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There Are Quantum Jumps

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Abstract: In this communication we take up the age-old problem of the possibility to incorporate quantum jumps. Unusually, we investigate quantum jumps in an extended quantum setting, but one of rigorous mathematical significance. The general background for this formulation originates in the Balslev-Combes theorem for dilatation analytic Hamiltonians and associated complex symmetric representations. The actual jump is mapped into a Jordan block of order two and a detailed derivation is discussed for the case of the emission of a photon by an atom. The result can be easily reassigned to analogous cases as well as generalized to Segrè characteristics of arbitrary order.

Keywords: dilation analytic family of operators; complex symmetric representation; Segrè characteristic; Jordan block

1. Introduction

In Walter Moore's celebrated Biography, Schrödinger life and thought [1], he reproduces the famous and passionate discussion between Bohr and Schrödinger during the latter's visit to Copenhagen in 1926. Schrödinger: "*You surely must understand, Bohr, that the whole idea of quantum jumps necessarily leads to nonsense.*" Bohr: "*Yes, in what you say, you are completely right. But that doesn't prove that there are no quantum jumps.*" Finally, Schrödinger: "*If we are still going to have to put up with these damn quantum jumps, I am sorry that I ever had anything to do with quantum theory.*"

The problem was reiterated by Schrödinger [2] in 1952, but without a definite resolution, see, e.g., Bell's reappraisal of the conundrum in the Centenary Celebration of the birth of the famous

scientist [3]. Although John Bell did borrow the same title as in [2], viz.: *Are there quantum jumps?* his answer was focused on physical models that propose such events as "local beables" of the theory leading, as discussed in an adjoined appendix, to reasonable probability time factors. Nevertheless such theories are only approximately Lorentz invariant besides assuming a non-fundamental jump scenario as an extra hypothesizing ingredient.

In the present contribution we will make use of the recent advances in non-Hermitian quantum mechanics [4–6] to demonstrate that a quantum jump can easily be bequeathed and controlled by rigorous mathematical techniques [7]. For the demonstration, we will first discuss a general situation, where an extended complex symmetric representation exhibits a so-called Jordan block, *i.e.*, a degenerate condition with a Segrè characteristic larger than one. To make this note self-contained a brief summary of a rigorous non-self-adjoint extension of standard Hermitian quantum mechanics is given in the Appendix. The theoretical approach [7] is particularly relevant for the present "jump scenario". In addition we portray the theoretical emergence and distinct role played by Jordan blocks and their associated physical consequences, including the importance played by the so-called Segrè characteristics of the actual degeneracy with particular significance for the process of decoherence.

To entrench a realistic setting, we will discuss, in some detail, the emission of a photon by an atom in which the "jump" follows as a rigorous consequence of the formulation without the need for making additional assumptions. Yet, the quantum transition, *i.e.*, the mechanism behind the excited atom in its spontaneous interaction with its environment, is properly specified and not portrayed as an instantaneous event, see, e.g., the classical book of Macomber [8]. Finally, the case of arbitrarily large Segrè characteristics is briefly mentioned [9] as well as generalizations to other "jump" scenarios.

2. Level Crossings by Analytic Extensions

Since there is a close connection between degeneracies and level crossings in atomic and molecular physics, see also the popular concept of conical intersections in photo-induced chemical dynamics [10], it is convenient to start with a simple 2×2 matrix and analyse its properties under the condition of a degeneracy.

Two extensions are of principal importance: (i) the Hamiltonian should belong to a self-adjoint family of dilation analytic operators—the latter a common characteristic of molecular problems in chemical physics, and (ii) the crossings should be discussed within a general multi-dimensional partitioning framework, for more details see references [11,12]. Within this framework we start out with the Hamiltonian matrix, illustrating a general quantum chemical system with dilatation analytic potentials (more details will be given in the next section), parameterized as follows

$$\begin{pmatrix} H_{11} & -iv \\ -iv & H_{22} \end{pmatrix} \tag{1}$$

where $H_{12} = H_{21} = -iv$ display the complex symmetric property of the representation, while the "$-i$" is just convention. We will return to this feature later on, when analytic continuation onto the so-called unphysical Riemann-sheet is administered. It is also trivial to invoke the generality of a partitioned effective Hamiltonian expressed as ($i, j = 1,2$)

$$H_{ij}(\varepsilon) = \overline{H}_{ij} + \overline{H}_{ib}(\varepsilon I_{bb} - \overline{H}_{bb})^{-1}\overline{H}_{bj} \tag{2}$$

with the $\overline{H}_{bb}, \overline{H}_{ib}, \overline{H}_{bj}$ being the appropriate partitions of an arbitrarily large *n*-dimensional matrix $\overline{H}$, assuming a unit metric and with ε finally becoming the eigenvalue (here assumed degenerate) of the matrix relation $Hc = Ec$ by solving the associated 2×2 secular equation for $\varepsilon = E$. Since the energy might be complex, we will use the notation $\varepsilon = E - i\epsilon$ for the general case. The eigenvalue relation corresponding to a degeneracy of Equation (1) is given by

$$\lambda_{\pm} = \tfrac{1}{2}\mathrm{Tr}\{H\} \pm \tfrac{1}{2}\sqrt{\mathrm{Tr}\{H\}^2 - 4\mathrm{Det}\{H\}} \tag{3}$$

and with $\lambda_+ = \lambda_- = \varepsilon$ provided

$$(H_{11} - H_{22})^2 = 4v^2 \tag{4}$$

This relation has an interesting solution in addition to he standard diagonal one, in that the eigenvalue $\varepsilon = \tfrac{1}{2}(H_{11} + H_{22})$ actually displays a Jordan block with Segrè characteristic equal to two, *i.e.*,

$$\begin{pmatrix} H_{11} & -iv \\ -iv & H_{22} \end{pmatrix} \rightarrow \begin{pmatrix} \varepsilon & 2v \\ 0 & \varepsilon \end{pmatrix} \tag{5}$$

under a similarity transformation to be decided below. In actual fact the formulation in Equation (5) is unitary and it follows simply, by rewriting $H_{11} = \varepsilon + v$; $H_{22} = \varepsilon - v$, and with I the unit matrix, that one obtains

$$H = \varepsilon I + 2vQ \tag{6}$$

with

$$Q = \tfrac{1}{2}\begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} \tag{7}$$

which under the unitary transformation U becomes

$$U^\dagger Q U = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = C \tag{8}$$

with

$$U = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}; \quad U^\dagger = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \tag{9}$$

displaying an eigenvector, the first column of U corresponding to the eigenvalue zero of Q, and the linearly independent, orthogonal vector, the root eigenvector, building up the unitary transformation. Introducing an orthonormal basis $|f\rangle = |f_1, f_2\rangle$, using the sesquilinear Dirac bra-ket notation, for the complex symmetric representation, our simple matrix problem reduces to, defining $|f\rangle U = |k\rangle$,

$$|f\rangle Q\langle f| = |k\rangle U^\dagger Q U\langle k| = |k_1\rangle\langle k_2| \tag{10}$$

Note, that according to Equation (5), the environment has "loaned" a virtual energy amount v to the system, which is "paid back", see the canonical form to the right of the arrow in Equation (5), and the "total transaction registered" in the (1,2) element above the diagonal. Although this is a rather straightforward derivation one needs to find the actual representations of the basis $|f\rangle$ and $|k\rangle$. This is moreover a choice that cannot be selected at will, since it depends on each specific case as will be seen in the next section.

3. The Case of Photon Emission by an Atom

In Macomber's book [8] on spectroscopic transitions, he asks the question: "*How does a photon get into an atom?*" In the same way as one wants to know the detailed mechanism, by which the electric field causes the atom to accept the energy or the photon, one would also want to understand how the atom, in its interaction with the environment gets aggravated to divulge the photon and return to a lower spectroscopic state. In this portrait, relaxation times, sizes and shapes enter the description.

For instance the emission of a photon by an atom is not an instantaneous event. Consider, e.g., the D_1 transition in rubidium, one of the two D-lines in ^{87}Rb (neglecting fine structure). The atom has a 5s electron outside a krypton closed shell, [Kr]. The process involves the $5^2S_{1/2}$ ground state, with energy E_0, and the $5^2P_{1/2}$ excited state, E_1, with the atom emitting a photon $\hbar\omega = E_1 - E_0$, where $h = 2\pi\hbar$ is Planck's constant, during the transition from upper to the lower electronic configurations. The transition-, or lifetime is $\tau = 26,24$ ns corresponding to an approximately 8 m long photon [13].

With this example in mind, we have a degeneracy concerning the ground state, $5^2S_{1/2}$, of the rubidium atom, including the absorbed photon, $|0, \hbar\omega\rangle$ and the excited $5^2P_{1/2}$ state, $|1\rangle$, with the energy relation given by $E_1 = E_0 + \hbar\omega = E$. Note that this scenario is compatible with allowed selection rules for dipole transitions. Considering further that the process of emitting the photon is characterized by the half width $\Gamma = \hbar/\tau$ or in energy terms $\varepsilon = E - i\epsilon$ with $\epsilon = \Gamma/2$. In the present case the half width is very small, *i.e.*, $\epsilon \sim 10^{-8}$ eV.

In summary, we have the rubidium atom emitting a photon – a process characterized by the FWHM, Γ, (full width at half maximum). During the emission process the energy lies in the interval $E - \Gamma/2 < E < E + \Gamma/2$. The resonance energy is $\varepsilon = E - i\Gamma/2$, corresponding to the decay constant Γ. To model this particular transition as a spontaneous process one must first "borrow" a virtual photon from the surrounding electromagnetic field, which must be "given back at the end of the process". Hence the self-adjoint Hamiltonian, including the perturbing electromagnetic field, is given by (the "*i*" in the off-diagonal matrix elements below is just for convenience)

$$H_0 = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} + \Gamma/2 \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \tag{11}$$

which is trivially diagonalized by the unitary transformation U in Equation (9), *i.e.*,

$$U^\dagger H_0 U = \begin{pmatrix} E + \Gamma/2 & 0 \\ 0 & E - \Gamma/2 \end{pmatrix} \tag{12}$$

with the eigenfunctions $f = f_1, f_2$ represented in the preferred basis $h = h_1, h_2$, with $h_1 = |1\rangle$ and $h_2 = |0, \hbar\omega\rangle$ given by

$$f_1 = \tfrac{1}{\sqrt{2}}(h_1 - ih_2); \; f_2 = \tfrac{1}{\sqrt{2}}(h_1 + ih_2) \tag{13}$$

The Equations (11)–(13) depict the zero order procedure, which "prepares" the atom for the actual non-instantaneous emission process. Note that we are describing the excited atom in its rest frame, while after the emission process the photon and the de-excited atom moves according to the law of total momentum conservation. The completion of the transition necessitates a more detailed description via the multidimensional partitioning technique. Before proceeding we note that the choice of basis has a certain order, reflecting the fundamental framework of a non-Hermitian time irreversal

dynamical situation. In passing we not that we have the following basis functions of relevance for the discussion: the preferred physical basis $|h\rangle$, the final interactive basis $|f\rangle$, and $|k\rangle$, the basis associated with the jump.

4. Partitioning Technique

The background, for the present formulation, can be found in many publications, see, e.g., [12]. The multidimensional formalism, presented in Section 2 above, can be given a succinct operator representation in terms of effective Hamiltonians, reduced resolvents and associated projection operators, *i.e.*,

$$(z - H)\boldsymbol{\psi}(z) = O\big(z - \mathcal{H}(z)\big)O\boldsymbol{\varphi} \tag{14}$$

with

$$\mathcal{H}(z) = H + HT(z)H \tag{15}$$

and

$$O = |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}|; \ |\boldsymbol{\varphi}\rangle = |f\rangle \tag{16}$$

with the reduced resolvent $T(z)$ given by, $P = I - O$,

$$T(z) = P(z - PHP)^{-1}P \tag{17}$$

and finally

$$|\boldsymbol{\psi}(z)\rangle = |\boldsymbol{\varphi}\rangle + T(z)H|\boldsymbol{\varphi}\rangle \tag{18}$$

Both sides of Equation (14) is zero for $z = \varepsilon$, *i.e.*, for a degenerate eigenvalue of the Hamiltonian describing the system. This holds for both the diagonal case, the Segrè characteristic equals one and the more general situation with the order of the Jordan block being two.

Focusing on the representation of the effective operator $\mathcal{H}(z)$ in the space spanned by $|\boldsymbol{\varphi}\rangle = |f\rangle$, with H parameterized as in Equations (11) and (12) one can prove that, $z = \varepsilon$

$$\mathcal{H}(z) = \begin{pmatrix} E + \Gamma/2 & 0 \\ 0 & E - \Gamma/2 \end{pmatrix} + \begin{pmatrix} -i\Gamma/2 & -i\Gamma/2 \\ -i\Gamma/2 & -i\Gamma/2 \end{pmatrix} \tag{19}$$

A simple proof follows from the fact that the second term above is a result of the dispersion relation for the operator $t(z) = HT(z)H$, *i.e.*,

$$\lim_{\epsilon \to +0} T(E + i\epsilon) = \mathcal{P}\int_{-\infty}^{+\infty} \frac{d\rho(\omega)}{E - \omega} - i\pi\delta(E - PHP) \tag{20}$$

with $\rho(\omega)$ equal to the spectral function of PHP. For instance one needs to determine the matrix elements $(i,j = 1,2)$

$$\langle f_i|H\delta(E - PHP)H|f_j\rangle = \langle f_i|H|\chi(E)\rangle\langle\chi(E)|H|f_j\rangle \tag{21}$$

where $|\chi(E)\rangle$ is an "eigenfunction", δ-function normalized, corresponding to the continuum of PHP at energy E. By assumption the interaction between the atom and the environment comes principally from $|h_1\rangle = |1\rangle$, and this implies that

$$\nu = \Gamma/2 = \pi\langle f_i|H|\chi(E)\rangle\langle\chi(E)|H|f_j\rangle$$

At the same time the real part of the dispersion relation in Equation (20) contributes nothing to the energy shift, since the closeness of the resonance to the real energy axis imparts a narrow resonance, which essentially allows the positive and negative parts of the principle value integral to cancel out. Hence analytic continuation of $\mathcal{H}(E)$ across the real energy axis into the "unphysical Riemann sheet" gives directly the result dependent only on $\varepsilon = E - i\Gamma/2$,

$$\mathcal{H}(\varepsilon) = \begin{pmatrix} E - i\Gamma/2 & 0 \\ 0 & E - i\Gamma/2 \end{pmatrix} + \Gamma/2 \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} \tag{22}$$

In the Equation (14) prompts that z should be iterated until self-consistency. This imparts the need for calculating $T(z)$ at complex values. However, expanding the resolvent around the real energy E shows that only the imaginary part is affected, provided the real energy shift is zero. Since the effective operator is solely dependent on $\Gamma/2$, the iterations will not influence our conclusion. Note the similarity between Equations (6)–(9) and the form Equation (22), *i.e.*,

$$\mathcal{H}(\varepsilon) = \langle f|\mathcal{H}(\varepsilon)|f \rangle = (E - i\,\Gamma/2)\boldsymbol{I} + \Gamma\boldsymbol{Q} \tag{23}$$

Moreover since, according to Equation (8), $\boldsymbol{Q} = \boldsymbol{U}\boldsymbol{C}\boldsymbol{U}^{\dagger}$, *i.e.*, that $|f\rangle\boldsymbol{U} = |k\rangle$ one obtains trivially

$$\boldsymbol{U}^{\dagger}\mathcal{H}(\varepsilon)\boldsymbol{U} = \langle k|\mathcal{H}(\varepsilon)|k \rangle = (E - i\,\Gamma/2)\boldsymbol{I} + \Gamma\boldsymbol{C} \tag{24}$$

or in operator form

$$\mathcal{H}(\varepsilon) = \varepsilon O + (\hbar/\tau)|k_1\rangle\langle k_2| \tag{25}$$

As can be seen, the effective operator $\mathcal{H}(\varepsilon)$ above exhibits the "jump" explicitly, where

$$|k_1\rangle\langle k_2| = -\frac{i}{2}|(h_1 + h_2)\rangle\langle(h_1 - h_2)| \tag{26}$$

Note that the zero order Hamiltonian, Equations (11) and (12) becomes in the $\boldsymbol{k}$-representation

$$\langle \boldsymbol{k}|H_0|\boldsymbol{k} \rangle = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} + \Gamma/2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which shows the restraint in choosing the preferred-, the actual gauge dependent resonance- and the jump basis. It is surprising that it is not possible to identify the basis $\boldsymbol{k}$ with $\boldsymbol{h}$, since such a choice will not be compatible with the analytic continuation procedure to be exercised with the basis $\boldsymbol{f}$.

By the use of Equation (18), the final wavefunctions will, without explicitly invoking the electromagnetic field, exhibit relevant resonance properties, like satisfying the correct outgoing boundary condition, displaying the proper imaginary part of the energy, or the lifetime of the state or transition, as well as depicting the precise analytic resonance structure on the appropriate second Riemann sheet. Equation (26) shows that the two wavefunctions, h_1 and h_2 superimpose (positively) by borrowing a virtual photon corresponding to $\nu = \Gamma/2$ and then returning it by negative interference.

In addition the "jump process" is not instantaneous as it relates to the lifetime, $\tau = \hbar/\Gamma$, of the excited atom and the size of the emitted photon. The parametrization refers exclusively to physical quantities that can be both measured and calculated. Together the derivation is commensurate with rigorous extensions of spectral theory to non-self adjoint Hamiltonians [7]. Advances to apply analogous continuations to electro-magnetic fields are given in Refs. [14,15].

5. Conclusions

In this document we have attempted to demonstrate that Schrödinger's discomfort regarding what he referred to as "*damn quantum jumps*" can be reformulated explicitly and rigorously within a slightly extended and more general framework. Note that conventional Coulomb atomic and molecular Hamiltonians belong to the class of dilatation analytic operators for which the Balslev-Combes theorem is valid. In our presented example this applies except for the interaction with the electromagnetic field. Although there exists general analytic structures also for interactions with an electromagnetic field, see, e.g., [14,15], the present investigation remains accurate in that the atomic states belong to the proper operator domain and further that only h_1 is employed as the sole partaker in the analytic continuation. Hence in the sense of perturbation theory to all orders the result should guarantee a degenerate pole in the analytically continued Green's function or resolvent.

There are several advantages, in addition to inclusions of actual transitions as a direct result of the dynamical situation, attached to this generalization, e.g., (i) a surprising relation between gravitational interaction and Gödel's incompleteness theorem(s) [16], (ii) generalizations of Segrè characteristics to arbitrary order and the paradigm of evolution [9,17], and (iii) a consistent zero energy universe scenario [17,18]. The general case prompts a correlation analysis based on density matrices and their reduced variants [9,16–19]. Such contexts invite decoherence scenarios, see the excellent anthology *Decoherence and the Appearance of a Classical World in Quantum Theory* [20], for more details regarding the implication of the present jump representation for decoherence protocols, see the Appendix. It is nonetheless interesting to observe that the extended "multi-jump" setting, see Equation (27) below, enacts decoherence code protection with profound consequences for complex enough, biological systems [17,19].

The possibility to reformulate quantum theory in terms of a complex symmetric ansatz of observables (operators) and their conjugate partners establishes further Lorentz invariance in the special theory and covariance and background independence in the general case [6,18]. It is also straightforward to show that an operator like $\boldsymbol{Q}$ or $\boldsymbol{C}$ imparts a temporal evolution proportional to time, which in the general case becomes a delayed decay rule, *i.e.*, of the Poissonian type

$$\left(\frac{t}{\tau}\right)^n \frac{1}{n!} e^{-t/\tau} \tag{27}$$

which, as already mentioned, might uncover interesting communication channels for cellular evolution in living systems [19].

The present discussion, focused on the atomic emission process, can obviously be transformed to other "jump" procedures as well as various collapse settings in quantum theory. For instance employing the rule of microscopic reversibility, which may not hold in general, one can in principle model the inverse process, *i.e.*, the absorption of an atom by a photon. In these archetypical, yet conventional, physical situations we emphasize again that there are no additional hypotheses and postulations necessary, except the rigorous mathematical extension of quantum theory to open dissipative systems.

Appendix

In this appendix we will briefly review some key components of non-Hermitian quantum mechanics and some of its surprising consequences. Space will not permit a full motivation of the necessity to accomplish a quantum mechanical extension, see, e.g., [4–6]. However, we will illustrate what we mean when we say that the Schrödinger equation is extended beyond Hermitian territory. As mentioned this extension rests on the so-called Balslev-Combes theorem for dilatation analytic operators [7].

The theory is particularly suited for applications in chemical physics, since the Coulomb operator belong to this family. Although other methods can be employed, see, e.g., [14,21], we will concentrate on the popular complex scaling or analytic dilation technique.

This method essentially amounts to multiplying the space coordinate x with a complex scale factor $\eta = e^{i\theta}$, with $\theta = \arg \eta$ for some $0 \leq \eta < \theta_0$, where θ_0 usually depends on the potential V in the Hamiltonian $H = T + V$ with T being the dominating kinetic operator, being related to the operator $\Delta = \nabla^2$. Under the scaling operation the spectrum of the Hamiltonian H changes in that the absolutely continuous part, σ_C, rotates an angle $-2 \arg \eta$ around the accumulation point(s), *i.e.*, at the onset of σ_C before scaling.

The Balslev-Combes theorem guarantees that the bound states of the unrotated operator are unaffected while the continuous part rotates as described above. In the sector between the rotated cut and the positive real axis (assuming a simple case with only one accumulation point and a σ_C on the positive real energy axis) there may emerge so-called resonance states. These resonances are represented by a complex energy with the imaginary part being proportional to the inverse of the life-time of the unstable state.

It is convenient to represent the complex rotated eigenvalue problem via complex symmetric matrices, orthogonal transformations and associated variational principles. Since any matrix can be transformed to a complex symmetric matrix via a similarity transformation, it follows that our extension imparts degenerate blocks that are not diagonalizable, so-called Jordan blocks. These blocks are characterized by their sub-dimensions and the largest order of such a sub-block is called the Segrè characteristic of the degeneracy. A convenient complex symmetric form of such a canonical block, with ones in the super diagonal above the diagonal containing the degenerate eigenvalue, was derived in [22] for the explicit use in situations which demand arbitrary large dimensions. The analytic continuation also imparts a transition from spaces with positive definite metrics to indefinite ones.

The occurrence of Jordan blocks in the structure of non-Hermitian Hamiltonians leads to surprising consequences. The Jordan block as represented in this article is in fact nothing but a transition matrix as shown in Equation (25). It further governs delayed time decays, introducing, in our example above in Section 4, a term linear in time. In general the degenerate irreducible Jordan block corresponds to a polynomial evolution, multiplying the decay factor, prolonging the actual lifetime of the transition state, see [17,19,21] for details. Another consequence is the straightforward derivation of Poisson type statistics from the related Dunford formula. Such formulations have been of focal relevance in biological, complex enough, systems, where the associated anomalous time evolution serves as a protection of decoherence [23]. It is also interesting to note that the present Poisson distribution of general space-time points is in analogy with the sprinkling of points into the Minkowski space as it can

be the embedding of a causal set into a Lorentzian manifold [24] and further commensurate with the operator array technique advanced in Refs. [16–19].

A straightforward extension of the ansatz of a matrix array of quantum mechanical operators and their conjugate partners yields proper covariance, including Lorentz invariance for the special case, and background independence, in concert with Einstein's equivalence principle, with a surprising relation to the formulation of Gödel's theorem [17,18].

Conflicts of Interest

The author declares no conflict of interest.

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