Interior eigenstates of strongly correlated quantum systems

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Abstract: We present a new method to compute states of quantum spin systems with high energy and low energy variance. Such states appear to play an important role in investigating current open problems in condensed matter physics. By minimizing the energy variance with a modification of the power method algorithm we obtain, from initial random states, states with low energy variance and their energy located in the middle of the spectrum. We test our method for a system of eight particles, four different instances of the Heisenberg model and one of the Ising model.

I. INTRODUCTION

Over the last decade or so, there has been an increasing interest in high energy eigenstates of strongly correlated Hamiltonian. They are key ingredients in the study of many-body quantum dynamics, in areas such as thermalization and many-body localization[1]. An example is the Eigenstate Thermalization Hypothesis (ETH). In a few words, this hypothesis stipulates that, given a Hamiltonian H, the mean value of a local observable for a high energy eigenstate is essentially the same as that of a thermal state, of this Hamiltonian, which temperature is tuned to have the same energy [1–4]. To test this hypothesis, a method to construct such high energy states, even if only approximately, would be welcome.

But such a construction seems to be a difficult task, especially for large systems of strongly correlated particles. This situation is in contrast with the investigation of low energy sectors of such systems, for which powerful methods such as tensor network algorithms can be used in a wide variety of situations [5, 6]. A central problem in computational condensed matter physics is to investigate high energy eigenstates of a Hamiltonian within this framework; that would allow to better study the phenomena evoked above. The present work is meant as a contribution to this larger issue.

We are going to present a method that produces states with high energy and low variance. For the sake of simplicity, we have not used the tensor network formalism to represent efficiently states with low entanglement, although we have aimed at a construction that could easily be adapted to that context. When states are represented exactly, exact diagonalization, the Lanczos method, and the like [7, 8] are the most common means to obtain eigenvectors and eigenvalues for a given Hamiltonian. The approach presented here shares some features with the Lanczos algorithm, but unlike this classical technique, we will not build a tower of eigenvectors until we get to the energy range we are interested in. Rather, we will take a random state from the middle of the spectrum, which is not an eigenstate of H, and convert it to an "interior state" by iteratively lowering its energy variance. Our construction is based on the fact that, given a Hermitian operator A, a state $|\psi\rangle$ is an eigenvector of A if and only if the variance of the operator on the state $|\psi\rangle$ is equal to zero. So, by minimizing the energy variance, we get states that are close to the energy eigenstates.

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II. METHOD

Let's consider a Hamiltonian H acting on some Hilbert space $\mathcal{H}$. The central element of our construction is the operator:

$$V(H) \equiv \frac{1}{2}\left(H^2 \otimes \mathbb{1} + \mathbb{1} \otimes H^2\right) - H \otimes H.$$

If we consider a normalized state $|\psi\rangle \in \mathcal{H}$, it is easily seen that

$$\langle\psi,\psi|V(H)|\psi,\psi\rangle = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2,$$

which corresponds to the energy variance of $|\psi\rangle$.

Let $\{\epsilon_i, |\epsilon_i\rangle\}$ denote the eigenvalues and eigenstates of H. The eigenvalues and eigenstates of $V(H)$ are:

$$\left\{\frac{1}{2}\left(\epsilon_i - \epsilon_j\right)^2, |\epsilon_i,\epsilon_j\rangle\right\}.$$

The reason behind this is that $V(H)$ is Hermitian, just like H, and commutes with $H \otimes H$. These two operators, therefore, have common eigenvectors and the eigenvectors of $H \otimes H$ are obviously $|\epsilon_i,\epsilon_j\rangle$.

To find states with low energy variance, the strategy we will follow is to construct states of the form $|\psi,\psi\rangle$ with low value of $V(H)$, *i.e.* $|\langle\psi,\psi|V(H)|\psi,\psi\rangle| \ll 1$, ideally lower than the eigenvalue gap of the operator $V(H)$. This is a minimization problem, which we address as follows.

Let's consider the operator $W = \mathbb{1} - \delta V(H)$, with a value of δ such that $W > 0$. To find this δ, we simply need to find an upper bound on $\|V(H)\|_\infty$. By using the infinity norm properties and the triangle inequality, we have:

$$\|V(H)\|_\infty \leq \frac{1}{2}\left(2\|H\|_\infty\|\mathbb{1}\|_\infty\right) + \|H\|_\infty\|H\|_\infty.$$

Typically, the Hamiltonian can be decomposed as a sum containing polynomially many terms, each of which with a bound easy to compute. That is, $H = \sum_{\alpha=1}^{p(N)} h_\alpha$, where $p(N)$ is a fixed degree polynomial and $\forall\alpha\ \exists M_\alpha$ finite such that $\|h_\alpha\|_\infty < M_\alpha$. Then $\|H\|_\infty$, and $\|V(H)\|_\infty$, can be easily upper bounded. In this case, if we set B as an upper bound on $\|V(H)\|_\infty$, it is sufficient for δ to satisfy $1 - \delta B > 0$. Then, for $\delta < \frac{1}{B}$ we guarantee that $W > 0$.

The power method [9, Ch. 5] is an algorithm that computes the largest eigenvalue, and its corresponding eigenvector, from a Hermitian matrix. In our case, the largest eigenvalue of the operator W coincides with the lowest of V, which is 0.

If we take W to the power of n, we have (baring degeneracies[10]):

$$(\mathbb{1} - \delta V(H))^n = \sum_j |\epsilon_j, \epsilon_j\rangle \langle \epsilon_j, \epsilon_j| + \sum_{\epsilon_{j_1} \neq \epsilon_{j_2}} \left(1 - \frac{(\epsilon_{j_1} - \epsilon_{j_2})^2}{2}\right)^n |\epsilon_{j_1}, \epsilon_{j_2}\rangle \langle \epsilon_{j_1}, \epsilon_{j_2}| .$$

Now, if we use the power method over W and a normalized state $|\psi\rangle = \sum_i \psi_i |\epsilon_i\rangle \in \mathcal{H}$, we obtain the following:

$$\lim_{n\to\infty} (\mathbb{1} - \delta V(H))^n |\psi, \psi\rangle = \sum_i \psi_i^2 |\epsilon_i, \epsilon_i\rangle .$$

In fact, in order to use this algorithm, we need some overlap between the initial state and the lowest eigenvalue subspace. In general, though, since we are considering random states, this will be the case.

There is no obvious way to extract an eigenstate of H from $\sum_i \psi_i^2 |\epsilon_i, \epsilon_i\rangle$. Hence, we need more than just the power method. Our solution will be to only consider states of the form $|\psi, \psi\rangle$. To do so, at each iteration t we will write the state $W |\psi(t), \psi(t)\rangle$ in a particular basis using a small matrix. We will then diagonalize this matrix and select the component of the state that corresponds to the largest eigenvalue. To select the initial state, we will take a random normalized state. By doing so, the energy of the initial state will be most probably located around the middle of the spectrum of H.

The algorithm works as follows:

1. Set $t = 0$ and let $|\psi(0)\rangle$ be a random normalized state of $\mathcal{H}$.
2. For $t < t_{\max}$, do:
   (i) Compute $|a_i(t)\rangle = H^i |\psi(t)\rangle$, normalized, for $i = 0, 1, 2$.
   (ii) Use the Gram–Schmidt algorithm to find a set of orthonormal states $\{|b_i(t)\rangle\}$ from $\{|a_i(t)\rangle\}$.
   (iii) Set $|\eta(t)\rangle = (\mathbb{1} - \delta V(H)) |\psi(t), \psi(t)\rangle$ and take $|\Phi(t)\rangle = |\eta(t)\rangle / \|\eta(t)\|$. Express this normalized state as $|\Phi(t)\rangle = \sum_{\alpha,\beta=0}^{2} M_{\alpha\beta} |b_\alpha, b_\beta\rangle$. It can be shown that M is real and symmetric.
   (iv) Diagonalize the 3×3 matrix M as:
   $$M_{\alpha\beta} = \sum_\mu Q_{\alpha\mu} \Lambda_\mu Q^t_{\mu\beta} = \sum_\mu \Lambda_\mu Q_{\alpha\mu} Q_{\beta\mu}.$$
   where Λ and Q are the eigenvalues and eigenvectors of M, respectively. Let μ_* be the index corresponding to the eigenvalue with the highest magnitude.
   (v) Expand $|\Phi(t)\rangle$ as:
   $$|\Phi(t)\rangle = \Lambda_{\mu_*} \sum_\alpha Q_{\alpha\mu_*} |b_\alpha(t)\rangle \otimes \sum_\beta Q_{\beta\mu_*} |b_\beta(t)\rangle + \sum_{\mu\neq\mu_*} \Lambda_\mu Q_{\alpha\mu} Q_{\beta\mu} |b_\alpha(t), b_\beta(t)\rangle .$$
   In order to avoid entangled states, we will only keep the first term of $|\Phi(t)\rangle$, as it is of the form of $|\psi, \psi\rangle$:
   $$|\psi(t+1)\rangle = \sum_\alpha Q_{\alpha\mu_*} |b_\alpha(t)\rangle .$$
   Since Q is an orthogonal matrix and $\{|b_i(t)\rangle\}$ is an orthonormal basis, the state $|\psi(t+1)\rangle$ has norm 1.
   (vi) Set $t := t + 1$.

III. CASE STUDY I: HEISENBERG MODEL

The Heisenberg model is a nearest neighbor Hamiltonian. For a system of N particles in 1D, it reads

$$H = -\frac{1}{2} J \sum_{j=1}^{N} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z\right) - \frac{1}{2} \sum_{j=1}^{N} h\sigma_j^z,$$

where J is the coupling constant, $\sigma^x = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, $\sigma^y = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$ and $\sigma^z = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ the Pauli matrices and h the constant representing the effect of an external magnetic field. We will also consider that $\sigma_{N+1} = \sigma_1$ (periodic boundary conditions).

In this work, we will be studying four different cases: ferromagnetic and antiferromagnetic cases with and without an external field. Their specifications can be found in Table I.

In addition, we will define an "interior energy zone" for each case. Let's consider a system of N particles and its energy spectrum. The interval $I(N) = [i_-(N), i_+(N)]$ of the spectrum, with $i_-(N) < i_+(N)$, is considered to be interior if the number of eigenvalues with energy value

	J	h
Ferromagnetic w/o field	1	0
Antiferromagnetic w/o field	-1	0
Ferromagnetic w/ field	1	1
Antiferromagnetic w/ field	-1	1

TABLE I: Values of the parameters J and h for four different Hamiltonians

lower than $i_-(N)$ and larger than $i_+(N)$ grows exponentially with N. In our case, we choose the "interior energy zone" to contain half of the spectrum. We define this window of energy to check whether the states stay in this region as the above algorithm is run or move to the other zones of the spectrum. To compute this zone, we use the power method over each H and obtain the largest and lowest eigenvalue.

Let's now consider a system with $N = 8$ and take a random normalized initial state for each of the four Hamiltonians.

In order to select the parameter δ, we run the algorithm with a small $t_{\max}$ using different values of δ. We will keep the δ that returns the lowest variance. Final results of the four experiments with the chosen δ can be seen in Table II. In all cases, a very low energy variance is reached.

$N = 8$	δ	var$(t = 0)$	var$(t = t_{\max})$
Ferromagnetic w/o field	0.041	6.02	7.15×10^{-14}
Antiferromagnetic w/o field	0.07	5.47	2.25×10^{-30}
Ferromagnetic w/ field	0.038	6.67	8.82×10^{-13}
Antiferromagnetic w/ field	0.039	6.19	1.29×10^{-13}

TABLE II: Chosen delta and variances results for the four different Hamiltonians and $t_{\max} = 5 \times 10^5$.

In Fig.(1) we see the evolution of the energy variance for the four Hamiltonians. In all cases, this value decreases with increasing t until it reaches a minimum and starts fluctuating around it due to the numerical precision. This minimum, though, depends on the value of δ and so does the fluctuation phase. We have no evidence to support that this is an absolute minimum of the final variance for a given initial state. Using another value of this parameter or modifying it during the process might result in a different outcome. We observe that, initially, this descent is very similar in all cases, but they all have a different breaking point where it becomes very steep and quickly reaches the minimum value.

In Fig.(2) we see the results of the state energy for the ferromagnetic case with external field, along with the whole energy spectrum, for $t_{\max} = 5 \times 10^5$ and $\delta = 0.035$. We observe that the state energy indeed remains in the "interior energy zone". In fact, it barely moves from the initial value.

In Fig.(3) we can see the evolution of the state energy for the ferromagnetic with field case during the first 7000 steps and different values of the parameter δ. For larger

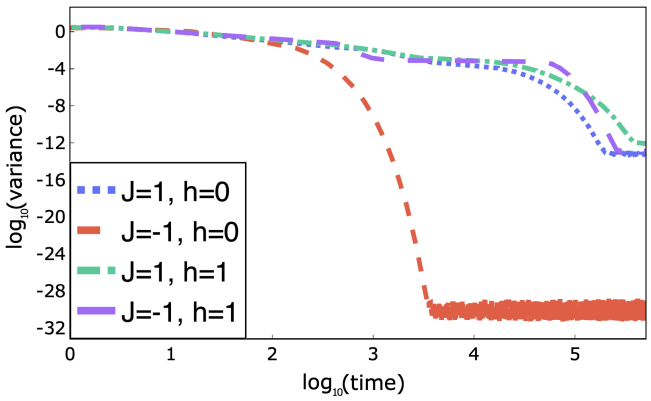

FIG. 1: Evolution of the variance as a function of time for the Hamiltonians in Table I (Log-log plot).

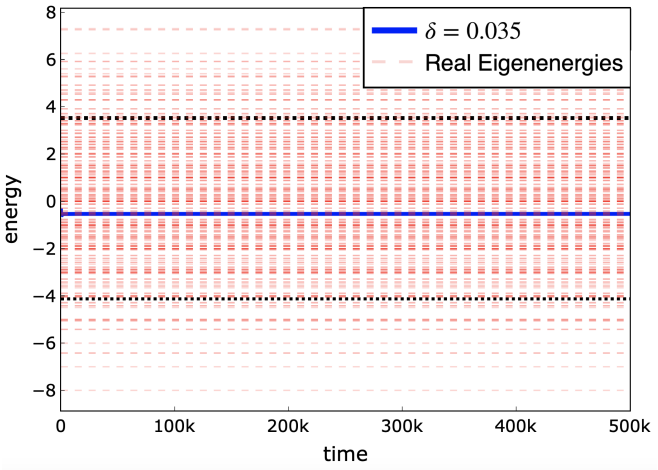

FIG. 2: Evolution of the state energy (blue line) as a function of time for $t_{\max} = 5 \times 10^5$ and $\delta = 0.035$, along with the real eigenergies of the system (red dotted lines) computed using exact diagonalization for the ferromagnetic case with external field. The black dotted lines define the "interior energy zone", which contains half of the energy spectrum.

values, the energy fluctuates and "misses" eigenvalues. In turn, for lower values of δ, the energy remains close to its initial value.

IV. CASE STUDY II: ISING MODEL

To further test our method, we have studied an instance of the Ising model. The Ising model is also a nearest neighbor quantum spin Hamiltonian. For a system of N particles, the Hamiltonian is defined as:

$$H = -\frac{1}{2}\sum_{j=1}^{N}\left(J^x\sigma_j^x\sigma_{j+1}^x + h^x\sigma_j^x + h^z\sigma_j^z\right).$$

We will study the antiferromagnetic case with parameters $J^x = -1$ and $h^x = h^z = 1$. The "interior energy zone" will be defined in the same way as in the previous section.

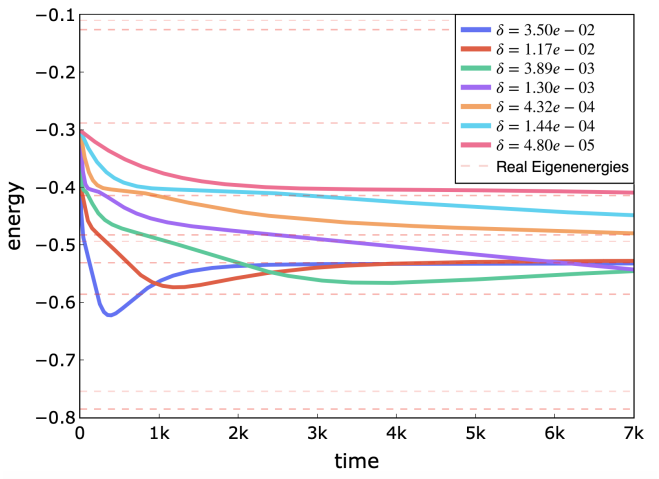

FIG. 3: Evolution of the state energy as a function of time for $t = 7000$ and different values of the parameter δ, along with the real eigenergies of the system (red dotted lines) computed using exact diagonalization for the ferromagnetic case with external field.

We have also considered a system with $N = 8$ and taken a random normalized initial state. This initial state has an energy variance of 5.68. Using $\delta = 0.043$, the variance at $t = 5 \times 10^5$ has a value of 4.55×10^{-14}.

In Fig.(4) we see the evolution of the energy variance for the Ising Hamiltonian. The behavior is the same as in the Heisenberg cases, the value of the variance decreases with increasing time until a minimum is reached.

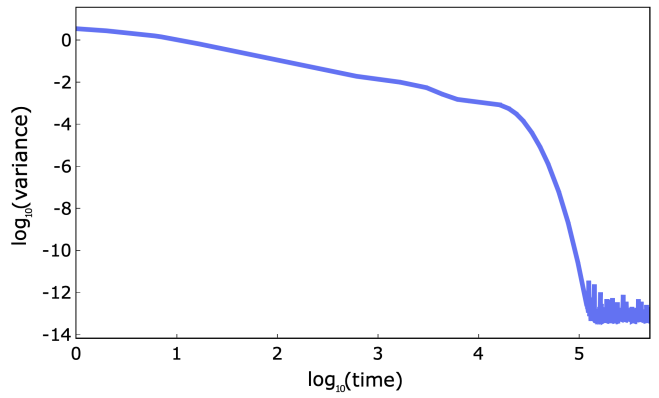

FIG. 4: Evolution of the variance as a function of time for the Ising Hamiltonian (Log-log plot).

In Fig.(5) we see the results of the state energy for the for $t_{\max} = 5 \times 10^5$ and $\delta = 0.043$. Again, the state energy remains in the "interior energy zone" during the whole process.

Finally, in Fig.(6) we can see the evolution of the state energy for the Ising Hamiltonian during the first 7000 steps and different values of the parameter δ. Same situation as in the Heisenberg model case study. The lower the value of δ is, the closer the final energy is to the initial one.

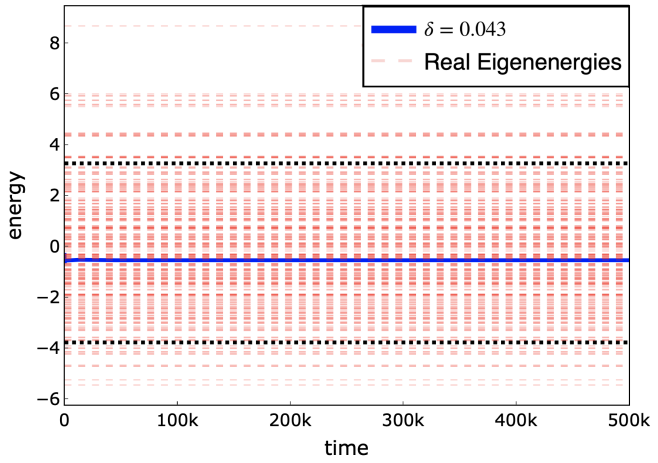

FIG. 5: Evolution of the state energy (blue line) as a function of time for $t_{\max} = 5 \times 10^5$ and $\delta = 0.043$, along with the real eigenergies of the system (red dotted lines) computed using exact diagonalization for the Ising Hamiltonian. The black dotted lines define the "interior energy zone", which contains half of the energy spectrum.

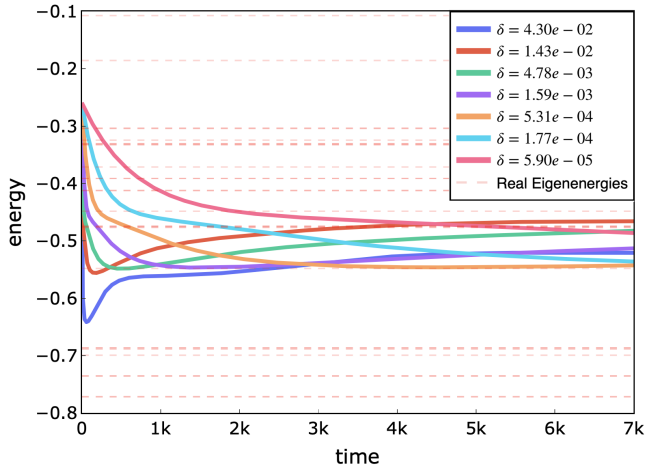

FIG. 6: Evolution of the state energy as a function of time for $t = 7000$ and different values of the parameter δ, along with the real eigenergies of the system (red dotted lines) computed using exact diagonalization for the Ising Hamiltonian.

V. CONCLUSIONS

We have presented a method that produces high energy states with low variance. A modification has been introduced in the power method applied over the operator W so it returns a state of the form $|\psi, \psi\rangle$ in each iteration. After testing this method in four instances of the Heisenberg model and one of the Ising model, we have seen it does indeed obtain states with low energy variance and an energy inside the "interior energy zone". Also, we have observed that, by changing the value of the parameter δ, the same initial state can converge to states with different final energies.

In addition, with this algorithm, we can obtain states with low energy variance from all over the spectrum and not only interior states. For example, if we define the Heaviside step function to have a value of 0 in a specific region and 1 everywhere else, with the use of the Monte Carlo algorithm or any other optimization technique we can easily obtain a state from this region if it is thick enough. Then, the presented method iteratively converts this state to another one with a close energy value and low energy variance.

The next step for this method would be to implement it using tensor network formalism, so larger systems can be tested. Another improvement that could be made is to vary the value of the parameter δ dynamically to check if lower variances can be obtained. Also, this algorithm could be used in non-spin models, such as fermionic systems, to test the limits of the presented technique.

As we stated previously, our results can be replicated with exact diagonalization, but this new approach opens the door to new developments in tensor network algorithms, which exact diagonalization cannot. It has the potential to overcome the bottleneck caused by the computational costs of diagonalizing large systems since it does not need to compute low energy eigenstates to reach high energy states.

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