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Quantum Approximation Optimization Algorithm for the Ising Model in an External Magnetic Field

Yu. Palii[a, b, *], A. Bogolubskaya[a], and D. Yanovich[a]

[a] *Joint Institute for Nuclear Research, Dubna, Russia*

[b] *Institute of Applied Physics, Moldova State University, Chişinău, Republic of Moldova*

**e-mail: palii@jinr.ru*

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Abstract—A representation of the Ising model in a longitudinal magnetic field on a quantum computer is introduced. The ansatz of the wave function of the model for a quantum approximation optimization algorithm is constructed. The scheme and the result of its operation for a lattice of size 2×2 are presented.

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INTRODUCTION

It is shown that in quantum field theory calculations, quantum algorithms can be more efficient than classical ones [1]. Therefore, they are supposed to be used for problems that are unsolvable for ordinary computers. Because of the imperfections of quantum computers today, the focus is on hybrid algorithms in which the role of a quantum computer is only to construct a wave function of the simulated system and to measure its observables. On a classical computer, the process of optimizing the parameters of quantum gates is performed to obtain the required value of the cost function, determined from measurements on the quantum computer [2]. The operation of such quantum variational algorithms is based on the Rayleigh–Ritz variational principle in quantum mechanics: for any trial wave function $|x(\alpha)\rangle$ with parameters $\alpha = (\alpha_1, \ldots, \alpha_n)$ the average value of the Hamiltonian is not less than the ground state energy,

$$\langle x(\alpha)|\mathcal{H}|x(\alpha)\rangle \geq E_0.$$

The quantum approximation optimization algorithm QAOA [3], discussed in this paper, is considered the most promising among hybrid algorithms.

REPRESENTATION OF THE ISING MODEL ON A QUANTUM COMPUTER

In the quantum register, a qubit is assigned to each lattice site. An arbitrary distribution of spin values over the lattice is specified by a set of one-bit length variables $z = z_1 z_2 \ldots z_n$. A variable z_i takes two values ± 1 and determines the spin orientation at the ith site. Note that the value of the variable z_i corresponds to the measurement of the Pauli operator $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$, acting on the ith qubit in the computational basis. If ith qubit is in one of the basis states, $|0\rangle$ or $|1\rangle$, then

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \leftrightarrow z_i = +1 \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \leftrightarrow z_i = -1,$$

that is, the value of z_i is nothing more than the eigenvalue of the operator Z for a given state. This means that the 2^n basis states of the quantum register exactly correspond to the 2^n possible spin configurations on the lattice,

$$\text{bitstring } z = z_1 z_2 \ldots z_n$$
$$\leftrightarrow \text{quantum register } |z\rangle = |z_1 z_2 \ldots z_n\rangle.$$

An arbitrary state of a quantum register $|\psi\rangle$ represents a superposition of all possible spin orientations on the lattice with different amplitudes.

The Hamilton operator of the Ising model is constructed from multiqubit operators $Z^{(i)}$,

$$Z^{(i)} = \mathbb{I} \otimes \ldots \otimes Z \otimes \ldots \otimes \mathbb{I},$$

where the operator Z stands on the ith place, that is, it acts on the ith qubit. In the case of nearest neighbor interaction, that is, the spin–spin interaction with the constant J and the interaction of spins with the external magnetic field h, the Hamiltonian takes the form:

$$\mathcal{H}_C(Z) = -J\sum_{\langle i,j\rangle} Z^{(i)}Z^{(j)} - h\sum_i Z^{(i)}, \qquad (1)$$

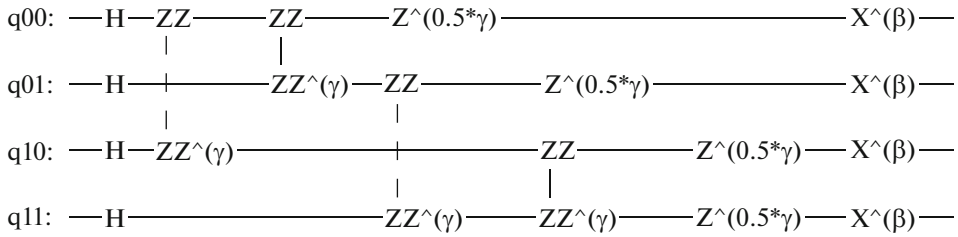

Fig. 1. Quantum circuit for the QAOA ansatz (2) with one layer ($p = 1$), created in the Cirq environment [4].

where $\langle i, j\rangle$ is the set of pairs of adjacent spins, and the second sum goes over all sites of the lattice. The index C means that the average value of the Hamiltonian is used as a cost function in the variational minimization process.

THE QAOA ANSATZ FOR THE ISING MODEL

The variational ansatz of the wave function $|x(\alpha)\rangle$ in the QAOA algorithm consists of several identical layers of operators. A layer includes the driving and mixing operators (driver and mixer). First of all, the qubits are transferred from the state $|0\rangle^{\otimes n}$ to the equal superposition state by the action of Hadamard operators H on each of the n qubits of the register

$$H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{2^{n/2}}\sum_{z\in\{0,1\}^n}|z\rangle,$$

as a result, all possible spin configurations have an equal probability of appearance.

• The driving operator is the evolutionary operator, corresponding to the Hamiltonian $\mathcal{H}_C(Z)$ ($J = 1$)

$$U(\gamma,\mathcal{H}_C) = e^{i\pi\gamma\mathcal{H}_C} = \prod_{\langle i,j\rangle} e^{-i\pi\gamma Z^{(i)}Z^{(j)}}\prod_i e^{-i\pi\gamma h Z^{(i)}},$$

and the variational parameter γ plays the role of evolution time.

• The mixing operator is constructed from the Pauli operators X:

$$U(\beta, B) = e^{i\pi\beta B} = \prod_{j=1}^{n} e^{i\pi\beta X^{(j)}}, \quad B = \sum_{j=1}^{n} X^{(j)},$$

where the variable β is the second variational parameter in this layer.

Thus, the entire QAOA ansatz, including p layers, has the form:

$$|\psi(\gamma,\beta)\rangle = \underbrace{U(\beta_p, B)U(\gamma_p,\mathcal{H}_C)}_{p}\ldots\underbrace{U(\beta_1, B)U(\gamma_1,\mathcal{H}_C)}_{1}H^{\otimes n}|0\rangle^{\otimes n}. \quad (2)$$

From the theorem proved in [3], it follows that with increasing number of layers minimum mean $E_p(\gamma,\beta)$ of the Hamiltonian $\mathcal{H}_C$, found using the QAOA algorithm, tends to the minimum value $\min_z \mathcal{H}_C(z)$ among all possible bit strings z:

$$\lim_{p\to\infty}\min_{\gamma,\beta} E_p(\gamma,\beta) = \min_z \mathcal{H}_C(z),$$
$$E_p(\gamma,\beta) \equiv \langle\psi(\gamma,\beta)|\mathcal{H}_C|\psi(\gamma,\beta)\rangle.$$

In reality, the number of layers p is finite, so the algorithm is approximate.

EXAMPLE: ISING MODEL ON A LATTICE 2 × 2

Consider one-layer QAOA ansatz (2) for the Ising model with the Hamiltonian (1) on the 2×2 lattice. The four qubits in the quantum circuit (Fig. 1, $h = 1/2$) represent spins in the four lattice sites. The gates implement the driving $U(\gamma,\mathcal{H}_C)$ and mixing $U(\beta, B)$ operators. The following optimization procedures were used to minimize the energy $E_1(\gamma,\beta)$ in the space of two parameters γ and β:

— iterating through the parameters on a two-dimensional grid;

— optimization using the gradient descent method.

The data derived in the grid search can be used in the gradient descent method to choose a starting point. The distribution plot of the average energy values $E_1(\gamma,\beta)$ for the Hamilton operator (1), found by preparing the wave function $|\psi(\gamma,\beta)\rangle$ (2) ($p = 1$) in the space of two parameters γ and β, is shown in Fig. 2. For parameter values $\gamma = 1.0$, $\beta = 0.5$ the wave function $|\psi(\gamma,\beta)\rangle$ has the form $[-0.9999999, 0, \ldots, 0]$. Only the first component related to the state of the register $|0000\rangle$ is different from zero, and it corresponds to the bit

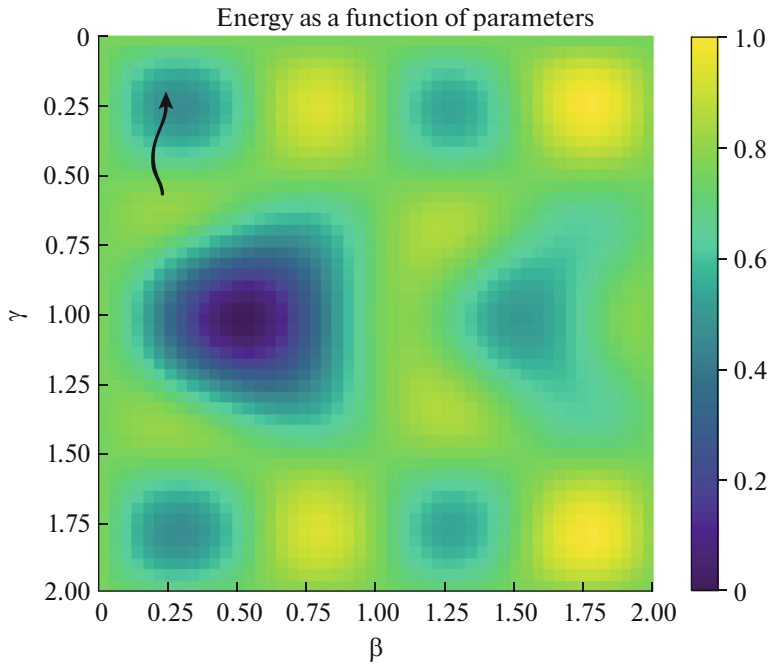

Fig. 2. Energy dependence $E_1(\gamma,\beta)$ on the parameters domain, derived from the circuit presented on Fig. 1. The gradient descent trajectory is indicated on the plot by a black line with an arrow.

string $z = 1111$. Such orientation of the spins really provides a minimum of energy for the Hamiltonian (1).

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CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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