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# Time-Conjugation in a Unified Quantum Theory for Hermitian and Non-Hermitian Electronic Systems under Time-Reversal Symmetry

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**Abstract:** We propose a reformulation of the mathematical formalism of many-electron quantum theory that rests entirely on the *physical* properties of the electronic system under investigation, rather than conventional mathematical assumption of Hermitian operators in Hilbert space. The formalism is based on a modified *dot-product* that replaces the familiar complex-conjugation in Hilbert space $\mathfrak{H}$ (fixed for all physical systems) by time-conjugation in $\mathfrak{T}$-space (as generated by the specific spin, magnetic field, or other explicit $t$-dependence of the system Hamiltonian $\mathcal{H}$ of interest), yielding *different spatial structure for different systems*. The usual Hermitian requirement for physical operators is thereby generalized to a self-$t$-adjoint ("$t$-reversible") character, leading to correspondingly generalized theorems of virial and hypervirial type. The $\mathfrak{T}$-space reformulation *preserves* the real values of measurable properties and the Born-probabilistic interpretations of state functions that underlie the present quantum theory of measurement, while also properly distinguishing "temporal" behavior of internal decay (tunneling-type) phenomena from that of applied fields with parametric $t$-dependence on an external clock. The $t$-product represents a further generalization of the "$c$-product" that was previously found useful in complex coordinate-rotation studies of autoionizing resonances.

**Keywords:** time-reversal symmetry; non-Hermitian quantum mechanics; time-dependent Hamiltonian; autoionizing resonances; tunneling phenomena

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**Citation:** Weinhold, F. Time-Conjugation in a Unified Quantum Theory for Hermitian and Non-Hermitian Electronic Systems under Time-Reversal Symmetry. *Symmetry* **2021**, *13*, 808. https://doi.org/10.3390/sym13050808

Academic Editor: Andrea Lavagno

Received: 31 March 2021
Accepted: 27 April 2021
Published: 5 May 2021

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## 1. Introduction

The title of Schrödinger's 1926 paper [1] ("Quantization as Eigenvalue Problem") aptly expresses the essence of the conceptual leap from classical to quantum mechanics. Schrödinger's time-independent eigenvalue equation

$$\mathcal{H}\psi_i = E_i\psi_i \tag{1}$$

restricts the energies $E_i$ of an $N$-particle system $\mathcal{H}$ to numerical values for which a corresponding state function $\psi_i$ satisfies Equation (1). As every student learns, the classical Hamiltonian (total energy) of the system is first made *operator*-valued by replacing each particle momentum $\mathbf{p}_\lambda$ of the kinetic energy ($\mathcal{K}$, energy of motion) with the differential operator $-i\hbar\nabla_\lambda$, then adding the classical-like potential energy ($\mathcal{V}$, energy of position) to obtain the quantal $\mathcal{H} = \mathcal{K} + \mathcal{V}$ whose eigenproperties (1) provide the quantal description.

In the present context, we focus on the quantum aspects of *electronic* systems, where the sharp distinctions from classical conceptions were first recognized [2]. More specifically, we adopt the conventional quantum chemical framework of non-relativistic $N$-electron theory in the Born–Oppenheimer approximation [3,4] where nuclei are treated as classical particles of fixed mass and charge that contribute (along with possible external electric and magnetic fields) to total potential energy $\mathcal{V}$. Of course, a parallel treatment might start with vibrational degrees of freedom (phonons) as the system of interest for quantization.

However, the electronic structure of atomic and molecular species more clearly illustrates the characteristic paradoxes ("spooky action at a distance") of quantized behavior in the profoundly non-classical regime of strictly conserved Fermi-Dirac antisymmetry.

Specification of electronic "position" in turn requires a suitable set of electronic coordinates. In the non-relativistic regime, each electronic coordinate must include both real-space location ($\mathbf{r}_\lambda$) and spin-space orientation ($\alpha$ ($\uparrow$) or $\beta$ ($\downarrow$)) in order to incorporate the all-important *exchange antisymmetry* of the electronic wavefunction $\psi_i$. We assume that the functional form of $\psi_i$ includes proper Slater-determinantal constraint of overall $N$-electron antisymmetry and total spin angular momentsum $\mathbf{S}$, allowing focus on its cartesian spatial dependence ($\psi_i(\mathbf{r}_1, \mathbf{r}_2,...,\mathbf{r}_N)$) in equations to follow. In particular, these constraints satisfy the symmetrization postulate ([4], p. 595) that insures Pauli-type *connectivity* of spatial variables and avoids formal difficulties that may arise in certain model problems [5,6].

Conventional interpretation of Equation (1) is based on the assumptions (initially formulated by mathematicians David Hilbert and John von Neuman [7,8]) that (i) the state functions $\psi_i(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N)$ and their linear combinations form a mathematical *Hilbert space* $\mathfrak{H}$, and (ii) the operators for $\mathcal{H}$ and other physical properties of the system are *Hermitian*. Both properties are based on a chosen form of *dot-product*, which provides the scalar measure of proximity that is characteristic of the space. In this description, allowed operators (including $\mathcal{H}$) must have domain and range properly matched to the space described by the chosen dot-product. The goal of the present work is to examine how alternative choices of dot product can achieve a more unified description of bound and dissipative (quasi-bound) states of general atomic and molecular systems. As we show below, the modified dot product is based on intrinsic *symmetries* of the physical system $\mathcal{H}$ (as specified by the associated complete set of commuting observables), and thereby is required to be consistent with *physical* details of the chosen system rather than of fixed mathematical type.

## 2. Coordinates and Dot Products for Stationary and Dissipative States of Many-Electron Systems

For Hilbert space, the well-known dot-product $d_{\mathfrak{H}}$ of two arbitrarily chosen elements ($\psi$, $\varphi$) is given by

$$d_{\mathfrak{H}}(\psi,\varphi) \equiv \int \psi^*(\mathbf{r}_1,\mathbf{r}_2, \ldots ,\mathbf{r}_N)\, \varphi(\mathbf{r}_1,\mathbf{r}_2, \ldots ,\mathbf{r}_N)\, d\mathbf{r}_1 d\mathbf{r}_2 \ldots d\mathbf{r}_N, \text{ all } \psi, \varphi \in \mathfrak{H} \tag{2}$$

where the integration is over all allowed values of real-space cartesian variables. The key characteristic of Hilbert space is that the dot-product of any function with itself is required to be real, positive, and finite,

$$0 \leq d_{\mathfrak{H}}(\psi, \psi) < \infty, \text{ all } \psi \in \mathfrak{H} \tag{3}$$

vanishing only if $\psi$ is everywhere zero. The Hermitian (self-adjoint) property for $\mathcal{H}$ (or other physical observable) is then stated as

$$d_{\mathfrak{H}}(\psi,\mathcal{H}\varphi) = d_{\mathfrak{H}}(\mathcal{H}\psi, \varphi), \text{ all } \psi, \varphi \in \mathfrak{H} \tag{4}$$

In Schrödinger's formulation (1), it is noteworthy that $d_{\mathfrak{H}}$-based conceptions are considered to apply only to stationary bound-state solutions of the $t$-independent regime. Description of more general scattering or resonance-type phenomena instead requires the *non*-eigenvalue form of Schrödinger's $t$-dependent wave equation, viz.,

$$(\mathcal{H} - i\hbar\, \partial/\partial t)\Psi = 0 \tag{5}$$

As shown by Dirac [9], the usual non-relativistic Hamiltonian must then be replaced with kinetic energy terms that depend linearly on momenta to avoid conflicts with special relativity in the high-energy limit. In either case, Equation (5) becomes the starting point for describing possible explicit or implicit time-dependence in $\mathcal{H}$. When all such $t$-dependence

is absent, solution of (5) reduces in well-known fashion to (1) by merely taking $\Psi$ and $\psi$ to be related by a phase factor ($\Psi = e^{-i\hbar t}\psi$) that cancels out of any $d_{\mathfrak{H}}$ evaluation.

The mathematical framework expressed by Equations (1)–(5) has enjoyed widespread success. In particular, the structural form of the eigenvalue-type Equation (1) for $t$-independent systems and the first-order differential form of Equation (5) for $t$-dependent systems appears secure [9]. However, in certain respects the $d_{\mathfrak{H}}$-dependent mathematical assumptions expressed by Equations (2)–(4) give an imperfect fit to the full range of quantum phenomena of the physical world, as we now wish to discuss.

The traditional Hilbert-space view (2) of quantum theory was most dramatically called into question by the remarkable work of Balslev and Combes [10,11] in the early 1970s. For a broad range of Coulombic and other analytic potentials of physical interest, their work showed that a complex-rotated eigenvalue equation

$$\mathcal{H}_\theta \ \psi_i = W_i \psi_i \tag{6}$$

gives *exact* eigenvalues both for the low-energy bound states (where $W_i = E_i$, cf. Equation (1)) as well as for the physically important quasi-bound resonance states $\psi_r$ that lie in the high-energy continuum region above the ionization threshold. In the latter case, $W_r$ becomes *complex*-valued,

$$W_r = E_r - (i/2)\Gamma_r \tag{7}$$

yielding both the position $E_r$ and width $\Gamma_r$ of the spectral feature as well as the corresponding *lifetime* $\tau_r$ of the quasi-bound species,

$$\tau_r = \hbar/\Gamma_r \tag{8}$$

spectral position $E_r$ and width $\Gamma_r$ are observable properties of a resonance spectral feature, and it was therefore quite surprising that a time-type observable $\tau_r$ could be extracted from what appears nominally to be the time-independent (eigenvalue-type) form (6) of Schrödinger's equation.

Moreover, the bonanza of additional spectral information in Equations (6)–(8) is achieved by *abandoning* the Hilbert space formulation (2) of dot-product and the Hermitian requirement (4) on $\mathcal{H}_\theta$. Specifically, $\mathcal{H}_\theta$ is constructed from $\mathcal{H}$ by complex-rotation of each particle coordinate $\mathbf{r}_\lambda$ by angle $\theta$ into the complex plane,

$$\mathbf{r}_\lambda \rightarrow \mathbf{r}_\lambda \ e^{i\theta} \tag{9}$$

thereby introducing non-Hermitian character in $\mathcal{H}_\theta$ and other violations of traditional mathematical assumptions.

It is noteworthy that the resonance-type (finite lifetime) phenomena encompassed by Balslev–Combes theory are not restricted to the high-energy spectroscopic domain of field-free atoms and molecules. Similar resonance characteristics extend to *all* states of atoms and molecules in the presence of an electric field, where the idealized field-free energy levels $E_i$ become Stark-shifted and broadened ($\Gamma_i > 0$) by the ionizing effect of even infinitesimal field strengths. Thus, the Balslev–Combes (*non*-Hermitian) formulation should be considered as the *more fundamental* mathematical conception underlying the quantum mechanics of atomic and molecular phenomena.

Superficially, the Hermitian condition (4) may seem indispensable to the quantum theory of measurement in two respects: (i) assuring real values of the expectation values $d_{\mathfrak{H}}(\psi,\mathcal{H}\psi)$ for $\mathcal{H}$ and other physical observables, and (ii) guaranteeing the independence of contributions from distinct states that is required for consistent application of the Born probability interpretation (orthonormality of non-degenerate state functions, $d_{\mathfrak{H}}(\psi_i,\psi_j) = \delta_{ij}$). Although mathematical Hermiticity (4) is sufficient to satisfy these two requirements, it admits many operators that have no conceivable relationship to measurable properties of a realistic physical system. However, as we show below, a consistent basis for the quantum theory of measurement can also be achieved in a properly generalized conception of dot-

product that departs from Hilbert's envisioned mathematical framework, but seamlessly incorporates both the Balslev–Combes domain of resonance phenomena (6)–(9) and the idealized resonance-free domain (1)–(4) of traditional bound-state applications.

The revised dot-product conception to be introduced below has an evident connection to the "*c*-product" formulation [12], as introduced in the late 1970s to derive generalized virial and hypervirial theorems for the Balslev–Combes domain that are fully analogous to those in the traditional Hermitian domain. In this complex ($\mathfrak{C}$) domain, the *c*-product $d_{\mathfrak{C}}$ is defined by merely *omitting* complex conjugation of the first function, viz.

$$d_{\mathfrak{C}}(\psi,\varphi) \equiv \int \psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\,\varphi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\,d\mathbf{r}_1 d\mathbf{r}_2\ldots d\mathbf{r}_N, \text{ all } \psi,\ \varphi \in \mathfrak{C} \tag{10}$$

As a result, there is no longer assurance that $d_{\mathfrak{C}}(\psi,\psi)$ is real or positive. The Hermitian condition (4) is similarly replaced by

$$d_{\mathfrak{C}}(\psi,\mathcal{H}\varphi) = d_{\mathfrak{C}}(\mathcal{H}\psi,\ \varphi), \text{ all } \psi,\ \varphi \in \mathfrak{C} \tag{11}$$

as the condition for "self-*c*-adjoint" (or "*c*-conjugate") character of $\mathcal{H}$ or other operators. The $d_{\mathfrak{C}}$-based formulation is contrary to traditional Hilbert-space and Hermitan operator conceptions, but allows the Balslev–Combes theory of dilation-analytic operators to be developed in remarkably parallel fashion for what has become a vast array of non-Hermitian quantum mechanical applications [13].

The present work aims at still further departures from traditional mathematical conceptions of Hermitian operators in Hilbert space as the intrinsic "home" of quantum mechanics. In effect, we abandon *all* associations with purely mathematical constructions of a dot-product, seeking instead a *physical*-based construction that depends on the system of interest, and more specifically on its explicit *t*-dependence. In this manner, the system itself dictates the *t*-dependent type of "conjugacy" between operators (or "proximity" between functions) that is characteristic of the associated $\mathfrak{T}$-space. The generalized formalism automatically reverts to the proper type of operator-conjugacy and function-proximity measure appropriate to the *t*-dependence of system $\mathcal{H}$, assuring consistent and unified description of all known system types.

The change in focus from states/functions to systems/operators in the $\mathfrak{T}$-space can be achieved by adopting an *operator*-based method to uniquely specify the state of the system, as we now describe. For a non-degenerate state, it is well-known that measurement of the eigenvalue $E_i$ is sufficient to identify the state function $\psi_i$ uniquely, whereas in the case of degeneracies, additional measurements of a complete set of commuting observables ("symmetries" of $\mathcal{H}$ [14]) serve to resolve the degeneracies and complete the unique specification of state. Operators of this $\mathcal{H}$-specific complete commuting set thus become the central focus of measurements on system $\mathcal{H}$, constituting only a small subset of the operators (many completely unphysical) meeting the mathematical Hermitian requirement of Equation (4).

"Spatial" aspects of quantum mechanical structure are most clearly exhibited in Dirac's elegant bra ("$\langle$")-ket ("$\rangle$") notation, without which coherent discussion of quantum mechanical fundamentals cannot proceed. For present notational needs, we employ *braces* to distinguish conventional $\mathfrak{H}$-space dot-products ("$\langle\psi\,|\,\varphi\rangle$") from $\mathfrak{T}$-space counterparts ("$\{\psi\,|\,\varphi\}$") in equations to follow. If further distinction between $\mathfrak{H}$-space (2), $\mathfrak{C}$-space (10), and $\mathfrak{T}$-space variants is required, alternative ${}^{\mathfrak{H}}\langle\varphi\,|\,\psi\rangle$, ${}^{\mathfrak{C}}\langle\varphi\,|\,\psi\rangle$, ${}^{\mathfrak{T}}\langle\varphi\,|\,\psi\rangle$ symbolism can be adopted.

## 3. Time-Conjugation in Systems with Time, Spin, or Magnetic Field Dependence

Consider a general Hamiltonian $\mathcal{H}$ in the coordinate representation,

$$\mathcal{H} = \mathcal{H}(\mathbf{r}, t, \mathbf{B}, \mathbf{S}) \tag{12}$$

with arguments that exhibit the explicit dependence (if any) on time $t$, magnetic field $\mathbf{B}$, and quantum-mechanical spin $\mathbf{S}$ [15], as well as spatial position $\mathbf{r}$ (now symbolizing the collective coordinates of the $N$-particle system). The $\mathbf{r}$-dependence which is to be rotated into the complex plane can be distinguished by defining a formal time-conjugated (overbar) Hamiltonian $\overline{\mathcal{H}}$,

$$\overline{\mathcal{H}} \equiv \mathcal{H}(\mathbf{r},\ -t,\ -\mathbf{B},\ -\mathbf{S}^*) \tag{13}$$

A similar procedure defines the time-conjugated operator $\overline{\mathcal{A}} \equiv \mathcal{A}(\mathbf{r}, -t, -\mathbf{B}, -\mathbf{S}^*)$ of a general dynamical variable $\mathcal{A}(\mathbf{r}, t, \mathbf{B}, \mathbf{S})$. All such operators necessarily have the properties $\overline{\overline{\mathcal{A}}} = \mathcal{A}$, $\overline{\mathcal{A}\mathcal{B}} = \overline{\mathcal{A}}\ \overline{\mathcal{B}}$ and so forth.

With a similar convention, it is also possible to define the t-conjugated counterpart $(\overline{\psi})$ of any physical wave function $\psi$ that could arise in the ordinary time-forward regime. To do so, let $\psi$ be uniquely specified in the usual manner by the complete commuting set of observables $\mathcal{A}, \mathcal{B}, \ldots$ for which it is the common eigenfunction. The $t$-conjugate $\overline{\psi}$ can then be defined as the corresponding common eigenfunction of the $t$-conjugated operators $\overline{\mathcal{A}}, \overline{\mathcal{B}}, \ldots$ [where Equation (27) below specifies the "corresponding" eigenvalue that completes the definition]. In particular, if $\psi$ satisfies the $t$-dependent Schrödinger equation (as suggested by the "equivalence" of $\Psi$, $\psi$ mentioned above)

$$(\mathcal{H} - i\hbar\,\partial/\partial t)\psi = 0 \tag{14}$$

then $\overline{\psi}$ must satisfy the time-conjugated equation

$$(\overline{\mathcal{H}}\ + i\hbar\,\partial/\partial t)\overline{\psi}\ =\ 0 \tag{15}$$

Although additional steps are required to find the specific $\overline{\psi}$ corresponding to a given "forward" wave function $\psi$, general time-reversal symmetry suggests that functions having the desired properties must exist, and must satisfy $\overline{\overline{\psi}} = \psi$, $\overline{\psi\varphi} = \overline{\psi}\ \overline{\varphi}$, $\overline{\mathcal{A}\psi} = \overline{\mathcal{A}}\ \overline{\psi}$, and so forth. Note particularly that the wave function $\overline{\psi}(\mathbf{r},t)$ need *not* be the same as $\psi(\mathbf{r},-t)$.

Given two wave functions $\psi(\mathbf{r},t)$, $\varphi(\mathbf{r},t)$ in $\mathfrak{T}$-space, we form their $t$-product $\{\psi \mid \varphi\}$ according to the definition

$$\{\psi|\varphi\}\ \equiv\ \int_{\text{all space}} \overline{\psi}(\mathbf{r},t)\ \varphi(\mathbf{r},t)\mathrm{d}\mathbf{r}\ \equiv\ d_{\mathfrak{T}}(\psi,\varphi)\ \text{all}\ \psi,\varphi \in \mathfrak{T} \tag{16}$$

where integration over spin variables (if any) is implicitly understood. The bilinear symbol $\{\psi \mid \varphi\}$ may be formally related to the ordinary Hermitian scalar product (which we now denote in standard bra-ket notation; cf. Equation (2)),

$$\langle\psi \mid \varphi\rangle \equiv \int_{\text{all space}} \psi^*(\mathbf{r},t)\ \varphi(\mathbf{r},t)\mathrm{d}\mathbf{r} \tag{17}$$

by the identity

$$\{\psi|\varphi\} = \langle\overline{\psi} * |\varphi\rangle \tag{18}$$

Equation (17) shows that the symbols $\{\psi \mid \varphi\}$ and $\langle\psi \mid \varphi\rangle$ coincide when $\overline{\psi} = \psi^*$, but in other cases their numerical values must be distinguished. While the $t$-products have familiar properties such as $\{\psi \mid \varphi\} = \overline{\{\varphi|\psi\}} = \{\ \overline{\varphi}\ |\ \overline{\psi}\}$ and $\{\psi \mid \varphi{+}\chi\} = \{\psi \mid \varphi\} + \{\psi \mid \chi\}$, the $t$-product $\{\psi \mid \psi\}$ of a function with itself is not necessarily real or positive, unlike the corresponding $\langle\psi \mid \psi\rangle$.

Although $\{\psi \mid \varphi\}$ is no longer the metric of a Euclidean-type geometry, the $t$-product of wave functions $\psi$ and $\varphi$ can nevertheless be interpreted as a probability amplitude in the usual manner, with absolute square $|\{\psi \mid \varphi\}|^2 = \{\psi \mid \varphi\}^*\{\psi \mid \varphi\}$ that is real and non-negative. The requirement that such $\{\psi \mid \varphi\}$ probability amplitudes (and thus, their summed absolute squares) be time-invariant ("conserved") quantities is expressed by the equation

$$\partial\{\psi \mid \varphi\}/\partial t = 0 \tag{19}$$

When the time evolution is governed by a Hamiltonian $\mathcal{H}$, Equations (14)–(16) show that condition (19) will be satisfied if

$$\{\mathcal{H}\psi \mid \varphi\} = \{\psi \mid \mathcal{H}\varphi\} \tag{20}$$

for any chosen $\psi, \varphi \in \mathfrak{T}$.

It is now convenient to introduce the *t*-adjoint, denoted $\mathcal{A}^{\ddagger}$, of an operator $\mathcal{A}$ by the definition

$$\{\mathcal{A}^{\ddagger}\psi \mid \varphi\} = \{\psi \mid \mathcal{A}\varphi\}, \text{ all } \psi, \varphi \in \mathfrak{T} \tag{21}$$

Equation (18) shows that the *t*-adjoint $\mathcal{A}^{\ddagger}$ is related to the ordinary Hermitian adjoint $\mathcal{A}^{\dagger}$ by the equation

$$\mathcal{A}^{\ddagger} = \mathcal{A}^{\dagger *} \tag{22}$$

The general conservation of probability, Equation (19), is thus equivalent to the requirement that the Hamiltonian be self-*t*-adjoint,

$$\mathcal{H}^{\ddagger} = \mathcal{H} \tag{23}$$

We may also call such operators "reversible" (or "*t*-reversible") to suggest their intimate relationship to time-reversal symmetry.

The reversibility property ($\mathcal{A} = \mathcal{A}^{\ddagger}$) characterizes observables that are even functions of time in the classical sense, while skew-reversibility ($\mathcal{A} = -\mathcal{A}^{\ddagger}$) characterizes those that are odd in time. We assume more generally that each $\mathcal{A}$ commutes with its own *t*-adjoint, $[\mathcal{A}, \mathcal{A}^{\ddagger}] = 0$, and hence shares with it a common set of eigenfunctions $\{u_k\}$. Let the corresponding eigenvalues of $\mathcal{A}$, $\mathcal{A}^{\ddagger}$ be denoted by $a_k$ and $a_k{}^{\ddagger}$, respectively,

$$\mathcal{A}u_k = a_k \cdot u_k \tag{24}$$

$$\mathcal{A}^{\ddagger}u_k = a_k{}^{\ddagger}\, u_k \tag{25}$$

and let the *t*-conjugate eigenvalue equation of $\mathcal{A}$ similarly be written as

$$\overline{\mathcal{A}}\overline{u}_k = \overline{a}_k \overline{u}_k \tag{26}$$

Consistency demands that the *t*-conjugate eigenvalues satisfy

$$\overline{a}_k = a_k{}^{\ddagger} \tag{27}$$

since Equations (16) and (21) require that, for every "non-exceptional" $u_k$ with non-zero *t*-product with itself ($\{u_k \mid u_k\} \neq 0$),

$$\overline{a}_k\{u_k|u_k\} = \{\mathcal{A}u_k|u_k\} = \left\{u_k\middle|\mathcal{A}^{\ddagger}u_k\right\} = a_k{}^{\ddagger}\{u_k|u_k\} \tag{28}$$

Equation (27) completes the definition of t-conjugate wave functions $\overline{\psi}$.

Table 1 summarizes the specific forms of common operators $\mathcal{A}$ for the variously defined "conjugacy" types ($\overline{\mathcal{A}}$, $\mathcal{A}^{*}$, $\mathcal{A}^{\dagger}$, $\mathcal{A}^{\ddagger}$). For example, if $\mathbf{r}$ (of length $r$) denotes the "ruler" (scale) for the collective position coordinate, the total electronic energy $\mathcal{H}(\mathbf{r}) = \mathcal{T}(\mathbf{r}) + \mathcal{V}(\mathbf{r})$ of an isolated atom or molecule includes kinetic energy $\mathcal{T}$ (homogeneous of degree $-2$; "scaling as $r^{-2}$") plus Coulombic potential energy $\mathcal{V}$ (scaling as $r^{-1}$) so that (cf. rows 8, 9 of Table 1)

$$\mathcal{H}_\theta = \mathcal{T}_\theta + \mathcal{V}_\theta = \mathcal{T}(\mathbf{r}e^{i\theta}) + \mathcal{V}(\mathbf{r}e^{i\theta}) = e^{-2i\theta}\ \mathcal{T}(\mathbf{r}) + e^{-i\theta}\ \mathcal{V}(\mathbf{r}) \tag{29}$$

and correspondingly

$$\mathcal{H}_\theta{}^{*} = \mathcal{H}_\theta{}^{\dagger} = e^{2i\theta}\ \mathcal{T}(\mathbf{r}) + e^{i\theta}\ \mathcal{V}(\mathbf{r}) \tag{30}$$

**Table 1.** Relationship of operators $\mathcal{A}$, $\overline{\mathcal{A}}$, $\mathcal{A}^*$, $\mathcal{A}^\dagger$, $\mathcal{A}^\ddagger$ for some common operators $\mathcal{A}$. An entry + or − signifies that the operator of the column heading is $+\mathcal{A}$ or $-\mathcal{A}$, respectively. For simplicity, spin operators in the lower portion of the table are given in Majorana representation (**S*** = −**S**; see [15]), but in no case does this affect the entry in the final column.

| $\mathcal{A}$ | $\overline{\mathcal{A}}$ | $\mathcal{A}^*$ | $\mathcal{A}^\dagger$ | $\mathcal{A}^\ddagger$ |
|---|---|---|---|---|
| **r** | + | + | + | + |
| **p** | + | − | + | − |
| **L** = **r**x**p** | + | − | + | − |
| **B** | − | + | + | − |
| **S** (Dirac rep.) | $-\mathbf{S}^*$ | $\mathbf{S}^*$ | + | − |
| **S** (Majorana rep.) | + | − | + | − |
| $c$ (complex constant) | + | $c^*$ | $c^*$ | + |
| $\mathcal{T} = \mathrm{p}^2/2\,\mathrm{m}$ | + | + | + | + |
| $\mathcal{V} = \mathrm{V}(\mathbf{r})$ | + | + | + | + |
| $\mathcal{T}(\mathbf{r}\mathrm{e}^{\mathrm{i}\theta})$ | + | $\mathrm{e}^{2\mathrm{i}\theta}\mathcal{T}$ | $\mathrm{e}^{2\mathrm{i}\theta}\mathcal{T}$ | + |
| $\mathcal{V}(\mathbf{r}\mathrm{e}^{\mathrm{i}\theta})$ | + | $\mathcal{V}(\mathbf{r}\mathrm{e}^{-\mathrm{i}\theta})$ | $\mathcal{V}(\mathbf{r}\mathrm{e}^{-\mathrm{i}\theta})$ | + |
| **L**·**S** | + | + | + | + |
| **B**·**S** | − | − | + | + |
| **B**·**L** | − | − | + | + |

If the potential energy includes an additional contribution ${}^{\mathrm{n}}\mathcal{K}(\mathbf{r})$ that scales as $r^{\mathrm{n}}$ (e.g., harmonic oscillator, $n = 2$), the corresponding complex-rotated ${}^{\mathrm{n}}\mathcal{V}_\theta$ is

$$ {}^{\mathrm{n}}\mathcal{V}_\theta = {}^{\mathrm{n}}\mathcal{V}(\mathbf{r}\mathrm{e}^{\mathrm{i}\theta}) = \mathrm{e}^{\mathrm{in}\theta}\,{}^{\mathrm{n}}\mathcal{V}(\mathbf{r}) \tag{31} $$

with ${}^{\mathrm{n}}\mathcal{V}_\theta{}^* = {}^{\mathrm{n}}\mathcal{V}_\theta{}^\dagger = \mathrm{e}^{-\mathrm{in}\theta}\,{}^{\mathrm{n}}\mathcal{V}(\mathbf{r})$, and so forth.

The reversibility condition (23) characterizes the Hamiltonian operators of known physical systems. One can verify from Table 1 that the t-adjoints of the fundamental dynamical variables **r**, **p**, **S** satisfy $\mathbf{r}^\ddagger = \mathbf{r}$, $\mathbf{p}^\ddagger = -\mathbf{p}$, $\mathbf{S}^\ddagger = -\mathbf{S}$, and thus coincide with the corresponding time-reversed operators ([4], pp. 667–669). Observables $\mathcal{A}$ that are real functions of such variables will similarly satisfy $\mathcal{A}^\ddagger = \mathcal{A}_{\mathrm{rev}}$, which suffices ([4], p. 645) to insure that the property $\mathcal{H}^\ddagger = \mathcal{H}$ is consistent with known time reversal symmetry of the Hamiltonian operator. Note however that $\mathcal{A}^\ddagger$ need not coincide with $\mathcal{A}_{\mathrm{rev}}$ for more general operators; for example, $c^\ddagger = c$ for a general complex number (regarded as a multiplicative operator), whereas $c_{\mathrm{rev}} = c^*$ ([4], p. 640). One could imagine many potentials that are formally Hermitian, but would violate fundamental time-reversal symmetry, such as $\mathbf{r} \times \mathbf{B}$, $\mathbf{r}\cdot\mathbf{S}$, $(\mathbf{r}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{r})/2$, and so forth (cf. Table 1). While the Hermitian condition $\mathcal{H}^\dagger = \mathcal{H}$ allows such unphysical possibilities, the reversibility condition (23) excludes these and similar terms (to any odd power) from the Hamiltonian. The class of reversible Hamiltonians is in this sense more restrictive and "physical" than that of Hermitian Hamiltonians.

In another sense, however, the reversible Hamiltonians are more general than Hermitian Hamiltonians, in that they properly *include* the complex-rotated kinetic ($\mathcal{T}$) and potential ($\mathcal{V}$) components of the Hamiltonian $\mathcal{H}(\mathbf{r}\mathrm{e}^{\mathrm{i}\theta}) = \mathrm{e}^{-2\mathrm{i}\theta}\mathcal{T} + \mathcal{V}(\mathrm{re}^{\mathrm{i}\theta})$ needed to treat resonance phenomena [10]. This follows from the fact, Equation (22), that a complex number is intrinsically reversible, $(\mathrm{e}^{\mathrm{i}\theta})^\ddagger = \mathrm{e}^{\mathrm{i}\theta}$, and from the observation that $\mathcal{V}_\theta(\mathbf{r}) = \mathcal{V}(\mathbf{r}\mathrm{e}^{\mathrm{i}\theta})$ is reversible whenever $\mathcal{V}(\mathbf{r})$ itself is. Thus, the formalism based on $t$-products and $t$-reversible Hamiltonians readily incorporates the dilatation analyticity of Balslev–Combes theory, whereas that based on conventional scalar products and Hermitian operators does not.

One can readily verify that the $t$-product reduces to the ordinary scalar product whenever the relevant Hamiltonian is Hermitian. Thus, whenever $\mathcal{H} = \mathcal{H}^\dagger = \mathcal{H}^\ddagger$, one finds

from Equation (22) that $\overline{\mathcal{H}} = \mathcal{H}^*$, and hence from Equations (14), (15) that $\overline{\psi} = \psi^*$, which makes the symbols $\{\psi \mid \varphi\}$ and $\langle \psi \mid \varphi \rangle$ equivalent.

The *t*-product also reduces properly in the resonance case. When the Hamiltonian is analytically continued to complex coordinates, $\mathcal{H}(\mathbf{r}) \rightarrow \mathcal{H}_\theta(\mathbf{r}) = \mathcal{H}(\mathbf{r}e^{i\theta})$, the complex-rotated $\mathcal{H}_\theta$, although still reversible, is no longer Hermitian and $\{\psi \mid \varphi\}$ is not a metric scalar product. In particular, when the potential $\mathcal{V}$ is a multiplicative function of coordinates only, one has $\mathcal{H}_\theta = \overline{\mathcal{H}}_\theta = \mathcal{H}_\theta{}^\ddagger$. In this case, the solutions of (15) differ from those of (14) only in the sign of the time variable ("complex conjugation of the time-dependent part of the solution"). In particular, when the time dependence is neglected in the usual manner, the *t*-product symbol $\{\psi \mid \varphi\}$ becomes equivalent to the *c*-product, as it must. Note however that the *t*-product also permits a convenient generalization of Ref. [10] for angular dependence, since the *t*-conjugated form of each spherical harmonic $Y_{\ell m}$ is the complex conjugate. Thus, the *t*-product formalism permits direct employment of the $Y_{\ell m}$'s (rather than their real linear combinations) as basis functions in complex-coordinate calculations.

One may now seek general theorems for reversible operators that encompass both Hermitian and complex-rotated special cases. Consider, for example, two solutions of the eigenvalue problem for general $\mathcal{H} = \mathcal{H}^\ddagger$,

$$\overline{\mathcal{H}}\,\overline{\psi} \;=\; \overline{W}_k \overline{\psi}_k \tag{32}$$

$$\mathcal{H}\psi_\ell = W_\ell\,\psi_\ell \tag{33}$$

where the first is written in t-conjugated form. Left-multiplying (32) by $\psi_\ell$ and (33) by $\overline{\psi}_k$ and subtracting, one finds, after integration over all space, that

$$0 = \left(\overline{W}_k \;-\; W_\ell\right)\{\psi_k|\psi_\ell\} \text{all } k, \ell \tag{34}$$

Since Equations (23), (27) guarantee that $W_k = W_k{}^\ddagger = \overline{W}_k$, one concludes that the eigenfunctions $\psi_k$, $\psi_\ell$ are automatically *t*-orthogonal if $W_k$, $W_\ell$ are non-degenerate, viz.,

$$\{\psi_k \mid \psi_\ell\} = 0, \text{ if } W_k \neq W_\ell \tag{35}$$

Similarly, one derives straightforwardly the generalized form of the hypervirial theorem [16],

$$\{\psi_k \mid [\mathcal{H},\Lambda]\psi_\ell\} = (W_k - W_\ell)\{\psi_k \mid \Lambda\psi_\ell\} \tag{36}$$

for an arbitrary operator $\Lambda$. For the special case $\Lambda = \mathbf{r}\cdot\mathbf{p}$ (or a sum of such terms in a many-particle system), Equation (36) leads to the generalized virial theorem for $\mathcal{H} = \mathcal{T} + \mathcal{V}$ (whether complex-rotated or not)

$$2\{\psi_k \mid \mathcal{T} \mid \psi_k\} = \{\psi_k \mid \mathbf{r}\cdot\boldsymbol{\nabla}\mathcal{V} \mid \psi_k\} \tag{37}$$

Related theorems were previously derived [12] for a restricted class of complex-rotated operators by the *c*-product formalism. The above examples suggest the many similarities, as well as key differences, that characterize the more general quantum mechanical formulation for *t*-reversible Hamiltonians.

## 4. Discussion

We have sketched a formal dot-product concept that departs from the purely mathematical Hilbert space prescription of conventional bound-state Schrödinger theory, but instead incorporates intrinsic dependence on the *physical system* ($\mathcal{H}$) of interest. The resulting *t*-product framework (and $\mathfrak{T}$-space) includes both the familiar Hilbert space of Hermitian operators as well as the related *c*-product space [12,13] of complex-rotated non-Hermitian operators. The *t*-product space and associated *t*-reversible operators ($\mathcal{A} = \mathcal{A}^\ddagger$) allow a unified quantum mechanical description of electronic bound (infinite lifetime) and resonance (finite lifetime) states, with sharpened restriction to physical Hamiltonian operators of proper time-reversal symmetry.

The unified $t$-product space yields normalizable probability amplitudes and other familiar virial- and hypervirial-type conservation laws of the Hermitian domain. Yet, it also incorporates the remarkable "exceptional points" [17–19]) of the non-Hermitian domain that correspond to spectral incompleteness (non-unitary dimensional collapse), with no counterpart in the Hilbert space of Hermitian operators. The $t$-product is also time-independent (Equation (18)), and hence distinguishable from the "F-product" [20] or other $t$-dependent analogs of the conventional scalar product of Hilbert space.

As discussed in the Introduction, the present treatment is framed rather narrowly in terms of non-relativistic *electronic* quantization in the Born–Oppenheimer framework, with semi-classical treatment of nuclei, electromagnetic radiation, or other "environmental" factors (along with the $t$, **B**, **S** factors explicitly included in Equation (12) and Table 1)) that may enter the potential energy $\mathcal{V}$. However, the treatment may be extended to perturbative corrections for relativistic effects (e.g., of Breit–Pauli type [21,22]), quantal effects (e.g., of nuclear structure, electromagnetic field, or radiative Lamb shift type [23,24]), or other weaker interactions (e.g., of gravitational type). In the spirit of common quantum chemical approximations, one may also include empirical descriptors of solvation (e.g., of Born type [25]), London dispersion (e.g., of Grimme type [26]), or other subtle aspects of electron correlation.

The formal integration of Hermitian and non-Hermitian domains in the $t$-product space provides a more general framework for relating the many available methods that have been employed for calculating resonance properties in one domain or the other, including stabilization [27], exterior scaling [28,29], Kohn S-matrix [30], complex absorbing potentials [31], Padé continuation of $\alpha$-derivatives [32], and related approaches [33,34]. The $t$-product framework somewhat alters the formal perception of the mathematical foundations of quantum mechanics [7,8], but provides broadened support for innovative non-Hermitian approaches that play an increasingly important role in describing the full range of $t$-dependent quantum mechanical phenomena, while retaining the original focus [1] on operator eigenvalue problems.

It is noteworthy that the $t$-product formulation draws a distinction between the "time" associated with spontaneous system evolution (e.g., through tunneling-type reactive or decay processes, even in the absence of "$t$"-dependent potential energy contributions) vs. that associated with an external clock (whose read-out "$t$"-value parametrically describes an external potential energy contribution applied to the system). Such distinction between "internal" ($t_{\mathrm{int}}$) measure of spontaneous system evolution vs. "external" ($t_{\mathrm{ext}}$) parametrization of an imposed external field may assist resolution of certain paradoxical issues of time-evaluation [35–38]. The $t$-product formulation also allows non-unitary dimensional collapse associated with exceptional-point degeneracy that may play a role in questions of information conservation (e.g., in the singular thermodynamic geometry of black-hole formation [39,40]). By offering a more physical (system-dependent) picture of quantal "spatial" structure, the present reformulation may cast light on formal ambiguities of the time-variable and other difficulties of reconciling quantum mechanics with classical descriptions of large-scale phenomena.

Although the present work focuses on $\mathfrak{T}$-space quantal structure in the Schrödinger equation (1) for isolated gas-phase atoms and molecules, we remark finally that the enriched spectrum of bound- and resonance-state eigenvalues may in principle introduce new features in thermodynamic-level description of chemical and phase behavior. In the standard quantum statistical thermodynamic theory of chemical equilibrium [41], the partition functions of reactant and product species (composed from quantal energy levels of the respective Schrödinger equations) may acquire *complex* character in certain ($T$,$P$) regimes, thereby mandating altered solutions for the equilibrium conditions. Similarly, in the cluster-based picture of fluid phases provided by quantum cluster equilibrium (QCE) theory [42], exotic resonance eigenvalues in any contributing cluster species may affect the self-consistent cluster populations that satisfy simultaneous equilibrium condi-

tions throughout the cluster reaction network. However, further speculations on possible applications of the unified $\mathfrak{T}$-space formalism are outside the scope of the present work.

**Funding:** The research was supported in part by National Science Foundation Grant CHE76-22760.

**Conflicts of Interest:** The author declares no conflict of interest.

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