The Transverse Ising Model: Exploring ground states and phase transitions with quantum eigensolvers

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We use a variational quantum eigensolver to explore the ground state behavior of the 1D Transverse Ising model. Some of the expected phase transitions are recovered.

I. INTRODUCTION

a. ***Quantum Simulation*** One of the first proposed applications of quantum computing is to simulate other quantum systems.[1–3] Quantum systems are difficult to simulate classically - in general, without approximations or special cases, the amount of resources required to classically simulate a quantum system grows exponentially with the number of degrees of freedom. [4] This is because a classical computer must keep track of the exponential number of terms in a general superposition state (or density matrix) - in contrast, a quantum computer naturally supports such superpositions, and one might hope to find algorithms with only linear resource scaling.

Simulation is not the only classically hard problem which is thought to be quantum easy. [5] Another example is integer factorization, a problem which is of great interest but which is believed to be classically hard, while admitting an easy quantum solution. [6] However, factoring integers large enough to be of interest will require at minimum several thousand logical qubits, which appears beyond the reach of near-term quantum computers. [7] Furthermore, because of the discrete nature of the problem, error rates are required to be low - which will probably incur addition overhead to implement error correcting codes, such as surface codes. [7]

Quantum simulation, on the other hand, is expected to be easy for many systems (including, importantly, local Hamiltonians, such as those only including nearest-neighbor and next-nearest-neighbor interactions). [3] In fact, not only do we obtain favorable scaling laws, but it is likely we will find interesting applications well before the widespread availability of thousand-qubit computers. A quantum computer with only tens of qubits might outperform modern simulations, and the error tolerance for these applications is likely much higher than in number-theoretic algorithms like Shor's. [8]

b. ***The Eigenproblem*** A (hermitian, finite-dimensional) quantum system is specified by a Hamiltonian, H, which is a hermitian matrix acting on a vector representing the state of the system, $|\psi\rangle$. While far from describing the full dynamics of a system, one of the first interesting questions to answer is: What is the ground state of this system? That is, what state, $|\psi_G\rangle$, minimizes the energy of the system, given by

$$E = \langle\psi| H |\psi\rangle$$

It is instructive to note that $|\psi_G\rangle$ must be an eigenvalue of the system - we denote its eigenvalue E_G. Therefore, one way to find the ground state (and the associated ground state energy) is to diagonalize H. However, full diagonalization is generally computationally expensive. Algorithms which find only the lowest or first few eigenvalues / eigenstates, such as the Lanczos algorithm [9], are faster, but still suffer from the exponential growth of the state space. Quantum computational approaches exist when the states of the system can be represented faithfully on a series of qubits. In general, this is a non-trivial problem, but such a representation always exists[3]. For spin systems the physical system is already in the form of qubits, so such a representation is trivial.

One of the first quantum approaches to solving this problem was quantum phase estimation (QPE). [10, 11] QPE assumes a starting state which has non-trivial overlap with the ground state. The state is then time evolved, using the time-evolution operator $U = e^{iHt}$, and the resulting time dependence of the state is fed into a quantum fourier transform (QFT). The QFT (after proper measurement) then returns information about the frequencies present in the time behavior, which are precisely the energy eigenvalues. This algorithm takes advantage of the fact that local Hamiltonians can be efficiently simulated (which is not true of general unitary operators!) and often has very good scaling. However, since this algorithm aims to coherently time evolve the system, the underlying qubit architecture requires long coherence times - requiring thousands or millions of gates between initialization and measurement. [4] Therefore this algorithm, while powerful, seems out of reach for near-term quantum computing hardware.

c. ***The Variational Quantum Eigensolver*** An alternative algorithm, called a Variational Quantum Eigensolver (VQE), is designed to work around the limits of near-term quantum computers. By representing the ground state as a minimization problem instead, one uses the quantum computer only to prepare and measure the energy of a state - which can be done efficiently - and a classical optimizer to search for the ground state. [12] Classical optimization is well understood and algorithms for it are widely available, but it requires a continuum of ansatz states parameterized by classical variables.

In particular, let us assume we have defined a continuum of states, $|\psi(\hat{\theta})\rangle$, parameterized by a vector of classical variables, $\hat{\theta}$. We can then define our optimization

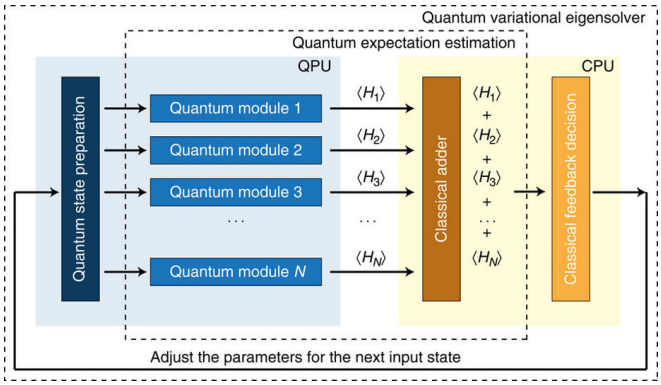

FIG. 1. A helpful diagram of the Variational Quantum eigensolver, borrowed from the 2014 original paper. [12]

as

$$E_G = \min_{\hat{\theta}} \langle\psi(\hat{\theta})| H |\psi(\hat{\theta})\rangle$$

This can be separated into two parts - the evaluation of $\langle\psi(\hat{\theta})| H |\psi(\hat{\theta})\rangle$, which is done quantum-mechanically, and the minimization, which is done classically.

Clearly, this minimization will only work if $|\psi(\hat{\theta})\rangle$ becomes (or approaches) the ground state for some value of $\hat{\theta}$. This means we will have to know something about our problem, at least enough to guess the states of interest. The more we know, the fewer variables we will need to parameterize the state, and the better our classical optimization results will be. Furthermore, like most optimization problems, the energy will likely be non-convex, with many local minima and a rich feature-scape. We must be careful not to let our optimization get trapped by these minima - which requires either a close guess of the starting parameters or many (random) starting positions.

Despite these caveats, if enough is known about the system, it is possible to run this algorithm to great success on currently available hardware. Ground states of simple molecules have been found using re-programmable photonic quantum processors [12], and more recently these results have been repeated on superconducting chips [13] We turn our attention, however, to another system, for which analytical solutions exist but for which the authors could find no published results from VQE simulations.

d. ***The Transverse Ising Model*** The basic Transverse Ising Model (TIM) assumes a lattice of spin-1/2 particles, on which the Hamiltonian is

$$H = -h\sum_i \sigma_i^z - J\sum_{\langle i,j\rangle} \sigma_i^x \sigma_j^x$$

Where $\sum_{\langle i,j\rangle}$ is taken over all nearest neighbor pairs. This represents spins with nearest neighbor lateral coupling, J, in an external field of strength h. In our simulations, we will also assume periodic boundary conditions.[14]

It is known that quantum phase estimation of the Transverse Ising model will scale polynomially in the number of spins, but exponentially in the precision. [15, 16] Trapped ions have been used to simulate frustration in the 2D TIM using a QPE algorithm, but this was only achieved for three spins. [17] The zero-temperature (quantum) phase transitions of this systems are known, for both 1 and 2 dimensions. [16] Since h and J are the only energy scales in the problem, the phase transitions occurs as a function of the dimensionless parameter $g = \frac{h}{J}$.

Spin models like the TIM are the basis of many fermion models, and since there is a natural direct mapping onto qubits it seems like a good candidate for quantum simulation on near-term hardware.

II. SETUP

a. ***QISKit*** In our simulations, we make use of the QISKit development environment provided by IBM.[18] An example VQE is provided with the package, which is a variation of that used to calculate bond lengths of small molecules[13, 19]. This example was used as the basis of the VQE for our simulations; the only major algorithmic change was the optimizer (as described below).

QISKit is designed to be portable between simulator backends and actual quantum hardware. While IBM does provide public access to their devices, the limitations of the publicly available devices, as well as limitation of the API and the large wait times involved, make it infeasible to currently run these algorithms on quantum hardware. However, the simulator provided with the package is sufficient to recapture the expected behavior of the system, as it simulates both the quantum mechanically expected behavior of the system and realistic errors that occur in experimental chips.

b. ***Spin Waves*** Since the Transverse Ising Model describes a lattice of spins with local interactions, a basis for the wavefunctions can be written as tensor products of spins, s_i, on lattice sites indexed by i. In particular, an obvious guess for the states of interest would be x-z spin waves, which are parameterized by

$$|\psi(\theta,\omega)\rangle = \bigotimes_i cos(\frac{\theta+\omega i}{2})|0_i\rangle + sin(\frac{\theta+\omega i}{2})|1_i\rangle$$

This describes a lattice of spins which rotate their spin in the $x-z$ plane of the Bloch-sphere as one moves along the lattice. The rotation moves from an initial offset at $i = 0$ at a constant rate. This simplistic ansatz is sufficient to capture the expected behaviors in 1-D. Of course, in a real problem of interest, a more general ansatz might be used - which allows for rotations into the y direction and non-constant rotations, as well as superpositions of these states. An important point to note is that this wavefunction is entirely separable, and so can actually be efficiently classically simulated.

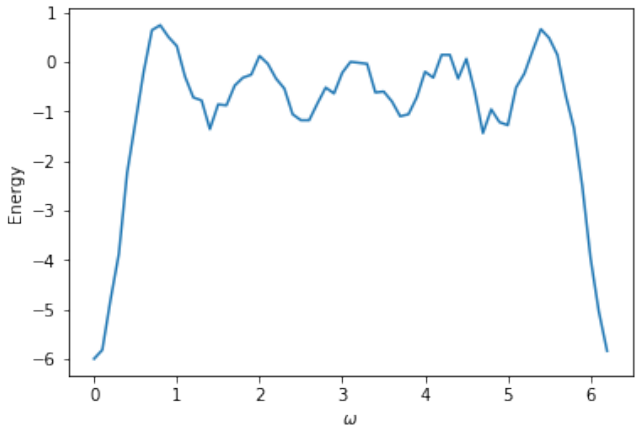

FIG. 2. One slice of the potential energy landscape for $h = 1$, $J = 0$. This is the cut corresponding to $\theta = 0$ on a six qubit chain.

c. ***Evaluating the Hamiltonian*** Evaluating the expectation of the Hamiltonian is simply equivalent to evaluating each individual term in the Hamiltonian.

$$\langle H \rangle = -h \sum_i \langle \sigma_i^z \rangle - J \sum_{\langle i,j \rangle} \langle \sigma_i^x \sigma_j^x \rangle$$

This can be performed by simply measuring each of these Pauli operators on their respective qubits. Note that measurements of individual terms will require averaging over many shots of measurement. Furthermore, because σ^x measurement requires a rotation followed by σ^z measurement, we expect lower fidelity from these measurements, and even more so from two-Pauli measurements. Therefore, we naively expect the $\sigma_i^x \sigma_j^x$ term measurements to be more prone to errors than the σ_i^z measurements.

Except where noted otherwise, measurements of this kind are averaged over 100 shots, which appears sufficient for good convergence.

d. ***Optimization*** While the QISKit example used a stochastic gradient descent algorithm, we expect a more complicated energy landscape with many local minima. As an example, a cut of the landscape for $h = 1$, $J = 0$ on a six-qubit chain is included in FIG. 2. This cut represents the energy for various values of ω, assuming that $\theta = 0$.[20] It includes the global minimum at $\theta = \omega = 0$, but also several local minima (at least in the ω behavior). Therefore, we use a Nelder-Mead simplex method, similar to the original photonic processor experiment, which is expected to be more well behaved in these situations.

III. RESULTS

a. ***1-Dimensional Ferromagnetic Ordering*** In 1 dimension, we analyze a 4 qubit chain with ferromagnetic coupling, $J > 0$. As the parameter $g = h/J$ is swept

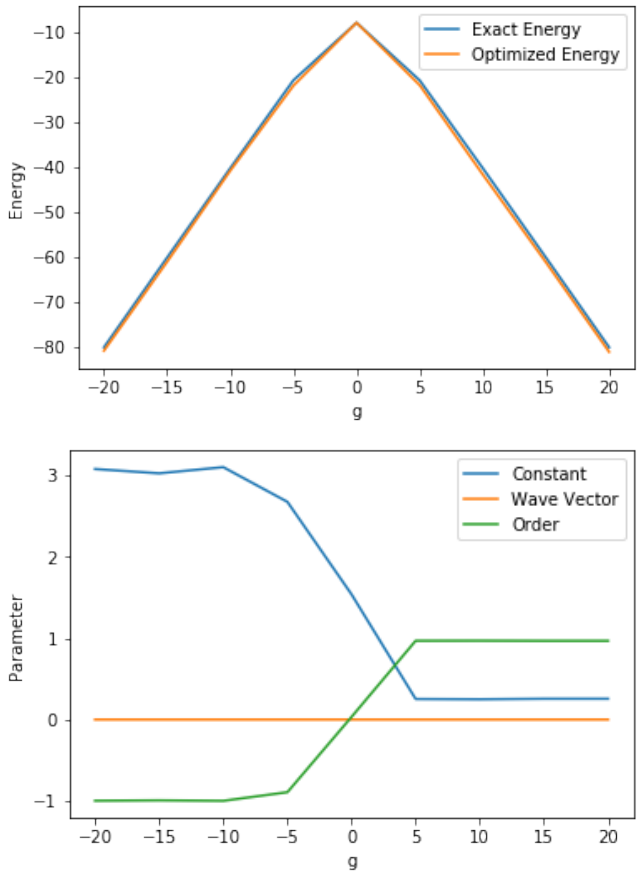

FIG. 3. Results from a 4 qubit chain with ferromagnetic nearest neighbor coupling. All energies are normalized so $|J| = 1$, and θ, ω, m are labeled as constant, wave vector, and order, respectively. As the external field, g, moves from $-\infty$ to ∞, the expected magnetization flip occurs. *Color online.*

from $-\infty$ to ∞, we expect a transition in the ground state from $|\psi_G\rangle = \bigotimes_i |1_i\rangle$ to $|\psi_G\rangle = \bigotimes_i |0_i\rangle$. These states correspond to our spin wave functions with $\theta = \pi$ and $\theta = 0$, respectively, both with $\omega = 0$. For intuition, we also we also define an order parameter, m, defined by

$$m = \langle \sigma_i^z \rangle$$

where the expectation value is taken both quantum-mechanically and over the qubits. This order parameter can be viewed as a classical magnetization, although we caution that this is not the only form of order in the system. We expect this order parameter to transition from -1 to 1 over the course of this alignment flip.

We report the results of our optimization, including both the optimized ground state energy (E_G) and the optimized wave function parameters (θ, ϕ), in FIG. 3 We also report the exact ground state energy (calculated through full diagonalization) and the order parameter corresponding to the optimized parameters. The expected behavior is recovered, and the optimization appears to be well-behaved based on the close match in energies. This result would have been easy to guess naively,

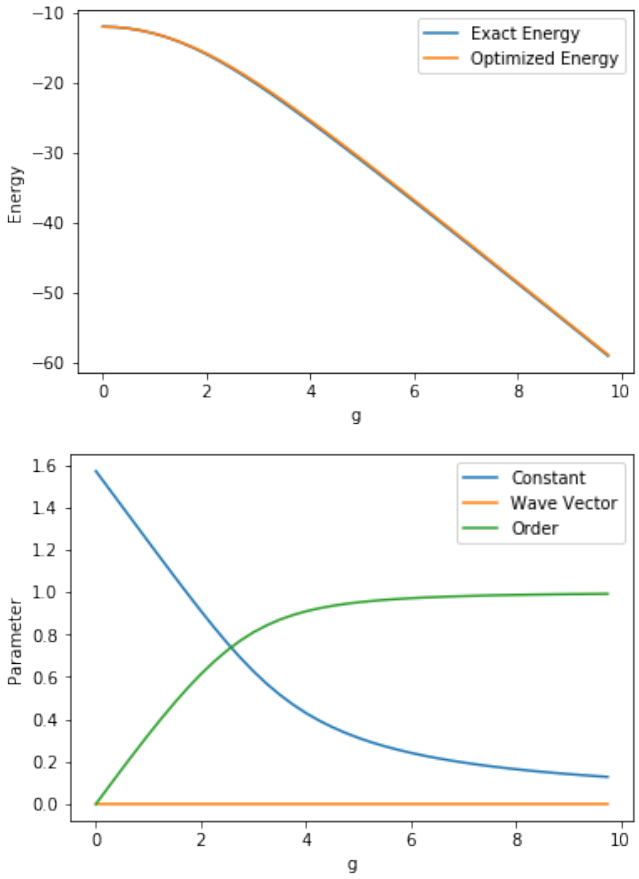

FIG. 4. The expected ferromagnetic phase transition is recovered, but required the elimination of measurement errors

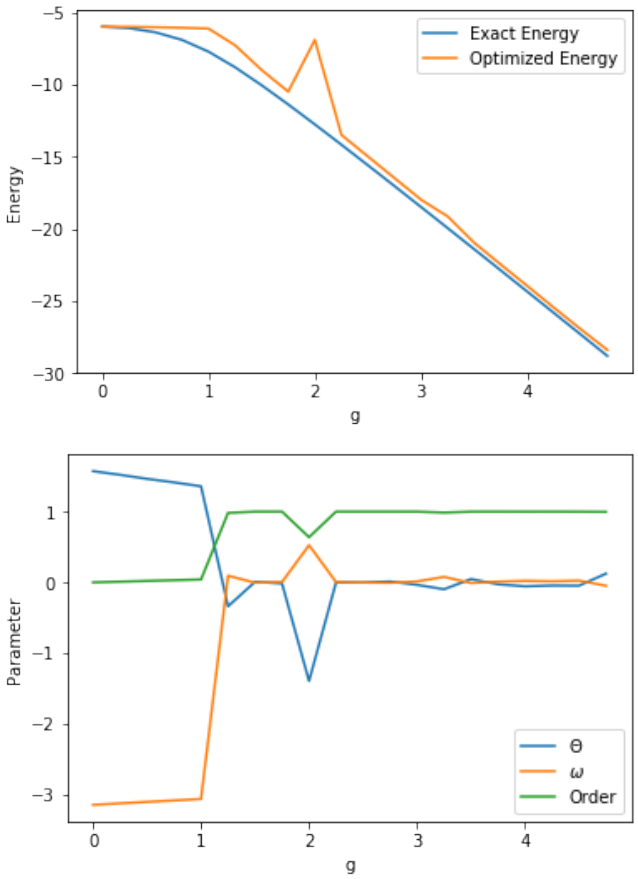

FIG. 5. The antiferromagnetic phase transition. Note that $\omega = -\pi$ is equivalent to $\omega = \pi$

but is still instructive. The optimized ground state energy sometimes drops below the exact ground state energy, which is of course physically impossible. This points to significant measurement errors - which appear to be on the order of J (with little h dependence). This agrees with our earlier intuition that measurement errors will be dominated by the $\sigma_i^x \sigma_j^x$ terms.

A more interesting transition occurs between $g = 0$ and $g >> 1$, where we expect a transition from x-direction ferromagnetism to z-direction alignment. These correspond to $\theta = \pm\pi/2$ and $\theta = 0$, respectively, and therefore $m = 0$ and $m = 1$, again with $\omega = 0$. This transition was more difficult to capture - initial attempts failed, likely due to the energy closeness of multiple states and measurement errors (c.f. FIG. 6, 7, after the bibliography). Since each parameter run was seeded with the optimized parameters from the previous, if the previous state was still low in energy and far away from the new ground state, it is likely to change only slowly. This is compounded by the fact that measurement errors cause the optimizer to be more susceptible to false minima.

This problem can be avoided by increasing the accuracy of measurement. For our purposes, we turn off measurement error for further simulations - but in actual experimental scenarios, one would either have to take more measurements or improve them. It also helps to take a finer sampling of g, which causes the correct parameters to change more slowly. We report the corrected transition in FIG. 4, where the simulation is run on a six qubit chain. Note that, because of our small system size, the transition is not very sharp, but the expected behavior is still recovered.

b. ***1-Dimensional Anti-Ferromagnetic Ordering*** We also here report results for anti-ferromagnetic coupling, $J < 0$, with the redefined $g = \frac{h}{|J|}$, on a six qubit chain. Here we expect a transition from anti-ferromagnetic x waves, corresponding to $\theta = \pi/2$, $\omega = \pi$, at $g = 0$, to the same $g >> 1$ behavior of z-alignment, with $\theta = \omega = 0$.

This behavior was even more difficult to recover than the ferromagnetic transition, likely due to the additional change in ω as well as θ. In addition to turning off measurement error and taking a fine sampling of g, we randomly seeded the parameters multiple times and took the lowest energy fit. To compensate for multiple fits, the number of optimizer iterations was reduced, which generally meant poorer convergence.

Still, the correct behavior is clearly recovered and we

declare the fit a success.

IV. DISCUSSION

The VQE does come with several caveats. It requires many repetitions of the circuit, and high fidelity measurements, which mean hardware considerations will become a factor. It also struggles precisely in the scenarios of interest, where there are competing ground states of greatly different character. Furthermore, we must know something about the states of interest to be able to efficiently parameterize them with classical variables, and we require that the states are able to be prepared efficiently using available gates - which may not always be possible and may defeat the scaling advantages over classical algorithms.

However, the VQE still seems to have great potential. Non-trivial ordering such as AFM spin waves are of great interest to the condensed matter community. The simulator used here could not handle more than about 8 spins on our hardware, which is not much smaller than more serious computational efforts (reaching at most 10-15 lattice sites). Given that chips with dozens of high-fidelity qubits seem on the horizon, it is possible that algorithms such as the variational quantum eigensolver will push simulations forward significantly.

Architectures such as photonic chips seem naturally suited to this, as they have high clock rates, can be reconfigured in hardware (almost like a quantum FPGA), and can be run at low cost at room temperature. General purpose quantum computing architectures, such as superconducting qubits and ion traps, seem less well suited, as they require much more significant hardware efforts for not much better results. Given the rapid advancement of quantum photonic processors[21], both in miniaturization and fidelity, it does not seem wildly optimistic to imagine something like a quantum co-processor, assisting powerful classical computers in simulating these systems to a high degree of accuracy.

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[5] Here we do not rigorously define these terms, but an easy (hard) problem is roughly one in which the required resources/time scale polynomially (exponentially) with the system size.

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[19] `https://github.com/QISKit/qiskit-tutorial/blob/master/reference/approximate/quantum_chemistry.ipynb`.

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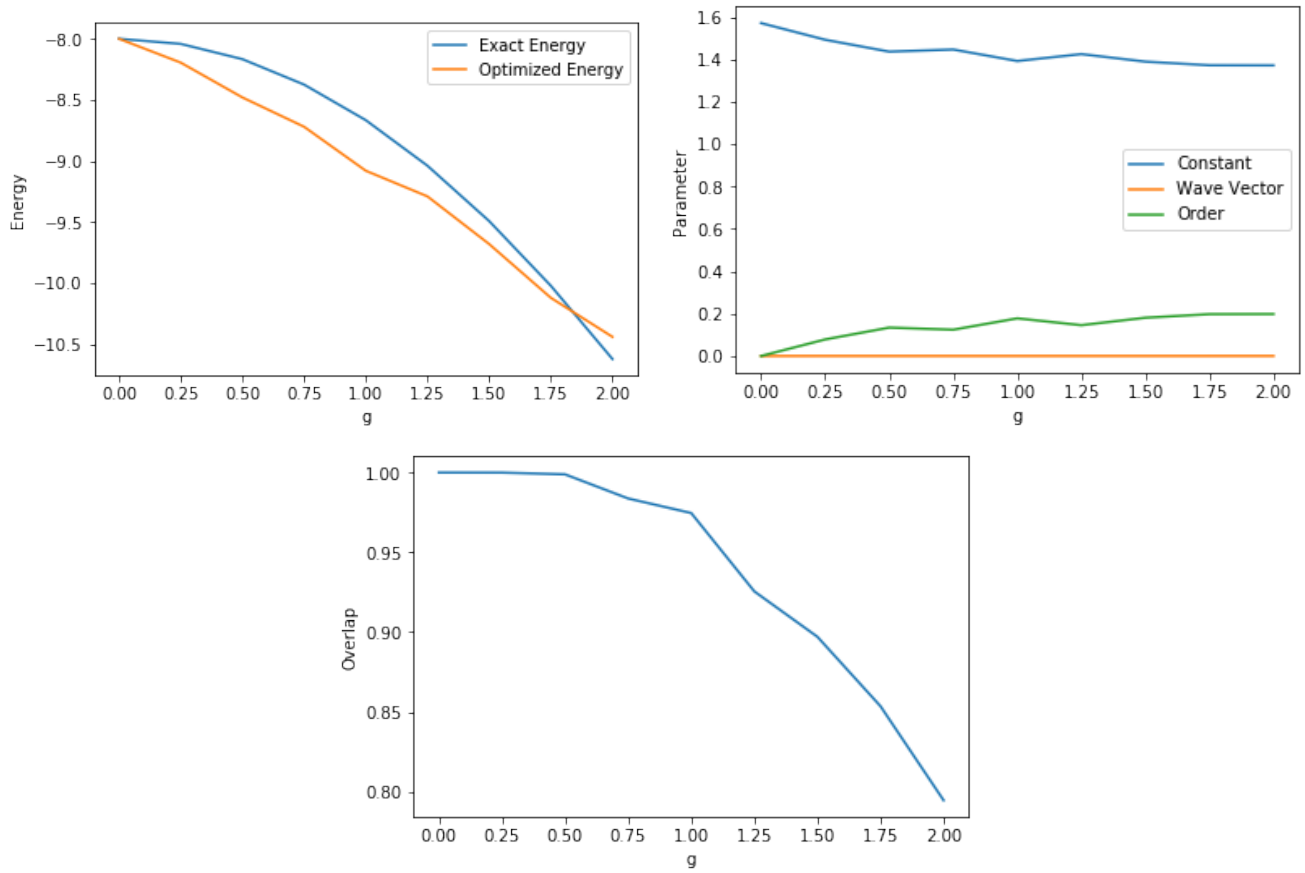

FIG. 6. Example of a bad fit to the ferromagnetic transition. This was likely due to measurement errors, causing the optimizer to fall into a false minimum. We also report the overlap, defined by $|\langle\psi_{exact}|\psi_{opt}\rangle|^2$

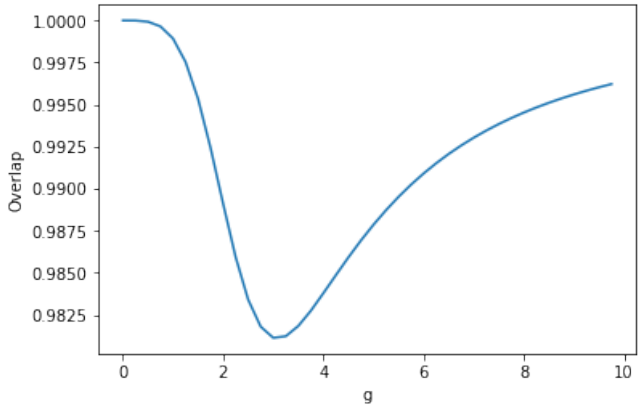

FIG. 7. The overlap of the correct ferromagnetic transition fit in FIG. 4, for comparison