EPFL Quantum Computing Association

Quantum Hackathon

Baptiste Claudon

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Contents

Part I
Algorithms for Quantum Simulation

I. VARIATIONAL QUANTUM EIGENSOLVER

A. Motivation

The Variational Quantum Eigensolver (VQE) is an algorithm aimed at computing the ground state of a physical Hamiltonian. Its optimization-based approach makes it suitable for applications on Noisy Intermediate-Scale Quantum (NISQ) computers. It is an example of a Variational Quantum Algorithm, sometimes considered the quantum analogues of the highly successful Machine Learning methods employed in classical computing [1].

B. Theory

The VQE bases itself on the so-called Variational principle in quantum mechanics.

Theorem 1. Variational principle Let $\mathcal{E}$ be the finite dimensional Hilbert space of states of a quantum system, and $H \in \mathcal{L}(\mathcal{E})$ be the Hamiltonian of this system. Then:

$$\forall \left|\psi\right\rangle \in \mathcal{E} : \left\langle\psi\right| H \left|\psi\right\rangle \geq E_0 \tag{1}$$

where $E_0 \in \mathbb{R}$ is the system's ground state energy.

Given a d parametrized circuit $C : \mathbb{R}^d \to \mathcal{L}(\mathcal{E})$, the VQE aims at finding:

$$\theta^* = \underset{\theta \in \mathbb{R}^d}{\arg\min} \left\langle 0\right| C(\theta)^* H C(\theta) \left|0\right\rangle \tag{2}$$

A common method to find such a minimum is the gradient descent algorithm.

Definition 1. Gradient Descent Algorithm Given $f \in C^1(\mathbb{R}^d, \mathbb{R})$. An algorithm to find:

$$x^* = \underset{x \in \mathbb{R}^d}{\arg\min} f(x) \tag{3}$$

is the following. Fix $x^{(0)} \in \mathbb{R}^d$. Then, iteratively compute $x^{(k+1)} = x^{(k)} - \eta \nabla f(x^{(k)})$, with $\eta > 0$, until either $k \in \mathbb{N}$ is large enough or $\parallel x^{(k+1)} - x^{(k)} \parallel$ is small enough.

As it turns out, certain parametrized quantum circuits allow for very efficient gradient calculations [2].

Theorem 2. The parameter-shift rule Let $\mathcal{E}$ be the 2^N dimensional state space of N qubits. Let $C : \mathbb{R}^d \to \mathcal{L}(\mathcal{E})$ be a unitary parametrized circuit and $B \in \mathcal{L}(\mathcal{E})$ a hermitian operator. If for each $\theta \in \mathbb{R}^d$, the circuit is of the form $U(\theta) = V e^{-i\theta_1 G} W$ with $V, W \in \mathcal{L}(\mathcal{E})$ independent of $\theta_1 \in \mathbb{R}$ the first component of θ, and $G \in \mathcal{L}(\mathcal{E})$ is a hermitian and unitary 1-spin operator, then:

$$\forall s \in \mathbb{R} : \partial_1 \left\langle 0\right| C(\theta)^* B C(\theta) \left|0\right\rangle = \frac{\left\langle 0\right| C(\theta + s e_1/2)^* B C(\theta + s e_1/2) \left|0\right\rangle - \left\langle 0\right| C(\theta - s e_1/2)^* B C(\theta - s e_1/2) \left|0\right\rangle}{2 \sin s} \tag{4}$$

In particular, the gradient can be calculated exactly by measuring the B operator only twice.

Definition 2. Variational Quantum Eigensolver Algorithm The VQE consists in minimizing the Hamiltonian expectation value as in equation 2 using the gradient descent algorithm and a parametrized circuit that is suitable for efficient gradient calculations.

C. Results

Consider a system of N spins of Hamiltonian:

$$H = J \sum_{i=1}^{N} Z_i Z_{i+1} + h \sum_{i=1}^{N} X_i \tag{5}$$

where J, h are respectively the coupling and field constants, and we assume boundary conditions $Z_{N+1} = Z_1$. In our case, consider $J = h = 1$. Our goal is to use the VQE algorithm to find the ground state of this Hamiltonian. The following ansatz is used [3]:

$$C(\omega) = \prod_{l=1}^{d} \left(\prod_{i=1}^{N} R_{\alpha}^{(i)}(\omega_{i,l}) \right) \left(\prod_{j=1}^{N-1} e^{-i\omega_{j,l} Z_j Z_{j+1}} \right) \tag{6}$$

where $\alpha = x$ if l is odd, $\alpha = y$ if l is even.

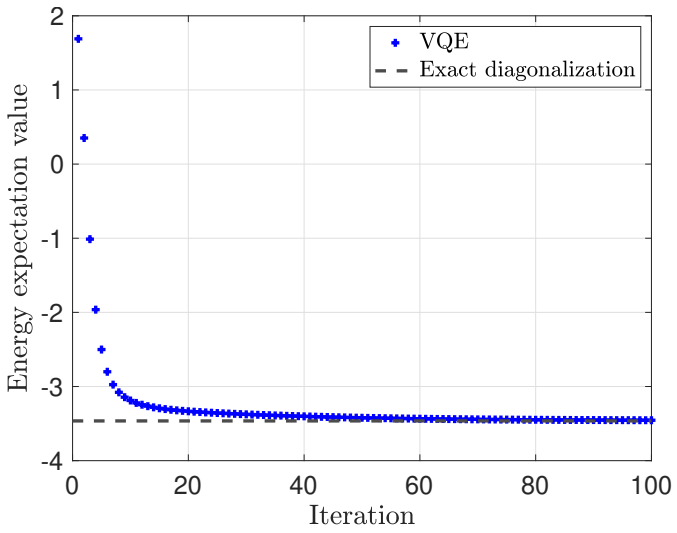

Figure 1: Calculation of the Ising model ground state via Variational Quantum Eigensolver

Figure 1 illustrates the ground state calculation using the VQE. After 100 steps, the ground state approximation is -3.454831823965546 whereas exact diagonalization yields -3.464101615137755.

II. TROTTERIZATION AND PROJECTED-VARIATIONAL QUANTUM DYNAMICS

A. Motivation

After focusing on the calculation of a time-independent property, one may wonder about the simulation of dynamics. This section aims at presenting two algorithms for the time evolution of a quantum system. The first one is the most naive and bases itself on the Trotter-Suzuki formula. The second one, more advanced, is named projected-Variational Quantum Dynamics (p-VQD) and realizes an iterative global projection of the exact time-evolution onto a well-chosen parametrized manifold.

B. Theory

This section on the simulation of unitary dynamics is taken from [3].

Definition 3. Let $\mathcal{E}$ be the Hilbert space of states, and $H \in \mathcal{L}(\mathcal{E})$ a time-independent Hamiltonian acting on it. Write the exact state at time $t \in \mathbb{R}$: $|\psi(t)\rangle \in \mathcal{E}$. Let $w(t) \in \mathbb{R}^p$ be a set of p parameters and $|\psi_{w(t)}\rangle \in \mathcal{E}$ be the approximation of the state vector. Also, define the evolved state:

$$\forall t, \delta t \in \mathbb{R} : |\phi(t+\delta t)\rangle = e^{-iH\delta t} |\psi_{w(t)}\rangle \in \mathcal{E} \tag{7}$$

Given an initial choice $w(t)$, the projected-Variational Quantum Dynamics (p-VQD) proposes to choose $w(t+\delta t) = w(t) + dw^*$, with dw^* satisfying:

$$dw^* = \underset{dw \in \mathbb{R}^p}{\arg\max} \left| \langle \phi(t+\delta t)| \, |\psi_{w(t)+dw}\rangle \right|^2 \tag{8}$$

Proposition 1. Define the step infidelity $L : \mathbb{R}^p \times \mathbb{R} \to \mathbb{R}$:

$$(dw, \delta t) \mapsto \frac{1 - \left| \langle \phi(t+\delta t)| \, |\psi_{w(t)+dw}\rangle \right|^2}{\delta t^2} \tag{9}$$

The, for all $dw \in \mathbb{R}^p$, the limit $\lim_{\delta t \to 0} L(dw, \delta t)$ exists.

Thus, at each time step, dw^* can be found by minimizing the step infidelity L. In practice, $d\omega^*$ can be found by using the gradient descent algorithm 1, and $|\phi(t+\delta t)\rangle$ by using an approximation inspired by the Trotter-Suzuki formula 2:

Proposition 2. Trotter-Suzuki formula Let $A, B \in \mathcal{M}_n(\mathbb{C})$. Then:

$$e^{A+B} = \lim_{m \to \infty} \left(e^{A/m} e^{B/m} \right)^m \tag{10}$$

C. Results

Let us consider the following open boundary Ising model:

$$H = \frac{1}{4} \sum_{k=0}^{1} Z_k Z_{k+1} + \sum_{k=0}^{2} X_k \tag{11}$$

Figure 2 illustrates the time evolution of the magnetization $\langle \sigma_z \rangle$ along the z direction, starting from $|000\rangle$ at time $t = 0$. Both methods capture the exact behaviour of the system.

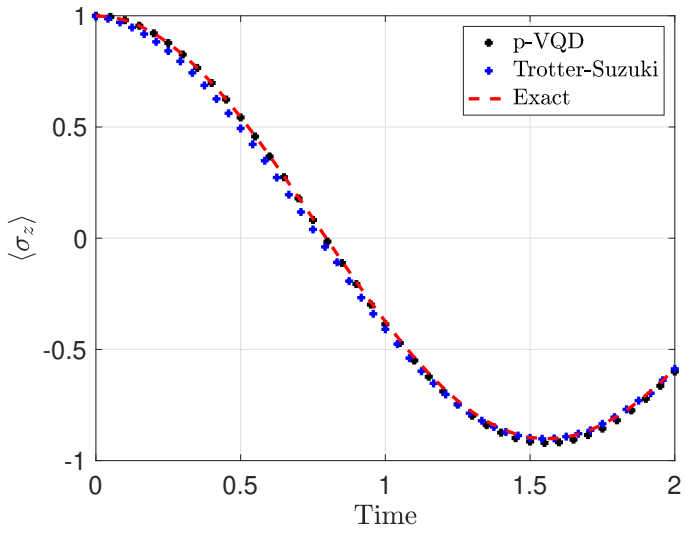

Figure 2: Time evolution of the $\langle\sigma_z\rangle$ magnetization.

III. OPEN QUANTUM SYSTEMS: DYNAMICS THROUGH SPECTRAL DENSITY AND NON-EQUILIBRIUM STEADY STATES

A. Motivation

Until now, each considered system was a so-called closed system. However, most physical systems are open in the sense that they present a coupling to their environment. This section starts with a simple method to simulate the dynamics of such a system, using the spectral density to approximate the interaction with the environment. Then, it introduces the Quantum Fourier Transform and the Quantum Phase Estimation algorithms to compute Non-Equilibrium Steady States.

B. Theory

1. *Dynamics through spectral density*

This algorithm on the simulation of dissipative dynamics is taken from [4].

Let $\mathcal{E}_S, \mathcal{E}_B, \mathcal{E}_I$ be the Hilbert space of states for the open system, the bath and the interaction between the two. For $H_{S,B,I} \in \mathcal{L}(\mathcal{E}_{S,B,I})$ the respective Hamiltonians, the global Hamiltonian is assumed to be $H = H_S + H_B + H_I \in \mathcal{L}(\mathcal{E}_S \otimes \mathcal{E}_B)$. Further assume there exists a sequence $(\omega_k, c_k)_{k\in\mathbb{N}} \subset \mathbb{R}^2$ of frequencies of the environment and coupling constants with the open system, such that:

$$H_B = \sum_{k=0}^{\infty} \omega_k (b_k b_k^\dagger + 1/2) \tag{12}$$

and

$$H_I = \sum_{k=0}^{\infty} c_k A_k \otimes (b_k^\dagger + b_k) \tag{13}$$

where $\left(b_k, b_k^\dagger\right)_{k\in\mathbb{N}} \in \mathcal{L}(\mathcal{E}_B)$ are the corresponding ladder operators, as well as a sequence $(A_k)_{k\in\mathbb{N}} \in \mathcal{L}(\mathcal{E}_S)$, depending on the corresponding coupling mechanism and spectral density [5] of the form:

$$\mathcal{D}(\mathbb{R}) \ni J : \omega \mapsto \pi \sum_{k=0}^{\infty} c_k^2 \delta(\omega - \omega_k) \tag{14}$$

where the δ can be the Dirac delta or an approximation of it.

Definition 4. Dynamics through spectral density
Given the initial density matrix for the total system $\rho^{(0)} \in \mathcal{L}(\mathcal{E}_S \otimes \mathcal{E}_B)$ and the thermalized bath density matrix at each time and temperature $t \in \mathbb{R}, T \in \mathbb{R}_+$: $\rho_B(t,T) \in \mathcal{L}(\mathcal{E}_B)$, the proposed algorithm consists in iteratively calculating the open system density matrix as:

$$\forall j \in \mathbb{N} : \rho_S^{(j+1)} = \mathcal{T}_B \left(U(t) \rho_S^{(j)} \otimes \rho_B(t,T) U^\dagger(t) \right) \in \mathcal{L}(\mathcal{E}_S) \tag{15}$$

where $\mathcal{T}_B$ denotes the partial trace over the bath and $U \in \mathcal{L}(\mathcal{E}_S \otimes \mathcal{E}_B)$ is the global system evolution operator.

2. Quantum Fourier Transform and Quantum Phase Estimation

The Quantum Fourier Transform (QFT) and Quantum Phase Estimation (QPE) circuits [6] will be useful in order to compute the Non-Equilibrium Steady State (NESS) of open quantum systems.

Definition 5. Quantum Fourier Transform Given a N-dimensional Hilbert space V with orthonormal basis $(|j\rangle)_j$, the QFT is defined by:

$$\mathcal{F} : V \to V, |j\rangle \mapsto \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i j k / N} |k\rangle \tag{16}$$

Proposition 3. If there exists $n \in \mathbb{N} : N = 2^n$, the QFT of j can be written:

$$\mathcal{F} |j\rangle = \frac{1}{2^{n/2}} \bigotimes_{l=1}^{n} \left(|0\rangle + e^{2\pi i j 2^{-l}} |1\rangle \right)$$

Proposition 4. Let R_k denote the gate $\begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i / 2^k} \end{pmatrix}$. Then, the following circuit, figure 3, performs $\mathcal{F} |j\rangle$.

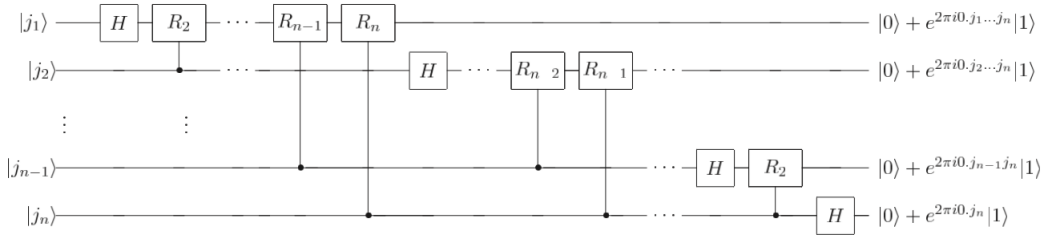

Figure 3: Quantum Fourier Transform circuit [6].

Definition 6. Phase Estimation Let $U \in \mathsf{U}(n)$. Let $|u\rangle$ be the eigenvector corresponding to the eigenvalue $e^{2\pi i \varphi}$ with $\varphi \in [0,1[$ unknown. Assume we are able to prepare $|u\rangle$ and perform $C(U^{2^j})$ for necessary $j \in \mathbb{N}$. The estimation uses two registers so that the first step is shown on figure 4. Then, the inverse QFT, $\mathcal{F}^\dagger$, is applied on the first register. Measurement on the first register yields the output.

Proposition 5. After the first step, the result is:

$$\frac{1}{2^{t/2}} \bigotimes_{k=0}^{t-1} \left(|0\rangle + e^{2\pi i 2^{t-1} \varphi} |1\rangle \right) = \frac{1}{2^{t/2}} \sum_{k=0}^{2^t - 1} e^{2\pi i \varphi k} |k\rangle \tag{17}$$

Proposition 6. The output of QPE is $|\varphi_1, ..., \varphi_t\rangle$.

Proposition 7. Let $\phi_0 \in \partial B_1(0) \subset \mathbb{C}$ be the eigenvalue of $U \in \mathsf{U}(n)$ to which is applied the QPE algorithm. The probability $p \in [0,1]$ of measuring the corresponding eigenvector $|\phi_0\rangle \in \mathcal{E}$ in the second registrer is:

$$p = \frac{|\langle \psi_0 | \phi_0 \rangle|^2}{2^{2t}} \frac{1 - \cos(2\pi \delta 2^t)}{1 - \cos(2\pi \delta)} \tag{18}$$

where $|\psi_0\rangle \in \mathcal{E}$ is the initial state of the second register and $\delta = \phi_0 - \lfloor 2^t \phi_0 \rfloor / 2^t$.

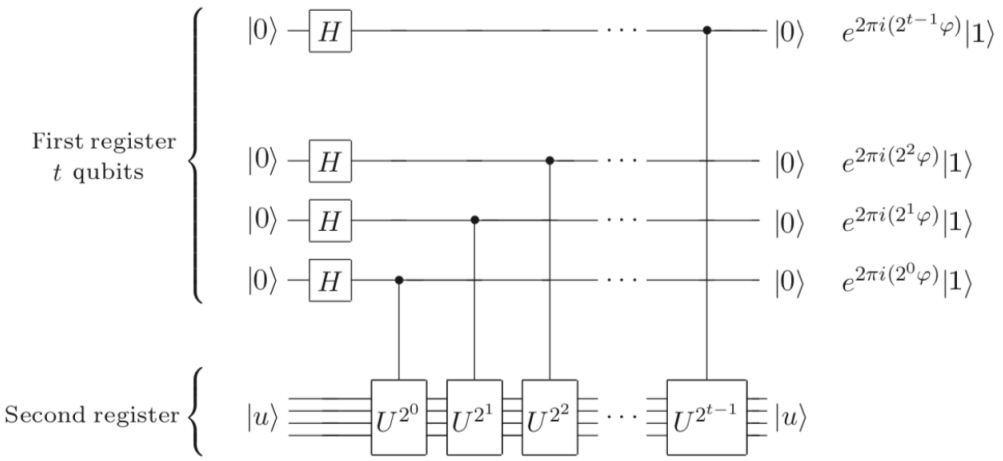

Figure 4: First stage of the Quantum Phase Estimation [6].

3. Non-Equilibrium Steady State

This section follows [7].

Definition 7. Let $\mathcal{E}$ be the finite dimensional Hilbert space of states for a given system of orthonormal basis $(|j\rangle)_j$. Given a density operator acting on $\mathcal{E}$ of the form $\rho = \sum_{jk} \rho_{jk} |j\rangle \langle k|$, the vectorized version of this operator is $\mathcal{E} \otimes \mathcal{E} \ni |\rho\rangle = \sum_{jk} \rho_{jk} |j\rangle \otimes |k\rangle$. The Liouvillian super-operator $\mathcal{L}$ such that $\frac{d}{dt} |\rho\rangle = \mathcal{L} |\rho\rangle$, as in the formalism for an open quantum system interacting with a Markovian environment, is vectorized the same manner.

Postulate 1. A Non-Equilibrium Steady State $|\rho_{ss}\rangle \in \mathcal{E} \otimes \mathcal{E}$, defined by the condition $\mathcal{L} |\rho_{ss}\rangle = 0$, exists and is unique.

Proposition 8. Let $\mathcal{L}$ be the vectorized Liouvillian super-operator and $|\rho_{ss}\rangle, |I\rangle$ respectively the vectorized NESS density matrix and vectorized identity matrix. Then, the following hold:

$$\mathcal{L} |\rho_{ss}\rangle = 0 \qquad\qquad \mathcal{L}^\dagger |I\rangle = 0 \tag{19}$$

Definition 8. Let $2^N \in \mathbb{N}$ be the dimension of the space $\mathcal{E}$. Define the following hermitian operator M by:

$$M = \begin{pmatrix} 0 & \mathcal{L} \\ \mathcal{L}^\dagger & 0 \end{pmatrix} \tag{20}$$

acting on a 2^{2N+1}-dimensional space.

Proposition 9. Under postulate 1, the operator M has exactly two eigenvectors associated to the 0 eigenvalue, namely $|\eta_0\rangle = |0\rangle |I\rangle$ and $|\eta_1\rangle = |1\rangle |\rho_{ss}\rangle$.

Definition 9. The M operator encoding Decompose the Liouvillian as $\mathcal{L} = \mathcal{L}_H - i\mathcal{L}_A$, with $\mathcal{L}_H = \mathcal{L}_H^\dagger$ and $\mathcal{L}_A = \mathcal{L}_A^\dagger$. The M operator is encoded as $M = X \otimes \mathcal{L}_H + Y \otimes \mathcal{L}_A$.

Definition 10. Quantum Circuit for NESS Solver The Quantum circuit of the gate $\mathcal{P}$ corresponds to the preparation of an estimate to the eigenvector corresponding to the 0 eigenvalue. The second part of the algorithm is the QPE circuit with $U = \exp(2\pi i t_0 M)$, $t_0 \in \mathbb{R}$ a normalizing factor for the spectrum of M.

Proposition 10. Let $|\psi\rangle$ be the circuit output state and O a hermitian operator to be measured. Then:

$$\langle O \rangle = \langle \psi | \, I_t \otimes X \otimes I_N \otimes O \, |\psi\rangle \tag{21}$$

where I_t is the identity operator acting on the first register, X the Pauli matrix acting on the first qubit of the second register, I_N the identity acting on the N following qubits and O acting on the N remaining qubits of the second register.

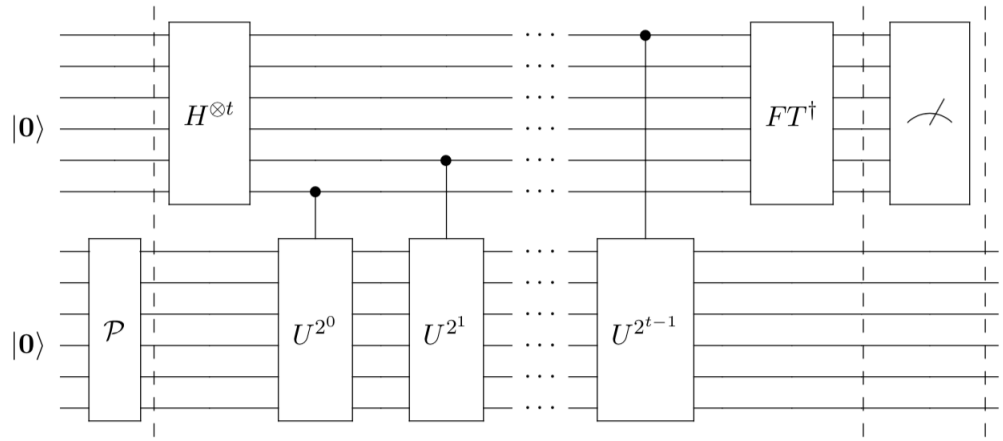

Figure 5: Quantum circuit for NESS solver [7].

C. Results

1. *A spin in a spin bath*

Consider the example of simulating the Markovian dynamics of a spin in a spin bath at thermal equilibrium. Assume the global system Hamiltonian is of the form:

$$H = -\frac{1}{2}Z_0 - \frac{1}{2}\sum_{k=1}^{8}\omega_k Z_k + \frac{1}{2}X \otimes \sum_{k=1}^{8} c_k X_k \tag{22}$$

where the index 0 refers to the system spin and indexes $k = 1, ..., 8$ refer to the bath spins. The $(\omega_k)_k$ coefficients are the frequencies of the environment modes and $(c_k)_k$ the coupling constants. Assume the spectral density of the spin bath is expressed as:

$$J(\omega) = 2\pi\alpha\omega e^{-\omega/\omega_c} \tag{23}$$

such that:

$$\int_{w_k-\Delta\omega/2}^{w_k+\Delta\omega/2} J(\omega)d\omega = \pi c_k^2 \tag{24}$$

Set $\alpha = 2 \cdot 10^{-4}$, $\omega_c/\Delta_0 = 100$, $\beta\Delta_0 = 1$. Furthermore, $\omega_k/\Delta_0 = 0.8 + 0.05k$ and $\Delta_0\tau = 30$. For an initial density matrix $\rho = |1\rangle\langle 1|$ corresponding to a purely excited state, the simulation results is given on figure 6, showing similar results to those presented in the original article [4].

2. *NESS of single spin subject to relaxation and external fields*

Let us consider the Linblad equation for a single spin subject to relaxation and external fields:

$$\dot{\rho} = -i[H, \rho] - \frac{1}{2}\{\sigma^+\sigma^-, \rho\} + \sigma^-\rho\sigma^+ \tag{25}$$

with $H = h\sigma_x$. After vectorization, the Liouvillian becomes:

$$\mathcal{L} = -i(I \otimes H - H^T \otimes I) - \frac{1}{2}(I \otimes \sigma^+\sigma^- + \sigma^+\sigma^- \otimes I - 2\sigma^- \otimes \sigma^+ -) \tag{26}$$

The decomposition writes:

$$\begin{aligned} \mathcal{L}_A &= I \otimes H - H^T \otimes I \\ \mathcal{L}_H &= \frac{1}{2}\left(\sigma^- \otimes \sigma^+ + \sigma^+ \otimes \sigma^- - I \otimes \sigma^+\sigma^- - \sigma^+\sigma^- \otimes I\right) \end{aligned} \tag{27}$$

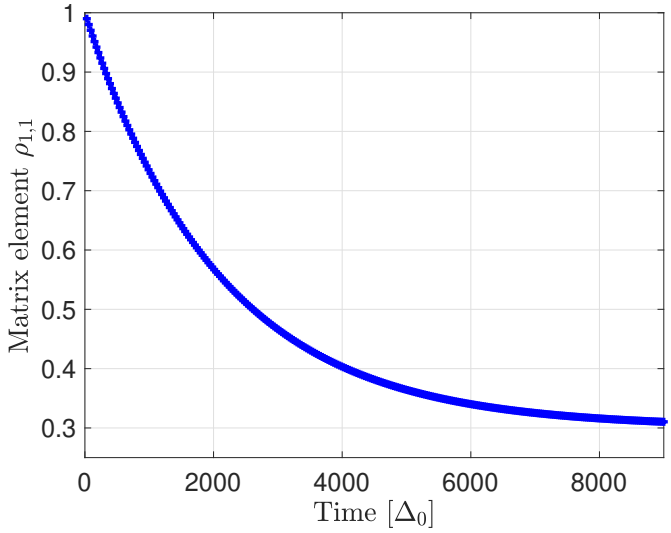

Figure 6: Evolution of the $\rho_{1,1}$ element through spectral density

from which the M operator can be obtained. The following Trotter-Suzuki approximation may be applied:

$$U^{2^j} \approx \left(\prod_\gamma \exp(2\pi i 2^j \alpha_\gamma M_\gamma / r) \right)^r$$

Running the algorithm with $t = 3$ qubits and $h = 1$ yields an expectation value $\langle \sigma_y \rangle = -0.14$, which is close to the value found in the original article [7].

IV. QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM

A. Motivation

Let us now see how Hamiltonians can appear, even when solving a non-physics-related problem. This section introduces an algorithm capable of producing approximate solutions to combinatorial problems: the Quantum Approximate Optimization Algorithm (QAOA).

B. Theory

Let us consider the general form of a combinatorial optimization problem: find $x^* \in S$ a set of discrete variables such that $x^* = \arg\max_{x \in S} C(x)$, given the cost function $C : S \to \mathbb{R}$. In this case, let $S = \{0,1\}^n$, $n \in \mathbb{N}$ and:

$$C(x) = \sum_{(Q,\bar{Q}) \in [\![n]\!]} \omega_{(Q,\bar{Q})} \prod_{i \in Q} x_i \prod_{j \in \bar{Q}} (1 - x_j) \tag{28}$$

where $\omega_{(Q,\bar{Q})} \in \mathbb{R}$. Denote by Z_i the Pauli operator acting on qubit i. Map the cost function C to the following n-qubit Hamiltonian:

$$H = \sum_{(Q,\bar{Q}) \in [\![n]\!]} \omega_{(Q,\bar{Q})} \frac{1}{2^{|Q|+|\bar{Q}|}} \prod_{i \in Q} (1 - Z_i) \prod_{j \in \bar{Q}} (1 + Z_i) \tag{29}$$

Definition 11. The weighted MAXCUT problem
Given a set of edges G. Assume $\omega_{(i,j)} = \chi_{(i,j) \in E}$. The problem Hamiltonian becomes:

$$H = \frac{1}{2} \sum_{(j,k) \in E} \omega_{jk} \left(1 - Z_j Z_k\right) \tag{30}$$

Definition 12. The QAOA trial state
Let $B = \sum_{i=1}^{n} X_i$. Given $\gamma, \beta \in \mathbb{R}^p$, define the trial state [8]:

$$|\psi_p(\gamma, \beta)\rangle = \prod_{j=n}^{1} \left(e^{-i\beta_j B} e^{-i\gamma_j H} \right) |+\rangle^n \tag{31}$$

with $|+\rangle$ eigenvector of X with eigenvalue 1.

It then remains to find:

$$(\gamma^*, \beta^*) = \underset{(\gamma,\beta) \in \mathbb{R}^p \times \mathbb{R}^p}{\arg\max} \langle \psi_p(\gamma, \beta)| H |\psi_p(\gamma, \beta)\rangle \tag{32}$$

Proposition 11. The following equality holds:

$$\lim_{p \to \infty} \langle \psi_p(\gamma^*, \beta^*)| H |\psi_p(\gamma^*, \beta^*)\rangle = \max_{x \in S} C(x) \tag{33}$$

Part II
Competition

V. CONSTRAINED VARIATIONAL QUANTUM EIGENSOLVER

Proposition 12 can help computing excited energy levels [1].

Proposition 12. The n-th excited state $|n\rangle \in \mathcal{E}$ of the Hamiltonian $H \in \mathcal{L}(\mathcal{E})$ is the ground state of the following Hamiltonian:

$$H' = H + a\sum_{j=0}^{n-1} |j\rangle\langle j| \in \mathcal{L}(\mathcal{E}) \tag{34}$$

for $a > 0$ is large enough.

VI. SIMULATE A MOLECULE

Let $\mathcal{E}$ be a single-particule Hilbert space and $\mathcal{F} = \overline{\oplus_{n=0}^{\infty} S_n \mathcal{E}^{\otimes n}}$, with S_n the anti-symmetrizing operator of tensor products, the corresponding Fock space. Let $(a_k)_{k\in\mathbb{N}}, (a_k^\dagger)_{k\in\mathbb{N}} \in \mathcal{L}(\mathcal{E})$ be the creation and annnihilation operators satisfying the fermionic Canonical Commutation Relations:

$$\forall j,k \in \mathbb{N}: \qquad \{a_j, a_k^\dagger\} = \delta_{j,k} \qquad \{a_j, a_k\} = \{a_j^\dagger, a_k^\dagger\} = 0 \tag{35}$$

Definition 13. Jordan-Wigner mapping 1 Mapping qubit operators to fermionic operators can be done the following way:

$$\forall j \in \mathbb{N}: a_j = -\left(\otimes_{k=1}^{j-1} Z_k\right) \otimes \sigma_j \tag{36}$$

where $\sigma_j = |0\rangle\langle 1|$.

Definition 14. Jordan-Wigner mapping 2 Mapping fermionic operators to qubit operators can be done the following way:

$$\begin{aligned} \forall j \in \mathbb{N}: \qquad Z_j &= [a_j, a_j^\dagger] \\ X_j &= -\left(\prod_{k=1}^{j-1} Z_k\right)(a_j + a_j^\dagger) \\ Y_j &= i\left(\prod_{k=1}^{j-1} Z_k\right)(a_j^\dagger - a_j) \end{aligned} \tag{37}$$

Proposition 13. Verify both transformations preserve the Canonical Commutation Relations 35.

Assume the annihilation operators correspond to a basis of one-particle states: $(|\phi\rangle_j)_{j\in\mathbb{N}}$.

Postulate 2. In the Born-Oppenheimer approximation, the absence of external fields, the second-quantization nonrelativistic and spin-free molecular electronic Hamiltonian is given by:

$$H = \sum_{j,k\in\mathbb{N}} h_{jk} a_j^\dagger a_k + \frac{1}{2}\sum_{i,j,k,l\in\mathbb{N}} g_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + H_{\text{nuc}} \tag{38}$$

where in atomic units:

$$\begin{aligned} h_{jk} &= \int \phi_j^* \left(-\frac{1}{2}\nabla^2 - \sum_l \frac{Z_l}{r_l}\right)\phi_k \\ g_{ijkl} &= \iint \frac{\phi_i^*(x_1)\phi_k^*(x_2)\phi_j(x_1)\phi_l(x_2)}{r_{12}} dx_1 dx_2 \\ H_{\text{nuc}} &= \frac{1}{2}\sum_{i\neq j} \frac{Z_i Z_j}{R_{ij}} \end{aligned} \tag{39}$$

Here, the Z_i are the nuclear charges, r_l the electron-nuclear separations, $r_{1,2}$ the electron-electron separation and R_{ij} the internuclear sepration.

VII. IMAGINARY TIME PROPAGATION

This section is taken from [9].

Proposition 14. Given a time-independent Hamiltonian $H \in \mathcal{L}(\mathcal{E})$, an arbitrary state $|\psi\rangle \in \mathcal{E}$ can be formally evolved in imaginary time $\tau = it \in i\mathbb{R}$:

$$|\psi(\tau)\rangle = \sum_{n=0}^{\infty} c_n e^{-E_n \tau} |\phi_n\rangle \tag{40}$$

with the $(c_n)_{n\in\mathbb{N}}$ complex coefficients and $|\phi_n\rangle$ the Hamiltonian eigenvectors.

By multiplying the imaginary time propagator by $e^{\tau E_T}$, for E_T the ground state, the normalization of the ground state is preserved, whereas the other components vanish.

Definition 15. Mapping to extended Hilbert space Let us map an arbitrary state $|\psi_s\rangle$ to $|\Psi_0\rangle = |0\rangle |\psi_s\rangle$ and define the following unitary operator acting on the total Hilbert space:

$$U(\tau) = \begin{pmatrix} Q_{ITP}(\tau) & \left(1 + e^{-2(H-E_T)\tau}\right)^{-1/2} \\ \left(1 + e^{-2(H-E_T)\tau}\right)^{-1/2} & -Q_{ITP}(\tau) \end{pmatrix} \tag{41}$$

where $Q_{ITP}(\tau) = \left(1 + e^{-2(H-E_T)\tau}\right)^{-1/2} e^{-(H-E_T)\tau}$.

Proposition 15. The application of $U(\tau)$ to $|\Psi_0\rangle$ yields:

$$|\Psi(\tau)\rangle \propto |0\rangle \otimes Q_{\mathrm{ITP}}(\tau) |\psi_s\rangle + |1\rangle \otimes \left(1 + e^{-2(H-E_T)\tau}\right)^{-1/2} |\psi_s\rangle \tag{42}$$

Proposition 16. If τ is large enough, performing a measurement along the reservoir state $|0\rangle$ pushes the system to collapse to the state $|\Psi_f\rangle$:

$$|\Psi_f\rangle = C |0\rangle \otimes |\phi_0\rangle \tag{43}$$

for $C \in \mathbb{C}$ a normalization coefficient.

VIII. USE OF SYMMETRY TO IMPROVE EIGENFUNCTION CALCULATIONS

Knowing a set of symmetries of a given Hamiltonian allows us to make use of group theory, see appendix A, to facilitate the diagonalization.

Proposition 17. Let (D, V) be, as in proposition 24, a representation of a finite group G, commuting with the Hamiltonian H. For $\mu > 0$ large enough, the eigenfunctions of H can be found by successively using the projectors $(\pi_i)_i$. These projectors force the ansatz to respect the desired symmetry.. More specifically, if $|\phi_i\rangle \in \mathcal{E}$ transforms like a basis function of the j-th irreducible representation V_j, $|\phi_i\rangle$ can be found as the ground state of:

$$H_i = H + \mu(1 - \pi_i) \in \mathcal{L}(\mathcal{E}) \tag{44}$$

Appendix A: A Summary of Group Representation Theory

This section is mainly taken from [10].

1. Representations of finite groups

Definition 16. A representation of a finite group G on a finite-dimensional complex vector space V is a homorphism $\rho : G \to \mathsf{GL}(V)$. A subrepresentation of a representation V is called irreducible if there is no proper nonzero invariant subspace W of V.

Definition 17. Direct sum, tensor product, dual and regular.

Proposition 18. If W is a subrepresentation of a representation V of a finite group G, then there is a complmentary invariant subspace W' of V, so that $V = W \oplus W'$.

Corollary 1. Any representation is a diect sum of irreducible representations

Theorem 3. Schur's lemma If V and W are irreducible representations of G and $\varphi : V \to W$ is a G-module homomorphism, then:

1. either φ is an isomorphism of $\varphi = 0$
2. if $V = W$, then $\varphi = \lambda$ for some $\lambda \in \mathbb{C}$

Proposition 19. For any representation V of a finite group G, there is a decomposition:

$$V = V_1^{\oplus a_1} \oplus ... \oplus V_k^{\oplus a_k} \tag{A1}$$

where the (V_i) are distinct irreducible representations . The decomposition of V into a direct sum of the k factors is unique, as are the V_i that occur and their mulitplicities a_i.

2. Characters and Projection Formulas

Definition 18. Let (D, V) be a finite-dimensional representation of the finite group G. Its character is the complex-valued function on the group defined by:

$$\forall g \in G : \chi_V(g) = \text{Trace}(D(g)) \tag{A2}$$

Proposition 20. Let V and W be representations of G. Then: $\chi_{V\oplus W} = \chi_V + \chi_W$ and $\chi_{V\otimes W} = \chi_V \chi_W$.

Notation For G a finite group and (D, V) one of its representation:

$$V^G = \{v \in V : D(g)v = v, \forall g \in G\} \tag{A3}$$

Proposition 21. The map

$$\text{End}(V) \ni \varphi : v \mapsto \frac{1}{|G|} \sum_{g\in G} D(g)v \tag{A4}$$

is a projector of V onto V^G.

Definition 19. Define $(\mathbb{C}_{\text{class}}(G), (\cdot, \cdot))$ the hermitian space with $\mathbb{C}_{\text{class}}(G)$ the set of class functions on G and the hermitian product:

$$(\alpha, \beta) = \frac{1}{|G|} \sum_{g\in G} \alpha(g)^* \beta(g) \tag{A5}$$

Theorem 4. The characters of the irreducible representations of G are orthonormal in $(\mathbb{C}_{\text{class}}(G), (\cdot, \cdot))$.

Lemma 1. If V is an irreducible representation, then $\dim \mathrm{Hom}(V,W)^G$ is the multiplicity of V in W.

Corollary 2. The number of irreducible representations of G is less than or equal to the number of conjugacy classes.

Corollary 3. Any representation is determined by its character.

Corollary 4. A representation V is irreducible if and only if $(\chi_V, \chi_V) = 1$.

Corollary 5. The mutiplicity a_i of the irreducible representation V_i in V is given by: $a_i = (\chi_V, \chi_{V_i})$

Definition 20. Let G be a group. A G-module consists of an abelian group $(M, +)$ with a left group action $\cdot : G \times M \to M$ verifying:

$$g \cdot (a + b) = g \cdot a + g \cdot b \tag{A6}$$

Proposition 22. Let $\alpha : \mathbb{C} \to \mathbb{C}$ be any function on the group G, and for any finite-dimensional representation (D, V) of G, set:

$$\varphi_{\alpha,V} = \sum_{g \in G} \alpha(g) D(g) : V \to V \tag{A7}$$

Then $\varphi_{\alpha,V}$ is a homomorphism of G-modules for all V if and only if α is a class function.

Proposition 23. The characters of irreducible representations of a finite group G form an orthonormal basis of $(\mathbb{C}_{\mathrm{class}}(G), (\cdot, \cdot))$.

Proposition 24. Let (D, V) be a finite-dimensional representation of the finite group G and write:

$$V = V_1^{\oplus a_1} \oplus ... \oplus V_k^{\oplus a_k} \tag{A8}$$

its decomposition. Then, the operator

$$\pi_i = \frac{\dim V_i}{|G|} \sum_{g \in G} \chi_{V_i}(g)^* D(g) \tag{A9}$$

is the projection of V onto $V_i^{\oplus a_i}$.

Appendix B: Aspects of dynamics of open quantum systems

This appendix follows [5].

1. Dynamics of open quantum systems

Let $\mathcal{E}_S, \mathcal{E}_B, \mathcal{E}_I$ be the Hilbert space of states for the open system, the bath and the interaction between the two. For $H_{S,B,I} \in \mathcal{L}(\mathcal{E}_{S,B,I})$ the respective Hamiltonians, the global Hamiltonian is assumed to be $H = H_S + H_B + H_I \in \mathcal{L}(\mathcal{E}_S \otimes \mathcal{E}_B)$.

Proposition 25. Let $A \in \mathcal{L}(\mathcal{E}_S)$ be an operator to be measured. Then:

$$\langle A \rangle = \mathcal{T}_S(A\rho_S) \tag{B1}$$

with $\rho_S = \mathcal{T}_B \rho \in \mathcal{L}(\mathcal{E}_S)$ the system's density matrix, for $\rho \in \mathcal{L}(\mathcal{E}_S \otimes \mathcal{E}_B)$ the total density matrix.

Proposition 26. The system's density matrix ρ_S verifies the following:

$$\forall t > 0 : \rho_S(t) = \mathcal{T}_B \left(U(t) \rho(t) U^\dagger(t) \right) \tag{B2}$$

where $t = 0$ is the initial time and U is the unitary evolution operator of the Schrödinger equation for the total system, assumed to be closed.

Proposition 27. A corollary from proposition 26 is the following equation:

$$\forall t > 0 : \frac{d}{dt}\rho_S(t) = -i\mathcal{T}_B[H(t), \rho(t)] \tag{B3}$$

Definition 21. Interaction picture von Neumann equation Decompose the global Hamiltonian as $H(t) = H_0 + H_I(t)$. Define $U_I(t) = U_0^\dagger(t)U(t)$ and finally $\rho_I(t) = U_I(t)\rho(0)U_I^\dagger(t)$. The von Neumann equation can be written for the interaction density matrix ρ_I as:

$$\frac{d}{dt} = -i[H_I(t), \rho_I(t)] \tag{B4}$$

From now on, we will denote by ρ the interaction density matrix ρ_I.

2. Weak-coupling limit

Proposition 28. Assuming $\mathcal{T}_B[H_I(t), \rho(0)] = 0$, the integral form of the interaction picture von Neumann equation takes the form:

$$\forall t > 0 : \frac{d}{dt}\rho_S(t) = -\int_0^t ds\mathcal{T}_B[H_I(t), [H_I(s), \rho(s)]] \tag{B5}$$

Definition 22. Born approximation Assume the density matrix takes the form:

$$\forall t > 0 : \rho(t) = \rho_S(t) \otimes \rho_B \tag{B6}$$

Proposition 29. Assuming we can replace, in the integrand, $\rho_S(s)$ by $\rho_S(t)$ (Markov approximation) and that this integrand vanishes rapidly when $s \to \infty$, the Markovian quantum master equation holds:

$$\forall t > 0 : \frac{d}{dt}\rho_S(t) = -\int_0^\infty ds\mathcal{T}_B[H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_B]] \tag{B7}$$

3. The Caldeira-Legett model

The model describes a particle of mass m with coordinate x which moves in a potential $V(x)$. The free Hamiltonian H_S of the particle is taken to be:

$$H_S = \frac{p^2}{2m} + V(x) \tag{B8}$$

with p the particle momentum. The bath is assumed to be governed by:

$$H_B = \sum_{n=0}^{\infty} \omega_n \left(b_n^\dagger b_n + \frac{1}{2} \right) \tag{B9}$$

with $b_n^\dagger$ and b_n the annihilation and creation operator of the bath, ω_n the mode frequency. The interaction is assumed to be of the form:

$$H_I = -x \sum_{n=0}^{\infty} \frac{\kappa_n}{(2m_n\omega_n)^{1/2}} (b_n^\dagger + b_n) \tag{B10}$$

In addition, the counter-term $H_C \in \mathcal{L}(\mathcal{E}_S)$ appears in this model, for renormalization reasons.

$$H_C = x^2 \sum_{n=0}^{\infty} \frac{\kappa_n^2}{2m_n\omega_n^2} \tag{B11}$$

yielding the final Hamiltonian $H = H_S + H_B + H_I + H_C$.

4. Von Neumann equation and spectral density

Proposition 30. For the Caldeira-Legett model, the Von Neumann equation can be written:

$$\frac{d}{dt}\rho_S(t) = -i[H_S + H_C, \rho_s(t)] - \int_0^\infty d\tau \mathcal{T}_B[H_I(\tau), [H_I(-\tau), \rho_S(t) \otimes \rho_B]] \tag{B12}$$

where the second term on the right hand side is denoted by $\mathcal{K}\rho_S(t)$.

Definition 23. Thermal equilibrium hypothesis Assume the bath at thermal equilibrium and temperature $T = \frac{1}{k_B\beta}$ has the following density matrix:

$$\rho_B = \frac{\exp(-\beta H_B)}{\mathcal{T}_B(\exp(-\beta H_B))} \tag{B13}$$

Averages with respect to the bath will be denoted by $\langle\cdot\rangle_B$.

Definition 24. Correlation functions It is convenient to introduce the following correlation functions:

$$\begin{aligned} D(\tau) &= i\langle[H_I(\tau)x, H_I(-\tau)x]\rangle_B \\ D_1(\tau) &= \langle\{H_I(\tau)x, H_I(-\tau)x\}\rangle_B \end{aligned} \tag{B14}$$

which are respectively called the dissipation and noise kernel.

Definition 25. Spectral density It is defined as:

$$J(\omega) = \sum_{n=0}^{\infty} \frac{\kappa_n^2}{2m_n\omega_n}\delta(\omega - \omega_n) \tag{B15}$$

Proposition 31. The bath correlation functions can be written in terms of the spectral density as:

$$\begin{aligned} D(\tau) &= 2\int_0^\infty d\omega J(\omega)\sin(\omega\tau) \\ D_1(\tau) &= 2\int_0^\infty d\omega J(\omega)\coth(\omega\beta/2)\cos(\omega\tau) \end{aligned} \tag{B16}$$

Proposition 32. The following expression for $\mathcal{K}\rho_S(t)$ holds:

$$\mathcal{K}\rho_S(t) = \int_0^\infty d\tau \left(\frac{i}{2}D(\tau)[x(\tau), [x(-\tau), \rho_S(t)]] - \frac{1}{2}D_1(\tau)[x(\tau), \{x(-\tau), \rho_S(t)\}]\right) \tag{B17}$$

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