Mathematical Physics

Study of a self-adjoint operator indicating the direction of time within standard quantum mechanics

Étude d’un opérateur auto-adjoint qui indique la direction du temps en mécanique quantique

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\textbf{ABSTRACT}

In [Y. Strauss, Self-adjoint Lyapunov variables, temporal ordering and irreversible representations of Schrödinger evolution, J. Math. Phys. 51 (2010) 022104] a self-adjoint operator was introduced that has the property that it indicates the direction of time within the framework of standard quantum mechanics, in the sense that as a function of time its expectation value decreases monotonically for any initial state. In this paper we study some of this operator’s properties. In particular, we derive its spectrum and generalized eigenstates, and treat the example of the free particle.

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\textbf{RÉSUMÉ}

Dans [Y. Strauss, Self-adjoint Lyapunov variables, temporal ordering and irreversible representations of Schrödinger evolution, J. Math. Phys. 51 (2010) 022104], un opérateur auto-adjoint a été introduit ayant la propriété d’indiquer la direction du temps dans le formalisme standard de la mécanique quantique, au sens où sa valeur moyenne décroît de façon monotone avec le temps pour tout état initial. Dans cet article, nous étudions les propriétés de cet opérateur. En particulier, nous dérivons son spectre et ses vecteurs propres généralisés et traitons en détail l’exemple de la particule libre.

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\textbf{Version française abrégée}

Nous étudions les propriétés d’un nouvel opérateur auto-adjoint $M$, dans l’espace d’Hilbert $K$ de la mécanique quantique standard, qui a la propriété de Lyapunov $(\psi(t_2), M\psi(t_2)) \leq (\psi(t_1), M\psi(t_1))$ pour $t_2 \geq t_1 \geq 0$, où $\psi(t) = U(t)\psi$ et $U(t)$ est l’opérateur unitaire représentant le groupe à un paramètre généré par l’hamiltonien auto-adjoint $H$ au spectre absolument...
Elles représentent une famille spectrale pour l’opérateur auto-adjoint, impliquant, avec le fait prouvé dans l’article qu’il n’y a pas de spectre ponctuel en 0 ni en 1, que le spectre de $M$ est absolument continu, c’est-à-dire $\sigma(M) = \sigma_{ac}(M) = [0, 1]$. La représentation de l’opérateur $M$ donnée par l’Eq. (16) (au sens de Dirac) est donc justifiée.

Pour illustrer le comportement de $M$, nous traitons l’exemple d’un paquet d’onde gaussien uni-dimensionnel représentant la propagation libre d’une particule de masse $\eta$ vers la droite. Voir Eq. (19), où $p_0$ et $q_0$ sont les position et largeur du paquet d’onde dans l’espace des impulsions à $t = 0$. La Fig. 1 montre l’évolution temporelle de la valeur moyenne de $M$, la Fig. 2, l’évolution temporelle de la densité de probabilité spatiale. On voit que si la suite de fenêtres temporelles est donnée en sens inverse, il n’est pas possible de dire si le temps s’écoule en arrière ou si on observe le paquet d’onde gaussien se propageant vers la gauche (avec le temps s’écoulant en avant). Cependant s’il a chaque fenêtre temporelle, nous attachons la valeur moyenne de $M$, alors il devient possible de distinguer ces deux scénarios. Cet exemple illustre bien l’ordre temporel introduit dans l’espace d’Hilbert par l’existence d’un opérateur de Lyapunov.

Dans [7–9] nous montrons que l’existence de l’opérateur $M$ conduit à une représentation irreversible de la dynamique quantique et à une nouvelle représentation des processus de diffusion dans laquelle la contribution de résonances est mise en évidence.

1. Introduction

Il est un fondamental question in standard quantum mechanics (SQM) of what type of restrictions the Schrödinger evolution imposes on the behavior in time of basic objects. In particular, it is of interest to ask if SQM allows for self-adjoint operators having the so-called Lyapunov property, that is, monotonicity of the expectation value irrespective of the initial state of the system. Clearly, such an operator would indicate the direction of time.

A natural candidate for a self-adjoint Lyapunov operator is a (self-adjoint) time operator $T$ canonically conjugate to the Hamiltonian $H$, such that $T$ and $H$ form an imprimivity system [3] (implying that each generates a translation on the spectrum of the other). However, a well-known theorem of Pauli tells us that this is impossible [6]. Recently, Galapon attempted to bypass Pauli’s arguments and found pairs of $T$ and $H$ satisfying the canonical commutation relations, but do not constitute an imprimivity system [1]. It can be shown that the $T$ operator obtained in this way does not have the Lyapunov property. Other authors do not insist on the conjugacy of $T$ and $H$. In this context, Unruh and Wald’s proof that a ‘monotonically perfect clock’ does not exist [10] should be noted, as well as Misra, Prigogine, and Courbage’s no-go theorem [4]. Still another solution, advocated by some authors, is to do away with the requirement of self-adjointness [2].

A Lyapunov self-adjoint operator acting within the framework of standard quantum mechanics was recently introduced in [7]. In this paper we study some of its properties. In particular, we derive its spectrum and generalized eigenstates, and treat the example of the free particle.

2. Main results

Let $\mathcal{H}$ be a separable Hilbert space and let $H$ be a self-adjoint operator generating a unitary evolution group $\{U(t)\}_{t \in \mathbb{R}}$, with $U(t) = \exp(-iHt)$, on $\mathcal{H}$. We take $\mathcal{H}$ to represent the Hilbert space corresponding to some given quantum system and $H$ its Hamiltonian. For an initial state $\psi(0) = \psi \in \mathcal{H}$, $\psi(t) = U(t)\psi$ denotes the state of the system at time $t$ and $\psi(t) := \{\psi(t)\}_{t \in \mathbb{R}}$ its trajectory. Let $B(\mathcal{H})$ be the space of bounded linear operators on $\mathcal{H}$. A (forward) Lyapunov operator is defined as follows [7]:

**Définition 2.1.** Let $M \in B(\mathcal{H})$ be a self-adjoint operator on $\mathcal{H}$. Let $\psi_M$ be the trajectory corresponding to an initial state $\psi$. Let $M(\psi) = \{\|\psi\|^{-2}(\psi, M\psi) \mid \psi \in \psi_M\}$ be the set of expectation values of $M$ in states in $\psi_M$. Then $M$ is a forward Lyapunov operator if the mapping $t_M, \psi : \mathbb{R}^+ \mapsto M(\psi_M)$ defined by
\( \tau_{M,\psi}(t) = \|\psi\|^{-2}(\psi(t), M\psi(t)) \) (1)

is one to one and monotonically decreasing for all non-recurring trajectories.

Let \( \mathcal{K} \) be a separable Hilbert space and \( L^2(\mathbb{R}^+; \mathcal{K}) \) the Hilbert space of Lebesgue square-integrable \( \mathcal{K} \) valued functions defined on \( \mathbb{R}^+ \), let \( H \) be the operator of multiplication by the independent variable on \( L^2(\mathbb{R}^+; \mathcal{K}) \), and let \( \{U(t)\}_{t\in\mathbb{R}} \) be the continuous one-unitary parameter evolution group generated by \( H \), i.e.,

\[
\left[ U(t)f \right](E) = e^{-iHt}f(E) = e^{-iEt}f(E), \quad f \in L^2(\mathbb{R}^+; \mathcal{K}), \quad E \in \mathbb{R}^+. 
\]

(2)

Denote by \( \mathcal{H}^2(\mathbb{C}^\pm; \mathcal{K}) \) the Hardy spaces of \( \mathcal{K} \) valued functions analytic in \( \mathbb{C}^\pm \). The Hilbert spaces \( \mathcal{H}^2(\mathbb{R}; \mathcal{K}) \) consisting of non-tangential boundary values on \( \mathbb{R} \) in \( \mathcal{H}^2(\mathbb{C}^\pm; \mathcal{K}) \) are, respectively, isomorphic to \( \mathcal{H}^2(\mathbb{C}^\pm; \mathcal{K}) \). The spaces \( \mathcal{H}^2(\mathbb{R}; \mathcal{K}) \) are orthogonal subspaces of \( L^2(\mathbb{R}; \mathcal{K}) \) with \( L^2(\mathbb{R}; \mathcal{K}) = \mathcal{H}^2_+(\mathbb{R}; \mathcal{K}) \oplus \mathcal{H}^2_-(\mathbb{R}; \mathcal{K}) \). We denote the orthogonal projections in \( L^2(\mathbb{R}; \mathcal{K}) \) on \( \mathcal{H}^2_+(\mathbb{R}; \mathcal{K}) \) and \( \mathcal{H}^2_-(\mathbb{R}; \mathcal{K}) \), respectively, by \( P_+ \) and \( P_- \). Let \( L^2(\mathbb{R}^+; \mathcal{K}) \) be the subspaces of \( L^2(\mathbb{R}; \mathcal{K}) \) consisting of square-integrable functions supported on \( \mathbb{R}^+ \).

There exists another orthogonal decomposition \( L^2(\mathbb{R}; \mathcal{K}) = L^2(\mathbb{R}^-; \mathcal{K}) \oplus L^2(\mathbb{R}^+; \mathcal{K}) \) with projections on \( P_{\mathbb{R}^+} \) and \( P_{\mathbb{R}^-} \). The following theorem is proved in [7]:

**Theorem 2.2.** Let \( M : L^2(\mathbb{R}^+; \mathcal{K}) \mapsto L^2(\mathbb{R}^+; \mathcal{K}) \) be the operator defined by

\[
M := (P_{\mathbb{R}^+} + P_{\mathbb{R}^-})(L^2(\mathbb{R}^+; \mathcal{K})). 
\]

Then \( M \) is a positive, contractive and injective operator on \( L^2(\mathbb{R}^+; \mathcal{K}) \). The following corollary to Theorem 2.2 casts Eq. (3) in a more useful form:

**Corollary 2.3.** Let \( M \) be the Lyapunov operator given in Eq. (3). Then, for any function \( f \in L^2(\mathbb{R}^+; \mathcal{K}) \) we have

\[
(Mf)(E) = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dE' \frac{1}{E - E' + i0^+} f(E'), \quad E \in \mathbb{R}^+, \quad f \in L^2(\mathbb{R}^+; \mathcal{K}). 
\]

(5)

**Proof.** For every function \( g \in \mathcal{H}^2(\mathbb{C}^\pm; \mathcal{K}) \) one has [5]

\[
\frac{1}{2\pi i} \int_{-\infty}^{\infty} dt \frac{1}{z - t} g_{\pm}(t) = \begin{cases} g(z), & \pm \text{Im } z > 0, \\ 0, & \pm \text{Im } z < 0. \end{cases} 
\]

(6)

where \( g_{\pm} \in \mathcal{H}^2_{\pm}(\mathbb{R}; \mathcal{K}) \) is the boundary value function of \( g \) on \( \mathbb{R} \). Hence, the orthogonal projection \( P_+ \) of \( L^2(\mathbb{R}^+; \mathcal{K}) \) on \( \mathcal{H}^2_+(\mathbb{R}; \mathcal{K}) \) is explicitly given by

\[
(P_+ g)(\sigma) = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\sigma' \frac{1}{\sigma - \sigma' + i0^+} g(\sigma'), \quad g \in L^2(\mathbb{R}; \mathcal{K}), 
\]

(7)

where Eq. (7) hold a.e. for \( \sigma \in \mathbb{R} \). From Eqs. (3), (7) we then immediately obtain Eq. (5). \( \square \)

**Theorem 2.4.** The spectrum of \( M \) satisfies \( \sigma(M) = \sigma_{ac}(M) = [0, 1] \). In \( L^2(\mathbb{R}^+; \mathcal{K}) \) choose an orthogonal basis \( \{\mathbf{e}_\lambda(E)\}_{E \in \mathbb{R}^+; \lambda \in \Lambda} \) with \( \Lambda \) an appropriate index set such that for every \( E \in \mathbb{R}^+ \) the set \( \mathbf{e}_\lambda(E) \) is a basis of \( \mathcal{K} \) and we have \( \mathbf{e}_\lambda(E), \mathbf{e}_\lambda'(E) \) is \( \delta(E - E') \delta_{\lambda,\lambda'} \), where \( \delta_{\lambda,\lambda'} \) stands for the Kronecker delta for discrete indices and the Dirac delta for continuous indices. Then for \( m \in (0, 1) \) the function defined by

\[
g_{m,\lambda} = \int_0^\infty dE \frac{E^{-\frac{1}{2}} \ln \frac{1-m}{1-m}}{2\pi \sqrt{m(1-m)}} \mathbf{e}_\lambda(E) 
\]

(8)

is a generalized eigenfunction of \( M \) satisfying \( M g_{m,\lambda} = mg_{m,\lambda} \). These eigenfunctions are normalized in such a way that \( (g_{m,\lambda}, g_{m',\lambda'})_{L^2(\mathbb{R}^+; \mathcal{K})} = \delta(m - m') \delta_{\lambda,\lambda'} \) and we have the eigenfunction expansion

\[
M = \sum_{\lambda \in \Lambda} \int_0^1 dm m g_{m,\lambda} g_{m,\lambda}^*. 
\]

(9)
Proof. Theorem 2.2 states that $M$ is positive and contractive, implying that $\sigma(M) \subseteq [0, 1]$. Consider the eigenvalue equation $Mg_{m, \lambda} = mg_{m, \lambda}$. In the basis $(e_x(E))_{x \in \mathbb{R}^+}$, the kernel of $M$ is given by $(e_x(E), Me_x(E')) = -(2\pi i)^{-1}(E - E' + i0^+)^{-1}\delta_{\lambda'}$. Hence, the eigenvalue equation for $M$ assumes the form

$$-\frac{1}{2\pi i} \int_0^\infty \frac{dE'}{E - E' + i0^+} g_{m, \lambda}(E') = mg_{m, \lambda}(E), \quad E \in \mathbb{R}^+,$$

(10)

where $g_{m, \lambda}(E) = (e_x(E), g_{m, \lambda})$. Any non-trivial solution of Eq. (10) is necessarily the boundary value on $\mathbb{R}^+$ from above of an analytic function defined on $\mathbb{C}\setminus\mathbb{R}^+$. Let $m \in (0, 1)$ and let $\tilde{g}_m(z)$ be such a continuation of an arbitrary solution $g_{m, \lambda}(E)$, so that $g_{m, \lambda}(E) = \tilde{g}_m(E + i0^+)$. We can now analytically continue Eq. (10) into the cut complex plane

$$-\frac{1}{2\pi i} \int_0^\infty \frac{1}{z - E} g_{m, \lambda}(E') = m\tilde{g}_m(z), \quad \text{Im} \ z \neq 0.$$  

(11)

Taking in Eq. (11) the difference between the limits from above and below $\mathbb{R}^+$ we get

$$g_{m, \lambda}(E) = \tilde{g}_m(E + i0^+) = m(\tilde{g}_m(E + i0^+) - \tilde{g}_m(E - i0^+)).$$  

(12)

The function $\tilde{g}_m(z)$ can now be continued to a second Riemann sheet by making use of the branch cut along $[0, \infty)$ in Eq. (11). Denoting this two sheeted function again by $\tilde{g}_m(z)$, Eq. (11), reduces to

$$\tilde{g}_m(z) = -\frac{1}{m} \tilde{g}_m(z).$$  

(13)

Eq. (13) admits solutions of the form $\tilde{g}_m(z) = N_m e^\beta$ with $\beta = k + \frac{1}{2} - \frac{i}{\pi} \ln(\frac{1}{m})$, $k \in \mathbb{Z}$, and $N_m$ a normalization factor dependent on $m$. Setting $k = -1$ and $N_m = (4\pi^2 m(1 - m))^{-1/2}$ the solutions of the eigenvalue equation, Eq. (10), satisfy

$$\int_0^\infty dE \tilde{g}_m(E)g_{m, \lambda}(E) = \delta(m - m')\delta_{\lambda, \lambda'}.$$  

With this choice of $k$ and $N_m$ the generalized eigenfunctions of $M$ are given by Eq. (8).

We proceed to show by construction that the set of generalized eigenfunctions, Eq. (8), forms a complete set for the operator $M$. Consider the following integral

$$\sum_{\lambda} \int_0^\infty \frac{dE}{4\pi^2}\sqrt{E} \int_0^\infty dE' \frac{e_x(E)e_x'(E')}{E - E'} \int_0^\infty \frac{dm}{1 - m} \frac{m}{1 - m} \ln(E/E') \int_0^\infty \frac{dm}{1 - m} \frac{m}{1 - m} \ln(E/E'),$$

(14)

where $dm$ is a Lebesgue measure on $[0, 1]$. The right-hand side of Eq. (14) is readily obtained from that of Eq. (8). Recall the definition of the Euler beta function $B(x, y) = \int_0^1 dm m^{x-1}(1 - m)^{y-1} = \Gamma(x)\Gamma(y)\Gamma^{-1}(x + y)$. $B(x, y)$ is well defined for $Re > 0$ and $Re > 0$, and can be analytically continued to other parts of the complex $x$ and $y$ planes. However, it is not well defined for $x = 0$ and $y = 0$, i.e. whenever $E = E'$ in Eq. (14). To avoid this problem we shift $E$ (or $E'$) away from the real axis. Hence, in the integration over $m$ on the right-hand side of Eq. (14) we take the limit

$$\frac{1}{4\pi^2}(EE')^{-1/2} \lim_{\theta \to 0^+} \int_0^1 \frac{dm}{1 - m} \frac{m}{1 - m} \ln(e^{\theta E}/E') \ln(e^{\theta E'/E'}),$$

$$= \frac{1}{4\pi^2}(EE')^{-1/2} \lim_{\theta \to 0^+} B \left(1 - \frac{\theta}{2\pi} + \frac{i}{2\pi} \ln\left(\frac{E}{E'}\right), \frac{\theta}{2\pi} - \frac{i}{2\pi} \ln\left(\frac{E}{E'}\right)\right),$$

$$= \frac{1}{4\pi^2}(EE')^{-1/2} \lim_{\theta \to 0^+} \frac{\pi}{\sin(-\frac{\theta}{\pi})} \left(\frac{E}{E'}\right) = -\frac{1}{2\pi i} E - E' + i0^+, $$

(15)

where in the last line in Eq. (15) we used the identity $\Gamma(z)\Gamma(1 - z) = \pi \sin^{-1}(\pi z)$. Thus, the integral on the spectrum of $M$ on the left-hand side of Eq. (15) reconstructs the kernel of $M$ in Eq. (5), i.e., we have reconstructed the operator $M$ using the set of generalized eigenfunctions $(g_{m, \lambda})_{m \in (0, 1), \lambda \in \mathcal{A}}$. Taken together with Eq. (14), Eq. (15) also shows that $M$ has no point spectrum at $m = 0$ and $m = 1$ and that $\sigma(M) = \sigma_{ac}(M) = [0, 1].$ 

Consider a quantum mechanical problem for which the Hamiltonian $H$, defined on an appropriate separable Hilbert space $\mathcal{H}$, satisfies the conditions: (i) Its ac spectrum is $\sigma_{ac}(H) = \mathbb{R}^+$. (ii) The multiplicity of $\sigma_{ac}(H)$ is uniform on $\mathbb{R}^+$. Let $\mathcal{H}_{ac}$ be the subspace of $\mathcal{H}$ corresponding to the ac spectrum of $H$. Then $\mathcal{H}_{ac}$ has a representation in terms of a function space $L^2(\mathbb{R}^+; K)$, where $K$ is a Hilbert space whose dimension corresponds to the multiplicity of $\sigma_{ac}(H)$ and the evolution
Fig. 1. Monotonic decrease of the expectation value of $M$ for a free Gaussian wave-packet with $p_0 = 0.64\eta$ and $\xi_0 = 0.3\eta$.

Fig. 2. Time frames of $|\psi(x, t)|^2$ and $|\langle m | \psi(t) \rangle|^2$ for the Gaussian wave-packet of Fig. 1.

generated by $H$ is represented by $[U(t)]_{t \in \mathbb{R}}$ defined in Eq. (2). For such models we can apply the results discussed above. Using the standard Dirac notation, Eq. (2) for $M$ can be rewritten as

$$M = -\frac{1}{2\pi i} \sum_{\lambda} \int_0^\infty dE \int_0^\infty dE' |E, \lambda\rangle \frac{1}{E - E' + i0^+} \langle E', \lambda|,$$

(16)

where the summation over $\lambda$ stands for summation over discrete degeneracy indices and appropriate integration over continuous degeneracy indices.

As an example we take a one-dimensional Gaussian wave-packet representing the propagation to the right of a free particle of mass $\eta$

$$\psi(x, t) = \left( \frac{\eta^2 \xi_0^2}{\pi (\eta + i\xi_0^2 t)^2} \right)^{1/4} \exp\left( -\frac{\eta^2 \xi_0^2 x^2 + ip_0 (p_0 t - 2\eta x)}{2(\eta + i\xi_0^2 t)} \right).$$

(17)

$p_0$ and $\xi_0$ are the location and width of the wave-packet in momentum space at $t = 0$. After obtaining the generalized eigenfunctions of the free Hamiltonian, constructing the Lyapunov operator $M$ according to Eqs. (16) and (14), and applying it to the wave-packet in Eq. (17) we obtain Fig. 1, showing the time evolution of the expectation value of $M$, and Fig. 2, showing the time evolution of the associated probability density function in the position basis and that of the eigenstates of $M$. We see that if the sequence of time frames is shown in reverse order one is unable to tell whether time is running backwards or whether one is observing a Gaussian wave-packet propagating to the left (with time running forward). However, if to all frames we attach the expectation value of $M$, then it possible to distinguish between these two scenarios. The example plainly illustrates the time-ordering of states introduced into the Hilbert space by the existence of a Lyapunov operator.

In [7–9] it is shown that the existence of the operator $M$ leads to an irreversible representation of the quantum dynamics, and to a novel representation of the scattering process, in which the contribution of the resonance is singled out.

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