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Original article

Simulating Ising-Like Models on Quantum Computer

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Abstract

Due to the complexity of lattice models of statistical physics, there is interest in developing new approaches to study them, including those using quantum technologies. In this paper, we describe and implement a scheme for applying the Variational Quantum Eigensolver to the problem of finding the free energy and magnetization in the thermodynamic limit of the n-chain generalized planar Ising model with the interaction of nearest neighbors, next nearest neighbors, and plaquette interactions. The calculation of Rayleigh quotient for transfer matrix is described in detail for n = 1,2,3. Using special parameterizations of the state of the system of qubits and transfer matrix decomposition, free energy and magnetization are calculated for 3-chain model on a quantum computer emulator. The entire computation process, including quantum computer emulation, is implemented using the Python programming language. Also, a method is proposed for significant acceleration of calculations (by about 10,000 times) on the emulator for considered models. Confidence intervals are constructed for the found characteristics of the model.

Keywords: quantum computing, variational quantum eigensolver, Ising model, Hamiltonian, transfer matrix, partition function, free energy

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Оригинальная статья

Исследование обобщенных моделей Изинга на квантовом компьютере

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Аннотация
В связи со сложностью исследования решеточных моделей статистической физики возникает интерес к разработке новых подходов к их изучению, в том числе с использованием квантовых технологий. В данной работе описывается и реализуется схема применения Variational Quantum Eigensolver (вариационный квантовый алгоритм для нахождения собственный значений) к задаче нахождения свободной энергии и намагниченности в термодинамическом пределе n-цепной обобщенной плоской модели Изинга с учетом взаимодействия ближайших соседей, следующих ближайших соседей и плакетных взаимодействий. Расчет отношения Рэлея для трансфер-матрицы подробно описан для n = 1,2,3. С помощью специальных параметризаций состояния системы кубитов и разложения трансфер-матрицы вычисляются свободная энергия и намагниченность для трехцепочечной модели на эмуляторе квантового компьютера. Весь процесс вычислений, включая эмуляцию квантового компьютера, реализован с использованием языка программирования Python. Также предлагается метод значительного ускорения вычислений (примерно в 10 000 раз) на эмуляторе для рассматриваемых моделей. Для найденных характеристик модели построены доверительные интервалы.

Ключевые слова: квантовые вычисления, вариационный квантовый алгоритм, модель Изинга, Гамильтониан, трансфер-матрица, статистическая сумма, свободная энергия

Конфликт интересов: авторы заявляют об отсутствии конфликта интересов.

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1. Introduction

The Ising model is a mathematical model of statistical physics designed to describe the magnetization of a material. Ising chain models are of interest in connection with the emergence and study of nanomaterials with one-dimensional or quasi-one-dimensional characteristics. Works [1, 2, 24, 25, 26] are devoted to the research in this area.Due to the complexity of such models, there is interest in developing new approaches to study them, including those using quantum technologies. This topic has been the subject of many works. The article [3] gives examples of calculating the energy of the ground state of the quantum Ising model with four spins and the partition function of the Potts model with three spins. In [4] authors present a quantum algorithm to prepare the thermal Gibbs state of interacting quantum systems. Paper [5] proposes a scheme to calculate the Gibbs function with the imaginary time evolution. An efficient quantum algorithm for the exact evaluation of either the fully ferromagnetic or anti-ferromagnetic q-state Potts partition function Z for a family of graphs related to irreducible cyclic codes is presented in [6]. In [7] establishes a relationship between IQP and computational complexity of calculating the imaginary-valued partition functions of Ising models. In [8] authors develop a hybrid quantum-classical algorithm to estimate the partition function, utilizing a novel Clifford sampling technique. A quantum algorithm for estimating partition functions of quantum spin Hamiltonians is presented in [9]. In [10] builds explicit quantum circuits that implement the actions of the transfer matrices on arbitrary many-qubit states. A linear-time algorithm is presented in [11] for the construction of the Gibbs distribution of configurations in the Ising model, on a quantum computer.

At this stage in the development of quantum computing, the capabilities of quantum computers are rather limited: the number of qubits is small, and the depth of a possible circuit is low due to strong noise. For computers of this period, the designation NISQ (Noisy intermediate-scale quantum, Noisy medium-scale quantum) is used. However, it has been shown that such quantum computers are superior to classical ones on a certain set of tasks that allow using the advantages of quantum computing [12-14]. Algorithms running on these devices can use a limited number of qubits and must be noise tolerant to some extent. Quite often, these are algorithms that use classical computations in addition to quantum ones.

VQE (Variational Quantum Eigensolver) is one of the most promising algorithms for computers of the NISQ era. VQE was first introduced in [15], its theoretical justification was extended and formalized in [16]. The scope of the algorithm is very wide, it includes: drug development [17, 18], materials science [19], chemical technology [20].

In this paper, we describe and implement a scheme for applying the Variational Quantum Eigensolver to the problem of finding the free energy and magnetization in the thermodynamic limit of the n-chain generalized planar Ising model with the interaction of nearest neighbors, next nearest neighbors, and plaquette interactions. Using special parameterizations of the state of the system of qubits, the highest eigenvalue of the transfer matrix is calculated for $n = 1, 2, 3$ on a quantum computer emulator. The entire computation process, including quantum computer emulation, is implemented using the Python programming language. Also, a method is proposed for significant acceleration of calculations (by about 10.000 times) on the emulator for considered models. Confidence intervals are constructed for the found characteristics of the model.

Chapters 2 and 3 describe the model under study and set the research task. Chapter 4 describes how VQE works. Chapter 5 describes a method for calculating the Rayleigh quotient for the transfer matrix. In the next three chapters, the method is described in more detail for specific cases. In chapter 7, the results of calculations for the three-chain Ising model are demonstrated.

2. Model description

In this paper, we consider the possibility of calculating the free energy of a generalized two-dimensional Ising-like model with cyclically closed boundary conditions in the thermodynamic limit on a quantum computer. The interaction between spins is given by the following Hamiltonian

$$H^n(\sigma) = -\sum_{i=0}^{L-1} H_i^n, \quad (1)$$

where

$$H_i^n = \sum_{j=0}^{n-1} \Big(\frac{J_1'}{2}\big(\sigma_{i,j}\sigma_{i,j+1} + \sigma_{i+1,j}\sigma_{i+1,j+1}\big) + J_2'\sigma_{i,j}\sigma_{i+1,j} + J_3'\big(\sigma_{i,j}\sigma_{i+1,j+1} + \sigma_{i,j+1}\sigma_{i+1,j}\big) + J_4'\sigma_{i,j}\sigma_{i+1,j}\sigma_{i,j+1}\sigma_{i+1,j+1} + \frac{h'}{2}\big(\sigma_{i,j} + \sigma_{i+1,j}\big)\Big)$$

$$\sigma_{i,j} = \pm 1,$$

$$\sigma_{0,j} \equiv \sigma_{L,j}, j = 0, \dots, n$$

$$\sigma_{i,0} \equiv \sigma_{i,n}, i = 0, \dots, L-1.$$

J_k' and h' are dimensionless coefficients characterizing the interaction of vertices with each other and with the external field, respectively.

It should be noted that with such a representation of the Hamiltonian at $n = 2$ interactions with the coefficients J'_1, J'_3, J'_4 are doubled, and at $n = 1$ we set $J'_1 = J'_3 = J'_4 = 0$.

3. Transfer-matrix method

To calculate the free energy in the thermodynamic limit, the transfer matrix method [1, 2, 24, 25, 26] is used, which is based on finding the largest eigenvalue λ_{max} of a certain matrix (transfer matrix) constructed from a given Hamiltonian.

The free energy in the thermodynamic limit $L \to \infty$ is calculated by formula

$$f = -\frac{k_B T}{n} ln(\lambda_{\max}),$$

where T is the temperature, k_B is the Boltzmann constant.

Elements of the transfer matrix Θ of size $2^n \times 2^n$ (Table 1) have the form

$$\theta_{kl} = e^{-\frac{H_0^n(\sigma_{0,0},\dots,\sigma_{0,n-1},\sigma_{1,0},\dots,\sigma_{1,n-1})}{k_B T}},$$

where

$$k = \sum_{j=0}^{n-1} 2^{j-1}(1 - \sigma_{0,j}),$$

$$l = \sum_{j=0}^{n-1} 2^{j-1}\big(1 - \sigma_{1,j}\big).$$

In the following calculations, we use the notation

$$J_k = \frac{J_k'}{k_b}, h = \frac{h'}{k_b}.$$

For the considered Hamiltonian, the transfer matrix will always be symmetric, and hence its eigenvalues are real.

T a b l e 1. **Structure of transfer matrix for n = 3**

			+				-				$\sigma_{1,2}$
			+		-		+		-		$\sigma_{1,1}$
			+	-	+	-	+	-	+	-	$\sigma_{1,0}$
+	+	+	θ_{00}	θ_{01}	θ_{02}	θ_{03}	θ_{04}	θ_{05}	θ_{06}	θ_{07}	
		-	θ_{10}	θ_{11}	θ_{12}	θ_{13}	θ_{14}	θ_{15}	θ_{16}	θ_{17}	
	-	+	θ_{20}	θ_{21}	θ_{22}	θ_{23}	θ_{24}	θ_{25}	θ_{26}	θ_{27}	
		-	θ_{30}	θ_{31}	θ_{32}	θ_{33}	θ_{34}	θ_{35}	θ_{36}	θ_{37}	
-	+	+	θ_{40}	θ_{41}	θ_{42}	θ_{43}	θ_{44}	θ_{45}	θ_{46}	θ_{47}	
		-	θ_{50}	θ_{51}	θ_{52}	θ_{53}	θ_{54}	θ_{55}	θ_{56}	θ_{57}	
	-	+	θ_{60}	θ_{61}	θ_{62}	θ_{63}	θ_{64}	θ_{65}	θ_{66}	θ_{67}	
		-	θ_{70}	θ_{71}	θ_{72}	θ_{73}	θ_{74}	θ_{75}	θ_{76}	θ_{77}	
$\sigma_{0,2}$	$\sigma_{0,1}$	$\sigma_{0,0}$									

Source: Compiled by the authors.

4. Variational quantum eigensolver

Due to the fact that the dimension of the matrix grows exponentially with the increase of lattice width, special algorithms are needed to calculate the largest eigenvalue. In this paper, we consider the possibility of applying VQE to this problem.

Let us describe the principle of its work.

Let Θ be a symmetric matrix with dimentions $2^n \times 2^n$. $|\psi\rangle$ is a state of a system of n qubits.

Consider the Rayleigh quotient for the transfer matrix, i.e. the dot product $\langle\psi|\Theta|\psi\rangle$ ($\langle\psi|\psi\rangle \equiv 1$).

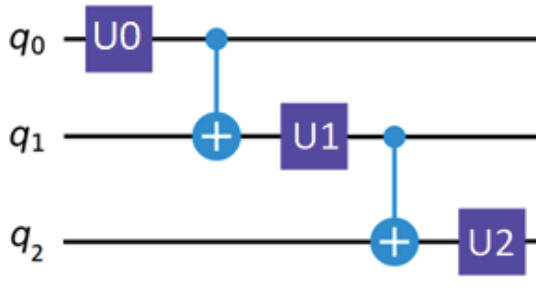
Representing $|\psi\rangle$ as a linear combination of orthonormal eigenvectors $|\phi_i\rangle$ of the matrix Θ, we obtain

$$\langle\psi|\Theta|\psi\rangle = \langle \sum_{i=0}^{2^n-1} a_i\phi_i\,|\Theta|\sum_{j=0}^{2^n-1} a_j\phi_j\ \rangle =$$
$$= \sum_{i=0}^{2^n-1}\sum_{j=0}^{2^n-1} a_i^* a_j\lambda_j\,\langle\phi_i|\phi_j\rangle =$$
$$= \sum_{i=0}^{2^n-1}\lambda_i|a_i|^2$$

Since $\sum|a_i|^2 = 1$, $\langle\psi|\Theta|\psi\rangle \le \lambda_{max}$, λ_{max} is the maximum eigenvalue. Moreover, there exists a state $|\psi_{\max}\rangle$, such that $\langle\psi_{\max}|\Theta|\psi_{\max}\rangle = \lambda_{max}$

We introduce a parameterized quantum circuit that will be used to obtain different states of qubits. An example of such circuit for $n = 3$ is shown in Fig. 1, where

$$U_i = U_i(x_{2i}, x_{2i+1}) = \begin{pmatrix} \cos\left(\frac{x_{2i+1}}{2}\right) & -\sin\left(\frac{x_{2i+1}}{2}\right) \\ e^{ix_{2i}}\sin\left(\frac{x_{2i+1}}{2}\right) & e^{ix_{2i}}\cos\left(\frac{x_{2i+1}}{2}\right) \end{pmatrix},$$
$$i = 0,1,2.$$



F i g. 1. Example of a parameterized quantum circuit for $n = 3$

Source: Hereinafter in this article all figures were drawn up by the authors.

By applying the circuit to the qubits, we get the parameterized state $|\psi(x_1, \dots, x_p)\rangle$.

Substituting into the dot product, we obtain a real function of p variables.

$$g(x_1, \dots, x_p) = \langle\psi(x_1, \dots, x_p)|\Theta|\psi(x_1, \dots, x_p)\rangle$$

It remains to find the maximum of this objective function equal to λ_{max} . Any optimization algorithm is suitable for solving this problem. In this work, the COBYLA algorithm[1] [21, 22] was used.

5. Computation of Rayleigh quotient on quantum computer

The Rayleigh quotient $\langle\psi|\Theta|\psi\rangle$ can be interpreted as the expected value $M(X)$ of some random variable X, corresponding to a given qubit state. In this case λ_i – are the possible values of this quantity, $|a_i|^2$ are the probabilities of obtaining them.

From here we get a method for its approximate calculation: to make a series of measurements of qubits and calculate the average. However, one needs to already know all the eigenvalues of the matrix to perform the computation.

To overcome this obstacle, we decompose the matrix Θ into a linear combination of matrices of a simpler form, independent of the model parameters.

$$\Theta = \sum c_i \cdot B_i, c_i = c_i(J_1, J_2, J_3, J_4, h, T)$$

To do this, identically equal coefficients are grouped, and for each of such groups a matrix is constructed with ones in the places of the elements of this group, the rest of the matrix is filled with zeros. Based on the construction, all matrices will be symmetrical. For a single-chain model, such a decomposition looks like this:

$$\begin{pmatrix} e^{J_2+h} & e^{-J_2} \\ e^{-J_2} & e^{J_2-h} \end{pmatrix} = e^{J_2+h}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + e^{J_2-h}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + e^{-J_2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Separately, we can consider the diagonal elements of the transfer matrix, since for a diagonal matrix composed of them, the eigenvalues and vectors are determined in an obvious way. This reduces the number of matrices in the decomposition.

In this case, the dot product also decomposes into a sum

$$\langle\psi|\Theta|\psi\rangle = \sum_{i=1}^{m} c_i\langle\psi|B_i|\psi\rangle$$

or

$$M(X) = \sum_{i=1}^{m} c_i M(Y_i),$$

[1] Powell M.J.D. A View of Algorithms for Optimization without Derivatives. Technical Report DAMTP2007/NA03. Cambridge: Department of Applied Mathematics and Theoretical Physics, University of Cambridge; 2007. 12 p. Available at: https://www.damtp.cam.ac.uk/user/na/NA_papers/NA2007_03.pdf (accessed 17.06.2023).

where Y_i is a random variable corresponding to B_i and the state $|\psi(x_1, \dots, x_p)\rangle$

For each matrix B_i we find eigenvalues and eigenvectors. From the found vectors we construct an orthonormal basis and a unitary operator A_i of transition to it.

Then, to calculate $M(Y_i)$, the state $|\psi(x_1, \dots, x_p)\rangle$ is first created using a parametrized circuit, after which the transition operator to eigenbasis A_i is applied and measurements are taken. As a result of the measurements, we obtain one of the eigenvectors $|v_j\rangle$ of the matrix B_i. This means that the random variable Y_i has taken a value equal to the eigenvalue $\lambda_{i,j}$ of the matrix B_i.

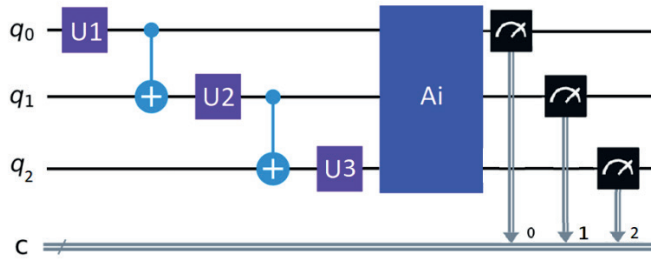


Fig. 2. Example of one measurement of Y_i for $n = 3$

After a series of such measurements, you can calculate the average value of the results $\overline{Y_i} = \frac{Y_{i,1}+\dots+Y_{i,k}}{k}$. Based on the law of large numbers $\overline{Y_i}$ approaches the expected value of Y_i, that is $\langle\psi|B_i|\psi\rangle$, as $k \to \infty$.

The accuracy of the estimate can be described using a confidence interval. Since $\overline{Y_i}$ for sufficiently large k has a normal distribution, the true expected value with a probability of 95 % lies in the interval

$$\left[\overline{Y_i} - 2\frac{s_i}{\sqrt{k}};\ \overline{Y_i} + 2\frac{s_i}{\sqrt{k}}\right],$$

where s_i is the standard deviation of Y_i.

After doing these calculations for all matrices B_i, we get

$$\langle\psi|\Theta|\psi\rangle = \sum_{i=1}^{m} c_i\langle\psi|B_i|\psi\rangle \approx \sum_{i=1}^{m} c_i\overline{Y_i} = \bar{X}.$$

Confidence interval $\left[\bar{X} - \frac{2s}{\sqrt{k}};\ \bar{X} + \frac{2s}{\sqrt{k}}\right]$, $s = \sqrt{\sum_{i=1}^{m} c_i^2 s_i^2}$.

6. Examples of objective function computation

1-chain model

In this example, we consider the Hamiltonian

$$H_i^1 = J_2'\sigma_{0,i}\sigma_{0,i+1} + \frac{h'}{2}(\sigma_{0,i} + \sigma_{0,i+1}).$$

We define the function $g(x,y) = \langle\psi(x,y)|\Theta_1|\psi(x,y)\rangle = (\boldsymbol{\psi}(x,y), \Theta_1\boldsymbol{\psi}(x,y))$ as follows. The qubit is initialized in the state $|0\rangle = \binom{1}{0}$. To obtain the state $|\psi(x,y)\rangle$, the parametrized unitary operator U_0 is applied to it.

$$U_0 = U_0(x,y) = \begin{pmatrix} \cos\left(\frac{y}{2}\right) & -\sin\left(\frac{y}{2}\right) \\ e^{ix}\sin\left(\frac{y}{2}\right) & e^{ix}\cos\left(\frac{y}{2}\right) \end{pmatrix}$$

$$|\psi(x,y)\rangle = U_0(x,y)\,|0\rangle$$

The dot product $\langle\psi(x,y)|\Theta_1|\psi(x,y)\rangle = (\boldsymbol{\psi}(x,y), \Theta_1\boldsymbol{\psi}(x,y))$ can be interpreted as the expected value $M(X)$ of some discrete random variable X, the values of which are the eigenvalues of the matrix Θ_1. To calculate $M(X)$ the transfer matrix is decomposed into a linear combination of matrices of a simpler form.

$$\Theta_1 = \begin{pmatrix} e^{\frac{(J_2+h)}{T}} & e^{\frac{-J_2}{T}} \\ e^{\frac{-J_2}{T}} & e^{\frac{(J_2-h)}{T}} \end{pmatrix}$$

$$= e^{\frac{-J_2}{T}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + e^{\frac{(J_2+h)}{T}}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$+ e^{\frac{(J_2-h)}{T}}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} == \sum_{i=1}^{3} c_i(J_2, h, T)\cdot B_i$$

$$B_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, B_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, B_3 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Then $\langle\psi(x,y)|\Theta_1|\psi(x,y)\rangle = (\boldsymbol{\psi}(x,y), \Theta_1\boldsymbol{\psi}(x,y)) = \sum_{i=1}^{3} c_i(\boldsymbol{\psi}(x,y), B_i\boldsymbol{\psi}(x,y)) =$

$$= \sum_{i=1}^{3} c_i\langle\psi(x,y)|B_i|\psi(x,y)\rangle$$

For each symmetric matrix B_i, a series of measurements is made in the basis formed by its orthonormal eigenvectors. To do this, the state of the qubit is transformed using the transition matrix into the new basis - the unitary operator A_i. A_i^{-1} is an operator whose columns are formed by orthonormal eigenvectors of the matrix B_i.

$$A_1^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, A_2^{-1} = A_3^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

In this case, the matrices A_i^{-1} are also symmetric, so $A_i = A_i^{-1}$. In general, this is not the case.

Let us present the eigenvalues of the matrices B_i. B_1: $\lambda_{1,0} = 1$, $\lambda_{1,1} = -1$. B_2: $\lambda_{2,0} = 1$, $\lambda_{2,1} = 0$. B_3: $\lambda_{3,0} = 0$, $\lambda_{3,1} = 1$.

After applying the operator A_i, the qubit is measured. The result of the measurement is either the state $|0\rangle$, or $|1\rangle$, which correspond to the eigenvectors of B_i. Let us define a discrete random variable Y_i as follows: if the state $|0\rangle$ is obtained as a result of the qubit measurement, then $Y_i = \lambda_{i,0}$, if $|1\rangle$, then $Y_i = \lambda_{i,1}$. The distribution of Y_i depends on the state of the qubit $|\psi(x,y)\rangle$.

Thus $M(X) = \sum_{i=1}^{3} c_i M(Y_i)$

For matrix B_i the scheme of one iteration is as follows (Fig. 3).

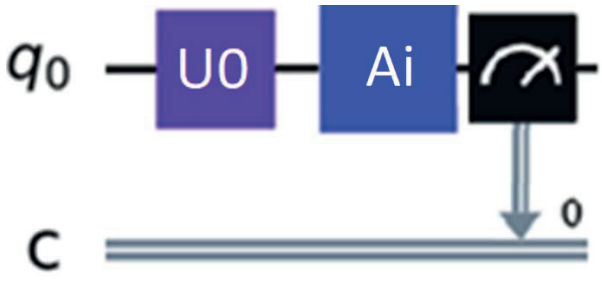


Fig. 3. Scheme of one iteration for matrix B_i with $n = 1$

k iterations are carried out and the average value of the results is calculated.

$$\bar{Y}_i = \frac{Y_{i,1} + \dots + Y_{i,k}}{k}$$

Then the approximate value of the function g is calculated.

$$g(x,y) = M(X) = \sum_{i=1}^{3} c_i M(Y_i) \approx \sum_{i=1}^{3} c_i\bar{Y}_i$$

2-chain model

We define the function $g(x_1,y_1,x_2,y_2) = \langle\psi(x_1,y_1,x_2,y_2)|\Theta_2|\psi(x_1,y_1,x_2,y_2)\rangle = \left(\boldsymbol{\psi}(x_1,y_1,x_2,y_2),\Theta_2\boldsymbol{\psi}(x_1,y_1,x_2,y_2)\right)$ as follows. The system of two qubits is initialized in the state $|00\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$. To obtain the state $|\psi(x_1,y_1,x_2,y_2)\rangle$, first, the parameterized unitary operator is applied to the null qubit

$$U_0 = U_0(x_1,y_1) = \begin{pmatrix} \cos\left(\frac{y_1}{2}\right) & -\sin\left(\frac{y_1}{2}\right) \\ e^{ix_1}\sin\left(\frac{y_1}{2}\right) & e^{ix_1}\cos\left(\frac{y_1}{2}\right)\end{pmatrix},$$

then the CNOT operator with zero controlling qubit, and after that the unitary operator is applied to the first qubit

$$U_1 = U_1(x_2,y_2) = \begin{pmatrix} \cos\left(\frac{y_2}{2}\right) & -\sin\left(\frac{y_2}{2}\right) \\ e^{ix_2}\sin\left(\frac{y_2}{2}\right) & e^{ix_2}\cos\left(\frac{y_2}{2}\right)\end{pmatrix}$$

$$|\psi(x_1,y_1,x_2,y_2)\rangle = \left(U_2(x_2,y_2)\right) CX \left(I\otimes U_1(x_1,y_1)\right)|00\rangle$$

The dot product $\langle\psi(x_1,y_1,x_2,y_2)|\Theta_2|\psi(x_1,y_1,x_2,y_2)\rangle = \left(\boldsymbol{\psi}(x_1,y_1,x_2,y_2),\Theta_2\boldsymbol{\psi}(x_1,y_1,x_2,y_2)\right)$ can be interpreted as the expected value $M(X)$ of some discrete random variable X, the values of which are the eigenvalues of the matrix Θ_2. To calculate $M(X)$ the transfer matrix is decomposed into a linear combination of matrices of a simpler form.

$$\Theta_2 = \begin{pmatrix} e^{\frac{2h+2J_1+2J_2+4J_3+2J_4}{T}} & e^{\frac{h-2J_4}{T}} & e^{\frac{h-2J_4}{T}} & e^{\frac{2J_1-2J_2-4J_3+2J_4}{T}} \\ e^{\frac{h-2J_4}{T}} & e^{\frac{-2J_1+2J_2-4J_3+2J_4}{T}} & e^{\frac{-2J_1-2J_2+4J_3+2J_4}{T}} & e^{\frac{-h-2J_4}{T}} \\ e^{\frac{h-2J_4}{T}} & e^{\frac{-2J_1-2J_2+4J_3+2J_4}{T}} & e^{\frac{-2J_1+2J_2-4J_3+2J_4}{T}} & e^{\frac{-h-2J_4}{T}} \\ e^{\frac{2J_1-2J_2-4J_3+2J_4}{T}} & e^{\frac{-h-2J_4}{T}} & e^{\frac{-h-2J_4}{T}} & e^{\frac{-2h+2J_1+2J_2+4J_3+2J_4}{T}} \end{pmatrix} =$$

$$= diag\left(e^{\frac{2h+2J_1+2J_2+4J_3+2J_4}{T}}, e^{\frac{-2J_1+2J_2-4J_3+2J_4}{T}}, e^{\frac{-2J_1+2J_2-4J_3+2J_4}{T}}, e^{\frac{-2h+2J_1+2J_2+4J_3+2J_4}{T}}\right) +$$

$$+e^{\frac{h-2J_4}{T}}B_2 + e^{\frac{-h-2J_4}{T}}B_3 + e^{\frac{2J_1-2J_2-4J_3+2J_4}{T}}B_4 + e^{\frac{-2J_1-2J_2+4J_3+2J_4}{T}}B_5 = \sum_{i=1}^{5} c_i(J_1,J_2,J_3,J_4,h,T)\cdot B_i$$

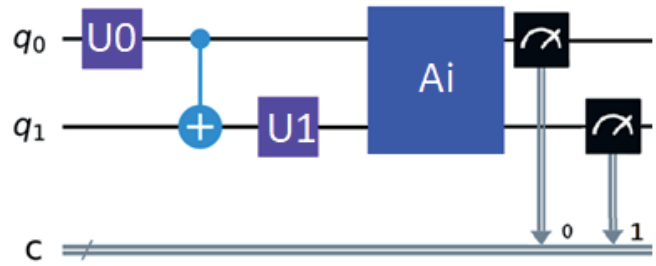
$$B_2 = \begin{pmatrix}0&1&1&0\\1&0&0&0\\1&0&0&0\\0&0&0&0\end{pmatrix}, B_3 = \begin{pmatrix}0&0&0&0\\0&0&0&1\\0&0&0&1\\0&1&1&0\end{pmatrix}$$

$$B_4 = \begin{pmatrix}0&0&0&1\\0&0&0&0\\0&0&0&0\\1&0&0&0\end{pmatrix}, B_5 = \begin{pmatrix}0&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&0\end{pmatrix}$$

Then $\langle\psi(x_1,y_1,x_2,y_2)|\Theta_2|\psi(x_1,y_1,x_2,y_2)\rangle = \left(\boldsymbol{\psi}(x,y),\Theta_2\boldsymbol{\psi}(x,y)\right) = \sum_{i=1}^{5} c_i\left(\boldsymbol{\psi}(x_1,y_1,x_2,y_2),B_i\boldsymbol{\psi}(x_1,y_1,x_2,y_2)\right) = \sum_{i=1}^{5} c_i\langle\psi(x_1,y_1,x_2,y_2)|B_i|\psi(x_1,y_1,x_2,y_2)\rangle$

For each symmetric matrix B_i, a series of measurements is made in the basis formed by its orthonormal eigenvectors. To do this, the state of the qubit is transformed using the transition matrix into the new basis - the unitary operator A_i. A_i^{-1} is an operator whose columns are formed by orthonormal eigenvectors of the matrix B_i. Eigenvalues of the matrix $B_i - \lambda_{i,j}, j = 0,1,2,3$.

After applying the operator A_i, the qubit is measured. The measurement result is one of the states $|0\rangle, |1\rangle, |2\rangle, |3\rangle$, which correspond to the eigenvectors of B_i. Let us define a discrete random variable Y_i as follows: if the state $|j\rangle$ is obtained as a result of measuring a qubit, then $Y_i = \lambda_{i,j}$. The distribution of Y_i depends on the state of the qubit$|\psi(x_1,y_1,x_2,y_2)\rangle$.
Thus $M(X) = \sum_{i=1}^{5} c_i M(Y_i)$
For matrix B_i the scheme of one iteration is as follows (Fig. 4).



F i g. 4. Scheme of one iteration for matrix B_i with $n = 2$

k iterations are carried out and the average value of the results is calculated.

$$\overline{Y_i} = \frac{Y_{i,1} + \cdots + Y_{i,k}}{k}$$

Calculations are carried out in turn for all matrices B_i.
Then the approximate value of the function g is calculated.

$$g(x_1,y_1,x_2,y_2) = M(X) = \sum_{i=1}^{3} c_i M(Y_i) \approx \sum_{i=1}^{3} c_i\overline{Y_i}$$

3-chain model

We define the function $g(x_1,y_1,x_2,y_2,x_3,y_3) = \langle\psi(x_1,y_1,x_2,y_2,x_3,y_3)|\Theta_3|\psi(x_1,y_1,x_2,y_2,x_3,y_3)\rangle = \big(\boldsymbol{\psi}(x_1,y_1,x_2,y_2,x_3,y_3),\Theta_3\boldsymbol{\psi}(x_1,y_1,x_2,y_2,x_3,y_3)\big)$ as follows. The system of three qubits is initialized in the state $|000\rangle = \begin{pmatrix}1\\0\\0\\0\\0\\0\\0\\0\end{pmatrix}$. To obtain the state $|\psi(x_1,y_1,x_2,y_2,x_3,y_3)\rangle$, first, a parameterized unitary operator is applied to the zero qubit (Fig. 5)

$$U_0 = U_0(x_1,y_1) = \begin{pmatrix} \cos\left(\frac{y_1}{2}\right) & -\sin\left(\frac{y_1}{2}\right) \\ e^{ix_1}\sin\left(\frac{y_1}{2}\right) & e^{ix_1}\cos\left(\frac{y_1}{2}\right)\end{pmatrix}.$$

Then a CNOT operator with zero control qubit acting on the first one. After that, the unitary operator is applied to the first qubit

$$U_1 = U_1(x_2,y_2) = \begin{pmatrix} \cos\left(\frac{y_2}{2}\right) & -\sin\left(\frac{y_2}{2}\right) \\ e^{ix_2}\sin\left(\frac{y_2}{2}\right) & e^{ix_2}\cos\left(\frac{y_2}{2}\right)\end{pmatrix}.$$

Then a CNOT operator with the first controlling qubit acting on the second. And finally, the unitary operator is applied to the second qubit

$$U_2 = U_2(x_3,y_3) = \begin{pmatrix} \cos\left(\frac{y_3}{2}\right) & -\sin\left(\frac{y_3}{2}\right) \\ e^{ix_3}\sin\left(\frac{y_3}{2}\right) & e^{ix_3}\cos\left(\frac{y_3}{2}\right)\end{pmatrix}$$

$$|\psi(x_1,y_1,x_2,y_2,x_3,y_3)\rangle = \\ = (U_1(x_2,y_2)\otimes I\otimes I)\; CX_{1,2}\;(I\otimes U_1(x_2,y_2)\otimes I)\cdot \\ \cdot CX_{0,1}\;(I\otimes I\otimes U_0(x_1,y_1))\;|000\rangle$$

Dot product $\langle\psi(x_1,y_1,x_2,y_2,x_3,y_3)|\Theta_3|\psi(x_1,y_1,x_2,y_2,x_3,y_3)\rangle = \big(\boldsymbol{\psi}(x_1,y_1,x_2,y_2,x_3,y_3),\Theta_3\boldsymbol{\psi}(x_1,y_1,x_2,y_2,x_3,y_3)\big)$ can be interpreted as the expected value $M(X)$ of some discrete random variable X, the values of which are the eigenvalues of the matrix Θ_3. To calculate $M(X)$ the transfer matrix is decomposed into a linear combination of matrices of a simpler form.

$$\Theta_3 = diag(e^{\frac{3h+3J_1+3J_2+6J_3+3J_4}{T}}, e^{\frac{h-J_1+3J_2-2J_3+3J_4}{T}}, e^{\frac{h-J_1+3J_2-2J_3+3J_4}{T}}, e^{\frac{-h-J_1+3J_2-2J_3+3J_4}{T}}, e^{\frac{h-J_1+3J_2-2J_3+3J_4}{T}}, \\ e^{\frac{-h-J_1+3J_2-2J_3+3J_4}{T}}, e^{\frac{-h-J_1+3J_2-2J_3+3J_4}{T}}, e^{\frac{-3h+3J_1+3J_2+6J_3+3J_4}{T}}) + +e^{\frac{2h+J_1+J_2+2J_3-J_4}{T}}B_2 + e^{\frac{h+J_1-J_2-2J_3-J_4}{T}}B_3 \\ + e^{\frac{h-J_1-J_2+2J_3-J_4}{T}}B_4 + e^{\frac{-J_1+J_2-2J_3-J_4}{T}}B_5 + e^{\frac{-J_1-3J_2+2J_3+3J_4}{T}}B_6 + e^{\frac{-h+J_1-J_2-2J_3-J_4}{T}}B_7 \\ + e^{\frac{-h-J_1-J_2+2J_3-J_4}{T}}B_8 + e^{\frac{-2h+J_1+J_2+2J_3-J_4}{T}}B_9 + e^{\frac{3J_1-3J_2-6J_3+3J_4}{T}}B_{10} = \sum_{i=1}^{10} c_i(J_1,J_2,J_3,J_4,h,T)\cdot B_i$$

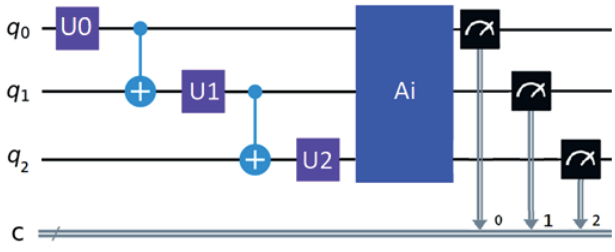
$$B_2 = \begin{pmatrix}0&1&1&0&1&0&0&0\\1&0&0&0&0&0&0&0\\1&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\1&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\end{pmatrix}, B_3 = \begin{pmatrix}0&0&0&1&0&1&1&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\1&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\1&0&0&0&0&0&0&0\\1&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\end{pmatrix}$$

$$B_4 = \begin{pmatrix}0&0&0&0&0&0&0&0\\0&0&1&0&1&0&0&0\\0&1&0&0&1&0&0&0\\0&0&0&0&0&0&0&0\\0&1&1&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\end{pmatrix}, B_5 = \begin{pmatrix}0&0&0&0&0&0&0&0\\0&0&0&1&0&1&0&0\\0&0&0&1&0&0&1&0\\0&1&1&0&0&0&0&0\\0&0&0&0&0&1&1&0\\0&1&0&0&1&0&0&0\\0&0&1&0&1&0&0&0\\0&0&0&0&0&0&0&0\end{pmatrix}$$

$$B_6 = \begin{pmatrix}0&0&0&0&0&0&0&0\\0&0&0&0&0&0&1&0\\0&0&0&0&0&1&0&0\\0&0&0&0&1&0&0&0\\0&0&0&1&0&0&0&0\\0&0&1&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\end{pmatrix}, B_7 = \begin{pmatrix}0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&1&1&0&1&0&0&0\end{pmatrix}$$

$$B_8 = \begin{pmatrix}0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&1&1&0\\0&0&0&0&0&0&0&0\\0&0&0&1&0&0&1&0\\0&0&0&1&0&1&0&0\\0&0&0&0&0&0&0&0\end{pmatrix}, B_9 = \begin{pmatrix}0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&0&1\\0&0&0&1&0&1&1&0\end{pmatrix}$$

$$B_{10} = \begin{pmatrix}0&0&0&0&0&0&0&1\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0\\1&0&0&0&0&0&0&0\end{pmatrix}$$



F i g. 5. Scheme of one iteration for matrix B_i with $n = 3$

Then $\langle\psi(x_1,y_1,x_2,y_2,x_3,y_3)|\Theta_3|\psi(x_1,y_1,x_2,y_2,x_3,y_3)\rangle = \big(\boldsymbol{\psi}(x_1,y_1,x_2,y_2,x_3,y_3),\Theta_3\boldsymbol{\psi}(x_1,y_1,x_2,y_2,x_3,y_3)\big) = \sum_{i=1}^{10} c_i\big(\boldsymbol{\psi}(x_1,y_1,x_2,y_2,x_3,y_3),B_i\boldsymbol{\psi}(x_1,y_1,x_2,y_2,x_3,y_3)\big) = = \sum_{i=1}^{10} c_i\langle\psi(x_1,y_1,x_2,y_2,x_3,y_3)|B_i|\psi(x_1,y_1,x_2,y_2,x_3,y_3)\rangle$

For each symmetric matrix B_i, a series of measurements is made in the basis formed by its orthonormal eigenvectors. To do this, the state of the qubit is transformed using the transition matrix into the new basis - the unitary operator A_i. A_i^{-1} is an operator whose columns are formed by orthonormal eigenvectors of the matrix B_i.
Eigenvalues of the matrix $B_i - \lambda_{i,j}, j = 0,1,2,\dots,7$.
After applying the operator A_i, the qubit is measured. The measurement result is one of the states $|0\rangle, |1\rangle, |2\rangle, \dots, |7\rangle$, which correspond to the eigenvectors of B_i. Let us define a discrete random variable Y_i as follows: if the state $|j\rangle$ is obtained as a result of measuring a qubit, then $Y_i = \lambda_{i,j}$. The distribution of Y_i depends on the state of the $|\psi(x_1,y_1,x_2,y_2,x_3,y_3)\rangle$.
Thus $M(X) = \sum_{i=1}^{10} c_i M(Y_i)$
For matrix B_i the scheme of one iteration is as follows (Fig. 5).

k iterations are carried out and the average value of the results is calculated.

$$\overline{Y_i} = \frac{Y_{i,1} + \dots + Y_{i,k}}{k}$$

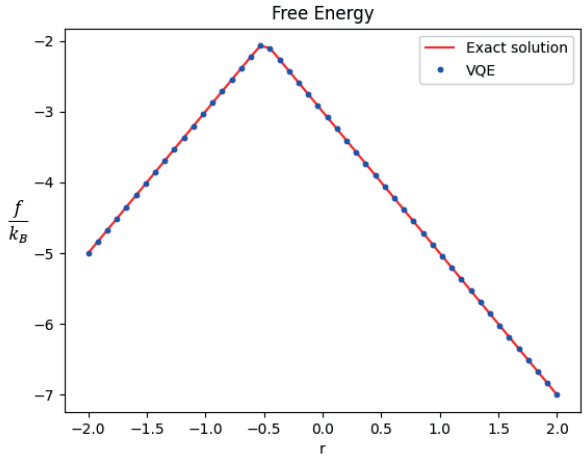
Calculations are carried out in turn for all matrices B_i.

Then the approximate value of the function g is calculated.

$$g(x_1,y_1,x_2,y_2,x_3,y_3) = M(X) = \sum_{i=1}^{10} c_i M(Y_i) \approx \sum_{i=1}^{10} c_i \overline{Y_i}$$

7. Computation results

The calculations were carried out using a quantum computer emulator [23] written in the Python programming language. Programs were also written to calculate the transfer matrix, its decomposition into a linear combination and the construction of unitary operators, and the calculation of the average value. The SciPy library was used to find the maximum mean value. The text of the program related directly to this work is presented in the appendices.
Using direct emulation of the circuit shown in Fig. 2, calculations were carried out (Fig. 6-7) for a three-chain model with parameters $h = -0.01, J_1 = J_2 = J_4 = 1, J_3 = r, T = 0.2$. The number of Y_i measurements $k = 10000$.



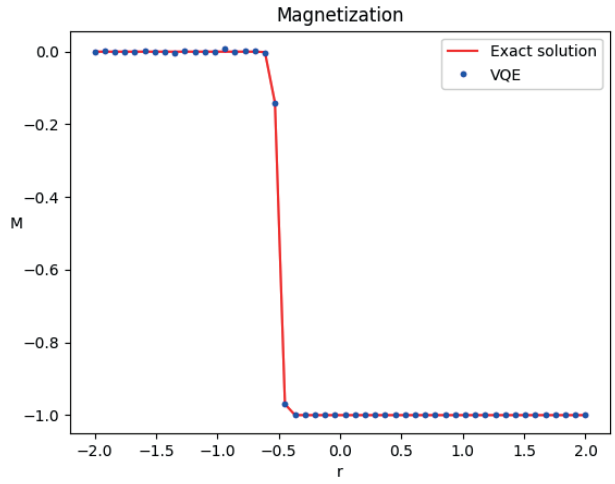
F i g. 6. Free energy for n=3 with parameters $h = -0.01, J_1 = J_2 = J_4 = 1, J_3 = r, T = 0.2$. The number of Y_i measurements $k = 10000$

The magnetization is calculated by the formula

$$M = -\frac{\partial f}{\partial h'} = -\frac{1}{k_B}\frac{\partial f}{\partial h}.$$

The derivative was calculated numerically.

$$\frac{\partial f}{\partial h} = \frac{f_{h+\Delta h} - f_h}{\Delta h} + o(\Delta h)$$



F i g. 7. Magnetization for $n = 3$ with parameters $h = -0.01, J_1 = J_2 = J_4 = 1, J_3 = r, T = 0.2$. The number of Y_i measurements $k = 10000$, $\Delta h = 0.01$

Confidence interval for the free energy with 95 % probability

$$\frac{f}{k_B} \in \left[-Tln\left(\bar{X} + 2\frac{s}{\sqrt{k}}\right);\ -Tln\left(\bar{X} - 2\frac{s}{\sqrt{k}}\right)\right].$$

Interval length

$$-Tln\left(1 - \frac{4s}{\bar{X}\sqrt{k} + 2s}\right) \sim T\frac{4s}{\bar{X}\sqrt{k} + 2s} \to 0\ as\ k \to \infty.$$

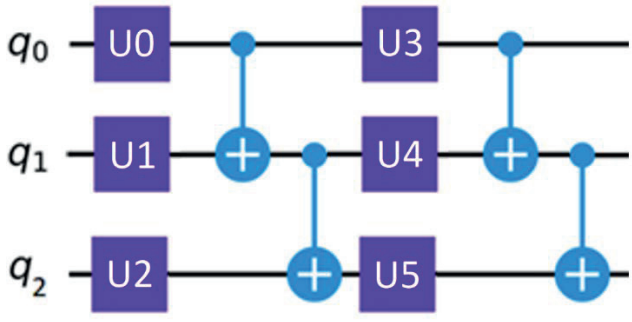
Confidence interval for magnetization with a probability of 91 %

$$[\,Tln\left(\bar{X}_{h=0} - 2\frac{S_{h=0.01}}{\sqrt{k}}\right) - Tln\left(\bar{X}_{h=-0.01} + 2\frac{S_{h=0}}{\sqrt{k}}\right);$$
$$Tln\left(\bar{X}_{h=0} + 2\frac{S_{h=0.01}}{\sqrt{k}}\right) - Tln\left(\bar{X}_{h=-0.01} - 2\frac{S_{h=0}}{\sqrt{k}}\right)\,].$$

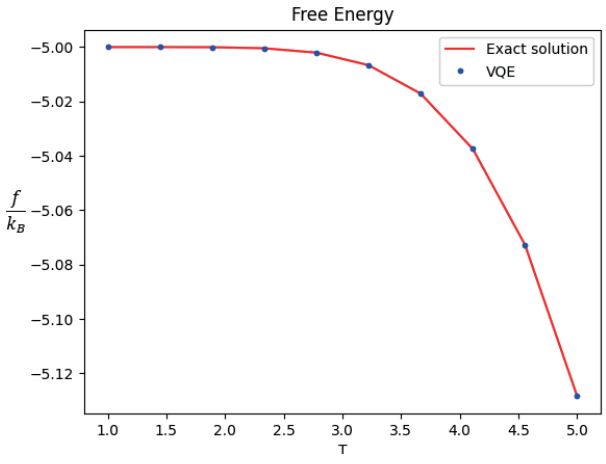
Remark. Since the approximate calculation of the Rayleigh quotient for the transfer matrix on a quantum computer requires extensive calculations, a method for accelerated calculation was developed to work on the emulator. The emulation of measuring the state of a system of qubits is carried out by calculating the distribution of a random variable and its subsequent realization. Based on the fact that the distribution of Y_i is known to us, a series of a large number of independent measurements can be replaced by a measurement of one random random variable with a normal distribution and the following parameters

$$\mu = \sum_{i=1}^{m} c_i M(Y_i), \sigma = \sqrt{\frac{1}{k}\sum_{i=1}^{m} c_i^2 D(Y_i)}.$$

Using accelerated emulation and the parametrized quantum circuit shown in Fig. 8, calculations were carried out (Fig. 9) for a three-chain model with parameters h $= -0.01, J_1 = J_2 = J_3 = J_4 = 1$ and $k = 10000$.



F i g. 8. Parameterized circuit for $n = 3$



F i g. 9. Free energy for n=3 with parameters

$h = -0.01, J_1 = J_2 = J_3 = J_4 = 1. k = 10000$

8. Conclusion

In this paper, the application of VQE to the problem of finding the free energy and magnetization of the *n*-chain generalized planar Ising model in the thermodynamic limit by the transfer matrix method was described. The process of calculating the objective function for $n = 1,2,3$ is described in detail. Using various parameterizations of the state of the system of qubits, the largest eigenvalue of the transfer matrix for the three-chain model was calculated on a quantum computer emulator. Graphs of free energy and magnetization in the thermodynamic limit are plotted. Confidence intervals are given for the found characteristics of the model. The entire calculation process, including quantum computer emulation, is implemented using the Python programming language. A method for significantly accelerating calculations on the emulator is also proposed.

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