Calculations on a quantum computer performed at IPCP RAS

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Quantum computers based on quantum phenomena such as superposition and entanglement [1] are expected to perform tasks which surpass the capabilities of modern classical digital computers [2]. First quantum computers were made quite recently and are limited to noisy intermediate-scale quantum (NISQ) technology. Quantum calculations open new possibilities for solving problems in various branches of science such as molecular and atomic calculations, structural chemistry, magnetic resonance and so on. Although the accuracy of today's calculations on quantum computers is insufficient owing to errors of quantum gates, it is still possible to perform quantum calculations for some relatively simple tasks. Taking into account fantastic advantages of quantum computers over their classical counterparts which is expected to be released in future, development of quantum algorithms is a challenging and useful task.

Quantum algorithms are based on Solovay-Kitaev theorem [1] according to which every unitary operator can be represented as a product of one- and two-qubit gates. A quantum algorithm can be represented as a circuit consisting of specially tailored gates which allows to solve the given problem. A lot of such algorithms were worked out in the Institute of Problems of Chemical Physics recently. In some cases we not only solved a concrete task but developed the method of correction of errors which were connected with errors of a quantum computer. All calculations were conducted on the 5-qubit quantum processor of IBM superconducting quantum computer. The following developed algorithms should be mentioned: algorithm for solving a system of three linear algebraic equations [3], calculation of the number π on quantum computer [4], simulation of multiple quantum NMR dynamics of a spin dimer on a quantum computer [5]. In all cases solutions obtained on quantum computer coincide with good accuracy with known theoretical results.

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