Introduction to Quantum Computing
VQE applied on quantum magnetism

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Abstract

In recent years due to the hardware limitations it isn't possible to implement fault tolerant algorithms. So hybrid algorithms that leverage the properties of state of the art quantum devices are implemented. As a result things are looking up for near term applications since long coherence times aren't necessary, which is one of the main drawbacks of the NISQ era[2]. In the following literature review I will examine basic principles of variational quantum algorithms (VQA) and in particular the variational quantum eigenvalue solver (VQE) in order to estimate the ground energies of several Hamiltonian's concerning Ising models.

Contents

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1. Theoretical background

1.1 Variational algorithms fundamentals

Variational (aka hybrid) quantum algorithms can be broken down in two subroutines Fig. 1. A shallow parameterized quantum circuit that computes the expectation value of a certain observable (or a POVM in general) and a classical optimizer that minimizes a cost function containing certain parameters. The quantum circuit is known as an ansatz and defines the optimization landscape (ansatz space) in which the algorithm works on. Most of the time it is implemented via controlled rotation gates and maximally entangled systems[18]. Keep in mind that VQA's are heuristic algorithms, so the trial circuit plays a crucial role in overall success. A large set of parameters may help navigate more finely around the ansatz space or expand the haystack to find the same needle (more on that later). When it comes to the optimizer the choice of algorithm varies according to the specific use case. For ideal quantum simulators, the COBYLA optimizer is often a preferred option, whereas in the case of noisy devices SPSA is more commonly used[18].

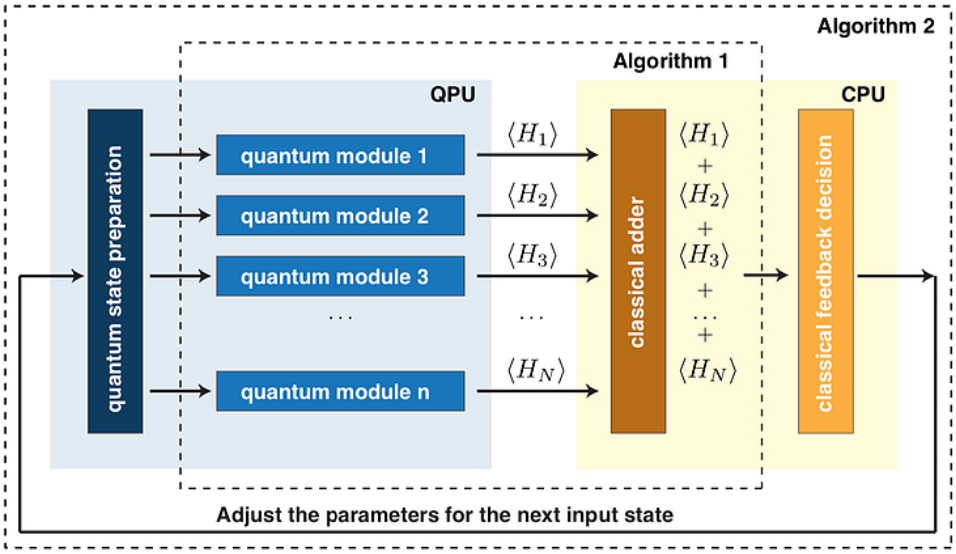

Figure 1: Schematic of the VQE which aims to minimize the energy (sum of Hamiltonian terms) by adjusting variational parameters through classical optimization. In each iteration, a quantum process (QPU) is prepared, and the expected values of the observables (one or more) are retrieved. These values are then passed through the classical process (CPU), which evaluates the cost function and updates the parameters until a convergence criteria is met. Figure adopted from [2].

1.2 The variational principal

In a more strict context the *variational principle*[16][7] is the theoretical underpinning that makes algorithms like this possible.

Definition

$$\langle \hat{\mathrm{H}} \rangle \equiv \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \geq E_0$$

The expectation value that we obtain, in every case, is an upper bound of E_0 (ground energy).

Proof Even though the corresponding to the ground state energy E_0 eigenstate isn't known, we may consider a trial state $|\psi(\vec{\theta})\rangle$ which can be expanded as

$$|\psi(\vec{\theta})\rangle = \sum_{k=0}^{\infty} |k\rangle\langle k|\psi(\vec{\theta})\rangle$$

where $\vec{\theta}$ is the vector of parameters and $|k\rangle$ is an eigenstate of $\hat{H}$:

$$\hat{\mathrm{H}}|k\rangle = E_k|k\rangle$$

The definition follows once we use $E_k = E_k - E_0 + E_0$ to evaluate $\langle \hat{H} \rangle$:

$$\langle \hat{H} \rangle = \frac{\sum_{k=0}^{\infty} \langle \psi(\vec{\theta})|k\rangle\langle k|\hat{H}|k\rangle\langle k|\psi(\vec{\theta})\rangle}{\sum_{k=0}^{\infty} \langle \psi(\vec{\theta})|k\rangle\langle k|k\rangle\langle k|\psi(\vec{\theta})\rangle} = \frac{\sum_{k=0}^{\infty} E_k \langle \psi(\vec{\theta})|k\rangle\langle k|\psi(\vec{\theta})\rangle}{\sum_{k=0}^{\infty} \langle \psi(\vec{\theta})|k\rangle\langle k|\psi(\vec{\theta})\rangle}$$

$$= \frac{\sum_{k=0}^{\infty} |\langle k|\psi(\vec{\theta})\rangle|^2 E_k}{\sum_{k=0}^{\infty} |\langle k|\psi(\vec{\theta})\rangle|^2} = \frac{\sum_{k=1}^{\infty} |\langle k|\psi(\vec{\theta})\rangle|^2 (E_k - E_0)}{\sum_{k=0}^{\infty} |\langle k|\psi(\vec{\theta})\rangle|^2} + E_0 \geq E_0$$

where the facts that $E_k - E_0 \geq 0$ (obviously equality is for $|k\rangle = |\psi_0\rangle$) have been used.

1.3 The transverse Ising model

The transverse Ising model (TIM) is the quantum analog of the classical Ising model known from statistical mechanics (and briefly discussed during the course). In a general sense, TIM is a many-body spin system with an external magnetic field acting perpendicularly to the direction of the spins. In the

majority of the cases the spins are oriented along the Z axis and the magnetic field across the X axis (as established by the Pauli observables). The model is defined[6], in terms of spin operators, by the following Hamiltonian:

$$\hat{\mathrm{H}} = -J \sum_{\langle i,j \rangle} S_i^z S_j^z - B \sum_i S_i^x$$

where i and j denote lattice sites, the subscript $_{\langle i,j \rangle}$ refers to all the nearest neighbour pairs, B denotes the external magnetic field and J nearest neighbour interactions (aka coupling). By transforming spin variables to qubit ones we obtain:

Definition

$$\hat{\mathrm{H}} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - B \sum_i \hat{\sigma}_i^x$$

This Hamiltonian possesses a $\mathbb{Z}_2$ *symmetry*[1], more specifically it's invariant under the rotation by π along the x axis:

$$R_x(\pi) H R_x(\pi)^\dagger = H$$

where $R_x(\pi)$ is the rotation operator with

$$R_x(\pi) \sigma^x R_x(\pi)^\dagger = \sigma^x$$
$$R_x(\pi) \sigma^z R_x(\pi)^\dagger = -\sigma^z.$$

The TIM has two phases (not including the gapless phase[6]) these are distinguished as the *ordered* and *disordered* one, depending on whether the value of $|B|$ conserves the previous symmetry. If $|B| < 1$ the system is said to be in the ordered phase thus exhibiting ferromagnetic properties (for $J > 0$), while the previous symmetry is broken. On the other hand if $|B| > 1$ the system is said to be in the disordered phase, it exhibits paramagnetic behavior and the symmetry is preserved. But what exactly means for the symmetry to be preserved? If the R_x symmetry is preserved then the ground state will be the same after applying the rotation. Otherwise, when applying the rotation we will end up with another state equivalent but different to the initial, this is called a degenerate energy state.

2. The ansatz and optimization loops

2.1 Ansatz structure

As discussed earlier (see 1.1) the ansatz is a very important part of VQA's implementation, because it defines the subspace in which VQE is gonna search in. Generally speaking, there are trade-offs between *speed*, *accuracy* and *noise* making essential the need for application specific ansatzes (which is an active area of research). An ansatz is a combination of two unitary operations shown in Fig. 2. The U_R operation, is not mandatory and initializes the circuit in a preferred state in order for the objective function to converge faster. Whereas, the $U_V(\vec{\theta})$ is referred to as the *variational form*[12] and it's our main interest. Some of the most general purpose ansatzes include: the N-Local and the Efficient SU2 among others.

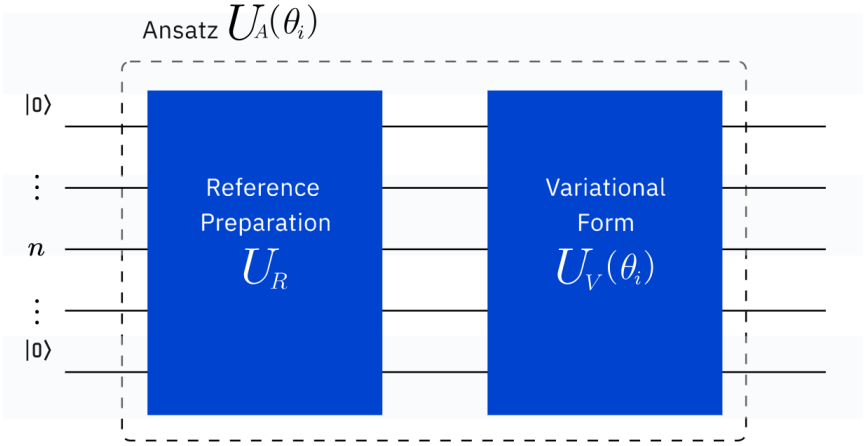

Figure 2: The abstract picture of an ansatz, constructed in general by two unitary operations. First, U_R that creates a reference state and second $U_V(\vec{\theta})$ which is to be updated in every iteration. Figure adopted from [12]

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Due to the need to be able to compare ansatzes, the need to have basic metrics[11] arises. The aspects (to describe) emerge intuitively from what we have covered up until now. In more detail, a quantitatively metric is needed to describe the noisiness of the circuit as well as one describing the overall runtime of the ansatz. Two relevant properties that express these are the *circuit depth* which is responsible for decoherence errors (and potential slowdowns) and the other is the number *entanglement gates* as a major source of error.

Another way to categorize trial circuits is either as *fixed structured* or as *adaptive structured* (from a systems perspective could be though as static and dynamic). The first are initialized at the beginning of the algorithm and are kept unchanged

ever since, not to be confused with the variational form. These include (but not limit to[11]): the unitary coupled cluster ansatz (UCC and it's extensions), the Hamiltonian variational ansatz, as well as the two mentioned earlier in this section. On the other hand, an adaptive ansatz is inherently preferred for application specific purposes since these develop along the iterative process. The ansatz could be optimized topologically by updating the gate structure of it or can expand in depth (as proposed by Harper R. Grimsley et al. [8]).

2.2 Optimizer categorization and the barren plateau

The barren plateau is an issue encountered in several optimization subroutines, both with local optimizers and global optimizers. It describes a deadlock situation under which the optimizer is unable to converge to a global minima. More precisely, this problem is associated with the risk of gradients vanishing exponentially with respect to the cost function's complexity (in other words the number of qubits). It seems that this is a downside only of *gradient-based optimizers*, which rely on gradient evaluations, surprisingly that's not the case.

Gradient-free optimizers is a class of optimization algorithms all depending on being able to distinguish cost function values at different landscape points. On the one hand, some of these are suited more for smooth (non noisy) landscapes, one well studied case of which is the Constrained Optimization BY Linear Approximation method (aka COBYLA). While on the other, there are methods such as the Nelder-Mead algorithm[3] (also applied on the original VQE paper[2]) that cope well with noise models. These have also shown to be effected by the barren plateau as demonstrated in Ref. [3].

There are applications in which we aren't able to have an appropriate picture of the parameter landscape thus a substandard set of initial parameters may lead to a inadequate solution. In such case one could utilize bootstrapping in order to reduce the overall optimization cost. *Bootstrapping* (in this context) is a process that leverages prior statistical knowledge about the problem. That could be, executing a cost efficient algorithm in order to obtain some meaningful advantage when running the main optimizer. For example, a local optimizer could be implemented at first with relatively low cost (possibly converging to a local solution) and afterwards pass it's optimal parameters as initial ones into a global optimizer, as a result boosting the main optimizer.

Continuing our overview of optimization routines, another class of optimizers with demonstrated capabilities in the VQE context are the gradient based optimizers. A remarkable mention is the *quantum natural gradient descent*[19] optimizer which is a variant of the typical gradient descent (GD):

$$\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla J(\vec{\theta}_i)$$

where J is the objective function that we try to minimize and η is the learning rate. The main idea is that while in basic GD the learning rate is related to the Euclidean distance in the parameter space, this distance shouldn't be equivalent for

different parameters because these can vary in different rates. In natural gradient optimization this distance has been replaced by the notion of the *Kullback-Leibler divergence* which in simple words describes how to probability distributions differ from one another (for additional reading see Ref.[19]).

3. Applied VQE

In this section I manage to carry out some simulations by utilizing the Qiskit Runtime service and Pennylane SDKs provided by IBM and Xanadu respectively. Based on a recent publication[10] the `ibm_qasm_simulator` is one of the better choices out there. Nevertheless in some cases Pennylane's general purpose `default.qubit` simulator is utilized, due to it's easy of use. The goal is to demonstrate a quantum advantage for otherwise resource consuming problems. No code is contained in this report, but such files can be provided upon request.

3.1 The 3D transverse Ising model

At first we look at the application of VQE in order to approximate the ground state energy of a cube lattice, whose Hamiltonian follows the TIM. The lattice (Fig. 3) is defined by the following Hamiltonian:

$$\hat{\mathrm{H}} = -\sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \frac{1}{4} \sum_i \hat{\sigma}_i^x.$$

As a note, same methods can of course be applied in different lattice patterns with different complexity. In this case, where every one of the eight lattice sites is mapped to a qubit, there will be $2^8 = 256$ basis states (in the computational basis), so the Hamiltonian will be a 256×256 square matrix.

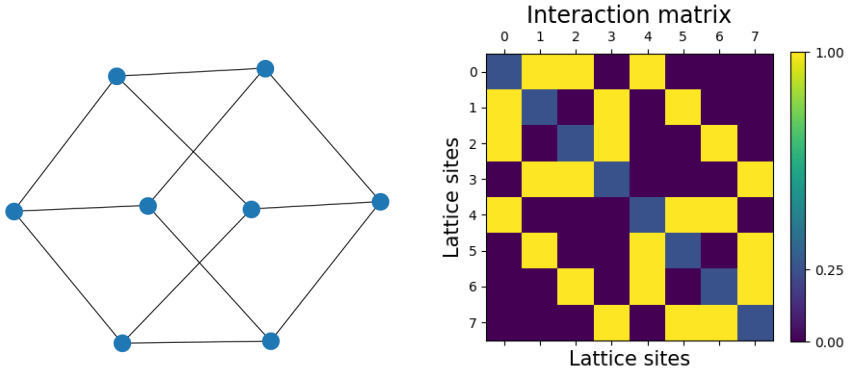

Figure 3: A 3 dimensional lattice with uniform particle interactions and open boundary conditions. On the **left** a simple network representation. On the **right** a graphical representation of the interaction matrix, note that the on-site interactions denote the transverse field.

In the first experiment used the COBYLA optimizer as it is a common choice among noiseless applications. The initial parameters are generated uniformly at random

$$0 < \theta_i < 1, \quad \forall \quad \theta_i \in \vec{\theta}$$

thus starting for sure with sub-optimal parameters while these are explicitly bounded them between -1 and 1. In order to have a point of reference the exact solution is computed by approaching the problem as a basic eigenvalue one. The ansatz of choice (see Fig. 4) consists of alternating rotation and two qubit entanglement layers with 3 repetitions in total. The entanglement strategy is refereed to as "`reverse_linear`"[9], this constructs an equivalent correlations as the "`full`" but with a shallower circuit. The rotation layers perform rotations along the Y axis only, thus not contributing to any imaginary part of the amplitude. The assumption has been made that this idea suites our use case since we are mapping fermions to qubits which don't present imaginary spins. Note that the ansatz is completely parameterized since a reference state isn't included.

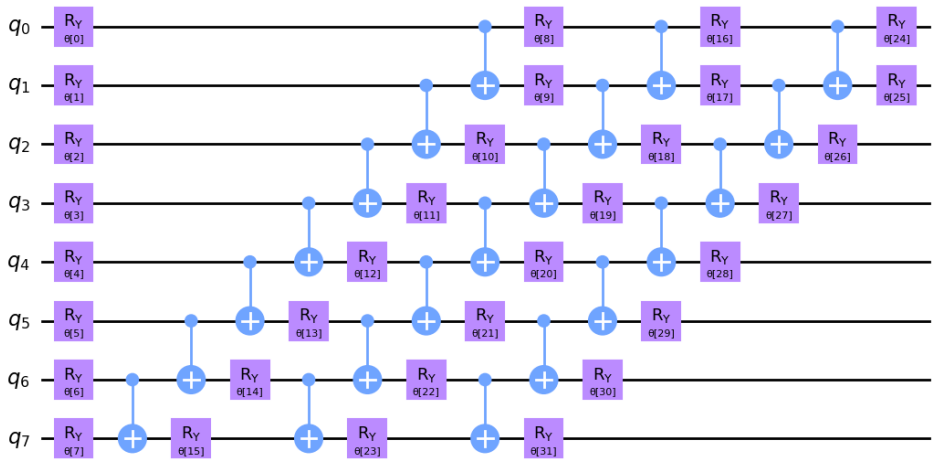

Figure 4: The variational circuit of choice with control-X as entanglers and R_θ in the rotation blocks in order to preserve only the real amplitudes. Shots per data point: 1000.

The result (see Fig. 5) obey the variational principal despite the notable fluctuations related to the variance. In addition, as it is clear the algorithm pretty much converges to the exact value after the passage of 100 iterations and one can say with confidence that it will continue to do so. This simulation was implemented on the the IBMQ cloud and serves as a first example.

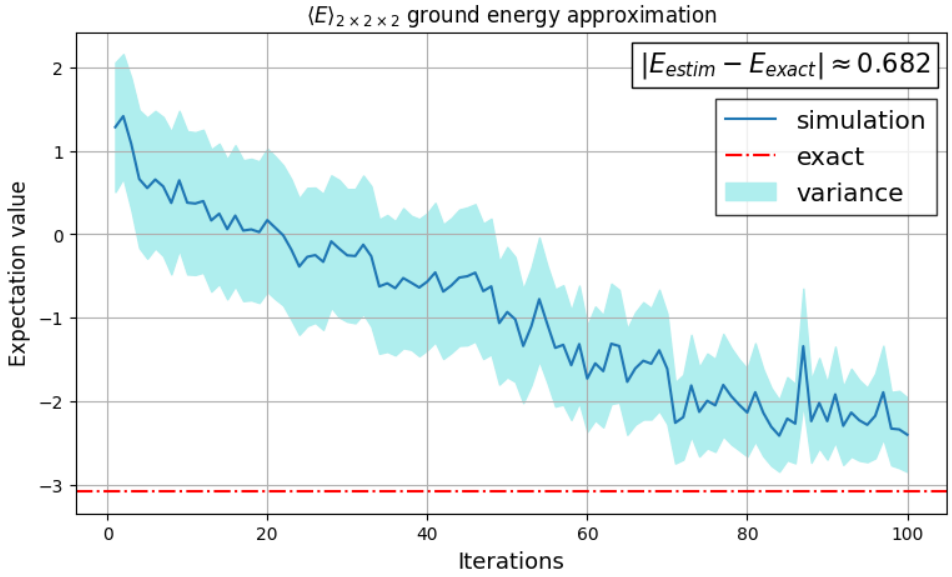

Figure 5: Expectation ground energy evolution of the Fig. 3 model with 1000 per data-point/experiment, implemented on the noiseless `ibmq_qasm_simulator`. At the top right a comparison between the last estimate and the exact energy has been made.

As a theoretical note, the overall implementation is based scenes the grounded energy is negative thus characterizing a bound system. Now comes the question on if and how this implementation can be improved. One may think to apply more sophisticated parameters, indeed we can do so and fast-forward the algorithm (and converge in the same way even prior to 30 iterations), but that's a subjective advantage since for different field intensities the Hamiltonian will differ significantly. Instead, quantum natural gradient descent (QNGD) is incorporated which was shortly mentioned above.

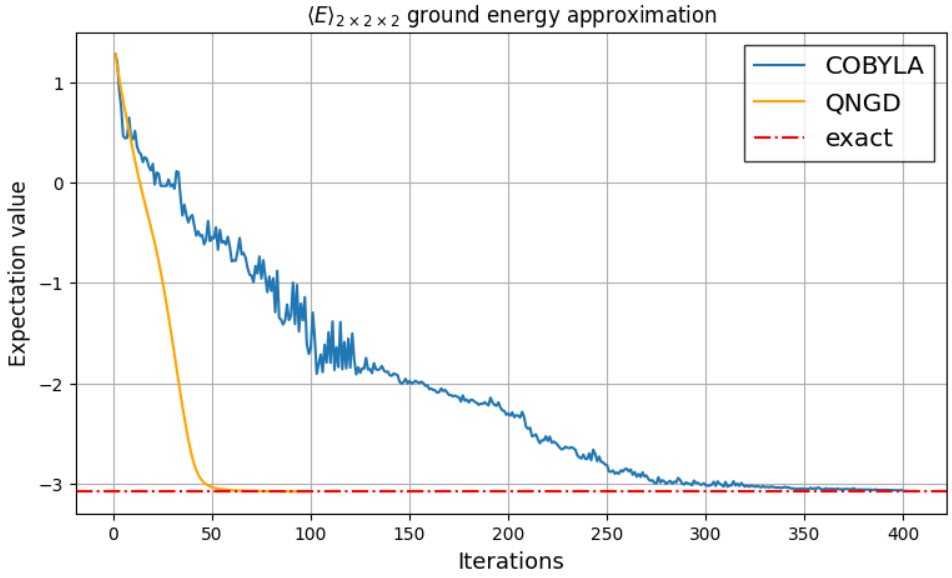

Figure 6: Expectation ground energy evolution of the Fig. 3 model implemented on the noiseless `default.qubit` simulator. The step size of the QNGD was 0.14 .

Looking at the outcomes (see Fig.6) of the two optimizers comparison are really clear. The gradient based optimizer converges significantly faster than COBYLA showcasing a substantial advantage of QNGD in some particular cases. Based on my intuitive understanding this is the case for relatively smooth landscapes where a local optimizer, with a quit generous step size (as the case here), will converge much faster compared to a global one which by definition takes a more rounded approach. Furthermore the same approach has been followed to leverage VQE in order to estimate the ground energy for different values of h (see Fig. 7). The algorithm utilizes some form of bootstrapping, in particular it starts with a random guess and as it evolves takes the optimal parameters from the previous data point as initial ones. The ground state energy decreases as the transverse field intensifies, proving that the system gradually gets more dependent to the field.

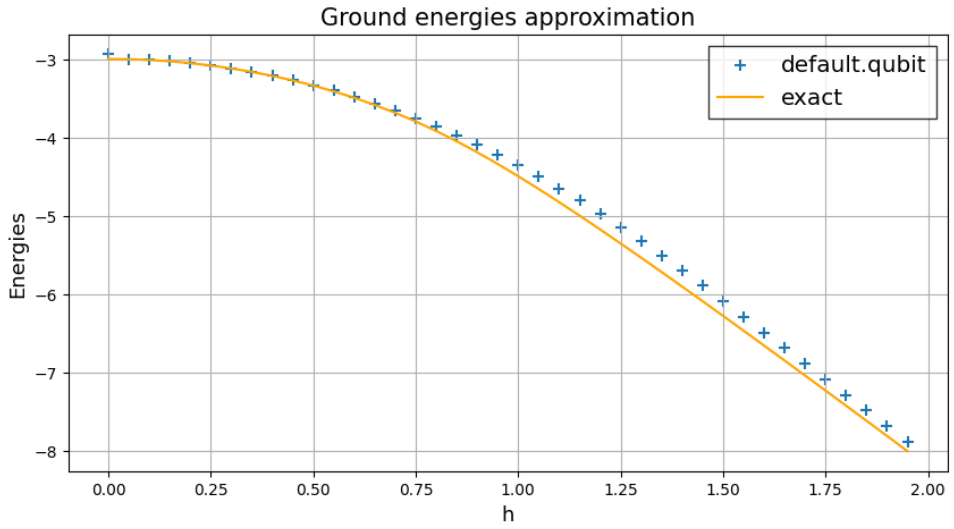

Figure 7: The ground energies of the lattice (see 3) approximated with VQE. The COBYLA optimizer was used with 250 iterations per data point.

3.2 The 1D quantum phase transition

As mentioned earlier the TIM undergoes a quantum phase transition, for relatively small fields it presenting ferromagnetic properties which convert to paramagnetic ones as the magnetic field increases. Calculating the critical point of this transition is beyond the scope of this review. However the study of such phase transitions in one dimension, is common among literature (and similar reviews). So in order to present that let's consider the following lattice with periodic boundary conditions.

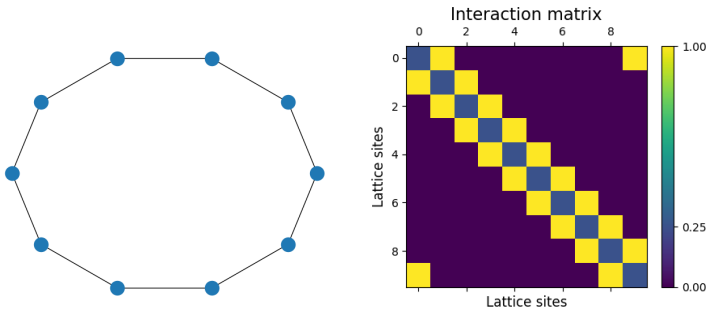

Figure 8: A 1 dimensional lattice with uniform particle interactions and periodic boundary conditions. On the **left** a simple network representation. On the **right** a graphical representation of the interaction matrix, note that the on-site interactions denote the transverse field.

Guided by similar literature[1] I noticed the phase transition taking place for $h \in [-1, 2]$ approximately. To be more detailed I followed the same procedure as in Fig. 7 to find the state of the ansatz in which the energy is the lowest and there I calculated the following expectation value:

$$M_x = \langle\psi| \sum_i {\sigma_i}^x |\psi\rangle$$

Intuitively speaking I was waiting for the expectation value to be negative after the transition, since that the spins should anti-align in order for the system to be in the ground state and as the field increases it would be more difficult for the particles to be in an excited state. In fact that's the case, as we see in Fig. 9. On the other hand M_x is positive prior to the transition, meaning that the magnetic moments align with the field, thus underlining the ferromagnetic behavior of the model.

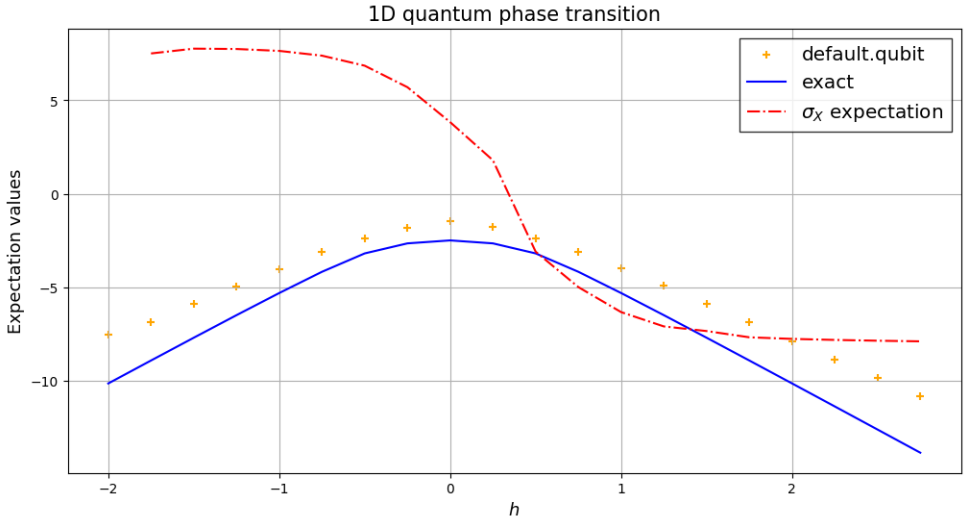

Figure 9: The quantum phase transition of the Fig. 8 lattice based on ground energies approximation executed on the `default.qubit` simulator. COBYLA was used with 250 iterations per data point.

3.3 VQE for the Kagome lattice

The Kagome structure is a more peculiar lattice structure often encountered in condense matter physics. In the simple form it's intriguing geometric is includes triangles arranged in a hexagonal pattern. In this review I undertake a lattice (see 10) with 2 rows, 2 colons and periodic boundary conditions, which is inherently resource consuming to study on a typical computer.

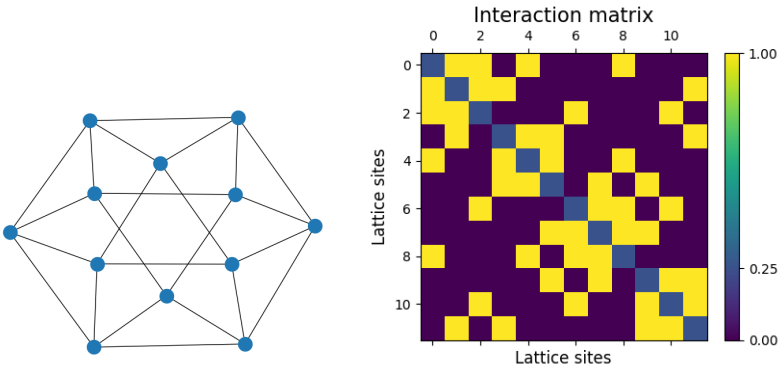

Figure 10: A 2×2 Kagome lattice with uniform particle interactions and periodic boundary conditions. On the **left** a simple network representation. On the **right** a graphical representation of the interaction matrix, note that the on-site interactions denote the transverse field.

At first I implemented VQE with a parameterized circuit including only rotations along the Y-axis (aka real-amplitudes) as done in previous cases. Although this didn't went very well as the algorithm converged in a local minima after several attempts to bootstrap it on previous parameter knowledge. Continuing, the obvious though was to implement a different ansatz, a common choice among similar reviews[17] is the Efficient SU2 which groups special unitary matrices of choice in groups of 2 per circuit block int his case I tried implementing this circuit under two cases: one with (σ_y, σ_x) and another with (σ_y, σ_z) as the SU2 pairs. However these circuits showed small differences from the initial with no notable performance improvement.

Afterwards, based on the fact that (regardless of the magnetic field), in the ground state the spins would be anti-aligned across the x axis, so it will be of our interest to add a reference block to the initial ansatz. So at the start of the circuit I added a σ_x gate every other qubit and I achieved the following improvement.

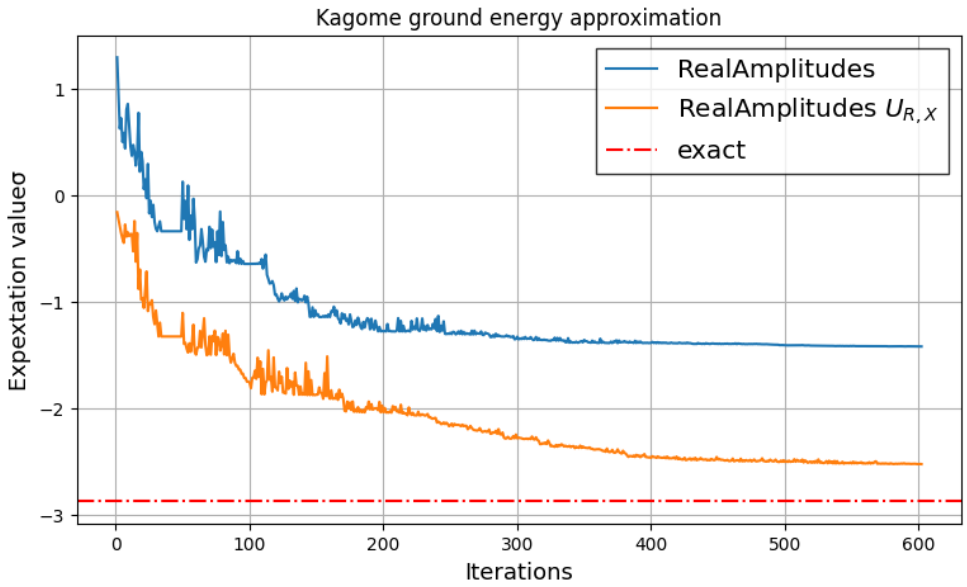

Figure 11: Simulation for the ground energy of the Kagome lattice (see 10) on the `default.qubit` and with COBYLA optimization. Both implementations converge to a local minima although the one with the reference stage clearly outperforms the initial.

A The Jordan-Wigner mapping

On this appendix I will make a short reference to the Jordan-Wigner (JW) mapping, as it is an essential concept in particle physics. This mathematical procedure (introduced in 1928) basically maps basically fermions to spin particles and vice versa. More in depth, in natural sciences many times problems are modeled with fermionic relations. In second quantization (see Ref. [5]) fermions are described in terms of creation and annihilation operators which act on the occupation number of the system, the JW transformation maps these onto our known Pauli spin operators.

Operator mapping

$$\sigma_j^+ = \frac{\sigma_j^x + i\sigma_j^y}{2} \equiv f_j^\dagger$$

$$\sigma_j^- = \frac{\sigma_j^x - i\sigma_j^y}{2} \equiv f^j$$

$$\sigma_j^z = 2f_j^\dagger f_j - I$$

Where the subscript $_j$ refers to different lattice sites, the σ^+ and σ^- are the raising and lowering operators respectively, while $f^\dagger$ is the creation and f the annihilation operators. Similar transformations can be applied between fermions and bosons (see Ref. [13]). In the case of quantum computing the fermion to spin transformation comes in hand in order to construct a spin Hamiltonian. Another useful transformation is the Bravyi-Kitaev mapping.

B Thoughts for additional study

In this literature review I gave an overview of the variational quantum eigensolver - although in many cases I followed a trial and error approach in order to cover a large area of latest research, as a result there is a great possibility for further investigation! Outside quantum magnetism (which is a whole science itself) there are several topics I did not cover including but not limited to: noise mitigation, different ansatzes, more theoretical background and measuring strategies. Especially on the ansatz part, I believe that there are few people that have an actual deep understanding of ansatz selection and construction, in this case theoretical avocation would be advised. As an instance, for the last part with the Kagome lattice the novel[15] Hamiltonian variational ansatz has shown great results[4].

Glossary

ansatz

An educated guess for the trial state of an optimization problem often described by a parameterized circuit. 3

boson

Group of elementary particles that describe interactions and have integer spins. 16

bound system

A physical system which is subject to a potential such that the particle has a tendency to remain localized in one or more regions of space. 10

creation and annihilation operators

In quantum field theory and in particular second quantization[5], these operators are introduced to add and remove a particle from the many-body system. 16

decoherence

The physical process of state "relaxation" from a non-ground state to a lower energy one. 6

degenerate energy state

Is an energy level to which two or more states are related. 5

fault tolerant algorithm

An algorithm is characterized as such if it's circuit depth is comparable to the computers coherence time. 1

fermion

Group of elementary particles that constitute matter, have odd number half spins and obey the Pauli exclusion principle. 9, 16

ferromagnetic

In contrast with paramagnetism, ferromagnetism is the property due to which certain structures are strongly attracted to a magnetic field. 5

global optimizer

These optimizers act on several subspaces in parallel thus making them relatively independent by the initial values. 7

gradient-based optimizer

These optimizers operate with the principal of evaluating the gradient of the cost function at different points and work their way along the landscape based on the sign. 7

gradient-free optimizer

These optimizers tend to be more robust compared to the gradient-based ones, although they seem to be more resource demanding[12]. 7

local optimizer

These optimizers act on a singe subspace at a time thus are heavily depended on the initial points. 7

NISQ

The Noisy Intermediate-Scale Quantum era is the current state of quantum computing characterize by limited hardware capabilities. 1

observable

A physical property described by an operator. 3

occupation number

Is a fundamental idea in second quantization[5], it denotes the number of particles in a certain state, thus making it unnecessary to label it's particle. 16

paramagnetic

The property due to which a structure is weakly attracted to a magnetic field. That's because the orientation of the dipoles relative to the field is practically random[20]. 5

POVM

A generalized mathematical notion of measurement[14]. 3

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