Title:
Algorithmic Cooling: Putting a New Spin on the Identification of Molecules

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Abstract:

In this talk I will present "Algorithmic Cooling of Spins", which is potentially the first near-future application of quantum computing devices. I will explain how straightforward quantum algorithms combined with novel entropy manipulations can result in a method to improve the identification of molecules.

Molecules are built from atoms, and the nucleus inside each atom has a property called "spin". The spin can be understood as the orientation of the nucleus, and when put in a magnetic field, certain spins are binary, either up (ZERO) or down (ONE). Several such bits (inside a single molecule) represent a binary string, or a register. A macroscopic number of such registers/molecules can be monitored in parallel, as is done, for instance, in Magnetic Resonance Imaging (MRI). Commonly, the purpose of such monitoring techniques is the identification of molecules for chemical or biomedical purposes. From the perspective of quantum computation, the spectrometric device that typically monitors and manipulates these bits/spins can be considered a simple "quantum computing" device.

Improving the molecule identification process is a Holy Grail in the area of Nuclear Magnetic Resonance (NMR). A common approach to this problem, known as "effective cooling", has been to reduce the entropy of spins. A spin with lower entropy is considered "cooler", and provides a better signal when used for identifying molecules. To date, effective cooling methods have been plagued by various limitations and feasibility problems.

We invented "Algorithmic Cooling", a novel and unconventional effective-cooling method that vastly reduces spin entropy. Algorithmic Cooling makes use of "data compression" algorithms (that are run on the spins themselves) in combination with "decoherence". Due to Shannon's entropy bound, data compression alone is highly limited in its ability to reduce entropy: the total entropy of the spins in a molecule is preserved, and therefore, cooling one spin is done at the expense of heating others. Entropy reduction is boosted drastically by taking advantage of the phenomenon of decoherence, the natural return of a spin's entropy to its thermal equilibrium value. Our entropy manipulation steps are designed such that the excess entropy is always placed on pre-selected spins, called "reset bits", which return very quickly to thermal equilibrium. Alternating data compression steps with decoherence of the reset spins thus reduces the total entropy of the spins in the system *far beyond* Shannon's bound. The Algorithmic Cooling of short molecules is experimentally feasible in conventional NMR labs; we, for example, recently cooled spins of a three-bit quantum computer beyond Shannon's entropy bound.