

# Ground State Energy Calculation

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This paper explores the potential of Model-Driven Engineering (MDE) in the realm of Quantum AI, particularly Quantum Machine Learning (QML) applications. Ground state calculations, crucial in quantum mechanics for various applications, pose challenges with the increasing complexity of multi-particle systems. To address this, the paper proposes an innovative approach leveraging diverse architectures to decode the intricacies of these systems. Beyond theoretical exploration, the paper provides a proof of concept for MDE in Quantum AI and analyzes classical and quantum hybrid solutions for ground state calculations in chemical simulations. The aim is to advance the practical applications of quantum computing in real-world problem-solving scenarios.

## I. INTRODUCTION

(MDE) paradigm emerges as a promising framework. MDE facilitates automated code generation, model checking, and analysis, providing a robust toolkit for Quantum AI applications. This paper delves into the analysis and proof of concept for MDE in Quantum AI, exploring its potential applications in Quantum Machine Learning (QML).

Ground state calculations in quantum mechanics are pivotal for diverse applications, spanning quantum physics, computation, and chemistry. They serve as a foundational step, laying the groundwork for advanced research and comprehension in these domains. Despite the existence of various methods for these calculations, the challenge intensifies with the growing complexity of multi-particle systems. As these systems evolve into intricate "black boxes," conventional methods encounter limitations.

To address this challenge, we propose a novel approach that harnesses diverse architectures to unravel the intricacies of multi-particle systems. This innovative strategy aims to overcome the complexities associated with traditional methods, offering a fresh perspective on ground state calculations.

The paper goes beyond theoretical exploration and delves into practical aspects, offering a proof of concept for MDE in Quantum AI. Furthermore, it analyzes classical and quantum hybrid solutions for the intricate problem of ground state calculations in chemical simulations. By leveraging the capabilities of both classical and quantum paradigms, this paper aims to contribute to the advancement of quantum computing applications in real-world problem-solving scenarios.

### A. Classical Algorithms for Ground State Calculation

#### 1. Network Representation of Multi-Particle Quantum States

Computing multi-particle quantum states in various fields, notably in condensed matter physics, becomes ex-

ponentially challenging with an increasing number of particles. An alternative method frequently used in related literature to overcome this difficulty is to employ network representations of quantum states.

#### 2. Tensor Networks and Density Matrix Renormalization Group (DMRG)

Tensor networks gained attention in the literature in the 1990s, offering a mathematical representation based on the local entanglement structure of multi-particle quantum states. This approach finds interdisciplinary applications, particularly at the intersections of condensed matter, quantum information, quantum gravity, quantum chemistry, and artificial intelligence.

The method is rooted in the principle that higher-rank tensors, such as the wave function  $\Psi$ , can be decomposed as a product of lower-rank tensors:

$$\Psi_{i_1, i_2, \dots, i_N} = \sum_{\alpha_1, \alpha_2, \dots, \alpha_N} A_{i_1; \alpha_1}^{[1]} A_{i_2; \alpha_1 \alpha_2}^{[2]} \dots A_{i_{N-1}; \alpha_{N-2} \alpha_{N-1}}^{[N-1]} A_{i_N; \alpha_{N-1}}^{[N]} \quad (1)$$

where  $i_k; \alpha_k$  represents indices corresponding to local properties, and the bond indices labeled with  $\alpha_k$  can encode correlations such as entanglement. The decomposition is a special case known as the matrix product state (MPS). The  $\alpha_k$  indices' maximum number of values, known as the bond size, serves as a quantitative measure of entanglement.

The invention of the Density Matrix Renormalization Group (DMRG) algorithm marks a significant development in the history of tensor networks. This algorithm is designed to target the low-energy eigenstates of one-dimensional Hamiltonians, strategically reducing the total number of degrees of freedom by retaining those specifically associated with entanglement through a renormalization procedure. DMRG performs variational optimization on Matrix Product State (MPS) states. Subsequently, the inventors extended the algorithm to quantum chemistry, leading to the utilization of tensor networks for calculating the electronic states of

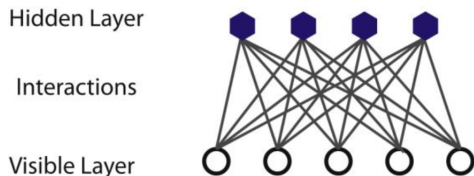


FIG. 1. The configuration of our network is represented such that  $a_i$  represents visible layers,  $b_i$  represents hidden layers, and  $W_{ik}$  is for weights. These are variational parameters that are adjusted to minimize the aimed energy.  $j_i$  represents the orthogonal vectors.

molecules. This process necessitates the proper realignment of all fermionic orbitals, a task facilitated by MPS affinities.

### 3. Artificial Neural Networks and Boltzmann Machine Algorithm

There are many studies pointing out that there is a strong relationship between hidden layer artificial neural networks and tensor networks, especially deep learning (DL) and Boltzmann machine (BM) networks. Hidden layers (in a sense acting as link indices in tensor networks) offer the possibility of computationally easy coding of complex relationships between visible layer neurons. In this context, it is also possible to find highly correlated multi-particle quantum system wave functions with classical neural network architectures as an alternative to tensor networks.

### 4. Restricted Boltzmann Machine (RBM)

For solving our system, we utilized the Python package Netket Employing the Restricted Boltzmann Machine (RBM) to address the system, illustrated in Fig. 1, we adopt an ansatz as the wave function. This ansatz consists of two layers: a visible layer with "L" 1/2 degrees of freedom and a hidden layer containing "M" different hidden units. Connections are established between all visible and hidden nodes. The ansatz is given by:

$$\psi_{\text{RBM}}(\mathbf{j}) = \exp \left( \sum_{i=1}^L a_i j_i \right) \prod_{i=1}^M \cosh \left( b_i + \sum_k W_{ik} j_k \right), \quad (2)$$

where  $\mathbf{j}$  represents the indices of the visible layer, and  $\psi_{\text{RBM}}$  is the restricted Boltzmann machine wave function.

it is also introduced the variable  $\alpha = M/L$  to investigate its impact on the convergence time to the calculated ground energy. To create a variational state with its parameters, we utilize a Monte Carlo-sampled Vari-

able State. This involves defining a suitable sampler in a Hilbert space for the system.

Next step is to determine the learning rate and diagonal shift ratio using the optimizer command. Subsequently, the solution minimize the following equation using the created variational state and Hamiltonian to reach the ground energy state after a certain number of iterations:

$$\text{Min}(H[\Psi]) = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$

Instead of solving the overall system, which is not efficient in minimization, we use a trick. By introducing local energies, we move towards the locality where the system tends towards the minimum energy:

$$E \approx \frac{\sum_x |\Psi|^2 E_{\text{loc}}}{\sum_x |\Psi|^2},$$

where  $E_{\text{loc}}(x) = \sum_y H_{xy}(\Psi(y))/\Psi(x)$ .

### B. Variational Quantum Eigensolver (VQE)

Exploring quantum computers reveals exciting possibilities, especially in the realm of chemical simulations. These simulations are essential for the development of new medicines and materials for various applications. When studying a chemical reaction, the focus lies in comparing the energy levels of interacting molecules. Higher energy molecules interact, leading the system to a lower energy state.

Simulating these processes involves calculating the ground states of the molecules. However, as the number of particles increases, the computational workload grows exponentially due to the complex interactions between them. Classical computers face challenges handling this complexity because of their limitations. Quantum computers, on the other hand, offer a unique advantage. Qbits, play a key role. Adding a qubit to the system doubles the computational capacity. So, with n qubits, the computational possibilities expand to  $2^n$ . This scalability provides quantum computers with an edge, offering a promising solution for handling the complexities of calculating ground states of the molecules.

The Variational Quantum Eigensolver (VQE) is a hybrid algorithm that combines variational methods with quantum mechanics. Its primary function is to estimate the ground state energy of a molecule. This is achieved through an iterative process of making educated guesses regarding the molecule's wave function and adjusting these conjectures to minimize the energy level. Ultimately it converges to the most stable state of the molecular system for given the model of Hamiltonian which describe the total energy of the system. The hybrid systems consist of a quantum component responsible for computing the energy of the system by solving the wave function for a particular Hamiltonian, and a classical component

dedicated to optimizing the variational parameters [? ? ].

As  $H$  is the Hamiltonian of a given quantum system, and it acts on the wave function  $\psi$  :

$$H|\psi\rangle = E|\psi\rangle \quad (3)$$

By Rayleigh–Ritz method, The inequality below provides an bound for the ground state energy  $E_0$  of the quantum system.

$$E_0 \leq \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \quad (4)$$

To find the ground state,  $\psi$  can parametrized the as  $\psi(\theta)$  with the set of parameters  $\theta$ . So, the main optimization problem become as follows:

$$\min_{\theta} \frac{\langle\Psi(\theta)|H|\Psi(\theta)\rangle}{\langle\Psi(\theta)|\Psi(\theta)\rangle} \quad (5)$$

The Hamiltonian  $\hat{H}$  defines the total energy in a quantum system, combining the kinetic and potential energy components. Mathematically, it is represented as the sum of the kinetic energy operator and the potential energy operator:

$$\hat{H} = \hat{T} + \hat{V} \quad (6)$$

For a single particle, the Hamiltonian can be expressed as:

$$\hat{H} = \frac{\hbar^2}{2m} \nabla^2 + V(r) \quad (7)$$

Where,  $\hbar$  is the reduced Planck's constant,  $m$  is the mass of the particle,  $\nabla^2$  represents the Laplacian operator associated with the kinetic energy, and  $V(r)$  is the potential energy function dependent on the position  $r$ .

The Hamiltonian operator for a quantum system, comprising electrons and nuclei, can be expressed as follows:

$$\begin{aligned} \hat{V} = & \sum_{i,j}^e \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{i,j}^n \frac{Z_i Z_j}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} \\ & - \sum_i^e \sum_j^n \frac{Z_j e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} \end{aligned} \quad (8)$$

$$\hat{T} = - \sum_{i=1}^e \frac{\hbar^2}{2m_i} \nabla_i^2 - \sum_{j=1}^n \frac{\hbar^2}{2m_j} \nabla_j^2 \quad (9)$$

Due to the Born-Oppenheimer assumption, which considers nuclei as stationary compared to electrons, certain terms are eliminated in  $\hat{T}$  and  $\hat{V}$ :

$$\hat{V} = \sum_{i,j=1}^e \frac{e^2}{4\pi\epsilon_0|r_i - r_j|} + c - \sum_{i=1}^e \sum_{j=1}^n \frac{Z_i e^2}{4\pi\epsilon_0|r_i - r_j|}$$

$$\hat{T} = - \sum_{i=1}^e \frac{\hbar^2}{2m_i} \nabla_i^2$$

The wave function can be seen as a Slater determinant from a classical perspective:

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_1(x_1) & \cdots & \chi_1(x_n) \\ \vdots & \ddots & \vdots \\ \chi_n(x_1) & \cdots & \chi_n(x_n) \end{vmatrix}$$

Where  $N$  is the normalizing constant,  $\chi_n$  provides the orbital information, and  $x_n$  provides the spin information.

In second quantization, we represent quantum states using occupation numbers and creation/annihilation operators. The wave function is expressed as a sum over different configurations, each associated with a set of occupation numbers.

$$\Psi = \sum_i c_i |n_1 \dots n_m\rangle$$

By introducing fermionic creation  $a_i^\dagger$  and annihilation  $a_j$  operators, we can simplify the representation. The wave function transforms into a concise form where the presence or absence of particles is represented by the occupation numbers.

$$\Psi = |011 \dots 0\rangle$$

To illustrate, we can express the Hamiltonian operator  $\hat{H}$  in atomic units. In this unit space, the Hamiltonian becomes:

$$\hat{H} \approx - \sum_{i=1}^e \frac{1}{2} \nabla_i^2 + \sum_{i,j=1}^e \frac{1}{|r_i - r_j|} - \sum_{i=1}^e \sum_{j=1}^n \frac{Z_j}{|r_i - r_j|}$$

This version incorporates the introduction of fermionic operators and makes the connection to expressing the Hamiltonian in atomic units clearer.

This reduced electronic Hamiltonian can be expressed in second quantized form, transitioning from its initial first quantized form. For single-particle operators  $h(x_i)$ , the conversion is given by:

$$\sum_i h(x_i) \Rightarrow \sum_{pq} \langle p|\hat{h}|q\rangle a_p^\dagger a_q$$

This notation succinctly captures the transformation, where  $a_p^\dagger$  and  $a_q$  are fermionic creation and annihilation operators, respectively, and  $\langle p|\hat{h}|q\rangle$  represents matrix elements of the operator in the basis of single-particle states.

$$h_{pq} = \int_{-\infty}^{\infty} \Psi_p(x) \left( \frac{1}{2} \nabla_i^2 - \sum_{j=1}^n \frac{Z_j}{|r_i - r_j|} \right) \Psi_q(x) dx$$

For the electron repulsion integral, a function of two electrons, a double integral is required:

$$\sum_i h(x_i, x_j) \Rightarrow \sum_{pqrs} \langle pq|\hat{h}|rs\rangle a_p^\dagger a_q^\dagger a_r a_s$$

The double integral is given by:

$$h_{pqrs} = \iint_{-\infty}^{\infty} \Psi_p^*(x_1) \Psi_q^*(x_1) \left( \frac{1}{|r_i - r_j|} \right) \Psi_r(x_2) \Psi_s(x_2) dx_1 dx_2$$

The final second quantized form of the Hamiltonian:

$$H = h_{pq} a_p^\dagger a_q + h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s + h_0$$

Where  $h_0$  represents the constant from the Born-Oppenheimer assumption.

Here, the main challenge lies in determining how to implement this representation on quantum qubits and their corresponding operators. Various techniques, such as parity mapping and Jordan-Wigner transformations, are employed for this purpose.

For instance, the Jordan-Wigner mapping is used to convert these fermionic operators to traditional Pauli expressions. One such method involves representing the fermionic operator  $a_p$  as:

$$a_p \rightarrow \frac{1}{2} (X_p + iY_p) Z_1 \dots Z_{p-1}$$

Here,  $X_p$  and  $Y_p$  are Pauli-X and Pauli-Y operators, respectively, and  $Z_1 \dots Z_{p-1}$  are Pauli-Z operators associated with different qubits in the context of Jordan-Wigner transformations.

With the Jordan-Wigner mapping and other techniques, it becomes possible to map the states of the molecular system to qubits.

The final step in this quantum computation process involves applying our molecular Hamiltonian to obtain an expectation value  $E_\theta$ .

$$E_\theta = \min_{\theta} \frac{\langle \Psi(\theta) | \hat{H} | \Psi(\theta) \rangle}{\langle \Psi(\theta) | \Psi(\theta) \rangle}$$

For the parametrized wave function  $|\Psi(\theta)\rangle$ , the output is obtained by passing the state through quantum gates

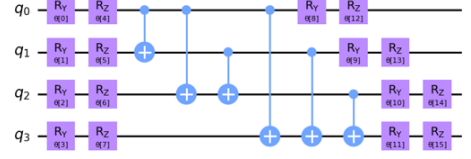


FIG. 2. Full-entangled ansatz circuit.

parametrized by  $\theta$ . The entire process is then iteratively repeated, optimizing the parameters to minimize the objective function.

In summary, the quantum algorithm involves encoding the molecular system into qubits, applying parametrized quantum gates to the wave function, and optimizing these parameters iteratively to minimize the expectation value of the molecular Hamiltonian. This iterative optimization process aims to find the best approximation of the ground state of the molecular system using quantum computation.

### 1. Model

In this research, I worked on 1-D Ising model, that is constructed by Pauli spins known as follows:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In the system, each of the spins on the x-axis affects the others that follows it. Those on the z-axis are also affected by the external magnetic field due to the  $\lambda$  effect. In this study,  $\lambda$  was constant and always was equal to 1. The equation for this hamiltonian is as follows.

$$H = \sum_{i=1}^n \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i=1}^n \sigma_i^z \quad (10)$$

### 2. Calculations

Unlike the section where I did entanglement analysis, A 4-qubit system used in this section. While performing these calculations, An ansatz with different types of entanglement is used to see the effect of the selected ansatz type.

Our first ansatz we used is called full-entangled ansatz that has entanglement in between all qubits as it can be

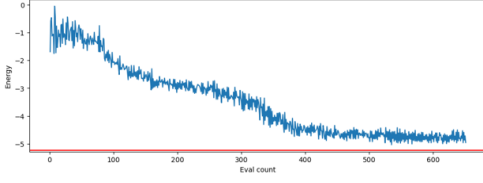


FIG. 3. This figure shows the step vs energy we have through iteration in blue line for full entangled ansatz. Red line is the exact ground state energy

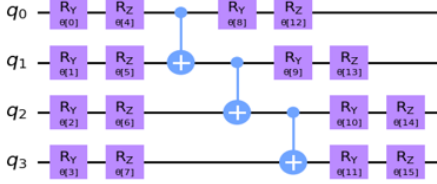


FIG. 4. Linear-entangled ansatz circuit.

in the Fig.2. The system got 0.27508 away from the exact ground state energy after the iteration as it can be seen in the Fig. 3.

The other ansatz we used is called linear-entangled ansatz that has entanglement in between qubits in linear increasing order as it can be in the Fig.4. The system got 0.27808 away from the exact ground state energy after the iteration as it can be seen in the Fig. 5.

The last ansatz we used is called circular-entangled ansatz that has entanglement in between qubits in linear increasing order and between the last qubit and the first qubit. This can be in the Fig. 4. The system got 1.93133 away from the exact ground state energy after the iteration as it can be seen in the Fig. 5.

### 3. Results

In conclusion, this application explored the 1-D Transverse Ising model using computational techniques to solve for ground state energy properties. Our investigation in the VQE via Qiskit has embodied our convergence to the ground state energy through optimization using quantum computing. As a result of the iterations in all ansatz

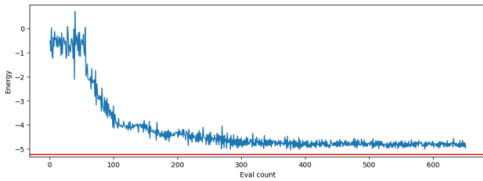


FIG. 5. This figure shows the step vs energy we have through iteration in blue line for linear entangled ansatz. Red line is the exact ground state energy

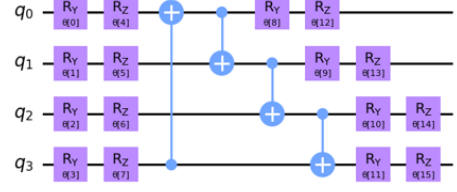


FIG. 6. Circular-entangled ansatz circuit.

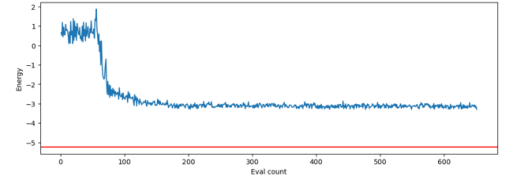


FIG. 7. This figure shows the step vs energy we have through iteration in blue line for circular entangled ansatz. Red line is the exact ground state energy

types, we saw that our energy converged to the ground state energy. In light of the results, our full-entangled ansatz achieved the closest value to the ground state energy at the end of the iteration.