

Estimation of Model Misspecification in Bayesian Quantum Phase Estimation

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Introduction

To analyze molecular characteristics, chemists often solve the following eigenvalue equation:

$$\mathbf{H}_{RV}\Psi(\vec{\theta}) = E\Psi(\vec{\theta}) \quad (1)$$

In this equation, \mathbf{H}_{RV} represents the Hamiltonian that accounts for the molecule's total ro-vibrational energy. The wavefunction Ψ , parameterized by the vector $\vec{\theta}$, serves as the eigenvector. The energy level E corresponds to the eigenvalue which represents the energy levels electrons can occupy. While simpler molecules like H_2 allow for straightforward single vector decompositions, larger molecules present computational challenges due to the increased size of \mathbf{H}_{RV} . This project aims to address these challenges by using quantum phase estimation to estimate a posterior distribution, which can then be used to estimate the eigenvalues of \mathbf{H}_{RV} for the Cr_2 molecule.

Literature Review

Taking the ro-vibrational Hamiltonian \mathbf{H}_{RV} and performing the following operation to form a matrix \mathcal{U} gives $\mathcal{U} = e^{i\mathbf{H}_{RV}t}$. The expression above allows for the application of the phase estimation algorithm, which estimates the eigenvalues of the unitary operators. The algorithm then uses these eigenvalues to approximate the eigenvalues of the original Hamiltonian. A matrix is denoted to be unitary if it follows the spectral theorem which is listed below.

Spectral Theorem: Let U be a normalized $K \times K$ complex matrix. There exists an orthonormal basis of K -dimensional complex vectors $\{|\psi_1\rangle, \dots, |\psi_K\rangle\}$, along with complex numbers $\lambda_1, \dots, \lambda_K$, such that $U = \lambda_1|\psi_1\rangle\langle\psi_1| + \dots + \lambda_K|\psi_K\rangle\langle\psi_K|$. This matrix U can be diagonalized in an orthonormal basis consisting of its eigenvectors, with the corresponding eigenvalues on the diagonal.

The main implementation of the phase estimation algorithm is shown below:

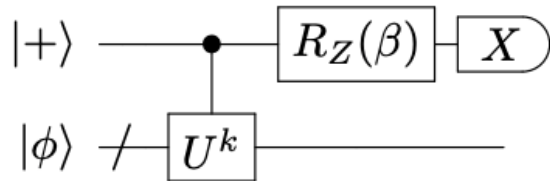
Quantum Phase Estimation Algorithm:

- **Input:** An n -qubit quantum state $|\psi\rangle$ and a unitary quantum circuit for an n -qubit operation U .
- **Promise/Assumptions:** $|\psi\rangle$ is an eigenvector of U .
- **Output:** An approximation to the number $\theta \in [0, 1)$ satisfying $U|\psi\rangle = e^{2\pi i\theta}|\psi\rangle$.

Quantum phase estimation can also take a probabilistic approach in the form of Bayesian optimization. Termed Bayesian Quantum Phase Estimation by Weibe and Granade in 2016¹. It was made efficient in a highly noisy environment by Yamamoto et al. (2024)². This method uses a quantum circuit to represent the posterior distribution of the phase estimation algorithm^{1,2}. For a two-qubit circuit, the authors used a quantum circuit which is an acyclic network of quantum gates connected by wires. The quantum gates are matrices that represent quantum operations while the wires represent the **qubits** (see appendix) on which the gates act. The pictorial representation of the circuit is shown in Figure 1 (below).

The quantum circuit is parameterized by $k \in \mathbb{N}$ and $\beta \in [0, 1]$. The circuit is measured in the Pauli X basis and the measurement is denoted as a probability of states (or a likelihood) in the computational basis such that $p(m|\phi, k, \beta) = \frac{1 + \cos(k\phi + \beta)}{2}$ where m is the measurement outcome in the computational basis, ϕ is the unknown where $p(\phi) \sim \text{Unif}[0, 2\pi)$, and R_Z is a rotational matrix described in the appendix below. With R possible measurement outcomes and a high number of iterations, a posterior distribution can be computed such that $p(\phi|m, k, \beta) \propto p(\phi) \cdot \prod_{r=1}^R p_r(m|\phi, k, \beta)$. Once converged, the probability distributions are then used to compute a posterior mean with respect to an observable or $\sum_R p(\phi|m, k, \beta) \langle R|\hat{H}|R \rangle$. Note that this work does not compute a posterior mean but instead creates the probabilities that will estimate the eigenvalues of the Hamiltonian matrix.

Problem Formulation



The data used in this project was generated by Asnaashari and is a discrete variable representation of the Hamiltonian³. First, an interpotential curve (measures the Coulombic interaction of two atoms) was generated from Fortran for the Cr₂ molecule (graph on the right). Afterwards, a Hamiltonian matrix was selected from the 32 points collected from the curve for each spin state. A combination of the **pennylane** and **phayes** Python 3.11.7 libraries were used to transform the Hamiltonian matrix into a unitary matrix as described in the literature review. The unitary matrix was then used to generate the quantum circuit by applying a transform:

The quantum circuit was then used to estimate the phases, ϕ , of each unitary matrix. The phase estimation algorithm itself can be described by the probabilistic model below.

The model used in this project is a Bayesian model that estimates the phases of the unitary matrices. The model is parameterized by the number of qubits, n , and the number of iterations, R . The model is defined as follows (using the \sim notation):

The quantum circuit provided in the literature review is used to estimate the phases of the unitary matrices. Note that we are trying to estimate ϕ and the error compared to the true value, ϕ_0 which is the angle(s) or phase that we are trying to estimate. The error is denoted as $\epsilon = \phi - \phi_0$. The error is then used to estimate the eigenvalues of the Hamiltonian matrix. Note that the phases will be estimated for multiple spin states of dichromium gas. The likelihood and prior are defined below:

- **Prior** This is the probability of phi or equivalently ϕ

Thus the posterior that is being estimated is described by:

The evaluation metric used for this model is $\epsilon = |\phi - \phi_0|$. This particular error metric is used as the model and the true phases are evaluated in the same basis for each spin state.

Results

References

- [1] Wiebe, N.; Granade, C. Efficient Bayesian Phase Estimation. *Phys. Rev. Lett.* **2016**, *117*, 010503.
- [2] Yamamoto, K.; Duffield, S.; Kikuchi, Y.; Muñoz Ramo, D. Demonstrating Bayesian quantum phase estimation with quantum error detection. *Phys. Rev. Res.* **2024**, *6*, 013221.
- [3] Asnaashari, K.; Krems, R. V. Compact quantum circuits for variational calculations of ro-vibrational energy levels of molecules on a quantum computer. *arXiv.org* **2023**,

Appendix

A: Glossary of Some Quantum Computing Terms

Bra A row vector defined by:

$$\langle\psi| = [\psi_1^\dagger, \psi_2^\dagger, \dots, \psi_K^\dagger] \quad (3)$$

where ψ^\dagger is the complex conjugate of ψ .

Ket A column vector defined by:

$$|\psi\rangle = [\psi_1, \psi_2, \dots, \psi_K]^T$$

Qubit Represented by a complex-valued, 2×1 vector. It can be written as a linear combination of $|0\rangle$ and $|1\rangle$ as follows:

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$$

where α and β are complex numbers, and $|\alpha|^2 + |\beta|^2 = 1$. Note that

$$|0\rangle = [1, 0]^T, |1\rangle = [0, 1]^T \quad (4)$$

One does not observe α and β . Instead $|\alpha|^2$ and $|\beta|^2$ are the coefficients that we observe. Each of $|\alpha|^2$ and $|\beta|^2$ and beta correspond to the probability of collapsing to a specific state.

Computational Basis States Refers to the standard orthonormal basis for the state space of n qubits and represents a complete set of orthonormal vectors for this space. For a single qubit, the computational basis consists of the two states $|0\rangle$ and $|1\rangle$. Each computational basis state for a system of n qubits can be described as a tensor product of n single-qubit states, where each qubit is independently in either $|0\rangle$ or $|1\rangle$. The computational basis states form an orthonormal basis, which implies that they are mutually orthogonal and each has unit norm. The completeness of this basis set means that any state $|\psi\rangle$ of the system can be uniquely expressed as a linear combination of these basis states, and no other states need to be added to fully describe the state space. Each basis state corresponds to a unique binary string of length n , which is particularly useful for encoding and manipulating information in quantum computation. The general form of a computational basis state for an n -qubit system is:

$$|i_1 i_2 \dots i_n\rangle = |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_n\rangle$$

where i_k is either 0 or 1, representing the state of the k -th qubit. For example, in a two-qubit system, the computational basis states are $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$, corresponding to the vector representations $[1, 0, 0, 0]^T$, $[0, 1, 0, 0]^T$, $[0, 0, 1, 0]^T$, and $[0, 0, 0, 1]^T$ respectively. Note that $|00\rangle = |1\rangle$, $|01\rangle = |2\rangle$, $|10\rangle = |3\rangle$, and $|11\rangle = |4\rangle$. This is because the number of computational basis states (k) is proportional to the number of qubits (N) such that

$$k = 2^N \quad (5)$$

Hardware Basis States Refers to the set of gates or operations that a quantum computer can physically rea

B: List of Quantum Gates Used in this Work

Pauli-Z Gate (Z)

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

RZ Gate

$$R_{z, x_k}(\theta) = \begin{bmatrix} e^{-i\theta \cdot x_k} & 0 \\ 0 & e^{i\theta \cdot x_k} \end{bmatrix}$$

C: Python Implementation