Simulating quantum systems in biology, chemistry and physics

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In principle, it is possible to model any physical system exactly using quantum mechanics; in practice, it quickly becomes infeasible. Recognising this, Richard Feynman suggested that quantum systems be used to model quantum problems [1]. For example, the fundamental problem faced in quantum chemistry is the calculation of molecular properties, which are of practical importance in fields ranging from materials science to biochemistry. Within chemical precision, the total energy of a molecule as well as most other properties, can be calculated by solving the Schrodinger equation. However, the computational resources required to obtain exact solutions on a conventional computer generally increase exponentially with the number of atoms involved [1, 2]. In the late 1990's an efficient algorithm was proposed to enable a quantum processor to calculate molecular energies using resources that increase only polynomially in the molecular size [2–4]. Despite the many different physical architectures that have been explored experimentally since that time—including ions, atoms, superconducting circuits, and photons—this appealing algorithm has not been demonstrated to date.

Here we take advantage of recent advances in photonic quantum computing [5] to present an optical implementation of the smallest quantum chemistry problem: obtaining the energies of H2, the hydrogen molecule, in a minimal basis [6]. We perform a key algorithmic step—the iterative phase estimation algorithm [7–10]—in full, achieving a high level of precision and robustness to error. We implement other algorithmic steps with assistance from a classical computer, explain how this non-scalable approach could be avoided, and provide new theoretical results which lay the foundations for the next generation of simulation experiments.

We also report on our recent results in simulating quantum systems in material science—phase transitions in topological insulators—and in biology—light-harvesting molecules in photosynthesis. Together this body of work represents early experimental progress towards the long term goal of exploiting quantum information to speed up calculations in biology, chemistry and physics.

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