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SYNERGY OF ARTIFICIAL INTELLIGENCE AND QUANTUM COMPUTING

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Abstract. The article examines theoretical and applied aspects of integrating artificial intelligence with quantum computing technologies, forming a new direction – quantum artificial intelligence. It is shown that quantum algorithms have the potential for exponential acceleration of computations in optimization problems, data analysis, machine learning, and image processing. Special attention is given to hybrid quantum-classical approaches demonstrating effectiveness in specific scientific and engineering problems such as catalyst selection and image clustering. Examples of quantum modeling of combinatorial problems and their transformation into quadratic binary programming formalism are presented. It is emphasized that quantum artificial intelligence is not a theoretical abstraction but a practically implementable technology with high potential in the era of NISQ computers.

Keywords: quantum artificial intelligence, quantum algorithms, Grover, quantum machine learning, hybrid computing, optimization, quantum image processing, quantum simulations, NISQ, intelligent systems.

1 Introduction

Modern science and technology are experiencing a stage of fundamental transformations driven by the rapid development of both artificial intelligence (AI) and quantum computing. AI is confidently penetrating the spheres of forecasting, diagnostics, optimization, and autonomous control, but as problem complexity increases, it encounters barriers of computational efficiency, especially when working with multidimensional, stochastic, or combinatorially complex systems. At the same time, quantum computing, relying on superposition, interference, and quantum entanglement, offers a revolutionary approach to information processing that surpasses classical algorithms in speed and resource efficiency. The merger of these two directions leads to the formation of a new scientific field – quantum artificial intelligence (Quantum AI), which combines the advantages of quantum data processing and the adaptability of AI models. Quantum algorithms such as the variational quantum solver (VQE), Grover's algorithm, quantum approximate optimization algorithm (QAOA), and variational quantum classifiers (VQC) are already finding applications in tasks previously considered unsolvable within reasonable timeframes. This suggests the beginning of a transition from classical to post-classical stage in the development of intelligent systems [1-2].

The relevance of the research is determined by the need to overcome fundamental limitations of classical AI systems associated with exponential complexity of optimization problems, learning on limited samples, and high sensitivity to noise. In the context of growing data volumes and increasingly complex decision-making models, traditional machine learning methods require significant computational resources and time. Quantum computing opens the way for implementing fundamentally new architectures and algorithms that can provide both acceleration and improved accuracy of analysis, especially in applied fields such as quantum chemistry, medicine, energy, and image processing. Moreover, quantum technologies are already implementable at the prototype level (NISQ era – Noisy Intermediate-Scale Quantum), making the research not only theoretically important but also practically reproducible. In conditions of increasing global competition in quantum development, the timely implementation of hybrid quantum-classical AI models represents a strategically important task [3].

The aim of this work is to analyze and demonstrate the advantages of the quantum-classical approach in artificial intelligence tasks based on the application of variational quantum algorithms, quantum optimization methods, and quantum machine learning [4-5].

To achieve this goal, the following tasks were formulated:

- Investigate the possibilities of integrating classical AI models with quantum computational schemes.
- Conduct comparative analysis of quantum algorithms (Grover, QAOA, VQE, VQC) with classical counterparts in optimization and data processing tasks.
- Develop and implement models for hybrid processing of images and texts using quantum methods.
- Test the proposed approaches on real problems such as nanocatalyst selection, traveling salesman problem, and route optimization.
- Evaluate the efficiency, accuracy, and scalability of quantum-classical AI solutions under limited quantum hardware (NISQ) conditions.

The presented work has scientific novelty through the integration of quantum computational algorithms (Grover, QAOA, VQE, VQC) with artificial intelligence models for solving problems of high computational complexity. For the first time, a hybrid architecture combining the classical self-consistent field method (SCF) with quantum energy corrections has been proposed, significantly improving the accuracy of selecting nanomaterials and catalysts. Quantum schemes for processing images and texts have also been developed and tested, demonstrating advantages in noise suppression, feature clustering, and resource efficiency reduction. For the first time, quantum optimization algorithms have been adapted to practical engineering tasks, including logistics (TSP, VRP) and traveling salesman problems, using formalization through quadratic binary programs (QUBO) and implementation on NISQ-era quantum simulators [6-8].

The practical value of the work lies in the fact that the proposed hybrid quantum-classical models can be implemented on modern quantum simulators and applied to real practical problems. The developed quantum image processing methods are promising for use in medicine, intelligent video surveillance, and automated diagnostics. Quantum solvers for catalyst selection tasks open possibilities for accelerated design of new functional materials in chemistry and energy. The obtained results can also be used in educational and research practice, promoting the introduction of courses and laboratory work on quantum artificial intelligence and its applications [9-10].

2 Methods

1. Variational Quantum Eigensolver (VQE).

The goal is to find the minimum eigenvalue of a Hamiltonian $\hat{H}$ based on a parameterized quantum state:

$$E(\vec{\theta}) = \langle \psi(\vec{\theta}) | \hat{H} | \psi(\vec{\theta}) \rangle \to \min_{\vec{\theta}},$$

where $|\psi(\vec{\theta})\rangle$ – is a quantum state created by a parameterized quantum circuit, $\vec{\theta}$ – is a vector of parameters selected by a classical optimizer.

2. Quantum Approximate Optimization Algorithm (QAOA).

An optimization problem of the form:

$$\min_{z \in 0,1^n} C(z)$$

is solved using alternating unitary evolution operators:

$$|\gamma, \beta\rangle = \prod_{j=1}^{p} e^{-i\beta_j H_M} e^{-i\gamma_j H_C} |s\rangle,$$

where H_C – is the cost Hamiltonian, H_M – is the mixer operator, and $|s\rangle$ – is the initial uniform state. Parameters (γ_j, β_j) are optimized to minimize:

$$\langle \gamma, \beta | H_C | \gamma, \beta \rangle .$$

3. Grover's Algorithm.

For accelerated quantum search in a database of $N = 2^n$ states, the number of iterations:

$$R \approx \left\lfloor \frac{\pi}{4} \sqrt{N} \right\rfloor,$$

where each step includes applying the oracle operator $\hat{O}$ and amplitude amplification (diffusion operator) $\hat{D}$:

$$\hat{G} = \hat{D} \cdot \hat{O} .$$

4. Variational Quantum Classifier (VQC).

The model implements mapping of input features $x \in R^n$ into quantum space through circuit $U(x)$, and the classification decision is made based on measurements:

$$y = \text{sign}\left(\langle 0 | U^{\dagger}(x) M U(x) | 0 \rangle \right),$$

where M is the observable operator (usually Pauli-Z or a combination of Pauli operators).

5. Transformation of problems into QUBO form.

For the traveling salesman problem and other discrete optimization problems, reduction to quadratic binary optimization form is applied:

$$\min_{x \in 0,1^n} x^T Q x ,$$

where $Q \in R^{n \times n}$ is a matrix of coefficients (costs and constraints), and x is a binary solution vector. This formulation is compatible with quantum solvers (QAOA, VQE) and hardware implementation in the form of the Ising model:

$$H = \sum_i h_i z_i + \sum_{i<j} J_{ij} z_i z_j \text{ где } z_i \in \{-1, +1\} .$$

6. Metric of expressibility of quantum circuits.

To evaluate the ability of a quantum circuit to represent different states, expressibility is used:

$$\mathcal{E} = \text{Tr}\left(\rho^2 \right), \quad \rho = \mathbb{E}_{\vec{\theta}} \left[|\psi(\vec{\theta})\rangle\langle\psi(\vec{\theta})| \right],$$

where ρ is the average density state across parameters.

3 Results

During the research, quantum and hybrid algorithms were implemented and tested on quantum computing simulators (Qiskit + AerSimulator), which allowed obtaining a number of important practical and numerical results.

1. Optimization of catalysts using a hybrid SCF+VQE algorithm. A variational quantum circuit (VQE) was implemented to evaluate quantum-corrected energy of catalysts selected after physicochemical filtration based on SCF. The scheme used included:

- Parameterized ansatz circuit stage based on RealAmplitudes.
- Measurement of the expected value of the Hamiltonian.
- Classical optimization of parameters.

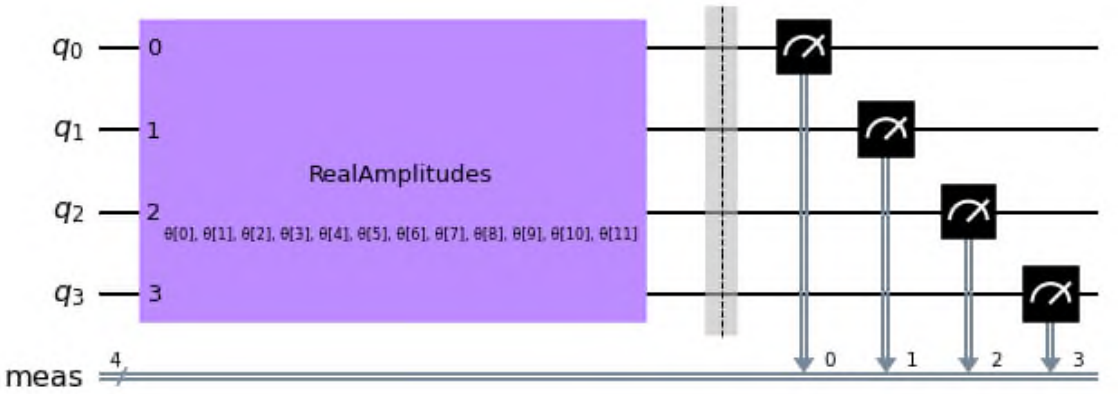


Fig. 1. Parameterized quantum VQE circuit using RealAmplitudes and energy measurement on AerSimulator

2. Quantum Approximate Optimization Algorithm (QAOA) for the traveling salesman problem.

The TSP was reduced to QUBO form, after which the QAOA algorithm with depth p=2 was applied. Binary solutions corresponding to optimal routes on graphs of 5 and 10 cities were obtained.

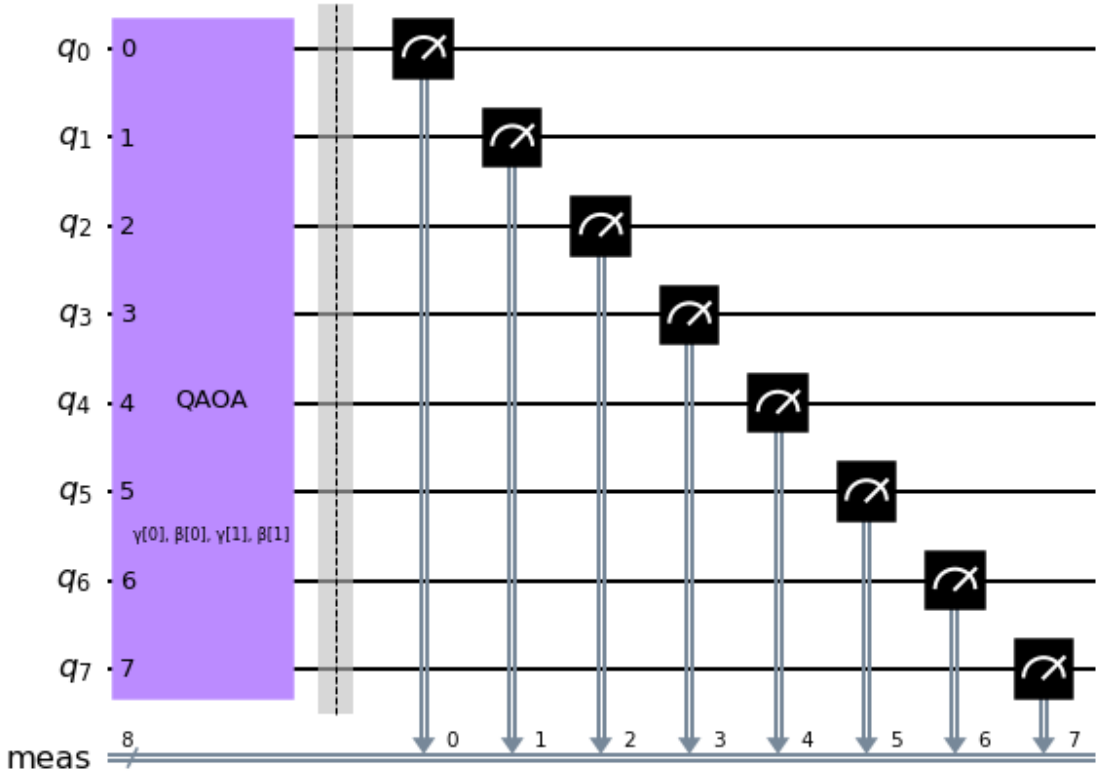


Fig. 2. QAOA scheme with two layers (p = 2) for solving the traveling salesman problem after transformation to QUBO

3. Quantum image enhancement.

Using quantum circuits, the following were implemented:

- Image filtering based on quantum superposition.
- Contrast enhancement through wavelet-quantum transformation.
- Quantum Sobel filter for edge detection.

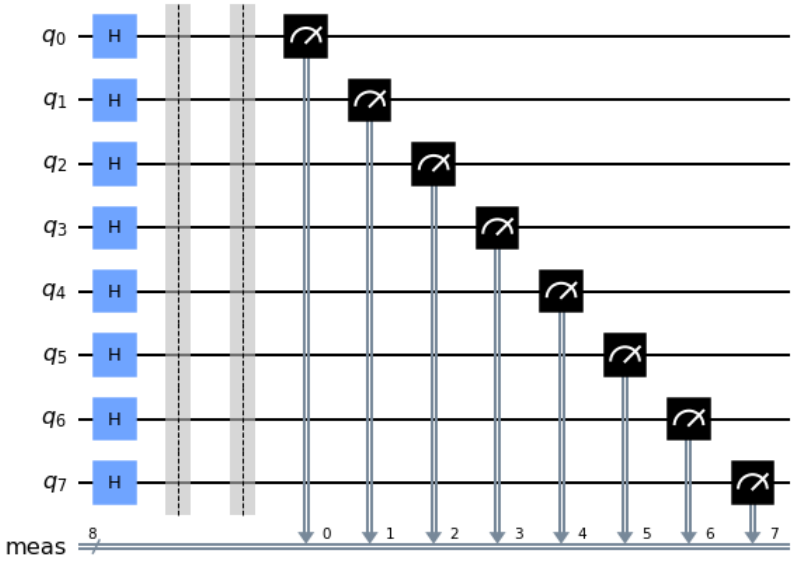


Fig. 3. Example of a quantum circuit for filtering an 8×8 image, simulating noise suppression

4 Conclusion

The conducted research confirms the high efficiency of integrating quantum computing and artificial intelligence methods in solving optimization problems, data analysis, and forecasting. The application of quantum algorithms such as QAOA, VQE, and Grover demonstrates a significant advantage compared to classical methods in conditions of exponential dimensionality of the state space and combinatorial complexity. Particularly promising was the implementation of hybrid quantum-classical schemes, allowing the combination of the accuracy of classical models (such as SCF) with the computational power of quantum ansatzes. The schemes developed and tested on simulators (Qiskit, AerSimulator) showed practical reproducibility of the approach already on existing NISQ era equipment. This opens the way for scalable application of quantum artificial intelligence in real-world tasks – from selection of functional materials and catalysts to intelligent image processing, logistics, and text analysis. In the future, it is expected that the development of quantum hardware will strengthen the role of such hybrid algorithms, laying the foundation for creating more accurate, fast, and adaptive intelligent systems.

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СИНЕРГИЯ ИСКУССТВЕННОГО ИНТЕЛЛЕКТА И КВАНТОВЫХ ВЫЧИСЛЕНИЙ

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Аннотация. В статье рассматриваются теоретические и прикладные аспекты интеграции искусственного интеллекта с технологиями квантовых вычислений, формируя новое направление – квантовый искусственный интеллект. Показано, что квантовые алгоритмы обладают потенциалом экспоненциального ускорения вычислений в задачах оптимизации, анализа данных, машинного обучения и обработки изображений. Особое внимание уделено гибридным квантово-классическим подходам, продемонстрировавшим эффективность в конкретных научных и инженерных задачах, таких как выбор катализаторов и кластеризация изображений. Приведены примеры квантового моделирования комбинаторных задач и их преобразования в формализм квадратичного бинарного программирования. Подчеркивается, что квантовый искусственный интеллект — это не теоретическая абстракция, а практически реализуемая технология с высоким потенциалом в эпоху квантовых компьютеров NISQ.

Ключевые слова: квантовый искусственный интеллект, квантовые алгоритмы, алгоритм Гровера, квантовое машинное обучение, гибридные вычисления, оптимизация, квантовая обработка изображений, квантовые симуляции, NISQ, интеллектуальные системы.

SUN’IY INTELLEKT VA KVANT HISOBLASHNING O‘ZARO UYG‘UNLIGI

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Annotatsiya. Maqolada sun’iy intellektni kvant hisoblash texnologiyalari bilan integratsiya qilishning nazariy va amaliy jihatlari ko‘rib chiqilib, “kvant sun’iy intellekti” deb nomlanuvchi yangi yo‘nalish shakllanishi yoritiladi. Kvant algoritmlar optimallashtirish masalalari, ma’lumotlarni tahlil qilish, mashinaviy o‘qitish va tasvirlarni qayta ishlashda hisoblash jarayonlarini eksponentsial tezlashtirish imkoniyatiga ega ekani ko‘rsatiladi. Katalizator tanlash va tasvirlarni klasterlash kabi aniq ilmiy va muhandislik masalalarida samaradorlikni namoyon etgan gibrid kvant-klassik yondashuvlarga alohida e’tibor qaratilgan. Kombinatorik masalalarning kvant modellashtirilishi va ularni kvadratik binar dasturlash (QBP) formalizmiga o‘tkazish bo‘yicha misollar keltiriladi. Kvant sun’iy intellekti nazariy abstraksiya emas, balki NISQ davri kompyuterlarida amalda tatbiq etilishi mumkin bo‘lgan yuqori salohiyatli texnologiya ekani ta’kidlanadi.

Kalit so‘zlar: kvant sun’iy intellekti, kvant algoritmlar, Grover algoritmi, kvant mashinaviy o‘qitish, gibrid hisoblash, optimallashtirish, kvant tasvirni qayta ishlash, kvant simulyatsiyalari, NISQ, intellektual tizimlar.