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Time asymmetry in quantum mechanics: a pure mathematical point of view

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Abstract
In the paper it is pointed out that 'time asymmetry in quantum mechanics' (TAQM) is an intrinsic element of the mathematical apparatus of quantum mechanics for semibounded Hamiltonians H with absolutely continuous spectrum coinciding with the positive half-line and of constant multiplicity. It is shown that the TAQM-semigroups are unsuitable for a spectral characterization of the resonances in terms of H.

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1. Introduction

The paper is intended to contribute to 'time asymmetry in quantum mechanics' (TAQM) from the mathematical point of view, based on the (essential) selfadjointness of the Hamiltonians in quantum mechanics. For general literature on the topic TAQM we refer to [1] and references therein (see also [2–4]).

In the paper it is pointed out that TAQM is, mathematically speaking, an intrinsic element of the mathematical apparatus of quantum mechanics for selfadjoint Hamiltonians which are semibounded with an absolutely continuous spectrum coinciding with the positive half-line and of homogeneous (constant) multiplicity. It is shown that in this case the so-called TAQM-semigroups act on the well-defined dense submanifolds of outgoing (or incoming) states of the subspace of all scattering states. The spectral structure of these semigroups changes totally as compared with that of the Hamiltonian. This implies that the TAQM-semigroups cannot contribute to a spectral characterization of the resonances because their eigenvalue spectrum coincides with the full lower (or upper) half-plane of the complex plane such that the resonances 'vanish' in the 'sea' of all eigenvalues. Furthermore, according to a theorem of Wollenberg [5] (see also [6]), it is not sufficient to characterize the resonances of a Hamiltonian only by their property to be poles of the scattering matrix. This means that a characterization in terms of the Hamiltonian itself is required.

2. Basic assumptions and properties of the Hamiltonians

The Hamiltonians H considered are selfadjoint and semibounded operators on a Hilbert space $\mathcal{H}$ with absolutely continuous spectrum $\mathbb{R}_+ := [0, \infty)$ of constant multiplicity. The projection onto the absolutely continuous subspace of H is denoted by P^{ac}. Since in the following only the absolutely continuous subspace $P^{ac}\mathcal{H}$ is of interest, for convenience we write simply $\mathcal{H}$ for $P^{ac}\mathcal{H}$ and H for $H \restriction P^{ac}\mathcal{H}$. We collect basic facts of the spectral theory of H: there is a *spectral representation* of H. This means there is an isometric operator Φ from $\mathcal{H}$ onto $L^2(\mathbb{R}_+, \mathcal{K}, \mathrm{d}E)$, where $\mathcal{K}$ is a Hilbert space and $\dim \mathcal{K}$ is the multiplicity of the absolutely continuous spectrum such that H respectively $\mathrm{e}^{-\mathrm{i}tH}$ is represented on $L^2(\mathbb{R}_+, \mathcal{K}, \mathrm{d}E)$ by M_+ respectively $\mathrm{e}^{-\mathrm{i}tM_+}$, where M_+ denotes the multiplication operator

$$M_+ f(E) := E f(E), \qquad f \in L^2(\mathbb{R}_+, \mathcal{K}, \mathrm{d}E),$$

i.e. one has

$$\Phi(\mathrm{e}^{-\mathrm{i}tH} f)(E) = \mathrm{e}^{-\mathrm{i}tE}(\phi f)(E), \qquad f \in \mathcal{H}$$

or

$$\Phi\, \mathrm{e}^{-\mathrm{i}tH} \phi^{-1} = \mathrm{e}^{-\mathrm{i}tM_+}. \tag{1}$$

Φ is not unique, however in general, for given concrete Hamiltonians there are distinguished canonical spectral transformations Φ.

For example, if H is the Hamiltonian for central-symmetric potentials with compact support and angular momentum quantum number $l = 0$, given on $L^2(\mathbb{R}_+, \mathrm{d}r)$, then the canonical spectral transformation Φ reads

$$(\Phi f)(E) = \frac{E^{1/4}}{\sqrt{\pi}|F(\sqrt{E})|} \int_0^\infty \varphi(r, E) f(r)\mathrm{d}r, \qquad f \in L^2(\mathbb{R}_+, \mathrm{d}r),$$

where $\varphi(\cdot, E)$ is the regular solution of the corresponding differential equation and $F(\cdot)$ denotes the Jost function. The inverse transformation Φ^{-1} is given by

$$(\Phi^{-1} g)(r) = \frac{1}{\sqrt{\pi}} \int_0^\infty \varphi(r, E) \frac{E^{1/4}}{|F(\sqrt{E})|} g(E)\, \mathrm{d}E, \qquad g \in L^2(\mathbb{R}_+, \mathrm{d}E).$$

By H_0 we denote a second, so-called 'free' selfadjoint Hamiltonian with the same absolutely continuous subspace as H and we assume that $\{H, H_0\}$ form an asymptotically complete scattering system. Then H and H_0 are necessarily unitarily equivalent on $\mathcal{H}$. For example, these conditions are satisfied if $H := H_0 + V$ where V is a trace class operator. In general, also H_0 has a canonical spectral transformation Φ_0. Then the operators $\tilde{W}_\pm := \Phi W_\pm \Phi_0^{-1}$, where $W_\pm$ are the unitary wave operators on $\mathcal{H}$, are multiplication operators on $L^2(\mathbb{R}_+, \mathcal{K}, \mathrm{d}E)$, acting by the so-called wave matrices $E \to W_\pm(E)$, where $W_\pm(E)$ are unitary operators on the multiplicity space $\mathcal{K}$. Then the scattering matrix is given by $S(E) = W_+(E)^* W_-(E)$.

In the following we do not use $W_\pm$ and S. However we recall that asymptotical completeness means that

$$W_+\mathcal{H} = W_-\mathcal{H} = \mathcal{H}.$$

In the physical literature usually $W_+\mathcal{H}$ is called the subspace of *out-states* and $W_-\mathcal{H}$ the subspace of *in-states*. That is, asymptotic completeness means that the subspaces of in- and out-states coincide with the absolutely continuous subspace $\mathcal{H}$, the space of all *scattering states*.

The starting point and the first ansatz for *time asymmetry* is the observation that there are sufficiently many scattering states with distinguished time properties w.r.t. the evolution $\mathbb{R} \ni t \to \mathrm{e}^{-\mathrm{i}tH}$. For the description of these states one has to point out the connection of the quantum-mechanical evolution with the unitary *shift evolution* on the Hilbert space $L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$. This approach requires the introduction of the Hardy spaces.

3. Hardy spaces and shift evolution

The Fourier transformation F is an isometric operator from $L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$ onto $L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}E)$, defined by

$$L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x) \ni f \to (Ff)(E) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}Ex} f(x)\, \mathrm{d}x$$

on an appropriate dense set (e.g. the Schwartz space). The projections on $L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$, acting by multiplication with the characteristic functions $\chi_{\mathbb{R}_\pm}(\cdot)$, where $\mathbb{R}_- := (-\infty, 0]$, are denoted by $P_\pm$. Then the Hardy spaces $\mathcal{H}^2_\pm(\mathbb{R}; \mathcal{K}) \subset L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$ are defined by

$$\mathcal{H}^2_\pm(\mathbb{R}, \mathcal{K}) := FP_\mp L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x).$$

The projections $Q_\pm$ onto these (mutually orthogonal) subspaces are given by

$$Q_\pm = FP_\mp F^{-1}.$$

Note that $Q_+ + Q_- = \mathbb{1}$, $Q_- Q_+ = 0$. On $L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$ the shift evolution $T(\cdot)$ is defined by

$$T(t)g(x) := g(x - t), \qquad g \in L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x).$$

It is well known that the subspaces $P_\mp L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$ are *incoming/outgoing subspaces* of the shift evolution (in the sense of Lax–Phillips [7]), i.e.

$$T(t)P_- L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x) \subseteq P_- L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x), \qquad t \leqslant 0, \tag{2}$$

$$T(t)P_+ L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x) \subseteq P_+ L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x), \qquad t \geqslant 0, \tag{3}$$

the intersection of all $T(t)P_+ L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$ is $\{0\}$, and their union is dense in $L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$ (similarly for P_-). Further, the spectral representation of the shift evolution is obtained by F, i.e.

$$FT(t)F^{-1} = \mathrm{e}^{-\mathrm{i}tM}, \tag{4}$$

where M denotes the multiplication operator on $L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}E)$. Note that the projections $P_\pm$ commute with the evolution $t \to \mathrm{e}^{-\mathrm{i}tM}$, they are spectral projections, i.e. elements from the spectral measure of M.

The decisive step to obtain the mentioned distinguished states in $\mathcal{H}$ is the application of results due to Halmos [8], van Winter [9, 10], refined by Kato [11], culminating in the following.

Lemma (Halmos, Kato). *Let P, Q be projections on subspaces of a Hilbert space $\mathcal{H}$ in generic position, i.e.*

$$P\mathcal{H} \cap Q\mathcal{H} = P\mathcal{H} \cap (\mathbb{1} - Q)\mathcal{H} = (\mathbb{1} - P)\mathcal{H} \cap Q\mathcal{H} = (\mathbb{1} - P)\mathcal{H} \cap (\mathbb{1} - Q)\mathcal{H} = \{0\}.$$

Then

(i) the linear manifold $\mathcal{M} := PQ\mathcal{H} \subset P\mathcal{H}$ is dense in $P\mathcal{H}$ w.r.t. the Hilbert space topology of $\mathcal{H}$;

(ii) the projection P on $Q\mathcal{H}$ is bijective, i.e. the inverse operator P^{-1} exists on $\mathcal{M}$;

(iii) if $\|P - Q\| = 1$ then P^{-1} is a closed and unbounded operator on $P\mathcal{H}$ and $\mathrm{dom}\, P^{-1} = \mathcal{M}$ is properly dense in $P\mathcal{H}$.

A proof can be found in [11]. The application of this lemma to the projections P_+ and $Q_\pm$ yields: the subspaces $P_+L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}E)$ and $Q_\pm L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}E)$ are in generic position and $\|P_+ - Q_\pm\| = 1$. This means

Corollary. *The assignment*

$$\mathcal{H}^2_\pm \ni f \rightarrow P_+ f \in \mathcal{M}_\pm := P_+\mathcal{H}^2_\pm(\mathbb{R}, \mathcal{K}) \tag{5}$$

is a bijection and $\mathcal{M}_\pm \subset L^2(\mathbb{R}_+, \mathcal{K}, \mathrm{d}E)$ *are dense in* $L^2(\mathbb{R}_+, \mathcal{K}, \mathrm{d}E)$.

In principle, to establish (5) the quotation of the result of van Winter is sufficient (it is related to this special case). However, only the much more deeper result of Kato brings into light the geometric roots of the matter.

4. Construction of scattering states with time asymmetric properties

Next we define the linear manifolds

$$\mathcal{F}_\pm := \Phi^{-1}\mathcal{M}_\pm \subset \mathcal{H}. \tag{6}$$

Then we obtain

Theorem. *The evolution* $\mathbb{R} \ni t \rightarrow \mathrm{e}^{-\mathrm{i}tH}$ *together with* $\mathcal{F}_\pm$ *satisfy the following properties:*

(i) The linear submanifolds $\mathcal{F}_\pm \subset \mathcal{H}$ *are dense in* $\mathcal{H}$ *w.r.t. its Hilbert space topology.*

(ii)

$$\mathrm{e}^{-\mathrm{i}tH} = \Phi^{-1}P_+FT(t)F^{-1}P_+\Phi, \qquad t \in \mathbb{R}.$$

(iii) Let $f_\pm \in \mathcal{F}_\pm$ *and* $g_\mp := F^{-1}P_+^{-1}\Phi f_\pm \in P_\mp L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$. *Then the assignment*

$$\mathcal{F}_\pm \ni f_\pm \leftrightarrow g_\mp \in P_\mp L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}x)$$

is a bijection, i.e. the scattering states $f_\pm$ *are bijectively represented by* $g_\mp$ *which are incoming/outgoing vectors w.r.t. the shift evolution.*

(iv) Correspondingly, the dense linear manifolds $\mathcal{F}_\pm$ *are incoming/outgoing manifolds w.r.t. the (quantum-mechanical) evolution* $\mathbb{R} \ni t \rightarrow \mathrm{e}^{-\mathrm{i}tH}$, *i.e.*

$$\mathrm{e}^{-\mathrm{i}tH}\mathcal{F}_+ \subseteq \mathcal{F}_+, \qquad t \leqslant 0,$$
$$\mathrm{e}^{-\mathrm{i}tH}\mathcal{F}_- \subseteq \mathcal{F}_-, \qquad t \geqslant 0.$$

Proof. (i) Obvious from the corollary. (ii) Obvious from (1) and (4). (iii) Obvious from the corollary. (iv) Obvious from (2) and (3). □

Remark

(i) Note that $\mathcal{F}_+ \cap \mathcal{F}_-$ is still dense in $\mathcal{H}$, i.e. there is a dense set of distinguished scattering states which are simultaneously incoming and outgoing for the quantum evolution (see [13]).

(ii) The construction of $\mathcal{F}_\pm$ uses only an isometric operator realizing the unitary equivalence of $\mathrm{e}^{-\mathrm{i}tH}$ and $\mathrm{e}^{-\mathrm{i}tM_+}$, the wave operators are not required, as well as Schwartz space arguments.

(iii) Mathematically speaking, the rational content and meaning of time asymmetric quantum mechanics is given by property (iv) of the theorem, i.e. there are dense linear manifolds of scattering states such that the restriction of the quantum-mechanical evolution onto these manifolds still acts as a semigroup for $t \geqslant 0$ or $t \leqslant 0$. However by this restriction the spectral structure of the semigroup evolutions changes totally such that there is no connection with the spectral structure of the Hamiltonian respectively the quantum-mechanical evolution. The conclusion is that TAQM and the (spectral) theory of resonances have to be sharply distinguished.

5. Resonances

The fact mentioned in (iii) of the remark, i.e. that the spectral structure of the semigroups

$$\mathbb{R}_{\mp} \ni t \to \mathrm{e}^{-\mathrm{i}tH} \restriction \mathcal{F}_{\pm} \tag{7}$$

and the spectral structure of the quantum evolution are completely different influences strongly the theory of the resonances. Strictly speaking, the restriction to the semigroups prevents an approach to establish the spectral properties of the resonances in dependence of the selfadjoint operator H. In the following it is pointed out that the semigroups cannot contribute to a characterization of the resonances.

The manifolds $\mathcal{F}_{\pm}$ are even Hilbert spaces w.r.t. stronger norms suggested by the corollary:

$$\mathcal{F}_{\pm} \ni f_{\pm} \to \|f_{\pm}\|_{\pm} := \|P^{-1}\Phi f_{\pm}\|, \tag{8}$$

where $\|\cdot\|$ denotes the Hilbert norm of $L^2(\mathbb{R}, \mathcal{K}, \mathrm{d}E)$. Note that $P^{-1}\Phi f_{\pm} \in \mathcal{H}^2_{\pm}(\mathbb{R}, \mathcal{K})$, i.e. the $\mathcal{F}_{\pm}$, considered as Hilbert spaces w.r.t. norm (8) are canonically isomorphic to $\mathcal{H}^2_{\pm}(\mathbb{R}, \mathcal{K})$. The semigroups (7) are strongly continuous w.r.t. norm (8). The inspection of the spectral theory of these semigroups yields the following result: the spectrum of the semigroup corresponding to $\pm$ is the closure of its pure point spectrum $\mathbb{C}_{\pm}$ (see e.g. [12]). This shows explicitly that the spectral structure of these semigroups has changed dramatically as compared with that of H. Already this fact indicates that they are unsuitable for a spectral characterization of the resonances in terms of H.

If one takes no note of this indication and wants to use the TAQM-semigroups and their Hilbert spaces as basic objects for this aim, one has to start with a Gelfand triplet, say in the +-case

$$\tilde{\mathcal{G}}_+ \subset \mathcal{H} \subset \tilde{\mathcal{G}}_+^{\times}, \qquad \tilde{\mathcal{G}}_+ \subseteq \mathcal{F}_+,$$

because (usually) resonances are nonreal and their spectral characterization as generalized eigenvalues requires extension techniques of this type. For convenience we work in the spectral representation, i.e.

$$\tilde{\mathcal{G}}_+ \subset L^2(\mathbb{R}_+, \mathcal{K}, dE) \subset \tilde{\mathcal{G}}_+^{\times}, \qquad \tilde{\mathcal{G}}_+ \subseteq \mathcal{M}_+, \tag{9}$$

where $\tilde{\mathcal{G}}_+$ is still invariant w.r.t. the semigroup $\mathbb{R}_+ \ni t \to \mathrm{e}^{\mathrm{i}tM_+}$. According to the corollary this ansatz is equivalent with

$$\mathcal{G}_+ \subset \mathcal{H}^2_+(\mathbb{R}, \mathcal{K}) \subset \mathcal{G}_+^{\times}, \qquad \mathcal{G}_+ \subseteq \mathcal{H}^2_+(\mathbb{R}, \mathcal{K}), \tag{10}$$

where $\mathcal{G}_+$ is still invariant w.r.t. the semigroup $\mathbb{R}_+ \ni t \to \mathrm{e}^{\mathrm{i}tM}$, like $\mathcal{H}^2_+(\mathbb{R}, \mathcal{K})$ itself. Then an extension of $\mathrm{e}^{-\mathrm{i}tM}$ w.r.t. triplet (10) is given by $(\mathrm{e}^{-\mathrm{i}tM})^{\times}$, defined by

$$\langle g_+|(\mathrm{e}^{-\mathrm{i}tM})^{\times} g_+^{\times}\rangle := \langle \mathrm{e}^{\mathrm{i}tM} g_+|g_+^{\times}\rangle, \qquad g_+ \in \mathcal{G}_+, g_+^{\times} \in \mathcal{G}_+^{\times}.$$

Now the Hardy functions $f \in \mathcal{H}^2_+(\mathbb{R}, \mathcal{K})$ are special continuous antilinear forms on $\mathcal{G}_+$ and one has in this case

$$\langle \mathrm{e}^{\mathrm{i}tM} g_+|f\rangle = (\mathrm{e}^{\mathrm{i}tM} g_+, f) = (g_+, \mathrm{e}^{-\mathrm{i}tM} f) = (g_+, Q_+\mathrm{e}^{-\mathrm{i}tM} Q_+ f), \qquad g_+ \in \mathcal{G}_+. \tag{11}$$

In other words, for $f \in \mathcal{H}^2_+(\mathbb{R}, \mathcal{K})$ the 'extension' of $e^{-itM}\lceil\mathcal{H}^2_+, t \geqslant 0$ (note that these operators do not form a semigroup w.r.t. $t \in \mathbb{R}_+$) is nothing else than the semigroup

$$\mathbb{R}_+ \ni t \to Q_+ e^{-itM}\lceil\mathcal{H}^2_+(\mathbb{R}, \mathcal{K}), \tag{12}$$

which is the adjoint semigroup of $\mathbb{R}_+ \ni t \to e^{itM}\lceil\mathcal{H}^2_+(\mathbb{R}, \mathcal{K})$. The spectral theory of this semigroup is well known. Its spectrum is the closure of its eigenvalue spectrum which coincides with the lower half-plane $\mathbb{C}_-$. The eigenspace corresponding to $\zeta \in \mathbb{C}_-$ is given by the subspace of all vectors

$$e_\zeta(E) := \frac{k}{E - \zeta}, \qquad k \in \mathcal{K}, \tag{13}$$

(see e.g. [12]). That is, already if one chooses $\mathcal{G}_+ := \mathcal{H}^2_+(\mathbb{R}, \mathcal{K})$, *all* points of the lower half-plane are 'generalized' eigenvalues with eigenspace (13) and it is not hard to see that by enlarging the set of continuous antilinear forms by the choice of a smaller Gelfand space $\mathcal{G}_+$ (e.g. by the requirement that the elements of $\mathcal{G}_+$ are Schwartz space functions) the manifold of 'generalized' eigenvectors w.r.t. an eigenvalue $\zeta \in \mathbb{C}_-$ cannot be enlarged.

The conclusion is that the Gelfand triplet approach finally leads to the spectral theory of (12), which is in [12] called the *characteristic semigroup*, and that $\mathcal{H}^2_+(\mathbb{R}, \mathcal{K})$ itself is sufficient to determine all relevant 'generalized' eigenvalues and eigenvectors. In other words: this approach applied to the TAQM-semigroups is unsuitable to obtain a characterization of the resonances of the quantum evolution because *all points* of the lower half-plane (in the +-case) appear as eigenvalues such that the resonances cannot be distinguished by this method. Therefore a spectral characterization of the resonances requires an inspection of the spectral theory of the Hamiltonian H and an ansatz with Gelfand triplets for H itself. (Note that the defining property of the resonances to be poles of the scattering matrix does not relate this concept to a single Hamiltonian H but to the vast class of all H which have the same scattering operator, see Wollenberg's theorem [5].)

For central-symmetric potentials with compact support and $l = 0$ this program is pointed out and a solution is presented in [13], for the finite-dimensional Friedrichs model on the half-line in [14–16].

On the other hand already the defining property of the resonances implies relations to the distinguished TAQM in/out-manifolds related to H_0. Without restriction of generality these manifolds can be assumed to be $\mathcal{M}_\pm$, this means that H_0 is identified with M_+. A relation of this type reads

$$\int_{-\infty}^{0} (f_+(\lambda), S(\lambda)g_-(\lambda))_\mathcal{K} d\lambda + (f_+, Sg_-) = -2\pi i \sum_\zeta (f_+(\overline{\zeta}), S_\zeta g_-(\zeta))_\mathcal{K}, \tag{14}$$

where $f_+ \in \mathcal{M}_+, g_- \in \mathcal{M}_-, E \to S(E)$ is holomorphic on $\mathbb{R}_+$ and it is analytically continuable into the complex plane. ζ runs through all poles of $S(\cdot)$ in the lower half-plane and S_ζ denotes the residuum of $S(\cdot)$ at the pole ζ. This relation is a simple application of the residual calculus and can be proved if $S(\cdot)$ satisfies suitable conditions at infinity and $\lambda = 0$ and if there are no resonances on $\mathbb{R}_-$. The term $\int_{-\infty}^{0} (f_+(\lambda), S(\lambda)g_-(\lambda))_\mathcal{K} d\lambda$ is sometimes called the 'background integral' (see e.g. [1]). Relations of type (14) and other similar relations are presented in [13] for the model considered there.

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