IRREVERSIBILITY IN QUANTUM MECHANICS

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Received 19 January 2004

Time asymmetry and irreversibility are signal features of our world. They are the reason of our aging and the basis for our belief that effects are preceded by causes. These features have many manifestations called arrows of time. In classical physics, some of these arrows are described by the increase of entropy or probability, and others by time-asymmetric boundary conditions of time-symmetric equations (e.g., Maxwell or Einstein). However, there is some controversy over whether probability or boundary conditions are more fundamental. For quantum systems, entropy increase is usually associated with the effects of an environment or measurement apparatus on a quantum system and is described by the von Neumann-Liouville equation. But since the traditional (von Neumann) axioms of quantum mechanics do not allow time-asymmetric boundary conditions for the dynamical differential equations (Schrödinger or Heisenberg), there is no quantum analogue of the radiation arrow of time. In this paper, we review consequences of a modification of a fundamental axiom of quantum mechanics. The new quantum theory is time asymmetric and accommodates an irreversible time evolution of isolated quantum systems.

1. Introduction

The study of irreversibility was a key focus of much of Prigogine's long and fruitful research career. Indeed, he often forcefully emphasized the mismatch between time-symmetric theories, on the one hand, and a world full of irreversible processes on the other.

Conventional quantum mechanics is such a time-symmetric theory. This means that solutions to the fundamental dynamical differential equations (Heisenberg and Schrödinger) are time-reversal invariant. That is to say, if $\phi(t)$ is a solution of the equations of motion, then so is $\phi(-t)$. In the conventional formulation of nonrelativistic quantum mechanics, these evolutions are taken to be governed by a one-parameter group of unitary operators

$$U(t) = e^{-iHt}, \quad -\infty < t < +\infty, \tag{1.1}$$

Discrete Dynamics in Nature and Society 2004:1 (2004) 75–83
2000 Mathematics Subject Classification: 47A70, 34L25
URL: http://dx.doi.org/10.1155/S1026022604401046

where H represents the selfadjoint Hamiltonian, and Planck's constant has been set to one.

In contrast to this picture, prominently emphasized in textbooks (e.g., by focusing almost exclusively on phenomena such as stationary states or cyclic evolutions), the physics of our world is, in the main, time asymmetric. In order to overcome this conflict, two approaches have been used. One of them is based on the idea that irreversible systems are never isolated but interact with the environment (so-called extrinsic irreversibility). For quantum mechanical systems, this approach implies that the evolution takes place in a Hilbert space (HS) which is a tensor product of the HS of the system and the HS of the environment, where the environment can act on the quantum system, but the quantum system does not act back on the environment. Then, the projection of the evolution operator into the former space may provide the irreversible evolution of this system.

The second approach to irreversible processes in quantum physics, defended by Prigogine, has its origin in the dynamical nature of the system itself without relying on any external interaction (so-called intrinsic irreversibility). Then, the question arises as to how it is possible to reconcile the irreversible behavior with the time-symmetric character of the dynamical differential equations, in particular with the Schrödinger equation. The resolution of this dilemma is given by noting that the dynamics of a system is not only solely determined by its differential equations of motion, but also by boundary conditions.

Typical irreversible processes in quantum mechanics are phenomena involving resonances and decay. Resonances are usually produced in scattering experiments, either in nature or in the laboratory. In addition, we can envisage irreversible scattering processes even without production of resonances, as in the scattering of two uncorrelated plane waves that emerge, after collision, as correlated spherical waves. But, the study of irreversibility in scattering phenomena is particularly important.

Here, we review recent developments in time-asymmetric quantum mechanics in scattering. In Section 2, we discuss time asymmetry in quantum mechanics, emphasizing quantum time arrows associated with scattering resonances and the need for a time-asymmetric generalization of quantum theory. We then give a brief overview of the necessary generalization, the rigged HS formulation of quantum mechanics, in Section 3, and conclude by highlighting some current work and prospects in Section 4.

2. Time asymmetry in quantum mechanics

Although textbooks in quantum mechanics focus mainly on stationary states of energy E_s, the vast majority of quantum states are quasistable. The latter resonance and decaying states are characterized by a resonance energy E_R (or resonance mass M in the relativistic case) and a resonance width Γ. Both of these features are combined to form the complex energy $z_R = E_R - i\Gamma/2$, which appears in the Breit-Wigner energy distribution. From this viewpoint, the difference between unstable and stable particles is that the latter have zero widths. Generally, particles decay unless there are selection rules for some quantum numbers preventing decay, so stable particles are relatively rare in comparison with the number of quasistable particles of interest in high energy and other areas of physics. So

there is every reason to consider quasistable particles on a par with stable particles as autonomous microphysical systems. Whereas stable particles are described by state vectors in HS, in von Neumann HS quantum mechanics there are no state vectors capable of describing resonances. So any generalization of quantum theory should also include generalized eigenvectors, such as Gamow vectors, with energy eigenvalues z_R. It must also support a natural analytic continuation into the complex energy plane required by such generalized eigenvectors. This analytic continuation is a familiar requirement of S-matrix theory [24, 30].

Furthermore, decaying phenomena like quasistable particles obey an exponential decay law. However, in conventional HS quantum mechanics, by theorem there exist no HS vectors corresponding to exact exponential time evolution [22, 23]. This means that, for example, Gamow and Dirac vectors, which have proven very useful for representing decaying phenomena, are not elements of the standard HS framework for quantum mechanics. Any time-asymmetric generalization of quantum theory should contain such elements and provide a rigorous derivation of the exponential decay law.

Clearly, quasistable particles and resonances have finite lifetimes, so the initial and boundary conditions suitable for describing such phenomena must be formulated for finite times. Additionally, intrinsically irreversible phenomena, such as kaon decay, require time-asymmetric initial and boundary conditions for their description. But conventional HS quantum mechanics accommodates neither finite-time nor time-asymmetric initial and boundary conditions. A time-asymmetric generalization of quantum theory naturally accommodates such conditions [7, 10, 13].

As a concrete example of time asymmetry in quantum mechanics, consider a simple scattering experiment consisting of an accelerator, which prepares a projectile in a particular state, a target, and detectors. The total Hamiltonian modeling the interaction of the particle with the target is $H = H_0 + V$, where H_0 represents the free particle Hamiltonian and V the potential in the interaction region. Scattering resonances are defined by the resonance poles of the analytically continued S-matrix [15, 24, 30]. Gamow vectors need to be associated with these resonance poles.

Following Ludwig [25, 26], an in-state of a particular quantum system (conceived of as an ensemble of individual systems such as each elementary particle) is prepared by a preparation apparatus (considered a macrophysical system). The detector (also considered to be macrophysical) registers the post-interaction particles, also called out-states. There is a natural quantum mechanical arrow of time associated with resonance scattering known as the *preparation/registration* arrow [8, 9]. The key intuition behind this arrow is that no observable properties can be measured in a state until the state has been prepared. For example, it makes no sense to speak of a measurement of an observable such as decay products in a detector at a particular scattering angle until there is a state prepared by the accelerator. The time $t = 0$ marks the moment in time at which the state preparation is completed and the registration of detector counts can begin (any detector counts before this time are discarded as noise). One of the consequences of the preparation/registration arrow is that some mathematical operations definable in HS are nonsensical. For example, one can calculate nonzero expectation values for an observable for $t < 0$ [21], meaning that an observable is predicted to have a nonzero expectation value

before the state has been prepared. Whereas the preparation/registration arrow embodies finite-time and time-asymmetric initial and boundary conditions, such conditions cannot be accommodated in HS. For example, in the case of scattering, one standard condition in HS is that states are not interacting with the scattering center in the asymptotic regime at $t \to -\infty$. Of course, this condition is unrealistic as the particles crucial to the experiment have yet to be created or properly prepared until some finite time before the interaction, but the mathematics of HS cannot accommodate realistic finite-time conditions.

The preparation/registration arrow also leads to a natural partition of mathematical spaces used to represent the time-asymmetric dynamics of scattering [7, 8, 9, 10, 13]. Sets of growing vectors and their associated semigroups represent the preparation of states by some apparatus defined in a vector space for $t < 0$, while sets of decaying vectors and their associated semigroups represent detectable observables defined in another vector space for $t > 0$. Semigroups are the kinds of evolution operators suitable for intrinsically irreversible phenomena, but it is not possible to have semigroup evolutions in von Neumann HS quantum mechanics unless one is dealing with open quantum systems (extrinsic irreversibility) [16]. So any time-asymmetric generalization of quantum theory should have semigroups as standard equipment so to speak.

A second-time arrow describing intrinsically irreversible dynamics, also resulting in semigroup evolutions, was proposed by George [20] and has been applied by Prigogine and coworkers to scattering phenomena [2]. This time arrow is defined by considering excitations to be events taking place before $t = 0$, while de-excitations are considered to be events taking place after $t = 0$. The Brussels-Austin arrow also leads to a natural splitting of mathematical spaces: excitations (e.g., formation of unstable states) and their associated semigroups are defined in one vector space for $t \leq 0$, and de-excitations (e.g., decay of unstable states) and their associated semigroups are defined in another vector space for $t \geq 0$. Although the excitation/de-excitation time arrow is more general than the preparation/registration time arrow, the two arrows have an interesting relationship and differ somewhat with respect to causality [3].

3. Time-asymmetric quantum theory of resonances and decay

Rigged Hilbert space (RHS) theories of quantum mechanics were originally developed [1, 5, 27, 29] in order to make the Dirac formalism of quantum mechanics mathematically rigorous [1, 5, 6, 27, 29]. An RHS or Gel'fand triplet [18, 19] is a triple of spaces

$$\Phi \subset \mathcal{H} \subset \Phi^{\times}, \tag{3.1}$$

where $\mathcal{H}$ is an HS with the standard norm topology $\tau_{\mathcal{H}}$, Φ is a vector space dense in $\mathcal{H}$ with a topology τ_{Φ} stronger than $\tau_{\mathcal{H}}$, and $\Phi^{\times}$ is the dual space of continuous antilinear functionals on Φ. Although this means that the limit points of converging Cauchy sequences are different in the three spaces, each space has properties allowing the kinds of manipulations to which physicists are accustomed from HS quantum mechanics. In particular, the very useful Dirac bra-ket formalism can be given a rigorous justification

within RHS, something that cannot be done on the basis of HS [1, 5, 27, 29]. For the Dirac kets, one usually chooses as Φ the Schwartz space.

Within the RHS framework, but using Hardy spaces in place of the Schwartz space, the exponential decay law can be made rigorous. The resonance lifetime τ_R of the exponential decay law and the width Γ of the Breit-Wigner energy distribution of a Gamow vector are conceptually and experimentally different quantities, but the identification of Γ with $1/\tau_R$ can be made rigorous in RHS quantum mechanics [7, 10, 13]. The Schwartz space and its dual are insufficient to describe decaying Gamow kets with complex eigenvalue $z_R = E_R - i\Gamma/2$, nor can the Schwartz space accommodate the plane wave solutions of the Lippmann-Schwinger equations $|E^{\pm}\rangle = |E \pm i\varepsilon^{\pm}\rangle$ which fulfill incoming and outgoing boundary conditions expressed by the infinitesimal imaginary part $+i\varepsilon$ and $-i\varepsilon$, respectively. Here, one needs Hardy spaces [7, 10, 13].

Boundary conditions can be imposed by careful analysis of scattering experiments. Any scattering process includes three parts: the preparation of a state to undergo scattering, the scattering itself, and the observation (or registration) of the scattering products (note that scattering is a natural process that does not require an observer to participate). Taking these stages into consideration allows us to define the boundary conditions using the following ideas.

(1) Causality conditions imply that no scattering products can be detected until the scattering has taken place and, therefore, until the scattering state has been prepared by a preparation apparatus (cf., preparation/registration arrow).

(2) The study of particular natural processes, such as the decay of the neutral kaon K^0, shows that the time t_0, at which the formation of the decaying state is completed and the decay starts, is meaningful [11, 12, 21]. This privileged value of time t_0 does not make sense in the conventional HS formulation of quantum mechanics, which does not distinguish any particular finite value of time because time evolution is given by the one-parameter group (1.1) with time evolving from $-\infty$ to ∞.

(3) A theorem by Hegerfeldt [21] shows that if the decay probability is zero in any time interval, then it is zero for all time if the decaying state is mathematically represented as a normalizable HS vector. On the other hand, causality implies that there is no decay before the time t_0 at which the formation of a resonance state is completed. Therefore, causality implies for an HS state that the decay probability be zero for all times. This means there is no HS state vector that starts decaying after the big bang.

(4) The basic elements of any physical theory are states and observables. In quantum mechanics, both are represented by operators on HS. For our scattering processes, prepared pure states are given by operators of the form $\rho^{\text{in}} = |\phi\rangle\langle\phi|$. After scattering has taken place, the observed scattering products are the projection P of the outgoing states in the region where the detection apparatus is located. If this projection is given by P, the registered observables are of the form $\eta^{\text{out}} = |\psi\rangle\langle\psi|$, with $\psi = P\psi^{\text{out}}$ and $\psi^{\text{out}} = S\phi$, where S is the scattering operator, and the set of vectors ψ does not need to be the whole HS.

In the HS formulation of von Neumann, this distinction cannot be made since the space of prepared states and the space of registered observables are the same. This is a consequence of the HS axiom, or the hypothesis of asymptotic completeness [7, 10]. If

one uses the RHS formulation of scattering theory, then the distinction between states and observables can be made in a very natural way. These considerations show that there is a conflict between the usual HS formulation of quantum mechanics (and/or asymptotic completeness) and causality.

Following this analysis, we can formulate appropriate boundary conditions for scattering phenomena:

(i) the set of preparable states $\{\phi\}$ is given by vectors ϕ of a space Φ_- so that $\rho^{\text{in}} = |\phi\rangle\langle\phi|$. As functions of the energy, the vectors in Φ_- are represented by Hardy functions analytic on the lower half of the complex plane (of the second sheet of the Riemann surface for the S-matrix);

(ii) the set of registrable observables $\{\psi\}$ is given by vectors ψ of a space Φ_+ so that $\eta^{\text{out}} = |\psi\rangle\langle\psi|$. As functions of the energy, the vectors in Φ_+ are represented by Hardy functions on the upper half of the complex plane.

Boundary conditions (i) and (ii) are a refinement of von Neumann's axiom on the nature of states and observables. In this refinement, not all states are vectors of $\mathcal{H}$, but only those in a dense set $\Phi_- \subset \mathcal{H}$ so that any vector in $\mathcal{H}$ can be approximated with arbitrary accuracy by a vector in the new space of states Φ_-. Thus, there is no experimental distinction between von Neumann's states and Hardy space states $\phi \in \Phi_-$. But the choice of the boundary conditions $\phi \in \Phi_-$ for the solutions of the Schrödinger equation eliminates the conflict with the causality condition. For the observables that fulfill the Heisenberg equation of motion, the boundary condition is $\psi \in \Phi_+$. These boundary conditions lead naturally to two separate RHSs for prepared states and observables [7, 10, 13]:

$$\Phi_- \subset \mathcal{H} \subset \Phi_-^\times, \qquad \Phi_+ \subset \mathcal{H} \subset \Phi_+^\times. \tag{3.2}$$

In the energy representation, Φ_- is the Hardy space of the lower complex energy half-plane intersected with the Schwartz class functions, and Φ_+ is the Hardy space of the upper complex energy half-plane intersected with the Schwartz class functions [7, 10]. Using this framework, a rigorous time-asymmetric theory of scattering can be worked out consistent with and extending the results of Lax and Phillips [24].

Time-asymmetric boundary conditions could not be introduced in the context of HS as they require an extension of HS to RHS [7, 10, 13]. In RHS, the group law for the evolution operator is, in general, no longer valid. As a consequence of the Hardy space axioms (3.2), time evolution is given by a semigroup valid for $t \geq 0$. For the semigroup $U_-(t) = e^{iH_-t}$ on Φ_-, there exists no inverse on Φ_-. Likewise, for the semigroup $U_+(t) = e^{iH_+t}$ on Φ_+, there exists no inverse on Φ_+.

Replacing the HS axiom with the Hardy space axioms leads to the following.

(1) We can fix the preparation time $t = 0$ as the time at which the state of a resonance is formed and starts to decay. The time evolution of resonance states then only makes sense for $t > 0$. Therefore, decay products cannot be observed before the resonance has been formed at $t = 0$, so causality is preserved.

(2) The time of formation of a resonance t_0 is meaningful and identified with $t_0 = 0$.

(3) No decay probability makes sense for $t < 0$ as there is no evolution for the decaying state (or scattered state) before $t = 0$. Hence, the Hegerfeldt problem [21] does not arise.

(4) The RHS formalism allows a clear distinction between prepared states and registered observables.

The semigroup evolution makes the theory irreversible since it predicts the quantum probabilities $|(\psi(t),\phi)|^2 = |(\psi,\phi(t))|^2$ only for time $t \geq 0$. This has been achieved by adding to the equations of motion the boundary conditions arising from the analysis of scattering experiments. Usually, when one uses Dirac kets $|E\rangle$ and gives them a mathematical definition, one uses the RHS (3.1), where $|E\rangle \in \Phi^{\times}$. However, when Hardy spaces are involved, as in (3.2), there are two kinds of energy eigenkets, $|E^+\rangle \in \Phi_-^{\times}$ and $|E^-\rangle \in \Phi_+^{\times}$ such that $|E^+\rangle$ represents the in-plane wave solutions of the Lippmann-Schwinger equation and $|E^-\rangle$ represents the out-plane wave solutions. Time asymmetry is then a consequence of (3.2). (In the case where Φ in (3.1) is the Schwarz space, the dynamical differential equations (Heisenberg and Schrödinger) integrate—as in conventional HS—to a unitary group and would not result in time asymmetry.)

4. Summary and new ideas

The RHS generalization of quantum theory using the Hardy RHS (3.2) is time asymmetric, but differs from the usual HS quantum theory only in the axioms regarding the asymptotic completeness of the mathematical spaces. Otherwise, the usual axioms of quantum theory to which physicists are accustomed remain unchanged and the mathematical tools remain much the same (e.g., inner products and linear operators). In contrast to the von Neumann HS framework, the RHS framework allows a rigorous formulation of the familiar ingredients of scattering and decay theory such as Gamow vectors, Lippmann-Schwinger (in- and out-plane wave) kets, the Breit-Wigner resonance amplitude, and the analytically continued S-matrix and its resonance poles.

More recently, the RHS framework has also proven useful for the study of relativistic resonances. In particular, the framework makes it possible to resolve the problem of mass and width definitions of Z^0 and other relativistic resonances [11, 12].

As mentioned in Section 2, the RHS framework naturally accommodates semigroup evolutions and time's arrow. Although only the forward-directed evolutions have been discussed here, a backward-directed set of evolutions are also mathematically possible in the RHS framework [3, 14, 17]. It has been speculated that the backward-directed evolutions and corresponding states might correspond abstractly to the domain of mental systems, while the forward-directed evolutions and corresponding states would correspond to the domain of material systems [4]. The key idea in this proposal is that these two domains might emerge from a more fundamental domain that is neutral with respect to any mental-material distinction and, as such, could represent a concrete realization of some of the ideas of Pauli and Jung [28]. And with these general speculations, of which Ilya was so fond and at which he was so good, we conclude our paper dedicated to his memory.

Acknowledgments

The first author would like to thank the Alexander von Humboldt Foundation as well as the Federal Ministry of Education and Research and the Program for the Investment in

the Future of the German Government for generous support. Financial support from the Junta de Castilla y Leon, Project VA 085/02, and the FEDER-Spanish Ministry of Science and Technology Projects DGI BMF 2002-0200 and DGI BMF2002-3773 is also acknowledged.

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