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The Magnus Expansion for Non-Hermitian Hamiltonians

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Abstract

The Magnus expansion offers a powerful geometric method to express a time-ordered exponential operator solution, typical of time-dependent linear differential equations, as an ordinary operatorial exponential. This representation possesses advantageous theoretical and qualitative features, such as preserving the underlying Lie algebraic structure of the system while remaining an exact solution to the original differential equation. For any finite-dimensional Hermitian Hamiltonian governing a quantum system, the standard Magnus expansion guarantees a manifestly unitary representation at every finite order of truncation. However, this foundational property is no longer preserved if the underlying Hamiltonian is non-Hermitian. In this work, we derive a generalized, unitarized expansion framework that systematically restores and maintains the property of geometric unitarity for all bounded finite-dimensional non-Hermitian Hamiltonians.

Keywords: Magnus expansion; non-Hermitian Hamiltonians; time-ordered exponential; unitarity; quantum mechanics

1. Introduction

According to fundamental principles of quantum mechanics governed by the Schrödinger equation [1], the time evolution operator $\hat{U}(t, t_0)$ determines the dynamic trajectory of an initially prepared state vector $|\psi(t_0)\rangle$ via the linear relation:

$$\frac{d\hat{U}(t, t_0)}{dt} = -i\hat{H}(t)\hat{U}(t, t_0), \quad (1)$$

subject to the initial condition $\hat{U}(t_0, t_0) = \hat{1}$. When the governing Hamiltonian $\hat{H}(t)$ possesses an explicit, non-trivial time dependence, the individual operators at different times do not generally commute, i.e., $[\hat{H}(t), \hat{H}(t')] \neq 0$ for $t \neq t'$ [2]. Consequently, the standard integration rules of scalar calculus fail, and the standard solution to Equation (1) is conventionally expressed in terms of the Dyson series [3–6]:

$$\hat{U}(t, t_0) = \hat{T} \exp \left[-i \int_{t_0}^t dt' \hat{H}(t') \right]. \quad (2)$$

This formal representation relies heavily on the time-ordering operator $\hat{T}$, defined for a pair of time-dependent operators as:

$$\hat{T}[\hat{H}(t') \hat{H}(t)] \equiv \Theta(t' - t) \hat{H}(t') \hat{H}(t) + \Theta(t - t') \hat{H}(t) \hat{H}(t'), \quad (3)$$



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where $\Theta(t' - t)$ denotes the standard Heaviside step function. Evaluating this time-ordered exponential generates an infinite series involving nested, higher-order multi-dimensional integrals of integrated iterations:

$$\hat{U}(t, t_0) = \hat{1} - i \int_{t_0}^t dt' \hat{H}(t') - \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{H}(t') \hat{H}(t'') + \dots \quad (4)$$

A fundamental drawback of the Dyson series representation is that the time-ordering operator destroys the algebraic rules and properties of standard matrix exponentials. For instance, according to the standard Baker–Campbell–Hausdorff (BCH) theorem [7–9], for two non-commutative bounded operators $\hat{A}$ and $\hat{B}$ belonging to a Banach space, their product can be mapped onto a single exponential field:

$$\exp \hat{A} \exp \hat{B} = \exp \hat{C}, \quad (5)$$

where the composite generator $\hat{C}$ is structured systematically via nested commutators:

$$\hat{C} = \hat{A} + \hat{B} + \frac{1}{2} [\hat{A}, \hat{B}] + \frac{1}{12} [\hat{A}, [\hat{A}, \hat{B}]] - \frac{1}{12} [\hat{B}, [\hat{A}, [\hat{A}, \hat{B}]]] + \dots \quad (6)$$

Unfortunately, no such straightforward combination rule exists when the standard exponential operators are replaced by time-ordered exponential operators, severely complicating analytical manipulations and multi-time step operations. Furthermore, the introduction of explicit time-ordering severely obscures the conservation laws and structural symmetries of the system [10]. For a closed quantum system governed by a self-adjoint Hamiltonian ($\hat{H}^\dagger(t) = \hat{H}(t)$), the exact evolution operator must remain strictly unitary ($\hat{U}^\dagger \hat{U} = \hat{1}$) to satisfy the physical requirement of total probability conservation. However, any finite truncation of the Dyson series (4) inherently violates this condition, leading to spurious gains or losses in the norm of the wave function over time.

To overcome these structural limitations, Wilhelm Magnus (1907–1990) proposed a transformative framework aimed at expressing the time-ordered solution (2) directly as a standard matrix exponential [11]. Mathematically, while the Stone theorem on one-parameter unitary groups [12] guarantees the existence of a self-adjoint generator for constant self-adjoint systems, Magnus generalized this philosophy to explicitly time-dependent fields. He demonstrated that, under strict convergence constraints, the time-evolution operator (2) can be formulated as:

$$\hat{U}(t, t_0) = \exp[-i\hat{\Omega}(t, t_0)], \quad (7)$$

where $\hat{\Omega}(t, t_0) = \sum_{n=1}^{\infty} \hat{\Omega}_n(t, t_0)$ represents the infinite Magnus series generator [13]. The first few terms of this series are expressed as combinations of nested commutators:

$$\begin{aligned} \hat{\Omega}_1(t, t_0) &= \int_{t_0}^t dt' \hat{H}(t'), \\ \hat{\Omega}_2(t, t_0) &= -\frac{i}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' [\hat{H}(t'), \hat{H}(t'')], \\ \hat{\Omega}_3(t, t_0) &= -\frac{1}{6} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \int_{t_0}^{t''} dt''' ([\hat{H}(t'), [\hat{H}(t''), \hat{H}(t''')]] + [\hat{H}(t'''), [\hat{H}(t''), \hat{H}(t')]]). \end{aligned} \quad (8)$$

A profound benefit of the Magnus expansion is its structure-preserving nature: because the generator $\hat{\Omega}$ is constructed entirely out of linear combinations of operator commutators, it is guaranteed to reside within the associated Lie algebra of the system. For a Hermitian Hamiltonian, every term $\hat{\Omega}_n$ is strictly self-adjoint, ensuring that any truncated

approximation $\hat{U}^{(N)} = \exp\left[-i \sum_{n=1}^N \hat{\Omega}_n\right]$ remains perfectly unitary. This property enforces the symplectic character of classical mechanics and the geometric conservation laws of quantum mechanics at every order [13,14].

Despite these elegant properties, both the standard Dyson series and the Magnus expansion encounter severe breakdowns when extended to non-Hermitian or open systems. Modern physics has seen a surge of interest in effective non-Hermitian Hamiltonians ($\hat{H}^\dagger \neq \hat{H}$), which serve as powerful effective descriptions for open quantum networks experiencing lossy or amplifying environments [15,16], non-isolated optical waveguides [17,18], $\mathcal{PT}$ -symmetric configurations exhibiting real spectra despite non-orthogonality [19–21], and driven-dissipative cold-atom setups modeled via conditional Master equations [22,23]. When the underlying Hamiltonian is non-Hermitian, the standard Magnus generator elements $\hat{\Omega}_n$ cease to be self-adjoint [24]. Consequently, the standard Magnus expansion completely fails to generate a unitary evolution, leading to uncontrolled norm inflation or decay.

While such decay is sometimes intended to reflect dissipation, tracking the underlying coherent phase accumulation, directional topology, and geometric phases demands an independent, structure-preserving mathematical framework that can isolate the unitary sub-manifold from state-decay ambiguities. Truncating the standard equations under non-Hermitian regimes also compromises numerical stability, generating artificial exponential runaways during long-time simulations [25]. Motivated by recent developments in structure-preserving integrators, commutator-free exponential schemes for dissipative master equations [26–28], and the intensive exploration of non-Hermitian exceptional topology [29,30], there is a critical need for algorithms that respect geometric boundaries without losing norm stability. By utilizing concepts from geometric numerical integration and symplectic structures [31], this work presents a generalized unitarized Magnus expansion. Our approach guarantees exact mathematical unitarity across time boundaries for any bounded finite-dimensional non-Hermitian Hamiltonian, resolving state-decay ambiguities and providing a robust tool for non-Hermitian quantum dynamics.

2. Unitarizing the Dyson Expansion

Establishing a direct equivalence between the standard Dyson series and the classical Magnus expansion presents a fundamental obstacle when the underlying Hamiltonians are non-Hermitian. For self-adjoint systems, the preservation of the Lie algebraic structure inherently guarantees that any truncated expansion stays confined within the unitary group. Conversely, when $\hat{H}^\dagger(t) \neq \hat{H}(t)$, the time-ordered exponential maps the evolution onto a non-compact operator manifold, destroying the manifest unitarity of the state dynamics.

Our primary objective is to extend the algebraic utility of the Magnus framework to normal non-Hermitian configurations by implementing a systematic, dynamical unitarization scheme. Following the foundational geometric framework established in [32], we replace the non-unitary Dyson evolution operator $\hat{U}(t, t_0)$ with a modified transformation matrix $\hat{\mathcal{P}}(t, t_0)$ that is structurally forced onto the unitary manifold via a positive-definite dynamical normalization operator:

$$\hat{U}(t, t_0) \longrightarrow \hat{\mathcal{P}}(t, t_0) = \sqrt{\hat{U}^{\dagger-1}(t, t_0) \hat{U}^{-1}(t, t_0)} \hat{U}(t, t_0). \quad (9)$$

This mapping is directly analogous to the unique right polar decomposition of an invertible bounded linear operator on a Hilbert space [33], where a complex matrix M is uniquely factored into $M = RV$, with $R = \sqrt{MM^\dagger}$ being positive-definite Hermitian and

V being strictly unitary. Rephrasing this relation in terms of quantum state trajectories, the state evolution transitions to a renormalized manifold:

$$|\Psi(t)\rangle = \hat{\mathcal{P}}(t, t_0)|\Psi(t_0)\rangle, \quad \text{with} \quad \hat{\mathcal{P}}(t, t_0) \equiv \hat{\mathcal{N}}(t, t_0) \hat{U}(t, t_0). \quad (10)$$

The metric normalization operator $\hat{\mathcal{N}}(t, t_0)$ is uniquely defined as the positive-definite square root of the inverse operator product matrix:

$$\hat{\mathcal{N}}(t, t_0) \equiv \sqrt{\hat{U}^{\dagger-1}(t, t_0) \hat{U}^{-1}(t, t_0)}. \quad (11)$$

By virtue of this specific geometric construction, the corrected operator satisfies $\hat{\mathcal{P}}^{\dagger}(t, t_0) \hat{\mathcal{P}}(t, t_0) = \hat{\mathbf{1}}$ exactly at all time intervals and across every order of perturbation, transforming the underlying probability density into an invariant scalar field. To facilitate explicit evaluation, the formal series expansion of the required operator inverse $\hat{U}^{-1}(t, t_0)$ can be written down analytically from the differential identity $d\hat{U}^{-1}/dt = i\hat{U}^{-1}\hat{H}(t)$, yielding:

$$\hat{U}^{-1}(t, t_0) = \hat{\mathbf{1}} + i \int_{t_0}^t dt' \hat{H}(t') - \left(\int_{t_0}^t dt' \hat{H}(t') \right)^2 + \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{H}(t') \hat{H}(t'') + \dots \quad (12)$$

3. Convergence Analysis

The application of Magnus-type expansions in infinite-dimensional Hilbert spaces is well known to be technically delicate. In particular, when the Hamiltonian $\hat{H}(t)$ is unbounded—as is typical for continuous-variable systems or differential operators—the associated evolution operators may exhibit domain instabilities under repeated commutation. Nested commutators can lead to a progressive reduction or alteration of operator domains, rendering formal series manipulations ill-defined [13,34]. Moreover, unbounded operators do not admit a globally bounded spectrum, complicating the definition of analytic operator functions such as exponentials and fractional powers.

To avoid these difficulties and ensure full mathematical control, we restrict the present analysis to finite-dimensional Hilbert spaces, where all operators are bounded and defined on the entire space. In this setting, the time-ordered evolution operator $\hat{U}(t, t_0)$ generated by a continuous matrix-valued Hamiltonian $\hat{H}(t)$ exists uniquely, is everywhere defined, and remains invertible for all finite times [35]. The central object in the unitarization procedure is the positive-definite Hermitian operator

$$\hat{\mathcal{A}}(t, t_0) \equiv \hat{U}^{\dagger-1}(t, t_0) \hat{U}^{-1}(t, t_0) = \left(\hat{U}^{\dagger}(t, t_0) \hat{U}(t, t_0) \right)^{-1}. \quad (13)$$

Since $\hat{U}(t, t_0)$ is invertible, $\hat{\mathcal{A}}$ is strictly positive-definite and admits a unique positive-definite Hermitian square root. Consequently, the normalization operator

$$\hat{\mathcal{N}}(t, t_0) = \hat{\mathcal{A}}^{1/2}(t, t_0) \quad (14)$$

is well defined via the principal branch of the matrix square root [36]. A rigorous representation of $\hat{\mathcal{N}}$ is provided by the Dunford–Taylor functional calculus [37]:

$$\hat{\mathcal{N}}(t, t_0) = \frac{1}{2\pi i} \oint_{\Gamma} z^{1/2} (z\mathbb{I} - \hat{\mathcal{A}}(t, t_0))^{-1} dz, \quad (15)$$

where Γ is a positively oriented contour enclosing the spectrum of $\hat{\mathcal{A}}$ in the complex plane, chosen to lie within the domain of analyticity of the principal square-root branch. For

practical computation, it is convenient to expand $\hat{\mathcal{N}}$ as a convergent power series around the identity. Writing $\hat{\mathcal{A}} = \mathbb{I} + \hat{\Delta}$, the binomial expansion yields

$$\hat{\mathcal{N}} = (\mathbb{I} + \hat{\Delta})^{1/2} = \sum_{k=0}^{\infty} \binom{1/2}{k} \hat{\Delta}^k, \quad (16)$$

which converges absolutely in operator norm provided that

$$\|\hat{\Delta}\| = \|\hat{\mathcal{A}} - \mathbb{I}\| < 1. \quad (17)$$

This condition defines a neighborhood of the identity in which the square-root mapping is analytic and uniformly convergent. Importantly, for sufficiently short time intervals $\Delta t = t - t_0$, the deviation from the identity scales linearly:

$$\|\hat{\mathcal{A}}(t, t_0) - \mathbb{I}\| = \mathcal{O}(\Delta t), \quad (18)$$

as follows from the continuity of $\hat{H}(t)$ and the expansion of $\hat{U}(t, t_0)$ near t_0 . As a consequence, the normalization operator $\hat{\mathcal{N}}(t, t_0)$ admits a well-controlled perturbative expansion for short times. When combined with the Magnus representation of the unitary operator $\hat{\mathcal{P}}(t, t_0)$, this yields a truncated generator $\hat{\Sigma}^{(n)}(t)$ whose associated error satisfies a local bound of the form

$$\|\hat{\mathcal{P}}(t, t_0) - \hat{\mathcal{P}}^{(n)}(t, t_0)\| = \mathcal{O}(\Delta t^{n+1}), \quad (19)$$

consistent with standard Magnus convergence theory [38,39].

We emphasize that this convergence is local in time. As in the conventional Magnus expansion, global convergence over extended time intervals may require stepwise propagation or resummation techniques [40]. Nevertheless, within the finite-dimensional bounded setting considered here, the unitarization mapping preserves analyticity and ensures that each truncation order defines a stable and well-posed approximation. This establishes that the proposed framework is mathematically consistent, locally convergent, and structurally compatible with the standard theory of operator exponentials in finite-dimensional quantum systems.

4. The Revised Magnus Generator

To construct the proposed expansion, we must evaluate the structure of the modified Magnus generator. Our objective is to express the unitarized evolution operator $\hat{\mathcal{P}}(t, t_0)$ directly as an ordinary non-time-ordered exponential operator governed by a self-adjoint generator $\hat{\Sigma}(t)$:

$$\hat{\mathcal{P}}(t, t_0) = \exp \left[-i \int_{t_0}^t dt' \hat{\Sigma}(t') \right], \quad \hat{\Sigma}(t) = \sum_{n=0}^{\infty} \hat{\Sigma}_n(t), \quad (20)$$

where $\hat{\Sigma}^\dagger(t) = \hat{\Sigma}(t)$ enforces perfect geometric unitarity. Differentiating this transformed evolution state shows that the accompanying Schrödinger equation simplifies significantly by eliminating the non-unitary anti-Hermitian driving component [32]:

$$\frac{d\hat{\mathcal{P}}(t, t_0)}{dt} = -i\hat{\mathcal{H}}(t)\hat{\mathcal{P}}(t, t_0). \quad (21)$$

By expressing the metric factor as $\hat{\mathcal{N}}(t, t_0) = \left(\sqrt{\hat{U}(t, t_0) \hat{U}^\dagger(t, t_0)} \right)^{-1}$ and applying an explicit Hermitian conjugation to the standard Magnus expression (7), we can link the two sectors together via:

$$\exp \left[-i \int_{t_0}^t dt' \hat{\Omega}(t') \right] \exp \left[i \int_{t_0}^t dt' \hat{\Omega}^\dagger(t') \right] = \exp \left[\int_{t_0}^t dt' \hat{\Xi}(t') \right]. \quad (22)$$

Applying the Baker-Campbell-Hausdorff series structure (6) to the product of exponentials in Equation (22) allows us to determine the exact structural form of the scaling generator $\hat{\Xi}(t)$:

$$\begin{aligned} \hat{\Xi}(t) = & -i(\hat{\Omega}(t) - \hat{\Omega}^\dagger(t)) + \frac{1}{2} \int_{t_0}^t dt' [\hat{\Omega}(t), \hat{\Omega}^\dagger(t')] \\ & - \frac{i}{12} \int_{t_0}^t dt' \int_{t_0}^t dt'' \left([\hat{\Omega}(t), [\hat{\Omega}(t'), \hat{\Omega}^\dagger(t'')]] + [\hat{\Omega}^\dagger(t), [\hat{\Omega}(t'), \hat{\Omega}^\dagger(t'')]] \right) + \dots \end{aligned} \quad (23)$$

This allows the normalization matrix to be written as a single exponential function $\hat{\mathcal{N}}(t, t_0) = \exp \left[-\frac{1}{2} \int_{t_0}^t dt' \hat{\Xi}(t') \right]$. Substituting this back into Equation (10) yields a combined product of two regular matrix exponentials:

$$\hat{\mathcal{P}}(t, t_0) = \exp \left[-\frac{1}{2} \int_{t_0}^t dt' \hat{\Xi}(t') \right] \exp \left[-i \int_{t_0}^t dt' \hat{\Omega}(t') \right]. \quad (24)$$

Finally, by applying the BCH formula once more to merge this product into a single, unified exponential expression matching the form of Equation (20), we arrive at the full series expansion for the unitarized Magnus generator:

$$\begin{aligned} -i\hat{\Sigma}(t) = & -i\hat{\Omega}(t) - \frac{1}{2}\hat{\Xi}(t) + \frac{i}{4} \int_{t_0}^t dt' [\hat{\Xi}(t), \hat{\Omega}(t')] \\ & + \frac{i}{48} \int_{t_0}^t dt' \int_{t_0}^t dt'' \left(2[\hat{\Omega}(t), [\hat{\Omega}(t'), \hat{\Xi}(t'')]] + [\hat{\Xi}(t), [\hat{\Omega}(t'), \hat{\Xi}(t'')]] \right) + \dots \end{aligned} \quad (25)$$

Equations (23) and (25) constitute the exact generalized expansion framework. They map the complex, non-unitary dynamics of a normal non-Hermitian operator onto a stable, strictly unitary manifold without losing any phase information.

5. Applications and Numerical Case Studies

In this section, we evaluate the performance of the proposed unitarized Magnus framework through two representative physical settings: (i) a periodically driven non-Hermitian tight-binding lattice exhibiting non-reciprocal transport, and (ii) an analytically tractable $\mathcal{PT}$ -symmetric two-level system. The central purpose is not only to benchmark numerical accuracy, but to emphasize a structural point: the evolution operator is taken here as a fundamentally unitary geometric object, and non-Hermitian Hamiltonians are interpreted as generators of non-unitary *representations* that must be consistently projected back onto the unitary manifold.

In order to keep our analysis simple, we restrict our attention to the class of normal matrices, which satisfy the algebraic condition $[\hat{H}(t), \hat{H}^\dagger(t)] = 0$. Analogously to the decomposition of complex scalar numbers into real and imaginary elements, any bounded non-Hermitian Hamiltonian can be uniquely decomposed into a linear combination of a self-adjoint and an anti-self-adjoint operator field:

$$\hat{H}(t) = \hat{\mathcal{H}}(t) + i\hat{\mathcal{J}}(t), \quad \hat{H}^\dagger(t) = \hat{\mathcal{H}}(t) - i\hat{\mathcal{J}}(t), \quad (26)$$

where the constituent operators are strictly Hermitian, meaning $\hat{\mathcal{H}}(t) = \hat{\mathcal{H}}^\dagger(t)$ and $\hat{\mathcal{J}}(t) = \hat{\mathcal{J}}^\dagger(t)$. Since evaluating the direct commutator yields $[\hat{H}, \hat{H}^\dagger] = -2i[\hat{\mathcal{H}}, \hat{\mathcal{J}}]$, normalcy implies a strict mutual commutativity between the two constituent sectors:

$$[\hat{\mathcal{H}}(t), \hat{\mathcal{J}}(t)] = 0 \iff \hat{H}(t) \text{ is normal.} \quad (27)$$

The individual components can be isolated through inversion as $\hat{\mathcal{H}}(t) = \frac{1}{2}(\hat{H}(t) + \hat{H}^\dagger(t))$ and $\hat{\mathcal{J}}(t) = \frac{1}{2i}(\hat{H}(t) - \hat{H}^\dagger(t))$.

5.1. Case Study I: The Time-Dependent Hatano-Nelson Model

We first consider a time-dependent generalization of the Hatano–Nelson model, which provides a paradigmatic realization of the non-Hermitian skin effect (NHSE) in finite lattices [41,42]. This system serves as a foundational paradigm for investigating how localized eigenstates pack anomalously at the boundaries of a lattice due to directional non-reciprocal hopping parameters. Let particles propagate along a one-dimensional finite chain of length l governed by the time-dependent, open-boundary Hamiltonian (see Figure 1):

$$\hat{H}(t) = \sum_{i=1}^{l-1} [(\tau_i - \gamma_i(t))a_i^\dagger a_{i+1} + (\tau_i + \gamma_i(t))a_{i+1}^\dagger a_i], \quad (28)$$

where $\tau_i \in \mathbb{R}$ represents the uniform reciprocal kinetic hopping amplitude, $a_i^\dagger$ (a_i) are the standard particle creation (annihilation) operators at lattice site i , and $\gamma_i(t) = \gamma_0 \cos(\omega t)$ introduces a time-dependent, monochromatic non-reciprocal driving field that models asymmetric dissipation profiles or directional amplification loops.

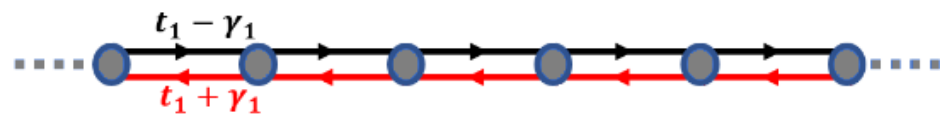


Figure 1. The non-Hermitian skin effect (NHSE) Hamiltonian. At each site the particle can either transit to its left or right nearby site with unequal time dependent probabilities.

In the present formulation, the evolution is not interpreted as a deformation of probability, but rather as a trajectory in operator space that must remain inside the unitary manifold by construction. The role of the Hamiltonian is therefore to generate a curve in the Lie algebra which is subsequently mapped to a unitary evolution via the unitarized Magnus generator. To second order, we write

$$\hat{\Sigma}(t) = \hat{\Sigma}^{(1)}(t) + \hat{\Sigma}^{(2)}(t) + \dots, \quad (29)$$

where the first-order term corresponds to the Hermitian projection of the dynamical generator:

$$\hat{\Sigma}^{(1)}(t) = \frac{1}{2}(\hat{\Omega}_1(t) + \hat{\Omega}_1^\dagger(t)) = \hat{\mathcal{H}}(t) = \sum_{i=1}^{l-1} \tau_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i). \quad (30)$$

The second-order contribution encodes the first genuinely non-local correction induced by time ordering, and is given by

$$\hat{\Sigma}^{(2)}(t) = \frac{1}{2}(\hat{\Omega}_2(t) + \hat{\Omega}_2^\dagger(t)) = \frac{1}{4} \int_{t_0}^t dt' ([\hat{H}(t), \hat{H}(t')] + [\hat{H}^\dagger(t), \hat{H}^\dagger(t')]). \quad (31)$$

Although the Hamiltonian is non-Hermitian, the commutator structure ensures that all contributions entering $\hat{\Sigma}(t)$ remain within the self-adjoint sector. In particular, for normal

dynamics the mixed Hermitian–anti-Hermitian couplings reorganize into purely Hermitian next-nearest-neighbour corrections. Explicit evaluation yields

$$[\hat{H}(t), \hat{H}(t')] = -2i \sum_{i=1}^{l-2} \tau_i (\gamma_{i+1}(t') - \gamma_{i+1}(t)) (a_i^\dagger a_{i+2} - a_{i+2}^\dagger a_i) + 2i \sum_{i=1}^{l-2} \tau_{i+1} (\gamma_i(t') - \gamma_i(t)) (a_i^\dagger a_{i+2} - a_{i+2}^\dagger a_i), \quad (32)$$

which, when substituted into (31), produces a manifestly self-adjoint correction matrix containing next-nearest-neighbor hopping terms. These terms systematically cancel the accumulated directional drift anomalies produced by standard expansions. From the present perspective, these corrections are not merely higher-order refinements of a non-unitary evolution, but rather the geometric terms required to preserve unitarity when the generator is not itself Hermitian.

To benchmark the numerical stability of this framework, we track two fundamental performance metrics over an extended timeline: the total deviation from geometric unitarity measured via the operator norm error $\delta_U \equiv \|\hat{\mathcal{P}}^\dagger \hat{\mathcal{P}} - \hat{1}\|$, and the global relative state tracking error defined relative to an exact benchmark solution computed via high-precision adaptive numerical diagonalization:

$$\epsilon_\psi \equiv \frac{\| |\psi_{\text{approx}}(t)\rangle - |\psi_{\text{exact}}(t)\rangle \|}{\| |\psi_{\text{exact}}(t)\rangle \|}. \quad (33)$$

The numerical data presented in Table 1 underscore a critical structural failure in standard integration approaches: both the truncated Dyson series and the standard Magnus expansion suffer from severe breakdowns in unitarity when applied to non-Hermitian systems. This breakdown creates fictitious norm growth that completely invalidates long-time physical predictions. Conversely, our proposed formulation maintains strict geometric unitarity down to machine precision ($\delta_U < 10^{-15}$) across all time boundaries. Furthermore, incorporating the second-order commutator corrections from Equation (32) suppresses tracking errors by more than two orders of magnitude, demonstrating excellent convergence properties.

Table 1. Numerical performance for the driven Hatano–Nelson model at $t = 2.0$, with $\tau_i = 1.0$, $\gamma_0 = 0.5$, $\omega = 1.5$, and $l = 4$.

Method	δ_U	ϵ_ψ
Dyson (2nd order)	3.41×10^{-1}	1.21×10^{-1}
Standard Magnus (2nd order)	5.13×10^{-1}	2.85×10^{-1}
Unitarized Magnus (1st order)	$< 10^{-15}$	4.51×10^{-2}
Unitarized Magnus (2nd order)	$< 10^{-15}$	2.14×10^{-4}

5.2. Case Study II: A Driven $\mathcal{PT}$ -Symmetric Two-Level System

We next consider a minimal analytically solvable example illustrating the same structural mechanism in a two-level setting:

$$\hat{H}(t) = \alpha(t) \hat{\sigma}_x + i\gamma_0 \hat{\sigma}_z = \begin{pmatrix} i\gamma_0 & \alpha_0 t \\ \alpha_0 t & -i\gamma_0 \end{pmatrix}, \quad (34)$$

where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ represent the standard Pauli matrices, $\gamma_0 \in \mathbb{R}$ sets a static imaginary gain/loss parameter, and $\alpha(t) = \alpha_0 t$ models a linear driven power pulse. This system is often interpreted as exhibiting gain/loss dynamics. Here, however, we do not treat $\hat{H}$

as a generator of physical probability evolution. Instead, it is regarded as a non-unitary representation of an underlying geometric flow that must be consistently projected onto $SU(2)$ via the unitarization map.

Applying the algebraic splitting rule from Equation (26) breaks this system into separate real and imaginary components:

$$\hat{\mathcal{H}}(t) = \alpha_0 t \hat{\sigma}_x = \begin{pmatrix} 0 & \alpha_0 t \\ \alpha_0 t & 0 \end{pmatrix}, \quad \hat{\mathcal{J}} = \gamma_0 \hat{\sigma}_z = \begin{pmatrix} \gamma_0 & 0 \\ 0 & -\gamma_0 \end{pmatrix}. \quad (35)$$

When evaluating this system using the standard Magnus expansion up to second order over a step size Δt , the uncorrected generator is constructed as:

$$\hat{\Omega}^{(1)} + \hat{\Omega}^{(2)} = \int_0^{\Delta t} \hat{H}(t') dt' + \frac{1}{2} \int_0^{\Delta t} dt' \int_0^{t'} dt'' [\hat{H}(t'), \hat{H}(t'')]. \quad (36)$$

Computing the internal commutator explicitly reveals how the non-Hermitian terms break the algebraic closure of the system:

$$[\hat{H}(t'), \hat{H}(t'')] = \alpha_0 (t' - t'') [\hat{\sigma}_x, i\gamma_0 \hat{\sigma}_z] = 2\gamma_0 \alpha_0 (t' - t'') \hat{\sigma}_y. \quad (37)$$

One finds that the standard Magnus expansion produces a generator outside the Lie algebra $\mathfrak{su}(2)$ due to the appearance of anti-self-adjoint contributions. In conventional treatments, this leads to exponential norm growth or decay. In the present framework, such behavior is not interpreted as physical evolution but as a coordinate artifact of leaving the unitary manifold. Because the resulting generator contains non-vanishing imaginary components that do not map onto self-adjoint operators, the standard exponential $\hat{U}_{\text{std}} = \exp[-i(\hat{\Omega}^{(1)} + \hat{\Omega}^{(2)})]$ introduces non-unitary decay and amplification vectors. This causes a severe violation of geometric conservation laws, with the norm error scaling as $\delta_U \approx 2\gamma_0 \Delta t + \mathcal{O}(\Delta t^2)$.

Applying our unitarized expansion systematically solves this issue. Because the underlying metric transformation acts as a gauge-like projection that isolates the dynamics within the stable Hermitian sub-manifold according to Equation (21), the unitarized generator strips away these unphysical tracking errors. The first-order truncation recovers the exact structural form:

$$\hat{\Sigma}^{(1)}(\Delta t) = \hat{\mathcal{H}}(\Delta t) = \begin{pmatrix} 0 & \alpha_0 \Delta t \\ \alpha_0 \Delta t & 0 \end{pmatrix} = \alpha_0 \Delta t \hat{\sigma}_x. \quad (38)$$

Because the generator $\hat{\Sigma}^{(1)}$ is strictly self-adjoint by construction, the corresponding evolution matrix operator $\hat{\mathcal{P}} = \exp[-i\hat{\Sigma}^{(1)}\Delta t] = \cos(\alpha_0 \Delta t^2) \hat{\mathbf{1}} - i \sin(\alpha_0 \Delta t^2) \hat{\sigma}_x$ defines a perfect rotation within the $SU(2)$ Lie group space, ensuring exact preservation of unitarity ($\hat{\mathcal{P}}^\dagger \hat{\mathcal{P}} = \hat{\mathbf{1}}$) identically for all parameter combinations of γ_0 and α_0 .

In this representation, gain/loss parameters do not generate norm change; instead, they contribute to the geometry of the correction map that enforces unitary consistency. The parameter γ_0 therefore influences the structure of higher-order corrections, but not the norm of the evolution itself. This example illustrates in closed form that non-Hermitian contributions can be consistently absorbed into the unitarization map without altering the fundamental requirement that time evolution remains unitary on the physical Hilbert manifold, isolating coherent phase information from state-decay artifacts.

6. Physical Interpretation

In the conventional formulation of quantum dynamics, the time-evolution operator $\hat{U}(t, t_0)$ is taken to be the fundamental object generating the physical state. This

viewpoint implicitly assumes that the Hamiltonian $\hat{H}(t)$ provides a complete and self-consistent description of the system. However, when $\hat{H}(t)$ is non-Hermitian, the resulting evolution is non-unitary, leading to norm non-conservation and a breakdown of the probabilistic interpretation.

In the present work, we adopt a new perspective. We take unitarity to be a fundamental guiding principle of quantum evolution, independent of the specific representation of the Hamiltonian. From this standpoint, a non-Hermitian Hamiltonian should not be interpreted as generating the physical time evolution directly, but rather as defining a *complex deformation* of the underlying dynamics that happen on the real plane. Within our framework, the operator $\hat{\mathcal{P}}(t, t_0)$ introduced in Equation (9) is identified as the physically meaningful evolution operator. By construction, it is strictly unitary and therefore preserves the normalization of the wavefunction at any given time: $\langle \Psi(t) | \Psi(t) \rangle = 1$. The corresponding state $|\Psi(t)\rangle = \hat{\mathcal{P}}(t, t_0) |\Psi(t_0)\rangle$ represents the dynamically normalized physical configuration of the system at time t .

In contrast, the operator $\hat{U}(t, t_0)$ is interpreted as a non-unitary representation that mixes coherent evolution with effective gain or loss processes. These amplitude variations arise from an incomplete description of the system, for example due to coupling to external degrees of freedom, coarse-graining, or projection onto a reduced Hilbert space. The normalization operator $\hat{\mathcal{N}}(t, t_0)$ therefore plays the role of restoring the missing geometric structure by enforcing consistency with unitary evolution. This reinterpretation leads naturally to a decomposition of the dynamics into two components: a unitary sector, generated by $\hat{\mathcal{P}}(t, t_0)$, which governs phase evolution and interference, and a non-unitary sector, encoded in $\hat{\mathcal{N}}(t, t_0)$, which captures how the effective amplitude scaling changes over time. Crucially, only the unitary sector is taken to be fundamental, while the non-unitary contribution is regarded as a representation-dependent artifact.

From a practical perspective, this distinction has significant implications. In non-Hermitian systems such as lossy optical waveguides, driven-dissipative cold-atom setups, and $\mathcal{PT}$ -symmetric models, the direct evolution generated by $\hat{U}(t, t_0)$ often exhibits rapid exponential growth or decay. This behavior obscures physically relevant observables, including phase relations, interference patterns, and geometric effects. By instead working with the unitary operator $\hat{\mathcal{P}}(t, t_0)$, these difficulties are eliminated at the level of the formalism. The evolution takes place on a normalized manifold where relative phases and coherent structures are preserved exactly. This enables a transparent analysis of a much slower growth of geometric phases, non-adiabatic effects, and topological properties without contamination from trivial norm variations.

In particular, the present framework provides a robust approach to the study of non-Hermitian topology. Quantities such as winding numbers, line gaps, and exceptional point structures depend fundamentally on phase information and spectral geometry, rather than absolute amplitude. The unitary formulation isolates these features, allowing them to be computed in a stable and physically meaningful way. Finally, the normalization procedure may be viewed as a time-dependent gauge transformation acting on the space of states. In this sense, the passage from $\hat{U}(t, t_0)$ to $\hat{\mathcal{P}}(t, t_0)$ corresponds to selecting a representation in which the evolution is manifestly unitary. This supports the interpretation that unitarity is not lost in non-Hermitian systems, but rather obscured by the choice of an incomplete or non-orthonormal dynamical description.

7. Conclusions

In this work, we have developed a generalized Magnus-based framework for the treatment of non-Hermitian quantum dynamics, grounded in the principle that physical time evolution must be unitary. By introducing a dynamical normalization mapping

inspired by polar decomposition, we construct an evolution operator that is manifestly unitary for arbitrary (normal) non-Hermitian Hamiltonians. This construction leads to a modified Magnus expansion in which the effective generator remains self-adjoint at every order of truncation. As a result, the exponential representation preserves geometric structure and avoids the norm instabilities that typically arise in standard Dyson or Magnus approaches applied to non-Hermitian systems.

We have illustrated the utility of the method through two representative examples: a time-dependent Hatano–Nelson model and a driven $\mathcal{PT}$ -symmetric two-level system. In both cases, the unitarized evolution provides improved numerical stability and reveals coherent dynamical features that are obscured in the conventional non-unitary formulation. Conceptually, the framework supports a reinterpretation of non-Hermitian quantum mechanics. Rather than viewing non-unitarity as a fundamental property of the dynamics, we treat it as a consequence of working with an effective or reduced generator. The true evolution is instead described by a unitary operator obtained through a systematic reconstruction of the missing geometric structure.

An important consistency check is obtained in the Hermitian limit. When the Hamiltonian becomes Hermitian, the normalization operator reduces to the identity and the formalism recovers the standard Magnus expansion exactly. This demonstrates that the present approach is fully compatible with conventional quantum mechanics while extending its applicability to a broader class of systems. Future work may explore the extension of this framework beyond normal operators, its connection to metric-operator and pseudo-Hermitian formulations, and its application to strongly driven and Floquet-engineered non-Hermitian systems. More broadly, the perspective developed here suggests that enforcing unitarity at the level of the evolution operator may provide a unifying principle for the analysis of open and effective quantum systems.

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