QUANTUM INFORMATION

Quantum search on a single-atom qudit

A terbium-based molecular magnet, containing four nuclear quantum states, or a qudit, experimentally validates the Grover algorithm for database searches.

Andrea Morello

Progress in quantum information science has often taken place in bursts, usually triggered by remarkable theoretical discoveries. A crucial one was due to Grover, who developed a quantum algorithm to search through an unsorted database of N items[1]. Classically, there exists no better search strategy than exhaustively checking every item, requiring on average $N/2$ attempts before finding the desired entry. The Grover algorithm works by identifying the items in the database with the basis states of a quantum system in an N-dimensional Hilbert space. The computation starts by creating an equal quantum superposition of all the N states, and then repeats an operation whereby the amplitude of the desired item is enhanced at each step. After a number of steps of order $\sqrt{N}$, the initial superposition collapses onto a state that contains almost exclusively the sought item, so it can be found with high probability by measuring the final state of the system. This was the first quantum algorithm whose complexity is provably lower than the best classical one.

Now, writing in *Physical Review Letters*, Godfrin *et al.* describe the experimental demonstration of Grover's search algorithm using a single nuclear spin, held within a single-atom magnet[2]. This experiment is noteworthy for many reasons. First, it implements a particular version of Grover's search, which constitutes what has been called an "analog analogue"[3] of the original algorithm. Second, it does so by using a single multi-level quantum system (called a qudit), instead of several coupled qubits.

In this case, the qudit is made of $d = 4$ energy levels generated from the $I = 3/2$ nuclear spin of a single terbium (Tb) atom. The Tb atom is surrounded by organic ligands and attached to a pair of electromigrated gold contacts to form a single-molecule transistor. Remarkably, the hyperfine interaction between the Tb nucleus and the surrounding electrons results in a process whereby the quantum state of the nucleus can be inferred by measuring the value of the magnetic field at which the total electron angular (spin plus orbital) momentum, J, flips direction[4]. This flipping event is itself a fascinating quantum effect, involving quantum tunnelling[5] of a large electronic angular momentum ($J = 6$ in this system) through a very high energy barrier. The electron spin orientation, in turn, affects the conductance through the molecule, which provides an electrical measurement of the combined electron and nuclear spin states. The final ingredient is an oscillating electric field which, thanks to the anisotropy of the electron–nuclear hyperfine coupling, provides coherent control of the nuclear spin states[6].

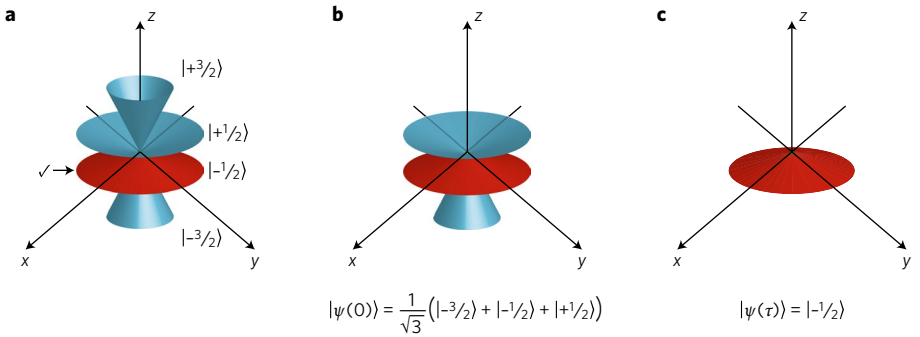

Fig. 1 | Analog Grover algorithm on a single-atom magnet. a, One of the four states of Tb nuclear spin is labelled by an energy shift in the rotating frame. **b**, The algorithm starts by preparing the system in an initial $|\psi(0)\rangle$ state that contains an equal superposition of $N = 3$ of the possible states — here, $|-3/2\rangle$, $|-1/2\rangle$, $|+1/2\rangle$. **c**, Driving the system with a multi-frequency alternating electric field causes it to oscillate between the initial state and the target state, which is reached after a time τ proportional to $\sqrt{N}$.

The way the quantum search algorithm proceeds is a beautiful example of how the natural evolution of quantum systems can be harnessed for computational tasks. First of all, what does it mean to search for something? The location of the wanted item — let's call it $|w\rangle$ — is unknown, but it must have some known property — a label — that allows us to recognize it when we encounter it. For quantum states, the natural label is their energy. Therefore, searching a quantum database means finding the only basis state that has a specific, known energy.

And here comes the magic of quantum mechanics. Instead of checking each item to inspect its label, we can create an equal superposition of all states — let's call it $|s\rangle$ — and impose that $|s\rangle$ and $|w\rangle$ have the same energy. This is obtained by adding energy to the system, that is, by driving it using an external field. As illustrated in the textbook example of the ammonia molecule[7], when two quantum states have the same energy, the system oscillates between the two. Therefore, a system prepared in $|s\rangle$ will naturally begin to oscillate and eventually reach $|w\rangle$, the wanted item (Fig. 1).

How long does this take? In the digital Grover algorithm, the item is found after $\sqrt{N}$ steps[1]. The analogue version implemented here is, at face value, a single-step operation, namely the driving that causes the system to oscillate from $|s\rangle$ to $|w\rangle$. However, one can show[3] that the period of oscillation is itself proportional to $\sqrt{N}$, unveiling the Grover-like dependence of the search time on the size of the database.

In the experiment of Godfrin *et al.*, three of the four nuclear spin states of the Tb nucleus are used as the database. The label of the wanted item is provided by its energy in a generalized rotating frame[8], in which the Hamiltonian appears time-independent while the system is subject to a carefully chosen multiple-frequency excitation. The advantage of working in a rotating frame is that the energy of each state is represented by its frequency detuning from the external drive. Therefore, labelling an item is as simple

as choosing the external frequency to be off-resonance with the desired state! Similarly, the superposition state and its subsequent driven evolution are obtained by tailoring a multi-frequency excitation signal, produced point-by-point with an arbitrary waveform generator.

This elegant and efficient way to perform quantum searches on a single qudit could be applied to any system in which the d levels are not equispaced, for example the nuclear spin $I > 1/2$ of a dopant in a semiconductor in the presence of strong quadrupolar interactions[8]. A typical criticism aimed at this approach is that it does not scale up: there is a limit to the maximum spin values one can find in nature, and this limit is quite low. Scaling up requires linking coherently multiple spins, a challenge that is being addressed in semiconductors[9] as well as single-atom magnets[10]. Meanwhile, experiments like that of Godfrin *et al.* provide inspiring examples of what can be achieved with the careful quantum control of individual systems with a large Hilbert space. ❐

Andrea Morello
Centre for Quantum Computation and Communication Technology, School of Electrical Engineering and Telecommunications, UNSW Sydney, Sydney, Australia.
e-mail: a.morello@unsw.edu.au

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