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Euclidean quantum mechanics: analytical approach

by

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ABSTRACT. — We give a Hilbert space picture of a novel probabilistic interpretation of the classical heat equation, realizing an idea of Schrödinger. By this we also obtain an Euclidean version of non relativistic Quantum Mechanics, distinct from the one obtained using the Feynman-Kac formula.

RÉSUMÉ. — Nous donnons une version Hilbertienne d'une nouvelle interprétation probabiliste de l'équation classique de la chaleur, ce qui réalise une idée de Schrödinger. Nous obtenons aussi une version Euclidienne de la Mécanique Quantique non relativiste distincte de celle obtenue par la formule de Feynman-Kac.

1. INTRODUCTION

The general problem considered in this paper concerns the relation between non-relativistic quantum mechanics and classical probability theory.

The unusual nature of these relations has been remarked since the beginning of quantum mechanics. In the fifties, R. Feynman [1] gave a remarkable heuristic description of non-relativistic (and relativistic) quantum theory in which the nature of the relations between probability theory and quantum mechanics is taken into account more directly than in other formulations. In the non-relativistic case, his theory was dealing directly with the Schrödinger equation. It has been quickly recognized, thanks to M. Kac [2], that it is technically much easier, especially when the interactions are singular, to deal with the corresponding heat equation, in which the time is regarded as "purely imaginary". This point of view is called Euclidean because, in the relativistic case, the Poincaré symmetry group of the theory is transformed into the Euclidean group.

The Feynman-Kac formula, which is an explicit probabilistic representation of the integral operator e^{-tH} , $t \geq 0$, for $H = -\frac{1}{2} \Delta + V$ the self-adjoint quantum mechanical Hamiltonian on $L^2(\mathbb{R}^d)$, and the theory associated to it, have been regarded, since the midsixties, as the natural Euclidean framework to be generalized in quantum field theory. This paper describes a quite different non-relativistic Euclidean version of quantum mechanics, whose relations with this theory are closer than in the previous approach via Feynman-Kac formula. It involves a new class of probability measures, whose construction has been suggested by an unfortunately forgotten idea of Schrödinger [3-4].

The organization of the present paper is the following:

Chapter 2 describes the construction of the Hilbert spaces associated with our approach. They are one-parameter families of Hilbert spaces resulting from the completion of subspaces of $L^2(\mathbb{R}^d)$ with respect to scalar products suggested by the probabilistic interpretation.

Chapter 3 is devoted to the construction of the most basic operators (observables) on these Hilbert spaces. They are densely defined, normal operators (mostly self-adjoint), whose definition is very close to the quantum mechanical ones.

The analytical description of the dynamics of the theory is described in Chapter 4, and is summarized in the coexistence of an (Euclidean) Heisenberg picture in which the observables evolve in time according to the (Euclidean) Heisenberg equation, and an (Euclidean) Schrödinger picture corresponding to the solutions of the heat equation in our Hilbert space.

The new resulting framework is called Euclidean quantum mechanics [4]. We devote the Chapter 5 to the investigation of the regularity conditions needed for our approach. They involve only conditions on the potential V , *i. e.* on the physical forces acting on the system, and boundary conditions for the dynamics. The class of allowed potential V is rather large: it describes most of the forces of physical interest.

Chapter 5 describes the probabilistic interpretation of Euclidean quantum mechanics, valid for cones of positive vectors in the Hilbert spaces. It involves a new class of diffusion processes, the Bernstein processes, associated in a natural way to the considered solutions of the heat equation. The most notable particularity of these processes is to be time-symmetric (in general not stationary). The existence and uniqueness of the underlying probability measure is provided by the construction.

The physical relevance of these Bernstein diffusions is founded on the fact that their moments (the “Schwinger Functions”)

$$E[Z(t_1)Z(t_2)\dots Z(t_n)], \quad -\frac{T}{2} \leq t_1 \leq t_2 \leq \dots \leq t_n \leq \frac{T}{2}$$

continued analytically in the variable t_j to $i\tau_j, j=1$ to n , yield the quantum mechanical expectation values

$$\langle \Psi | Q(\tau_1) Q(\tau_2) \dots Q(\tau_n) \Psi \rangle_2$$

when $\langle . | . \rangle_2$ is the scalar product in the Hilbert space of quantum mechanics and Q the position operator. This holds not only when Ψ is the vacuum state but also when Ψ is any other (regular) solution of the underlying Schrödinger equation.

A short chapter (Chapter 7) summarizes the comparison with quantum mechanics in order to shed more light on the nature of the classical analogy proposed here.

At last, Chapter 8 is a brief review both of the origin of Euclidean quantum mechanics and of the main alternative approaches of the relations between quantum physics and probability theory. We hope that it will help the reader to better understand the spirit of the present attempt.

Since the dynamical content of the theory has already been investigated in probabilistic terms ([12], [4]) the present paper focuses on the analytical counterpart of this dynamics, and the probabilistic results are mostly expository. The reader should consult [33] for a more detailed presentation of this part of the theory.

2. CONSTRUCTION OF THE HILBERT SPACES

Let us consider the Schrödinger equation on $L^2(\mathbb{R}^d, dx) \equiv L^2(\mathbb{R}^d)$, the Hilbert space of square integrable complex-valued functions over \mathbb{R}^d ,

$$i(\partial/\partial\tau)\psi = H\psi \quad (2.1)$$

for an initial condition $\psi(x, 0) = \chi(x)$ in the domain $D(H)$ of H in $L^2(\mathbb{R}^d)$. H is the Hamiltonian, realized as a lower bounded self-adjoint operator on $L^2(\mathbb{R}^d)$ and $\frac{\partial}{\partial\tau}$ is understood as strong derivative in $L^2(\mathbb{R}^d)$.

That H is lower bounded means that there exists a finite real number e_0 such that $\langle \psi | H \psi \rangle_2 \geq e_0 \langle \psi | \psi \rangle_2$ for all ψ in $\mathcal{D}(H)$, where $\langle \cdot | \cdot \rangle_2$ denotes the inner product in $L^2(\mathbb{R}^d)$, linear on the right.

In the situation of N nonrelativistic particles interacting through a potential V (a real valued measurable function over \mathbb{R}^n), one has $d = sN$, H is a self-adjoint extension of $-\frac{1}{2}\Delta + V$, with Δ the Laplacian in \mathbb{R}^d , $-\frac{1}{2}\Delta + V$ is understood in the sense of form sums or in the sense of operator sum provided suitable assumptions on V are satisfied.

Many sufficient conditions for this are known, e. g. $V = V_1 + V_2$, $c \leq V_1$ in $L^1_{loc}(\mathbb{R}^d)$ for some number $c > \infty$, V_2 form-bounded with respect to $H_0 = -\frac{1}{2}\Delta$, with domain $\mathcal{D}(H_0) = H^{2,1}(\mathbb{R}^d)$ (the Sobolev space of generalized functions with square integrable derivatives), and with bound strictly less than 1. For example, for $d = 3$, we can take $V_2 = V_3 + V_4$, with V_3 in the Rollnik class and V_4 in $L^\infty(\mathbb{R}^3)$. (See e. g. [5].) Under such conditions, H is uniquely defined by closure of the form sum of $-\frac{1}{2}\Delta$ and V on $C_0^\infty(\mathbb{R}^d)$. More generally, H could be defined using Dirichlet forms, see e. g. ([5], [6], [34]). Much of what we shall do in this paper is independent of the particular way H is obtained. From now on, unless stated otherwise, H will be any self-adjoint lower bounded operator.

From the spectral theorem for unbounded self-adjoint operators we have, for $\{E^H(\lambda)\}$ the spectral family of H ,

$$U(\tau) = e^{-i\tau H} = \int_{-\infty}^{\infty} e^{-i\tau\lambda} dE^H(\lambda), \quad \tau \text{ in } \mathbb{R} \quad (2.2)$$

The solution ψ_χ of the initial value problem (2.1), with $\chi \in \mathcal{D}(H)$, can be written

$$\psi_\chi(x, \tau) = e^{-i\tau H} \chi(x) = \left(\int_{-\infty}^{\infty} e^{-i\tau\lambda} dE^H(\lambda) \chi \right)(x). \quad (2.3)$$

Since H is bounded below by e_0 , the functional calculus also shows that $U(\tau)$ can be analytically continued in the time parameter to a self-adjoint semigroup on $L^2(\mathbb{R}^d)$, denoted by $T(t)$, $t \in [0, \infty[$, for $\tau = -it$,

$$T(t) = e^{-tH},$$

bounded in norm by e^{-te_0} .

Let, for any $\chi \in L^2(\mathbb{R}^d)$,

$$\eta_x^*(x, t) \equiv (e^{-tH}\chi)(x), \tag{2.4}$$

well defined for a. e. x and all t .

We have

$$\eta_x^*(x, t) = \left(\int_{-\infty}^{\infty} e^{-t\lambda} dE^H(\lambda) \chi \right)(x). \tag{2.4'}$$

η_x^* solves the initial value problem for the heat equation on $L^2(\mathbb{R}^d)$, t in $[0, \infty[$, if, as before, $\chi \in \mathcal{D}(H)$. In other words

$$\begin{aligned} -\frac{\partial \eta_x^*}{\partial t}(\cdot, t) &= H \eta_x^*(\cdot, t) \\ \eta_x^*(\cdot, 0) &= \chi(\cdot). \end{aligned} \tag{2.5}$$

Remarks. — (a) If H is of the form $H = -\frac{1}{2}\Delta + V$ with e. g. V bounded below, continuous, and χ in $\mathcal{D}(H) \cap C(\mathbb{R}^d)$ then $\psi_x(x, \tau)$, given by (2.3), is in $\mathcal{D}(H) \cap C(\mathbb{R}^d)$ and this pointwise solution of (2.1) can be analytically continued, $\tau \rightarrow i\tau = t$, to a pointwise solution $\eta_x^*(x, t)$ of (2.5).

(b) Here and in the following, the $*$ of η_x^* should not be confused with the operation of taking complex conjugate, which will be denoted by $-$. Let $T > 0$ be fixed. Let χ in $L^2(\mathbb{R}^d)$ be such that χ is an analytic vector

for H with convergence radius $\frac{T}{2}$ (Cf. [7]), in the sense that $\chi \in \bigcap_{n=1}^{\infty} \mathcal{D}(H^n)$

and $\sum_{n=0}^{\infty} \frac{\|H^n \chi\|_2}{n!} |t|^n < \infty$ for any t in $I \equiv \left[-\frac{T}{2}, \frac{T}{2}\right]$. Here $\|\cdot\|_2$ means the norm of $L^2(\mathbb{R}^d)$.

We call $\mathcal{D}(e^{(T/2)H})$ the set of all such vectors χ . A vector ψ in $L^2(\mathbb{R}^d)$ is called an entire vector for H if $\sum_{n=0}^{\infty} \frac{\|H^n \psi\|_2}{n!} |t|^n < \infty$ for all real t .

We call $\varepsilon(H)$ the set of all entire vectors for H . Let $\varepsilon_0(H) \equiv \bigcup_{K \geq 0} E^H([-K, -K])$. Then $\varepsilon_0(H) \subset \varepsilon(H) \subset \mathcal{D}(e^{(T/2)H})$ and $\varepsilon_0(H)$ is dense in $L^2(\mathbb{R}^d)$. *A fortiori* $\varepsilon(H)$ and $\mathcal{D}(e^{(T/2)H})$ are dense in $L^2(\mathbb{R}^d)$.

We observe that for χ in $\mathcal{D}(e^{(T/2)H})$ we have, for any t in I , that

$$\left(\int_{-\infty}^{\infty} e^{t\lambda} dE^H(\lambda) \chi \right) (x) \equiv \eta_x(x, t) \tag{2.6}$$

is a well defined element of $L^2(\mathbb{R}^d)$, with norm bounded by $\sum_{n=0}^{\infty} \frac{|t|^n}{n!} \|H^n \chi\|_2 < \infty$.

It is natural to write

$$(e^{tH} \chi) (x) \equiv \eta_x(x, t) \tag{2.6'}$$

because of (2.6).

Notice that for $H = -\frac{1}{2} \Delta + V$ with V a smooth Fourier transform of a bounded measure, e. g., $\eta_x(x, t)$ is the pointwise analytic continuation of $(e^{i\tau H} \chi) (x)$ for τ in \mathbb{R} , $t = i\tau$, $0 \leq t \leq T/2$ (see for example, [32]). e^{tH} , $t \geq 0$, is a semigroup of unbounded self-adjoint operators defined on the dense invariant subset $\varepsilon(H)$ of $L^2(\mathbb{R}^d)$. Of course, e^{-tH} , $t \geq 0$, is a bounded self-adjoint semigroup on $L^2(\mathbb{R}^d)$. Clearly, for χ in $\mathcal{D}(e^{(T/2)H})$, $\eta_x(x, t)$ solves the backward heat equation

$$\begin{aligned} \frac{\partial}{\partial t} \eta_x(\cdot, t) &= H \eta_x(\cdot, t), & t \text{ in } I & \tag{2.6''} \\ \eta_x(\cdot, 0) &= \chi \end{aligned}$$

in the strong L^2 -sense.

We remark that χ is in $\mathcal{D}(e^{(T/2)H})$ implies that $\bar{\chi}$ is in $\mathcal{D}(e^{(T/2)H})$. Later on, we shall see that it is natural to consider the pair of vectors $\eta_{\bar{x}}(\cdot, t)$, $\eta_x^*(\cdot, t)$ in $L^2(\mathbb{R}^d)$, for t in I and χ in $\mathcal{D}(e^{(T/2)H})$.

Let us suppose, as an example, that $H = -\frac{1}{2} \Delta + V$, with V such that H is well defined and has a pure point spectrum, with $\{\varphi_j\}$, $j = \{0\} \cup \mathbb{N}$ a complete orthonormal system of real eigenfunctions of H , and eigenvalues E_j (the reality of the φ_j is not a restriction, H being self-adjoint). The assumptions are satisfied e. g. when V is in $L^1(\mathbb{R}^d)$, lower bounded, and $V(x) \rightarrow +\infty$ for $|x| \rightarrow \infty$; see e. g. [5], XIII. 67, for more general conditions.

We have $\chi = \sum_{j=0}^{\infty} \alpha_j \varphi_j$ for $\alpha_j \in \mathbb{C}$, with convergence in $L^2(\mathbb{R}^d)$, hence the above mentioned condition $\chi \in \mathcal{D}(e^{(T/2)H})$ is satisfied if the α_j satisfy, besides $\sum_{j=0}^{\infty} |\alpha_j|^2 < \infty$, also $\sum_{j=0}^{\infty} |\alpha_j|^2 e^{E_j T} < \infty$.

On the other hand, χ belongs to $\mathcal{D}(H)$ iff $\|H\chi\|_2^2 = \sum_{j=0}^{\infty} |E_j \alpha_j|^2 < \infty$.

In this case, (2.4) respectively (2.6) read

$$\eta_x^*(x, t) = \sum_{j=0}^{\infty} \alpha_j e^{-t E_j} \phi_j(x) \tag{2.7}$$

and

$$\eta_{\bar{x}}(x, t) = \sum_{i=0}^{\infty} \bar{\alpha}_i e^{t E_i} \phi_i(x) \tag{2.8}$$

with convergence in $L^2(\mathbb{R}^d)$ for any t in I .

By the orthogonality of the spectral family, we have for any χ in $\mathcal{D}(e^{(T/2)H})$

$$\langle \bar{\eta}_{\bar{x}} | \eta_x^* \rangle_2 = \int_{\mathbb{R}^d} \eta_{\bar{x}} \eta_x^*(x, t) dx = \int_{\sigma(H)} d \|E^H(\lambda) \chi\|_2^2 = \|\chi\|_2^2 \tag{2.9}$$

where $\sigma(H)$ is the spectrum of H . In particular, for $\chi \neq 0$ in $\mathcal{D}(e^{(T/2)H})$,

$$0 < \langle \bar{\eta}_{\bar{x}} | \eta_x^* \rangle_2 = \|\chi\|_2^2 < \infty. \tag{2.10}$$

Remark. — Clearly, $\|\eta_x^*\|_2^2 = \|e^{-tH} \chi\|_2^2$ is, in general, different from $\|\chi\|_2^2$. Also, if H is of the Schrödinger form $-\frac{1}{2} \Delta + V$ with V , say, bounded and continuous, $e^{-tH} \chi \neq 0$ a. e. for $\chi \neq 0$ a. e. as seen e. g. by the Lie-Trotter formula, hence $\|\eta_x^*\|_2^2 > 0$ for $\chi \neq 0$. We summarize over our results by

PROPOSITION 2.1. — Let H be a self-adjoint operator in $L^2(\mathbb{R}^d)$, lower bounded with lower bound e_0 . Then $e^{-t(H-e_0)}$, $t > 0$, is a strongly continuous contraction self-adjoint semigroup in $L^2(\mathbb{R}^d)$. For any $t \geq 0$, χ in $L^2(\mathbb{R}^d)$, $\eta_x^*(x, t) = (e^{-tH} \chi)(x)$ is a well defined element in $L^2(\mathbb{R}^d)$. When χ is in $\mathcal{D}(H)$, $\eta_x^*(x, t)$ solves, in the strong $L^2(\mathbb{R}^d)$ sense, $-\frac{\partial}{\partial t} \eta_x^*(\cdot, t) = H \eta_x^*(\cdot, t)$, with $\eta_x^*(\cdot, 0) = \chi(\cdot)$. Let $T > 0$ be fixed and $\mathcal{D}(e^{(T/2)H})$ denotes the dense set of vectors ϕ in $L^2(\mathbb{R}^d)$ s. t.

$$\sum_{n=0}^{\infty} \frac{1}{n!} \|H^n \phi\|_2 |t|^n < \infty \text{ for any } t \text{ in } I = \left[-\frac{T}{2}, \frac{T}{2}\right]. \text{ Then, for}$$

$\chi \in \mathcal{D}(e^{(T/2)H})$, we have strong convergence in $L^2(\mathbb{R}^d)$ of $\sum_{n=0}^{\infty} \frac{H^n \bar{\chi}}{n!} t^n$ for all t in I . For any t in I , χ in $\mathcal{D}(e^{(T/2)H})$, $\eta_{\bar{x}}(x, t) = \sum_{n=0}^{\infty} \frac{H^n \bar{\chi}}{n!}(x) t^n \equiv e^{tH} \bar{\chi}(x)$

solves, in the strong L^2 -sense, for t in I ,

$$\frac{\partial}{\partial t} \eta_{\bar{x}}(\cdot, t) = H \eta_{\bar{x}}(\cdot, t), \text{ with } \eta_{\bar{x}}(\cdot, 0) = \bar{\chi}(\cdot).$$

Moreover (2.9) and (2.10) hold.

Remark. — The definitions of $\eta_x^*(\cdot, t)$ and $\eta_{\bar{x}}(\cdot, t)$ are unsymmetric inasmuch as $\eta_x^*(\cdot, t)$ exists for all $t \geq 0$, χ in $L^2(\mathbb{R}^d)$, whereas $\eta_{\bar{x}}(\cdot, t)$ is only defined for t in I , χ in $\mathcal{D}(e^{(T/2)H})$. Actually, the possibility of defining $\eta_x^*(\cdot, t)$ by $\eta_x^*(\cdot, t) = (e^{-tH} \chi)(\cdot)$ for all $t \geq 0$, χ in $L^2(\mathbb{R}^d)$, comes from the lower bound of H , a natural assumption for Schrödinger operators. In a more abstract setting, we could have dropped the assumption H lower bounded and defined $\eta_x^*(\cdot, t)$ for t in I and χ in $\mathcal{D}(e^{(T/2)H})$. Then we would have the above evolution equation for $\eta_x^*(\cdot, t)$ satisfied for χ in $\mathcal{D}(e^{(T/2)H})$, t in I . We also observe that under the assumptions of the Proposition 2.1 (lower bound on H), $\eta_x^*(\cdot, t)$ is also defined for $-\frac{T}{2} \leq t \leq 0$ (hence in particular for all t in I) provided χ is taken in $\mathcal{D}(e^{(T/2)H})$.

We are now ready to define several Hilbert spaces over \mathbb{R}^d , denoted by \mathcal{V}_t^* , \mathcal{V}_t and \mathcal{H}_t .

Consider η_x^* defined by (2.4) with t in $I \cup [-\frac{T}{2}, \infty[$, χ is $\mathcal{D}(e^{(T/2)H}) \subset L^2(\mathbb{R}^d)$. Let $\tilde{\mathcal{V}}_t^* \equiv \{\eta_x^*(t), \chi \text{ in } \mathcal{D}(e^{(T/2)H})\}$. Then $\tilde{\mathcal{V}}_t^*$ is a dense linear subspace of $L^2(\mathbb{R}^d)$, the range of $e^{-tH} \upharpoonright \mathcal{D}(e^{(T/2)H})$, or, equivalently, the domain of $e^{(t+(T/2)H)}$.

Let us define a linear operator A_t from $\tilde{\mathcal{V}}_t^*$ onto $\mathcal{D}(e^{(T/2)H}) \subset L^2(\mathbb{R}^d)$ by

$$A_t \eta_x^*(t) \equiv \chi. \tag{2.11}$$

We have, of course, $A_t = e^{tH} \upharpoonright \tilde{\mathcal{V}}_t^*$. Let us define a scalar product $(\cdot \mid \cdot)_t$, in $\tilde{\mathcal{V}}_t^*$ by

$$\begin{aligned} (\eta_{x_1}^*(t) \mid \eta_{x_2}^*(t))_t &\equiv \langle A_t \eta_{x_1}^*(t) \mid A_t \eta_{x_2}^*(t) \rangle_2 \\ &= \langle \chi_1 \mid \chi_2 \rangle_2. \end{aligned} \tag{2.12}$$

That $(\cdot \mid \cdot)_t$ is a scalar product, linear on the right, follows from the linearity of A_t and the fact that $\langle \cdot \mid \cdot \rangle_2$ is a scalar product. From (2.12) we have $\|\eta_x^*(t)\|_t = \|\chi\|_2$. In particular $\eta_x^*(t)$ is the zero element in $\tilde{\mathcal{V}}_t^*$ iff χ is the zero element in $\mathcal{D}(e^{(T/2)H})$.

Define $B_t: \mathcal{D}(e^{(T/2)H}) \rightarrow \tilde{\mathcal{V}}_t^*$ by

$$B_t \chi \equiv \eta_x^*(t). \tag{2.13}$$

Hence $B_t = e^{-tH} \mathcal{D}(e^{(T/2)H})$, t in $I \cup [\frac{T}{2}, \infty[$. Clearly B_t is onto and we have $A_t B_t = 1$ on $\mathcal{D}(e^{(T/2)H})$, and $B_t A_t = 1$ on $\tilde{\mathcal{V}}_t^*$.

We shall denote by \mathcal{V}_t^* the Hilbert space which is the completion of $\tilde{\mathcal{V}}_t^*$ with respect to the scalar product $(\cdot | \cdot)_t$. \mathcal{V}_t^* is called the forward Hilbert space. We shall now see that we can extend A_t to a unitary operator from \mathcal{V}_t^* onto $L^2(\mathbb{R}^d)$ and B_t to a unitary operator from $L^2(\mathbb{R}^d)$ onto \mathcal{V}_t^* , so that $B_t = A_t^+ = A_t^{-1}$ (where A_t^+ denotes the adjoint of A_t).

PROPOSITION 2.2. — For all $t \in 0 \cup [\frac{T}{2}, \infty[$, $(\mathcal{V}_t^*, (\cdot | \cdot)_t)$ can be identified with $(L^2(\mathbb{R}^d), \langle \cdot | \cdot \rangle_2)$ by the unitary map A_t from \mathcal{V}_t^* onto $L^2(\mathbb{R}^d)$ defined by $A_t \psi(t) \equiv \chi$ for $\psi(t) \equiv e^{-tH} \chi \equiv \eta_\chi^*(t)$, $\chi \in \mathcal{D}(e^{(T/2)H})$ (so that $\psi(t) \in \mathcal{D}(e^{(t+(T/2)H})$ i. e. $\psi(t) \in \tilde{\mathcal{V}}_t^*$). For arbitrary $\psi(t) \in \mathcal{V}_t^*$ s. t. $\psi(t) = \mathcal{V}_t^* - \lim_{n \rightarrow \infty} \psi_n(t)$, with $\psi_n(t) = e^{-tH} \chi_n \in \tilde{\mathcal{V}}_t^*$, $\chi_n \in \mathcal{D}(e^{(T/2)H})$, A_t is defined by $A_t \psi(t) \equiv \chi$, with $\chi = L^2 - \lim_{n \rightarrow +\infty} \chi_n$, which exists by the existence of $\tilde{\mathcal{V}}_t^* - \lim_{n \rightarrow \infty} \psi_n(t)$. (All limits are taken in the strong sense.)

Proof. — Let $\chi \in \mathcal{D}(e^{(T/2)H})$, then $\eta_\chi^*(t) = \psi(t) \equiv e^{-tH} \chi$ is a well defined element of $\tilde{\mathcal{V}}_t^* \subset L^2(\mathbb{R}^d)$.

We have by definition $A_t \psi(t) \equiv \chi$. We know already, by what we said in relation with (2.11), that A_t is isometric from $\tilde{\mathcal{V}}_t^*$ into $L^2(\mathbb{R}^d)$. Now let $\psi(t) \in \mathcal{V}_t^*$ arbitrary. Since \mathcal{V}_t^* is the completion of $\tilde{\mathcal{V}}_t^*$, there exists a sequence $\psi_n(t) \in \tilde{\mathcal{V}}_t^*$ s. t. $\psi(t) = \mathcal{V}_t^* - \lim_{n \rightarrow +\infty} \psi_n(t)$. We have $\psi_n(t) = e^{-tH} \chi_n$ with $\chi_n \in \mathcal{D}(e^{(T/2)H})$ and we observe that for any $m, n \in \mathbb{N}$, by (2.12): $\|\chi_n - \chi_m\|_2 = \|\chi_n(t) - \chi_m(t)\|_t$. But $\{\psi_n(t), n \in \mathbb{N}\}$ is a Cauchy sequence in \mathcal{V}_t^* (since it converges), hence by the latter equality we see that $\{\chi_n, n \in \mathbb{N}\}$ is a Cauchy sequence in $L^2(\mathbb{R}^d)$, hence, $L^2(\mathbb{R}^d)$ being complete, there exists $\chi \in L^2(\mathbb{R}^d)$ s. t. $\chi = L^2 - \lim \chi_n$.

Let us set $A_t \psi(t) \equiv \chi$. We then have $A_t \psi(t) = L^2 - \lim \chi_n$ and hence, by the definition of A_t on \mathcal{V}_t^* , $A_t \psi(t) = L^2 - \lim_{n \rightarrow +\infty} A_t \psi_n(t)$.

In particular

$$\|A_t \psi(t)\|_2 = \|\chi\|_2 = \lim_{n \rightarrow +\infty} \|A_t \psi_n(t)\|_2 = \lim_{n \rightarrow +\infty} \|\chi_n\|_2 = \lim_{n \rightarrow +\infty} \|\psi_n(t)\|_t,$$

by the isometry of A_t on $\tilde{\mathcal{V}}_t^*$. On the other hand $\|\psi(t)\|_t = \lim_{n \rightarrow +\infty} \|\psi_n(t)\|_t$, by the fact that $\psi(t)$ is the strong \mathcal{V}_t^* -limit of $\psi_n(t)$. Hence we have proven $\|A_t \psi(t)\|_2 = \|\psi(t)\|_t$, and thus A_t is isometric from the whole \mathcal{V}_t^* into $L^2(\mathbb{R}^d)$. It remains to show that the range of A_t is the whole $L^2(\mathbb{R}^d)$.

Let χ be an arbitrary element of $L^2(\mathbb{R}^d)$, then, $\mathcal{D}(e^{(T/2)H})$ being dense in $L^2(\mathbb{R}^d)$, there exist $\chi_n \in \mathcal{D}(e^{(T/2)H})$ s. t. $\chi_n \rightarrow \chi$ strongly in $L^2(\mathbb{R}^d)$. Set $\psi_n(t) \equiv e^{-tH} \psi_n$, then $\psi_n \in \tilde{\mathcal{V}}_t^*$ and $A_t \psi_n(t) = \chi_n \rightarrow \chi$ in $L^2(\mathbb{R}^d)$. On the other hand $\psi_n(t)$ is Cauchy in \mathcal{V}_t^* , since $\|\psi_n(t) - \psi_m(t)\|_t = \|\chi_n - \chi_m\|_2$ and χ_n converges, hence there exists $\psi(t) \in \mathcal{V}_t^*$ s. t. $\psi_n(t) \rightarrow \psi(t)$ strongly in \mathcal{V}_t^* . But A_t is bounded (even isometric) hence

$$\begin{aligned} A_t \psi(t) &= A_t(\mathcal{V}_t^* - \lim_{n \rightarrow +\infty} \psi_n(t)) = L^2 - \lim_{n \rightarrow +\infty} A_t \psi_n(t) \\ &= L^2 - \lim_{n \rightarrow +\infty} \chi_n = \chi, \end{aligned}$$

which shows that χ is in the range of A_t , hence A_t is onto. A_t is thus isometric from \mathcal{V}_t^* onto $L^2(\mathbb{R}^d)$. A_t^{-1} has then domain $L^2(\mathbb{R}^d)$ and is again isometric, and A_t is unitary from \mathcal{V}_t^* onto $L^2(\mathbb{R}^d)$ with $A_t^+ = A_t^{-1}$ its inverse, so that $A_t^+ A_t$ is the identity in \mathcal{V}_t^* and $A_t^+ A_t$ is the identity in $L^2(\mathbb{R}^d)$. \square

If we recall the definition of B_t given in (2.13), we see that $A_t^+ = A_t^{-1}$ is an extension of B_t (preserving isometry) to the whole of $L^2(\mathbb{R}^d)$. In the following we shall write U_t for the unitary operator A_t^+ from $L^2(\mathbb{R}^d)$ onto \mathcal{V}_t^* , $t \in I \cup [\frac{T}{2}, \infty[$. We then have $U_t^{-1} = U_t^+$ as the unitary operator A_t from \mathcal{V}_t^* onto $L^2(\mathbb{R}^d)$. By (U_t, U_t^{-1}) the Hilbert spaces \mathcal{V}_t^* , $L^2(\mathbb{R}^d)$ are then identified (in the sense of unitary equivalence).

Remark. — If H is of the form $H = -\frac{1}{2}\Delta + V$, for V smooth with all derivatives bounded and continuous, and with domain $\mathcal{D}(H) = \mathcal{D}(\Delta)$, we observe that the set $\xi(\mathbb{R}^d)$ of Hermite functions (eigenfunctions of $-\frac{1}{2}\Delta + \frac{1}{2}|x|^2$) is dense in \mathcal{V}_t^* for any $t \in I \cup [\frac{T}{2}, \infty[$. Indeed, for any $\psi(t)$ in \mathcal{V}_t^* , $\exists \{\chi_n\}_{n \in \mathbb{N}}$ in $\mathcal{D}(e^{(T/2)H})$ such that $\|\psi(t) - e^{-tH} \chi_n\|_t \xrightarrow[n \rightarrow \infty]{} 0$ [$\xi(\mathbb{R}^d)$ being dense in $L^2(\mathbb{R}^d)$]. But, for any χ_n , there is a sequence $\tilde{\chi}_{n,m}$ in $\xi(\mathbb{R}^d)$ such that $\|\chi_n - \tilde{\chi}_{n,m}\|_2 \xrightarrow[m \rightarrow \infty]{} 0$. Moreover, it is easy to show, by direct estimates, that $\xi(\mathbb{R}^d) \subset \mathcal{D}(e^{(T/2)H})$. Since

$$\|e^{-tH} \chi_n - e^{-tH} \tilde{\chi}_{n,m}\|_t = \|\chi_n - \tilde{\chi}_{n,m}\|_2,$$

an $\varepsilon/2$ argument shows that $\|\psi(t) - e^{-tH} \tilde{\chi}_{n,m}\|_t \rightarrow 0$. Therefore $\xi(\mathbb{R}^d)$ is dense in \mathcal{V}_t^* . We also remark that for any dense subset $\mathcal{F}(\mathbb{R}^d)$ of $L^2(\mathbb{R}^d)$ we have that $U_t \mathcal{F}(\mathbb{R}^d)$ is a dense subset of \mathcal{V}_t^* .

Let us now introduce another family of linear subspaces of $L^2(\mathbb{R}^d)$ by

$$\tilde{\mathcal{V}}_t \equiv \{\eta_\chi(t), \chi \text{ in } \mathcal{D}(e^{(T/2)H})\}, \text{ with } \eta_\chi(t) \text{ defined by (2.6')},$$

for all t in I . We give $\tilde{\mathcal{V}}_t$ the scalar product

$$\begin{aligned} (\eta_{x_1}(t) \mid \eta_{x_2}(t))_t &\equiv \langle C_t \eta_{x_1}(t) \mid C_t \eta_{x_2}(t) \rangle_2 \\ &= \langle \chi_1 \mid \chi_2 \rangle_2, \end{aligned} \tag{2.14}$$

where the linear operator C_t from $\tilde{\mathcal{V}}_t$ onto $\mathcal{D}(e^{(T/2)H})$ is defined by

$$C_t \eta_x(t) \equiv \chi.$$

Similarly as above, we verify that $C_t D_t = 1$ on $\mathcal{D}(e^{(T/2)H})$ and $D_t C_t = 1$ on $\tilde{\mathcal{V}}_t$, where $D_t \equiv e^{tH} \mid \mathcal{D}(e^{(T/2)H})$, t in I .

By definition, the backward Hilbert space \mathcal{V}_t is the completion of $\tilde{\mathcal{V}}_t$ with respect to the scalar product (2.14). Similarly as in Proposition 2.2 we can extend C_t to an unitary operator from \mathcal{V}_t onto $L^2(\mathbb{R}^d)$ and identify in this way \mathcal{V}_t with $L^2(\mathbb{R}^d)$. In fact we have the

PROPOSITION 2.3. — *For all $t \in I$, $(\mathcal{V}_t, (\mid)_t)$ can be identified with $(L^2(\mathbb{R}^d), \langle \mid \rangle_2)$ by the unitary map C_t from \mathcal{V}_t onto $L^2(\mathbb{R}^d)$ defined by $C_t \psi(t) \equiv \chi$ for $\psi(t) \equiv e^{tH} \chi = \eta_\chi(t)$, $\chi \in \mathcal{D}(e^{(T/2)H})$ and for arbitrary $\psi(t) \in \mathcal{V}_t$ by $C_t \psi(t) \equiv \chi$, where $\psi(t) = \mathcal{V}_t - \lim \psi_n(t)$ with*

$$\psi_n(t) = e^{tH} \chi_n \in \tilde{\mathcal{V}}_t, \quad \chi_n \in \mathcal{D}(e^{(T/2)H}), \quad \chi = L^2 - \lim_{n \rightarrow \infty} \chi_n. \quad \square$$

It follows from this Proposition that $C_t^+ = C_t^{-1}$ is an extension of D_t (preserving isometry) to the whole of $L^2(\mathbb{R}^d)$. In the following we shall write V_t for the unitary operator C_t^+ from $L^2(\mathbb{R}^d)$ onto \mathcal{V}_t , for $t \in I$. We then have $V_t^{-1} = V_t^+$ as the unitary operator C_t from \mathcal{V}_t onto $L^2(\mathbb{R}^d)$. By (V_t, V_t^{-1}) the Hilbert spaces \mathcal{V}_t and $L^2(\mathbb{R}^d)$ are then identified (in the sense of unitary equivalence). From Proposition 2.2, 2.3 we also notice that $J_t \equiv U_t V_t^{-1}$ is a unitary map from \mathcal{V}_t onto \mathcal{V}_t^* and $J_t^{-1} \equiv V_t U_t^{-1}$ is a unitary map from \mathcal{V}_t^* onto \mathcal{V}_t .

Finally, another useful family of Hilbert spaces is defined by considering the direct sum of the vector space \mathcal{V}_t^* and \mathcal{V}_t , t in I ,

$$\mathcal{H}_t = \mathcal{V}_t^* \oplus \mathcal{V}_t. \tag{2.15}$$

Then \mathcal{H}_t is a one-parameter family of vector spaces, whose vectors, at a fixed time t in I , are ordered pairs $(f(t), f'(t))$ with $f(t)$ in \mathcal{V}_t^* , $f'(t)$ in \mathcal{V}_t , and with scalar product

$$\begin{aligned} (f(t) \mid f'(t))_t &\equiv ((f^1(t), f^{1'}(t)) \mid (f^2(t), f^{2'}(t)))_t \\ &\equiv (f^1(t) \mid f^2(t))_t + (f^{1'}(t) \mid f^{2'}(t))_t. \end{aligned} \tag{2.16}$$

Let $\| \cdot \|_t$ denote the corresponding norm. Thus we denote by the same symbols the scalar products of \mathcal{V}_t^* , \mathcal{V}_t and \mathcal{H}_t . By Proposition 2.2, 2.3 we have a unitary map $\tilde{U}_t \equiv U_t \oplus V_t$ from $L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$ onto \mathcal{H}_t and an unitary map $\tilde{U}_t^{-1} = U_t^{-1} \oplus V_t^{-1}$ from \mathcal{H}_t onto $L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$. Hence $(\mathcal{H}_t, (\cdot , \cdot)_t)$ is unitary equivalent to $L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$ (with its natural

scalar product), and these spaces can thus be identified. Henceforth, we shall work mainly in the forward Hilbert space \mathcal{V}_t^* .

For each fixed t in I , we define $K_t: \mathcal{V}_t^* \rightarrow \mathcal{V}_t$ by

$$K_t \equiv V_t C U_t^{-1}, \tag{2.17}$$

where C is the usual complex conjugation in $L^2(\mathbb{R}^d)$. We then have, from Proposition 2.2, 2.3 that K_t is an isometric antilinear operator from \mathcal{V}_t^* onto \mathcal{V}_t . We shall call K_t the forward Euclidean conjugation. We see from the definition of U_t, V_t , that C commutes with V_t and U_t .

Using the definition (2.17) of K_t we easily see that for any $\chi_1, \chi_2 \in L^2(\mathbb{R}^d)$:

$$(K_t \bar{\Psi}_1(t), J_t \Psi_2(t))_{\mathcal{V}_t} = (V_t \chi_1 \mid V_t \chi_2)_{\mathcal{V}_t} = (\Psi_1(t) \mid \Psi_2(t))_{\mathcal{H}} = \langle \chi_1 \mid \chi_2 \rangle_2,$$

with $\Psi_i(t) \equiv U_t \chi_i, i=1, 2$. Here, for clarity, we have appended suffixes \mathcal{V}_t resp. \mathcal{V}_t^* to the scalar products in \mathcal{V}_t resp. \mathcal{V}_t^* ; we also recall that $J_t \equiv U_t V_t^{-1}$ maps unitarily \mathcal{V}_t onto \mathcal{V}_t^* .

Remark. — We have constructed \mathcal{V}_t^* by closure, in $\| \cdot \|_t$ -norm, of $\tilde{\mathcal{V}}_t^*$. $\tilde{\mathcal{V}}_t^*$ can be looked upon as a subspace of \mathcal{V}_t^* as well as of $L^2(\mathbb{R}^d)$. By definition, U_t maps $L^2(\mathbb{R}^d)$ onto \mathcal{V}_t^* . It is sometimes useful to think of the restriction of U_t to $\mathcal{D}(e^{(T/2)H})$ as the operator e^{-tH} acting on $\mathcal{D}(e^{(T/2)H})$, $t \in I \cup [\frac{T}{2}, \infty[$. This is possible in the following way. Let α_t^F be the linear map from $\tilde{\mathcal{V}}_t^*$, as a subspace of \mathcal{V}_t^* , into $L^2(\mathbb{R}^d)$ given by

$$\begin{aligned} \alpha_t^F U_t \chi &\equiv \chi^F(t), & \chi \in \mathcal{D}(e^{(T/2)H}), \\ \chi^F(t) &\equiv e^{-tH} \chi \equiv \eta_\chi^*(t). \end{aligned}$$

Similarly let α_t^B be the linear map from $\tilde{\mathcal{V}}_t^*$ as a subspace of \mathcal{V}_t^* , into $L^2(\mathbb{R}^d)$ given by

$$\alpha_t^B V_t \chi \equiv \chi^B(t) \equiv e^{tH} \chi = \eta_\chi(t), \quad \chi \in \mathcal{D}(e^{(T/2)H}).$$

Let us consider for $\chi_i, i=1, 2$, in $\mathcal{D}(e^{(T/2)H})$, $t \in I$:

$$\langle \alpha_t^B V_t \chi_1 \mid \alpha_t^F U_t \chi_2 \rangle_2 = \langle \chi_1^B(t) \mid \chi_2^F(t) \rangle_2. \tag{2.12'}$$

From the definition of $\chi_2^F(t), \chi_1^B(t)$, and the symmetry of e^{-tH} on the chosen domain, we have that the r.h.s. of (2.12') is equal to $\langle \chi_1 \mid \chi_2 \rangle_2$.

On the other hand from the definition of U_t and its unitarity we have

$$(\Psi_1(t) \mid \Psi_2(t))_{\mathcal{V}_t} = (U_t \chi_1 \mid U_t \chi_2)_{\mathcal{V}_t} = \langle \chi_1 \mid \chi_2 \rangle_2 \tag{2.12''}$$

with $\Psi_i(t) \equiv U_t \chi_i(t)$.

Hence, from (2.12'), (2.12'') and the equality of (2.12') with $\langle \chi_1 | \chi_2 \rangle_2$ we get

$$\begin{aligned} \langle \alpha_t^B V_t \chi_1 | \alpha_t^F U_t \chi_2 \rangle_2 &= \langle \chi_1^B(t) | \chi_2^F(t) \rangle_2 = (U_t \chi_1 | U_t \chi_2)_{\mathcal{V}_t} \\ &= \langle \chi_1 | \chi_2 \rangle_2 = \langle \alpha_t^B K_t U_t \bar{\chi}_1 | \alpha_t^F U_t \chi_2 \rangle_2 \\ &= \langle \alpha_t^B K_t \eta_{\chi_1}^*(t) | \alpha_t^F \eta_{\chi_2}^*(t) \rangle_2, \end{aligned}$$

where we used $K_t U_t \bar{\chi}_1 = V_t C \bar{\chi}_1 = V_t \chi_1 = \eta_{\chi_1}(t)$. Similarly we have the corresponding formulae with $U_t \leftrightarrow V_t$, $B \leftrightarrow F$, $K_t \leftrightarrow K_t^{-1}$:

$$\begin{aligned} (V_t \chi_1 | V_t \chi_2)_{\mathcal{V}_t} &= \langle \chi_1 | \chi_2 \rangle_2 = \langle \alpha_t^F U_t \chi_1 | \alpha_t^B V_t \chi_2 \rangle_2 \\ &= \langle \chi_1^F(t) | \chi_2^B(t) \rangle_2 = \langle \alpha_t^F K_t^{-1} V_t \bar{\chi}_1 | \alpha_t^B V_t \chi_2 \rangle_2. \end{aligned}$$

It is worth noticing that K_t is not simply a complex conjugation. It should rather be interpreted as a time reversal operator. Indeed, in analogy with Quantum Mechanics, where a natural time reversal operator $T_\tau: L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ is defined by $T_\tau: \psi_\chi(x, \tau) \rightarrow \overline{\psi_\chi(x, -\tau)}$ [for $\psi_\chi(x, \tau)$ given by (2.3)], a natural Euclidean time reversal operator is

$$T_t: \left. \begin{aligned} \tilde{\mathcal{V}}_t^* &\rightarrow \tilde{\mathcal{V}}_t \\ \eta_{\chi}^*(t) &\rightarrow \eta_{\chi}^*(-t) \end{aligned} \right\} \quad (2.18)$$

for χ in $\mathcal{D}(e^{(T/2)H})$. The image of T_t is $\overline{\eta_{\chi}^*(-t)} = \eta_{\bar{\chi}}(t)$ which is $K_t \eta_{\chi}^*(t)$. Hence $T_t = K_t$ and K_t is the Euclidean time reversal.

We can extend the pair (K_t, K_t^{-1}) to a conjugation operator C_t from $\mathcal{H}_t \equiv \mathcal{V}_t^* \oplus \mathcal{V}_t$ onto $\mathcal{H}_t^c \equiv \mathcal{V}_t \oplus \mathcal{V}_t^* \cong \mathcal{H}_t$ in a natural way: $C_t = K_t$ on \mathcal{V}_t^* and $C_t = K_t^{-1}$ on \mathcal{V}_t . In particular we have

$$C_t(\eta_{\chi}^*(t) \oplus \eta_{\chi'}(t)) \equiv \eta_{\bar{\chi}}(t) \oplus \eta_{\bar{\chi}'}(t) \quad (2.19)$$

C_t is again antilinear, isometric, from \mathcal{H}_t onto \mathcal{H}_t^c , and is called the Euclidean conjugation.

Let us define the cone in $\tilde{\mathcal{V}}_t^*$ of the positive vectors:

$$\tilde{S}_+^*(t) = \{f_t \text{ in } \tilde{\mathcal{V}}_t^* \text{ such that } f_t(x) \geq 0 \text{ as an element of } L^2(\mathbb{R}^d)\}.$$

We extend, by closure in \mathcal{V}_t^* , $\tilde{S}_+^*(t)$ to a closed subset $S_+^*(t)$ of \mathcal{V}_t^* .

If e^{-tH} is positively preserving (which is the case of Schrödinger operators for $t \geq 0$, cf. Chapter 5) then $0 \leq \chi$ (a. e.) in $\mathcal{D}(H)$ implies $\eta_{\chi}^*(t)$ is in $S_+^*(t)$. We also denote by $S_-^*(t)$ the cone in \mathcal{V}_t^* of negative vectors:

$S_-^*(t) = \{g_t \text{ in } \mathcal{V}_t^* \text{ such that } -g_t \text{ belongs to } S_+^*(t)\}$ and by $S^*(t)$ the set $S_+^*(t) \cup S_-^*(t)$ in \mathcal{V}_t^* .

Notice that $S_+^*(t) \cap S_-^*(t) = \{0\}$ (0 being the zero element of $L^2(\mathbb{R}^d)$). S^* will be called the set of physical states for the heat equation. Its elements have a probabilistic interpretation, discussed in Chapter 6.

In complete analogy, two cones $S_{\pm}(t)$ in \mathcal{V}_t are defined by closure from $\tilde{S}_+(t) = \{f_t \text{ in } \tilde{\mathcal{V}}_t \text{ such that } f_t(x) \geq 0 \text{ in } L^2(\mathbb{R}^d)\}$ and $S_-(t) = \{g_t \text{ in } \mathcal{V}_t \text{ such that } -g_t \text{ is in } S_+(t)\}$. We also introduce $S(t) \equiv S_+(t) \cup S_-(t)$.

3. LINEAR OPERATORS ASSOCIATED WITH PHYSICAL OBSERVABLES

Let us first discuss the general situation. Let A be an operator mapping a dense domain $D(A)$ of $L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^d)$. By the unitary mapping $U_t, t \in I \cup [\frac{T}{2}, \infty[$, from $L^2(\mathbb{R}^d)$ onto \mathcal{V}_t^* we can associate to A a unitarily equivalent operator A_t^F from a dense domain $D(A_t^F) \subset \mathcal{V}_t^*$ into \mathcal{V}_t^* by $D(A_{-t}^F) = U_t D(A)$ and

$$A_{-t}^F U_t \chi = U_t A \chi \tag{3.1}$$

for all $\chi \in D(A) \subset L^2(\mathbb{R}^d)$.

Thus we have

$$U_t^+ A_{-t}^F U_t = A. \tag{3.2}$$

If A is normal (resp. self-adjoint, resp. skew-adjoint, respectively closed) we notice that A_t^F is normal (resp. self-adjoint, resp. skew-adjoint, resp. closed), by the unitarity of U_t .

Remark. — If $D(A) \subset \mathcal{D}(e^{(T/2)H})$ we can look upon $U_t D(A)$ as a subset of $L^2(\mathbb{R}^d)$, consisting of those $\eta_{\chi}^*(t) \in \tilde{\mathcal{V}}_t^*$ (as embedded in $L^2(\mathbb{R}^d)$, with $\chi \in D(A)$). More precisely, in the notations of Section 2, $\alpha_t^F U_t D(A) \subset L^2(\mathbb{R}^d)$ with

$$\alpha_t^B U_t \chi = \chi(t), \quad \chi \in \mathcal{D}(e^{(T/2)H}),$$

$\chi(t) \equiv e^{-tH} \chi$. $\alpha_t^F U_t D(A)$ is dense in $L^2(\mathbb{R}^d)$. (Since U_t is isometric, hence $\langle \psi | \alpha_t^F U_t \varphi \rangle_2 = 0$ for all $\varphi \in D(A)$ implies $\alpha_t^{F-1} U_t^{-1} \psi = 0$ and then $\psi = 0$ since α_t^F is 1-1 and U_t^{-1} is isometric.)

If A maps $\mathcal{D}(e^{(T/2)H})$ into $\mathcal{D}(e^{(T/2)H})$ we have, on the other hand, that $U_t A \chi$ can be looked upon as the element $\eta_{A\chi}^*(t)$ in $\tilde{\mathcal{V}}_t^* \subset L^2(\mathbb{R}^d)$, more precisely $\alpha_t^F U_t A \chi = \eta_{A\chi}^*(t)$. In this case we can look upon A_{-t}^F as the densely defined operator A_{-t}^F in $L^2(\mathbb{R}^d)$, with domain $\{\eta_{\chi}^*(t), \chi \in D(A)\}$, such that

$$\tilde{A}_{-t}^F \eta_{\chi}^*(t) = \eta_{A\chi}^*(t), \tag{3.3}$$

for all $\chi \in D(A)$. In fact we have $(\alpha_t^F)^{-1} \tilde{A}_{-t}^F \alpha_t^F = A_{-t}^F$. We call $A_{-t}^F, \tilde{A}_{-t}^F$ the forward operators corresponding to A . We can repeat corresponding considerations with U_t replaced by $V_t, t \in I$. Thus, to the operator A with dense domain $D(A)$ in $L^2(\mathbb{R}^d)$, there corresponds the unitarily equivalent

backward operator A_{-t}^B , from the dense domain $D(A_{-t}^B) \equiv V_t D(A) \subset \mathcal{V}_t$ into \mathcal{V}_t by:

$$A_{-t}^B V_t \chi = V_t A_x \chi \tag{3.4}$$

If $D(A) \subset \mathcal{D}(e^{(T/2)H})$ and $AD(A) \subset \mathcal{D}(e^{(T/2)H})$ then we can look upon A_{-t}^B as the densely defined \tilde{A}_{-t}^B given by

$$\tilde{A}_{-t}^B \eta_x(t) = \eta_{A_x}(t), \tag{3.5}$$

for all $\chi \in D(A)$, $\eta_x(t)$, $\eta_{A_x}(t)$ being regarded as elements of $\tilde{\mathcal{V}}_t \subset L^2(\mathbb{R}^d)$. We have

$$(\alpha_t^B)^{-1} \tilde{A}_{-t}^B \alpha_t^B = A_{-t}^B. \tag{3.6}$$

Let us now look more closely at some particularly important operators.

3.1. Position operator

Let Q_i , $i=1, \dots, d$ be the self-adjoint operator multiplication by x_i in $L^2(\mathbb{R}^d)$, i.e. the operator $f(x) \rightarrow x_i f(x)$, for $f \in D(Q_i) \subset L^2(\mathbb{R}^d)$. Let Q be the self-adjoint operator from the dense domain $D(Q) \subset L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^d) \otimes \mathbb{R}^d$ given by $f(x) \rightarrow (x_i f(x), i=1, \dots, d)$. (Q can be looked upon as the position operator for a quantum mechanical particle in the Schrödinger representation of the Hilbert space.)

Let us define the "position operator" in the forward Hilbert space $\mathcal{V}_t^*(\mathbb{R}^d)$, $t \in I \cup [\frac{T}{2}, \infty[$, as the map Q_t from a dense subset of $\mathcal{V}_t^*(\mathbb{R}^d) \otimes \mathbb{R}^d$ given by

$$Q_{-t} \equiv U_t Q U_t^{-1} \tag{3.7}$$

on the natural domain

$$\begin{aligned} D(Q_{-t}) &\equiv \{ \psi(t) \in \mathcal{V}_t^* \mid U_t^{-1} \psi(t) \in D(Q) \}. \\ &= U_t D(Q) \subset \mathcal{V}_t^*. \end{aligned}$$

Since U_t is unitary and Q is self-adjoint we have immediately that Q_{-t} is self-adjoint from $D(Q_{-t})$ into $\mathcal{V}_t^*(\mathbb{R}^d) \otimes \mathbb{R}^d$.

Similarly one defines $(Q_{-t})_i \equiv U_t Q_i U_t^{-1}$, and $(Q_{-t})_i$ are self-adjoint operators from $D(Q_{-t})_i \equiv U_t D(Q_i)$ into $\mathcal{V}_t^*(\mathbb{R}^d)$. The $(Q_{-t})_i$ are the components of Q_{-t} .

The spectral representations of $(Q_{-t})_i$ and Q_{-t} are, of course, given by the above unitary equivalence and the spectral representation of Q_i resp. Q . In particular, by the unitary equivalence, $(Q_{-t})_i$ has purely continuous spectrum \mathbb{R} . The realisation of the position operator $Q_{-t}^B \equiv V_t Q V_t^{-1}$ in the backward Hilbert space \mathcal{V}_t is, of course, analogous. For $t=0$, notice that $Q_0 = Q_0^B = Q$. The position operator in \mathcal{H}_t will be defined by $Q \oplus Q^B$.

3.2. Momentum operator

Let \dot{P} be the operator defined in the dense subset $C_0^\infty(\mathbb{R}^d)$ of $L^2(\mathbb{R}^d)$ by

$$\left. \begin{aligned} \dot{P}: C_0^\infty(\mathbb{R}^d) &\rightarrow L^2(\mathbb{R}^d) \otimes \mathbb{R}^d \\ \chi &\rightarrow -\nabla\chi \end{aligned} \right\} \quad (3.8)$$

i. e. $\dot{P} = -\nabla$ on $C_0^\infty(\mathbb{R}^d)$. We have $\dot{P}^+ = -\nabla^+$ (with $+$ denoting adjoints) and $\dot{P}^+ \supset -\dot{P} = \nabla$.

It is well known that $iP = -i\nabla$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d)$ (see e. g. [5]). Hence $\dot{P}^+ = -\dot{P}$, where \dot{P} is the closure of $\dot{P} = -\nabla$. Thus \dot{P} is skew-adjoint. Its domain is $\mathcal{D}(P) = \left\{ \chi \text{ in } L^2(\mathbb{R}^d); \int_{\mathbb{R}^d} |\nabla\chi|^2 dx < \infty \right\}$, (where the derivatives are taken in distributional sense).

We shall henceforth set $P \equiv \dot{P}$.

It is also well known that the spectrum and spectral decomposition of P are given by

$$(P\hat{f})(k) = i \int_{\mathbb{R}^d} k\hat{f}(k) dk$$

We define the momentum operator P_{-t} in \mathcal{V}_t^* by

$$P_{-t} \equiv U_t P U_t^{-1} \quad (3.9)$$

P_{-t} is skew-adjoint from $D(P_{-t}) = U_t D(P) \subset \mathcal{V}_t^*$ into $\mathcal{V}_t^* \otimes \mathbb{R}^d$, with skew-adjoint components $(P_{-t})_i \equiv U_t P_i U_t^{-1}$, and P_i the closure of $\frac{-\partial}{\partial x_i} \cdot (P_i)_i$ has an absolutely continuous spectrum, the line \mathbb{R} .

Similarly one defines $P_{-t}^{\mathbb{B}} = ((P_{-t}^{\mathbb{B}})_i, i=1, \dots, d)$, $(P_{-t}^{\mathbb{B}})_i = V_t P_i V_t^{-1}$ as the momentum operator in \mathcal{V}_t . $P_{-t} \oplus P_{-t}^{\mathbb{B}}$ is then the momentum operator in \mathcal{H}_t . Let us also observe that for $\chi \in D(QP) \cap D(PQ)$

$$\begin{aligned} [Q_{-t} P_{-t} - P_{-t} Q_{-t}] U_t \chi &= U_t (QP - PQ) \chi \\ &= U_t \chi \end{aligned}$$

$D(QP) \cap D(PQ)$ is dense in $L^2(\mathbb{R}^d)$ [it contains e. g. $C_0^\infty(\mathbb{R}^d)$]. Also $U_t [D(Q_i P_j) \cap D(P_i Q_j)]$ is dense in \mathcal{V}_t^* , since U_t is unitary. Hence we have

$$[Q_{-t} P_{-t} - P_{-t} Q_{-t}] = 1 \quad (3.10)$$

on a dense domain of \mathcal{V}_t^* .

3.3. Hamiltonian operators

We consider first the kinetic energy operator. Let $\mathcal{D}(H_0)$ be the subspace of $L^2(\mathbb{R}^d)$ given by

$$\mathcal{D}(H_0) = \left\{ \chi \text{ in } \mathcal{V}_0^*(\mathbb{R}^d) = L^2(\mathbb{R}^d) \text{ such that } \int_{\mathbb{R}^d} |\nabla \chi|^2 dx < \infty \right\}$$

and define

$$\begin{aligned} H_0: \mathcal{D}(H_0) &\rightarrow L^2(\mathbb{R}^d) \\ \chi &\rightarrow -\frac{1}{2} \Delta \chi. \end{aligned} \tag{3.11}$$

We call H_0 the kinetic energy operator in $\mathcal{V}_0^*(\mathbb{R}^d)$. It is obvious that $H_0 = -\frac{1}{2} P^2$, where P is the momentum operator of paragraph 3.2 defined on $\mathcal{V}_0^*(\mathbb{R}^d) = L^2(\mathbb{R}^d)$. Moreover

$$H_0 = \frac{1}{2} P^+ P$$

for P^+ the adjoint of P . H_0 is self-adjoint, positive, unbounded. The restriction of H_0 to $C_0^\infty(\mathbb{R}^d)$ is essentially self-adjoint (see, e. g. [5]). Let now V be the operator of multiplication by a measurable function $V(x)$ in $L^2(\mathbb{R}^d)$, s. t. $H = H_0 + V$ exists (in the form sense sum or operator sum) as a self-adjoint operator on a dense domain $D(H)$ of $L^2(\mathbb{R}^d)$ (for sufficient conditions for this see e. g. [5]). We define the energy operator, or Hamiltonian, in \mathcal{V}_t^* by

$$H_{-t} = U_t H U_t^{-1}. \tag{3.12}$$

H_{-t} is self-adjoint, with the same spectrum as H . The Hamiltonian H_{-t}^B in \mathcal{V}_t is defined similarly by $H_{-t}^B = V_t H V_t^{-1}$, as a self-adjoint operator with the same spectrum as H . The Hamiltonian \mathbb{H}_{-t} in \mathcal{H}_t is then defined by $\mathbb{H}_{-t} = H_{-t} \oplus H_{-t}^B$.

Let us remark that for $\chi, \chi' \in \mathcal{D}(e^{(T/2)H})$ we have

$$\begin{aligned} \mathbb{H}_{-t} \{U_t \chi, V_t \chi'\} \\ = \{U_t H \chi, V_t H \chi'\} = \{(\alpha_t^F)^{-1} \eta_{\mathbb{H}}^*(t), (\alpha_t^B)^{-1} \eta_{H \chi'}(t)\} \end{aligned} \tag{3.13}$$

We also remark that it follows from (3.12) and the property that H is essentially self-adjoint on $\varepsilon(H) \subset L^2(\mathbb{R}^d)$ that \mathbb{H}_{-t} is essentially self-adjoint on the dense subset $U_t \varepsilon(H) \oplus V_t \xi(H)$ of \mathcal{H}_t .

We summarise the above results in the following:

THEOREM 3.1. — *Let A be any operator mapping a dense domain $D(A) \subset L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^d)$. Define, for $t \in I \cup [\frac{T}{2}, \infty[$, the forward operator associated with A by $A_{-t}^F = U_t A U_t^{-1}$ on $D(A_{-t}^F) \equiv U_t D(A)$. If A is normal (resp. self-adjoint, resp. skew-adjoint) then A_{-t}^F is also normal (resp. self-adjoint, resp. skew-adjoint). A_{-t}^F has the same spectrum as A.*

If $A \mathcal{D}(e^{(T/2)H}) \subset \mathcal{D}(e^{(T/2)H})$ we have $A_{-t}^F = (\alpha_t^F)^{-1} A_{-t}^F \alpha_t^F$, with α_t^F the map from $U_t \mathcal{D}(e^{(T/2)H}) \subset \mathcal{V}_t^$ into $L^2(\mathbb{R}^d)$ given by $\alpha_t^F U_t \chi \equiv e^{-tH} \chi$, $\chi \in \mathcal{D}(e^{(T/2)H})$, and \tilde{A}_{-t}^F the map from $e^{-tH} \mathcal{D}(e^{(T/2)H}) \subset L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^d)$ given by*

$$\tilde{A}_{-t}^F e^{-tH} \chi \equiv e^{-tH} A \chi.$$

Similarly, one defines for $t \in I$ the backward operator associated with A by (3.4). A_{-t}^B has all corresponding properties as A_{-t}^F . In particular if $AD(A) \subset \mathcal{D}(e^{(T/2)H})$ then (3.6) holds, with α_t^B the map from $V_t \mathcal{D}(e^{(T/2)H}) \subset \mathcal{V}_t$ into $L^2(\mathbb{R}^d)$ given by $\alpha_t^B V_t \chi \equiv e^{tH} \chi$, $\chi \in \mathcal{D}(e^{(T/2)H})$. One also defines the operator corresponding to A in \mathcal{H}_t by $A_{-t}^F \oplus A_{-t}^B$.

For $A = Q_i$ we have that A_{-t}^F is the i -th component $(Q_{-t})_i$ of the position operator $Q_{-t} \equiv U_t Q U_t^{-1}$ in \mathcal{V}_t^ . For $A = P_i = -\frac{\partial}{\partial x_i}$, A_{-t}^F is the i -th component $(P_{-t})_i$ of the momentum operator $P_{-t} \equiv U_t P U_t^{-1}$ in \mathcal{V}_t^* . One verifies the commutation relations $Q_{-t} P_{-t} - P_{-t} Q_{-t} = 1$ on a dense domain of \mathcal{V}_t^* . For $A = H$, A_{-t}^F is the Hamiltonian H_{-t} in \mathcal{V}_t^* . For $\chi \in \mathcal{D}(e^{(T/2)H})$ we have*

$$H_{-t} U_t \chi = (\alpha_t^F)^{-1} e^{-tH} H \chi.$$

H_{-t} is essentially self-adjoint on the dense subset $U_t \varepsilon(H)$ of \mathcal{V}_t^ . Corresponding results hold for \mathcal{V}_t^* replaced by \mathcal{V}_t or \mathcal{H}_t . \square*

Remark. — Define for any χ in $\mathcal{D}(Q)$,

$$\langle Q^2 \rangle_0 \equiv \int (x - \langle Q \rangle_0)^2 |\chi(x)|^2 dx, \tag{3.14}$$

$$\langle Q \rangle_0 \equiv \int_{\mathbb{R}^d} x |\chi(x)|^2 dx$$

and for any χ in $\mathcal{D}(P)$, $\langle P^2 \rangle_0 \equiv \int_{\mathbb{R}^d} |\nabla(\chi(x) e^{i \langle P \rangle_0 x})|^2 dx,$

$$\langle P \rangle_0 \equiv - \int_{\mathbb{R}^d} \bar{\chi}(x) \nabla \chi(x) dx. \tag{3.15}$$

We observe that for α any positive constant, the substitution $\tilde{\chi} = \alpha^{1/2} \chi(\alpha x)$ in the definitions of $\langle Q^2 \rangle_0$ and $\langle P^2 \rangle_0$ gives $\langle \tilde{Q}^2 \rangle_0 = \alpha \langle Q^2 \rangle_0$ and

$\langle \tilde{P}^2 \rangle = \alpha^{-1} \langle P^2 \rangle_0$ so that $\langle \tilde{Q}^2 \rangle_0 \langle \tilde{P}^2 \rangle_0 = \langle Q^2 \rangle_0 \langle P^2 \rangle_0$. Let us choose α such that $\langle Q^2 \rangle_0 \doteq \langle P^2 \rangle_0$, i. e. $(\langle Q^2 \rangle_0^{1/2} - \langle P^2 \rangle_0^{1/2})^2 = 0$. Then

$$\begin{aligned} \langle Q^2 \rangle_0^{1/2} \langle P^2 \rangle_0^{1/2} &= \frac{1}{2} (\langle P^2 \rangle_0 + \langle Q^2 \rangle_0) \\ &= \int \left\{ \frac{1}{2} |\nabla \chi|^2 + \frac{1}{2} |x|^2 |\chi|^2 \right\} dx. \end{aligned}$$

This positive functional is minimised in $L^2(\mathbb{R}^d)$ by

$$\chi_0 = \pi^{-d/4} \exp \left\{ -\frac{1}{2} |x|^2 \right\}$$

and its minimal value is $\frac{1}{2}$. Using the unitarity of U_t , we see that the following (Euclidean) uncertainty principle holds:

PROPOSITION 3.2. — For each χ in $\mathcal{D}(Q) \cap \mathcal{D}(P) \subset L^2(\mathbb{R}^d)$, if $(\Delta Q)_0^2 \equiv \langle Q^2 \rangle_0 - \langle Q \rangle_0^2$ and $(\Delta P)_0^2 \equiv \langle P^2 \rangle_0 - \langle P \rangle_0^2$ then

$$(\Delta Q)_0 (\Delta P)_0 \geq \frac{1}{2}.$$

The same holds with $\langle Q^2 \rangle_0, \langle Q \rangle_0$ replaced by $(U_t \chi | Q_{-t}^2 U_t \chi)_t$ resp. $(U_t \chi | Q_{-t} U_t \chi)_t$ and correspondingly for P .

3.4. Conjugation and observables

First, let us observe that $\mathcal{D}(e^{(T/2)H}) = \bigcap_{t \in I} \text{Ran} \{ e^{-tH} |_{\mathcal{D}(e^{(T/2)H})} \}$.

PROPOSITION 3.3. — Let A be any densely defined operator in $\mathcal{V}_t^*(\mathbb{R}^d) t \in I$, with $\mathcal{D}(A) \supset U_t \mathcal{D}(e^{(T/2)H})$. Then we have, for any χ_1, χ_2 in $\mathcal{D}(e^{(T/2)H})$,

$$\begin{aligned} (U_t \chi_1 | A U_t \chi_2)_{\mathcal{V}_t} &= (K_t U_t \chi_2 | (K_t A + K_t^{-1}) K_t U_t \chi_1)_{\mathcal{V}_t} \\ &= (V_t \bar{\chi}_1 | \bar{A}_t V_t \bar{\chi}_2)_{\mathcal{V}_t} \end{aligned}$$

where K_t is the Euclidean conjugation, $+$ denotes the adjoint in $\mathcal{V}_t^*(\mathbb{R}^d)$, and $\bar{A}_t \equiv K_t A + K_t^{-1} = J_t^+ C A^+ C J_t$, with $J_t \equiv U_t V_t^{-1}$ (the unitary map from \mathcal{V}_t onto \mathcal{V}_t^*).

Proof. — Let us set $\gamma^+(t) \equiv A^+ U_t \chi_1$. This is well defined since $A^+ \supset A$ and $U_t \chi_1$ is in $\mathcal{D}(A)$ for any t in I , by our assumption on χ_1 .

The r.h.s. of the claimed equality is

$$(K_t U_t \chi_2 | K_t \gamma^+(t))_t = (\gamma^+(t) | \eta_{\chi_2}^*(t))_t,$$

by the isometric antilinearity of K_t . This proves the proposition.

We can look upon \tilde{A}_t as the time reversal of A . We observe that $CA^+C = CAC$ if A is self-adjoint, $CA^+C = -CAC$ if A is skew-adjoint. If A is real, i.e. commutes with C , we have $CA^+C = A$ resp. $CA^+C = -A$, for A self-adjoint, resp. skew-adjoint. In the former case we have $\tilde{A}_{-t} = J_t^+ A J_t$; in the latter case $\tilde{A}_{-t} = -J_t^+ A J_t$.

For $A = Q_{-t}$, resp. P_{-t} , resp. H_{-t} we have $\tilde{A}_{-t} = J_t^+ Q_{-t} J_t$, resp. $\tilde{A}_{-t} = -J_t^+ P_{-t} J_t$, resp. $\tilde{A}_{-t} = J_t^+ H_{-t} J_t$. Thus:

$$\begin{aligned} (U_t \chi_1 \mid Q_{-t} U_t \chi_2)_{\mathcal{V}_t^*} &= (V_t \tilde{\chi}_1 \mid J_t^+ Q_{-t} J_t V_t \tilde{\chi}_2)_{\mathcal{V}_t} \\ (U_t \chi_1 \mid P_{-t} U_t \chi_2)_{\mathcal{V}_t^*} &= -(V_t \tilde{\chi}_1 \mid J_t^+ P_{-t} J_t V_t \tilde{\chi}_2)_{\mathcal{V}_t} \\ (U_t \chi_1 \mid H_{-t} U_t \chi_2)_{\mathcal{V}_t^*} &= (V_t \tilde{\chi}_1 \mid J_t^+ H_{-t} J_t V_t \tilde{\chi}_2)_{\mathcal{V}_t} \end{aligned} \tag{3.16}$$

We shall say that the position and the Hamiltonian operators are even, and the momentum operator is odd under time reversal.

The Euclidean Heisenberg commutation relation of paragraph 3.2,

$$Q_{-t} P_{-t} - P_{-t} Q_{-t} = I$$

is invariant under time reversal. In fact

$$\begin{aligned} J_t^+ (Q_{-t} P_{-t} - P_{-t} Q_{-t})^+ J_t &\supset -J_t^+ (P_{-t} Q_{-t} - Q_{-t} P_{-t}) J_t \\ &= J_t^+ (Q_{-t} P_{-t} - P_{-t} Q_{-t}) J_t \end{aligned} \tag{3.17}$$

where $Q_{-t}^+ = Q_{-t}$, $P_{-t}^+ = -P_{-t}$ has been used. The corresponding property is true for the Heisenberg commutation relation in the backward Hilbert space $\mathcal{V}_t(\mathbb{R}^d)$ and in the total Hilbert space \mathbb{H}_t .

Remark. — Using the fact that Q, iP are self-adjoint, Stone theorem shows that the Weyl form of the commutation relation also holds:

$$e^{i\alpha Q_{-t}} e^{-\beta P_{-t}} = e^{-\beta P_{-t}} e^{i\alpha Q_{-t}} e^{-\alpha\beta} \tag{3.18}$$

4. EQUATIONS OF MOTION

Let A be as in Theorem 3.1 and let A_{-t}^F be the corresponding operator in $\mathcal{V}_t^*(\mathbb{R}^d)$:

$$A_{-t}^F \equiv U_t A U_t^{-1} \tag{4.0}$$

By definition $D(A_{-t}^F) = U_t D(A) \subset \mathcal{V}_t^*(\mathbb{R}^d)$.

Let us assume $D(A) \supset \mathcal{D}(e^{(T/2)H})$ in $L^2(\mathbb{R}^d)$. Then

$$D(A_{-t}^F) \supset U_t D(e^{(T/2)H}) \quad \text{and} \quad U_t D(e^{(T/2)H}) = \tilde{\mathcal{V}}_t^*$$

can be looked upon as subsets of $L^2(\mathbb{R}^d)$. Therefore we can look upon $A_{-t}^F \mid U_t D(e^{(T/2)H})$ as an operator \tilde{A}_{-t}^F from the dense subset $\tilde{\mathcal{V}}_t^*$ in $L^2(\mathbb{R}^d)$ into \mathcal{V}_t^* [note that \tilde{A}_{-t}^F coincides with the operator discussed in Section 3, denoted by the same symbol, if $D(A) = D(e^{(T/2)H})$].

Let $\psi_t = U_t \chi \in \tilde{\mathcal{V}}_t^*$, $\chi \in D(e^{(T/2)H})$.

Then

$$\tilde{A}_{-t}^F \psi_t = U_t A \chi. \tag{4.1}$$

Let us assume that $AD(e^{(T/2)H}) \supset D(e^{(T/2)H})$. In this case $U_t A \chi \in \tilde{\mathcal{V}}_t^*$ and \tilde{A}_{-t}^F maps $\tilde{\mathcal{V}}_t^*$ into $\tilde{\mathcal{V}}_t^*$. We can then look in this case at \tilde{A}_{-t}^F as a densely defined map from a dense domain $D(\tilde{A}_{-t}^F) = \tilde{\mathcal{V}}_t^*$ of $L^2(\mathbb{R}^d)$ into $\tilde{\mathcal{V}}_t^* \subset L^2(\mathbb{R}^d)$.

Since A_{-t}^F is symmetric (resp. skew symmetric, resp. normal), it follows easily that \tilde{A}_{-t}^F is a symmetric (resp. skew symmetric, resp. normal) operator in $L^2(\mathbb{R}^d)$.

We also observe that

$$\tilde{\mathcal{V}}_t^* = D(e^{(t+(T/2))H}) \supset D(e^{tH}).$$

We can thus restrict, if we wish, \tilde{A}_{-t}^F to the t -independent dense domain

$$D(e^{tH}) \text{ of } L^2(\mathbb{R}^d), \quad \forall t \in I.$$

Now let $\varphi \in D(e^{tH})$ and consider $\tilde{A}_{-t}^F \varphi$. This is given by (4.1) with $\chi \equiv U_t^{-1} \varphi = e^{tH} \varphi$. Thus

$$\tilde{A}_{-t}^F \varphi = U_t A U_t^{-1} \varphi. \tag{4.2}$$

From our assumptions, this can also be written as

$$\tilde{A}_{-t}^F \varphi = e^{-tH} A e^{tH} \varphi. \tag{4.3}$$

Let $\varphi' \in D(H e^{(T/2)H})$ and consider

$$\langle \varphi' | \tilde{A}_{-t}^F \varphi \rangle_2 = \langle e^{-tH} \varphi' | A e^{tH} \varphi \rangle_2.$$

The r.h. side is differentiable with respect to t if $A e^{tH}$ is strongly differentiable with respect to t , which is the case e.g. if φ is in the dense domain $D(H e^{-tH})$ (as seen using the previous assumptions on A). The derivative is easily seen to be equal to

$$\begin{aligned} \frac{d}{dt} \langle \varphi' | \tilde{A}_{-t}^F \varphi \rangle_2 &= \langle -e^{-tH} H \varphi' | A e^{tH} \varphi \rangle_2 \\ &+ \langle e^{-tH} \varphi' | A H e^{tH} \varphi \rangle_2. \end{aligned} \tag{4.4}$$

Using $A e^{tH} D(e^{tH}) \subset D(H)$, the r.h. side can be written as

$$\langle e^{-tH} \varphi' | [A, H] e^{tH} \varphi \rangle_2, \tag{4.5}$$

where $[A, H]$ is the commutator $AH - HA$.

If $[A, H] e^{tH} \varphi \in D(e^{-tH})$, (4.5) is also

$$\langle \varphi' | U_t [A, H] U_t^{-1} \varphi \rangle_2, \tag{4.6}$$

hence, from (4.4),

$$\frac{d}{dt} \tilde{A}_{-t}^F = B_{-t}^F,$$

where $B_{-t}^F = U_t B U_t^{-1}$, and $B \equiv [A, H]$.

Hence we have proven the following

PROPOSITION 4.1. — *Let A be as in Theorem 3.1 and let A_{-t}^F be the corresponding operator in $\mathcal{V}_t^*(\mathbb{R}^d)$ given by $A_{-t}^F = U_t A U_t^{-1}$, $t \in I$. Assume $D(A) \supset D(e^{(T/2)H})$. We can look upon A_{-t}^F as an operator \tilde{A}_{-t}^F from the closed subset $\tilde{\mathcal{V}}_t^*$ in $L^2(\mathbb{R}^d)$ into \mathcal{V}_t^* .*

If $AD(e^{(T/2)H}) \subset D(e^{(T/2)H})$, the range of \tilde{A}_{-t}^F is contained in $\tilde{\mathcal{V}}_t^ \subset L^2(\mathbb{R}^d)$ and we can look upon \tilde{A}_{-t}^F as an operator acting in the fixed Hilbert space $L^2(\mathbb{R}^d)$, densely defined on a domain containing the dense t -independent domain $D(e^{TH}) \subset L^2(\mathbb{R}^d)$. Equation 4.3 holds for any $\varphi \in D(e^{TH})$. For $\varphi \in D(He^{TH})$, $\varphi' \in D(He^{(T/2)H})$, we have*

$$\frac{d}{dt} \langle \varphi' | \tilde{A}_{-t}^F \varphi \rangle_2 = \langle e^{-tH} \varphi' | [A, H] e^{tH} \varphi \rangle_2.$$

If $[A, H] e^{tH} \varphi \in D(e^{-tH})$, then

$$\frac{d}{dt} \tilde{A}_{-t}^F = [A, \tilde{H}]_{-t}^F,$$

on the dense domain $D(He^{TH})$ of $L^2(\mathbb{R}^d)$, where $[A, \tilde{H}]_{-t}^F$ is the restriction of $[A, H]_{-t}^F$ to $\tilde{\mathcal{V}}_t^*$.

Remarks.

(a) The formulae for $\frac{d}{dt} \tilde{A}_{-t}^F$ give the equations of motion for the observable \tilde{A}_{-t}^F . In fact, the equation of motion relates the observable A_{-t}^F , associated with A, with the observable $[A, H]_{-t}^F$, associated with $[A, H]$.

(b) The assumption $D(A) \supset D(e^{(T/2)H})$ is, of course, satisfied if A is bounded.

(c) $D(e^{(T/2)H})$ and $D(He^{TH})$, in the statement of Proposition 4.1, can be replaced by subsets D_1 of $D(e^{(T/2)H})$, resp. D_2 of $D(He^{TH})$, which are still dense in $L^2(\mathbb{R}^d)$. E. g. for $H = -\frac{1}{2}\Delta + V$, V smooth with bounded derivatives and A the observables position and momentum, discussed in Section 3, it is useful to take $D_1 = D_2$ as the linear space of Hermite functions (eigenfunctions of $-\frac{1}{2}\Delta + \frac{1}{2}x^2$). Then all assumptions are satisfied and the conclusions hold, yielding the equations of motion for these observables.

(d) Of course for $A = H$ the equation of motion is trivial: $\frac{d}{dt} \tilde{A}_{-t}^F = 0$.

(e) Using $[Q, H] = -P$ on a dense domain, as follows from Section 3, we get easily

$$\frac{d}{dt} \tilde{Q}_{-t}^F = -\tilde{P}_{-t}^F, \text{ i. e. } \frac{d}{dt} \tilde{Q}_t^F = \tilde{P}_t^F. \tag{4.7}$$

For this reason it is useful to look upon $\tilde{Q}_t^F, \tilde{P}_t^F$ as the Euclidean analogue of the Heisenberg operator corresponding in quantum mechanics to the position, and momentum observables.

More generally, we look upon \tilde{A}_t^F as the Euclidean analogue to the quantum mechanical Heisenberg operator giving the evolution, at time t , of the observable A . We call \tilde{A}_t^F the *Euclidean Heisenberg operator* associated with A . The Euclidean equation of motion is

$$\frac{d}{dt} \tilde{A}_t^F = [H, \tilde{A}_t^F]. \text{ Similarly as above, using, for } H = -\frac{1}{2} \Delta + V,$$

$$[P, H] = \nabla V,$$

which follows from Section 3, we get

$$\frac{d}{dt} \tilde{P}_t^F = \nabla \tilde{V}_t^F. \tag{4.8}$$

It is also natural to look upon (4.2), (4.8) as the Euclidean analogues of the (Heisenberg picture) Hamilton equation of motion in quantum mechanics.

We shall call \tilde{A}_t^F a constant of motion if A does not depend on t and $\frac{d}{dt} \tilde{A}_t^F = 0$. This, by the above, is equivalent with $[H, \tilde{A}_t^F] = 0$ and is implied by $[H, A] = 0$. An example is given by $A = [Q, P]$. Obviously, any bounded function of H is a constant of motion.

(f) In the case $d = 1, H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{\omega^2}{2} x^2, \omega$ a constant, we have

$$\left. \begin{aligned} \tilde{Q}_t^F &= Q \cos h \omega t + P \sin h \omega t \\ \tilde{P}_t^F &= Q \sin h \omega t + P \cos h \omega t \end{aligned} \right\} \tag{4.9}$$

with Q as the operator of multiplication by x and P is $-\frac{\partial}{\partial x}$.

5. REGULARITY CONDITIONS ON THE POTENTIAL

In this chapter, we give sufficient regularity conditions for our constructions, in particular in the perspective of the probabilistic interpretation summarized in Chapter 6.

First we remind of the definition of a class of potentials $V: \mathbb{R}^d \rightarrow \mathbb{R}$ introduced by Kato [8].

A real measurable potential $V: \mathbb{R}^d \rightarrow \mathbb{R}$ belongs to the Kato class K^d if

- (a) For $d=1$, $\sup_x \int_{|x-y| \leq 1} |V(y)| dy < \infty$
- (b) For $d=2$, $\lim_{\varepsilon \downarrow 0} \sup_x \int_{|x-y| \leq \varepsilon} |V(y)| \ln \frac{1}{|x-y|} dy = 0$ (5.1)
- (c) For $d \geq 3$, $\lim_{\varepsilon \downarrow 0} \sup_x \int_{|x-y| \leq \varepsilon} \frac{|V(y)|}{|x-y|^{d-2}} dy = 0$

The potential V belongs to the local Kato class K_{loc}^d if for any L , $V \chi_L$ is in the Kato class K^d , where χ_L is the characteristic function of the sphere of radius L centered at the origin. A natural condition, for a physical potential, is that $V_- \equiv \max(-V, 0)$ is in K^d , but $V_+ \equiv \max(V, 0)$ is only in K_{loc}^d . For example, if $d=3$, the harmonic oscillator potential $V(x) \equiv V_+(x) = \frac{1}{2}|x|^2$ is in K_{loc}^3 , and the Coulomb potential

$$V(x) \equiv V_-(x) = -\frac{1}{|x|} \text{ is in } K^3.$$

The definition (5.1) is the analytical translation of the following property, independent of the dimension, involving a Brownian process $X_x(t)$, starting at $x \in \mathbb{R}^d$ at time 0 and its associated conditional expectation denoted by $E_{0,x}$,

$$\lim_{t \downarrow 0} \sup_x E_{0,x} \int_0^t |V(X_x(s))| ds = 0. \quad (5.2)$$

The above class of potentials K^d has been used for several technical problems, e. g. [9].

THEOREM 5.1. — *If $V_- \in K^d$ and $V \in K_{loc}^d$, the semigroup $e^{-(t-s)H}$, for $H = -\frac{1}{2}\Delta + V$, is a well defined family of integral operators, for every $t \geq s$. The kernel $h(x, t-s, y)$ of $e^{-(t-s)H}$, $t \geq s$, is jointly continuous in x, y and $(t-s)$, and non-negative. Moreover, for any $\varepsilon > 0$,*

$$h(x, t-s, y) \leq C(\varepsilon, t-s) \exp \left\{ -\frac{(y-x)^2}{2(1+\varepsilon)(t-s)} \right\}$$

for some positive C ($\varepsilon, t-s$).

Proof. — Cf. [9].

Under additional assumptions, it is possible to show that $h > 0$. For example, this holds if H is such that e_0 is a simple eigenvalue (which is the case, e. g. when $V \in \mathcal{R} + (L^\infty)_\varepsilon$, where \mathcal{R} denotes the Rollnik class and $(L^\infty)_\varepsilon$ the L^∞ functions with norm less than ε , or when V_+ is bounded and such that the Lie-Trotter formula applies. A sufficient condition for the application of Lie-Trotter formula is $V \in L^2_{loc}$ outside a set of capacity zero.

The strict positivity of h can also be shown using Feynman-Kac formula when, e. g. V is continuous, lower bounded and such that $-\frac{1}{2}\Delta + V$ is essentially self-adjoint. Sufficient conditions for this are given in [9], for instance.

Remarks. — 1. The positivity of h , in addition to the conclusions of Th. 5.1, are satisfied if $V(x) = \frac{1}{2}|x|^2$ (harmonic oscillator) or, e. g. for

$d=3, V(x) = \frac{\alpha}{|x|}$ for a real constant (Coulomb potential).

2. Under general assumptions on V , one has that e^{-tH} maps $L^2(\mathbb{R}^d)$ into any $L^p(\mathbb{R}^d)$, $p \geq 2$, for $t > 0$. See, e. g. [5], [9]. Also, for V as in theorem 5.1, it is known that $e^{-tH} L^2(\mathbb{R}^d)$ consists of continuous functions for all $t \geq 0$.

Henceforth we call *Schrödinger class* the class of potentials V such that h has the properties of Theorem 5.1 and, in addition, is strictly positive. As observed in 1 it contains potentials of physical interest.

6. PROBABILISTIC INTERPRETATION

6.1. Bernstein processes

Let χ in $D(e^{(T/2)H}) \subset L^2(\mathbb{R}^d)$. (6.1)

By the construction given before, $\eta_x^* = e^{-tH}\chi$ and $\eta_x^- = e^{tH}\bar{\chi}$ are well defined for any t in I . Set

$$p_{-T/2}(x) \equiv (\eta_x^- \eta_x^*) \left(x, -\frac{T}{2} \right) \tag{6.2}$$

$$p_{T/2}(y) \equiv (\eta_y^- \eta_y^*) \left(y, \frac{T}{2} \right). \tag{6.3}$$

We observe that if $\|\chi\|_2 = 1$, then $\int p_{-T/2}(x) dx = \int p_{T/2}(x) dx = 1$ since, using (2.12),

$$\int_{\mathbb{R}^d} p_{\pm T/2}(x) dx = \left(\eta_x^* \left(\pm \frac{T}{2} \right) \middle| \eta_x^* \left(\pm \frac{T}{2} \right) \right)_{\pm T/2} = \|\chi\|_2^2.$$

We assume that h is as in Theorem 5.1, with V in the Schrödinger class.

Now let us denote by $h(s, x, t, y) \equiv h(x, t-s, y)$ the integral kernel of $e^{-(t-s)H}$, as an integral operator on $L^2(\mathbb{R}^d)$, like in Chapt. 5. For $-\frac{T}{2} < s < t < u < \frac{T}{2}$, x, ξ , and y in \mathbb{R}^d , and B any Borel set in \mathbb{R}^d , we define

$$H(s, x, t, B, u, y) \equiv \int_B h(s, x, t, \xi, u, y) d\xi \tag{6.4}$$

where the density with respect $d\xi$ is the positive function

$$h(s, x, t, \xi, u, y) \equiv \frac{h(s, x, t, \xi) h(t, \xi, u, y)}{h(s, x, u, y)}. \tag{6.5}$$

Notice that the kernel H should not be confused with the Hamiltonian H . The kernel H will be called a *Bernstein transition function*. (See [12].)

Let us introduce some probabilistics notions and notations. When Z is an integrable random variable on a probability space (Ω, σ, P) , $E[Z]$ denotes its expectation. If \mathcal{P} is a sub-sigma-algebra of σ , $E[Z | \mathcal{P}]$ denotes the conditional expectation of Z given \mathcal{P} , defined for $Z \geq 0$ or $Z \in L^1(P)$.

We shall consider stochastic processes indexed by $I = \left[-\frac{T}{2}, \frac{T}{2} \right]$, $Z(t) = Z_t$,

defined as functions from I to the set of random variables on the underlying probability space. \mathcal{P}_t , for t in I , will denote an increasing family of sigma-algebras such that each Z_t is \mathcal{P}_t -measurable and \mathcal{F}_t a decreasing family of sigma-algebras such that Z_t is \mathcal{F}_t -measurable. \mathcal{P}_t is interpreted as the past information about Z_t and \mathcal{F}_t the future information.

Under the above mentioned assumptions, one proves [10] easily the

LEMMA 6.1. – (a) For any x, y in \mathbb{R}^d , $-\frac{T}{2} < s < t < u < \frac{T}{2}$, the set function $B \rightarrow H(s, x, t, B, u, y)$ is a probability measure on the Borel sigma algebra of \mathbb{R}^d , $\mathcal{B}(\mathbb{R}^d)$.

(b) For any B in $\mathcal{B}(\mathbb{R}^d)$, $-\frac{T}{2} < s < t < u < \frac{T}{2}$, $(x, y) \mapsto H(s, x; t, B; u, y)$ is $\mathcal{B}(\mathbb{R}^d) \times \mathcal{B}(\mathbb{R}^d)$ -measurable

(c) For any couple B_1, B_2 in $\mathcal{B}(\mathbb{R}^d)$, $-\frac{T}{2} < s < t < u < \frac{T}{2}$,

$$\int_{B_2} H(s, w, t, B_1, u, y) H(s, w; u, dy, v, z) \\ = \int_{B_1} H(s, w, t, dx, v, z) H(t, x, u, B_2, v, z)$$

As a path space, a possible choice is $\Omega = \prod_{t \in I} \mathbb{R}^d$, compact in the product topology, with \mathbb{R}^d a compactification of \mathbb{R}^d . We denote by σ_I the Borel sigma algebra of Ω .

DEFINITION. — A stochastic process $Z_t: \Omega \rightarrow \mathbb{R}^d$ is a *Bernstein process* ([10]-[12]) if the following relation between conditional expectations holds for any bounded Borel measurable f and $-\frac{T}{2} < s < t < u < \frac{T}{2}$

$$E[f(Z_t) \mid \mathcal{F}_s \cup \mathcal{F}_u] = E[f(Z_t) \mid Z_s, Z_u]. \tag{6.6}$$

Then, we have the following

THEOREM 6.2. — Let $H(s, x, t, B, u, y)$ be a Bernstein transition function as before, for $-\frac{T}{2} < s < t < u < \frac{T}{2}$ and m a probability measure on

$\mathcal{B}(\mathbb{R}^d) \times \mathcal{B}(\mathbb{R}^d)$. Then there is a unique probability measure P_m such that with respect to (Ω, σ_I, P_m) , $Z_t, t \in I$, is a Bernstein process and

- (a) $P_m(Z_{-T/2} \in B_S, Z_{T/2} \in B_E) = m(B_S \times B_E)$, B_S and B_E in $\mathcal{B}(\mathbb{R}^d)$
- (b) $P_m(Z_t \in B \mid Z_s, Z_u) = H(s, Z_s, t, B, u, Z_u)$, for B in $\mathcal{B}(\mathbb{R}^d)$.
- (c) The finite dimensional distributions of Z_t are given by

$$P_m(Z_{-T/2} \in B_S, Z_{t_1} \in B_1, \dots, Z_{t_n} \in B_n, Z_{T/2} \in B_E) \\ = \int_{B_S \times B_E} dm(x, y) \int_{B_1} H\left(-\frac{T}{2}, x, t_1, dx_1, \frac{T}{2}, y\right) \dots \\ \times \int_{B_n} H\left(t_{n-1}, x_{n-1}, t_n, dx_n, \frac{T}{2}, y\right).$$

The proof of this Theorem can be found in [10] (and in the context of the present construction for quantum physics in [12]).

According to this result, a Bernstein transition function H and a joint probability measure m determine a Bernstein process $Z_t, t \in I$, in general not Markovian. It turns out that a particular choice of m characterizes a

Markovian Bernstein process:

THEOREM 6.3. — Let V be a potential in the Schrödinger class, $H(s, x, t, B, u, y)$ be a Bernstein transition function, and m be a probability measure on $\mathcal{B}(\mathbb{R}^d) \times \mathcal{B}(\mathbb{R}^d)$. If $Z_t, t \in I$, denotes the Bernstein process of Theorem 6.2, then $Z_t, t \in I$ is also a Markovian process iff $m \equiv M$ (M for Markovian) is of the form

$$M(B_S \times B_E) = \int_{B_S \times B_E} \mathcal{O}_{-T/2}^*(x) h(x, T, y) \mathcal{O}_{T/2}(y) dx dy, \\ B_S \text{ and } B_E \text{ in } \mathcal{B}(\mathbb{R}^d), \quad (6.7)$$

for $\mathcal{O}_{-T/2}^*$ and $\mathcal{O}_{T/2}$ two bounded real measurable functions having the same sign on \mathbb{R}^d .

Proof. — cf. [10] and [12].

We shall call the process Z_t of Th. 6.3 the Markovian Bernstein process. The main consequence of this Theorem is the following. After substitution of the particular joint density $m = M$ given by Eq. (6.7) in the general expression of the finite dimensional distribution for a Bernstein process $Z_t, t \in I$ [Th. 6.2(c)] we obtain, for $-\frac{T}{2} < t_1 < t_2 < \dots < t_n < \frac{T}{2}$,

$$P_M(dx_1, t_1, \dots, dx_n, t_n) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \mathcal{O}_{-T/2}^*(x) h\left(x, t_1 + \frac{T}{2}, dx_1\right) \dots \\ \times h\left(dx_n, \frac{T}{2} - t_n, y\right) \mathcal{O}_{T/2}(y) dx dy \quad (6.8)$$

where the notation $f(dx) = f(x) dx$ has been used.

Notice that the functions $\mathcal{O}_{-T/2}^*$ and $\mathcal{O}_{T/2}$ are not yet specified in the conclusion of the Theorem 6.3. By definition of the joint probability measure M , the marginals of M have to satisfy the following constraints:

$$\mathcal{O}_{-T/2}^*(x) \int_{\mathbb{R}^d} h(x, T, y) \mathcal{O}_{T/2}(y) dy = p_{-T/2}(x) \\ \mathcal{O}_{T/2}(y) \int_{\mathbb{R}^d} \mathcal{O}_{-T/2}^*(x) h(x, T, y) dx = p_{T/2}(y) \quad (6.9)$$

where $p_{-T/2}$ and $p_{T/2}$ are the boundary probability densities of the Markovian Bernstein process $Z_t, t \in I$.

If we assume that $p_{-T/2}$ and $p_{T/2}$ are given, and since the integral kernel h is known by hypothesis, Eq. (6.9) is clearly a (complicated) system of nonlinear functional equations for $\mathcal{O}_{-T/2}^*, \mathcal{O}_{T/2}$. Afterwards, (6.9) will be called *Schrödinger's system* (because it was initially formulated by Schrödinger for the one-dimensional free case, $V=0$, in 1932 [3]: Cf. § 8.1).

The following Theorem gives the conditions for the existence and uniqueness of positive solutions of Schrödinger's system (6.9).

THEOREM 6.4. — *Let $P_{-T/2}(dx)$ and $P_{T/2}(dy)$ be two probability measures on \mathbb{R}^d with strictly positive densities with respect to Lebesgue measure,*

$$P_{-T/2}(dx) = p_{-T/2}(x) dx \quad \text{and} \quad P_{T/2}(dy) = p_{T/2}(y) dy.$$

Let $h(x, T, y)$ be a bounded and strictly positive integral kernel on $\mathbb{R}^d \times \mathbb{R}^d$. Then positive (but not necessarily integrable) solutions $\{\theta^, \theta\}$ of Schrödinger's system (6.9) exist and are unique.*

Jamison gave a proof in [10] which is an adaptation and an extension of an abstract result of Beurling [13].

Remark. — What can happen if $p_{-T/2}$ or $p_{T/2}$ are not strictly positive is illustrated by the following one dimensional example:

Let H be the Hamiltonian on $L^2(\mathbb{R}, dx)$

$$H_{os} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2. \tag{6.10}$$

The (positive) integral kernel of $e^{-(t-s)H_0}$ is given explicitly by Mehler's formula. Let us denote it by $h_{0s}(x, t-s, y)$.

Let us consider Schrödinger's system (6.9) for h_{0s} , and the particular data

$$p_{-T/2}(x) = \left(\frac{2}{\pi^{1/2}}\right) x^2 e^{-x^2} = p_{T/2}(x). \tag{6.11}$$

Then it is easy to check that

$$\theta_{-T/2}^*(x) = \left(\frac{2}{\pi^{1/2}}\right)^{1/2} x e^{-x^2/2} e^{(3/2)T} \tag{6.12}$$

and

$$\theta_{T/2}(y) = \left(\frac{2}{\pi^{1/2}}\right)^{1/2} y e^{-y^2/2} e^{(3/2)T}$$

are solutions of the system. Nevertheless, they are not positive. This is due to the fact that the choice of data (6.11) violates the hypothesis of Theorem 6.4: $p_{-T/2} (\equiv p_{T/2})$ has a zero at the origin $x=0$. This case is, however, relevant for our physical application. See § 6.5 and [12].

6.2. The Markovian Bernstein process

THEOREM 6.5. — *Let $H = -\frac{1}{2} \Delta + V$, with V in the Schrödinger class and let $h(x, t-s, y)$ be the kernel of $e^{-(t-s)H}$, $t \geq s$.*

For any pair (χ, χ') with $\chi = e^{-(T/2)H} \varphi$, $\chi' = e^{(T/2)H} \varphi'$, and φ, φ' strictly positive functions in $L^2(\mathbb{R}^d)$, there exists an unique Markovian Bernstein process $Z_t, t \in I \equiv [-\frac{T}{2}, \frac{T}{2}]$, corresponding to the data

$$P_{-(T/2)}(x) = (\eta_{\chi'} \eta_{\chi}^*) \left(x, -\frac{T}{2} \right), \tag{6.13}$$

$$P_{T/2}(y) = (\eta_{\chi'} \eta_{\chi}^*) \left(y, \frac{T}{2} \right). \tag{6.14}$$

Z_t will be called the Markovian Bernstein process associated with the pair χ, χ' . The finite dimensional distributions of the process are given by

$$P_M(dx_1, t_1, \dots, dx_n, t_n) = \int_{\mathbb{R}^d \times \mathbb{R}^d} (e^{(T/2)H} \chi)(x) h \left(x, t_1 + \frac{T}{2}, dx_1 \right) \dots \times h \left(dx_n, \frac{T}{2} - t_n, y \right) (e^{(T/2)H} \chi')(y) dx dy \tag{6.15}$$

for $-\frac{T}{2} < t_1 < t_2 < \dots < t_n < \frac{T}{2}$.

The proof of this Theorem is given in [12].

Remarks. – (a) The statements hold in particular for $\varphi = \varphi'$ i. e. $\chi = \chi'$. In this case we have that $(e^{(T/2)H} \chi)(x) = \eta_{\chi}^* \left(x, -\frac{T}{2} \right)$, and

$$(e^{(T/2)H} \chi')(x) = \eta_{\chi'} \left(x, \frac{T}{2} \right)$$

coincide, i. e. (6.15) is expressed by h and the initial and final solutions $\eta_{\chi}^* \left(x, -\frac{T}{2} \right), \eta_{\chi'} \left(x, \frac{T}{2} \right)$ of Schrödinger's system (6.9) for the data (6.2), (6.3).

(b) The probabilistic meaning of (6.15) imposes $\chi, \chi' > 0$. In general, even for complex χ , the data (6.2), (6.3) satisfy the conditions of Theorem 6.4 and $\eta_{\chi}^* \left(x, -\frac{T}{2} \right), \eta_{\bar{\chi}} \left(y, \frac{T}{2} \right)$ are solutions of the Schrödinger system (6.9) with data (6.2), (6.3). For χ not real, these solutions are not real.

Now we are going to describe explicitly the unique Markovian Bernstein process of Th. 6.5.

Using (6.14) and the strict positivity of $\eta_x^*(x, s)$, let us define, for B in $\mathcal{B}(\mathbb{R}^d)$, $-\frac{T}{2} \leq s \leq t \leq \frac{T}{2}$

$$Q^*(s, B, t, y) = \frac{1}{\eta_x^*(y, t)} \int_B \eta_x^*(x, s) h(x, t-s, y) dx \quad (6.16)$$

and the associated density

$$q^*(s, x, t, y) = \frac{\eta_x^*(x, s)}{\eta_x^*(y, t)} h(x, t-s, y). \quad (6.16')$$

LEMMA 6.6. — $Q^*(s, B, t, y)$, for B in $\mathcal{B}(\mathbb{R}^d)$, $-\frac{T}{2} \leq s \leq t \leq \frac{T}{2}$, is the backward transition probability of a Markov process, with density $q^*(s, x, t, y)$.

Proof. — This is a straightforward verification. The positivity of q^* is obvious since $\chi = e^{-(T/2)H} \varphi$, $\varphi > 0$ and h is strictly positive. Also $Q^*(s, \cdot, t, y)$ is a probability, and $Q^*(s, B, t, \cdot)$ is $\mathcal{B}(\mathbb{R}^d)$ -measurable. The Chapman-Kolmogorov equation for Q^* follows from the semigroup property of h . Cf. [12]. \square

LEMMA 6.7. — The finite-dimensional distributions (6.15) of the Markovian Bernstein process $Z_t, t \in I$, can also be written as

$$P_M(dx_1, t_1, \dots, dx_n, t_n) = \int_{\mathbb{R}^d} Q^*(t_1, dx_1, t_2, x_2) Q^*(t_2, dx_2, t_3, x_3) \dots \times Q^*\left(t_n, dx_n, \frac{T}{2}, y\right) p\left(y, \frac{T}{2}\right) dy \quad (6.15')$$

for the final distribution probability

$$p_{T/2}(y) dy \equiv p\left(y, \frac{T}{2}\right) dy \equiv \eta_x^*\left(y, \frac{T}{2}\right) \eta_{x'}\left(y, \frac{T}{2}\right) dy.$$

Proof. — The substitution of (6.16) into (6.15') gives (6.15). \square

LEMMA 6.8. — The probability density of the Markovian Bernstein process $Z_t, t \in I$, reduces to

$$P_M(dx, t) \equiv p(dx, t) = \eta_x^*(x, t) \eta_{x'}(x, t) dx. \quad (6.17)$$

Proof. — This is (6.15) for $n=1$. \square

From lemma 6.7 we observe that the Bernstein process of Th. 6.5 can be regarded as a (backward) Markov process. It follows that a very explicit

description of Z_t is possible:

PROPOSITION 6.9. — *Let V be as in Th. 6.5 and, in addition, smooth. Let $\chi = e^{-(T/2)H} \varphi$, $\varphi > 0$ in $L^2(\mathbb{R}^d)$, then $\eta_x^*(x, t)$ is smooth. The Markovian Bernstein process Z_t , t in I , of Th. 6.5 is an \mathbb{R}^d -valued diffusion process whose (backward) drift and diffusion coefficients are given respectively by*

$$B_*(y, t) \equiv \lim_{\Delta t \downarrow 0} \frac{1}{\Delta t} \int_{S_\varepsilon(y)} (y-x) q^*(t-\Delta t, x, t, y) dx = -\frac{\nabla \eta_x^*}{\eta_x^*}(y, t) \quad (6.18)$$

$$C_*(y, t) \equiv \lim_{\Delta t \downarrow 0} \frac{1}{\Delta t} \int_{S_\varepsilon(y)} (y-x)^2 q^*(t-\Delta t, x, t, y) dx = I \quad (6.19)$$

where $S_\varepsilon(y)$ is the sphere of centre y and radius ε , and I is the $d \times d$ identity matrix. Notice that for $d > 1$, the term $(y-x)^2$ in the definition of the diffusion coefficient means $(y-x) \otimes (y-x)$.

Idea of proof. — The conclusion is a straightforward consequence of the fact that, for the class of potentials V considered in Chapter 5, the integral kernel $h(s, x, t, y)$ of $e^{-(t-s)H}$ also satisfies

$$(\alpha) \quad \lim_{\Delta t \downarrow 0} \int_{S_\varepsilon(y)} h(t-\Delta t, x, t, y) dx = 1$$

$$(\beta) \quad \lim_{\Delta t \downarrow 0} \frac{1}{\Delta t} \int_{S_\varepsilon(y)} (y-x) h(t-\Delta t, x, t, y) dx = 0$$

$$(\varphi) \quad \lim_{\Delta t \downarrow 0} \frac{1}{\Delta t} \int_{S_\varepsilon(y)} |y-x|^2 h(t-\Delta t, x, t, y) dx = I$$

and, moreover,

(δ) There is an $\delta > 0$ such that

$$\int_{S_\varepsilon(y)} |y-x|^{2+\delta} h(t-\Delta t, x, t, y) dx = o(\Delta t).$$

The properties (α)-(δ) are most easily derived from the integral equation solved by the kernel $h(s, x, t, y)$, *i.e.* by following Kac's original method [2].

Remark. — The smoothness condition on V can be relaxed when (6.18-19) are interpreted in the distributional sense.

The striking particularity of any Bernstein process is its time symmetry, displayed in (6.6). To analyze this aspect for the Markovian Bernstein process Z_t of Theorem 6.5, we introduce the

DEFINITION. — Let $Z_t = Z(t)$, $t \in I$ be a Markovian Bernstein process defined according to Theorem 6.5. Then, the time reversed process of Z_t is defined by $\hat{Z}(t) = Z(-t)$.

PROPOSITION 6.10. — *The time reversal $\hat{Z}(t)$ of the Markovian Bernstein process of Prop. 6.9, t in I , is a Bernstein diffusion process with values in \mathbb{R}^d and same diffusion coefficient as $Z(t)$. The (backward) drift of $\hat{Z}(t)$ is such that*

$$\hat{B}_*(\hat{Z}(t), t) = -B(Z(-t), -t) \tag{6.20}$$

where

$$B(x, s) \equiv \frac{\nabla \eta_{x'}}{\eta_{x'}}(x, s). \tag{6.21}$$

Moreover, if P is the probability of $Z(t)$ and \hat{P} the probability of $\hat{Z}(t)$, we have

$$P(Z(-t) \in dx) = \hat{P}(\hat{Z}(t) \in dx)$$

or equivalently, if p and \hat{p} are the respective probability densities,

$$p(x, -t) dx = \hat{p}(x, t) dx$$

Proof. — One starts from the permuted boundary probabilities [(6.13)-(6.14)], namely

$$\left. \begin{aligned} \hat{p}_{-T/2}(x) &= p_{T/2}(x) \\ \hat{p}_{T/2}(y) &= p_{-T/2}(y) \end{aligned} \right\} \tag{6.22}$$

Since the pair $\eta_x^* \left(x, -\frac{T}{2}\right) = (e^{(T/2)H} \chi)(x)$ and $\eta_{x'} \left(y, \frac{T}{2}\right) = (e^{(T/2)H} \chi')(y)$ of (6.13) is solution of the associated Schrödinger system (6.9) it is clear that the pair

$$\hat{\eta}_x^* \left(x, -\frac{T}{2}\right) = (e^{(T/2)H} \chi')(x) \quad \text{and} \quad \hat{\eta}_x \left(y, \frac{T}{2}\right) \equiv (e^{(T/2)H} \chi)(y)$$

is solution of the Schrödinger system with permuted data (6.22). This means that for any time t in I , we have

$$\left. \begin{aligned} \hat{\eta}_x^*(x, t) &= \eta_{x'}(x, -t) \\ \hat{\eta}_x(x, t) &= \eta_x^*(x, -t) \end{aligned} \right\} \tag{6.23}$$

Therefore

$$\hat{p}(x, t) = \hat{\eta}_x^* \hat{\eta}_x(x, t) = p(x, -t). \tag{6.24}$$

Moreover, using (6.18) and (6.23),

$$\hat{B}_*(x, t) = \frac{-\nabla \hat{\eta}_x^*}{\hat{\eta}_x^*}(x, t) = -\frac{\nabla \eta_{x'}}{\eta_{x'}}(x, -t). \tag{6.25}$$

So if we define

$$B(x, t) = \frac{\nabla \eta_{x'}}{\eta_{x'}}(x, t) \tag{6.26}$$

the relation (6.25) reduces indeed to

$$\hat{B}_*(x, t) = -B(x, -t) \quad (6.25')$$

i. e., in terms of the Markovian Bernstein processes,

$$\hat{B}_*(\hat{Z}(t), t) = -B(Z(-t), -t). \quad \square \quad (6.25'')$$

It is clear from Eqns. (6.23) that $\mathcal{V}_{-t}(\mathbb{R}^d)$ plays the same role for $\hat{Z}(t)$ as $\mathcal{V}_t^*(\mathbb{R}^d)$ plays for $Z(t)$. A very convenient interpretation of the backward drift is suggested by the following definition of the mean backward derivative

$$D_* Z(t) = \lim_{\Delta t \downarrow 0} E \left[\frac{Z(t) - Z(t - \Delta t)}{\Delta t} \middle| \mathcal{F}_t \right]. \quad (6.27)$$

Using the Markovian property of $Z(t)$, it is easy to verify that

$$D_* Z(t) = B_*(Z(t), t). \quad (6.28)$$

Clearly, $-\hat{B}_*(\hat{Z}(t), t)$ is the mean derivative of $\hat{Z}(t)$ in the other sense of the time. According to (6.25''), we can interpret $B(Z(t), t)$ as the mean derivative of $Z(t)$ in the usual (forward) sense of time, but with a conditioning with respect to the past \mathcal{P}_t , denoted by

$$\begin{aligned} DZ(t) &= \lim_{\Delta t \downarrow 0} E \left[\frac{Z(t + \Delta t) - Z(t)}{\Delta t} \middle| \mathcal{P}_t \right] \\ &= B(Z(t), t) \end{aligned} \quad (6.29)$$

6.3. Probabilistic interpretation of observables

Let us consider first the position operator Q_{-t} in $\mathcal{V}_t^*(\mathbb{R}^d)$ defined by (3.7). Assume $H = -\frac{1}{2}\Delta + V$, with V smooth with bounded derivatives so that we are in the conditions of the remark (c) after Prop. 4.1. The Euclidean Heisenberg operator \tilde{Q}_t^F associated with Q_{-t} satisfies

$$\tilde{Q}_t^F \chi = e^{tH} Q e^{-tH} \chi,$$

for any χ in the linear span D of products of Hermite functions (eigenfunctions of $-\frac{1}{2}\Delta + \frac{1}{2}x^2$). Let us consider for $\chi, \chi' \in D$.

$$\chi, \chi' > 0: \quad \langle \chi' | \tilde{Q}_t^F \chi \rangle_2 = (\eta_{\chi'}^*(t) | U_t \tilde{Q}_t^F U_{-t} \eta_{\chi}^*(t))_t \quad (6.30)$$

[where we used (2.12)].

The left-hand side of (6.30) is equal to

$$\begin{aligned} \langle \chi' \mid e^{tH} Q e^{-tH} \chi \rangle_2 &= \langle \eta_{\chi'}(t) \mid Q \eta_{\chi}^*(t) \rangle_2 \\ &= \int \eta_{\chi'}(x, t) \eta_{\chi}^*(x, t) x \, dx, \end{aligned} \tag{6.31}$$

which, by Lemma 6.8, can be written as

$$\int x P_M(dx, t) = E[Z(t)], \tag{6.31}$$

according to the definition of the Markovian Bernstein process $Z(t)$. Hence we have proven the

LEMMA 6.11. — *Let H be as in Theorem 6.5, with V with bounded derivatives (of all orders). Then for any strictly positive χ', χ in a dense subset D of $L^2(\mathbb{R}^d)$ we have*

$$(\eta_{\chi'}^*(t) \mid U_t \tilde{Q}_t^F U_{-t} \eta_{\chi}^*(t))_t = \langle \chi' \mid \tilde{Q}_t^F \chi \rangle_2 = E[Z(t)],$$

with \tilde{Q}_t^F the Euclidean Heisenberg position operator in $L^2(\mathbb{R}^d)$ (associated with the position operator Q_{-t} in $\mathcal{V}_t^*(\mathbb{R}^d)$). $Z(t)$ is the Markovian Bernstein process of Theor. 6.5 (associated with the pair χ, χ'). \square

Remark. — Notice that

$$\hat{E}[\hat{Z}(-t)] = E[Z(t)], \tag{6.30}$$

if we denote by \hat{E} the (absolute) expectation with respect to the measure \hat{P} . The relation (6.30) is the probabilistic counterpart of the fact that the position operator Q_t is even under time reversal (Cf. §3.4). Indeed, more generally we have the

PROPOSITION 6.12. — *Let H, χ', χ be as in Lemma 6.11. Let A be a densely defined operator in $L^2(\mathbb{R}^d)$ and let \tilde{A}_t^F be the Euclidean Heisenberg operator associated to it as in Prop. 4.1. We assume that there are Borel functions a, \hat{a} on $\mathbb{R}^d \times I$ such that*

$$(\eta_{\chi'}^*(t) \mid U_t \tilde{A}_t^F U_{-t} \eta_{\chi}^*(t))_t = E[a(Z(t), t)] \tag{6.31}$$

and

$$(\hat{\eta}_{\chi'}^*(-t) \mid U_t \tilde{A}_t^F U_{-t} \hat{\eta}_{\chi}^*(-t))_{-t} = E[\hat{a}(\hat{Z}(-t), -t)]. \tag{6.32}$$

Then, if A is even (odd) under time reversal (in the sense of Section 3) we have $E[a(Z(t), t)] = (\pm) \hat{E}[\hat{a}(\hat{Z}(-t), -t)]$.

Proof. — Since $\hat{\eta}_{\chi'}^*(-t) = \eta_{\chi'}(t)$ by (6.23), this relation between expectations is the analytical definition of paragraph 3.4 for the parity under time reversal. \square

Remark. — For any t in I , the condition $\eta_x^*(t)$ is in $\mathcal{D}(Q_{-t})$, the domain of Q_{-t} , in $\mathcal{V}_t^*(\mathbb{R}^d)$, means

$$0 < \int_{\mathbb{R}^d} x^2 \eta_{x'}(x, t) \eta_x^*(x, t) dx < \infty \quad (6.33)$$

or equivalently, since $\hat{Z}(-t) = Z(t)$,

$$0 < E[Z^2(t)] \equiv E[\hat{Z}(-t)Z(t)] < \infty. \quad (6.34)$$

Entirely similar formulae hold for forward operators replaced by backward ones.

For the momentum operator P in $\mathcal{V}_t^*(\mathbb{R}^d)$ we have

$$\begin{aligned} \langle P_t^F \rangle &\equiv (\eta_x^*(t) | U_t \hat{P}_t^F U_{-t} \eta_x^*(t))_t = \langle \chi' | \hat{P}_t^F \chi \rangle_2 = - \langle \chi' | e^{tH} \nabla e^{-tH} \chi \rangle_2 \\ &= - \int_{\mathbb{R}^d} \eta_{x'} \nabla \eta_x^*(x, t) dx \\ &= - \int_{\mathbb{R}^d} \frac{\nabla \eta_x^*}{\eta_x^*}(x, t) \eta_x^*(x, t) \eta_{x'}(x, t) dx \\ &= \int_{\mathbb{R}^d} B_*(x, t) p(x, t) dx \\ &= E[B_*(Z(t), t)] \end{aligned} \quad (6.35)$$

where the lemma 6.8 and the proposition 6.9 have been used. Notice that according to Th. 3.1, the values of (6.35) could be regarded as purely imaginary. Up to the sign, the definition (3.18) of the momentum P^B in $\mathcal{V}_t(\mathbb{R}^d)$ is the same and we obtain, with (6.21),

$$\langle P_t^B \rangle = E[B(Z(t), t)]. \quad (6.36)$$

The momentum operator \mathbb{P} on $\mathcal{H}_t(\mathbb{R}^d)$ satisfies

$$(f_x | \mathbb{P} f_x)_t = E \left[\frac{1}{2} (B(Z(t), t) + B_*(Z(t), t)) \right]. \quad (6.37)$$

It is convenient to give a name to the integrand on the right hand side:

DEFINITION. — We call

$$\bar{v}(x, t) \equiv \frac{1}{2} (B(x, t) + B_*(x, t)) \quad (6.38)$$

the current velocity of the Markovian Bernstein process Z_t . From (6.37) and (6.38) we also have

$$(f_x | \mathbb{P} f_x)_t = E[\bar{v}(Z(t), t)].$$

It is also immediate to check that

$$\hat{E}[\bar{v}(\hat{Z}(-t), -t)] = -E[\bar{v}(Z(t), t)]. \quad (6.39)$$

By lemma 6.11, this expresses the fact that the momentum operator is odd under time reversal.

Remark. — For any t in I , the condition that $\eta_x^*(t)$ is in $\mathcal{D}(P_t^F)$, the domain of P_t^F in $\mathcal{V}_t^*(\mathbb{R}^d)$, means

$$0 < \int \nabla \eta_{x'} \nabla \eta_x^*(x, t) dx < \infty$$

i. e., using (6.18), (6.20) and (6.21),

$$0 < \int \frac{\nabla \eta_{x'}}{\eta_{x'}} \frac{\nabla \eta_x^*}{\eta_x^*}(x, t) \eta_{x'} \eta_x^*(x, t) dx < \infty$$

$$0 < -E[B(Z(t), t) B_*(Z(t), t)]$$

$$\equiv E[\hat{B}_*(\hat{Z}(-t), -t) B_*(Z(t), t)] < \infty. \tag{6.40}$$

At last, for the Hamiltonian operator \hat{H}_t^F in $\mathcal{V}_t^*(\mathbb{R}^d)$, we have

$$\begin{aligned} \langle \hat{H}_t^F \rangle &= (e^{-tH} \chi' | U_t H_t U_t^{-1} e^{-tH} \chi)_t = \langle \chi' | e^{tH} H e^{-tH} \chi \rangle_2 \\ &= \int_{\mathbb{R}^d} \eta_{x'} \left(-\frac{1}{2} \Delta + V \right) \eta_x^*(x, t) dx \\ &= \int_{\mathbb{R}^d} \left(\frac{1}{2} \nabla \eta_{x'} \nabla \eta_x^* + V \eta_{x'} \eta_x^* \right) (x, t) dx \tag{6.41} \\ &= \int_{\mathbb{R}^d} \left(-\frac{1}{2} \mathbf{B} \mathbf{B}_* + V \right) (x, t) p(x, t) dx \\ &= E \left[-\frac{1}{2} \mathbf{B} \mathbf{B}_*(Z(t), t) + V(Z(t)) \right] \end{aligned}$$

where an integration by parts and the definitions of \mathbf{B} , \mathbf{B}_* have been used. In particular, of course, this expectation $\langle \hat{H}_t^F \rangle$ is time independent. Since the definition of \hat{H}_t^B in $\mathcal{V}_t(\mathbb{R}^d)$ is similar, it is clear that we also have

$$(f_x | \mathbb{H} f_x)_t = E \left[-\frac{1}{2} \mathbf{B} \mathbf{B}_*(Z(t), t) + V(Z(t)) \right]. \tag{6.42}$$

6.4. Probabilistic interpretation of the dynamics

Let A as in Prop. 4.1 and χ as in Section 6.3. We have

$$(\eta_x^*(t) | U_t \tilde{A}_t^F U_{-t} \eta_x^*(t))_t = \langle \chi | A_H(t) \chi \rangle_2 \equiv \langle A_H(t) \rangle_x \tag{6.43}$$

with $A_H(t) \chi \equiv e^{tH} A e^{-tH} \chi$, the Euclidean Heisenberg operator associated with A .

According to Prop. 4.1, the evolution, for t in I , is given by the expectation of the (Euclidean) Heisenberg equation of motion (in the sense of quadratic forms),

$$-\frac{d}{dt} \langle A_H(t) \rangle_x = \langle [A_H(t), H] \rangle_x. \quad (6.44)$$

The most interesting case, for us, is the one of the Hamiltonian operator H of the form $-\frac{1}{2} \Delta + V$, $V \in C^1(\mathbb{R}^d)$, and $A = Q$, respectively $A = P$.

Using $[Q, H] = -P$, $[P, H] = -\nabla V$, which follows from Chapter 3, we get

$$\frac{d}{dt} \langle Q_H(t) \rangle_x = \langle P_H(t) \rangle_x \quad (6.45)$$

$$\frac{d}{dt} \langle P_H(t) \rangle_x = \langle \nabla V(Q_H(t)) \rangle_x. \quad (6.46)$$

We interpret these equations as the Euclidean version of Ehrenfest theorem. Moreover,

$$\frac{d^2}{dt^2} \langle Q_H(t) \rangle_x = \langle \nabla V(Q_H(t)) \rangle_x \quad (6.47)$$

suggesting the existence of some probabilistic version of Newton equation for the underlying Bernstein process $Z(t)$. This is indeed the case:

PROPOSITION 6.14. — *Under the above mentioned regularity conditions on V , the Markovian Bernstein process $Z(t)$ of the proposition 6.9 satisfies, for t in I , the stochastic Newton equation*

$$D_* D_* Z(t) = \nabla V(Z(t)). \quad (6.48)$$

Proof. — Cf. [12, 33].

Remark. — By definition of the mean backward derivative

$$D_* f(Z(t), t) = \lim_{\Delta t \downarrow 0} E \left[\frac{f(Z(t), t) - f(Z(t - \Delta t), t - \Delta t)}{\Delta t} \middle| \mathcal{F}_t \right] \quad (6.49)$$

for any f in $C_0^\infty(\mathbb{R}^d \times \mathbb{R})$, when the trajectories of the process are smooth (i. e. when its diffusion constant is zero), the l.h.s. of (6.48) reduces to an ordinary second derivative. Hence (6.48) reduces to Newton's law of motion of classical mechanics, with V replaced by $-V$, as expected since this theory is Euclidean.

Let us recall that the Lagrangian of classical (Euclidean) mechanics corresponding to the elementary Euclidean Newton equation with scalar potential V in $C^1(\mathbb{R}^d)$,

$$\frac{d^2}{dt^2} q(t) = \nabla V(q(t)) \tag{6.50}$$

is the $\mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ function

$$L(\dot{q}, q) = \frac{1}{2} |\dot{q}|^2 + V(q). \tag{6.51}$$

In [12] it is shown that the Markovian Bernstein process $Z(t)$ solution of the stochastic Newton equation (6.48) minimizes the (finite) regularized action functional

$$J[Z(\cdot)] = E_t \left[\int_{-T/2}^t L(D_* Z(s), Z(s)) ds \right] + E_t A^* \left(Z\left(-\frac{T}{2}\right), -\frac{T}{2} \right) \tag{6.52}$$

with $A^*(z, s) = -\log \eta_x^*(z, s)$, $s \in I$.

(Here $E_t \equiv E[\cdot | \mathcal{F}_t]$ on a one-parameter family of diffusion processes Z^e such as

$$D_* Z^e \left(-\frac{T}{2} \right) = \nabla A^* \left(Z^e \left(-\frac{T}{2} \right), -\frac{T}{2} \right) \quad \text{and} \quad Z^e(t) = x.$$

The initial gradient condition, in this result, is preserved during the evolution, as follows from the equality

$$B_*(Z(s), s) = \nabla A^*(Z(s), s) = -\nabla \log \eta_x^*(Z(s), s), \quad s \in I.$$

In [12] the following path integral representation of η_x^* is given (together with a corresponding one for $\eta_x(x, t)$). Under the conditions of validity

of (6.52), for $-\frac{T}{2} \leq s \leq t \leq \frac{T}{2}$,

$$\eta_x^*(x, t) = \exp - \left\{ E_t \int_{-T/2}^t L(D_* Z(s), Z(s)) ds + E_t A^* \left(Z\left(-\frac{T}{2}\right), -\frac{T}{2} \right) \right\}. \tag{6.53}$$

Remark. — The idea of the stochastic calculus of variation sketched here is due to one of us, in another context [14].

Let us also notice that both the stochastic Newton equation (6.48) and the action functional (6.52) are not time symmetric, as they use only the decreasing filtration \mathcal{F}_t . But one shows easily that their time reversed versions also hold, restoring in this way the time symmetry of the theory. A direct (probabilistic) discussion of (6.48) is certainly possible, because

of its simplicity. It would provide an appealing approach of (Euclidean) quantum dynamics, independent of the data of a solution of the (Euclidean) Schrödinger equation. The variational principle associated with (6.52) should play a natural role in such an approach.

6.5. Time invariant states

Let us assume, for simplicity, $d = 1$. Suppose that the starting continuous potential V is such that H has a lowest energy eigenvalue E_0 with strictly positive eigenfunction φ_0 and has a further eigenvalue $E > E_0$ [for the former, it is sufficient, e. g., that V is positive, in L^p , $\forall p < \infty$, or $V \geq 0$, $V \in L^2_{loc}$ with $\lim_{x \rightarrow \infty} V(x) = \infty$], and consider

$$\psi(x, \tau) = e^{-i\tau E} \varphi(x), \tag{6.54}$$

for φ an eigenfunction of H in $L^2(\mathbb{R})$, which we may assume to be real.

By orthogonality of the eigenfunctions for different eigenvalues, φ necessarily changes its sign on the real line, at some points Z_α , called zeros of $\varphi(x)$. We denote by $\tilde{\varphi}$ the truncated function

$$\tilde{\varphi}(x) = \varphi(x) \chi_\Lambda(x) \tag{6.55}$$

for Λ any one of the two possible kinds of intervals on the line, $\Lambda_a =]Z_a, \infty[$ (or $] -\infty, Z_a[$) or $\Lambda_{bc} =]Z_b, Z_c[$, with Z_b, Z_c two successive zeros. It is clear that the whole line can be decomposed in such domains Λ . In Ref. [12], it is shown that for the natural choice of boundary positive (invariant) probability densities on such an interval Λ ,

$$p_{-T/2}(x) = p_{T/2}(x) = \frac{|\tilde{\varphi}|^2(x)}{\int_\Lambda |\tilde{\varphi}|^2(\xi) d\xi} \tag{6.56}$$

and for the relevant integral kernel of e^{-tH} , $h_\Lambda(x, t, y)$, whose domain takes care of the different boundary conditions associated with each interval Λ for the fixed pair of data (6.56), one can construct a unique homogeneous Bernstein diffusion process with drift

$$B_*(x) = -\frac{\nabla \eta_{\tilde{\varphi}}^*(x, t)}{\eta_{\tilde{\varphi}}^*(x, t)} = -\frac{\nabla \tilde{\varphi}}{\tilde{\varphi}}(x) \tag{6.57}$$

with

$$\eta_{\tilde{\varphi}}^*(x, t) = e^{-tE} \tilde{\varphi}(x). \tag{6.58}$$

The only possible singularities of the drift B_* are on the boundaries of Λ . In probabilistic terms, the left boundary of $\Lambda_a =]Z_a, \infty[$ is an entrance boundary, the right one a natural boundary. For Λ_b , both boundaries are entrance. We can also observe that, on some intervals Λ , $\eta_{\tilde{\varphi}}^*(t)$ are in $S_+^*(t)$ since $\tilde{\varphi}$ are negative.

In this way, a unique Markovian Bernstein process $Z(t)$ is indeed constructed on the line, but its probability transition is different on each connected domain Λ between the nodes of φ . Cf. also [15].

7. COMPARISON WITH QUANTUM MECHANICS

Let us discuss the quantum mechanical analogue of the structure developed in Chapter 2. In quantum mechanics [16], the central dynamical object is the evolution group

$$U_\tau = e^{-i\tau H}: L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d). \tag{7.1}$$

This defines a unitary isomorphism, in other words a one-parameter group of unitary operators on $L^2(\mathbb{R}^d)$. If $\psi_\chi(\tau) = e^{-i\tau H}\chi$, we have

$$\langle \psi_{\chi_1}(\tau) | \psi_{\chi_2}(\tau) \rangle_2 = \langle U_\tau^{-1} \psi_{\chi_1}(\tau) | U_\tau^{-1} \psi_{\chi_2}(\tau) \rangle_2 = \langle \chi_1 | \chi_2 \rangle_2. \tag{7.2}$$

Since the analytical vectors for H are dense in $L^2(\mathbb{R}^d)$ and $e^{-i\tau H}[L^2(\mathbb{R}^d)]$ is all of $L^2(\mathbb{R}^d)$, for any real time τ , the analog of the crucial condition $\chi \in \mathcal{D}(e^{(T/2)H})$ in the definition of $\mathcal{V}_T^*(\mathbb{R}^d)$ and of its completion $\mathcal{V}_T^*(\mathbb{R}^d)$, is not a restriction anymore since $\mathcal{D}(e^{i(T/2)H}) = L^2(\mathbb{R}^d)$. Let us assume

$H = -\frac{1}{2}\Delta + V$, and V smooth with bounded derivatives. Then the condition that χ in $L^2(\mathbb{R}^d)$ be an analytic vector for the (self-adjoint) operator H means simply that $\psi_\chi(\tau)$ is the restriction to the real axis of a function analytic in a strip of width T .

The same argument is obviously valid for the backward Hilbert space, so in particular for any real τ ,

$$\mathcal{V}_\tau(\mathbb{R}^d) = \mathcal{V}_\tau^*(\mathbb{R}^d) = L^2(\mathbb{R}^d). \tag{7.3}$$

Since the two Hilbert spaces coincide, there is no need for a direct sum \mathcal{H}_τ like in (2.15). This basic difference explains why the underlying diffusion process in "imaginary time", $Z(t)$, is only defined on bounded intervals I , in general (in contrast, for example, with stochastic mechanics, § 8.5). If we start from any $\chi \in L^2(\mathbb{R}^d)$, it is clear that after analytical continuation in the time parameter, χ cannot be in $\mathcal{D}(e^{(T/2)H})$ for arbitrary T , and that the largest possible T depends on the chosen χ . For

example, if $d=1$, $H \equiv H_0 = -\frac{1}{2} \frac{d^2}{dx^2}$, and

$$\chi = (\pi a)^{-1/4} \exp \left\{ -\frac{x^2}{2a} + iv_0 x \right\},$$

the resulting Markovian Bernstein process $Z(t)$ is Gaussian with mean $V_0 t$ (where $V_0 = -iv_0$) and variance $\frac{a^2 - t^2}{2a}$, and therefore is well defined

for any t in $I = \left[-\frac{T}{2}, \frac{T}{2} \right]$, with

$T < 2a$. (This corresponds to the fact that χ is analytical for H_0 with convergence radius a).

In quantum mechanics, the conjugation operator

$$\begin{aligned} K_\tau: L^2(\mathbb{R}^d) &\rightarrow L^2(\mathbb{R}^d) \\ \varphi_\chi(\tau) &\mapsto \overline{\varphi_\chi(\tau)} \end{aligned} \quad (7.4)$$

can be written in term of the usual complex conjugation C as $K_\tau = e^{i\tau H} C e^{i\tau H}$ by analogy with (2.17). But since $C e^{i\tau H} = e^{-i\tau H} C$, we get

$$K_\tau = C. \quad (7.5)$$

This shows why the scalar product in $\mathcal{V}_t^*(\mathbb{R}^d)$ is the most natural Euclidean version of the quantum mechanical scalar product. The quantum mechanical version of (4.0), for any real τ and any densely defined self-adjoint operator A on $L^2(\mathbb{R}^d)$, is

$$A_H(\tau) = e^{i\tau H} A e^{-i\tau H}. \quad (7.6)$$

Its infinitesimal form

$$i \frac{dA_H(\tau)}{d\tau} = [A_H(\tau), H] \quad (7.7)$$

is the Heisenberg picture of the quantum dynamics.

In summary, the dynamical structure of the theory presented here is indeed related to the structure of quantum mechanics by an analytical continuation in the time parameter, valid *also* for the function spaces. In addition, the associated probabilistic structure of the theory is as close as possible to the probabilistic structure of quantum mechanics since, according to lemma 6.8, it is founded on the fact that, for any t in I , the product

$$\eta_\chi^*(x, t) \eta_{\chi'}(x, t) dx \quad (7.8)$$

is a probability density, in complete analogy with the quantum mechanical expression

$$\Psi_\chi(x, t) \overline{\Psi_{\chi'}(x, t)} dx \quad (7.9)$$

whose probabilistic interpretation is due to Born.

For such reasons our framework has been called Euclidean quantum mechanics (EQM) [4].

8. COMPARISON WITH OTHER APPROACHES

The history of the relations between quantum physics and probability theory is long and intricate. It is not our aim here to give an extensive discussion of it but rather to compare Euclidean quantum mechanics with some other related frameworks.

Let us start with Schrödinger's paper [3] giving origin to Euclidean quantum mechanics.

8.1. Schrödinger's idea

Schrödinger has never been convinced by the Copenhagen interpretation of quantum mechanics. Five years after the discovery of his famous equation (2.1), he described what he regarded as a very striking classical analogy with wave mechanics [3], involving Brownian motion.

He considers, for simplicity, the one-dimensional free case where the (already) classical Fokker-Planck equation reduces to an initial value problem

$$-\frac{\partial \mathcal{O}^*}{\partial t} = -D \frac{\partial^2 \mathcal{O}^*}{\partial x^2} \quad (8.1)$$

for \mathcal{O}^* a real function of position and time such that

$$\mathcal{O}^* \left(x, -\frac{T}{2} \right) = p_{-T/2}(x),$$

a probability density, and where D is the (real) diffusion coefficient of the underlying medium. Now, assuming that the observer had also an information on another probability density, for example $p_{T/2}(y)$, Schrödinger asks for the probability density at any $-\frac{T}{2} \leq t \leq \frac{T}{2}$. Observing that

for an initial data only, the problem is well posed and that for a final data only it would also be well posed for the backward equation

$$\frac{\partial \mathcal{O}}{\partial t} = -D \frac{\partial^2 \mathcal{O}}{\partial y^2}. \quad (8.2)$$

Schrödinger shows heuristically that for both data $\{p_{-T/2}(x), p_{T/2}(y)\}$ the problem is new and that its solution is given by a product

$$p(x, t) = \mathcal{O}^*(x, t) \mathcal{O}(x, t), \quad -\frac{T}{2} \leq t \leq \frac{T}{2} \quad (8.3)$$

where \mathcal{O}^* is the solution of an initial value problem (8.1) and \mathcal{O} the solution of a final value problem (8.2), chosen in such a way that their product at $t = -\frac{T}{2}$ and $t = \frac{T}{2}$ coincide with the data $p_{-T/2}(x)$ respectively $p_{T/2}(y)$.

The key constraint to fulfill this last condition is expressed by Eq. (6.9), for $h(x, T, y) = \text{kernel} \{e^{-TH_0}\}(x, y)$, and H_0 the self-adjoint free Hamiltonian on $L^2(\mathbb{R})$, namely by what we have called a Schrödinger's system in § 6.1.

In 1932, S. Bernstein (who was a precursor of the theory of stochastic differential equations) gave a rigorous definition of the property characterizing such processes. This is (6.6), in modern terms a version of local Markov property. Several mathematicians were able to show the kinematical consistency of Schrödinger's idea ([10], [11], [13], [17]) but this idea was forgotten by theoretical and mathematical physicists. The completion of the probabilistic part of the program, in a physically natural dynamical context, has been done in [12] and [4]. It has been the purpose of the present paper to show that the analytical structure of the theory suggested by Schrödinger's idea is indeed what can be expected from a Euclidean version of quantum mechanics.

From a technical point of view, Schrödinger's original idea is much more general than the version used in this paper. For instance, one constructs the probability measure of a unique Markovian Bernstein process $Z(t)$ for any couple of probability measures $\{p_{-T/2}(dx), p_{T/2}(dy)\}$ fulfilling the regularity conditions of Theorem 6.4. But, in order to exhibit any explicit example, one needs to solve Schrödinger's system (6.9).

The aim of the construction given here is to involve exclusively the particular Markovian Bernstein processes relevant for (Euclidean) quantum mechanics. This enables us to introduce extra analytical structures, indispensable in this perspective, and to use Theorem 6.4 only to assure the existence of the probability measure, the solutions of Schrödinger system (6.9) being known by construction (Cf. § 6.2).

8.2. Feynman's space-time approach to quantum mechanics

Feynman's 1948 paper [1] was at the origin of the revival of interest for the relations between quantum physics and probability theory. He was able to show heuristically that the quantum description of the dynamics

in terms of the evolution group U_t can be replaced by a path integral representation or "sum over histories".

These "Feynman path integrals" have been constructed, *see* for instance ([18], [19]). For some recent developments, *see* [20]. However they are not directly associated to a stochastic process, the main tool of Feynman's strategy.

The physical interpretation of Feynman's theory is not trivial. Its author was mainly interested in the development of a very heuristic tool for quantum physics and, in this sense, he fully succeeded.

The real stake of the method (and the original motivation of Feynman) was its generalization to quantum field theory, in particular Quantum Electrodynamics. For some results in this direction *see* [19].

This approach is most effective in expressing probability amplitudes but the construction of a physical Hilbert space often presents difficulties. The latter is best constructed through Euclidean functional approaches. For alternative discussions on the role of probability in quantum mechanics *see*, for example, [31].

8.4. The Euclidean functional approach

M. Kac discovered in 1950 that after an analytical continuation $\tau \rightarrow it$, possible for a large class of potentials V , Feynman's formula for the group $e^{-i\tau H}$ becomes what we now call Feynman-Kac formula for the heat semigroup. This is a probabilistic formula with an underlying stochastic process, often more appropriate as a technical tool than the original Feynman's formula involving formal path integrals.

Notice, however, that the dynamical meaning of the underlying process is left unclear.

As an element of $L^2(\mathbb{R}^d)$, a solution of the heat equation is, for a large class of potentials, analytic in $\text{Re}t > 0$, continuous for $\text{Re}t \geq 0$ and its value on the imaginary axis indeed solves the Schrödinger equation. Notice that the underlying function space is, for any time t , the same as in quantum mechanics, in contrast with EQM where a one-parameter family of Hilbert spaces, $\mathcal{V}_t^*(\mathbb{R}^d)$, is used.

The Feynman-Kac formula is the nonrelativistic starting point of Euclidean field theory, a program initiated by Schwinger, Nakano and Symanzik in which the physical Minkowski space becomes Euclidean space, the Poincaré group becomes the Euclidean group and noncommuting operators become random variables.

In 1971 Nelson [22] gave a rigorous formulation of this program involving the theory of Markov fields, the proof of this Markov property in a specific model being the difficult part of the method. Nelson's approach became an efficient constructive tool, *see* e. g. [23].

A short time later, Osterwalder and Schrader [24] found a weaker positivity condition sufficient to recover relativistic fields from Euclidean ones. In the one dimensional case, that is for stochastic processes, this property is related to Bernstein positivity for (stationary) Markovian Bernstein processes [35].

A number of models in 2 or 3 space-time dimensions have been constructed along these lines [23-26]. See also [27] for recent discussions in 4 dimensions.

In these constructions, probability theory plays only a technical role, the relations between quantum physics and probability theory being only indirectly taken care, by an analytical continuation in the time parameter distinct from the one used here in the passage from quantum mechanics to EQM.

8.5. Nelson's stochastic mechanics

This theory, inspired by an early paper of Féynes [28], is an original attempt to find some classical interpretation of quantum processes. It shows that to each, regular enough, solution $\psi(x, \tau)$ of Schrödinger equation (2.1) there can be associated an \mathbb{R}^d -valued Markovian diffusion process $X(\tau)$, with drift and diffusion coefficients given in terms of ψ . In addition, each such process satisfies a stochastic Newton law of motion.

Very natural regularity conditions for Nelson's theory have been discovered by Carlen [29]. They involve a class of potentials (the Kato-Rellich class) closely related to the class relevant for EQM. For further discussions of Nelson's ideas, *cf.*, for example, [30], [36].

The origin of the above mentioned stochastic Newton equation, in Nelson's theory, lies in a change of dependent variables in the starting solution $\psi(x, \tau)$ of the Schrödinger equation (2.1). Here is the Euclidean version of this argument.

Let us define a pair of real scalar fields R and S on \mathbb{R}^d by

$$\psi_x(x, \tau) = (e^{R+iS})(x, \tau) \equiv \rho^{1/2} e^{iS}(x, \tau). \quad (8.4)$$

We can regard this ψ_x in its dependence on $v_0 = \nabla S(x, 0)$ and denote it by $\psi_x^v(x, \tau)$. The "Euclidean" wave function η_x^* corresponding to ψ_x is defined formally by

$$\begin{aligned} \eta_x^*(x, t) &= \psi_x^{iv_0}(x, -it) \\ &\equiv e^{\bar{R}-\bar{S}}(x, t) \equiv p^{1/2} e^{-S}(x, t), \end{aligned} \quad (8.5)$$

(The bar should not be confused here with a complex conjugation) where

$$\bar{R}(x, t) = R_{-iv_0}(x, \tau) \quad \text{and} \quad \bar{S}(x, t) = -iS_{-iv_0}(x, \tau).$$

We also define

$$\eta_{\chi'}(x, t) = e^{\bar{R} + \bar{S}}(x, t) \equiv p^{1/2} e^{+\bar{S}}(x, t). \tag{8.5'}$$

From the formal analytical continuation of (2.1) we get the coupled system of equations

$$\frac{\partial \bar{R}}{\partial t} = -\frac{1}{2} \Delta \bar{S} - \nabla \bar{R} \cdot \nabla \bar{S} \tag{8.6}$$

$$\frac{\partial \bar{S}}{\partial t} = -\frac{1}{2} \Delta \bar{R} - \frac{1}{2} (\nabla \bar{R})^2 - \frac{1}{2} (\nabla \bar{S})^2 + V. \tag{8.7}$$

We notice that since these equations are real, we can get real solutions. Taking gradient and using the definition

$$\bar{v}(x, t) = \nabla \bar{S}(x, t), \bar{u}(x, t) = \frac{1}{2} \nabla \ln p = \nabla \bar{R}(x, t),$$

one checks that the first equation reduces to the continuity equation for the probability density p , (7.8), of a Markovian Bernstein process $Z(t)$, t in I , and the second one to the Euclidean Newton equation (6.48). In fact, if $p_{-T/2}(x) = e^{2\bar{R}}(x, -T/2)$ and $p_{T/2}(y) = e^{2\bar{R}}(y, T/2)$ fulfil the conditions of Theorem 6.4, an unique Markovian Bernstein process $Z(t)$, t in $[-\frac{T}{2}, \frac{T}{2}]$ can indeed be obtained in this way. By Theorem 6.5 this process can be identified with the pair $\chi = e^{\bar{R}} \cdot e^{-\bar{S}}$ and $\chi' = e^{\bar{R}} e^{\bar{S}}$ since $\chi \chi' = e^{2\bar{R}}$ at $t=0$.

Let us consider the moments of this process, for $t_1 \leq t_2 \leq \dots \leq t_n$, $t_j \in I$,

$$\begin{aligned} & E[Z(t_1)Z(t_2) \dots Z(t_n)] \\ &= \int_{\mathbb{R}^d} \eta_{\chi}^*(x, -T/2) h(x, t_1 + T/2, x_1) x_1 h(x_1, t_2 - t_1, x_2) \\ & \quad x_2 \dots x_n h(x_n, T/2 - t_n, y) \eta_{\chi'}(y, T/2) dx dx_1 \dots dx_n dy. \end{aligned} \tag{8.8}$$

Setting $S = -iT$, $\tau_j = -it_j$, for $j=1$ to n , using (8.5) and the fact that $\psi_{\chi}^{v_0}$, respectively $\bar{\psi}_{\chi}^{v_0}$ are formally the analytical continuation of η_{χ}^* respectively $\eta_{\chi'}$, we obtain, by formal analytical continuation of (8.8),

$$\begin{aligned} & \int_{\mathbb{R}^d} \psi_{\chi}(x, -S/2) e^{i(\tau_1 + S/2)H}(x, x_1) x_1 e^{-i(\tau_2 - \tau_1)H}(x_1, x_2) \dots \\ & \quad x_n e^{-i(S/2 - \tau_n)H}(x_n, y) \bar{\psi}_{\chi}(y, S/2) dx dx_1 \dots dx_n dy. \end{aligned} \tag{8.9}$$

Such expressions have been introduced formally by Feynman [1]. See also, for a mathematical interpretation [19]. It is well known that they do *not* correspond to the moments of any stochastic process. Nevertheless they describe completely quantum dynamics. This is another reason to regard

the theory associated with (8.8) as a natural Euclidean version of quantum dynamics.

If $\tau_1 = \tau_2 = \dots = \tau_n = \tau$, however, (8.9) reduce to the single time moments $E[X^n(\tau)]$, where $X(\tau)$ is Nelson's diffusion process associated to the wave function ψ . This means that the symbolic relation $Z(i\tau) = X(\tau)$ makes sense as long as only one time expectations are involved. In particular, it is clear from (8.4) and (8.5) that the following symbolic relation between the probability densities of the two diffusion processes holds:

$$p(x, i\tau) = \rho(x, \tau), \quad t = i\tau \text{ in } I. \quad (8.10)$$

For expectations involving several times, the relations between the two processes $Z(t)$ and $X(\tau)$ are not as simple because Euclidean Quantum Mechanics and Stochastic Mechanics differ essentially by their dynamical structures.

9. CONCLUSION

It is not the scope of the present paper to discuss the possible physical interpretations of EQM. This has been initiated elsewhere [4]. The key point of EQM is that it is a classical (stochastic) theory in which most of the puzzling aspects of Quantum Mechanics are present. In particular, it shows that Kolmogorovian probabilities are sufficient to describe these effects; hence the specificity of Quantum Mechanics must be found elsewhere.

The key idea of EQM is very general: it is preserved in all the realizations of quantum dynamics, and will be discussed in forthcoming publications.

An extension of EQM to field theory will be very interesting in view of the very close similarity of nonrelativistic quantum mechanics with EQM.

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