

Hamiltonian Learning Through Lie-Theoretic Methods

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ABSTRACT

This paper presents a method for identifying unknown coefficients of basis elements in an effective Hamiltonian of single-qubit cases. This is done directly from the measurement statistics of a quantum system's unitary evolution, utilizing a unique method of Lie algebra coefficient recovery. The method exploits the fact that repeated application of a unitary operator amplifies the generator coefficient linearly in the exponent. The result produces measurement probabilities that constrain the unknown coefficient differently at each power tested. Inversion of any single measurement probability yields a multivalued set of candidates due to the periodic nature of the trigonometric functions involved. However, the true coefficient can be identified as the unique true value satisfying a consistency criterion across all powers simultaneously. The method is demonstrated numerically for the single-generator Hamiltonian ($H_e = aX$) and extended analytically to the two-generator case ($H_e = aX + bZ$), where geometric conjugation reduces the Hamiltonian to an effective single-generator form. Numerical simulations further verify the geometric reduction and the subsequent coefficient reconstruction for representative two-generator Hamiltonians, given a known rotation angle. In both cases, the correct coefficients are recovered from measurement statistics, without ancilla qubits, coherent control circuits, or prior knowledge of the system's spectrum; for the two-generator case, the rotation angle used to align the Hamiltonian is currently taken as given rather than estimated from data.

INTRODUCTION

A. CONTEXT

At the most fundamental level, a quantum system is any physical object whose properties can only be defined in relation to a measuring device, observer, or other system that interacts with it. Unlike classical physics, where the precise position and speed of an object can be precisely known, quantum systems exist in multiple configurations until a measurement is made and an outcome is observed. This behavior is now experimentally confirmed and lays the foundation for modern quantum physics and the basis of an entirely new generation and class of technologies. One are quantum computers, which exploit superposition and related phenomena to process information in ways that are provably impossible for classical machines. Quantum sensors use the extreme sensitivity of quantum states to detect signals such as magnetic fields, gravitational waves, and chemical concentrations, far below the limits of any classical

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instrument. Yet each of these technological expansions fundamentally relies on the ability to control how quantum systems evolve over time.

That evolution is governed by the Hamiltonian, which encodes every physically meaningful parameter of a quantum system, such as how strongly different parts of the system interact, how fast they oscillate, or how they respond to external fields. If the Hamiltonian is known, one can predict, at least in principle, how the system will behave. However, in practice, the Hamiltonian is seldom perfectly known. Components are fabricated with slight imperfections, and the more complex the device becomes, the harder it is to characterize what is happening inside it. The problem of how we can then characterize the Hamiltonian of a quantum device directly from the data it produces becomes a central one that this work aims to address.

B. MOTIVATION

The mathematical language best suited to answer this question is Lie theory. In Lie Theory, a Lie algebra is, in general terms, a mathematical structure whose elements generate the transformations a system can undergo when exponentiated. For a quantum system, these generators are the terms in the Hamiltonian, and the transformations they produce are unitary operators describing how the state of a system evolves over time.

The key insight of Lie theory in this context is that the Hamiltonian can always be written as a combination of generators with real-valued coefficients, and those coefficients correspond precisely to the physical parameters required to characterize the Hamiltonian.

Resultantly, the central question becomes: if we can only observe the outcomes of measurements performed on a quantum system, can we work backwards to identify the key elements determining its evolution? The current gap becomes evident when examining the existing literature addressing this problem.

C. LITERATURE REVIEW

A substantial body of existing work attempts to understand Lie-algebraic structure analytically or numerically in order to solve dynamical problems, without necessarily concerning itself with the inverse problem

of inferring the Hamiltonian directly from measurement data. This leaves a significant gap in the literature.

One classical line of work concerns Lie-algebraic decoupling methods for solving time-dependent Schrödinger equations. If the Hamiltonian at all times belongs to a finite-dimensional Lie algebra, then the evolution operator can be written as an ordered product of exponentials of Lie algebra elements,

commonly classified as a Wei-Norman decomposition [1]. These methods require complete knowledge of the Hamiltonian and its Lie-algebraic structure as input and produce the full time evolution as output. While they are undeniably powerful tools for solving dynamics, they remain fundamentally forward methods.

The Magnus expansion offers a similar approach by representing the time-ordered evolution operator as a single exponential

$$U(t, t_0) = \text{Exp} \left(-\frac{i}{\hbar} \int_{t_0}^t H(t') dt' \right) U(T) = e^{\Omega(T)}$$

Where Ω is expressed as an infinite series of nested commutators and time-ordered integrals involving the Hamiltonian at different times. Studies of the Magnus expansion in Lie-algebraic settings establish that the effective Hamiltonian remains within the dynamical Lie algebra generated by the original operators [2].

Research combining Lie algebras and Hamiltonian systems has similarly examined how the structure constants of the algebra, simply the numerical coefficients that appear in the commutation relations between the Lie algebras, constrain the resulting dynamics and admissible transformations [3].

One of the most prominent examples of Hamiltonian parameter inference is Quantum Phase Estimation (QPE), which extracts eigenphases of a unitary operator and thereby infers spectral properties of its generator. In the standard formulation, an ancilla qubit is prepared in superposition and used to coherently control repeated applications of U_m , after which interference measurements reveal phase information [4, 5]. QPE and related Fourier-based methods provide powerful spectral estimation techniques but generally require coherent control circuitry, large ancilla systems, and deep quantum circuits.

Recent work on Bayesian Hamiltonian learning adopts a different perspective by treating Hamiltonian parameters as unknown random variables updated through experimental observations [6]. Such approaches can achieve highly efficient parameter scaling but often rely on extensive classical optimization and probabilistic inference.

A closely related non-ancilla approach is Robust Phase Estimation (RPE), which characterizes the rotation angle of a single-qubit gate by applying the unitary a variable number of times and measuring in the computational basis, then combining estimates across power levels to resolve the periodic ambiguity inherent in any single measurement [7]. Like the present method, RPE requires no ancilla qubits or coherent control, and its core mechanism, using repeated applications of a unitary to amplify an unknown parameter and cross-referencing multiple power levels to eliminate spurious solutions, is mathematically analogous to the cross-power consistency procedure developed here. RPE, however, is typically created as an estimator for a single eigenphase of an arbitrary gate for calibration purposes, generally using powers chosen adaptively (e.g., doubling at each round) to achieve Heisenberg-limited precision scaling. It is not

generally framed in terms of recovering multiple structured coefficients of a Hamiltonian expressed in a fixed Lie algebra basis, nor does it address the multi-generator case through geometric conjugation.

From the preceding discussion, a specific gap becomes apparent. Lie-theoretic approaches are highly effective for the forward problem: given a Hamiltonian expressible as a linear combination in the Lie algebra generators with known coefficients, they efficiently characterize and simulate the resulting dynamics. Quantum phase estimation, Bayesian methods, and RPE-style non-adaptive phase estimation all address aspects of the inverse problem, but none are generally formulated in terms of direct coefficient reconstruction in a known, fixed Lie algebra basis, nor do they provide an explicit geometric procedure, such as the conjugation-based rotation developed in Section III, for decoupling multiple simultaneously present generators before applying single-parameter estimation.

The present work thus investigates whether repeated powers of a unitary evolution operator may themselves serve as a computational resource for recovering Hamiltonian coefficients directly from measurement statistics.

When multiple generators are present, for example

$$V = aX + bZ$$

the method may be extended through unitary conjugation,

$$U_1(\theta) = e^{-i\theta X} U e^{i\theta X}$$

with strategically chosen rotations used to eliminate unwanted basis components and reduce the Hamiltonian to a single-generator form before coefficient extraction.

While forward methods and spectral estimation techniques are well developed, relatively little work has examined the direct recovery of Lie algebra coefficients from repeated measurement statistics alone. The present work investigates this setting precisely, whether a quantum system evolving under a unitary generated by a known Lie algebra element with unknown coefficients can be reconstructed by the linear amplification of the unknown parameter, and whether this case can be further expanded and generalized to multiple coefficients of the Lie algebra.

D. METHODS

I. Introduction

The method begins with the introductory set up that is derived as follows. We begin with the simplest quantum system, which is a qubit, the quantum analogue of a classical bit. Where a classical bit is either 0 or 1, a qubit can exist in a superposition of both. The two computational basis states are written as $|0\rangle$ and $|1\rangle$, and a general qubit state is

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad (1)$$

where α and β are complex numbers. Upon measurement, the probability of obtaining $|0\rangle$ is $|\alpha|^2$ and the probability of obtaining $|1\rangle$ is $|\beta|^2$. Since one of the two outcomes must occur, the normalization condition holds:

$$|\alpha|^2 + |\beta|^2 = 1 \quad (2).$$

This state vector $|\psi\rangle$ lives in a two-dimensional complex vector space, and all system dynamics are described by transformations on this vector.

The time evolution of a quantum system is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \quad (3)$$

where H is the Hamiltonian operator encoding the physical interactions of the system.

Working in natural units where $\hbar = 1$, this simplifies notation. For a time-independent Hamiltonian, the solution is

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle \quad (4)$$

The operator

$$U(t) = e^{-iHt} \quad (5)$$

is unitary and preserves normalization. It describes the full physical evolution of a closed quantum system.

The matrix exponential is defined by its Taylor series:

$$e^M = I + M + \frac{M^2}{2!} + \frac{M^3}{3!} + \dots \quad (6)$$

where I is the identity matrix.

For a single qubit, the standard generators are the Pauli operators:

$$X = \begin{pmatrix} 0 & 1 & 1 & 0 \end{pmatrix}, Y = \begin{pmatrix} 0 & -i & i & 0 \end{pmatrix}, Z = \begin{pmatrix} 1 & 0 & 0 & -1 \end{pmatrix} \quad (7)$$

These operators satisfy

$$X^2 = Y^2 = Z^2 = I \quad (8)$$

Because of this property, their exponentials simplify to

$$e^{iaP} = \cos(a)I + i\sin(a)P, P \in \{X, Y, Z\} \quad (9)$$

The Pauli operators also satisfy the commutation relations:

$$XY = iZ, YZ = iX, ZX = iY \quad (10)$$

and reversing the order introduces a minus sign:

$$YX = -iZ, ZY = -iX, XZ = -iY \quad (11)$$

Because of the normalization condition and the irrelevance of global phase, a qubit state is fully described by two real parameters. It can be written as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle \quad (12)$$

The angle θ defines the polar position and ϕ defines the azimuthal angle on the Bloch sphere.

Unitary evolution corresponds to rotations of this state vector around an axis determined by the Hamiltonian.

Measurement in the computational basis yields either $|0\rangle$ or $|1\rangle$. The Born rule gives:

$$P_0 = |\alpha|^2, P_1 = |\beta|^2 = 1 - P_0 \quad (13)$$

Repeated experiments allow estimation of these probabilities via frequencies.

For the specific evolution

$$U_0 = e^{iaX} \quad (14)$$

acting on $|0\rangle$, we obtain

$$e^{iaX}|0\rangle = \cos(a)|0\rangle + i\sin(a)|1\rangle \quad (15)$$

Thus,

$$P_0 = \cos^2(a) \quad (16)$$

II. Single-Basis Coefficient Identification

Now we begin with the simplest instance of the Lie algebra coefficient identification problem, in which the effective Hamiltonian is proportional to a single known generator. This case establishes the core structure that will later be generalized to higher-dimensional Lie algebras and multi-parameter Hamiltonians. The method relies on repeated unitary application and the resulting inverse-trigonometric degeneracy, which is resolved through cross-power consistency conditions.

Consider a finite-dimensional quantum system with effective Hamiltonian

$$H_e = aX \quad (17)$$

where X denotes a Pauli operator and $a \in \mathbb{R}$ is an unknown coefficient to be identified.

The corresponding unitary evolution operator is

$$U_0 = e^{iaX} \quad (18)$$

We apply U_0 to the computational basis state $|0\rangle$. Since Pauli operators satisfy

$$X^2 = I \quad (19)$$

the exponential may be expanded through its Taylor series as seen in the background section,

$$e^{iaX} = \cos(a)I + i\sin(a)X. \quad (20)$$

the evolved state becomes

$$e^{iaX}|0\rangle = \cos(a)|0\rangle + i\sin(a)|1\rangle \quad (21)$$

The probability of measuring the outcome $|0\rangle$ is therefore

$$P_0 = |\langle 0|e^{iaX}|0\rangle|^2 = \cos^2(a). \quad (22)$$

The function $P_0(a)$ oscillates periodically between 0 and 1, implying that multiple values of a correspond to the same measurement probability. Inverting the relationship gives

$$a = \arccos(\sqrt{P_0}) + k\pi, \forall k \in \mathbb{Z} \quad (23)$$

which is multivalued at every factor, of π due to the periodicity and symmetry of the cosine function. Consequently, a single measurement with one application of the unitary is insufficient to uniquely determine a .

To resolve this ambiguity, we consider repeated applications of the unitary operator. Applying U_0 a total of m times yields

$$(U_0)^m = (e^{iaX})^m = e^{imaX} \quad (24)$$

where the exponent scales linearly because powers of the same matrix exponential commute trivially.

Acting on $|0\rangle$, the resulting state is

$$e^{imaX}|0\rangle = \cos(ma)|0\rangle + i\sin(ma)|1\rangle. \quad (25)$$

The corresponding measurement probability becomes

$$P_0^{(m)} = \cos^2(ma). \quad (26)$$

Thus, repeated application amplifies the unknown coefficient by a factor of m in the argument of the cosine.

For each value of m , inversion of the measured probability produces a candidate estimate

$$m\theta_m = \arccos\left(\sqrt{P_0^{(m)}}\right) + k\pi \quad (27)$$

or equivalently,

$$\theta_m = \frac{1}{m}\arccos\left(\sqrt{P_0^{(m)}}\right) + k\pi \quad (28)$$

Because the inverse cosine remains multivalued, each m generates multiple candidate solutions for a . The physically correct coefficient is identified as the unique value that is simultaneously consistent across all powers m :

$$\theta_1 = \theta_2 = \dots = \theta_m = a \quad (29)$$

Spurious solutions arising from the inverse trigonometric ambiguity fail to satisfy this consistency relation for other values of m . By collecting measurement data across multiple powers and identifying the common intersection among all candidate sets, the true coefficient a can therefore be uniquely reconstructed.

The full reconstruction procedure is implemented numerically in Julia, and the resulting simulations are presented in subsequent sections.

This relationship forms the basis for extracting unknown Hamiltonian parameters from measurement statistics.

III. Two-Coefficient Identification via Geometric Rotation

We now extend the previous construction to the case where the effective Hamiltonian contains two unknown coefficients,

$$H_e = aX + bZ \quad (30)$$

where a and b are real-valued unknown parameters. Geometrically, the Hamiltonian corresponds to a vector in the x - z plane of the Bloch sphere. The purpose of the following transformation is to demonstrate analytically that the two-generator Hamiltonian can be rotated into a form proportional to a single Pauli generator, after which the single-generator reconstruction procedure can be applied.

Define

$$V = aX + bZ \quad (31)$$

with associated unitary evolution

$$U_0 = e^{iV} \quad (32).$$

For the present case, we first rotate about the X -axis and define

$$U_1(\theta) = e^{(-i\theta X)} U_0 e^{(i\theta X)} \quad (33)$$

Using unitary similarity of the exponential,

$$U_1(\theta) = \exp(i e^{(-i\theta X)} V e^{(i\theta X)}) \quad (34)$$

The rotated generator is therefore

$$e^{(-i\theta X)} V e^{(i\theta X)} = e^{(-i\theta X)} (aX + bZ) e^{(i\theta X)} \quad (35)$$

The X component is unchanged because it commutes with the rotation operator,

$$e^{(-i\theta X)} X e^{(i\theta X)} = X \quad (36)$$

Using the Pauli rotation identity,

$$e^{(-i\theta X)} Z e^{(i\theta X)} = \cos(2\theta)Z + \sin(2\theta)Y \quad (37)$$

the transformed Hamiltonian becomes

$$H_1(\theta) = aX + b \cos(2\theta)Z + b \sin(2\theta)Y. \quad (38)$$

Choosing

$$\theta = \pi/4 \quad (39)$$

eliminates the Z-component and gives

$$H_1 = aX + bY \quad (40).$$

A second rotation about the Z-axis can then rotate the vector in the X-Y plane. Define

$$U_2(\varphi) = e^{(-i\varphi Z)} U_1 e^{(i\varphi Z)} \quad (41)$$

The corresponding Hamiltonian is

$$H_{rot} = (a \cos(2\varphi) - b \sin(2\varphi))X + (a \sin(2\varphi) + b \cos(2\varphi))Y \quad (42)$$

If the rotation angle is selected so that the coefficient of Y vanishes,

$$a \sin(2\varphi) + b \cos(2\varphi) = 0 \quad (43)$$

then

$$\tan(2\varphi) = b/a. \quad (44)$$

Under this choice, the transformed Hamiltonian becomes

$$H_{rot} = \sqrt{(a^2 + b^2)}X. \quad (45)$$

Defining

$$r = \sqrt{(a^2 + b^2)} \quad (46)$$

the transformed unitary therefore has the single-generator form

$$U_{rot} = e^{(irX)} \quad (47)$$

The repeated-power procedure developed in Section II can then be applied to U_{rot} . Applying the unitary m times to $|0\rangle$ gives the measurement probability

$$P_0^{(m)} = \cos^2(mr) \quad (48).$$

Cross-power consistency can therefore be used to identify the magnitude r . Once r and the rotation angle φ are known, the original coefficients are reconstructed according to

$$a = r \cos(2\varphi) \quad (49)$$

$$b = r \sin(2\varphi) \quad (50)$$

The analytical derivation establishes the geometric reduction from the two-generator Hamiltonian to the single-generator form. To validate this reduction numerically, we compare the unitary obtained by directly applying the two conjugations with the unitary obtained from the analytically predicted rotated Hamiltonian. We then test the cross-power reconstruction for representative values of a and b .

In this numerical validation, the rotation angle φ is treated as the selected control parameter used to align the Hamiltonian vector. Thus, the simulation validates the geometric reduction and the subsequent coefficient reconstruction conditional on the selected rotation angle, rather than claiming an independent procedure for estimating φ itself.

E. RESULTS

This section presents the numerical validation of the identification procedure in three stages. First, we validate the single-generator method of Section II using simulated measurement data, illustrating how the periodic ambiguity of a single measurement is resolved through cross-power consistency across increasing powers m (Figures 1–3). Second, we validate the two-generator geometric reduction of Section III, confirming numerically that the predicted rotation reproduces the target unitary to machine precision and that the resulting coefficients a and b are recovered accurately once the rotation angle φ is specified (Table A). Third, we extend this validation to more realistic conditions by introducing finite measurement statistics and systematic depolarizing noise, and report how reconstruction accuracy for a and b degrades as a function of shot count and noise strength (Tables B–C). Unless otherwise stated, all simulations were implemented in Julia, and the two-generator results in Part II assume the rotation angle φ is known rather than estimated from measurement data, as noted in Section III.

I. Single-coefficient Numerical Validation

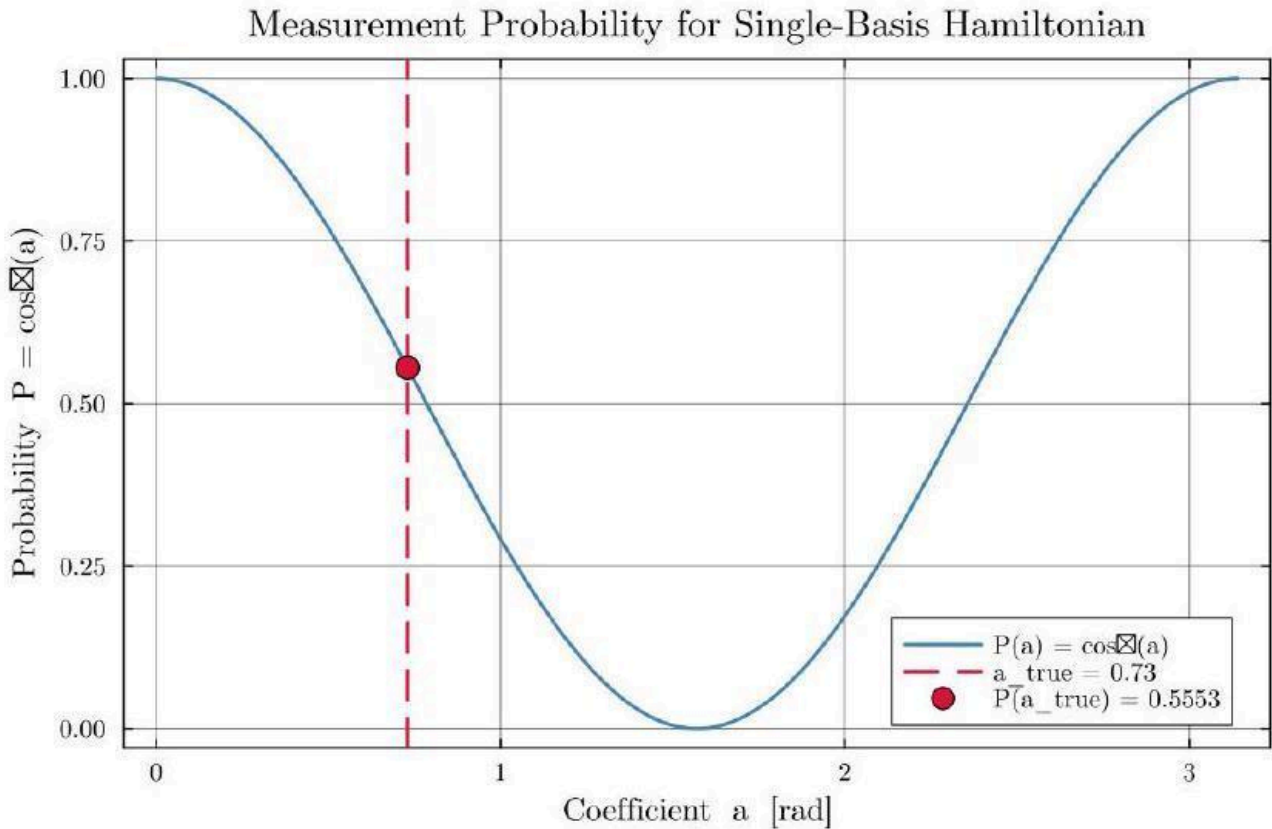


Figure 1. Measurement probability $P(a) = \cos^2(a)$ for the single-basis Hamiltonian.

The dashed red line indicates the true coefficient $a_{true} = 0.73rad$, with the corresponding probability $P(a_{true}) = 0.5553$ marked by the filled circle.

Figure 1 illustrates the central challenge the paper aims to resolve. Showing the theoretical measurement probability curve for the single basis Hamiltonian, defined by $P(a) = \cos^2(a)$ over the domain $[0, \pi]$. The curve exhibits the expected sinusoidal structure with $P(a) = 1$ at $a = 0$ and $a = \pi$. For any observed probability value in the range $(0, 1)$, there exist several candidate values for a that produce an identical measurement outcome, creating an inherent two-fold degeneracy in estimation.

The true coefficient was set to $a_{true} = 0.73rad$, yielding a theoretical probability of $P(a_{true}) = 0.5553$. This point lies on the descending slope of the probability curve, in a region of moderate sensitivity, where the curve provides sufficient local gradient to distinguish nearby candidate values while remaining susceptible to the global degeneracy problem discussed above.

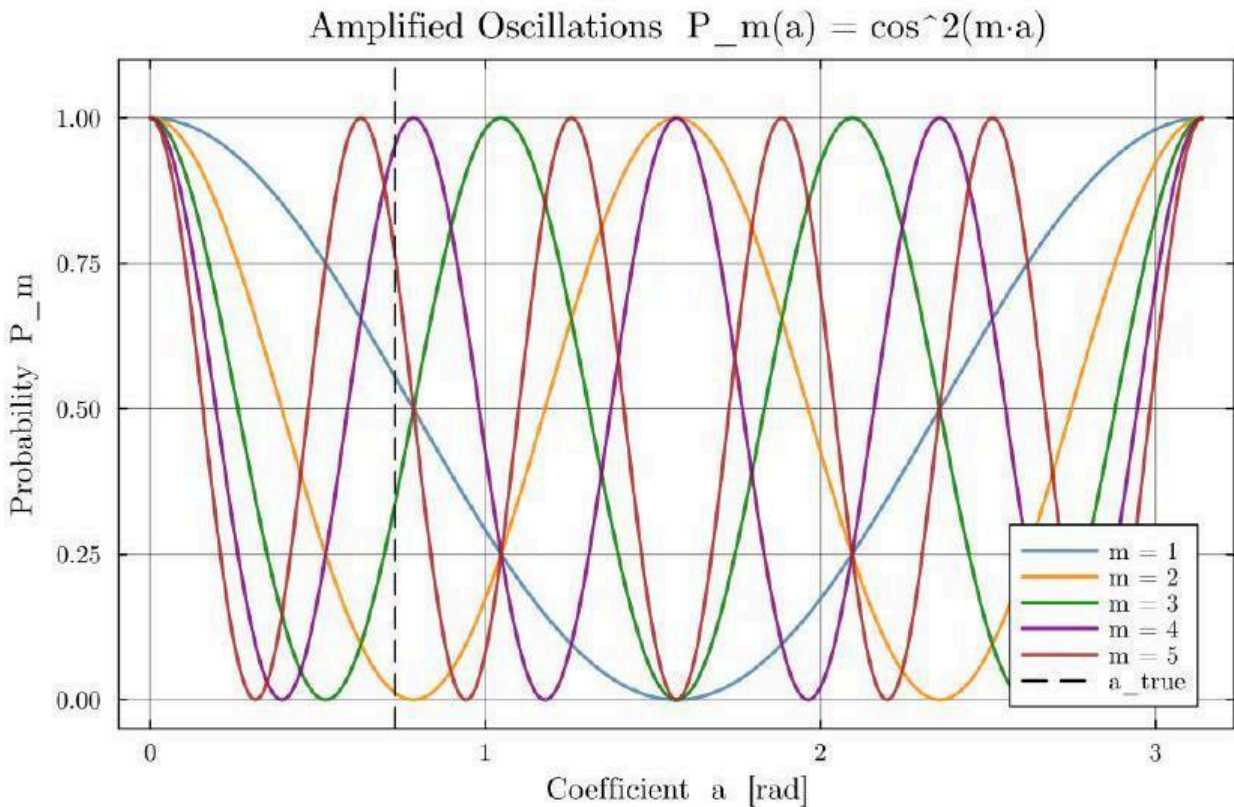


Figure 2. Amplified oscillations $P_m(a) = \cos^2(m \cdot a)$ for powers $m = 1$ to 5.

Higher powers introduce additional oscillation frequency, increasing the selectivity of the cross-power intersection near a_{true} (dashed black line).

Figure 2 illustrates how applying successive m powers amplifies the oscillation frequency of the measurement probability function, with each power producing full cycles across the parameter domain. This frequency amplification is the theoretical foundation of the crosspower consistency method: while the curve alone admits many candidate values consistent with any observed probability, each additional power introduces a finer oscillation grid whose intersections with the observed probability become increasingly sparse. The true coefficient rad (dashed black line) lies at a point where all five curves simultaneously pass through consistent probability values, visually confirming that it satisfies the measurement constraint at every power level shown. This behaviour motivates the use of higher powers as a disambiguation tool - spurious candidates that accidentally satisfy the constraint at low will generically fail to do so as increases, leaving the true value as the unique survivor of the cross-power consistency check detailed in Figure 3.

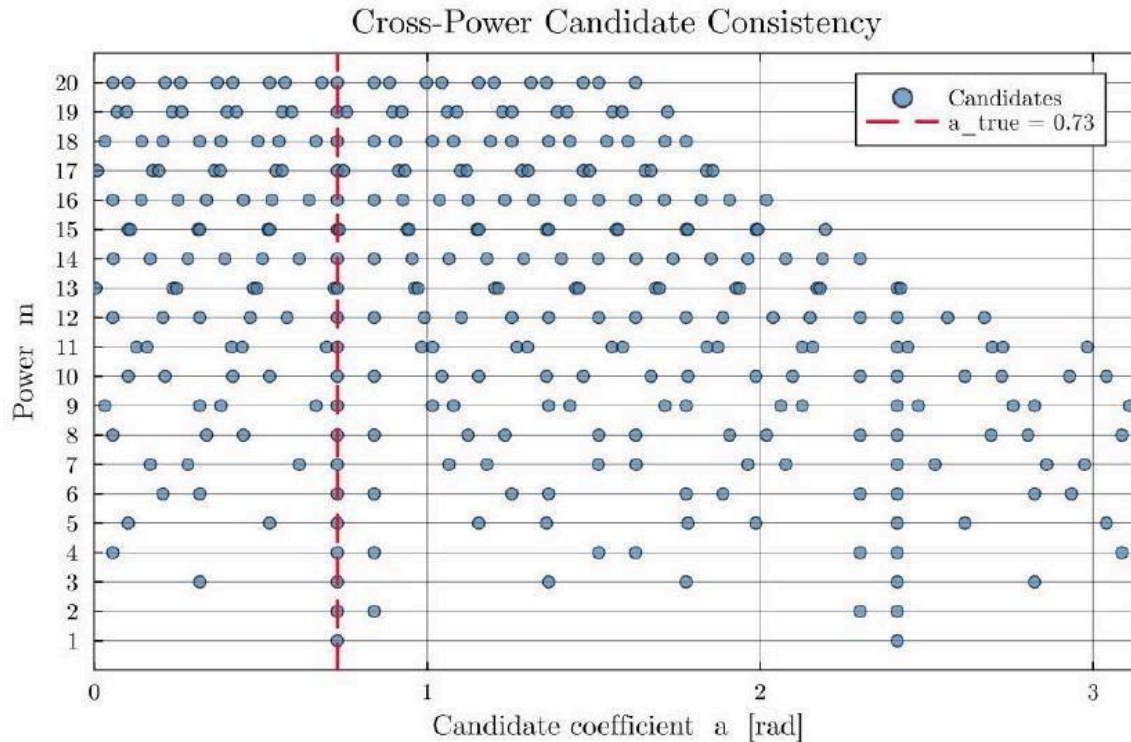


Figure 3. Cross-power candidate consistency across powers $m = 1$ to 20 .

Each point represents a candidate coefficient consistent with the observed measurement at that power level. The dashed red line at 0.73 rad is the only value maintaining consistency across all power levels.

Figure 3 demonstrates the cross-power consistency method by displaying the full set of candidate coefficients recovered at each power level, $m = 1$ to 20 . At low powers, the candidate solutions are broadly distributed across the parameter domain, reflecting the strong degeneracy inherent in single-basis measurements. As m increases, the candidate positions shift, and the set of values satisfying the consistency condition across all powers simultaneously is progressively reduced.

The true coefficient at $a_{\text{true}} = 0.73 \text{ rad}$, shown by the dashed red line, is the only value that remains a consistent candidate at every power level, appearing as a vertically coherent column in the scatter plot. All other candidate clusters fail to maintain this consistency as m grows, either drifting away from a_{true} or disappearing entirely at higher powers.

This convergence toward a single surviving candidate demonstrates that the cross-power method successfully resolves the degeneracy inherent in single-basis estimation, uniquely identifying the true Hamiltonian coefficient.

II. Two-Coefficient Numerical Validation

To numerically validate the geometric reduction introduced in Section III, we consider a two-generator Hamiltonian with the representative coefficients

$$H_e = aX + bZ,$$

with

$$a_{true} = 0.73$$

and

$$b_{true} = 0.41.$$

The corresponding Hamiltonian magnitude is

$$r_{true} = \sqrt{(a_{true}^2 + b_{true}^2)} = 0.8372574276.$$

Using the rotation angle

$$\varphi = 0.2558694212 \text{ rad}$$

and the first rotation angle

$$\theta = \pi/4,$$

the two conjugations reduce the Hamiltonian to the predicted single-generator form

$$H_{rot} = rX.$$

We numerically compare the unitary obtained by applying the two rotations directly with the unitary generated by the predicted reduced Hamiltonian. The Frobenius norm of their difference is

$$\|U_{direct} - U_{predicted}\|_F = 2.322 \times 10^{-16},$$

which is effectively zero at numerical precision. This confirms that the implemented geometric rotations produce the analytically predicted single-generator Hamiltonian.

We next apply the cross-power consistency procedure to the reduced unitary. Measurement probabilities are generated for powers $m = 1, \dots, 20$ according to

$$P_0^{(m)} = \cos^2(mr).$$

The resulting probability sequence provides the measurement data used for reconstruction. Applying the cross-power procedure gives

$$r_{est} = 0.8372580041,$$

compared with the true value

$$r_{true} = 0.8372574276.$$

The recovered coefficients are then obtained from

$$a_{est} = r_{est} \cos(2\varphi)$$

and

$$b_{est} = -r_{est} \sin(2\varphi),$$

giving

$$a_{est} = 0.7300005027$$

and

$$b_{est} = 0.4100002823.$$

The corresponding absolute reconstruction errors are

$$|a_{est} - a_{true}| = 5.027 \times 10^{-7}$$

and

$$|b_{est} - b_{true}| = 2.823 \times 10^{-7}.$$

Thus, for this representative two-generator Hamiltonian, the numerical implementation reproduces the predicted rotation to machine precision and recovers both coefficients with errors below 10^{-6} . These results provide numerical validation of the geometric reduction and of the subsequent cross-power reconstruction when the rotation angle is specified.

Table A. Numerical validation of the two-generator reconstruction

Quantity	True Value	Recovered value	Absolute Error
r	0.8372574276	0.8372580041	5.765×10^{-7}
a	0.7300000000	0.7300005027	5.027×10^{-7}
b	0.4100000000	0.4100002823	2.823×10^{-7}

The Frobenius-norm difference between the directly rotated unitary and the predicted reduced unitary was 2.322×10^{-16} .

III. Measurement Uncertainty and Noise Robustness

The preceding simulations use ideal measurement probabilities. In an experimental setting, however, the probabilities are estimated from a finite number of measurements and are therefore subject to statistical fluctuations. To investigate the effect of finite measurement statistics on coefficient recovery, we repeat the reconstruction procedure using simulated measurement outcomes rather than exact probabilities.

For each power m , let $P_0^{(m)}$ denote the ideal probability of measuring the state $|0\rangle$. For a finite number N of independent measurements, the observed number of $|0\rangle$ outcomes is sampled from a binomial distribution,

$$n_0^{(m)} \sim \text{Binomial}(N, P_0^{(m)}),$$

where N is the number of measurement shots and $P_0^{(m)}$ is the ideal probability. The estimated probability supplied to the reconstruction procedure was therefore

$$P_{\text{hat } 0}^{(m)} = n_0^{(m)} / N.$$

Using the two-generator example with $a_{\text{true}} = 0.73$ and $b_{\text{true}} = 0.41$, the reconstruction was evaluated for $N = 100, 1,000, 10,000$, and $100,000$ measurement shots. For each value of N , 100 independent trials were performed. The mean absolute reconstruction errors for a and b are shown in Table B

Table B. Mean absolute reconstruction for a and b at varying N values.

N	Mean reconstructed a	Mean reconstructed b	MAE(a)	MAE(b)
100	0.729792	0.409883	7.899×10^{-4}	4.436×10^{-4}
1,000	0.729957	0.409976	2.794×10^{-4}	1.569×10^{-4}
10,000	0.729981	0.409989	8.383×10^{-5}	4.708×10^{-5}
100,000	0.730007	0.410004	2.830×10^{-5}	1.590×10^{-5}

The results show that the reconstruction error decreases systematically as the number of measurement shots increases. In particular, increasing the number of shots from 100 to 100,000 reduces the mean absolute error in a from 7.899×10^{-4} to 2.830×10^{-5} , while the corresponding error in b decreases from 4.436×10^{-4} to 1.590×10^{-5} . This demonstrates that the reconstruction remains stable under finite-shot measurement uncertainty and improves as the statistical uncertainty in the measured probabilities is reduced.

To investigate the effect of systematic noise, a simple depolarizing noise model was also introduced at the probability level,

$$P_{noisy}^{(m)} = (1 - \eta)P_0^{(m)} + \eta/2,$$

where η denotes the noise strength. For each noise level, $N = 10,000$ measurement shots were used and the reconstruction was repeated over 100 independent trials. The resulting mean absolute errors are shown in Table C.

Table C. Mean absolute errors at varying noise levels

η	MAE(a)	MAE(b)
0.00	8.444×10^{-5}	4.743×10^{-5}
0.01	7.986×10^{-5}	4.485×10^{-5}
0.05	1.070×10^{-4}	6.009×10^{-5}

0.10	1.692×10^{-4}	9.501×10^{-5}
0.20	3.231×10^{-4}	1.815×10^{-4}

The reconstruction error generally increases as the systematic noise strength increases. At $\eta = 0.20$, the mean absolute errors reach 3.231×10^{-4} for a and 1.815×10^{-4} for b , compared with 8.444×10^{-5} and 4.743×10^{-5} , respectively, in the $\eta = 0$ case. The degradation arises because the noise drives the measured probabilities toward 1/2, reducing the contrast of the probability oscillations used for coefficient identification.

Together, these simulations extend the ideal numerical validation by quantifying the effect of finite measurement statistics and systematic noise on coefficient recovery. The results indicate that the method remains accurate for the noise levels examined, while also showing the expected degradation as measurement noise increases.

F. DISCUSSION AND FUTURE OUTLOOK

This work has presented a systematic and transparent method for identifying unknown coefficients in effective Hamiltonians directly from the measurement statistics of a quantum system's evolution. The approach was validated numerically in Julia for the single-basis coefficient case and extended analytically to the two coefficient case through a geometric rotation procedure.

Repeated application of the Hamiltonian unitary

$$U = e^{-iHt}$$

at integer powers m amplifies the unknown coefficient linearly in the exponent, producing measurement probabilities of the form

$$P_m(a) = \cos^2(ma),$$

which impose increasingly selective constraints on candidate values of a . The degeneracy inherent in inverting a single measurement is fully resolved by enforcing consistency across multiple powers:

spurious candidates that satisfy the constraint at low m generically fail to do so as m increases, leaving the true coefficient as the unique surviving solution. The implemented algorithm successfully recovered the true coefficient

$$a_{\text{true}} = 0.73\text{rad},$$

in numerical simulation, confirming the theoretical prediction.

For the two-generator Hamiltonian

$$H = aX + bZ,$$

the single-generator method was extended by introducing a geometric rotation that collapses H to an effective single-generator form. Conjugating H by a unitary rotation about a chosen axis at angle φ on the circle of radius

$$r = \sqrt{a^2 + b^2},$$

eliminates the Z -component, reducing the Hamiltonian to a form proportional to X . The single-generator identification method can then be applied directly to recover the individual coefficients from the reduced Hamiltonian. This establishes a general two-step procedure: first rotate to eliminate one generator, then apply crosspower consistency to identify the remaining coefficient.

The method shares its ancilla-free, non-adaptive character with existing techniques such as RPE, so this alone is not a distinguishing advantage. Its distinct contribution lies in explicitly casting coefficient recovery as a Lie-algebra problem and providing a geometric conjugation strategy for reducing multi-generator Hamiltonians to a sequence of single-generator estimation problems. Unlike RPE's typical adaptive power selection, which is designed to achieve Heisenberg-limited scaling, the present implementation uses a fixed, non-adaptive range of powers ($m = 1$ to 20); we have not analyzed the scaling of estimation precision with the number or choice of powers used, and make no claim of matching Heisenberg-limited performance.

Additionally, the robustness analysis provides an initial quantitative assessment of finite measurement statistics and systematic noise. The simulations show that coefficient recovery improves with increasing measurement shots and degrades as the strength of the applied noise increases.

The work reveals several directions that present themselves as natural extensions of the present method

The most immediate extension is the generalisation of the identification method to the full single-qubit Hamiltonian

$$H = aX + bZ + cY,$$

incorporating all three Pauli generators. Successfully establishing this three-generator pipeline would complete the identification framework for arbitrary single qubit Hamiltonians, representing both a practically significant and theoretically complete result.

Secondly, the robustness of the method under the full range of experimental imperfections warrants further investigation. As these results were obtained using a simplified probability-level noise model, a more detailed treatment of gate-dependent errors, decoherence, and correlated experimental noise remains an important direction for future work.

$$\cos^2(ma)$$

form, potentially introducing systematic bias into the recovered coefficients. Incorporating a noise model into the inversion procedure, for example by treating the decoherence rate as an additional unknown parameter, could make the method viable on near-term quantum hardware.

Finally, the geometric rotation approach used for the two-generator case has a natural interpretation in terms of the Lie algebraic structure of the Hamiltonian. Exploring this connection more formally may reveal deeper links between the present method and established techniques in quantum process tomography and Hamiltonian learning, potentially combining the transparency and efficiency of the cross-power approach with the statistical rigour of tomographic methods.

CONCLUSION

This work has demonstrated that the coefficients of an effective single-qubit Hamiltonian can be recovered directly and uniquely from computational-basis measurement statistics, without requiring deep ancilla systems, coherent control circuits, or prior spectral knowledge. The core mechanism-repeated unitary applications that amplify the unknown coefficient linearly in the exponent-transforms the Hamiltonian identification problem into a cross-power consistency condition that is both computationally lightweight and transparently interpretable.

For the single-generator case, $H_e = aX$, the method was validated numerically, successfully recovering the true coefficient $a_{true} = 0.73 \text{ rad}$, from simulated measurement data. For the two-generator case, $H = aX + bZ$, an analytic geometric rotation strategy was developed that reduces the problem to an effective single-generator form. The individual coefficients are then recovered from the magnitude $r = \sqrt{a^2 + b^2}$ and the rotation angle φ , where φ was numerically validated as a specified control parameter rather than one estimated independently from measurement data. Together, these results establish an identification pipeline for Hamiltonians in the x-z plane of the single-qubit Lie algebra that is complete for the magnitude r and conditionally complete for the individual coefficients a and b , pending a data-driven procedure for determining φ .

The natural next step is the extension of the method to the full single-qubit algebra, incorporating all three Pauli generators. Achieving this would complete the identification framework for arbitrary single-qubit Hamiltonians. Physical systems such as spin-1/2 particles in external fields or superconducting qubits with two-parameter drift are natural candidate applications of this framework, since their dynamics are generated by the same Pauli algebra. Realizing this in practice, however, still requires a data-driven method for determining the rotation angle φ , which the present work has not yet demonstrated. We therefore present the method as a candidate building block for lightweight, ancilla-free characterization rather than a ready-made alternative to existing tomographic approaches.

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