - f^{(t)}}{\Delta t} \in \mathcal{H},$$

where the limit is taken in the strong $\mathcal{H}$ sense. Let us define the partial differential operator

$$\mathcal{Q} = \frac{\partial}{\partial t} - \frac{1}{i\hbar}H$$

on the subset $\mathcal{K}_H$ of $\mathcal{K}$ consisting of those $(f^{(t)})_{t\in\mathbb{R}}$ such that the mapping $x \in \mathbb{R}^n \mapsto f^{(t)}(x)$ belongs to $\mathcal{D}_H$ for all $t \in \mathbb{R}$. We can also define the Hilbert space $W^2_1(\mathbb{R}, \mathcal{H})$, consisting of the functions $f = (f^{(t)})_{t\in\mathbb{R}}$, with $f \in \mathcal{K}$ such that $f^{(t)}(x), (\partial/\partial t)f^{(t)}(x) \in L^2(\mathbb{R}, \mathrm{d}t)$ for $\mathrm{d}x$ a.e., $x \in \mathbb{R}^n$. The operator $i\mathcal{Q}$ is well defined on $\mathcal{K}^0_H \equiv \{f^{(t)} \in \mathcal{K}_H, t \mapsto f^{(t)} \in C^1_0(\mathbb{R})\}$. This operator is symmetric in $W^2_1(\mathbb{R}^n, \mathcal{H})$, on a dense domain $\mathcal{K}^S_H \equiv \mathcal{D}_S$ (S for "Schrödinger"), independent of time.

Let $\mathcal{K}_t$ be the "tth copy" of $L^2(\mathbb{R}^n, \mathrm{d}x)$ so that $f^{(t)} \in \mathcal{K}_t$ for any $t \in \mathbb{R}$. Let us consider the image under $U^{-1}_{\varphi_t}$ of $\mathcal{K}_t$. $U^{-1}_{\varphi_t}\mathcal{K}_t$ is made of all functions of the form $f^{(t)}(x)/\varphi_t(x)$, with $f^{(t)} \in \mathcal{K}_t$ and $(x,t) \notin \mathcal{N}^{\varphi}_t$.

$U^{-1}_{\varphi_t}$ can be extended to an operator $\tilde{U}^{-1}_{\varphi_t}$ from $\mathcal{K}$ into $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\,\mathrm{d}x)$, defined by

$$(\tilde{U}^{-1}_{\varphi_t} f^{(s)})(x) = \frac{f^{(s)}(x)}{\varphi_t(x)}, \quad (x,t) \notin \mathcal{N}^{\varphi}_t, \quad s \in \mathbb{R}.$$

Restricted to $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\,\mathrm{d}x), \tilde{U}^{-1}_{\varphi_t}$ is unitary from $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\,\mathrm{d}x)$ to $L^2(\mathbb{R}^n, \mathrm{d}x)$, since

$$\|\tilde{U}_{\varphi_t}^{-1} f^{(s)}\|_{L^2(\mathbb{R}^n, |\varphi_t(x)|^2 \, dx)} = \|f^{(s)}\|_{L^2(\mathbb{R}^n, dx)}, \qquad \forall\, s,t \in \mathbb{R},$$

and its inverse is $\tilde{U}_{\varphi_t} f^{(s)} = \varphi_t f^{(s)}$.

We can look at the image of the operator $\mathcal{Q}_t$ in $\mathcal{K}$ under $\tilde{U}_{\varphi_t}^{-1}$ as an operator $\hat{\mathcal{Q}}_t$ whose action on elements of $L^2(\mathbb{R}^n, |\varphi_t(x)|^2 \, dx)$ is given by $\tilde{U}_{\varphi_t}^{-1} \mathcal{Q}_t \tilde{U}_{\varphi_t} = \hat{\mathcal{Q}}_t$ on $D \subset L^2(\mathbb{R}^n, |\varphi_t(x)|^2 \, dx), D$ being such that $\tilde{U}_{\varphi_t} D \in \mathcal{D}_{\mathcal{Q}t}$. Since $i\mathcal{Q}_t = i\partial/\partial t - (1/\hbar)H$ is symmetric on the dense domain $\mathcal{D}_S$ of $W_1^2(\mathbb{R}, \mathcal{H})$, this means that $i\mathcal{Q}_t$ is symmetric on the dense domain $\tilde{U}_{\varphi_t}^{-1}\mathcal{D}_S$ in $L^2(\mathbb{R}^n \times \mathbb{R}, dx\, dt)$. On this domain, $\hat{\mathcal{Q}}_t$ is given by

$$\hat{\mathcal{Q}}_t \tilde{U}_{\varphi_t}^{-1} f = \frac{1}{\varphi_t}\left(\frac{\partial}{\partial t} - \frac{1}{i\hbar} H\right) f,$$

with $f = (f^{(t)})_{t\in\mathbb{R}} \in \mathcal{D}_S$.

$\mathcal{D}_S$ contains, for example, the subset $\mathcal{D}_S^0$ consisting of all families $f = (f^{(t)})_{t\in\mathbb{R}}$ such that $f^{(t)}(\cdot)$ as well as $(\partial/\partial t) f^{(t)}(\cdot)$ are both in $C_0^\infty(\mathbb{R}^n)$ [if $\mathcal{D}_H \supset C_0^\infty(\mathbb{R}^n)$].

Setting $h = \tilde{U}_{\varphi_t}^{-1} f$ for $f \in \mathcal{D}_S^0$ we see that

$$\hat{\mathcal{Q}}_t h = \frac{1}{\varphi t}\left(\frac{\partial}{\partial t} - \frac{1}{i\hbar} H\right)(\varphi_t h).$$

Comparing with (2.11), this means that, on $\tilde{U}_{\varphi_t}^{-1}\mathcal{D}_S^0$ we have indeed

$$\hat{\mathcal{Q}}_t = D_t. \tag{2.12}$$

□

Remarks:

(1) Suppose that H is the Hamiltonian for a unit mass and charged particle in an electromagnetic field, i.e., $H = -(\hbar^2/2)[\nabla - (i/\hbar)A]^2 + V$ on $C_0^\infty(\mathbb{R}^n)$ or

$$H = -\frac{\hbar^2}{2}\Delta + i\hbar A \cdot \nabla + \frac{i\hbar}{2} \nabla \cdot A + \frac{1}{2}\|A\|^2 + V, \tag{2.13}$$

where $A: \mathbb{R}^n \mapsto \mathbb{R}^n$ is the vector potential and $V: \mathbb{R}^n \mapsto \mathbb{R}$ the scalar potential, both continuous, A being C^1, and such that H has a unique self-adjoint extension, also denoted by H (cf., for example, Ref. 4 for sufficient conditions such that this holds). In this case, using (2.11), we obtain explicitly a quantum derivative along φ_t (in the sense of Lemma II.4) given by

$$D_t = \frac{\partial}{\partial t} + \left(-i\hbar \frac{\nabla \varphi_t}{\varphi_t} - A\right) \cdot \nabla - \frac{i\hbar}{2}\Delta \tag{2.14}$$

on the domain of functions of the form $\varphi \cdot \mathcal{D}_S$, which is dense in $L^2(\mathbb{R}^n, |\varphi_t(x)|^2 \, dx)$. According to our Remark 1 after Corollary II.3, D_t is also defined on a larger set of functions in $L^2(\mathbb{R}^n, |\varphi_t(x)|^2 \, dx)$. For example, denoting by q the function

$$\begin{aligned} \mathbb{R}^n \times \mathbb{R} &\to \mathbb{R}^n, \qquad \forall\, t, \quad \text{we have } D_t q = i\hbar \frac{\nabla \varphi_t}{\varphi_t} - A \\ (x,t) &\mapsto x \end{aligned}$$

which is well defined, provided

$$\int \bar{\varphi}_t(x) x (H\varphi_t)(x) dx < \infty .$$

This is the case under weak restrictions on the vector and scalar potentials A and V.

(2) We shall also need the complex conjugate of the operator D_t, denoted by $\bar{D}_t$. On complex space–time observables of the form $a^A_{\varphi_t}$, one has, by definition,

$$\bar{D}_t a^A_{\bar{\varphi}_t} = \frac{1}{\bar{\varphi}_t}\left(\frac{\partial}{\partial t} + \frac{1}{i\hbar}H\right)(\bar{\varphi}_t a^A_{\bar{\varphi}_t}).$$

Proceeding as before in connection with (2.12), i.e., considering vectors h of the form $\tilde{U}^{-1}_{\bar{\varphi}_t} f$, with $f \in \mathcal{D}^0_S$, we have

$$\bar{D}_t h = \frac{1}{\bar{\varphi}_t}\left(\frac{\partial}{\partial t} + \frac{1}{i\hbar}H\right)(\bar{\varphi}_t h). \tag{2.15}$$

In particular, when the Hamiltonian H is of the form (2.13), $\bar{D}_t$ reduces on $\tilde{U}^{-1}_{\bar{\varphi}_t}\mathcal{D}^0_S$ to the differential operator

$$\bar{D}_t = \frac{\partial}{\partial t} + \left(i\hbar\,\frac{\nabla\bar{\varphi}_t}{\bar{\varphi}_t} - A\right)\cdot\nabla + \frac{i\hbar}{2}\Delta \tag{2.16}$$

defined on the elements $\{\tilde{U}^{-1}_{\bar{\varphi}_t}\mathcal{D}^0_S\}_{t\in\mathbb{R}}$ of $W^2_1(\mathbb{R}^n,\mathcal{H})$. These elements form a dense domain of $W^2_1(\mathbb{R}^n,\mathcal{H})$, as discussed in the proof of the Lemma II.4. Using the terminology introduced there, $\bar{D}_t$ will simply be called the *quantum derivative along* $\bar{\varphi}_t$.

(3) It follows clearly from (2.11) and (2.15) that

$$\overline{D_t g} = \bar{D}_t \bar{g},$$

where the lhs denotes the complex conjugate of $D_t g$.

Motivated by Born's probabilistic interpretation of the wave function, let us introduce the natural definition.

Definition II.5: Let $f=(f^{(t)})_{t\in\mathbb{R}}$, *with* $f^{(t)}(\cdot)$ *in* $L^1(\mathbb{R}^n,|\varphi_t(x)|^2\,\mathrm{d}x)$ *and* $f^{(t)}$ *measurable in* t. *The* quantum (absolute) expectation of f in the state φ_t *solving* (2.1), *denoted by* $\langle f\rangle_{\varphi_t}$, *is the integral*

$$\langle f\rangle_{\varphi_t} = \int f^{(t)}(x)|\varphi_t(x)|^2\,\mathrm{d}x \tag{2.17}$$

and we shall refer to $|\varphi_t(x)|^2$ *as the density* (*with respect to* dx) *of the quantum probability in the state* φ_t.

The terminology chosen for D_t and $\bar{D}_t$ is due to the crucial observation that, under this quantum expectation, these differential operators behave like derivations.

Proposition II.6:

Let $f=(f^{(t)})_{t\in\mathbb{R}}$, $g=(g^{(t)})_{t\in\mathbb{R}}$ *be in the domains of the quantum derivatives* D_t *and* $\bar{D}_t$ *and with compact support in the space variables. Then* $\langle f\cdot g\rangle_{\varphi_t}$ *is differentiable with respect to the time variable and the following Leibniz rule holds:*

$$\frac{d}{\mathrm{d}t}\langle f\cdot g\rangle_{\varphi_t} = \langle D_t f\cdot g + f\cdot\bar{D}_t g\rangle_{\varphi_t}. \tag{2.18}$$

In particular,

$$\frac{d}{\mathrm{d}t}\langle f\rangle_{\varphi_t} = \langle D_t f\rangle_{\varphi_t} = \langle\bar{D}_t f\rangle_{\varphi_t}. \tag{2.19}$$

Corollary II.7:

If f, g *have supports with respect to the time variable strictly contained in the interior of an interval* $[t_0,t_1]$ *for some* $t_0,t_1\in\mathbb{R}$, *then* $\mathcal{D}^+_t = -\bar{D}_t$ *where* $^+$ *denotes the adjoint with respect to* $|\varphi_t(x)|^2\,\mathrm{d}x\,\mathrm{d}t$ *on* $\mathbb{R}^n\times[t_0,t_1]$.

Proof: Integrating (2.18), we obtain

$$\int_{t_0}^{t_1} \langle D_t f \cdot g \rangle_{\varphi_t} \, \mathrm{d}t = - \int_{t_0}^{t_1} \langle f \cdot \bar{D}_t g \rangle_{\varphi_t} \, \mathrm{d}t.$$

□

Proof of Proposition II.6: By definition, $(d/\mathrm{d}t)\langle f \cdot g \rangle_{\varphi_t}$ denotes

$$\lim_{\Delta t \downarrow 0} \frac{\langle f^{(t+\Delta t)} g^{(t+\Delta t)} \rangle_{\varphi_{t+\Delta t}} - \langle f^{(t)} g^{(t)} \rangle_{\varphi_t}}{\Delta t}.$$

The term under $\lim_{\Delta t \downarrow 0}$ means explicitly

$$\begin{aligned} \frac{1}{\Delta t} & \left[\int f^{(t+\Delta t)} g^{(t+\Delta t)} |\varphi_{t+\Delta t}(x)|^2 \, \mathrm{d}x - \int f^{(t)} g^{(t)} |\varphi_t(x)|^2 \, \mathrm{d}x \right] \\ &= \frac{1}{\Delta t} \left[\int (f^{(t+\Delta t)} - f^{(t)}) g^{(t+\Delta t)} |\varphi_{t+\Delta t}(x)|^2 \, \mathrm{d}x \right. \\ &\quad + \int f^{(t)} (g^{(t+\Delta t)} - g^{(t)}) |\varphi(x)_{t+\Delta t}|^2 \, \mathrm{d}x \\ &\quad \left. + \int f^{(t)} g^{(t)} (|\varphi_{t+\Delta t}(x)|^2 - |\varphi_t(x)|^2) \mathrm{d}x \right]. \end{aligned}$$

The first term on the rhs converges, when $\Delta t \downarrow 0$, to $\int (\dot{f}^{(t)} g^{(t)})(x) |\varphi_t(x)|^2 \, \mathrm{d}x$ by the dominated convergence theorem and the hypothesis that $f^{(t)}$ is strongly differentiable in $L^2(\mathbb{R}^n, \mathrm{d}x)$ [here we denote $(\partial/\partial t) f^{(t)}$ by $\dot{f}^{(t)}$ for simplicity]. Similarly we see that the second term of the rhs converges to $\int f^{(t)} \dot{g}^{(t)} |\varphi_t(x)|^2 \, \mathrm{d}x$.

For the third term we use again the dominated convergence theorem and the fact that, in the strong $L^2(\mathbb{R}^n, \mathrm{d}x)$ sense,

$$\frac{d}{\mathrm{d}t} |\varphi_t|^2 = \frac{d}{\mathrm{d}t} \bar{\varphi}_t \cdot \varphi_t = - \frac{1}{i\hbar} H \bar{\varphi}_t \cdot \varphi_t + \dot{\bar{\varphi}}_t \frac{1}{i\hbar} H \varphi_t,$$

where the Schrödinger equation has been used, together with the fact that $\dot{\bar{\varphi}}_t \cdot H\varphi_t$ as well as $H\bar{\varphi}_t \cdot \varphi_t$ are in $L^1(\mathbb{R}^n, \mathrm{d}x)$ and $f^{(t)}, g^{(t)}$ have compact support as functions of the space variable. In other words the rhs above becomes

$$\begin{aligned} & \int \left\{ \dot{f}^{(t)} g^{(t)} + f^{(t)} \dot{g}^{(t)} + f^{(t)} g^{(t)} \left(\frac{1}{i\hbar} \frac{H\varphi_t}{\varphi_t} - \frac{1}{i\hbar} \frac{H\bar{\varphi}_t}{\bar{\varphi}_t} \right) \right\} (x) |\varphi_t(x)|^2 \, \mathrm{d}x \\ &= \int (D_t f^{(t)} \cdot g^{(t)} + f^{(t)} \bar{D}_t g^{(t)})(x) |\varphi_t(x)|^2 \, \mathrm{d}x, \end{aligned}$$

where the definition of $D_t, \bar{D}_t$ have been used together with the self-adjointness of H, in order to simplify the term involving $H(f^{(t)} \varphi_t)$.

The second part of the calculation follows from the first one by approaching in the $L^2(\mathbb{R}^n, |\varphi_t(x)|^2 \, \mathrm{d}x)$-norm $f^{(t)} = 1$, respectively, $g^{(t)} = 1$ through $C_0^\infty(\mathbb{R}^n)$ functions. □

Remarks:

(1) When the Hamiltonian H is of the explicit form (2.13), the relation (2.18) can be given a more illuminating form if we use exclusively one of the quantum derivatives,

$$\frac{d}{dt}\langle f\cdot g\rangle_{\varphi_t}=\langle (D_tf)\cdot g+f(D_tg)\rangle_{\varphi_t}-i\hbar\,\langle \nabla f\cdot\nabla g\rangle_{\varphi_t} \tag{2.20}$$

$$=\langle (\bar{D}_tf)\cdot g+f(\bar{D}_tg)\rangle_{\varphi_t}+i\hbar\,\langle \nabla f\cdot\nabla g\rangle_{\varphi_t}. \tag{2.21}$$

Proof: This follows directly from Proposition II.6, using the explicit expressions (2.14) and (2.16) of D_t and $\bar{D}_t$ available for the Hamiltonian (2.13). □

(2) Relations like (2.20) and (2.21) hold, in fact, also without integration with respect to $|\varphi_t(x)|^2\,\mathrm{d}x$.

Proposition II.8:

For f,g in a dense domain of the form $\varphi_t\cdot\mathcal{D}_S\subset L^2(\mathbb{R}^n,|\varphi_t(x)|^2\,\mathrm{d}x)$ (cf. Lemma II.4) and an Hamiltonian of the form (2.13), *one has*

$$D_t(f\cdot g)=(D_tf)\cdot g+f(D_tg)-i\hbar\,\nabla f\cdot\nabla g, \tag{2.20$'$}$$

$$\bar{D}_t(f\cdot g)=(\bar{D}_tf)\cdot g+f(\bar{D}_tg)+i\hbar\,\nabla f\cdot\nabla g, \tag{2.21$'$}$$

for any (t,x) such that $\varphi_t(x)\neq 0$.

Proof: Equations (2.20) and (2.21) can be written, for any $\varphi_t=U_t\varphi$, and any (t,x) s.t. $\varphi(t,x)\neq 0,\int A(x,t)|\varphi_t(x)|^2\,dx=0$ with $A(x,t)=\bar{D}(f\cdot g)-(\bar{D}_tf)g-f(\bar{D}_tg)-i\hbar\nabla f\cdot\nabla g$, and so equations (2.20′) and (2.21′) hold a.e. with respect to $\mathrm{d}x$. Alternatively, one can use directly the definitions (2.14) and (2.16) to show that the conclusion holds. □

Equations (2.20′) and (2.21′) show that the quantum derivatives behave, in fact, like quantum *deformations* of derivatives in the (commutative) algebra of families of functions $f=(f^{(t)})_{t\in\mathbb{R}}$ with $f^{(t)}\in C_0(\mathbb{R}^n)$. To regard D_t and $\bar{D}_t$ as quantum deformations of derivations will prove, later on, to be a very natural interpretation.

Now we are going to introduce the quantum counterpart of the probabilistic concept of conditional expectation given a space point $x\in\mathbb{R}^n$ in the past time $t\geq 0$.

Definition II.9:

Let $g=(g^{(\tau)})_{\tau\in\mathbb{R}}$ be complex valued, measurable functions defined on $\mathbb{R}^n$ and such that $g^{(\tau)}\times(\cdot)\psi_\tau(\cdot)\in L^2(\mathbb{R}^n,\mathrm{d}x)$ where, as before, $\psi_\tau=U_\tau\psi$. For $0\leq t\leq\tau$ and (t,x) such that $\underline{\psi}_t(x)\neq 0$ [or, for short, (t,x) "ψ-admissible"] let us define the quantum conditional expectation $M_{t,x}^{\bar{\psi}}$ in the state ψ, given (t,x) and evaluated at $g^{(\tau)}$ *by*

$$M_{t,x}^{\bar{\psi}}\,[g^{(\tau)}]=(\bar{\psi}_t(x))^{-1}(U_{\tau-t}(g^{(\tau)}\bar{\psi}_\tau))(x). \tag{2.22}$$

Let us first assume that the Hamiltonian H is time-independent and that the evolution group $U_{\tau-t}$ has an integral kernel, denoted by

$$k(x,\tau-t,q)=(e^{-(i/\hbar)(\tau-t)H})(x,q),\quad x,q\in\mathbb{R}^n,\ \tau>t.$$

Then the definition (2.22) means

$$M_{t,x}^{\bar{\psi}}[g^{(\tau)}]=(\bar{\psi}_t(x))^{-1}\int k(x,\tau-t,q)g^{(\tau)}(q)\bar{\psi}_\tau(q)\mathrm{d}q, \tag{2.22$'$}$$

which is well defined for any ψ-admissible $(t,x)\in\mathbb{R}^+\times\mathbb{R}^n$. We shall denote by

$$\hat{p}(t,x,\tau,\mathrm{d}q)=(\bar{\psi}_t(x))^{-1}k(x,\tau-t,q)\bar{\psi}_\tau(q)\mathrm{d}q,\quad t\leq\tau,\ x,q\in\mathbb{R}^n, \tag{2.23}$$

the integral kernel associated with (2.22′) and refer to it as the *forward quantum transition* kernel ["forward" because the conditioning x is in the past $t\leq\tau$ and also because the initial quantum probability density $|\psi_t(x)|^2$ is propagated towards the future by $\hat{p}$]. More precisely since, for $\tau > t$ the kernel $k(x,\tau-t,q)$ coincides with the retarded (or "casual") propagator

$$k_+(x,\tau-t,q) = \theta(\tau-t)(e^{-(i/\hbar)(\tau-t)H})(x,q),$$

(where θ is Heaviside's distribution) i.e., the distribution solving

$$\left(-i\hbar\frac{\partial}{\partial\tau}+H\right)k_+(x,\tau-t,q) = -i\hbar\,\delta(q-x)\delta(\tau-t),$$

Eq. (2.23) means that

$$\hat{p}(t,x,\tau,\mathrm{d}q) = (\bar{\psi}_t(x))^{-1}k_+(x,\tau-t,q)\bar{\psi}_\tau(q)\mathrm{d}q. \tag{2.23$'$}$$

Let us observe that sufficient conditions for the existence of k and therefore $\hat{p}$ as continuous functions in all the variable are known; cf., e.g., Refs. 5, 6, and 60.

We remark that when H is time dependent, Eq. (2.23) still holds with k replaced by the integral kernel of the two-parameter family of unitary operators $U(t,\tau)$, $t,\tau \in \mathbb{R}$ defining the corresponding time evolution.

The main properties of the quantum conditional expectation of Definition 2.9 are expressed by the following:

Proposition II.10:

For all ψ-admissible $(t,x) \in \mathbb{R}\times\mathbb{R}^n$ and $g=(g^{(\tau)})_{\tau\in\mathbb{R}}$ as in (2.22$'$), with $\tau \geq t$,

(1) *the quantum mechanical conditional expectation is linear: if $\alpha_i \in \mathbb{C}$ and $g_i=(g_i^{(\tau)})_{\tau\in\mathbb{R}}$, $i=1,2$ as above,*

$$M_{t,x}^{\bar{\psi}}[\alpha_1 g_1^{(\tau)} + \alpha_2 g_2^{(\tau)}] = \alpha_1 M_{t,x}^{\bar{\psi}}[g_1^{(\tau)}] + \alpha_2 M_{t,x}^{\bar{\psi}}[g_2^{(\tau)}];$$

(2) $M_{t,x}^{\bar{\psi}}[\alpha]=\alpha$, $\alpha \in \mathbb{C}$;

(3) $M_{t,x}^{\bar{\psi}}[g^{(\tau)}]=g^{(t)}(x)$, $\tau \geq t$;

(4) $\langle M_t^{\bar{\psi}}[g^{(\tau)}]\rangle_{\psi_\tau} = \langle g^{(\tau)}\rangle_{\psi_\tau}$, $\tau \geq t$;

(5) *when $M_{s,x}^{\bar{\psi}}[g_1^{(s)}g_2^{(t)}]$, $s \leq t$, is well defined, then*

$$M_{s,x}^{\bar{\psi}}[g_1^{(s)}g_2^{(t)}] = g_1^{(s)}(x)M_{s,x}^{\bar{\psi}}[g_2^{(t)}].$$

Proof: This follows from direct computations using the definitions (2.17) and (2.22). □

Remarks:

(1) We shall also need, for the same class of $g=(g^{(\tau)})_{\tau\in\mathbb{R}}$ as in Proposition II.10, and any ψ-admissible $(t,x) \in \mathbb{R}\times\mathbb{R}^n$, the definition (2.22) with ψ replaced by $\bar{\psi}$ and $U_{\tau-t}$ replaced by $U_{\tau-t}$, $0<\tau\leq t$, i.e.,

$$M_\psi^{t,x}[g^{(\tau)}] = (\psi_t(x))^{-1}(U_{t-\tau}(g^{(\tau)}\psi_\tau))(x). \tag{2.24}$$

The properties of $M_\psi^{t,x}$ are, of course, similar to the ones of $M_{t,x}^{\bar{\psi}}$.

Let us stress that, for the latter quantum conditional expectation in the state ψ, the conditioning x is lying in the future of the time interval under consideration [i.e., $t \geq \tau$; this justifies our alteration of notation with respect to (2.22)]. For this reason, we shall occasionally call backward (respectively, forward) the conditional expectation (2.24) [respectively (2.22)] when a confusion is possible between these two concepts. When needed, we shall denote by $p(\tau,\mathrm{d}q,t,x)$ the *backward quantum transition* kernel associated with (2.24), i.e.,

$$p(\tau,\mathrm{d}q,t,x) = \psi_\tau(q)k_-(q,t-\tau,x)(\psi_\tau(x))^{-1}\,\mathrm{d}q, \quad \tau \leq t, \tag{2.25}$$

for any (t,x) ψ-admissible. Here, we denote by k_- the advanced propagator defined in terms of the causal one by

$$k_-(x_1,s-u,x_2)=\overline{k_+(x_2,u-s,x_1)}. \tag{2.26}$$

(2) Comparing the definitions (2.23′) and (2.25), it is clear that the relation between the forward and backward quantum transition kernels can be expressed as

$$\overline{\hat{p}(t,x,s,y)}=p(s,y,t,x), \quad s\leq t,\ x,y\in\mathbb{R}^n. \tag{2.27}$$

Definition II.11:
Let $f=(f^{(t)})_{t\in\mathbb{R}}$, $(g^{(s)})_{s\in\mathbb{R}}$ *as in the definitions* (2.22′) and (2.23). *The* quantum (absolute) expectation of their product $f^{(t)}\cdot g^{(s)}$ *in the state* ψ, *for* $t\geq s$, *is defined by*

$$\langle f^{(t)}g^{(s)}\rangle_\psi=\langle M^{\bar{\psi}}_{s,\cdot}[f^{(t)}]\cdot g^{(s)}\rangle_{\psi_s} \tag{2.28}$$

$$=\langle f^{(t)}M^{t,\cdot}_{\psi}[g^{(s)}]\rangle_{\psi_t}, \tag{2.28′}$$

when $M^{\bar{\psi}}_{s,\cdot}[f^{(t)}]\cdot g^{(s)}\in L^2(|\psi_s(x)|^2\,\mathrm{d}x)$ *and* $f^{(t)}M^{t,\cdot}_{\psi}[g^{(s)}]\in L^2(|\psi_t(q)|^2\,\mathrm{d}q)$.

The consistency of this definition is verified by observing that equation (2.28) reduces, after simplification, to

$$\int\int \psi_s(x)g^{(s)}(x)k(x,t-s,q)f^{(t)}(q)\bar{\psi}_t(q)\mathrm{d}q\,\mathrm{d}x,$$

when the integral kernel (2.23′) exists (since $t\geq s$). On the other hand, using the forward conditional expectation of (2.28′), this absolute expectation in the state ψ_t reduces to

$$\int\int \psi_s(x)g^{(s)}(x)k_-(x,t-s,q)f^{(t)}(q)\bar{\psi}_t(q)\mathrm{d}q\,\mathrm{d}x,$$

i.e., to the same expression as before, by definition of the advanced propagator k_- when $t\geq s$.

This duality with respect to the time parameter suggests to introduce the following two-parameters family of operators $P^*_{s,t}, s\leq t$ associated with quantum conditional expectations:

$$\begin{aligned} P^*_{s,t}&:L^2(|\psi_s(x)|^2\,\mathrm{d}x)\to L^2(|\psi_t(q)|^2\,\mathrm{d}q)\\ g^{(s)}(\cdot)&\mapsto\int g^{(s)}(x)p(s,\mathrm{d}x,t,q)\equiv M^{t,q}_{\psi}[g^{(s)}], \end{aligned} \tag{2.29}$$

where the backward transition kernel (2.25) has been introduced and its "time reversed" family $P_{t,s}$, $s\leq t$,

$$\begin{aligned} P_{t,s}&:L^2(|\psi_t(q)|^2\,\mathrm{d}q)\to L^2(|\psi_s(x)|^2\,\mathrm{d}x),\\ f^{(t)}(\cdot)&\mapsto\int f^{(t)}(q)\hat{p}(s,x,t,\mathrm{d}q)\equiv M^{\bar{\psi}}_{s,x}[f^{(t)}], \end{aligned} \tag{2.29′}$$

so that the equality between (2.28) and (2.28′) can be rewritten as

$$\langle (P_{t,s}f^{(t)})\cdot g^{(s)}\rangle_{\psi_s}=\langle f^{(t)}\cdot(P^*_{s,t}g^{(s)})\rangle_{\psi_t}. \tag{2.30}$$

The properties of the operators $P^*_{s,t}$ (or $P_{t,s}$) for $s\leq t$ are as follows:

(a) $P^*_{s,t}$ are linear operators; as a map from $\mathbb{R}_+\times\mathbb{R}_+$ into densely defined, bounded operators from $L^2(|\psi_s(x)|^2\,\mathrm{d}x)$ into $L^2(|\psi_t(q)|^2\,\mathrm{d}q)$, $(s,t)\mapsto P^*_{s,t}$ is continuous;

(b) $\|P^*_{s,t}g^{(s)}\|_{L^2(|\psi_t(q)|^2\, dq)}=\|g^{(s)}\|_{L^2(|\psi_s(x)|^2\,\mathrm{d}x)}$;

(c) $P^*_{s,t}1_{(s)}=1_{(t)}$ where $1_{(s)}$ is the function identically 1 in $L^2(|\psi_s(x)|^2\,\mathrm{d}x)$ [with $1_{(t)}$ the same in $L^2(|\psi_t(q)|^2\,\mathrm{d}q)$] and $P_{t,s}1_{(t)}=1_{(s)}$;

(d) $P^*_{s,s}=\mathrm{Id}$, the identity operator from $L^2(|\psi_s(x)|^2\,\mathrm{d}x)$ into $L^2(|\psi_s(x)|^2\,\mathrm{d}x)$;

(e) $P^*_{t,u}\cdot P^*_{s,t}=P^*_{s,u}, \quad s\le t\le u$;

(f) $P^*_{s,t}\cdot P_{t,s}=1_{(t)}$ and $P_{t,s}\cdot P^*_{s,t}=1_{(s)}$.

We may summarize the situation as follows:

Proposition II.12:

The two-parameters family of bounded operators $P^*_{s,t}$ and $P_{t,s}$ are dual from $L^2(|\psi_s(x)|^2\,\mathrm{d}x)$ into $L^2(|\psi_t(q)|^2\,\mathrm{d}q)$ in the sense that for any $f^{(t)}\in\mathcal{D}_{P_{t,s}}$ and $g^{(s)}\in\mathcal{D}_{P^*_{s,t}}$, the relation (2.30) *holds. Moreover, the properties* (*a*) *to* (*f*) *are satisfied* [*where* (*a*) *to* (*e*) *have their natural counterparts for $P_{t,s}$*].

The proof follows directly from the definitions (2.23′) and (2.25) of the forward and backward quantum transition kernels.

Remarks:

(1) Let $f^{(s)}(\cdot)$ be non-negative in $L^2(|\psi_s(x)|^2\,\mathrm{d}x)$. Then, clearly $P^*_{s,t}$ does not, in general, transform $f^{(s)}(\cdot)$ into a non-negative element of $L^2(|\psi_t(q)|^2\,\mathrm{d}q)$ since the backward quantum transition kernel p is not even real. In particular, $p(s,\cdot,t,q)$ is not a measure, although it shares manifestly a number of properties with probability measures.

(2) The equality between (2.28) and (2.28′) can be rewritten infinitesimally using the quantum derivatives D_t and $\bar{D}_t$. To do this, we need another property of these derivatives, which will be the first result of the next section.

Let $P^*_{s,t}$ and $P_{t,s}$ a pair of 2-parameters family of operators satisfying the properties of Proposition II.12 and $p,\bar{p}$, respectively, their associated quantum transition kernels.

Definition II.13:

The two dual kernels define a quantum diffusion if $\forall s<t, x\in\mathbb{R}^n, \varepsilon>0$, we have

(1) $\hat{p}(s,x,t,S_\varepsilon(x)^c)=o(t-s)$, *where $S_\varepsilon(x)^c$ is the complement of the sphere $S_\varepsilon(x)$ of radius ε and center x.*

(2) *There is a $\mathbb{C}^n$-valued function $\hat{B}(x,s)$ s.t.,*

$$\int_{S_\varepsilon(x)}(q-x)\hat{p}(s,x,t,\mathrm{d}q)=\hat{B}(x,s)(t-s)+o(t-s).$$

There is an $n\times n$ complex-valued function $\hat{C}(x,s)$ s.t.

$$\int_{S_\varepsilon(x)}(q-x)(q-x)^T\hat{p}(s,x,t,\mathrm{d}q)=\hat{C}(x,s)(t-s)+o(t-s).$$

$\hat{C}$ will be called the quantum diffusion matrix *and $\hat{B}$ the* (forward) drift of the quantum diffusion.

(3) *There is a $\mathbb{C}^n$-valued function $B(x,t)$ s.t.*

$$\int_{S_\varepsilon(x)}(q-x)p(s,\mathrm{d}x,t,q)=B(q,t)(t-s)+o(t-s),$$

and an $n\times n$ complex-valued function $C(x,s)$ s.t.

$$\int_{S_\varepsilon(x)}(q-x)(q-x)^Tp(s,\mathrm{d}x,t,q)=C(q,t)(t-s)+o(t-s).$$

These properties are satisfied, e.g., for the kernels associated with the Hamiltonians (2.13) Compare also Refs. 5 and 6. Indeed we have the following.

Proposition II.14:

Let H be of the form (2.13) *and its associated kernel k be such that*

$$\lim_{\Delta s \downarrow 0} \frac{1}{\Delta s} \int (q-x) R(q,x,\Delta s) k(x,\Delta s,q) \mathrm{d}q = 0,$$

where $R(q,x,\Delta s)=0((q-x)^2)+0(\Delta s)^2$ *is a term in the Taylor expansion of the integrand of* $\hat{B}(x,s)$ *in the proof below. Let* $(q,t) \in \mathbb{R}^n \times \mathbb{R}$ *be* ψ*-admissible, where* ψ_t *is a regular solution of the Schrödinger equation for H, admitting a Taylor expansion in powers of the space and time variables around* $\psi_t(q)$. *Then a quantum diffusion corresponds to this solution, whose drifts and diffusion matrix are, respectively, given by*

$$\hat{B}(q,t) = i\hbar \frac{\nabla \bar{\psi}_t}{\bar{\psi}_t}(q) - A(q),$$

$$B(q,t) = -i\hbar \frac{\nabla \psi_t}{\psi_t}(q) - A(q), \tag{2.31}$$

$$C(q,t) = \hat{C}(q,t) = i\hbar \mathbb{1},$$

where $\mathbb{1}$ *denotes the* $n \times n$ *identity matrix.*

Proof: By (3) and (2.23),

$$\begin{aligned}
\hat{B}(x,s) &= \lim_{\Delta s \downarrow 0} \frac{1}{\Delta s} \int_{s_\varepsilon(x)} (q-x) \hat{p}(s,x,s+\Delta s,q) \mathrm{d}q \\
&= \lim_{\Delta s \downarrow 0} \frac{1}{\Delta s} \int_{s_\varepsilon(x)} (q-x) (\bar{\psi}_s(x))^{-1} k(x,\Delta s,q) \bar{\psi}_{s+\Delta s}(q) \mathrm{d}q \\
&= \lim_{\Delta s \downarrow 0} \frac{1}{\Delta s} \int_{s_\varepsilon(x)} (q-x) \left[1 + \frac{\nabla \bar{\psi}_s}{\bar{\psi}_s}(x)(q-x) + \frac{\dot{\bar{\psi}}_s}{\bar{\psi}_s}(x)\Delta s + O((q-x)^2) + O(\Delta s^2) \right] k(x,\Delta s,q) \mathrm{d}q.
\end{aligned}$$

We can easily verify the following properties of the integral kernel $k(x,\tau,q)$ of the evolution group U_τ for the Hamiltonian (2.13):

$$\lim_{\tau \downarrow 0} \frac{1}{\tau} \left[1 - \int_{\mathbb{R}^n} k(x,\tau,q) \mathrm{d}q \right] = \frac{1}{2} \nabla \cdot A(x) + \frac{i}{2\hbar} \|A(x)\|^2 + \frac{i}{\hbar} V(x),$$

$$\lim_{\tau \downarrow 0} \frac{1}{\tau} \int_{\mathbb{R}^n} (q-x) k(x,\tau,q) \mathrm{d}q = A(x),$$

$$\lim_{\tau \downarrow 0} \frac{1}{\tau} \int_{\mathbb{R}^n} (q-x)(q-x)^T k(x,\tau,q) \mathrm{d}q = i\hbar \mathbb{1}.$$

Using these in the above rhs of the expression of $\hat{B}(x,s)$ we obtain the expected result. The other results follow in a similar way. □

Proposition II.15:

Let $\nabla \psi_t / \psi_t$ *and* $A(q)$ *be given and continuous, for a Hamiltonian of the form* (2.13). *Assume* *that, in the representations* (2.29) and (2.29′), *the partial derivatives with respect to* (t,q) [*respectively* (s,x)] *of the quantum conditional expectations are well defined and continuous, and can be exchanged with the integrals. Then the quantum equation of Kolmogorov for the transition kernel* $\hat{p}$ *for* $s \le t \in \mathbb{R}$, $x,y \in \mathbb{R}^n$, *is given by*

(a)

$$-\frac{\partial \hat{p}}{\partial s}(s,x,t,q) = \frac{i\hbar}{2}\frac{\partial^2 \hat{p}}{\partial x^j\,\partial x^j}(s,x,t,q) + \left(i\,\hbar\,\frac{\nabla^j \bar{\psi}_t}{\bar{\psi}_t}(q) - A^j(q)\right)\frac{\partial}{\partial x^j}\hat{p}(s,x,t,q) \qquad (2.32)$$

(*with the usual summation convention over the indices* j). *Equivalently, regarded as a function of the past variable*, $\hat{p}$ *is the fundamental solution of*

$$\bar{D}_s u = 0, \quad for \quad u \in \mathcal{D}_{\bar{D}_s}, \qquad (2.33)$$

with $\bar{D}_s$ *defined in* (2.16).

(b) *If all the involved partial derivatives exist and are continuous*, $\hat{p}$, *regarded as a function of the future variables, solves the quantum Fokker-Planck equation*

$$\frac{\partial \hat{p}}{\partial t}(s,x,t,q) = \frac{i\hbar}{2}\frac{\partial^2 \hat{p}}{\partial q^j\,\partial q^j}(s,x,t,q) - \frac{\partial}{\partial q^j}\left[\left(i\,\hbar\,\frac{\nabla^j \bar{\psi}_t}{\bar{\psi}_t}(q) - A^j(q)\right)\hat{p}(s,x,t,q)\right]. \qquad (2.34)$$

Similarly, the transition kernel $p(s,x,t,q)$ *solves*

(c)

$$-\frac{\partial p}{\partial s}(s,x,t,q) = -\frac{i\hbar}{2}\frac{\partial^2 p}{\partial x^j\,\partial x^j}(s,x,t,q) + \left(-i\,\hbar\,\frac{\nabla^j \psi_t}{\psi_t}(q) - A^j(q)\right)\frac{\partial}{\partial x^j}p(s,x,t,q). \qquad (2.35)$$

So that p *is the fundamental solution of*

$$D_s v = 0 \quad for \quad v \in \mathcal{D}_{D_s}, \qquad (2.36)$$

with D_s *given by* (2.14) *and the following backward quantum Fokker-Planck equation holds*:

(d)

$$\frac{\partial p}{\partial t}(s,x,t,y) = -\frac{i\hbar}{2}\frac{\partial^2 p}{\partial q^j\,\partial q^j}(s,x,t,y) - \frac{\partial}{\partial q^j}\left[\left(-i\,\hbar\,\frac{\nabla^j \psi_t}{\psi_t}(q) - A^j(q)\right)p(s,x,t,y)\right]. \qquad (2.37)$$

Proof: (*a*) Let us consider (2.29′)

$$(P_{t,s}f^{(t)})(x) = \int f^{(t)}(q)\hat{p}(s,x,t,\mathrm{d}q) \equiv u(s,x), \quad s < t,$$

for any $f^{(t)}$ of compact support in the class used to define (2.22). By hypothesis, we can differentiate with respect to (s,x) under the integral sign. Using Proposition II.12 (c) and the properties of the quantum transition kernels before Proposition II.14,

$$
\begin{aligned}
u(s_1,x)-u(s_2,x) &= \int_{S_\varepsilon(x)} [u(s_2,q)-u(s_2,x)]\hat{p}(s_1,x,s_2,q)\mathrm{d}q + o(s_2-s_1) \\
&= \int_{S_\varepsilon(x)} \left\{ (q-x)\,\nabla\, u(s_2,x) + (q-x)(q-x)^T \frac{1}{2}\nabla^2 u(s_2,x) + R \right\} \hat{p}\,\mathrm{d}q + o(s_2-s_1) \\
&= \Bigg[\nabla u(s_2,x) \int_{S_\varepsilon(x)} (q-x)\hat{p}(s_1,x,s_2,q)\mathrm{d}q \\
&\quad + \frac{1}{2}\nabla^2 u(s_2,x) \int_{S_\varepsilon(x)} (q-x)(q-x)^T \hat{p}(s_1,x,s_2,q)\,\mathrm{d}q + R \Bigg] (s_2-s_1) + o(s_2-s_1) \\
&= \left[\hat{B}(x,s_2)\,\nabla\, u(s_2,x) + \frac{1}{2}\hat{C}(s_2,x)\nabla^2 u(s_2,x) + R \right](s_2-s_1) + o(s_2-s_1),
\end{aligned}
$$

where $\hat{B}$ and $\hat{C}$ have been computed in Proposition II.14 and $R \equiv R(s_1,s_2,q,x)$ is a remainder $O(|q-x|^2)$. Dividing by (s_2-s_1) and taking $\lim_{s_2 \downarrow s}$, $\lim_{s_1 \uparrow s}$ one verifies that $u(s,x)$ solves the quantum Fokker-Planck equation (2.34).

According to (2.29′), the boundary condition of this equation is provided by

$$
u(s,x) - f^{(s)}(x) = \int_{S_\varepsilon(x)} [f^{(t)}(q) - f^{(s)}(x)]\hat{p}(s,x,t,q)\mathrm{d}q + o(t-s).
$$

So

$$
\lim_{s \uparrow t} u(s,x) \equiv \lim_{s \uparrow t} M^{\bar{\psi}}_{s,x}[f^{(t)}] = f^{(t)}(x). \tag{2.33′}
$$

(b) Let $f^{(t)}$ be of compact support, twice continuously differentiable in the class used to define (2.22). As before, one verifies that

$$
\lim_{s_1 \uparrow s, s_2 \downarrow s} \frac{1}{s_2 - s_1} \left[\int f^{(s_2)}(q)\hat{p}(s_1,x,s_2,q)\mathrm{d}q - f^{(s)}(x) \right] = \hat{B}(x,s)\,\nabla\, f^{(s)}(x) + \frac{1}{2}\hat{C}(x,s)\nabla^2 f^{(s)}(x). \tag{2.38}
$$

Now let us write

$$
\begin{aligned}
\frac{\partial}{\partial t}\int f^{(t)}(q)\hat{p}(s,x,t,q)\mathrm{d}q &= \lim_{s_1 \uparrow t, s_2 \downarrow t} \frac{1}{s_2 - s_1} \int [\hat{p}(s,x,s_2,q) - \hat{p}(s,x,s_1,q)] f^{(t)}(q)\mathrm{d}q \\
&= \lim_{s_1 \uparrow t, s_2 \downarrow t} \int \hat{p}(s,x,s_1,q) \left[\frac{1}{s_2 - s_1} \int f^{(s_2)}(z)\hat{p}(s_1,q,s_2,z)\mathrm{d}z - f^{(s_2)}(q) \right] \mathrm{d}q.
\end{aligned}
$$

Using (2.38) this reduces to

$$
\int \hat{p}(s,x,t,q) \left[\hat{B}(q,t)\,\nabla\, f^{(t)}(q) + \frac{1}{2}\hat{C}(q,t)\nabla^2 f^{(t)}(q) \right] \mathrm{d}q.
$$

After integration by parts, we get

$$
\int \frac{\partial}{\partial t}\hat{p}(s,x,t,q)\cdot f^{(t)}(q)\mathrm{d}q = \int \mathrm{d}q\, f^{(t)}(q) \left[-\nabla_q \left(\hat{p}(s,x,t,q)\hat{B}(q,t) - \frac{1}{2}\nabla_q \left(\hat{C}(q,t)\hat{p}(s,x,t,q) \right) \right) \right].
$$

□

Introducing $\hat{B}$, $\hat{C}$ of Proposition II.14, (2.34) holds since $f^{(t)}$ is arbitrary in the chosen dense class.

Starting from (2.29), one proves (c) and (d) in the same way.

Proposition II.16:

Under the same conditions as in Proposition II. 15, the density of the quantum probability in the state $\psi_t, \rho(x,t)\,\mathrm{d}x = |\psi_t(x)|^2\,\mathrm{d}x$, *solves the continuity equation*

$$\frac{\partial \rho}{\partial t} + \nabla_j\left[\frac{i\hbar}{2}(\psi_t \nabla^j \bar{\psi}_t - \bar{\psi}_t \nabla^j \psi_t) - A^j \rho\right] = 0,$$

or

$$\frac{\partial \rho}{\partial t} + \nabla_j\left[\frac{i\hbar}{2}\left(\frac{\nabla^j \bar{\psi}_t}{\bar{\psi}_t} - \frac{\nabla^j \psi_t}{\psi_t} - A^j\right)\rho\right] = 0. \tag{2.39}$$

Proof: It follows from the definition (2.23′) of the forward quantum transition kernel $\hat{p}(s,x,t,q)$ that, if $\rho^{(s)}(\mathrm{d}x)$ denotes the quantum probability density at time $s<t$, then

$$\rho(q,t) = \int \rho^{(s)}(\mathrm{d}x)\hat{p}(s,x,t,q). \tag{2.40}$$

Applying the integration with respect to $\rho^{(s)}(\mathrm{d}x)$ to the quantum Fokker-Planck equation (2.34) one can see that $\rho(q,t)$ satisfies the same equation, namely

$$\frac{\partial \rho}{\partial t} = -\nabla_j\left[\left(i\hbar\frac{\nabla^j \bar{\psi}_t}{\bar{\psi}_t} - A\right)\rho\right] + \frac{i\hbar}{2}\Delta\rho. \tag{2.41}$$

But the quantum probability density ρ is also propagated backward in time by the transition kernel p solving (2.37). This means that ρ solves as well

$$\frac{\partial \rho}{\partial t} = -\nabla_j\left[\left(-i\hbar\frac{\nabla^j \psi_t}{\psi_t} - A\right)\rho\right] - \frac{i\hbar}{2}\Delta\rho. \tag{2.42}$$

It follows that ρ also solves the average of (2.41) and (2.42), i.e., the usual quantum continuity equation (2.39), as claimed. □

III. THE QUANTUM ACTION FUNCTION AND ITS DYNAMICAL CONTENT

Let us show first why, in relation with the quantum conditional expectation in a given state, it is legitimate to call $\bar{D}_\tau$ a quantum (time) derivative. The next proposition can be regarded as a quantum version of the fundamental theorem of calculus.

Proposition III.1: Let $f=(f^{(\tau)})_{\tau\in\mathbb{R}}$ *be any function continuous in the time variable* τ, *and in the domain of* $\bar{D}_\tau$. *Then, for any* $t \le u$ *we have*

$$M_{t,x}^{\bar{\psi}}\left[\int_t^u \bar{D}_\tau f^{(\tau)}\,\mathrm{d}\tau\right] = M_{t,x}^{\bar{\psi}}[f^{(u)}] - f^{(t)}(x), \tag{3.1}$$

where $\bar{D}_\tau$ *is defined by* (2.15), *for* φ *replaced by* ψ.

Proof: By the definition (2.22) of $M_{t,x}^{\bar{\psi}}$, the lhs of (3.1), for (t,x) ψ-admissible, is

$$(\bar{\psi}_t(x))^{-1}\left(\int_t^u U_{\tau-t}[\bar{D}_\tau f^{(\tau)}\cdot\bar{\psi}_\tau]\mathrm{d}\tau\right)(x).$$

Introducing the definition (2.15) of $\bar{D}_\tau$, this means

$$(\bar{\psi}_t(x))^{-1}\left(\int_t^u U_{\tau-t}\cdot\left[\frac{1}{\bar{\psi}}\left(\frac{\partial}{\partial\tau}+\frac{1}{i\hbar}H\right)(\bar{\psi}_\tau f^{(\tau)})\cdot\bar{\psi}_\tau\right]\mathrm{d}\tau\right)(x)$$

$$=[\bar{\psi}_t(x)]^{-1}\left(\int_t^u U_{\tau-t}\left[\left(\frac{\partial}{\partial\tau}+\frac{1}{i\hbar}H\right)(\bar{\psi}_\tau\cdot f^{(\tau)})\right)\mathrm{d}\tau\right](x).$$

By an integration by parts with respect to $\mathrm{d}\tau$ and using the self-adjointness of H in $L^2(\mathbb{R}^n,\mathrm{d}x)$ we obtain

$$(\bar{\psi}_t(x))^{-1}\left\{-\int_t^u\left(\frac{\partial}{\partial\tau}U_{\tau-t}\right)(\bar{\psi}_\tau f^{(\tau)})\mathrm{d}\tau+U_{\tau-t}(\bar{\psi}_\tau f^{(\tau)})\bigg|_t^u(x)+\frac{1}{i\hbar}\int_t^u(HU_{\tau-t})(\bar{\psi}_\tau f^{(\tau)})\mathrm{d}\tau\right\}.$$

Since $U_{\tau-t}$ solves, for $\tau>t$, $(\partial/\partial\tau)U_{\tau-t}\chi=(1/i\hbar)HU_{\tau-t}\chi$ for all χ in $\mathcal{D}_H$, this reduces to

$$(\bar{\psi}_t(x))^{-1}U_{\tau-t}(\bar{\psi}_\tau f^{(\tau)})\big|_t^u=(\bar{\psi}_t(x))^{-1}\{U_{u-t}(\bar{\psi}_u f^{(t)})(x)-\bar{\psi}_t(x)f^{(t)}(x)\}.$$

By definition of the quantum conditional expectation, this is the rhs of Eq. (3.1). □

Remark:

When U_τ admits an integral kernel k, as in Sec. II, then the lhs of Eq. (3.1) becomes

$$(\bar{\psi}_t(x))^{-1}\int_t^T\int k(x,\tau-t,q)\bar{D}_\tau f^{(\tau)}(q)\bar{\psi}_\tau(q)\mathrm{d}q\,\mathrm{d}\tau.$$

The integration by parts with respect to $\mathrm{d}\tau$ mentioned in Proposition III.1 is done using the fact that k coincides with the retarded (or causal) distribution k_+ solving, for $\tau\geq t$, in the sense of distributions

$$\left(-i\hbar\frac{\partial}{\partial\tau}+H\right)k_+(x,\tau-t,q)=-i\hbar\,\delta(q-x)\delta(\tau-t).$$

□

Corollary III.2:

Let $f=(f^{(t)})_{t\in\mathbb{R}}$ strongly continuously differentiable from $\mathbb{R}$ into $L^2(\mathbb{R}^n,\mathrm{d}x)$, with $f^{(t)}(\cdot)\in\mathcal{D}_H$, $\forall t$. Assume that $(Hf^{(t)})_{t\in\mathbb{R}}$ is continuous in the time variable t. Then

$$\bar{D}_t f^{(t)}(x)=\lim_{\Delta t\downarrow 0}M_{t,x}^{\bar{\psi}}\left[\frac{f^{(t+\Delta t)}(\cdot)-f^{(t)}(x)}{\Delta t}\right].\qquad(3.2)$$

Proof: By Proposition III.1 for $u=t+\Delta t$ and property (3) of Proposition II.10,

$$\Delta t M_{t,x}^{\bar{\psi}}[\bar{D}_{t^*}f^{(t^*)}]=M_{t,x}^{\bar{\psi}}[f^{(t+\Delta t)}(\cdot)-f^{(t)}(x)],\qquad(3.3)$$

for some $t^*\geq t$. The lhs is

$$\Delta t(\bar{\psi}_t(x))^{-1}U_{t^*-t}\left[\left(\frac{\partial}{\partial t^*}+\frac{1}{i\hbar}H\right)(\bar{\psi}_{t^*}f^{(t^*)})\right].$$

Now $f^{(t^*)}\in\mathcal{D}_H$ and $H(\bar{\psi}_{t^*}f^{(t^*)})=\bar{\psi}_{t^*}Hf^{(t^*)}\to_{t^*\to t}\bar{\psi}_t Hf^{(t)}=H(\bar{\psi}_t f^{(t)})$. By Lemma II.4 $(\partial/\partial t^*)f^{(t^*)}$ is continuous in time, thus $\lim_{t^*\to t}M_{t,x}^{\bar{\psi}}[\bar{D}_{t^*}f^{(t^*)}]$ exists. After division by Δt, the rhs limit of (3.3) is the rhs of (3.2).

Corollary III.2 provides another proof of Proposition II.14 regarding the forward quantum transition kernel $\hat{p}$.

Corollary III.3:

Let us assume that $f=(f^{(\tau)})_{\tau\in\mathbb{R}}$ is as before and, moreover, admits a Taylor expansion up to the second order around a ψ-admissible $(t,x)\in\mathbb{R}\times\mathbb{R}^n$. Then if the Hamiltonian H is of the form

(2.13), *equation* (3.2) *implies, for* $f^{(t)}(x)=x$,

$$\bar{D}_t x = \lim_{\Delta t\downarrow 0} M_{t,x}^{\bar{\psi}}\left[\frac{f^{(t+\Delta t)}(\cdot)-x}{\Delta t}\right] = i\hbar\,\frac{\nabla\bar{\psi}_t}{\bar{\psi}_t}(x) - A(x), \tag{3.4}$$

and

$$\lim_{\Delta t\downarrow 0} M_{t,x}^{\bar{\psi}}\left[\frac{(f^{(t+\Delta t)}(\cdot)-x)^2}{\Delta t}\right] = i\hbar\,\mathbb{1}, \tag{3.5}$$

where $(f^{(t+\Delta t)}(\cdot)-x)^2$ *refers to the tensor product* $(f^{(t+\Delta t)}(\cdot)-x)\otimes(f^{(t+\Delta t)}(\cdot)-x)$ *and* $\mathbb{1}$ *is the* $n\times n$ *identity matrix.*

In equations (3.4) and (3.5) *the dummy variable* $(\cdot)$ *is the one denoted by* q *in* (2.23′). *All such "quantum moments" of order higher than 2 vanish.*

Proof: Let us consider the Taylor expansion up to the second order,

$$M_{t,x}^{\bar{\psi}}[f^{(t+\Delta t)}(q)-f^{(t)}(x)] = M_{t,x}^{\bar{\psi}}\left[\frac{\partial f}{\partial t}(x,t)\,\nabla\, t + (q-x)\cdot\Delta f(x,t) + \frac{1}{2}\sum_{i,j}((q_i-x_i)(q_j-x_j))\frac{\partial^2 f}{\partial x^i\,\partial x^j}(x,t) + o(\Delta t)\right].$$

Using the linearity of the quantum conditional expectation, as well as the properties (3) and (5) of Proposition II.15, the conclusion follows from the comparison with the explicit form (2.16) of $\bar{D}_t$ (with ψ replacing φ) for the Hamiltonian (2.13). □

In a similar way one proves the following.

Proposition III.4:

Let $f=(f^{(\tau)})_{\tau\in\mathbb{R}}$ *be continuous in the time variable* τ *and in the domain of* D_τ. *Then,* $\forall t\geq s$,

$$M_{\psi}^{t,x}\left[\int_s^t D_\tau f^{(\tau)}\mathrm{d}\tau\right] = f^{(t)}(x) - M_{\psi}^{t,x}[f^{(s)}], \tag{3.6}$$

where D_τ *is defined by* (2.11), *with* φ *replaced by* ψ.

Corollary III.5:

Under the same conditions as in Corollary III.2 we have

$$D_t f^{(t)}(x) = \lim_{\Delta t\downarrow 0} M_{\psi}^{t,x}\left[\frac{f^{(t)}(x)-f^{(t-\Delta t)}(\cdot)}{\Delta t}\right]. \tag{3.7}$$

If f *admits a Taylor expansion up to the second order around a* ψ*-admissible* $(t,x)\in\mathbb{R}\times\mathbb{R}^n$, *with* H *as in* (2.13) *we have, for* $f^{(t)}(x)=x$,

$$D_t x = \lim_{\Delta t\downarrow 0} M_{\psi}^{t,x}\left[\frac{x-f^{(t-\Delta t)}(\cdot)}{\Delta t}\right] = -i\hbar\,\frac{\nabla\psi_t}{\psi_t}(x) - A(x), \tag{3.8}$$

and

$$\lim_{\Delta t\downarrow 0} M_{\psi}^{t,x}\left[\frac{(x-f^{(t-\Delta t)}(\cdot))^2}{\Delta t}\right] = i\hbar\,\mathbb{1}, \tag{3.9}$$

where $(\cdot)$ *is the dummy space variable of the definition* (2.24). *As before, all such moments of order higher than 2 vanish.*

As mentioned in Remark 2 after Proposition II.12, in the conditions of Propositions III.1 and III.4, the definitions of the quantum (absolute) expectation of $f^{(t)}\cdot g^{(s)}$ in the state ψ, $t\geq s$, given in (2.28) and (2.28′) can be reexpressed in terms of the quantum derivatives D_t and $\bar{D}_t$ as follows.

Corollary III.6:

$$\langle f^{(t)}g^{(s)}\rangle_{\psi}=\left\langle M_{s,\cdot}^{\bar{\psi}}\left[\int_s^t \bar{D}_\tau f^{(\tau)}\,\mathrm{d}\tau\right]\cdot g^{(s)}+f^{(s)}g^{(s)}\right\rangle_{\psi_s}$$
$$=\left\langle f^{(t)}g^{(t)}-f^{(t)}M_{\psi}^{t,\cdot}\left[\int_s^t D_\tau g^{(\tau)}\,\mathrm{d}\tau\right]\right\rangle_{\psi_t},\quad t\geq s.$$

This relation could define, actually, the proper concept of time-dependent Dirichlet form relevant to quantum dynamics (or its Euclidean counterpart—cf. Ref. 7).

Let us apply the Proposition III.1 to a $f=(f^{(\tau)})_{\tau\in\mathbb{R}}$ in the domain of $\bar{D}_\tau$ which is, in fact, time independent and of the form $f^{(\tau)}(\cdot)=F(\cdot)$ for some regular F. Then the lhs of (3.1) can be made explicit using (2.16) for the Hamiltonian (2.13), as well as (3.4),

$$M_{t,x}^{\bar{\psi}}\int_t^T \bar{D}_\tau F\,\mathrm{d}\tau=M_{t,x}^{\bar{\psi}}\int_t^T\left(\bar{D}_\tau q\cdot\nabla F+\frac{i\hbar}{2}\Delta F\right)\mathrm{d}\tau=M_{t,x}^{\bar{\psi}}[F(\cdot)]-F(x). \tag{3.10}$$

This relation clearly displays a quantum deformation of the fundamental theorem of calculus for line integrals along C^1 trajectories

$$\begin{aligned}\gamma:[t,T]\subset\mathbb{R}&\to\mathbb{R}^n\\ \tau&\mapsto q(\tau).\end{aligned}$$

We shall henceforth denote the lhs of (3.10) by

$$M_{t,x}^{\bar{\psi}}\int_t^T \nabla F\circ\mathrm{d}q \tag{3.11}$$

in order to remind ourselves that it coincides simply with the rhs of (3.10) but involves the mentioned deformation of the classical calculus.

Using (3.6) instead of (3.1), we shall write as well, when $s\leq t$,

$$M_{\psi}^{t,x}\int_s^t \nabla F\circ\mathrm{d}q=F(x)-M_{\psi}^{t,x}[F(\cdot)], \tag{3.11'}$$

understanding now the lhs as

$$M_{\psi}^{t,x}\int_s^t\left(D_\tau q\cdot\nabla F-\frac{i\hbar}{2}\Delta F\right)\mathrm{d}\tau. \tag{3.10'}$$

More generally, for any $A:\mathbb{R}^n\to\mathbb{R}^n$ regular such that

$$M_{t,x}^{\bar{\psi}}\int_t^T\left(\bar{D}_\tau q\cdot A+\frac{i\hbar}{2}\nabla A\right)\mathrm{d}\tau \tag{3.12}$$

makes sense, we shall denote the expression (3.12) simply by

$$M_{t,x}^{\bar{\psi}}\int_t^T A\circ\mathrm{d}q. \tag{3.13}$$

We preserve, however, the boundary value in the time variable, in order to stress that (3.13) is only a short notation for (3.12) and that, in particular, *no* assumption on the existence of some underlying continuous trajectories $\tau\mapsto q(\tau)$ is made. The same remark applies to

$$M_{\psi}^{t,x}\left[\int_s^t A \circ \mathrm{d}q\right] = M_{\psi}^{t,x}\int_s^t \left(D_\tau q \cdot A - \frac{i\hbar}{2}\,\nabla\,\cdot A\right)\mathrm{d}\tau, \tag{3.13$'$}$$

so, with the conventions (3.13) and (3.13′), this "quantum calculus" satisfies the rules of the classical (Riemann-Stieltjes) calculus.

Let us come back to the special Lagrangian system whose quantum Hamiltonian is (2.13), i.e., a unit mass and charge particle in an electromagnetic field. Its associated classical action S_L with initial condition $S^{(s)}$ is defined by

$$S_L(x,t) = S^{(s)}(q(s)) + \int_\gamma \left(\frac{1}{2}|\dot{q}|^2 + \dot{q}\cdot A - V(q)\right)\mathrm{d}\tau, \tag{3.14}$$

for $s<t$. It is a real valued function of $x\in\mathbb{R}^n$, $t\in\mathbb{R}$ and a functional along a bundle of solutions γ in $C^2([s,t];\mathbb{R}^n):\tau\mapsto q(\tau)$ of the classical Lagrangian equations of motion, with the mixed boundary conditions on $[s,t]$,

$$\dot{q}(s) = \left.\frac{\partial S^{(s)}}{\partial q}\right|_{q(s)} \quad \text{and} \quad q(t) = x.$$

It is well known (cf., e.g., Ref. 8) that for $|t-s|$ small enough [and A and V as in (2.13)], S_L is a well-defined function. Notice that the Lagrangian L of S_L [i.e., the integrand of (3.14)] can be rewritten as

$$\int_\gamma L\,\mathrm{d}\tau = \int_\gamma \left(\frac{1}{2}|\dot{q}|^2 - V(q)\right)\mathrm{d}\tau + \int_\gamma A\,\mathrm{d}q. \tag{3.15}$$

We are going to show that, using various regularizations provided by the quantum mechanical conditional expectation, we can define a quantization of the above classical action functional S_L which will prove to be natural later on.

For any $(\tau,q)\psi$-admissible, let us define

$$S(q,\tau) = -i\hbar\,\ln\psi_\tau(q), \tag{3.16}$$

where ψ_τ is a regular solution of the Schrödinger equation (2.2) with Hamiltonian (2.1), such that $S=(S^{(\tau)})_{\tau\in\mathbb{R}}$ is continuous in the domain of D_τ. [We may choose the principal determination of the logarithm in the definition (3.16).]

According to (3.8), we observe that

$$D_\tau q = \nabla S(q,\tau) - A(q) \tag{3.17}$$

is an element of $L^2(\mathbb{R}^n, |\psi_\tau(q)|^2\,\mathrm{d}q)$ when $\int|\nabla\psi_\tau|^2\,\mathrm{d}q<\infty$ as well as $\int A^2(q)|\psi_\tau(q)|^2\,\mathrm{d}q<\infty$. Using the definition (2.14) for our situation, we compute

$$D_\tau S(q,\tau) = \frac{\partial S}{\partial\tau} + \left(-i\hbar\,\frac{\nabla\psi_\tau}{\psi_\tau} - A\right)\cdot\nabla S - \frac{i\hbar}{2}\Delta S = \frac{1}{2}(D_\tau q)^2 - \frac{i\hbar}{2}\,\nabla\,\cdot A + A\cdot D_\tau q - V(q), \tag{3.18}$$

where the relation (3.16) and the fact ψ_i solves the Schrödinger equation with H as in (2.13) have been used. The rhs of (3.18) is interpreted as the Lagrangian $L(D_\tau q, q)$ of our quantum system. Then, by Proposition III.4,

$$M_{\psi}^{t,x}\left[\int_s^t \left(\frac{1}{2}(D_\tau q)^2 - V(q)\right)\mathrm{d}\tau + \int_s^t \left(A\cdot D_\tau q - \frac{i\hbar}{2}\,\nabla\,\cdot A\right)\mathrm{d}\tau\right] = S(x,t) - M_{\psi}^{t,x}[S^{(s)}(\cdot)].$$

With the convention (3.13), this means that we have defined a regularized action function by

$$S(x,t) = M_{\psi}^{t,x}[S^{(s)}(\cdot)] + M_{\psi}^{t,x}\left[\int_s^t \left(\frac{1}{2}(D_\tau q)^2 - V(q)\right)\mathrm{d}\tau\right] + M_{\psi}^{t,x}\left[\int_s^t A \circ \mathrm{d}q\right], \tag{3.19}$$

to be compared with the corresponding classical action (3.14) and (3.15). The relation (3.19) provides us with an exact representation of the solution ψ_t of the Schrödinger equation.

Theorem III.7:

Let ψ_t be the solution of the Cauchy problem in $L^2(\mathbb{R}^n, \mathrm{d}x), t \geq s$,

$$i\hbar \frac{\partial \psi_t}{\partial t} = H\psi_t,$$

$$\psi_s(x) = e^{(i/\hbar)S^{(s)}(x)} \in \mathcal{D}_H, \quad \textit{with } S^{(s)} \textit{ such that } S^{(s)} = -i\hbar \ln \psi_s(x) \textit{ exists},$$

for $H=-(\hbar^2/2)[\nabla-(i\hbar)A]^2+V$, with A,V continuous as in Remark 1 after Lemma II.4. We also assume that $\int|\nabla\psi_\tau(q)|^2\,\mathrm{d}q<\infty$ and $\int A^2|\psi_\tau(q)|^2\,\mathrm{d}q<\infty$, $\forall\,\tau\geq s$. Then the following exact integral representation of the solution ψ_t holds:

$$\psi_t(x) = \exp\left(\frac{i}{\hbar}M_{\psi}^{t,x}\left[\int_s^t \left(\frac{1}{2}(D_\tau q)^2 - V(q)\right)\mathrm{d}\tau + \int_s^t A\circ \mathrm{d}q + S^{(s)}(\cdot)\right]\right) = e^{(i/\hbar)S(x,t)}, \tag{3.20}$$

$\forall(t,x)\,\psi$-admissible, where S is the (complex-valued) solution of the quantum Hamilton Jacobi equation on $\mathbb{R}^n\times[s,\infty[$

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S - A)^2 + V + \frac{i\hbar}{2}\nabla\cdot A - \frac{i\hbar}{2}\Delta S = 0,$$

$$S^{(s)}(x) = -i\hbar \ln \psi_s(x). \tag{3.21}$$

Remark: The kinetic energy term in (3.20) (i.e., the term with $V=0, A=0$) involves the scalar product of real vectors and not an Hermitian product. So, since $D_\tau q$ is a complex function, the kinetic energy term is, in general, a complex function, denoted here by $(D_\tau q)^2$.

Proof: When $t=s$ the representation (3.20) holds trivially, according to the property (3) of Proposition II.10 of the quantum mechanical conditional expectation. When $t>s$, using the relation (3.17), Eq. (3.18) means

$$\frac{\partial S}{\partial t} + (\nabla S - A)\cdot\nabla S - \frac{i\hbar}{2}\Delta S = \frac{1}{2}(\nabla S - A)^2 - \frac{i\hbar}{2}\nabla\cdot A + A\cdot(\nabla S - A) - V.$$

After simplification, this reduces to (3.21). The integral representation (3.20) follows from the definition (3.16) and the relation (3.19).

Remarks: We shall interpret (3.20) as a rigorous substitute for Feynman's path integral representation of the wave function ψ_t.[2] Like this one, (3.20) is built in term of the Lagrangian of the underlying classical system. We are going to need this for our study of quantum symmetries. However, the mathematical status of (3.20) is quite distinct from Feynman's heuristic (and, in some cases, rigorous[9,10] sum over a path space, as it involves in an essential way the regularizations provided by the quantum conditional expectation and no underlying path space whatsoever (cf. Sec. VII).

Corollary III.8:

Let $\bar{\psi}_t$ be the solution of the boundary problem in $L^2(\mathbb{R}^n, \mathrm{d}x)$ which is complex conjugate to the one of Theorem III.7,

$$\begin{cases} -i\hbar \dfrac{\partial \bar{\psi}_t}{\partial t} = H\bar{\psi}_t, \quad 0 \le t \le T, H \textit{ as in Theorem III.7}, \\ \bar{\psi}_T(x) = e^{(i/\hbar)S^{(T)}(x)}. \end{cases}$$

Then the following representation holds under the same assumptions as Theorem III.7:

$$\bar{\psi}_t(x) = \exp\left(\frac{i}{\hbar} M_{(t,x)}^{\bar{\psi}}\left[\int_t^T \left(\frac{1}{2}(\bar{D}_\tau q)^2 - V(q)\right)\mathrm{d}\tau + \int_t^T A \circ \mathrm{d}q + S^{(T)}(\cdot)\right]\right) = e^{(i/\hbar)\hat{S}(x,t)}, \tag{3.22}$$

where $\hat{S}$ *solves the equation adjoint to* (3.21) *on* $\mathbb{R}^m \times [-\infty, T]$,

$$\begin{gathered} -\frac{\partial \hat{S}}{\partial t} + \frac{1}{2}(-\nabla \hat{S} - A)^2 + V - \frac{i\hbar}{2}\nabla \cdot A - \frac{i\hbar}{2}\Delta \hat{S} = 0, \\ \hat{S}(x,T) = \hat{S}^{(T)}(x) = -i\hbar \ln \bar{\psi}_T(x). \end{gathered} \tag{3.23}$$

Proof: Starting from the logarithmic transformation of (3.22), Eq. (2.16) shows that $\bar{D}_\tau q = -\nabla \hat{S} - A$. Also $\bar{D}_i \hat{S}(q,\tau) = -(1/2)(\bar{D}_\tau q)^2 + V(q) - \bar{D}_\tau q \cdot A - (i\hbar/2)\nabla$. A reduces to (3.23). The conclusion follows from the definition (3.10) and Proposition III.1. □

Notice the change of signs in the two Hamilton-Jacobi equation (3.21) and (3.23). In the heuristic classical limit $\hbar = 0$, this is a well-known observation when the action is computed as a function of the future or past configurations (Ref. 11). This limit could be computed rigorously using, e.g., the methods of Ref. 12.

Also notice that, up to the convention (3.10) and (3.11) and the fact that the classical norm $|\dot{q}|^2$ of (3.14) is replaced by the square of a complex-valued quantum derivative, the Lagrangian of (3.22) is indeed the classical one, but evaluated on regularized variables.

The regularized action (3.19) used in our integral representation (3.20) satisfies the following additivity property along an admissible family of states ψ_τ, $s \le \tau \le u$.

Corollary III.9:

For any $t \in [s,u]$ *and under the conditions of Theorem III.7*,

$$M_\psi^{u,z}\left[\int_s^t L\, \mathrm{d}\tau + A \circ \mathrm{d}q\right] + M_\psi^{u,z}\left[\int_t^u L\, \mathrm{d}\tau + A \circ \mathrm{d}q\right] = M_\psi^{u,z}\left[\int_s^t L\, \mathrm{d}\tau + A \circ \mathrm{d}q\right].$$

Proof: According to the property (c) of the operator P^* defined by (2.29), using (3.19), and for $S^{(s)}$ like in the definition (3.21),

$$\begin{aligned} P_{t,u}^* \cdot P_{s,t}^*[S^{(s)}] &= M_\psi^{u,z}[M_\psi^{t,\cdot}[S^{(s)}]] \\ &= M_\psi^{u,z}\left[S^{(t)}(\cdot) - M_\psi^{t,\cdot}\left[\int_s^t L\mathrm{d}\tau + A \circ \mathrm{d}q\right]\right] \\ &= M_\psi^{u,z}[S^{(t)}(\cdot)] - M_\psi^{u,z}\left[M_\psi^{t,\cdot}\left[\int_s^t L\mathrm{d}\tau + A \circ \mathrm{d}q\right]\right] \\ &= S^{(u)}(z) - M_\psi^{u,z}\left[\int_t^u L\, \mathrm{d}\tau + A \circ \mathrm{d}q\right] - M_\psi^{u,z}\left[\int_s^t L\, \mathrm{d}\tau + A \circ \mathrm{d}q\right] \\ &= P_{s,u}^*[S^{(s)}] \\ &= S^{(u)}(z) - M_\psi^{u,z}\left[\int_s^u L\, \mathrm{d}\tau + A \circ \mathrm{d}q\right]. \end{aligned}$$

□

Let us see what the fundamental gauge invariance of quantum mechanics means in the context of our integral representation (3.20).

Proposition III.10:

Let ψ_t *be the solution of the Cauchy problem of Theorem III.7. Let* $\chi=(\chi^{(\tau)})_{\tau\in\mathbb{R}}$ *be real continuous and differentiable in the domain of* D_τ*. Then the gauge transformation*

$$A \mapsto A' = A + \nabla\chi,$$
$$V \mapsto V' = V - \frac{\partial\chi}{\partial\tau} \tag{3.24}$$

leaves the form of the Schrödinger equation invariant provided that the integral representation (3.20) *becomes*

$$\psi_t(x) \mapsto \psi_t'(x) = \exp\left(\frac{i}{\hbar}M_\psi^{t,x}\left[\int_s^t\left(\frac{1}{2}(D_\tau q)^2 - V(q)\right)\mathrm{d}\tau + \int_s^t A\circ \mathrm{d}q + \int_s^t D_\tau\chi^{(\tau)}\mathrm{d}\tau + (S^{(s)}+\chi^{(s)})(\cdot)\right]\right). \tag{3.25}$$

Proof: According to (2.14), for φ_t replaced by ϕ_t, and (3.11),

$$M_\psi^{t,x}\left[\int_s^t D_\tau\chi^{(\tau)}\,\mathrm{d}\tau\right] = M_\psi^{t,x}\left[\int_s^t \nabla\chi\circ\mathrm{d}q + \int_s^t\frac{\partial\chi}{\partial\tau}\,\mathrm{d}\tau\right] = \chi^{(t)}(x) - M_\psi^{t,x}[\chi^{(t)}(\cdot)]. \tag{3.26}$$

Using the representation of $\psi_t(x)$ in Theorem III.7 and (3.26), the representation (3.25) reduces to

$$\psi_t'(x) = \psi_t(x)e^{(i/\hbar)\chi^{(t)}(x)}. \tag{3.27}$$

When the starting wave function ψ_t is subject to the phase transformation (3.27), it is well know that the Schrödinger equation is form invariant under the gauge transformation (3.24). And indeed, (3.25) coincides with the representation (3.20) of $\psi_t'(x)$ in term of V' and A' defined by (3.24). □

We shall need, later on, a dynamical characterization of what plays, for our regularized action (3.19), the role of the critical points of the classical action (3.15), regarded as a functional of the C^2 path $\gamma:\tau\mapsto q(\tau)$.

Proposition III.11:

For the action (3.19), *the regularized equations of motion and conservation of energy in the admissible state* ψ_τ *solving the Schrödinger equation* (2.2) *with Hamiltonian H* (2.13) *in* $L^2(\mathbb{R}^3,\mathrm{d}q)$ *are, respectively, when* $D_\tau q$ *is in the domain of* D_τ,

$$D_\tau D_\tau q = -\operatorname{rot} A\wedge D_\tau Z - \frac{i\hbar}{2}\operatorname{rot}(\operatorname{rot} A) - \nabla V, \tag{3.28}$$

when $\wedge$ *denotes the exterior product in* $\mathbb{R}^n$ *and*

$$D_\tau h_{\psi_\tau}^H(q,\tau) = \frac{\partial h_{\psi_\tau}^H}{\partial\tau}, \tag{3.29}$$

where $h_{\psi_\tau}^H$ *is the space–time observable associated by* (2.5) *with the Hamiltonian* (2.13), *i.e.,*

$$h_{\psi_\tau}^H = \frac{1}{2}p^2 - p\cdot A + \frac{i\hbar}{2}\nabla\cdot(A-p) + \frac{1}{2}A^2 + V$$

for p the vector $p^j=-i\hbar(\nabla^j\psi_\tau/\psi_\tau)=B^j-A^j, j=1,2,3$ *and* $B(q,\tau)=D_\tau q$. *In* (3.29), $\partial h_{\psi_\tau}^H/\partial\tau$ *denotes the space–time observable associated with* $\partial H/\partial\tau$, *i.e., here,* $\partial V/\partial\tau$. *In particular, for V time independent,* $h_{\psi_\tau}^H$ *is a quantum martingale along* ψ_τ, *i.e.,* $D_\tau h_{\psi_\tau}^H=0$.

Proof: According to (2.14), we have $D_\tau q = -i\hbar(\nabla\psi_\tau/\psi_\tau) - A$. If $D_\tau q$ is in the domain of $\mathcal{D}_\tau$ we can compute $D_\tau D_\tau q$. Using the fact that ψ_τ solves the Schrödinger equation of Theorem III.7 one gets, after some simplification, the rhs of (3.28). Alternatively, taking the gradient ∇ of the quantum Hamilton-Jacobi equation (3.21) and, by (3.17),

$$D_\tau q = \nabla S(q,\tau) - A(q) \equiv B(q,\tau),$$

where we introduced the notation $B = -i\hbar(\nabla\psi_\tau/\psi_\tau) - A$ for the space–time observable $a_{\psi_\tau}^{P-A}$ associated by (2.5) with the quantum velocity observable $P - A(Q)$ (P being the momentum and Q the position observable). We verify that the resulting equation coincides with (3.28). The additional "quantum" deformation on the rhs of (3.28) comes from the vector identity in $\mathbb{R}^3 : \nabla(\nabla\cdot A) = \mathrm{rot}(\mathrm{rot}\, A) + \Delta A$ for the potential vector A. Besides this extra term, the rhs of (3.28) is the quantum regularization of the classical Lorentz force acting, at the singular limit $\hbar = 0$, on the system with Hamiltonian (2.13) (cf. remark below). Concerning (3.29), the space–time energy function h associated with the Hamiltonian (2.13) is, by (2.5), $(H\psi_\tau/\psi_\tau)$ for $\psi_\tau \in \mathcal{D}_H$. After substitution in (2.11) and using the fact that $i\hbar(\partial\psi_\tau/\partial\tau) = H\psi_\tau$, we obtain the conclusion. □

Remark: Using $\bar{D}_\tau$, as defined in (3.2), instead of D_τ, we would find that

$$\bar{D}_\tau \bar{D}_\tau q = \bar{D}_\tau q \wedge \mathrm{rot}\, A + \frac{i\hbar}{2}\mathrm{rot}(\mathrm{rot}\, A) - \nabla V, \tag{3.30}$$

instead of (3.28). In particular, only the average of $D_\tau D_\tau q$ and $\bar{D}_\tau \bar{D}_\tau q$ can provide a regularization of the classical Lorentz force free of quantum corrections but involving, instead, the symmetric velocity $(1/2)(D_\tau q + \bar{D}_\tau q)$, namely

$$\tfrac{1}{2}(D_\tau D_\tau q + \bar{D}_\tau \bar{D}_\tau q) = \tfrac{1}{2}(D_\tau q + \bar{D}_\tau q) \wedge \mathrm{rot}\, A - \nabla V. \tag{3.31}$$

Let us stress that our quantum calculus over space–time observables is perfectly commutative. For example, $-\mathrm{rot}\, A \wedge D_\tau q = D_\tau q \wedge \mathrm{rot}\, A$ in contrast with its operator counterpart,

$$-\mathrm{rot}\, A \wedge (P - A) = (P - A) \wedge \mathrm{rot}\, A + i\hbar\ \mathrm{rot}(\mathrm{rot}\, A), \tag{3.32}$$

but the quantum correction associated with the noncommutativity of the operators reappears now in (3.28) as a consequence of the definition (2.14) of D_τ. Also we remark that the use of both $\bar{D}_\tau$ and D_τ is really necessary for our quantum calculus. For example, as expressed by (3.32), $-\mathrm{rot}\, A \wedge q$ and $q \wedge \mathrm{rot}\, A$ differ after canonical quantization and, in fact, they do not even define, individually, symmetric operators. So our symmetrization leading to (3.31) is the space–time counterpart of the canonical (symmetrized) Lorentz equations of motion[13]

$$\frac{d^2 Q}{\mathrm{d}\tau^2} = \frac{1}{2}[(P - A) \wedge \mathrm{rot}\, A - \mathrm{rot}\, A \wedge (P - A)] - \nabla V, \tag{3.33}$$

for Q and P, respectively, the position and momentum quantum observables in the sense of Heisenberg.

IV. SYMMETRIES OF THE QUANTUM ACTION FUNCTION AND THE THEOREM OF NŒTHER

Let $\mathbb{R}^n$ be the configuration manifold of the classical system associated with the quantum Hamiltonian H of (2.2). The corresponding Lagrangian is

$$\begin{aligned} L:\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} &\to \mathbb{R} \\ (q,\dot{q},t) &\mapsto L(q,\dot{q},t). \end{aligned} \tag{4.1}$$

Let us consider a one-parameter local Lie group of transformations of the extended configuration space $\mathbb{R}^n \times \mathbb{R}$, of the form

$$U_\alpha : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n \times \mathbb{R}$$

$$(q,t) \mapsto (Q,\tau),$$

where

$$Q = q + \alpha X(q,t) + o(\alpha); \quad \tau = t + \alpha T(t) + o(\alpha); \tag{4.2}$$

the generators $X : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ and $T : \mathbb{R} \to \mathbb{R}$ are real analytical functions and α is a real parameter.

Let us write the action function (3.19) associated with the special Hamiltonian H of Theorem III.7. With an appropriate choice of the gauge $\chi^{(t)}(x)$ (Proposition III.10), we can get rid of the initial condition in the representation (3.19) for, say, $s=t_0$ and $t=t_1$,

$$S_L(x,t_1) = M_\psi^{t_1,x}\left[\int_{t_0}^{t_1}\left(\frac{1}{2}(D_t q)^2 - V(q)\right)\mathrm{d}t + \int_{t_0}^{t_1} A \circ \mathrm{d}q\right] \tag{4.3}$$

where ψ denotes the underlying solution of the associated Cauchy problem of Theorem III.7.

In analogy with the concept of invariance of the action involved in the classical Theorem of Nœther[14] we want to use the change of space–time variables, defined by (4.2), for defining the invariance of our regularized action (4.3).

Let us assume the existence of a further, complex analytic, generator $\varphi^{(t)}$ in the domain of D_τ, called the "divergence."

Definition IV.1: The action (4.3) *is divergence invariant under the one-parameter group of transformations* (4.2) *if, any interval* $[t_0,t_1]$, *we have*

$$\begin{aligned} M_\psi^{t_1,x_1}&\left[\int_{t_0}^{t_1}\left(\frac{1}{2}(D_\tau q)^2 - V(q)\right)\mathrm{d}t + \int_{t_0}^{t_1} A \circ \mathrm{d}q\right] + \alpha M_\psi^{t_1,x_1}\left[\int_{t_0}^{t_1} D_\tau \varphi^{(t)}\mathrm{d}t\right] \\ &= M_{\tilde\psi}^{\tau_1,Q_1}\left[\int_{\tau_0}^{\tau_1}\left(\frac{1}{2}(D_\tau Q)^2 - V(Q)\right)\mathrm{d}\tau + \int_{\tau_0}^{\tau_1} A \circ dQ\right] + o(\alpha), \end{aligned} \tag{4.4}$$

where $\tilde\psi$ denotes the associated solution of the same Cauchy problem as in Theorem III.7 but for the new space–time variables (Q,τ) resulting from the transformation U_α.

We remark that the definition (4.2) implies, up to the first order in α,

$$q + \alpha X(q,t) = Q, \tag{4.5}$$

where Q refers to the new configuration at the new time τ (we do not denote Q by Q_τ only to avoid the suggestion that paths $\tau \mapsto Q_\tau$ are involved).

Clearly, the invariance condition (4.4) can only hold under severe restrictions on the generations X,T, and φ. These conditions are easier to find in terms of the two solutions ψ and $\tilde\psi$ of the underlying Cauchy problem.

First, Proposition III.10 suggests that the addition in (4.4) of the divergence term $D_t\varphi^{(t)}$ to the given Lagrangian should correspond to a relation similar to (3.27) between ψ and $\tilde\psi$. So, to the first order in the parameter α, it should hold that

$$\tilde\psi = \psi - \alpha\frac{i}{\hbar}\varphi \cdot \psi. \tag{4.6}$$

Now let us consider (4.2) and (4.6) together with the linear generator of the associated local group of transformations of the Schrödinger equation (2.2) (as before, Einstein's sum convention is used)

$$\mathcal{L} = X^j \frac{\partial}{\partial x^j} + T\frac{\partial}{\partial t} + \frac{i}{\hbar}\varphi, \quad j = 1, \ldots, n.$$

For further purposes, it will be more natural to consider, instead, the formal symmetry generator

$$\hat{N}(t) = -i\hbar\,\mathcal{L} = X^j(x,t)\left(-i\hbar\frac{\partial}{\partial x^j}\right) - T(t)\left(i\hbar\frac{\partial}{\partial t}\right) + \varphi(x,t), \tag{4.7}$$

as well as the Schrödinger partial differential operator [cf. (2.2)], already used in Lemma II.4 (up to a factor i),

$$\mathbb{Q} = i\frac{\partial}{\partial t} - \frac{1}{\hbar}H. \tag{4.8}$$

Definition IV.2: $\hat{N}(t)$ is a symmetry operator for the Schrödinger equation (2.2) *provided*

$$[\hat{N}(t), \mathbb{Q}] = \lambda_{\hat{N}}(x,t)\mathbb{Q}, \tag{4.9}$$

where the complex analytic function $\lambda_{\hat{N}}(x,t)$ will depend, in general, on $\hat{N}(t)$ and is s.t. $\lambda_{\hat{N}}\mathbb{Q}D_{\mathbb{Q}} \subset L^2(\mathbb{R}^n \times \mathbb{R}, \mathrm{d}x\,\mathrm{d}t)$.

The domain $\mathcal{D}_{\mathbb{Q}}$ of $\mathbb{Q}$ has been defined in Lemma II.4. For the time being, we assume that $\mathcal{D}_{\mathbb{Q}} \supset \mathbb{Q}\mathcal{D}_{\mathbb{Q}}$ and $\hat{N}(t)\mathcal{D}_{\mathbb{Q}} \subset \mathcal{D}_{\mathbb{Q}}$ so that the lhs commutator of (4.9) is well defined on $\mathcal{D}_{\mathbb{Q}}$. We shall be more specific about $\mathcal{D}_{\hat{N}}$ in Sec. V.

In Refs. 15 and 67 it was shown that, in the algebraic sense, we have the following:

A symmetry operator $\hat{N}(t)$ generates a group, mapping solutions of the Schrödinger equation (2.2) into other solutions. The collection $\mathfrak{g}$ of such symmetry operators $\hat{N}(t)$ is a complex Lie algebra, i.e., if $\hat{N}_1, \hat{N}_2 \in \mathfrak{g}$, then (1) $\beta_1\hat{N}_1 + \beta_2\hat{N}_2 \in \mathfrak{g}, \forall \beta_1, \beta_2 \in \mathbb{C}$, (2) $[\hat{N}_1, \hat{N}_2] \in \mathfrak{g}$.

The formal symmetry group $G \equiv \exp \mathfrak{g}$ of Eq. (2.2) results from products of formal exponentials of symmetry operators; it is a local Lie group.

Let us stress that, in order to make this claim analytical rigorous, we have first to define the symmetrization $N(t)$ of such a formal generator $\hat{N}(t)$ then a self-adjoint extension $\hat{N}(t)$ and finally the unitary group generated by $\hat{N}(t)$. This will be done in Sec. V.

For a given Hamiltonian H, the property (4.9) implies the explicit conditions on the coefficients X, T, and φ that we are looking for.

Proposition IV.3:

$\hat{N}(t)$ is a symmetry operator for the Schrödinger equation in $L^2(\mathbb{R}^n)$, with Hamiltonian (2.13) *(where V may depend on time), if and only if*

(1)

$$\frac{\mathrm{d}T}{\mathrm{d}t}\delta^{jk} = \frac{\partial X^k}{\partial x^j} + \frac{\partial X^j}{\partial x^k}, \quad 1 \le j, \quad k \le n,$$

(2)

$$\frac{\partial X^j}{\partial t} = -\frac{\partial \varphi}{\partial x^j} - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t}A^j - X^k\frac{\partial A^j}{\partial x^k},$$

(3)

$$\frac{\partial \varphi}{\partial t} - A^j\frac{\partial \varphi}{\partial x^j} - \frac{i\hbar}{2}\Delta\varphi = X^j\frac{\partial}{\partial x^j}\left(\frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V\right) + \frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V\right) + T\frac{\partial V}{\partial t},$$

where Einstein's sum convention has been used, $\nabla.\,A$ denotes the divergence of the vector field A *and n is the dimension of the configuration space of the underlying classical system.*

Remark: If we allow space–dependent time transformation $\tau = t + \alpha T(q,t) + o(\alpha)$ in (4.2) then, for the associated $\hat{N}(t)$ to be a symmetry operator it is necessary, in addition to (1), (2), (3), that

$$\frac{\partial T}{\partial x^j} = 0, \quad j = 1, \ldots, n.$$

In other words, our initial choice of $T = T(t)$ was not a restriction.

Proof: Using the definitions (4.7) and (4.8), the conclusion follows from (4.9), after a laborious computation. One verifies that the coefficient $\lambda_{\hat{N}}(x,t)$ in (4.9) is

$$\lambda_{\hat{N}}(x,t) = -\frac{\mathrm{d}T}{\mathrm{d}t}(t). \tag{4.10}$$

In particular $\lambda_{\hat{N}}$ is not space dependent. □

Notice that the "determining equations" (1)–(4) (Ref. 16) for the coefficients X^j, T, and φ of the symmetry operator (4.7) are linear. We shall come back later to discuss their integrability conditions.

According to Theorem III.7, when $\hat{N}$ is a symmetry operator for (2.2) with Hamiltonian H of the form (2.13), $\tilde{\psi}$ solves the same Schrödinger equation but in the new variables (Q, τ). Therefore it follows from (3.16) and (3.19) that

$$-i\hbar \ \ln \tilde{\psi}(Q,\tau) = M_{\tilde{\psi}}^{\tau,Q}\left[\int_{\tau_0}^{\tau}\left(\frac{1}{2}(D_sQ)^2 - V(Q)\right)\mathrm{d}s + \int_{\tau_0}^{\tau} A \circ \mathrm{d}Q\right].$$

On the other hand, taken together, the relations (4.2) and (4.6) defining the Lie groups of transformation around the identity $\alpha = 0$ mean that ψ and $\tilde{\psi}$ are related, up to the first order in α, by

$$\psi(q,t)\exp\left(-\frac{i\alpha}{\hbar}\varphi(q,t)\right) = \tilde{\psi}(q + \alpha X(q,t), t + \alpha T(t)).$$

By considering $(-i\hbar \ \ln)$ of this equality for the principal determination of ln, taking into account the relation (4.5), valid for α small enough, as well as the representations (3.20) and (3.26), we verify that the invariance condition (4.4) of the action (4.3) is satisfied. In other words, the following proposition holds.

Proposition IV.4:

When the determining equations (1)–(3) *are satisfied for the Schrödinger equation with Hamiltonian* (2.13) *i.e., when the operator* $\hat{N}$ *of* (4.7) *is a symmetry operator for this equation, the associated action* (4.3) *is divergence invariant under the Lie groups of transformations defined by* (4.2) *and* (4.6).

We shall need:

Proposition IV.5:

Let us denote by $L = L(D_t q, q, t)$ *the Lagrangian involved in* (3.18)–(3.20). *Then, a necessary condition for the divergence invariance* (4.4) *of the action is that*

$$\frac{\partial L}{\partial t}T + \frac{\partial L}{\partial q^j}X^j + \frac{\partial L}{\partial (D_t q)^j}\left(D_t X^j - (D_t q)^j \frac{\mathrm{d}T}{\mathrm{d}t}\right) + L\frac{\mathrm{d}T}{\mathrm{d}t} = -D_t\varphi. \tag{4.11}$$

Proof: For the Hamiltonian of Theorem III.7 we have, according to the definition (2.14) of D_t, densely defined in $L^2(\mathbb{R}^n, |\psi_t(x)|^2 \,\mathrm{d}x)$,

$$D_t X^j = \frac{\partial X^j}{\partial t} + B^k \frac{\partial X^j}{\partial q^k} - \frac{i\hbar}{2}\Delta X^j, \tag{4.12}$$

where

$$B^k = -i\hbar \frac{\nabla^k \psi_t}{\psi_t} - A^k, \quad k = 1, \ldots, n.$$

By (1) and (2) of Proposition IV.3,

$$D_t X^j = -\frac{\partial \varphi}{\partial q^j} - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t}A^j - X^k \frac{\partial A^j}{\partial q^k} + B^k \frac{\partial X^j}{\partial q^k}.$$

In particular,

$$D_t X^j = -(D_t q)^j \frac{\mathrm{d}T}{\mathrm{d}t} = i\hbar \frac{\nabla^j \psi_t}{\psi_t} \cdot \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t} - \frac{\partial \varphi}{\partial q^j} - X^k \frac{\partial A^j}{\partial q^k} + \frac{1}{2}B^k\left(\frac{\partial X^j}{\partial q^k} - \frac{\partial X^k}{\partial q^j}\right).$$

After substitution of $L(D_t q, q, t) = (1/2)(D_t q)^2 + A \cdot D_t q - (i\hbar/2)\nabla \cdot A - V$ in (4.11) we verify that this relation reduces to the condition (3) of Proposition IV.3 and therefore to one of the conditions ensuring that the generator $\hat{N}$ of (4.7) is a symmetry operator for the Schrödinger equation of Theorem III.7. □

Proposition IV.6:

When the generator $\hat{N}(t)$ *is a symmetry operator for the Schrödinger equation* (2.2) *s.t.* $(\varphi_t, \hat{N}(t)\varphi_t)$ *is well defined and the assumption for* (4.9) *is satisfied, then we have* $\forall \varphi_t \in \mathcal{D}_{\hat{N}(t)}$,

$$\frac{d}{\mathrm{d}t}(\varphi_t, \hat{N}(t)\varphi_t) = 0.$$

Proof: The equation (2.3) for $A(t) = \hat{N}(t)$ holds even when the members of the one-parameter family of operators $\hat{N}(t)$ are not self-adjoint as long as H is, and if the $\hat{N}(t)$ are densely defined and such that $(\varphi_t, \hat{N}(t)\varphi_t)$ makes sense.

Then, for any $\varphi_t \in D_{\hat{N}(t)}$, using (2.3) for $\psi_t = \varphi_t$,

$$\frac{d}{\mathrm{d}t}(\varphi_t, \hat{N}(t)\varphi_t) = \int \bar{\varphi}_t \left(\frac{\partial \hat{N}(t)}{\partial t} + \frac{i}{\hbar}[H, \hat{N}(t)]\right)\varphi_t \, \mathrm{d}x$$
$$= -i \int \bar{\varphi}_t \{\mathbb{Q}(\hat{N}(t)\varphi_t) - \hat{N}(t)\mathbb{Q}\varphi_t\}\mathrm{d}x,$$

where the operator $-i\mathbb{Q} = [(\partial/\partial t) - (1/i\hbar)H]$ of Lemma II.4 has been introduced.

On the other hand, it follows from the definition (4.9) that when $\hat{N}$ is a symmetry operator for (2.2) then $\mathbb{Q}\varphi_t = 0 \Rightarrow \mathbb{Q}(\hat{N}(t)\varphi_t) = 0$. So the conclusion follows. □

Let us prove a stronger version of Proposition IV.6 (without expectation) in terms of space–time observables.

Theorem IV.7 (Theorem of Nœther):

When $\hat{N}(t)$ *is a symmetry operator for the Schrödinger equation* (2.2) *with Hamiltonian* (2.13), *and when the action* (4.3) *is divergence invariant under the Lie group of transformations generated by* $\hat{N}(t)$, *the associated space–time observable* $n_{\psi_t}^{\hat{N}}$ *in the state* ψ_t *satisfies* $D_t n_{\psi_t}^{\hat{N}} = 0$, for all ψ_t*-admissible elements in* $\mathcal{D}_{\hat{N}(t)}$. *In this case we shall say that* $n_{\psi_t}^{\hat{N}}$ *is a* quantum martingale *for this Schrödinger equation.*

Proof: According to the definition (4.7), writing n instead of $n_{\psi_t}^{\hat{N}}$ for simplicity, we have

$$D_t n(x,t) = D_t(X^j p_j - Th + \varphi)(x,t), \tag{4.13}$$

where the space–time functions associated with $\hat{N}$, the momentum observable P_j and the Hamiltonian observable H of (2.13) have been introduced.

Using the relation (4.12) and Proposition II.8, the derivative of the scalar product in (4.13) can be written as

$$D_t(X^j p_j) = (D_t X^j)p_j + X^j(D_t p_j) - i\hbar \frac{\partial X^j}{\partial x^k}\frac{\partial p_j}{\partial x^k}, \tag{4.14}$$

where we notice the quantum deformation of Leibniz rule. Since $p_j = -i\hbar(\nabla_j \psi_t/\psi_t)$, $\partial p_j/\partial x^k$ is symmetric in j and k, so

$$\begin{aligned} D_t(X^j p_j) &= (D_t X^j)p_j + X^j(D_t p_j) - i\hbar \frac{1}{2}\left(\frac{\partial X^k}{\partial x^j} + \frac{\partial X^j}{\partial x^j}\right)\frac{\partial p^j}{\partial x^k} \\ &= (D_t X^j)p_j + X^j(D_t p_j) - \frac{\hbar^2}{2}\frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{\Delta\psi_t}{\psi_t} - \left(\frac{\nabla\psi_t}{\psi_t}\right)^2\right), \end{aligned}$$

since, by (1) of Proposition IV.3,

$$\frac{\partial X^k}{\partial x^j} + \frac{\partial X^j}{\partial x^k} = \frac{\mathrm{d}T}{\mathrm{d}t}\delta^{jk}. \tag{4.15}$$

On the other hand, coming back to (4.13), we have

$$h = -\frac{\hbar^2}{2}\frac{\Delta\psi_t}{\psi_t} + i\hbar\frac{\nabla\psi}{\psi}\cdot A + \frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V. \tag{4.16}$$

Using (2.11) it is easy to verify (cf. also Proposition III.11) that

$$D_t h = \frac{\partial V}{\partial t}. \tag{4.17}$$

We have already found, in Proposition IV.5, that

$$D_t X^j = (D_t q)^i \frac{\mathrm{d}T}{\mathrm{d}t} + i\hbar\frac{\nabla^j\psi_t}{\psi_t}\cdot\frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t} - \frac{\partial\varphi}{\partial x^j} - X^k\frac{\partial A^j}{\partial x^k}.$$

Also, by (3) of Proposition IV.3,

$$\begin{aligned} D_t\varphi &= \left(\frac{\partial\varphi}{\partial t} - A^j\frac{\partial\varphi}{\partial x^j} - \frac{i\hbar}{2}\Delta\varphi\right) - i\hbar\frac{\nabla^j\psi_t}{\psi_t}\frac{\partial\varphi}{\partial x^j} \\ &= X^j\frac{\partial}{\partial x^j}\left(\frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V\right) + \frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V\right) + T\frac{\partial V}{\partial t} - i\hbar\frac{\nabla^j\psi_t}{\psi_t}\frac{\partial\varphi}{\partial x^j}. \end{aligned}$$

By (3.28), we also have, since $p_j = (D_t q)_j + A_j$,

$$D_t p_j = (D_t q \wedge \operatorname{rot} A)_j - \frac{i\hbar}{2}\operatorname{rot}(\operatorname{rot} A)_j - \nabla_j V + D_t A_j,$$

where

$$D_t A_j = \left(-i\hbar\frac{\nabla\psi_t}{\psi_t}\cdot\nabla\right)A_j - (A\cdot\nabla)A_j - \frac{i\hbar}{2}\Delta A_j.$$

After substitution of all this in

$$D_t n = (D_t X^j)p_j + X^j(D_t p_j) - \frac{\hbar^2}{2}\left[\frac{\Delta\psi_t}{\psi_t} - \left(\frac{\nabla\psi_t}{\psi_t}\right)^2\right] - hD_t T - D_t h \cdot T + D_t\varphi,$$

we obtain, indeed, zero. □

Let us come back to the explicit definition (4.7) of a symmetry operator $\hat{N}(t)$ for the Schrödinger equation (2.2). Introducing the definitions of the momentum and energy quantum observables P and H (in Heisenberg's picture) we observe that

$$\hat{N}(t) = X^j P_j - TH + \varphi, \tag{4.18}$$

where the coefficients X^j, T, and φ solve the partial differential equations of Proposition IV.3.

Let us denote by $Q(t)$ the time (Heisenberg) evolution of the position observable under an Hamiltonian H of the form (2.13). Then we define the following symmetrization of $\hat{N}(t)$:

$$N(t) = X^j(Q(t),t) \circ P_j(t) - T(t)H(t) + \hat{\varphi}(Q(t),t), \tag{4.19}$$

where $\circ$ denotes Jordan's multiplication of operators, i.e., $C\circ B=(1/2)(CB+BC)$. Then the phase φ should be redefined by

$$\hat{\varphi} = \varphi + \frac{i\hbar}{2}\nabla \cdot X. \tag{4.20}$$

Proceeding heuristically, without worrying about domains (cf. Sec. V for precise definitions), we see that by the Corollary II.3 and Theorem IV.7, $n_{\varphi_t}^{\hat{N}}$ satisfies

$$D_t n_{\varphi_t}^{\hat{N}} = \frac{1}{\varphi_t}\left(\frac{\partial\hat{N}}{\partial t} + \frac{1}{i\hbar}[\hat{N},H]\right)\varphi_t = 0, \tag{4.21}$$

or, equivalently, for $n_{\varphi_t}^{N}$. So we can also verify, using the definition (4.19) of $N(t)$, the following Heisenberg equations of motion for the Hamiltonian (2.13):

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = P - A(Q),$$

$$\frac{\mathrm{d}P}{\mathrm{d}t} = [P,H] = \frac{1}{2}\{(P-A)\wedge \operatorname{rot} A - \operatorname{rot} A \wedge (P-A)\} - \nabla V + \frac{1}{i\hbar}[A,H], \tag{4.22}$$

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t},$$

and the equations (1), (2), and (3) of Proposition IV.3, that $N(t)$ is indeed a constant of motion, i.e., satisfies

$$\frac{\partial N(t)}{\partial t} + \frac{1}{i\hbar}[N(t),H] = 0. \tag{4.23}$$

So we have heuristically checked that the family of operators $N(t)$ defined by (4.19) in terms of any solution $\{X^j, T, \varphi_s\}$ of the system of determining equations of Proposition IV.3 are constants of motion of the system with Hamiltonian H (2.13), associated with the Lie groups of space–time transformations generated by $\hat{N}(t)$.

From now on, we shall refer to $N(t)$ as above as a Nœtherian operator. We must now prove that any Nœtherian operator is indeed a respectable quantum observable, in the sense of Von Neumann.

V. STUDY OF THE NŒTHERIAN OPERATORS

A. Quadratic Hamiltonians

We shall start from the special class of Hamiltonian observables used in Theorem III.7, i.e., of the form

$$H(Q,P,t) = \tfrac{1}{2}[P - A(Q)]^2 + V(Q,t) \quad \text{on } C_0^\infty(\mathbb{R}^n) \tag{5.1}$$

but where, in addition, H is a real-valued polynomial of degree ≤ 2 in Q and P, which may be time dependent.

Let us denote by H_c the classical observable (or symbol) on the phase space $\mathbb{R}^{2n}\times\mathbb{R}$ to which $H \equiv H^W$ is associated by the Weyl calculus[17] of pseudodifferential operators. The set of quadratic inhomogeneous polynomials in q,p on $\mathbb{R}^{2n}$, denoted by $IQ(2\mathrm{n})$, constitutes a Lie algebra under the classical Poisson bracket of observables

$$\{F_c, G_c\} = \sum_{j=1}^{n} \frac{\partial F_c}{\partial q^j}\frac{\partial G_c}{\partial p_j} - \frac{\partial F_c}{\partial p_j}\frac{\partial G_c}{\partial q^j}. \tag{5.2}$$

Since the algebra generated under (5.2) by $IQ(2n)$ and any additional polynomial of order >2 is the set of all polynomials, $IQ(2n)$ will be maximal for our purpose.

Let us consider a smooth family of initial conditions $\psi^\alpha \in \mathcal{D}_H \subset L^2(\mathbb{R}^n, \mathrm{d}x), \alpha \in \mathbb{R}$, for the Schrödinger equation of a quadratic Hamiltonian (5.1), such that $\psi^0 = \psi$. The infinitesimal generator $\mathcal{N}$ of the associated one-parameter group in $\mathcal{D}_H$ is defined formally by

$$\mathcal{N}\psi = \left.\frac{d}{\mathrm{d}\alpha}\psi^\alpha\right|_{\alpha=0}. \tag{5.3}$$

Using the notation (4.7) for the symmetry operator $\hat{N}(t)$ of this Schrödinger equation, we consider the family of transformations $\mathcal{N}$ of the initial conditions ψ such that, under the quantum evolution generated by the quadratic Hamiltonian H,

$$(\mathcal{N}\psi)_t(x) = \hat{N}(t)\psi_t(x), \tag{5.4}$$

where, as before, ψ_t denotes the solution of the above-mentioned Cauchy problem of Schrödinger with initial condition $\psi \in \mathcal{D}_H$.

On the other hand, the ("Weyl") quantization $(-i/\hbar)F^W(Q,P)$ of any observable $F(q,p) \in IQ(2n)$ provides a linear map between Lie algebras, preserving the Lie bracket operation, i.e., a *representation* of such quadratic polynomials by skew-symmetric operators, such that Dirac's correspondence holds,

$$[F^W(Q,P), G^W(Q,P)] = \frac{i}{\hbar}\{F_c, G_c\}^W(Q,P) \tag{5.5}$$

for Q and P the quantum position and momentum observables, respectively. We consider first the simplest quadratic Hamiltonian (5.1), i.e., the free case $A = V = 0$. This will prove to be sufficient for any quadratic case (cf. Proposition V.4).

Proposition V.1:

The above (faithful) representation of $IQ(2n)$ can be exponentiated to a representation of a Lie group, called the inhomogeneous (or extended) metaplectic group and denoted $iMp(n)$, which is the semidirect product of $Mp(n)$, the ("metaplectic") group generated by the quadratic observables and W_n, the Heisenberg group generated by the linear and constant observables. In particular, any generator $\mathcal{N}$ satisfying (5.4) *belongs to the inhomogeneous metaplectic algebra, denoted by $imp(n)$.*

Proof: Let us denote by $k_0(q,t,x)$ the propagator of the free Schrödinger equation (2.2) [i.e., with $H=H_0$ in (5.1), where $A=V=0$]. Using the definition (4.7) of $\hat{N}(t)$, the rhs of Eq. (5.4) can be written as

$$\int_{\mathbb{R}^n} \psi(q)\left\{X^j(x,t)\left(-i\hbar\frac{\partial k_0}{\partial x^j}\right) - T(t)i\hbar\frac{\partial k_0}{\partial t} + \varphi(x,t)k_0\right\}(q,t,x)\mathrm{d}q$$
$$= \int_{\mathbb{R}^n}\left\{i\hbar X^j(x,t)\frac{\partial\psi(q)}{\partial q^j} + T(t)\frac{\hbar^2}{2}\frac{\partial^2\psi(q)}{\partial(q^j)^2} + \varphi(x,t)\right\}k_0(q,t,x)\mathrm{d}q,$$

where the space translation invariance of k_0 has been used. Taking $\lim_{t\downarrow 0}$, this provides the following explicit form of $\mathcal{N}$ defined on $C_0^\infty(\mathbb{R}^n)$ by (5.4):

$$\mathcal{N} = -X^j(Q,0)P_j - \tfrac{1}{2}T(0)P_j^2 + \varphi(Q,0). \tag{5.6}$$

□

Clearly, the maximal Lie algebra generated by such infinitesimal operators is a subalgebra, denoted by $\mathcal{G}_s(n)$, of the above-mentioned Weyl quantization of $IQ(2n)$.

Equivalently, each $X^j(x,0)$ can be an inhomogeneous polynomial of degree 1, $T(0)$ is a constant and $\varphi(x,0)$ an inhomogeneous polynomial of degree 2. Taking into account the restrictions imposed by (5.4) and the special form of our free Schrödinger equation, one computes that the dimension of this ("symmetry") Lie algebra $\mathcal{G}_s(n)$ of skew-symmetric operators is $(n/2)(n+3)+4=l$.

Here is a basis of $\mathcal{G}_s(n)$, for $j,k=1,2,\ldots,n$:

$$B_s(n) = \left\{ i, iq^k, \hbar\frac{\partial}{\partial q^k}, i\sum_k (q^k)^2, i\frac{\hbar^2}{2}\sum_k\frac{\partial^2}{\partial(q^k)^2} \quad , \quad \hbar\sum_k q^k\frac{\partial}{\partial q^k} + \frac{\hbar}{2}n, \hbar\left(q^j\frac{\partial}{\partial q^k} - q^k\frac{\partial}{\partial q^j}\right)\right\}. \tag{5.7}$$

We shall denote by $\mathcal{N}_j, j=1,2,\ldots,(n/2)(n+3)+4\equiv l$, the skew-Hermitian operators of $B_s(n)$ on $L^2(R^n)$. A necessary condition for exponentiating this representation of the Lie algebra $\mathcal{G}_s(n)$ is that all the generators $\mathcal{N}_j$ should be essentially skew-adjoint on a common domain in the Hilbert spaces. We shall use the following general result of Nelson[18] (cf. also Ref. 19):

Let G be a simply connected Lie group with an ℓ-dimensional Lie algebra $\mathcal{G}$, and a given representation of $\mathcal{G}$ by unbounded skew-Hermitian operators $\mathcal{N}_j, j=1,\ldots,\ell$, on a Hilbert space $\mathcal{H}$. Then this representation of $\mathcal{G}$ arises by differentiation of a unique unitary representation of $\mathcal{G}$ if there is dense set vectors ψ in the domain of any product $\mathcal{N}_{j_1},\ldots,\mathcal{N}_{j_m}$ and such that

$$\frac{\|\mathcal{N}_{j_1}\cdots\mathcal{N}_{j_m}\psi\|_{\mathcal{H}}}{m!} \le CK^m, \tag{5.8}$$

$\forall m\in\mathbb{N}$ and $\forall j_i\in\{1,\ldots,\ell\}$, for C,K two positive constants. Such a $\psi\in\mathcal{H}$ is called "analytic for $\{\mathcal{N}_j\}_{j=1}^{\ell}$."

In our case we have the following.

Lemma V.2:

The finite linear combinations of the Hermite functions on $\mathbb{R}^n$ (i.e., the products of one-dimensional Hermite functions) are analytic vectors for any products $\mathcal{N}_{j_1}\ldots\mathcal{N}_{j_m}$ of the generators listed in the basis (5.7) *of* $\mathcal{G}_s(n)$.

Proof: Since the set of finite linear combinations of Hermite functions is dense in $L^2(\mathbb{R}^n)$, one needs only to show that each Hermite function is an analytic vector for any $\mathcal{N}_{j1}\cdots\mathcal{N}_{jm}$. Instead of the standard basic $\{i, iq^k, \hbar\partial/\partial q^k\}, k=1,\ldots,n$, used in (5.7) for the Heisenberg algebra (of constant and linear observables in q and p), consider the linear combinations called creation and annihilation operators:

$$\left\{ i, A_k \equiv \frac{1}{\sqrt{2}}\left(q^k + \hbar\,\frac{\partial}{\partial q^k}\right), \quad A_k^+ \equiv \frac{1}{\sqrt{2}}\left(q^k - \hbar\,\frac{\partial}{\partial q^k}\right)\right\}. \tag{5.9}$$

Expressing the Hermite function in terms of A_k^+, one shows that those functions are analytical vectors for q^k and $-i\hbar(\partial/\partial q^k)$ (see, e.g., Ref. 4, p. 204). On the other hand, the operators of $B_s(n)$ quadratic in q and p are generated by all possible double products of creation and annihilation operators and it is known that the Hermite functions are analytic vectors as well for such quadratic observables (Ref. 19, p. 190). □

So there is indeed a unique representation of a Lie group $G_s(n)$ whose infinitesimal version (or differential) is the symmetry algebra $\mathcal{G}_s(n)$. The representation is included in the so-called extended metaplectic representation[19] which is the semidirect product of the $n(2n+1)$-dimensional metaplectic group $Mp(n)$, generated by all quadratic observables, and the $(2n+1)$-dimensional Heisenberg group W_n generated by the constant and liner observable.

In particular, let us consider matrices D in the symplectic Lie algebra $\mathcal{S}p(2n)$, i.e., of the form

$$D = \begin{pmatrix} W^T & Z \\ Y & -W \end{pmatrix}, \tag{5.10}$$

where Y and Z are $n \times n$ real matrices of the form $Y=\gamma\mathbb{1}, Z=\beta\mathbb{1}$, with γ, β two real constants, $\mathbb{1}$ the $n \times n$ identity matrix, and W is a $n \times n$ real matrix of the form

$$W = \begin{pmatrix} \delta & -W_{21} & -W_{31} & \dots & \dots & -W_{n1} \\ W_{21} & \delta & -W_{32} & \dots & \dots & -W_{n2} \\ W_{32} & W_{32} & \delta & \dots & \dots & -W_{n3} \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & -W_{nn-1} \\ W_{n1} & W_{n2} & \dots & \dots & W_{nn-1} & \delta \end{pmatrix} \tag{5.11}$$

for δ a constant. Then we use the faithful representation of $\mathcal{S}p(2n)$ by skew-Hermitian quadratic operators associated with the names of Segal, Shale, and Weil,[20]

$$D \mapsto -iP_D^W(Q,P) \equiv \beta\frac{i\hbar^2}{2}\frac{\partial^2}{\partial q_k^2} - \hbar\, q_k W_{jk}\frac{\partial}{\partial q^j} - \frac{\hbar}{2}n\delta + \gamma\frac{i}{2}q_k^2, \tag{5.12}$$

which is the infinitesimal version of the representation of some elements M_α of the symplectic groups $\mathcal{S}p(2n)$ by unitary groups $U_\alpha, \alpha \in R$, on $L^2(R^n)$,

$$M_\alpha = e^{\alpha D} \mapsto U_\alpha = e^{\alpha P_D^W(Q,P)}.$$

On the classical side, each M_α is a one-parameter group of linear difeomorphisms of the classical phase space $\mathbb{R}^{2n}$, whose associated quadratic Hamiltonian vector field v_D is defined by

$$\begin{aligned} v_D(F_c) &= \frac{\mathrm{d}}{\mathrm{d}\alpha}F_c(M_\alpha(q,p))\big|_{\alpha=0} = (W^T q + \beta p)\nabla_q F_c + (\gamma q - Wp)\nabla_p F_c = \nabla_p P_D^c \cdot \nabla_q F_c - \nabla_q P_D^c \cdot \nabla_p F_c \\ &= \{F_c, P_D^c\} \end{aligned} \tag{5.13}$$

on any F^c in the Schwartz space of smooth and rapidly decreasing functions, which are C^∞ vectors for the metaplectic representation. Equation (5.13) holds since the classical observable P_D^c in $IQ(2n)$ associated with $D \in \mathcal{S}p(2n)$ is

$$P_D^c(q,p) = \frac{\beta}{2}p^2 + qWp - \frac{\gamma}{2}q^2. \tag{5.14}$$

Notice that the only additional constant term in the representation (5.12) with respect to (5.14) is due to the Weyl (Jordan) symmetrization of the classical qWp term in (5.14).

The relation $D \in \mathcal{S}p(2n) \mapsto v_D$ preserves the respective Lie parentheses, i.e., is a Lie algebra homomorphism. As mentioned before, the Heisenberg algebra W_n adds to the previous picture the representation of the linear observable on $\mathbb{R}^{2n}$,

$$ap - bq + c \mapsto - i\,\hbar\, a_k \frac{\partial}{\partial qk} - b_k q^k + c, \tag{5.15}$$

where $a, b \in \mathbb{R}^n$ and $c \in \mathbb{R}$, so that, finally, the classical quadratic observable

$$P_D^c(q,p) = \frac{\beta}{2}p^2 + qWp - \frac{\gamma}{2}q^2 + ap - bq + c \tag{5.16}$$

of Hamiltonian vector field v_P associated with the (affine) equation of Hamilton,

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} \nabla_p P^c \\ -\nabla_q P^c \end{pmatrix} = \begin{pmatrix} W^T & \beta\mathbb{1} \\ \gamma\mathbb{1} & -W \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} + \begin{pmatrix} a \\ b \end{pmatrix},$$

is quantized, according to Weyl, by

$$P_D^W(Q,P) = -\frac{\beta}{2}\hbar^2\frac{\partial^2}{\partial q_k^2} - i\,\hbar\, q_k W_{jk}\frac{\partial}{\partial q_j} - \frac{\gamma}{2}q_k^2 - i\,\hbar\, a_k\frac{\partial}{\partial q_k} - b_k q^k + \left(c - \frac{i\hbar}{2}n\,\delta\right) \tag{5.17}$$

(with the usual convention of summing over repeated indices). We can now be more specific about the comments at the beginning of this section: The Lie algebra $IQ(2n)$ associated with the semi-direct product of the metaplectic group $Mp(n)$ and the Heisenberg group W_n is isomorphic to the algebra of all polynomial observables of degree ≤ 2 on $\mathbb{R}^{2n}$ equipped with the Poisson bracket (5.2) and the representation of the classical observables is Weyl quantization procedure.

Let us observe that some subgroups of $S_p(2n)$ have, under this representation, explicit integral formulations. We will not need them here. See Ref. 19 for some particular cases.

In particular, let us consider $D = \begin{pmatrix} 0 & \mathbb{1} \\ 0 & 0 \end{pmatrix} \in \mathcal{S}p(2n)$, i.e., the case $\beta=1, \gamma=0, W=0$ in (5.14). So the associated classical observable reduces to our free Hamiltonian

$$P_A^c(q,p) = \tfrac{1}{2}p^2 \equiv H_0(p),$$

and its Weyl quantization is, of course,

$$P_A^W(Q,P) = -\frac{i}{\hbar}H_0(P)$$

or $i\mathcal{N}_{(2n+3)}$ in term of the $(2n+3)$th element of the basis $B_s(n)$ (5.7). Denoting the associated parameter α by t, let us consider

$$U_t = e^{tP_A^W} = e^{-(i/\hbar)tH_0}, \quad t \in \mathrm{R},$$

i.e., the strongly continuous unitary group evolution in $L^2(\mathbb{R}^n)$, solving the free Schrödinger equation, and defined on $\mathcal{D}_{H_0}$. This groups acts on the symmetry algebra $\mathcal{G}_s(n)$ generated by the symmetry operators $\mathcal{N}_j, j=1, \cdots (n/2)(n+3)+4$ via the adjoint representation

$$\mathcal{N} \mapsto U_t \mathcal{N} U_t \equiv \hat{N}(t). \tag{5.18}$$

Since this representation sends analytic vectors into analytic vectors, the domains are preserved, $\mathcal{D}_{\mathcal{N}} = \mathcal{D}_{\hat{N}(t)}$. In other words, although H_0 and the operators $-i\mathcal{N}$ are unbounded symmetric operators, they are essentially self-adjoint and defined on a common dense invariant domain of analytic vectors in $L^2(\mathbb{R}^n)$. By a variant of the commutator theorem,[4] the Baker-Campbell-Hausdorff formula still holds. The image of the basis $B_s(n)$ under (5.18) is, therefore, computed as follows:

$$\Bigg\{ i, iq^k - t\hbar\frac{\partial}{\partial q^k}, \hbar\frac{\partial}{\partial q^k}, i\sum_k (q^k)^2 - 2t\left(\sum_k q^k \hbar\frac{\partial}{\partial q^k} + \frac{\hbar}{2}n\right) - 2t^2\hbar\frac{\partial}{\partial t}, \hbar\frac{\partial}{\partial t},$$
$$\hbar\sum_k q^k\frac{\partial}{\partial q^k} + \frac{\hbar}{2}n + 2t\hbar\frac{\partial}{\partial t}, \hbar\left(q^j\frac{\partial}{\partial q^k} - q^k\frac{\partial}{\partial q^j}\right)\Bigg\}, \tag{5.19}$$

where $j,k=1,\cdots,n$. We shall denote by $\hat{N}_j(t), j=1,\cdots,\ell$, any of those $\ell=(n/2)(n+3)+4$ resulting skew-symmetric operators.

Theorem V.3:

For fixed $t\in\mathbb{R}$, let us define by $U_t V_0^j(\alpha) U_{-t} = V_t^j(\alpha)$, $\alpha\in\mathbb{R}$, a one-parameter family of operators in $L^2(\mathbb{R}^n)$, with $V_0^j(\alpha)=e^{(\alpha/\hbar)\mathcal{N}_j}$ and $V_t^j(\alpha)=e^{(\alpha/\hbar)\hat{N}_j(t)}$, $\hat{N}_j(t)$ being any of the skew-symmetric operators of (5.19), *image under the adjoint representation* (5.18) *of the one-parameter group of operators $V_0^j(\alpha)$, $j=1,\ldots,\ell$, generated by the basis* (5.7) *of the symmetry algebra $\mathcal{G}_s(n)$. Then, the $V_t^j(\alpha)$ are symmetry operators of the free, Schrödinger equation $i\hbar(\partial/\partial t)\psi_t = H_0\psi_t$ in $L^2(\mathbb{R}^n)$, i.e., they map any regular solution ψ_t of this equation in another solution of the same equation $\tilde{\psi}_t = V_t^j(\alpha)\psi_t$, and the $i\hat{N}_j(t)$ are constant observables of the free quantum system.*

Proof: Let us consider $\psi_t = U_t\psi$, $\psi\in\mathcal{D}_H$ for $U_t = e^{-(i/\hbar)tH_0}$, $t\in\mathbb{R}$. Then $V_t^j(\alpha)\psi_t \equiv e^{-(i/\hbar)tH_0}\psi^\alpha$, $\alpha\in\mathbb{R}$, is, by construction, solution of the same free Schrödinger equation, for the one-parameter family of initial conditions in $\mathcal{D}_H \subset L^2(\mathbb{R}^n)$ defined by $\psi^\alpha \equiv e^{(\alpha/\hbar)\mathcal{N}_j}\psi$.

It follows from the definition of $V_t^j(\alpha)$ and the computation of $(\partial/\partial\alpha)|_{\alpha=0}$ in the relation above that

$$(\mathcal{N}_j\psi)_t(x) = \hat{N}_j(t)\psi_t(x), \quad j=1,\ldots,\frac{n}{2}(n+3)+4, \tag{5.20}$$

is the infinitesimal version of this relation, as required by the definition (5.4) of a symmetry operator.

Now by (5.18), $U_t\mathcal{N}_j U_t^{-1} = \hat{N}_j(t)$. Proceeding like in Sec. II (or observing, as before, that the Baker-Campbell-Hausdorff formula holds here), we see that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\psi_t, \hat{N}_j(t)\varphi_t) = \left(\psi_t, \left(\frac{\partial\hat{N}_j}{\partial t} + \frac{1}{i\hbar}[\hat{N}_j, H_0]\right)\varphi_t\right).$$

But, by definition (4.9) of a symmetry operator $\hat{N}(t)$ for the free Schrödinger operator

$$\mathbb{Q}\varphi_t \equiv \left(i\frac{\partial}{\partial t} - \frac{1}{\hbar}H_0\right)\varphi_t, \tag{5.21}$$

we had

$$[\hat{N}(t), \mathbb{Q}]\varphi_t = \lambda_N \mathbb{Q}\varphi_t = 0 \tag{5.22}$$

for any $\varphi_t \in \mathcal{D}^{\hat{N}}(t)$ (in the notations of Proposition II.2). In particular, for any $\hat{N}_j(t)$ as before we find, by Proposition IV.6,

$$i\frac{\mathrm{d}}{\mathrm{d}t}(\varphi_t,\hat{N}_j(t)\varphi_t)=0, \tag{5.23}$$

i.e., that $i\hat{N}_j(t)$ is a constant observable of the free Schrödinger equation. □

Any quadratic Hamiltonian H of the form (5.1) can, in fact, be handled in the same way since the infinitesimal generators of $B_s(n)$ [cf. (5.7)] form a vector space. Let us see how, in the special case $n=2$ for the simplicity of the illustration (and notations).

Proposition V.4:

All Schrödinger equations in $L^2(\mathbb{R}^2)$, of the form

$$i\hbar\frac{\partial}{\partial t}\psi_t=\left[-\frac{\hbar^2}{2}\Delta+c_1((x^1)^2+(x^2)^2)+c_2\left(-i\hbar\frac{\partial}{\partial x^1}\right)+c_3\left(-i\hbar\frac{\partial}{\partial x^2}\right)+c_4\left(-i\hbar\left(x^1\frac{\partial}{\partial x^2}-x^2\frac{\partial}{\partial x^1}\right)\right)\right.$$
$$\left.+c_5x^1+c_6x^2+c_7\left(-i\hbar\left(x^1\frac{\partial}{\partial x^1}+x^2\frac{\partial}{\partial x^2}\right)\right)+c_8\right]\psi_t, \tag{5.24}$$

with $c_k\in\mathbb{R}$ such that the Hamiltonian is essentially self-adjoint on $C_0^\infty(\mathbb{R}^2)$, have isomorphic symmetry algebras and are equivalent to the free equation

$$i\hbar\frac{\partial}{\partial t}\psi_t=H_0\psi_t, \tag{5.25}$$

where H_0 is the two-dimensional free Hamiltonian

$$H_0=-\frac{\hbar^2}{2}\left(\frac{\partial^2}{\partial(x^1)^2}+\frac{\partial^2}{\partial(x^2)^2}\right).$$

Proof: Given in Ref. 15. □

In order to illustrate this isomorphism, let us consider the following linear combination of elements of $\mathcal{G}_s(2)$ [using the notations of (5.7)]:

$$\mathcal{N}=-\mathcal{N}_6+\frac{1}{2}\mathcal{N}_7=i\left(-\frac{\hbar^2}{2}\Delta+\frac{1}{2}((x^1)^2+(x^2)^2)\right)\equiv iH_{0s}. \tag{5.26}$$

H_{0s} is the Hamiltonian observable of the isotropic two-dimensional harmonic oscillator. So, for any $\psi\in\mathcal{D}_{H_{0s}}$,

$$\psi_t(x)=\left(e^{-(i/\hbar)tH_{0s}}\psi\right)(x) \tag{5.27}$$

solves in $L^2(\mathbb{R}^2)$

$$\begin{aligned} i\hbar\frac{\partial\psi_t}{\partial t}&=H_{0s}\psi_t,\\ \psi_0(x)&=\psi(x). \end{aligned} \tag{5.28}$$

Now pick any $\mathcal{N}_j$, $j=1,\ldots,9$ in $B_s(2)$, the basis (5.7) of the free symmetry algebra $\mathcal{G}_s(2)$. Then, according to (5.18), but now for $U_t^{0s}=\exp(-(i/\hbar)tH_{0s})$,

$$\hat{N}_j^{0s}(t)=U_t^{0s}\mathcal{N}_j(U_t^{0s})^{-1} \tag{5.29}$$

is a symmetry generator of the harmonic oscillator, for the same reason as in Theorem V.3. Therefore $i\hat{N}_j^{0s}(t)$ is a constant observable of the quantum harmonic oscillator (5.28). All such harmonic symmetry operators $\hat{N}_j^{0s}(t)$, $j=1,\ldots,9$, are linear combinations of the $\mathcal{N}_j$ in $B_s(2)$, with time-dependent coefficients denoted by $X^k(x,t)$, $k=1,2,T(t)$ and $\varphi(x,t)$ in (4.7).

By Proposition IV.3, we already know the system of partial differential equations solved by these coefficients X^k, T, and φ regarded as functions. In our case, since $V(q)=\frac{1}{2}((x^1)^2+(x^2)^2)$ and the vector field A in (5.26) vanishes, they reduce to

$$\frac{\partial X^1}{\partial x^2}+\frac{\partial X^2}{\partial x^1}=0, \quad \frac{\partial X^1}{\partial x^1}+\frac{\partial X^2}{\partial x^2}=\frac{\mathrm{d}T}{\mathrm{d}t},$$
$$\frac{\partial X^j}{\partial t}=-\frac{\partial \varphi}{\partial x^j}, \quad j=1,2, \tag{5.30}$$
$$\frac{\partial \varphi}{\partial t}-\frac{i\hbar}{2}\Delta\varphi = X^1x^1+X^2x^2+\frac{\mathrm{d}T}{\mathrm{d}t}\cdot\frac{1}{2}((x^1)^2+(x^2)^2).$$

In particular, instead of solving (5.30), we could use the Baker-Campbell-Hausdorff formula in (5.29), for $\mathcal{N}_j$ any explicit element of the free basis $B_s(2)$ of (5.7). Let us take, for example, $\mathcal{N}_4=\hbar\,\partial/\partial x^1$. According to (5.19) this generator is invariant under (5.18), i.e., $\hat{N}_4(t)=\hbar\,\partial/\partial x^1$. On the other hand, under (5.29) we obtain, on $C_0^\infty(\mathbb{R}^2)$,

$$\hat{N}_4^{0s}(t)=\exp\left(-\frac{i}{\hbar}tH_{0s}\right)\mathcal{N}_4\exp\left(\frac{i}{\hbar}tH_{0s}\right)=\left(1-\frac{t^2}{2!}+\frac{t^4}{4!}-\cdots\right)\left(\hbar\frac{\partial}{\partial x^1}\right)-x^1\left(t-\frac{t^3}{3!}+\frac{t^5}{5!}-\cdots\right).$$

Comparing with the general form (4.7), this means that the coefficients of $\hat{N}_4^{0s}(t)$ are, respectively,

$$X^1(x,t)=\cos t, \quad X^2(x,t)=0, \quad T(t)=0, \quad \varphi(x,t)=x^1\sin t. \tag{5.31}$$

One verifies easily that (5.31) makes up a solution of the system (5.30). In other words,

$$\cos t\cdot P_1(t)+\sin t\cdot Q^1(t) \tag{5.32}$$

is a constant of motion of the quantum harmonic oscillator. This can also be easily verified otherwise: Consider the solution of the equation of motion of this system, in the Heisenberg picture. Those (linear) equations are, for $j=1,2$,

$$\begin{pmatrix} Q^j(t) \\ P_j(t)\end{pmatrix}=\Omega(t)\begin{pmatrix} Q^j \\ P_j\end{pmatrix}, \quad \text{with } \Omega(t)=\begin{pmatrix}\cos t & \sin t \\ -\sin t & \cos t\end{pmatrix}\in \mathrm{SO}(2). \tag{5.33}$$

In particular, the (constant) operators which are initial conditions of this solution are given by

$$\begin{pmatrix} Q^j \\ P_j\end{pmatrix}=\begin{pmatrix}\cos t & -\sin t \\ \sin t & \cos t\end{pmatrix}\begin{pmatrix} Q^j(t) \\ P_j(t)\end{pmatrix}, \quad j=1,2. \tag{5.34}$$

So the constant of motion (5.32) provided by Nœther's theorem coincides, in this elementary case, with the initial momentum P_1 of the solution (5.33). Another trivial example of symmetry generator is

$$\cos tQ^2(t)-\sin tP_2(t)\equiv Q^2, \tag{5.35}$$

associated with the following solution of the system (5.30)

$$X^1(x,t)=0, \quad X^2(x,t)=-\sin t, \quad T(t)=0, \quad \varphi(x,t)=x^2\cos t.$$

Fortunately, many nontrivial examples follow as well from this constructions (cf. Sec. VIII). In this way, the free basis $B_s(2)$ allows us to compute the basis of the symmetry Lie algebra of any quadratic Hamiltonian of the form (5.24) and then their associated symmetry operators $\hat{N}(t)$. We summarize this result (in two dimensions, for simplicity) as follows.

Proposition V.5:

Let us consider any essentially self-adjoint quadratic Hamiltonian H_Q in $L^2(\mathbb{R}^2)$, as in the rhs of equation (5.24), i.e., resulting from a linear combination of elements of $\mathcal{G}_s(2)$. For any ψ

$\in \mathcal{D}_{H_Q}$, $\psi_t=(e^{-(i/\hbar)tH_Q}\psi)(x)$ *solves the Cauchy problem for the associated Schrödinger equation. If* $\mathcal{N}_j$, $j=1,\ldots,9$, *denotes any element of the basis* $B_s(2)$ *of the free symmetry algebra* $\mathcal{G}_s(2)$ *then, on the dense invariant domain of analytic vectors of Lemma V.2,*

$$\hat{N}_j^{H_Q}(t) = U_t^Q \mathcal{N}_j (U_t^Q)^{-1} \tag{5.36}$$

is a symmetry generator of the H_Q*-system, where* U_t^Q, $t\in\mathbb{R}$, *denotes the one-parameter strongly continuous group of unitary operators*

$$U_t^Q = e^{-(i/\hbar)tH_Q}:L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2).$$

In particular, $i\hat{N}_j^{H_Q}(t)$ *is a constant of the motion of the* H_Q*-system. By construction, the time-dependent coefficients* $X^j(x,t),T(t)$ *and* $\varphi(x,t)$ *of this constant observable solve the system of equations of Proposition IV.3, for the quadratic Hamiltonian* H_Q.

Moreover, if W_t *denotes the one-parameter, strongly continuous, group of unitary operators in* $L^2(\mathbb{R}^2)$ *defined by*

$$W_t = U_t^Q \cdot e^{(i/\hbar)tH_0} \tag{5.37}$$

on the invariant domain of Lemma V.2, and for H_0 *as in* (5.25), *then* W_t *provides the time-dependent canonical transformation from the free system* (5.25) *to the one of Hamiltonian* H_Q. *In particular, we have*

$$H_Q = W_t H_0 W_t^{-1} + i\hbar \frac{\mathrm{d}W_t}{\mathrm{d}t} W_t^{-1}. \tag{5.38}$$

Proof: The Hamiltonian defined by the rhs of (5.24) is of the general quadratic form (5.18) with

$$\begin{gathered}\beta=1, \quad W_{21}=-c_4, \quad \gamma=-2c_1, \quad a_1=c_2, \quad a_2=c_3, \\ b_1=-c_5, \quad b_2=-c_6, \quad \delta=c_7, \quad c-i\hbar c_7=c_8\end{gathered} \tag{5.39}$$

and results indeed from a linear combination of elements of $\mathcal{G}_s(2)$. Let H_Q denote a self-adjoint extension of this (lower-bounded) operator in $L^2(\mathbb{R}^2)$. By Stone's theorem, $U_t^Q=e^{-(i/\hbar)tH_Q}$ is a strongly continuous unitary group of evolution in $L^2(\mathbb{R}^n)$ solving the associated Schrödinger equation. Using (5.36), any $\mathcal{N}_j\in B_s(2), j=1,\ldots,9$, evolves into a symmetry generator $\hat{N}_j^{H_Q}(t)$ of the H_Q-system, as in the above-mentioned example.

Let us define a time-dependent unitary operator W_t on the invariant domain of Lemma V.2 by

$$W_t = U_t^Q e^{(i/\hbar)tH_0}.$$

Clearly, if ψ_t is a solution of the free Schrödinger equation (5.25) with initial condition $\psi_0=\psi \in \mathcal{D}_{H_0}$ then $\phi_t=W_t\psi_t$ solves the Schrödinger equation with quadratic potential H_Q and the same initial condition. Equivalently, an H_Q-solution ϕ_t is given by a quadrature from a solution ψ_t of the free equation. (One could also introduce an extra unitary generator M acting as well on the initial condition ψ, so that

$$W_t' = U_t^Q M e^{(i/\hbar)tH_0}$$

is unitary.)

Then, it is well known that such a time-dependent unitary transformation W_t the Hamiltonian H_0 is transformed into H_Q given by (5.38). Precisely, this goes as follows.

Let us write $H_Q=H_0+(H_Q-H_0)$ and denoted by $\mathcal{D}_Q$ the above-mentioned common dense domain of analytic vectors of H_0 and H_Q. Then $H_Q=U_t^Q H_0 (U_t^Q)^{-1}+U_t^Q(H_Q-H_0)(U_t^Q)^{-1}$ on $\mathcal{D}_Q$. By the definition (5.37) of W_t this is also $H_Q=W_tH_0W_t^{-1}+U_t^Q(H_Q-H_0)(U_t^Q)^{-1}$ on $\mathcal{D}_Q$. Now on $\mathcal{D}_Q$ [in the strong $L^2(\mathbb{R}^n)$ sense]

$$i\hbar \frac{\mathrm{d}W_t}{\mathrm{d}t} \cdot W_t^{-1} = ih\frac{\mathrm{d}}{\mathrm{d}t}(U_t^Q e^{(i/\hbar)tH_0})e^{-(i/\hbar)tH_0}(U_t^Q)^{-1}$$
$$= H_Q - U_t^Q H_0 (U_t^Q)^{-1}$$
$$= U_t^Q (H_Q - H_0)(U_t^Q)^{-1},$$

so $H_Q = W_t H_0 W_t^{-1} + i\hbar(\mathrm{d}W_t/\mathrm{d}t)W_t^{-1}$ on $\mathcal{D}_Q$.

Since $\mathcal{D}_Q$ is a domain of essential self-adjointness, this implies (5.38). □

Let us make a remark on the problem of the zeroes set $\mathcal{N}_t^{\psi} = \{x \in \mathbb{R}^n \mid \psi_t(x) = 0\}$.

As mentioned in Sec. II, our construction [see the definitions (2.5) and (2.14), for example] requires to consider (t,x)-admissible states ψ, i.e., such that $\psi_t(x) \neq 0$.

The study of the zeroes of $\psi_t(x)$ amounts to investigate the wave front set WF of the integral kernel of Schrödinger,

$$k(x,t,y) = \mathrm{kernel}(e^{-(i/\hbar)tH})(x,y)$$

for fixed initial configuration x and time t. This problem has been considered by Zelditch[21] and Weinstein[22] for H slight perturbations of a quadratic Hamiltonian H_Q.

For example, in the case of the classical harmonic oscillator Hamiltonian $P_A^c(q,p) = (1/2)p^2 + (\omega^2/2)q^2$ [i.e., the case $\beta = 1, \gamma = -\omega^2$ and $W = 0$ in (5.14)] the initial zero (cf. Mehler formula) of the associated ψ_t reappears at times $k\pi/\omega$ and positions $(-1)^k x = y, k \in \mathbb{Z}$.

For more about this, see also Fujiwara (Ref. 23).

Under bounded perturbations with bounded derivative, the singularities of ψ_t behave as if H was the harmonic Hamiltonian, i.e., the wave front sets are stable under these weak perturbations.

The study of these singularities is made using the geometry of the underlying Hamiltonian flow on the classical phase space.

B. General Hamiltonians

When the Hamiltonian H of our given quantum system is not of the quadratic form H_Q considered in Sec. V A (cf., for example, Proposition V.5), the symmetry operators $N(t)$ defined formally in (4.19) with coefficients X, T, φ solving the PDE of Proposition IV.3 are still quantum constants of motion.

However, Dirac's correspondence (5.5) does not hold anymore and the metaplectic representation used in Sec. V B is of no help. In general, no explicit basis of the associated symmetry algebra can be found. But since, by hypothesis, the coefficients X, T, and φ of the symmetry operator $N(t)$ are analytic functions, it is easy to show that $N(t)$ is well defined for a large class of Hamiltonians H.

Proposition V.6: *Let us consider* $H = -(\hbar^2/2)\Delta + V$, *with* $V: \mathbb{R}^n \to \mathbb{R}$ *as in the Kato-Rellich theorem, so that H is self-adjoint in* $L^2(\mathbb{R}^2)$. *Let* $X: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n, \varphi: \mathbb{R}^n \times \mathbb{R} \to \mathbb{C}$ *and* $T: \mathbb{R} \to \mathbb{R}$ *be analytic functions, respectively, of the form* $X(q,t) = \Sigma_{n=0}^{\infty} \alpha_n(t) q^n$, *with* α_n *real-valued smooth functions,* $\varphi(q,t) = \Sigma_{n=0}^{\infty} \gamma_n(t) q^n$ *with* γ_n *complex-valued and smooth. If* $\Sigma_{n=0}^{\infty} |\alpha_n(t)| \|Q^n P \varphi\| < \infty$ *and* $\Sigma_{n=0}^{\infty} |\gamma_n(t)| \, \|Q^n \varphi\| < \infty, \forall \varphi \in \mathcal{A}(H)$, *the set of analytic vectors for H, then the Nœtherian symmetry operator*

$$N(t) = X^j(Q(t),t) \circ P_j(t) - T(t)H(t) + \hat{\varphi}(Q(t),t) \tag{5.40}$$

is a densely defined operator in $L^2(\mathbb{R}^n)$.

VI. THE QUANTUM THEOREM OF NŒTHER IN A RIEMANNIAN MANIFOLD

Let us consider now a classical system like the one of Sec. IV but with a configuration space which is, instead of $\mathbb{R}^n$, any n-dimensional smooth Riemannian manifold M, with positive-definite metric tensor $g_{i,j}$.

The state ψ of the associated quantum system evolves in $L^2(M,\mathrm{d}\mathcal{M})$, with volume element $\mathrm{d}\mathcal{M}(q)=\sqrt{g}\,\mathrm{d}q$, where $g=\det(g_{ij})$, according to

$$i\hbar\frac{\partial\psi_t}{\partial t}=H\psi_t \tag{6.1}$$

for the Hamiltonian of the form (2.13)

$$H=-\frac{\hbar^2}{2}\nabla^j\nabla_j+i\hbar A^j\nabla_j+\frac{i\hbar}{2}\nabla_kA^k+\frac{1}{2}\|A\|^2+V, \tag{6.2}$$

where $\|\cdot\|$ denotes the Riemannian norm and ∇_j is the covariant derivative with respect to the Levi-Civita connection. Let us recall that for this connection, the Christoffel symbols are symmetric: $\Gamma^i_{jk}=\Gamma^i_{kj}$, i.e., we are in the torsion-free case.

Conditions on the vector and scalar potentials V and A ensuring the self-adjointness of H on a dense domain of $L^2(M,\sqrt{g}\mathrm{d}q)$ are known; see, e.g., Refs. 24–27.

The relevant one-parameter group $U_\alpha, \alpha\in\mathbb{R}$, of transformations of the extended configuration space will be denoted, like in the flat case, by

$$U_\alpha{:}M\times\mathbb{R},(q^i,t)\mapsto(Q^i_\alpha=q^i+\alpha X^i(q,t)+o(\alpha),\tau_\alpha=t+\alpha T(t)+o(\alpha)), \tag{6.3}$$

where q^i are local configuration coordinates and

$$X{:}M\times\mathbb{R}\to M,\quad T{:}\mathbb{R}\to\mathbb{R},$$

are real analytic. For g any scalar field on $M\times\mathbb{R}$ such that $g\psi_t\in\mathcal{D}_H$ and such that $\dot{g}$ exists, let us define, like in (2.11), the quantum derivative along ψ_t by

$$D_tg=\frac{1}{\psi_t}\left(\frac{\partial}{\partial t}-\frac{1}{i\hbar}H\right)(g\psi_t). \tag{6.4}$$

Introducing (6.1) and (6.2), this means that

$$D_tg=\left(\frac{\partial}{\partial t}+\left(-i\hbar\frac{\nabla^j\psi_t}{\psi_t}-A^j\right)\nabla_j-\frac{i\hbar}{2}\nabla^j\nabla_j\right)g. \tag{6.5}$$

Since this can be interpreted as a quantum deformation of the classical "absolute" (or "intrinsic") derivative of the scalar g along a smooth continuous curve $q^j=q^j(t)$, we shall define D_tq^j by the vector

$$D_tq^j=-i\hbar\frac{\nabla^j\psi_t(q)}{\psi_t(q)}-A^j(q)\equiv B^j(q,t), \tag{6.6}$$

in analogy with what we have done in the proof of Theorem III.7 of Sec. III. Choosing, like in Eq. (3.16), $g(q,\tau)=S(q,\tau)$, with

$$S(q,\tau)=-i\hbar\ \ln\psi_\tau(q) \tag{6.7}$$

for any τ,q ψ-admissible solution of the Schrödinger equation (6.1), we can compute

$$D_\tau S(q,\tau)=\frac{1}{2}D_\tau q^jD_\tau q_j-\frac{i\hbar}{2}\nabla_jA^j+A_jD_\tau q^j-V(q). \tag{6.8}$$

The rhs of (6.8) defines the Lagrangian $L(D_\tau q,q)$ associated with the quantum system (6.1). Defining, for any $g=(g^{(s)})_{s\in\mathbb{R}}$ complex-valued, measurable and such that $g^{(s)}(\cdot)\psi_s(\cdot)\in L^2(M,\mathrm{d}\mathcal{M})$, the (forward) quantum conditional expectation in the state ψ by

$$E_{\psi}^{t,x}[g^{(s)}] = \int g^{(s)}(\xi)p(s,\xi,t,x)\mathrm{d}\mathcal{M}(\xi), \tag{6.9}$$

where, for any (t,x) ψ-admissible, $s \leq t$,

$$p(s,\xi,t,x)\mathrm{d}\mathcal{M}(\xi) = \psi_s(\xi)k_-(\rho,t-s,x)(\psi_t(x))^{-1}\,\mathrm{d}\mathcal{M}(\xi) \tag{6.10}$$

with k_- the advanced propagator of the Schrödinger equation (6.1), one verifies that Theorem III.7 still holds. So, canceling the boundary term without loss of generality, the regularized action functional (6.3) becomes

$$\begin{aligned} S_L(x,t_1) &= M_{\psi}^{t_1,x}\left[\int_{t_0}^{t_1}\left(\frac{1}{2}(D_t q)^2 - V(q)\right)\mathrm{d}t + \int_{t_0}^{t_1}\left(A_j D q^j - \frac{i\hbar}{2}\nabla_j A^j\right)\mathrm{d}t\right] \\ &= M_{\psi}^{t_1,x}\left[\int_{t_0}^{t_1}\left(\frac{1}{2}(D_t q)^2 - V(q)\right)\mathrm{d}t + \int_{t_0}^{t_1} A \circ \mathrm{d}q\right], \end{aligned} \tag{6.11}$$

where we have used on M the same notations as in the Euclidean case of equations (3.10) and (3.11).

Given an additional analytic generator $\varphi : M \times \mathbb{R} \to \mathcal{C}$, called the divergence, the invariance of the action (6.11) (up to this divergence term) is defined as in (4.4).

The formal symmetry operator on M becomes, instead of (4.7),

$$\hat{N}(t) = X^j(x,t)(-i\hbar\,\nabla_j) - T(t)\left(i\hbar\,\frac{\partial}{\partial t}\right) + \varphi(x,t), \tag{6.12}$$

and it is defined by the same commutation property (4.9) with the Schrödinger equation as in the Euclidean case. This property implies the following conditions on X, T, and φ.

Proposition VI.1:

$\hat{N}(t)$ *is a symmetry operator for the Schrödinger equation* (6.1) *in* $L^2(M,\mathrm{d}\mathcal{M})$, *with Hamiltonian* (6.2) (*where V may depend smoothly on time*) *if and only if the following determining equations hold*:

(1)

$$\frac{\mathrm{d}T}{\mathrm{d}t}g^{jk} = \nabla^j X^k + \nabla^k X^j,$$

(2)

$$\frac{\partial X^j}{\partial t} = -\nabla^j\varphi - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t}A^j - X^k\nabla_k A^j,$$

(3)

$$\frac{\partial\varphi}{\partial t} - A^j\nabla_j\varphi - \frac{i\hbar}{2}\nabla_j\nabla^j\varphi = X^j\nabla_j\left(\frac{i\hbar}{2}\nabla_k A^k + \frac{1}{2}\|A\|^2 + V\right)$$

$$+ \frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{i\hbar}{2}\nabla_k A^k + \frac{1}{2}\|A\|^2 + V\right) + T\frac{\partial V}{\partial t}.$$

Proof: This is based on a simple computation of $[\hat{N}(t),\mathbb{Q}] = \lambda_{\hat{N}}(x,t)\mathbb{Q}$, where $\mathbb{Q} = (\partial/\partial t) - (i/\hbar)H$ with the Hamiltonian (6.2). Like in the flat Euclidean case, one finds that

$$\lambda_{\hat{N}}(x,t) = -\frac{\mathrm{d}T}{\mathrm{d}t}(t). \tag{6.13}$$

□

Remark: As in the flat Euclidean case, if we allow space-dependent time transformations in (6.3), a further condition is needed for $\hat{N}(t)$ to be a symmetry operator for (6.1). This is

$$\nabla_j T = 0. \tag{6.14}$$

In other words (6.3) is indeed the most general space–time transformation for our purpose.

The integrability conditions of the determining equations (1)–(3) are not as obvious as in the flat Euclidean case, but they have already been investigated.[28]

When the determining equations (1)–(3) hold, the divergence invariance of the action (6.11) [in the sense of the relation (4.4)] is guaranteed by construction.

In order to obtain the general form of the invariance of the Lagrangian under our groups of transformations (Proposition IV.5) we need first to define the quantum derivative along ψ_t of a vector field Y^j on $M \times \mathbb{R}$.

In classical mechanics on a Riemannian manifold M, it is well known that the time derivative of the velocity field is, in general, not a tensor. In consequence, the acceleration is defined as the "absolute" (or "intrinsic") derivative of the velocity.[29] The result is indeed a contravariant tensor of rank one.

Definition VI.2: *Let R_k^j be the Ricci tensor of the Riemannian manifold M. Then the quantum ("absolute") derivative of the complex-valued vector field Y, on $M \times \mathbb{R}$ is defined by*

$$D_t Y^j = \frac{\partial Y^j}{\partial t} + B^k \nabla_k Y^j - \frac{i\hbar}{2}(\nabla^k \nabla_k Y^j + R_k^j Y^k), \tag{6.15}$$

where B^k is given by (6.6).

To be short, we shall denote simply by Δ the operator $\nabla^k\nabla_k + R$, so that

$$D_t Y^j = \frac{\partial Y^j}{\partial t} + B^k \nabla_k Y^j - \frac{i\hbar}{2} \triangle Y^j. \tag{6.15$'$}$$

On scalars and covariant vectors, the Laplacian $\triangle$ coincides with the Laplace-Kodaira-de Rham operator.[30] One easily shows that this Laplacian commutes with the gradient and the divergence, i.e., for g a scalar field as before,

$$\nabla_j \triangle g = \triangle \nabla_j g,$$

and for Y a vector field,

$$\nabla_j \triangle Y^j = \triangle \nabla_j Y^j.$$

Notice, in contrast, that $[\nabla^j \nabla_j, \nabla_i]$ is not zero, in general.

Proposition VI.3:

Let $L(D_t q, q, t)$ be the Lagrangian, defined by the rhs of (6.8), *of the quantum system, when the potential V is allowed to be a smooth function of the time. A necessary condition for the divergence invariance of the action functional* (6.11) *is*

$$\frac{\partial L}{\partial t}T + \frac{\partial L}{\partial q^j}X^j + \frac{\partial L}{\partial (D_t q)^j}\left(D_t X^j - (D_t q)^j \frac{\mathrm{d}T}{\mathrm{d}t}\right) + L\frac{\mathrm{d}T}{\mathrm{d}t} = -D_t \varphi. \tag{6.16}$$

Proof:

$$D_tX^j = \frac{\partial X^j}{\partial t} + B^k\nabla_kX^j - \frac{i\hbar}{2}(\nabla^k\nabla_kX^j + R^j_kX^k). \tag{6.17}$$

From the determining equation (1) (Proposition VI.1) and $(\mathrm{d}T/\mathrm{d}t)=(2/n)\nabla_jX^j$ (where $n=\dim M$) we have

$$\nabla_l\nabla_kX_j + \nabla_l\nabla_jX_k = 0.$$

Using this in the Ricci identity we get

$$\nabla_l\nabla_kX_j = R^m_{kjl}X_m, \tag{6.18}$$

where R^m_{kjl} denotes the Riemannian-Christoffel curvature tensor. The rhs of (6.18) coincides with $R_{kn,jl}X^n$, so

$$\nabla^n\nabla_kX_j = g^{n,l}R_{kn,jl}X^n$$

and

$$\nabla^k\nabla_kX^j = -R^j_kX^k. \tag{6.19}$$

After introduction of the determining equation (2) (Proposition VI.1) and of (6.19) in the definition (6.17) we obtain

$$D_tX^j = -\nabla^j\varphi - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t}\cdot A^j - X^k\nabla_kA^j + B^j\nabla_kX^j.$$

In particular,

$$D_tX^j - (D_tq)^j\frac{\mathrm{d}T}{\mathrm{d}t} = -\nabla^j\varphi - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t}\cdot A^j - X^k\nabla_kA^j - \frac{1}{2}B^j\frac{\mathrm{d}T}{\mathrm{d}t} + \frac{1}{2}B^k(\nabla_kX^j - \nabla^jX_k). \tag{6.20}$$

Now consider the invariance condition (6.16). Using the rhs of (6.8) as a definition of the Lagrangian (for V smoothly time dependent) this condition means explicitly, after simplification,

$$\frac{\partial\varphi}{\partial t} - A^j\nabla_j\varphi - \frac{i\hbar}{2}\nabla_j\nabla^j\varphi = X^j\nabla_j\left[\frac{i\hbar}{2}\nabla_kA^k + \frac{1}{2}\|A\|^2 + V\right] + \frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{i\hbar}{2}\nabla_kA^k + \frac{1}{2}\|A\|^2 + V\right) + T\frac{\partial V}{\partial t}.$$

This is the determining equation (3) of Proposition VI.1 and, therefore, the invariance condition (6.16) constitutes indeed a necessary condition for the divergence invariance of the action (6.11) under the Lie group of transformations (6.13). □

The main results of the flat case are, now, easily generalized. Using the definition of the quantum derivative along ψ_t of the scalar field $\boldsymbol{S}$ defined by (6.7), one verifies that S solves the quantum Hamilton-Jacobi equation on $M\times\mathbb{R}$,

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S - A)^2 + V + \frac{i\hbar}{2}\nabla_jA^j - \frac{i\hbar}{2}\nabla^j\nabla_jS = 0, \tag{6.21}$$

where the same remark as after (3.21) applies, as far as our notations are concerned. The quantum Hamilton-Jacobi equation (6.21) provides us with a direct derivation of the regularized equation of motion generalizing (3.28) and the Riemannian version of conservation of energy (3.29).

Let us compute

$$\nabla_jS = B_j + A_j. \tag{6.22}$$

We first notice that

$$\nabla_j \tfrac{1}{2}(\nabla S - A)^2 = \tfrac{1}{2}\nabla_j (B^k B_k) = B^k \nabla_k B_j + (\nabla_j B_k - \nabla_k B_j) B^k.$$

Since, for the Levi-Civita connection, there is no torsion, $\nabla_j B_k - \nabla_k B_j$ is the exterior derivative of B_k, generalizing the curl operator of Proposition III.11. By (6.22) this coincides with $-(\nabla_j A_k - \nabla_k A_j)$ so

$$\nabla_j \tfrac{1}{2}(\nabla S - A)^2 = B^k \nabla_k B_j - (\nabla_j A_k - \nabla_k A_j) B^k. \tag{6.23}$$

On the other hand, as observed after (6.15′), $[\Delta, \nabla_j]S = 0$ implies that

$$\nabla_j \nabla^k \nabla_k S = \nabla^k \nabla_k \nabla_j S + R_j^k \nabla_k S.$$

Finally, using (6.15) and (6.22), the covariant derivative of the quantum Hamilton-Jacobi equation (6.21) reduces to

$$D_t D_t q_j = -(\nabla_j A_k - \nabla_k A_j) B^k - \frac{i\hbar}{2}(\nabla_j \nabla_k A^k - \nabla A_j) - \nabla_j V. \tag{6.24}$$

Now let us consider the space–time observable of energy $h_{\psi_t}^H$ associated with (6.2), namely

$$h_{\psi_t}^H = \frac{H\psi_t}{\psi_t} = -\frac{\hbar^2}{2}\frac{\nabla^j \psi_t}{\psi_t}\frac{\nabla_j \psi_t}{\psi_t} - \frac{\hbar^2}{2}\nabla^j\left(\frac{\nabla_j \psi_t}{\psi_t}\right) + i\,\hbar\, A^j \frac{\nabla_j \psi_t}{\psi_t} + \frac{i\hbar}{2}\nabla_k A^k + \frac{1}{2}\|A\|^2 + V. \tag{6.25}$$

According to (6.6), it is consistent to denote the space–time momentum by

$$p^j = B^j + A^j, \tag{6.26}$$

so that the energy becomes

$$h_{\psi_t}^H = \frac{1}{2}p^2 - A^j p_j + \frac{i\hbar}{2}\nabla^j A_j - \frac{i\hbar}{2}\nabla^j p_j + \frac{1}{2}A^2 + V. \tag{6.25′}$$

Associated with the quantum Hamilton-Jacobi equation (6.21) we notice the following integrability condition:

$$\nabla_j h_{\psi_t}^H = -\frac{\partial B_j}{\partial t}. \tag{6.27}$$

Indeed, from the definition (2.5) and Schrödinger equation (6.1), $h_{\psi_t}^H = -(\partial/\partial t)S$, where the relation (6.7) has been used. In other words, according to (6.6), the relation (6.27) holds. Since the energy space–time observable is a scalar, its quantum derivative along ψ_t is given by (6.5),

$$D_t h_{\psi_t}^H = \frac{\partial h}{\partial t} - B^j \frac{\partial B_j}{\partial t} + \frac{i\hbar}{2}\nabla^j \frac{\partial B_j}{\partial t}, \tag{6.28}$$

where the integrability condition (6.27) was used. On the other hand, by the definition (6.25′) of $h_{\psi_t}^H$,

$$\frac{\partial H_{\psi_t}^H}{\partial t} = B^j \frac{\partial B_j}{\partial t} - \frac{i\hbar}{2}\nabla^j \frac{\partial B_j}{\partial t} + \frac{\partial V}{\partial t}.$$

After substitution in (6.28) we obtain the conservation of the energy

$$D_t h_{\psi_t}^H = \frac{\partial V}{\partial t}. \tag{6.29}$$

Let us collect this information in the

Proposition VI.4:

For the action functional S_L defined by (6.11), *the regularized equation of motion and conservation of energy in an admissible state ψ_t, solution of the Schrödinger equation* (6.1) *in $L^2(M,\sqrt{g}\mathrm{d}q)$, are given respectively by*

$$D_t D_t q_j = -(\nabla_j A_k - \nabla_k A_j)B^k - \frac{i\hbar}{2}(\nabla_j \nabla_k A^k - \triangle A_j) - \nabla_j V \tag{6.30}$$

and

$$D_t h^H_{\psi_t} = \frac{\partial V}{\partial t}. \tag{6.31}$$

In particular, when the scalar potential V is time independent, the energy space–time observable is a quantum martingale.

More generally, one shows, like in the flat case (cf. Ref. 31 and 32 for the probabilistic case), the following.

Theorem VI.5 (Theorem of Nœther):

Let us consider the Jordan symmetrization of the formal symmetry operator $\hat{N}(t)$ in $L^2(M,d\mathcal{M})$ defined in (6.12), *i.e., the Nœtherian operator*

$$N(t) = X^j(Q(t),t) \circ P_j(t) - T(t)H(t) + \hat{\varphi}(Q(t),t), \tag{6.32}$$

where $\circ$ denotes Jordan's multiplication of operators,

$$\hat{\varphi} = \varphi + \frac{i\hbar}{2}\nabla_j X^j \tag{6.33}$$

and X, T, and φ are solutions of the determining equations (1), (2), *and* (3) *of Proposition VI.1, for the symmetry groups of the Schrödinger equation* (6.1). *In* (6.32) *P_j and H are, respectively, the momentum and Hamiltonian observable in Heisenberg's picture [cf.* (6.26) *and* (6.2)*].*

Then N(t) is a quantum constant observable, densely defined on $\mathcal{D}_{N(t)} \subset L^2(M,\mathrm{d}\mathcal{M})$ and the associated space–time (scalar) observable $n^N_{\psi_t}$ is a quantum martingale, i.e., $D_t n^N_{\psi_t} = 0$, $\forall\, \psi_t$ admissible.

VII. QUANTUM PHYSICS, FEYNMAN PATH INTEGRAL AND STOCHASTIC ANALYSIS

Von Neumann axiomatization of quantum mechanics in Hilbert space is the mathematical form of the original version of this theory.[33] It can be regarded as a generalization of classical Hamiltonian mechanics, where the commutative algebra of the (real) observables in phase space is replaced by a noncommutative one.

It is well known that there is no mathematically rigorous Lagrangian version of quantum theory. To construct such a framework was precisely one of Feynman's original motivations.[2] But, in spite of its success (founded on its extraordinary heuristic power), Feynman's path integral theory still cannot be regarded as such a satisfactory framework, from the mathematical point of view. Let us recall that Feynman represents the solution of the initial value problem (2.2) by the symbolic expression

$$\psi_t(x) = \int_{\Omega^{t,x}} \psi(\omega(0)) e^{(i/\hbar)S[\omega;t]} \mathcal{D}\omega, \tag{7.1}$$

where $\Omega^{t,x}$ denotes the path space $\{\omega \in C([0,t],\mathbb{R}^n) \mid \omega(t)=x\}$. $S[\omega;t]$ is the action functional of the underlying classical Lagrangian system. For example, when H is as in (2.13), with $A=0$,

$$S[\omega;t]=\int_0^t\left(\frac{1}{2}|\dot{\omega}(\tau)|^2-V(\omega(\tau))\right)\mathrm{d}\tau\equiv S_0[\omega;t]-\int_0^t V(\omega(\tau))\mathrm{d}\tau, \tag{7.2}$$

$\mathcal{D}\omega$ is the heuristic "flat measure" on the path space $\Omega^{t,x}$ (used as a Lebesgue measure)

$$\mathcal{D}\omega=\prod_{0\leq\tau\leq t}\mathrm{d}\omega(\tau),$$

and

$$e^{(i/\hbar)S[\omega;t]}\equiv e^{-(i/\hbar)\int_0^t V(\omega(\tau))\mathrm{d}\tau}e^{(i/\hbar)S_0[\omega;t]}$$

is a complex weight.

Note that to make sense of the kinetic energy term in S_0 one should *a priori* assume that the paths $\tau\mapsto\omega(\tau)$ are absolutely continuous and in the Cameron-Martin Hilbert space $\mathcal{H}_{\mathrm{CM}}$ with (finite) norm

$$(\omega,\omega)_{\mathcal{H}}=\int_0^t|\dot{\omega}(\tau)|^2\mathrm{d}\tau. \tag{7.3}$$

Using Lie-Trotter's formula, Nelson has shown that the rhs of (7.1) can be reinterpreted as the strong limit $j\to\infty$ in $L^2(\mathbb{R}^n)$ of a discretization of the time interval $0<t_1<t_2<\cdots<t_j=t$ along polygonal paths interpolating linearly between the corresponding configurations $\omega(t_k)=x_k$, $k=1,\ldots,j,\omega(t)=x$. But the heuristic expression for the limit of

$$e^{(i/\hbar)S_0[\omega,t]}\prod_{\tau\in\{t_1,\ldots,t_j=t\}}\mathrm{d}\omega(\tau) \tag{7.4}$$

is not σ-additive (cf. Ref. 18) and therefore cannot be used for the construction of a basic complex measure on $\Omega^{t,x}$. However, it is possible, but very hard, to construct a rigorous (nonprobabilistic) functional calculus on path space, using the time discretization approximation (cf. Ref. 34). For various other approaches, cf. also Ref. 35. Let us see (in the free case, for simplicity) how the lack of complex measure is reinterpreted in our distinct construction.

We consider a finite product of complex-valued functions like the ones used in our definition (2.28),

$$F=f_n^{(t)}\cdot f_{n-1}^{(t_j-1)}\cdots f_1^{(t_1)},\quad n\in\mathbb{N},\quad t>t_{j-1}>t_{j-2}>\cdots>t_1. \tag{7.5}$$

By iteration of the argument used there for only two such functions, the quantum (absolute) expectation of F in the state ψ becomes

$$\langle f_j^{(t)}\cdots f_1^{(t_1)}\rangle_\psi=\int\psi_{t_1}(x_1)f_1^{(t_1)}(x_1)k_0(x_1,t_2-t_1,x_2)f_2^{(t_2)}(x_2)k_0(x_2,t_3-t_2,x_3)\cdots k_0(x_{j-1},t-t_{j-1},x_j)$$
$$f_j^{(t)}(x_j)\bar{\psi}_t(x_j)\mathrm{d}x_1\cdots\mathrm{d}x_j, \tag{7.6}$$

where $k_0(x,t-s,y)$ denotes the integral kernel of the evolution group U_{t-s} when $V=0$.

The rhs of (7.6) is a multilinear functional of $f_1^{(t_1)},\ldots,f_j^{(t)}$ which is well defined. But the corresponding finite additive measure is not σ-additive (the proof goes back to Cameron.[36] See also Ref. 37) and, therefore, there is no way to look at such an additive measure as the path space measure of some diffusion process, i.e., a Markovian stochastic process with continuous sample paths $\tau\to\omega(\tau)$.

What we have called the forward quantum transition kernel $\hat{p}$ in (2.23), for example, is not positive in contrast with a crucial requirement of the existence proof of such a probability measure.[38] However, regarded only as defining a continuous complex-valued functional on a reasonable domain of integrable functions and satisfying some basic properties needed otherwise for quantum theory, the limit of (7.4) makes sense and allows to obtain a number of results (see Refs. 39, 40, 37, 41, 42, and 61).

If we are insistent about interpreting Feynman's type of formula (7.1) as an integral over a space of continuous paths, the traditional way, in mathematical physics, is to appeal to Kac's approach (but cf. also Refs. 62–66). First one replaces Schrödinger's initial value problem (2.2) by its "Euclidean" (or "imaginary time") counterpart, say

$$-\hbar\frac{\partial\eta^*}{\partial t}=H\eta^* \tag{7.7}$$

with a bounded continuous initial condition χ in $L^2(\mathbb{R}^n)$. Then the counterpart of (7.4), i.e.,

$$e^{-(1/\hbar)\mathcal{S}_0[\omega;t]}\prod_{\tau\in\{t_1,\cdots\ldots,t_j=t\}}\mathrm{d}\omega(\tau), \tag{7.8}$$

converges to the Wiener measure with diffusion coefficient $\hbar$, denoted by $\mathrm{d}\mathcal{M}_W^{\hbar}$, on the path space $\Omega^{t,x}$ (cf., e.g., Ref. 38). The measure $\mathcal{M}_W^{\hbar}$ has support on continuous but not differentiable paths [in particular $\mathcal{M}_W^{\hbar}(\mathcal{H}_{\mathrm{CM}})=0$] so neither the first factor in (7.8) nor the second one are well defined but their product is. After a discrete absorption of the a.s. singular kinetic energy term in the measure, the probabilistic counterpart of (7.1) is Feynman-Kac formula,[43]

$$\eta_t^*(x)=\int_{\Omega^{t,x}}\chi(\omega(0))e^{-(1/\hbar)\int_0^t V(\omega(\tau))\mathrm{d}\tau}\mathrm{d}\mathcal{M}_W(\omega)=E^{t,x}\Big[\chi(W(0))e^{-(1/\hbar)\int_0^t V(W(\tau))\mathrm{d}\tau}\Big], \tag{7.9}$$

where the last expression adopts the probabilities notation for the conditional expectation given that the Wiener process satisfies $W(t)=x$ (our superscript t,x indicates that the condition lies in the future of the time interval of integration), as well as another notation η_χ^* for the solution of (7.7) stressing its dependence on the initial condition χ.

The process $W(\tau)$ is used exclusively as a technical tool in (7.9). We shall not insist here on the fact, underlined time and time again[44,45] that its (irreversible) dynamical properties have little to do with the (reversible) ones of free quantum dynamics. There is no surprise here: the way probability theory enters in (7.7)–(7.9) has nothing to do with the way it enters in quantum dynamics, where, in particular, no direct probabilistic concept of conditional expectation is defined but Born interpretation of ψ_t is fundamental to the absolute expectation.

The above-mentioned support of $\mathcal{M}_W^{\hbar}$ makes rather tricky the construction of any "stochastic (Euclidean) Lagrangian calculus" along the line suggested by Feynman in Ref. 2, since the irregularities of the "quantum paths" turn any classical action functional into a divergent one.

Any quantum observable should be defined as a function of the basic underlying "stochastic process." It is easy to check (see Chap. 7 of Ref. 2) that Feynman's implicit relation between self-adjoint operators in Hilbert space and associated "random variables" is precisely of our form (2.5) (although formulated by the authors in the time discretized context, i.e., before taking $\lim_{j\to\infty}$ in the above-mentioned construction, in order to avoid flagrant singularities). But the specific rules for handling these "random variables" are not established at all in Ref. 2. Their calculus seems to be plagued by the same kind of singularities as in naive computations along the paths of diffusion processes before the advent of Itô's calculus.

The first problem is, of course, that the precise nature of the underlying formal stochastic process itself (for a given H) is never specified. This may be due to the fact that, after the above-mentioned nonexistence proof of the "Feynman's process," the specific properties it should have were not, understandably, investigated. Is it clear, for example, that this process should be the one associated with the real time version of the Wiener measure or, instead, of the counterpart of some measure absolutely continuous with respect to the Wiener measure?

Also even if, given a quantum observable A, one admits (2.5) as a rule for the associated space–time observable, there are, of course, many other candidates providing the same quantum mechanical expectation $\langle\psi_t,A(t)\psi_t\rangle$. For example, Feynman gives two distinct space–time observables for the Hamiltonian H of the form (2.13) with zero vector potential (Ref. 2, p. 194). He does not indicate any way to choose which of those is more natural, for instance as defining the proper space–time counterpart of the quantum constant of motion. It is also worthwhile to observe here that Feynman's path integral approach does not provide, curiously, any Nœther Theorem although its whole point is to be a Lagrangian approach.

Nevertheless, Feynman's formal computations suggest that the abelian nature of the classical algebra of observables should be preserved under quantization but that other basic rules of Newtonian calculus should be "deformed in $\hbar$" so as to preserve the compatibility with regular (noncommutative) quantum mechanics in Hilbert space.

The point of our present work has been to investigate systematically the properties of the above-mentioned "process," beyond what Feynman did, without ever using what it certainly cannot provide, a well-defined probability measure on the path space, compatible with Born interpretation of the wave function ψ_t and all quantum mechanical predictions.

Our main improvement with respect to Feynman's original framework is the introduction of the quantum version(s) of conditional expectation(s) for his heuristic process. Indeed, this supplies us with a natural regularization of the many divergent terms in his formal computation, for example the kinetic energy term [cf. (3.20)] of the classical action function.

Introducing the quantum derivatives along an L^2-state associated with this quantum conditional expectation, our calculus of space–time observables follows directly, as well as the definition of quantum martingale, underlying Nœther theorem.

The key deformations of the rules of the classical calculus are, therefore, the ones of the derivations, given by Proposition II.8.

With this procedure, we have embedded regular quantum mechanics (more precisely, the class of elementary systems considered here) into a framework which, we claim, is much closer to probability theory and stochastic analysis than Feynman's path integral approach and, a fortiori, than quantum theory in Hilbert space.

Let us now recall why this claim is justified.

A solution of the Cauchy problems for Schrödinger's equation can be regarded as the value on the imaginary axis of a solution of the heat equation (7.7). This is the famous "Euclidean" relation (or "Wick rotation")

$$\psi_\chi(x,-it) = \eta_\chi^*(x,t) \tag{7.10}$$

for any $\chi \in \mathcal{D}_H \subset L^2(\mathbb{R}^n)$.

Let us restrict ourselves, for a fixed $T>0$, to χ in the dense set of vectors in $L^2(\mathbb{R}^n)$, denoted by $\mathcal{D}(e^{(T/2)H})$, such that

$$\sum_{n=0}^{\infty} \frac{1}{n!} \|H^n\chi\|_2 |t|^n < \infty, \quad \forall\, t \in I = \left[-\frac{T}{2},\frac{T}{2}\right].$$

Then, together with the solution of (7.7), we can consider the solution, in the strong L^2-sense of the adjoint equation with respect to the time parameter

$$\begin{aligned} \hbar \frac{\partial \eta_{\bar\chi}}{\partial t} &= H\eta_{\bar\chi}, \quad t \in I \\ \eta_{\bar\chi}(\cdot,0) &= \bar\chi(\cdot), \end{aligned} \tag{7.11}$$

where the overbar denotes, now, the complex conjugate.

Clearly we have

$$\int_{\mathbb{R}^n} \eta_{\bar{\chi}} \eta_{\chi}^{*}(x,t) \mathrm{d}x = \|\chi\|_2^2, \tag{7.12}$$

in a striking analogy with Born's "probabilistic" interpretation of the associated wave function ψ_t [cf. definition (2.17)]. This observation is due to Schrödinger (cf. Refs. 44 and 45) and lies at the foundations of Euclidean quantum mechanics.

The identity (7.12) suggests the introduction of various Hilbert spaces associated with the pair of heat equations (7.7)–(7.11) and allowing to mimic what happens in regular quantum mechanics. For each $t \in I$, consider the solution space of (7.7), namely

$$\tilde{\vartheta}_t^* \equiv \tilde{\vartheta}_t^*(\mathbb{R}^n) = \left\{ \eta_\chi^*(t), \chi \in \mathcal{D}(e^{(T/2)H}) \right\},$$

and define

$$\begin{gathered} U_t^{-1} : \tilde{\vartheta}_t^* \to \mathcal{D}(e^{(T/2)H}), \\ \eta_\chi^*(t) \mapsto \chi. \end{gathered} \tag{7.13}$$

Equation (7.12) suggests as well the definition of the following scalar product in $\tilde{\vartheta}_t^*$:

$$(\eta_{\chi_1}^*(t) | \eta_{\chi_2}^*(t))_t = \langle U_t^{-1} \eta_{\chi_1}^*(t) | U_t^{-1} \eta_{\chi_2}^*(t) \rangle_2 = \langle \chi_1 | \chi_2 \rangle_2, \tag{7.14}$$

and to complete $\tilde{\vartheta}_t^*$ with respect to $(\cdot|\cdot)_t$. The resulting space, denoted by ϑ_t^*, is called forward Hilbert space. As a matter of fact, $(\vartheta_t^*, (\cdot|\cdot)_t)$ is unitarily equivalent to $(L^2, \langle\cdot|\cdot\rangle_2)$ since U_t^{-1} can be extended unitarily from ϑ_t^* onto L^2. Using U_t, the Euclidean version of Heisenberg time evolution of observables will be, for any densely defined A,

$$A_{-t}^F = U_t A U_t^{-1}, \quad t \in I, \tag{7.15}$$

where F stands for forward (space).

So the familiar (Heisenberg's) quantum formulas will be valid, but without the factor $i = \sqrt{-1}$. For the same reason, the observables, in this framework, are densely defined normal operators (not necessarily self-adjoint). For example, the momentum observable in $\vartheta_0^*(\mathbb{R}^n) = L^2(\mathbb{R}^n)$ is defined as $-\hbar\nabla$ on its usual domain. A symmetric construction for equation (7.11) would introduce another one-parameter family of ("backward") Hilbert space, ϑ_t.

Before continuing, it is worth stressing that the "reciprocal" analytical continuation in time of the above construction adds nothing to regular quantum theory. Since the analytical vectors are dense in $L^2(\mathbb{R}^n)$ and $e^{-(i/\hbar)tH}(L^2(\mathbb{R}^n)) = L^2(\mathbb{R}^n)$ $\forall t$, the real time version of the key restriction $\chi \in \mathcal{D}(e^{(T/2)H})$ disappears since

$$\mathcal{D}(e^{i(T/2)H}) = L^2(\mathbb{R}^n), \quad \forall\, T \in \mathbb{R}.$$

Let us see that the probabilistic interpretation suggested by (7.12) and (7.14) is indeed fully justified on positive vectors in ϑ_t^*, if $e^{-(t/\hbar)H}$ is positively preserving. For H as in Theorem III.7, with $A=0$, this is the case when V belongs to a subset of a class of potentials introduced by Kato (cf. Ref. 45). The integral kernel of $e^{-(1/\hbar)(t-s)H}$ in $L^2(\mathbb{R}^n)$, denoted by

$$h(x, t-s, q), \tag{7.16}$$

is, then, known to be jointly continuous and strictly positive.

For $\chi > 0$ fixed as before, and $\eta_s^*(\cdot) = \eta_\chi^*(\cdot, s)$, the Euclidean counterpart of the quantum transition kernel (2.25) becomes

$$q^*(\tau, \mathrm{d}q, t, x) = \eta_\tau^*(q) h(q, t-\tau, x) (\eta_t^*(x))^{-1} \, \mathrm{d}q, \quad \tau \le t \text{ in } I. \tag{7.17}$$

In contrast with (2.25), q^* satisfies all the properties of the backward transition probability of a real-valued Markov process in I, for a given final probability distribution $p_{T/2}(y)\mathrm{d}y$.

For another fixed $\chi' > 0$, and $\eta_t(\cdot) = \eta_{\chi'}(\cdot, t)$ in $\vartheta_t(\mathbb{R}^n)$ one gets the Euclidean version of the quantum transition kernel (2.23), i.e.,

$$q(t,x,\tau,\mathrm{d}q) = \eta_t^{-1}(x)h(x,\tau - t,q)\,\eta_\tau(q)\mathrm{d}q, \quad t \leq \tau \text{ in I}, \tag{7.18}$$

namely the (forward) transition probability of a Markov process for a given initial probability distribution $p_{-T/2}(x)\mathrm{d}x$. The existence of this Markov process $Z_t, t \in I$, introduced in 1984–1985 under the name of Bernstein diffusion[45] has been proved since then in more general settings (see Ref. 46 for a recent review, using the tools of statistical physics).

Notice that the quantum problem of the zeroes of the wave function disappears here since, by hypothesis on the potential V, $\exp(-(1/\hbar)(t-s)H)$ is positivity preserving. Using (7.17) and (7.18), one verifies easily that Z_t, $t \in I$, is a real valued inhomogeneous diffusion process whose drifts and diffusion matrix are given by the Euclidean version of Proposition II.14, i.e.,

$$B^*(q,t) = -\,\hbar\,\frac{\nabla \eta_t^*}{\eta_t^*}(q),$$

$$B(q,t) = \hbar\,\frac{\nabla \eta_t}{\eta_t}(q), \tag{7.19}$$

$$C(q,t) = C^*(q,t) = \hbar\,\mathbb{1},$$

with $\mathbb{1}$ the $n \times n$ identity matrix.

The particularity of such diffusions is that, in contrast with the traditional one-sided notion of Markov processes, they take seriously the fact that the Markov property itself is invariant under time reversal. If $\mathcal{P}_t$ denotes the σ-algebra generated by the past of Z_t, i.e., $\mathcal{P}_t = \sigma\{Z_s, s \in I, s \leq t\}$ and $\mathcal{F}_t$ the future, $\mathcal{F}_t = \{Z_u, u \epsilon I, u \geq t\}$, then, for any events $A \in \mathcal{P}_t$ and $B \in \mathcal{F}_t$,[38]

$$P(AB|\mathcal{N}_t) = P(A|\mathcal{N}_t) \cdot P(B|\mathcal{N}_t) \tag{7.20}$$

almost surely, where $\mathcal{N}_t$ denotes the present $\sigma\{Z_t\}$ and $P(\cdot|\mathcal{N}_t)$ is the conditional probability given $\mathcal{N}_t$.

The time symmetry of $Z_t, t \in I$, shows up in the multiplicative aspect of the integrand of (7.12), for a pair of positive analytic vectors χ, χ', since Eqs. (7.7) and (7.11) are formally time reversed of each other.

The Euclidean version of the relation (2.5) between operators in Hilbert space and space–time observables provides us with well-defined random variables, functions of Z_t. For example, the above-mentioned momentum observable at time t corresponds to $-\hbar(\nabla \eta_t^* / \eta_t^*)(Z_t)$, i.e., the drift $B_*(z_k, t)$ already known by (7.19).

It follows that the Euclidean counterparts of the quantum derivatives (2.14) and (2.16) along the quantum state ψ_t and $\bar{\psi}_t$ are given, respectively, by

$$D_t^* = \frac{\partial}{\partial t} + \mathcal{L}^*, \tag{7.21}$$

$$D_t = \frac{\partial}{\partial t} + \mathcal{L}, \tag{7.22}$$

where $\mathcal{L}^*$ and $\mathcal{L}$ are backward and forward generators of $Z_t, t \in I$, namely the elliptic operators

$$\mathcal{L}^* = -\,\hbar\,\frac{\nabla \eta_t^*}{\eta_t^*} \cdot \nabla - \frac{\hbar}{2}\Delta, \tag{7.21$'$}$$

and

$$\mathcal{L} = \hbar \frac{\nabla \eta_t}{\eta_t} \cdot \nabla + \frac{\hbar}{2} \Delta. \tag{7.22$'$}$$

The derivatives (7.21) and (7.22) are better defined as limits (whenever they exist) of conditional expectations, for f smooth real valued with compact support on $\mathbb{R}^{n+1}$, namely

$$D_t^* f(Z_t,t) = \lim_{\Delta t \downarrow 0} E_t \left[\frac{f(Z_t,t) - f(Z_{t-\Delta t}, t - \Delta t)}{\Delta t} \right] \tag{7.23}$$

and

$$D_t f(Z_t,t) = \lim_{\Delta t \downarrow 0} E_t \left[\frac{f(Z_{t+\Delta t}, t + \Delta t) - f(Z_t,t)}{\Delta t} \right], \tag{7.24}$$

where E_t denotes the conditional expectation given Z_t in the future or in the past of the time interval, computed in terms of the kernels (7.17) or (7.18), respectively. These conditional expectations make sense from the probabilistic viewpoint, since the process Z_t does, in contrast with our quantum definitions (2.24) and (2.22).

Let us stress that, although the definitions (7.23) and (7.24) coincide with Nelson's ones in Ref. 47, the processes Z_t have little in common with the ones introduced by him in order to interpret probabilistically (2.2) (cf. Ref. 44 for more about that).

By definition of D_t^* and D_t, notice that $f(Z_t,t)$ is an $\mathcal{F}_t$ (respectively, $\mathcal{P}_t$) martingale if and only if $D_t^* f(Z_t,t)=0$ [respectively, $D_t f(Z_t,t)=0$].

The probabilistic counterpart of Proposition III.1, involving the derivative (7.24), is generally known in stochastic analysis, as Dynkin's formula (cf., e.g., Ref. 48). The fact that the counterpart of (3.4), using (7.23), holds as well is due to the time symmetry of Bernstein measures.

The infinitesimal operators D_t and D_t^* are keystones of Itô's stochastic calculus.[49,68] Although it is not as widely known in mathematical physics as it should, this calculus can indeed be formulated in a time-symmetric way as well as with respect to the usual increasing filtration $\mathcal{P}_t$. This requires the introduction of the time-reversed filtration $\mathcal{F}_t$, (Refs. 45, 47, and 50), used here. The quantum deformations (2.20′) and (2.21′) of Leibniz rule (for our class of Hamiltonians) become, respectively, in stochastic analysis, for f,g smooth and real valued,

$$D_t(f \cdot g) = (D_t f) \cdot g + f(D_t g) + \hbar \nabla f \cdot \nabla g, \tag{7.25}$$

$$D_t^*(f \cdot g) = (D_t^* f) \cdot g + f(D_t^* g) - \hbar \nabla f \cdot \nabla g, \tag{7.26}$$

The relations (3.13) and (3.13′) are the quantum counterparts of the relations between Itô and Stratonovich stochastic integrals [also denoted by $\circ$ (Ref. 50)] with respect to $\mathcal{P}_t$ and $\mathcal{F}_t$. It is well known that the latter relation had already been discovered by Feynman in his path integral approach to quantum theory.[2,44]

Using this, one shows that positive solutions of the two adjoint heat equations (7.7) and (7.11) admit two path integral representations in terms of $Z_t, t \in I$. These are the probabilistic counterparts of the integral representations (3.20) and (3.22).

The study of the symmetries of the action functionals involved in these path integrals results in the probabilistic version of the quantum theorem of Nœther, proved in paper I, which is in fact the origin of the present Lagrangian formulation of quantum theory for elementary systems.

One can further develop Feynman's ideas using the rigorous tools of stochastic analysis.[69] For example, his functional calculus[2] is well defined for the class of Bernstein diffusions and allows to prove the Euclidean version of his heuristic results.[51] The aim of Euclidean quantum mechanics, in the sense of Refs. 44 and 45 and for the present paper, is to transfer along this line, as much as possible of mathematical structures from stochastic analysis to regular quantum theory. The point of this indirect approach is to make the best of the irreducible probabilistic content of this theory and discover more easily new conceptual and technical aspects of quantum dynamics which have been muddled along the years by the superficial role of probability in the traditional Hilbert space framework.

VIII. SOME CONCRETE EXAMPLES

A. One-dimensional free fall

Let the configuration manifold M of Sec. VI be simply $\mathbb{R}$ and consider the free fall Hamiltonian,

$$H=-\frac{\hbar^2}{2}\frac{\partial^2}{\partial q^2}+gq, \tag{8.1}$$

where g is a real constant. This is the (one dimensional) case $A=0, V(q,t)=gq$ of (6.2). In particular, H belongs to the quadratic class (5.1) and it follows from Sec. V that it is sufficient to compute the free case $V=0$. The basis $\mathcal{B}_s(1)$ of the symmetry Lie algebra $\mathfrak{g}_s(1)$ is six dimensional and, according to (5.7), given by

$$\mathcal{B}_s(1)=\left\{i,iq,\hbar\frac{\partial}{\partial q},iq^2,i\frac{\hbar^2}{2}\frac{\partial^2}{\partial q^2},\hbar q\frac{\partial}{\partial q}+\frac{\hbar}{2}\right\}\equiv\{\mathcal{N}_j,j=1,\ldots,6\}. \tag{8.2}$$

We observe that the free fall Hamiltonian (8.1) results from a linear combination of elements of $\mathcal{B}_s(1)$.

By (5.19) we know that the constant observables of the one-dimensional free system are

$$\left\{i,i\left(q+i\hbar t\frac{\partial}{\partial q}\right),\hbar\frac{\partial}{\partial q},iq^2-2t\left[iq\left(-i\hbar\frac{\partial}{\partial q}\right)+\frac{\hbar}{2}\right]+2it^2\left(i\hbar\frac{\partial}{\partial t}\right),\right.$$
$$\left.\hbar\frac{\partial}{\partial t},q\hbar\frac{\partial}{\partial q}+\frac{\hbar}{2}-2it\left(i\hbar\frac{\partial}{\partial t}\right)\right\} \tag{8.3}$$

Equivalently the coefficients of the symmetry generator defined in (4.18) for the one-dimensional free case are

X	T	φ
0	0	1
$-t$	0	q
1	0	0
$-qt$	$-t^2$	$\frac{1}{2}(i\hbar t+q^2)$
0	1	0
q	$2t$	$-\frac{i\hbar}{2}.$

(8.4)

According to the method of Proposition V,5 each of these generators is unitarily equivalent to one generator of the free fall Hamiltonian H via the strongly continuous one parameter groups of unitary operators in $L^2(\mathbb{R})$ defined by

$$W_t=e^{-(i/\hbar)tH}\cdot e^{(i/\hbar)tH_0}. \tag{8.5}$$

Using this, one computes the corresponding coefficients for the free fall symmetry generators. The results are

X	T	φ
0	0	1
$-t$	0	$q-\frac{g}{2}t^2$
1	0	gt
$-qt+\frac{g}{2}t^3$	$-t^2$	$\frac{1}{2}(i\hbar t+q^2)-\frac{3g}{2}t^2q+\frac{g^2}{8}t^4$
0	1	0
$q-\frac{3g}{2}t^2$	$2t$	$-\frac{i\hbar}{2}+3gtq-\frac{g^2}{2}t^3.$

(8.6)

As they should, the constant observables of the free fall system reduce clearly to the ones of the pure free case (8.4) when the constant g vanishes.

We also observe that the second and third of those constants are "trivial" (although consistently forgotten) since they correspond to the initial position and momentum observables expressed, in the Heisenberg picture, in terms of $Q(t)$ and $P(t)$. On the other hand, the fourth and last observables are nontrivial constants for this elementary system with purely continuous spectrum σ_H.

B. The free particle on the sphere $S^2\subset\mathbb{R}^3$

Now take for the configuration manifold M of Sec. VI the sphere S^2 of radius R in $\mathbb{R}^3$.

It is natural to introduce the spherical coordinates $(q^j)=(\theta,\phi)$ in $]0,\pi[\times[0,2\pi]$. Then, since $A=V=0$ here, the Lagrangian of the classical system reduces to the kinetic part

$$L(\dot\theta,\dot\phi,\theta,\phi)=\frac{R^2}{2}(\dot\theta^2+\sin^2\theta\dot\phi^2), \tag{8.7}$$

since the metric of S^2 is of the form

$$\mathrm{d}s^2=R^2(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2), \tag{8.8}$$

or, equivalently,

$$g_{ij}=\begin{pmatrix} R^2 & 0\\ 0 & R^2\sin^2\theta\end{pmatrix}. \tag{8.9}$$

The associated Christoffel symbols and covariant derivatives are easily computed,

$$\begin{gathered}\Gamma^1_{11}=\Gamma^1_{12}=\Gamma^1_{21}=\Gamma^2_{11}=\Gamma^2_{22}=0,\\ \Gamma^2_{12}=\Gamma^2_{21}=\mathrm{cotg}\,\theta,\\ \Gamma^1_{22}=-\sin\theta\cos\phi,\end{gathered} \tag{8.10}$$

and

$$\begin{gathered}\nabla_\theta=\frac{\partial}{\partial\theta},\quad \nabla_\phi=\frac{\partial}{\partial\phi},\\ \nabla^\theta=\frac{1}{R^2}\frac{\partial}{\partial\theta},\quad \nabla^\phi=\frac{1}{R^2\sin^2\theta}\frac{\partial}{\partial\phi}.\end{gathered} \tag{8.11}$$

The quantum momentum observables in $L^2(S^2,R^2\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi)$ are

$$P_\theta = -i\hbar\nabla_\theta - i\hbar \cot g\theta, \qquad P_\phi = -i\hbar\nabla_\phi, \tag{8.12}$$

and the Hamiltonian observable is

$$H = -\frac{\hbar^2}{2R^2}\left[\left(\frac{\partial^2}{\partial\theta^2} + \text{cotg } \theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]. \tag{8.13}$$

It is known that for this case with constant curvature $K = R^{-2} > 0$ and potentials $A = V = 0$ the dimension of the symmetry algebra is maximal; here this is five. The table of the coefficients of the symmetry generator $\hat{N}(t)$ for the Schrödinger equation with Hamiltonian (8.13) is the following:

$X=(X^\theta,X^\phi)$	T	φ
$(0,0)$	1	0
$(0,0)$	0	1
$\left(\sin\phi, \dfrac{\cos\phi}{tg\ \theta}\right)$	0	0
$\left(-\cos\phi, \dfrac{\sin\phi}{tg\ \theta}\right)$	0	0
$(0,-1)$	0	0.

(8.14)

Given the definition (6.12) of the symmetry generator $\hat{N}(t)$, it is clear that the first symmetry corresponds to the conservation of the energy observable. The three last ones are interesting, but also of a purely classical origin.

$(X_j^\theta, X_j^\phi), j=1,2,3$ form a basis of the Killing vector field Lie algebra for S^2, an homogeneous manifold. Those vectors X_j are proportionals to the quantum angular momenta, known to be a basis of SO(3), the group of isometries (rotations) of S^2:

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\text{tg }\theta}\frac{\partial}{\partial\phi}\right) \equiv i\hbar\left(\sin\phi, \frac{\cos\phi}{\text{tg }\theta}\right) \equiv i\hbar X_1, \tag{8.15}$$

and correspondingly for L_y, L_z. The three vectors X_j solve the determining equation (1) of Proposition VI.1 which reduces here to Killing's equation

$$\nabla^\theta X_j^\phi + \nabla^\phi X_j^\theta = 0, \quad j = 1,2,3. \tag{8.16}$$

The last symmetry of the table (8.14) corresponds to the conservation of the angular momentum P_ϕ.

The integrability of the underlying classical system is built on the existence of the two constants of motion H and P_ϕ allowing to foliate the data space by a two parameter family of two-dimensional tori.

C. An example of Goldstein

In Goldstein's *Classical Mechanics* (1980), (p. 430), the problem 2a) consists in showing that, for a one-dimensional classical system with Hamiltonian

$$H(q,p) = \frac{p^2}{2} - \frac{1}{2}q^{-2}, \tag{8.17}$$

there is a time-dependent constant of motion of the form

$$n = \frac{q}{2}p - tH. \tag{8.18}$$

This is the case where $M=\mathbb{R}, A(q)=0$, $V(q)=-\frac{1}{2}q^{-2}$and (8.18) shows that

$$X(q,t) = \frac{q}{2}, \quad T(t) = t, \quad \varphi(q,t) = 0.$$

The determining equations (1) and (2) of Proposition IV.3 are trivially satisfied and the "classical limit $\hbar=0$" of (3) holds as well, so n is indeed a (classical) constant of motion. Let us recall that there is nothing exotic about time-dependent classical first integrals, as shown by the ones associated with Galilean boosts.

D. Lewis and Riesenfeld invariant

This is a quantum invariant, discovered in 1969 (Ref. 52) for the harmonic oscillator with time-dependent frequency, i.e., with classical Hamiltonian ($M=\mathbb{R}$)

$$H(q,p,t) = \frac{1}{2}p^2 + \frac{\omega^2(t)}{2}q^2. \tag{8.19}$$

It can be shown that this invariant is of the form (6.32), with

$$X(q,t) = \frac{\dot{T}}{2}q, \quad \hat{\varphi}(q,t) = -\frac{\ddot{T}}{4}q^2, \quad T(t) = \rho^2(t),$$

where $\rho(t)$ solves the nonlinear equation

$$\ddot{\rho} + \omega^2(t)\rho - \frac{1}{\rho^3} = 0.$$

Details can be found in Ref. 53.

IX. CONCLUSIONS

Our framework is founded on a dynamic reinterpretation of the symmetry group of the Schrödinger equation, itself very close to the one of the associated heat equation.

Given the fact that this group was computed by Lie around 1890, a number of the tools we used here are, indeed, quite old. The free Lie algebra can be found in most of the textbooks on Lie groups analysis of PDE published since 1970 (for example Refs. 15, 16, and 54), often with commentaries about the obscure physical interpretation of most explicitly time-dependent transformations, notably those presented as trivial in our Section V. Kuwabara's result[28] (1984) (discovered by us after the redaction of the present work was almost finished) is especially relevant, as it shows that the Lie algebraic structure for quantum (and classical) symmetries is time-dependent. He found, in particular, the form (6.12) of the symmetry operator, without regarding it as a consequence of a Nœther theorem or trying to relate it with a Lagrangian framework. Although we could not find a clear statement that the associated quantum first integrals should be understood in the sense of the Heisenberg picture of quantum dynamics, such a statement may well already exist in the vast literature on the subject, but is certainly not common knowledge in mathematical or theoretical physics.

The specific contribution of our indirect Euclidean approach lies, curiously, in the physical interpretation it provides of many time-dependent symmetries, through their elementary meaning in stochastic analysis.[69]

The simplest illustration is provided by the one-dimensional ($n=1$) free case ($A=V=0$) and the symmetry associated with the coefficients $X=-t, T=0, \varphi=x$ of the symmetric generator $\hat{N}(t)$ in (4.7), corresponding to a simple solution of the system of equations of Proposition IV.3. This symmetry corresponds to the one-parameter family of solutions

$$\psi_\alpha(x,t) = e^{(i/\hbar)(\alpha x-(\alpha^2/2)t)}\psi(x-\alpha t,t), \quad \alpha \in \mathbb{R} \tag{9.1}$$

of the free equation $i\hbar(\partial\psi/\partial t)=-(\hbar^2/2)\Delta\psi$, quite familiar in the context of the Galilean invariance of this equation.[55]

Let us rewrite (9.1) as

$$\psi_\alpha(x,t) = (e^{\alpha\hat{N}(t)}\psi)(x,t), \tag{9.2}$$

and expand in α this expression when ψ is the trivial (unnormalizable) free solution if $\psi_t=1$. On this "state," the space–time observables of momentum and energy vanish and the one associated with $\hat{N}(t)$ reduces to the phase φ [cf. (4.18)]. We find

$$\psi_\alpha(x,t) = 1 + \alpha x + \frac{\alpha^2}{2!}(x^2 + i\hbar t) - \frac{\alpha^3}{3!}(x^3 + 3i\hbar tx) + \cdots . \tag{9.3}$$

By successive taking of $(\partial/\partial\alpha)$ at $\alpha=0$ we obtain a collection of constant space–time observables $n_1^{\hat{N}^n}(x,t) \equiv \varphi_n(x,t), n \in \mathbb{N}$, each, indeed, solution of $D_t\varphi_n=0$.

Now $\hat{N}(t)=(-tP(t)+Q(t))$ itself is certainly a trivial quantum first integral, namely the initial position observable [since $Q(t)$ and $P(t)$ are solutions of the free Heisenberg equation of motion] and the $\hat{N}^n(t), n \in \mathbb{N}$, reduce to the successive powers of this trivial dynamical information on the free quantum system.

On the Euclidean side, we are dealing instead of (9.1) with the one parameter family

$$\eta_\alpha(q,t) = e^{(1/\hbar)(\alpha q-(\alpha^2/2)t)}\eta(q-\alpha t,t), \quad \alpha \in \mathbb{R} \tag{9.4}$$

of (positive) solutions of the free heat equation (7.11). It corresponds to the Euclidean counterpart (cf. paper I)

$$N_E(t) = t\frac{\partial}{\partial q} - q \tag{9.5}$$

of the real time symmetry generator $\hat{N}(t)$. The above unphysical state ψ_t turns into the trivial solution $\eta_t=1$ of the free equation (7.11) whose probabilistic role becomes fundamental. Indeed, according to (7.19) and (7.22′) the associated well-defined diffusion Z_t reduces to the one-dimensional Wiener process with diffusion coefficient $\hbar$. Notice that the corresponding solution of the free adjoint heat equation (7.7) is, then, the integral kernel $\eta_t^*=h_0(x,t,q)$ of this equation. Since the relation between η_t and η_t^* is manifestly not the Euclidean counterpart of a complex conjugacy, this means that for the Wiener process itself, the time invariance of the lhs of (7.12) (with an appropriate pair of positive boundary conditions) is the basis of our probabilistic interpretation of a complex quantum probability amplitude.

Now let us consider

$$h_\alpha(q,t) = \frac{\eta_\alpha}{\eta}(q,t). \tag{9.6}$$

If Z_t is the diffusion, of law P, built from η using (7.19), it is easy to show that h_α is a strictly positive $\mathcal{P}_t$-martingale of Z_t, i.e., satisfies $D_t\, h_\alpha(Z_t,t)=0$. Denoting by Z_t^α the new diffusion, of law P_α, built from η_α, one shows easily that P_α is absolutely continuous with respect to P, with Radon-Nikodym derivative $\mathrm{d}P_\alpha/\mathrm{d}P=h_\alpha$. In the case of the Wiener process, h_α is the exponential martingale of this process, a basic tool dating[44,49] back to the foundations of stochastic analysis.

The family of $\mathcal{P}_t$-martingales resulting from the successive taking of derivatives $\partial/\partial\alpha$ at $\alpha=0$, namely $\{1,q,q^2-\hbar t,q^3-3\hbar tq,\ldots\}$, coincides with the familiar Wick product of the Brownian motion[56] which is, therefore, reinterpreted as the probabilistic counterpart of the above-mentioned trivial dynamical information on the free quantum system provided by Nœther's theorem.

Thus stochastic analysis may help, indeed, to understand some conventional aspects of quantum dynamics.

The version of Euclidean quantum mechanics advocated in paper I is known to be valid for a class of Hamiltonians much larger than the one considered here (cf. Ref. 57) and it is expected that many ideas expressed here will survive in more general contexts (cf. Refs. 70 and 71).

Although, as shown here, the Riemannian formulation of our results is quite natural, the proper geometrical framework of this method is distinct. It should be regarded, in fact, as deformation of classical contact geometry.[58] This viewpoint also has serious computational advantages when adopted in the Euclidean context where the probability measures make sense, and quantum symmetries are reinterpreted as symmetries of families of diffusion processes.

X. ERRATA FOR PAPER I

(1) In Proposition 3.6 of Ref. 1 (cf. also Ref. 59), the term $\nabla\phi-X_q\cdot B$, i.e., the variation of the drift, is ambiguous. It should be understood as

$$\frac{\partial\phi}{\partial q^i}-\frac{\partial X^k}{\partial q^i}B^k$$

(where the summation convention is used).

(2) The "illustration of the central role of time symmetry," mentioned in p. 331 of Ref. 1 is wrong: the function $n(q,t)$ [respectively $n_*(q,t)$] solves our heat equation (7.11) [respectively, (7.7)] and so are $\mathcal{P}_t$ (respectively, $\mathcal{F}_t$) martingales of the starting process Z_t, $t\in I$. But they are not strictly positive and so cannot be used as h-functions, in the sense of Doob's h-transform. However, when the Nœtherian symmetry operator $\hat{N}$ is positivity preserving, $\eta_\alpha(q,t)=e^{-\alpha\hat{N}}\eta(q,t)$, where η is the positive solution of (7.11) associated with Z_t, is a one-parameter family of solutions of the same equation. Then $h_\alpha(q,t)=(\eta_\alpha/\eta)(q,t)$ is, indeed, the positive martingale needed for the h-transform producing the family of Bernstein diffusions Z_t^α associated with this symmetry (cf. Conclusion here, Sec. 6, Part 2 of Ref. 44, and Refs. 31, 32, and 58 for much more).

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