Day 3 (Poster D)

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Title: Improving accuracy of energy estimation by combining quantum annealing with classical computation

Abstract:
Quantum chemistry calculations are important applications of the quantum annealing(QA). Especially，the energy of the chemical molecule contains essential information. However，when we use the QA，there is no guarantee about the accuracy of the energy estimation. In this talk，we propose a way to improve the accuracy of the estimate of the ground state energy by combining quantum annealing with a classical computer. In our scheme，before running the QA，we need a pre-estimation of the energies of the ground state and first excited state with some error bars (corresponding to possible estimation error) by performing classical computation with some approximations. We show that，if an expectation value and variance of the energy of the state after the QA are smaller than certain threshold values (that we can calculate from the pre-estimation)，the QA provides us with a better estimate of the ground state energy than that of the pre-estimation. Our scheme would be useful to measure the energy of molecules with chemical accuracy when quantum annealing with long-lived qubits becomes available. Our talk is based on arXiv 2102.05323.