

Optimising control over nuclear spin transitions

- Controlling transitions between the spin states of atomic nuclei is a fundamental aspect of modern technologies as wide-ranging as medical imaging, chemical analysis, and quantum computing.
- Through new analysis, a team led by Professor Navin Khaneja at Indian Institute of Technology Bombay (IIT Bombay) shows how the efficiency of these transitions can be linked to the basic mathematics of rotating points.
- Building on these principles, the team shows how control over these transitions can be optimised in both NMR spectroscopy and quantum computing.

Many quantum particles possess a property, called 'spin', which can either point 'up' or 'down' along an axis of rotation running through the particle. Spin plays a vital role in many cutting-edge technologies, including Nuclear Magnetic Resonance (NMR) spectroscopy and quantum computing.

Spin states in two different technologies

NMR spectroscopy uses strong, steady magnetic fields to align the spins of the atomic

nuclei in the sample being imaged, and then probes the sample with a range of radio frequency pulses. At specific frequencies, nuclei will absorb the energy contained in these pulses, causing their spins to flip direction. Whether or not this absorption occurs depends on the type of nucleus as well as those of other nuclei in its surrounding chemical environment.

As they relax back to their original spin states, the nuclei in the sample will re-emit the energy they absorbed. By recording the

frequency and intensity of these re-emitted signals, researchers can then make accurate measurements of the sample's chemical composition. This approach is now employed

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across a diverse array of applications, helping researchers to analyse chemical samples on molecular scales, and providing detailed images of internal body structures, making it an invaluable imaging technique in medicine.

Along with NMR spectroscopy, spin states also play an immensely important role in quantum computing. Whereas the bits in a regular computer can occupy one of the two states, either a 0 or a 1, the quantum bits, or 'qubits' in a quantum computer can exist in a superposition of both states simultaneously, allowing quantum computers to perform certain calculations far more quickly.

Quantum computers can use a variety of different properties of quantum particles as qubits, but spin states are especially desirable for a variety of reasons – including their ability to retain quantum information over extended periods, and for their ease of manipulation into desired states.

Rotation between two points

Although it may not appear to be relevant at first glance, Navin Khaneja, Professor of Systems and Control at IIT Bombay, India,

argues that the performance of both of these technologies is directly affected by a basic mathematical rule. No matter their relative positions, the shortest path between two points will always be a straight line. If you change direction while travelling between them, the path will no longer be optimal.

As Khaneja explains, the same is true if you want to rotate a point from the north pole of a sphere to its south pole. 'To rotate the point at a fixed rate, it is necessary to choose a transverse axis to rotate around and stick with it,' he says. If this axis were changed along the way, the rotation would become less efficient.

According to Khaneja and his colleagues, rotations are a fundamental aspect of both quantum computing and NMR spectroscopy. In these technologies, data is stored in the form of up and down states. 'Quantum gates are used to transform these states, which essentially involves rotating them around specific axes,' explains Khaneja.

Quantum gates are directly analogous to the gates in regular computers, which perform logic operations on one or more bits. Through

their research, Khaneja's team aim to show how rotation-like spin state operations can be carried out more efficiently in both qubits and NMR samples.

Combining Hamiltonians

In the context of quantum mechanics, rotations are generated by mathematical operators named 'Hamiltonians', which effectively define the axes about which particles rotate. In systems containing two different types of quantum spin, there are essentially two different types of Hamiltonians. The first of these are 'control' Hamiltonians, which rotate the two spins and occur very quickly. The second are the 'coupling' Hamiltonians through which the two spins interact with each other and occur far more slowly.

In practical technologies like quantum computing and NMR spectroscopy, these two types of Hamiltonians often need to be combined, allowing researchers to encode, process, and retrieve information from nuclear spins. Khaneja explains that when looking to combine the two Hamiltonians, choosing the axes that 'commute' with each other is vital. This ensures that the rotations can then be performed in any order with no change in the outcome. Since there are only a finite number of available axes, it is of crucial importance to choose them optimally.

By taking this into account, Khaneja's team could then describe how quantum gates in both technologies can be created by changing how nuclear spins interact with each other. Importantly, they show that through the careful consideration of optimal rotations, generated by control and coupling Hamiltonians which commute with each other, interactions can be set up so that they can be carried out in any order, without changing the final result of the operation.

In doing this, the researchers show how complex rotation operates as efficiently

as possible. 'This principle of optimality extends to control systems where rotations can be split into slow, interaction-like directions and fast, control-like directions,' Khaneja adds. Moving along Hamiltonian-commuting directions is the most efficient way to achieve the desired rotations.

Khaneja's team now hopes that the insights gathered through their analysis will provide useful guidance for researchers in future studies. Ultimately, this may help to improve efficiency in both quantum computing and NMR spectroscopy, as well as other technologies involving transitions between nuclear spin states.

Personal response

How could your findings be implemented in real-life quantum computing and NMR apparatus?

In NMR, the commuting Hamiltonians can be produced by controlling the phase of the radiofrequency pulses we apply.

How much more efficient do you anticipate these technologies could become if your findings are implemented?

We expect and have demonstrated time improvements ranging from 10–100% in NMR methods in spectroscopy and quantum computing compared to conventional techniques.

What other technologies could your insights be applied to?

These methods will also find use in superconducting qubits and trapped ion quantum computers.

Details



e: navinkhaneja@gmail.com
w: www.sc.iitb.ac.in/~nkhaneja

Funding

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Collaborators

• Steffen Glaser
• Haidong Yuan

Bio

Navin Khaneja received his BTech in electrical engineering from IIT Kanpur (1994), MA and MSc in mathematics and electrical engineering from Washington University, St. Louis (1997), and PhD in Applied Mathematics from Harvard University (2000). He is the recipient of the NSF career award, The Sloan fellowship, and the Bessel Prize of the Humboldt Foundation. His research focuses on areas of control theory and NMR spectroscopy. He is the author of about 90 journal papers.

Further reading

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- Khaneja, N, Brockett, R, Glaser, SJ, (2001) Time optimal control in spin systems. *Physical Review A*, 63(3), 032308.

