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Recent Advances

Q-Bits & Pieces

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1. Nature isn't classical, dammit!

If you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy! This was what Richard Feynman's take on simulating real-life problems. Now, many decades after his words of wisdom we actively discuss simulating processes such as photosynthesis an important job only a Quantum Computer (QC) can take up. Now, if one says the QC can revolutionize the fertilizer industry, save you 100s of billions of dollars per year and prevent a huge amount of greenhouse gas emission, it is not a propaganda, do not laugh it off. Ammonia is an unavoidable component in any commercially available fertilizers. For more than a century it has been manufactured using Haber-Bosch process where the atmospheric nitrogen is combined with hydrogen derived from methane or other fossil fuels under extreme pressure and temperature conditions. Approximately 3% of the world's total energy is budgeted for this process, also contributing the largest greenhouse gas and carbon foot print. Surprisingly the ammonia is also produced in the roots of plants at ambient temperature and pressure with help of a tiny nitrogen fixing bacteria with help of enzyme nitrogenase present in them, the process called *nitrogen fixation*, is still not decoded.

2. What is the complexity of the problem?

The important player here is a cofactor (FeMoco) embedded in a protein (MoFe protein) which can split the N_2 to form two Ammonia molecules.[1] To understand the process, one need to have a good grasp of the structure and configuration of the protein, more importantly the cofactor. Surprisingly this is a daunting task given the complexity of the molecule which contains multiple transition metal ions with multiple charge stages and complex spin couplings. The configurations and intermediate states for simple molecules can be calculated using toady's computer, but as the number of electrons and interactions grows the complexity scales exponentially and the very best one could do today is about 50 strongly interacting electrons! But to get even a qualitative picture of the cofactors role one need to consider at least 103 electrons in 71 orbitals which is too much to handle for any imaginable computer in any imaginable timeframe.[2] Classical computers often take various approximations and simplifications to make similar problems solvable. Though this

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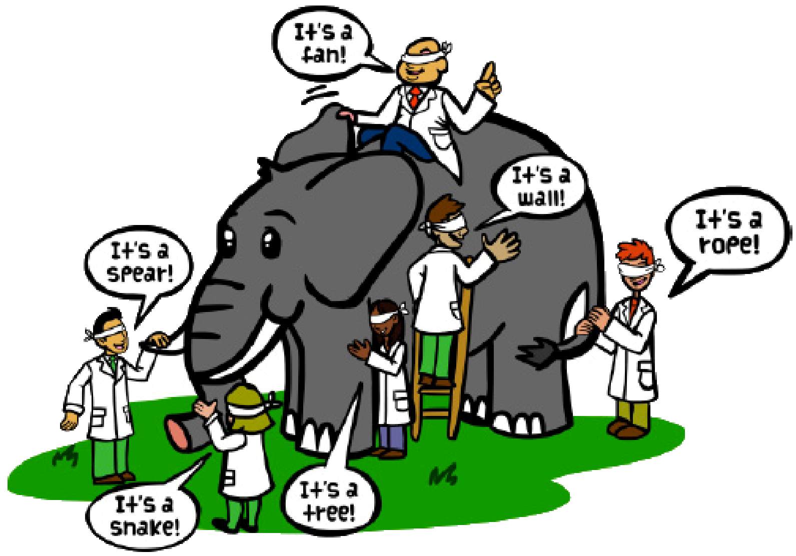
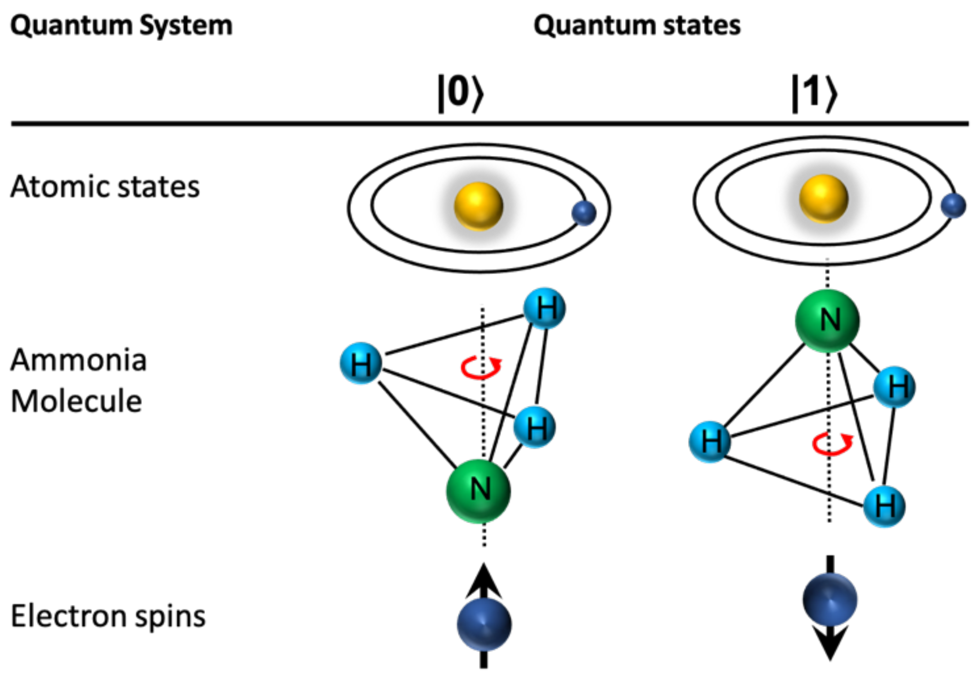


Probing quantum chemistry problems with a classical computer is similar to six blind men trying to visualize the elephant by touching.

might work for simple organic chemistry problems, when it comes to inorganic processes often masks the entire flavour of the problem and you will end up in a situation comparable to Six blind men seeing an elephant. Another stellar example where quantum chemistry at its best is photosynthesis where plants combine CO_2 and water to form starch using the energy available in the sunlight. If we could crack this recipe, one can artificially produce starch and enter a hunger-free world. Needless to say, a classical computer cannot solve these problems, even in best of its dreams.

3. What makes quantum computers superior?

Processes which are inherently quantum mechanical need a quantum system to bring out the full physics flavour. Classical computer works in the premise of deterministic nature while Quantum mechanics has its foundations built on uncertainty, superposition and entanglement. The building blocks of classical computers, the transistors or **the bits** assume two well defined states, **0** and **1**. The bits in a quantum computers, **the qubits**, are also two-state systems, but follow the laws of quantum mechanics. These qubits outmuscle classical-bits owing to two quantum effects: the superposition and the entanglement. Superposition allows a qubit to have both states, the **0** and the **1** at the same time enabling simultaneous computation while, entanglement enables one qubit to share its state with another distant one. An algorithm using, say, five entangled qubits can effectively do 32, computations in parallel, while the classical computer would have to do these 32 computations sequentially. For a 64 qubit system there are 2^{64} = 18,446,744,073,709,600,000 possibilities! While 64 regular bits can also represent this huge number (2^{64}) of states, but only one at a time. To cycle through all these combinations with a two GHz clock speed would take about 400 years. A regular computer tries to solve a problem the same way you might try to escape a maze – every path sequentially, turning back when you hit a wall - start again, till you eventually find the way out. But superposition allows the quantum



computer to try all the paths at once – Another way to say this is these paths are mutually dependent, while the classical paths are mutually independent. This power enables the QC to tackle problems requiring large amount of computational resources such as the nitrogen fixation or photosynthesis.[3]

4. The start, the hype, and the prospects

Qubits are two-state quantum systems. Ground and excited states of an atom, states of ammonia molecule or the UP and DOWN spin states of an electron are good examples of such systems. In a classical computer, the states of the bits are accessed by varying the gate voltages taking the bit from an OFF state to the ON state or vice versa. In a quantum computer, the states are accessed via the exchange of appropriate energy quanta between the qubit and the driving circuit. During the initial stage of the revolution there were a number of candidates proposed for hosting qubits. All are bistable quantum states of molecules, atoms, ions, electrical circuits or spin states of electrons.

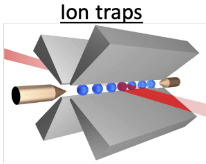
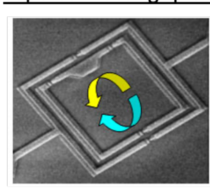
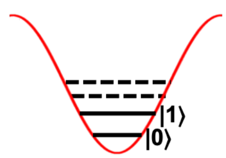
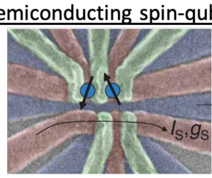
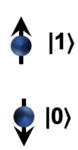
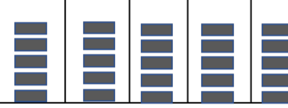
Now, comes the practical question - Can any bi-state quantum system form qubits? The answer is negative! The concept of quantum computation was triggered by Feynman, a proper frame work of Quantum computers was proposed by David DiVincenzo who put forth a set of criteria for candidate systems to qualify for hosting Quantum computers, popularly known as DiVincenzo criteria, listed in the associated table.[4]

Over the time, it has been realized that only less than a handful among the many aspiring qubit candidates satisfy the criteria. The major contenders are the ion-traps, superconducting circuits and semiconducting quantum dot circuits- summarized in the associated table with their concurrence to the DiVincenzo criteria.[5] A word of caution, among these finalists, there are no clear winners; It is a swiftly evolving field. Apart from these three, any other surprising system may evolve as the leading candidate.

Being an emerging technology, projected to bring multifaceted revolution in many

DiVincenzo Criteria for the practical realization of qubits

1	Scalability	The physical system should be scalable to large number of Qubit
2	Initialization	Should be able to address the Qubits individually and initialize
3	Coherence	Long coherence time to run the computation
4	Universal gates	Should be able to realize one and two qubit gates
5	Measurement	Facilitate Reading out the result by a single quantum measurement

<table>
<tr><th rowspan="2">System</th><th rowspan="2">Quibt states
|0⟩ & |1⟩</th><th colspan="5">DiVincenzo criteria Score</th></tr>
<tr><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr>
<tr><td>Ion traps
</td><td>Two stable electronic states of the each ion form the qubit states.
➢ Ground state and excited states
➢ Two Hyperfine levels</td><td colspan="5"></td></tr>
<tr><td>Superconducting qubits
</td><td>Anharmonic quantum oscillator realized by superconducting tunnel junction systems. The lowest two levels forms the qubit state.
</td><td colspan="5"></td></tr>
<tr><td>Semiconducting spin-qubits
</td><td>Spin states of single electrons trapped using electrostatic gates on a piece of semiconducting materials such as Silicon or GaAs.
</td><td colspan="5"></td></tr>
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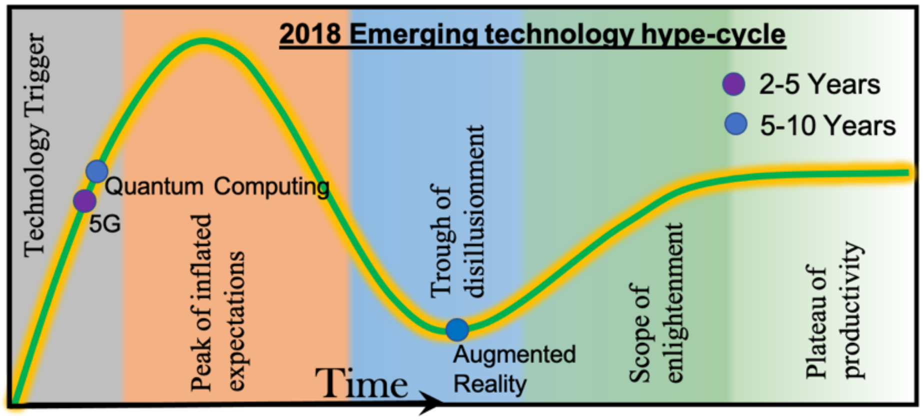
Leading candidate-systems for the realization of quantum computers.

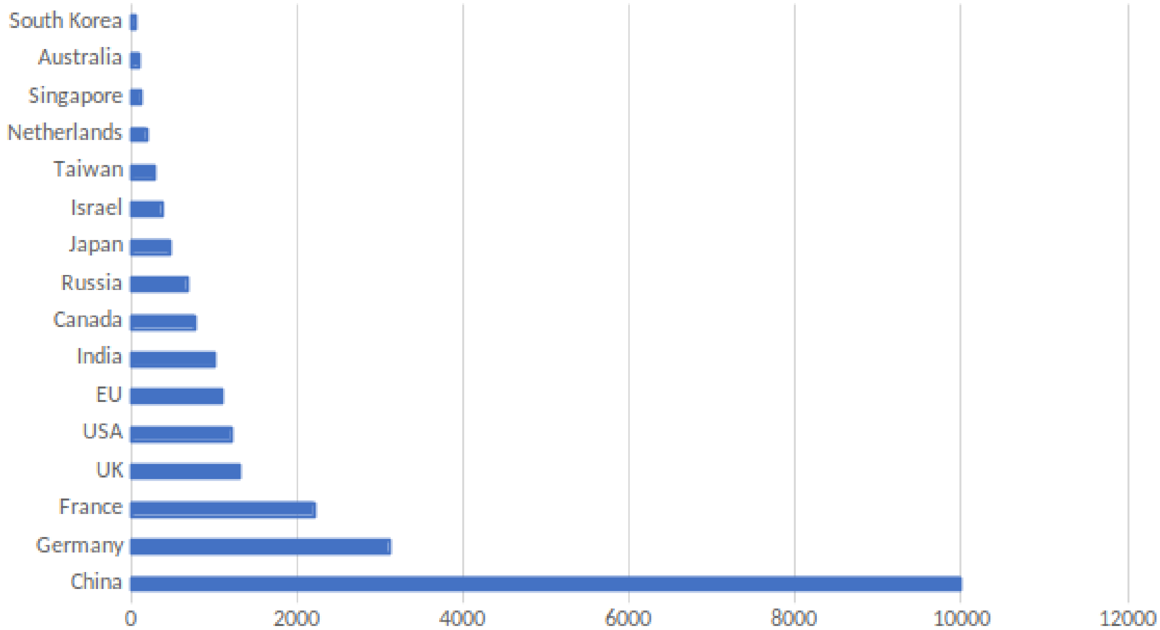


aspects of human life, starting from banking through chemical engineering to defense applications, the **hype-factor** around quantum computing has been running high ever since its proposal. The journey taken by any emerging technology to mature to the stage of social application has been observed to take more or less a common pattern, referred to as the **hype cycle.** This concept has been developed and used by the American research, advisory and information technology firm Gartner as a guide to the investors .[6] Quantum computing and quantum technologies have occupied spots on the hype-cycle multiple times suggesting that the business world has been seeing this as a serious financially viable future-technology. The 2018 and 2019 hype cycle predicts that the quantum computing would take around 5-10 years to mature. This is not a long-time compared to many of the other technologies figured out on the hype cycle. For example, the 5G communication technology figure just ahead of the quantum computing in the 2018 cycle and predicts a maturity time of 2-5 years which puts a time-line of 2023 to have the 5G technology available to the public. We all know that 5G has now been launched in many countries already and has been deployed and about launch in a matter of an year or so in the rest of the world including our Nation.[7]

Preliminary results emerging from various labs, including the latest quantum supremacy claims by Google's quantum computer have also justified these hypes to a great extent.[8] Many of the private companies such as IBM, Google, D-wave and Honeywell have invested a huge amount of money in this field. The global public funding also witnessed a great deal of increase in this field .[9] Public investments by major countries around the globe is shown in the associated figure, among which our Nation's contribution is also substantial.

5. The national scenario & footprint

As a nation we lag a clear 10-12 years behind other developed nations in this area. The National Mission of Quantum Technologies & Applications (NM-QTA) is one of the 9 missions of national importance, under Prime Minister's Science and Technology Innovation Advisory Council (PM-STIAC) to make swift progress in this field and bridge the gap between other global players in this field. Department of science and technology (DST) has been entrusted with the practical implementation of the mission .[10] An Rs 8000 Cr package for the next 5-year period has been announced for this mission. NM-QTA has an apex committee taking all its decisions which includes one chairman, one member secretary



Global public Investment for Quantum Technologies (in Crores).

and 6 members.

The mission will focus both the fundamental science and developing technology platforms in 4 different themes enabled by quantum mechanics.

(1) Quantum Computing & Simulations
(2) Quantum Materials & Devices
(3) Quantum Communications
(4) Quantum Sensor & Metrology

Announcement of a detailed road map for the mission is on its final stage. Apart from accelerated science and technology development, generation of human and infrastructural resources is an important component of this mission.

The leading quantum computing architectures depend on three specialized branches of quantum physics and technology. (i) Trapped atoms/ions in optical or magneto-optical traps. (ii) Superconducting circuits and, (iii) semiconducting quantum dot circuits. Atom/ion trapping technologies have substantial presence in the country while the combined expertise on both the superconducting circuits and semiconducting quantum-dot circuits are less than a hand full. It is important to identify the available expertise and facilities in the country and identify the gap areas in this field prior to start the intensive mission mode project NM-QTA. This has been the main idea behind the project call **QuST** (Quantum enabled science and technology) spearheaded by DST/ICPS division. This proposal came with the broad objective of the development of a few Qubit quantum processor and associated and technologies with a budget close to Rs. 270 Crores .[11] The project has been divided into four thematic/technology areas and one group developing theoretical expertise while maintaining close ties with the experimental groups.

(1) Quantum information technologies with photonic devices.
(2) Quantum information technologies with solid state, nitrogen vacancy, Magnetic Resonance.

(3) Quantum information technologies with ion-trap and optical-lattice devices.
(4) Quantum information technologies with superconducting qubit devices and quantum dot devices.
(5) Mathematical and fundamental aspects of quantum computation and quantum information.

The associated table provides a short list of Institutions pan-India carrying out experimental research on these technologies.

Quantum Communication	**Ion-traps and optical lattices**	**Superconducting Qubits**	**Semiconducting Spin Qubits**
IIT Delhi	IISc Bangalore	TIFR Mumbai	IISER Thiruvananthapuram
IIT Madras	IISER Pune	IISc Bangalore	IIT Bombay
RRI, Bangalore	IIT Roorkee		
PRL Ahmadabad	IISER Mohali		
IGCAR Kalpakkam			

This is a very short list who work on area directly related to the fields under the focused field of quantum computation and communication. There are many other institutions and research groups working on projects which are related to the above mentioned area. In addition, a large number of theoretical physicists spanning across various institutes in the country also work on various aspects of quantum computation; the list is large and beyond the scope of this short article.

The Quantum computer, once realized, could take different physical forms and mode of operation depending on its technological platform. For e.g., a QC realized using ion traps would require ultra-high-vacuum systems with state of the art electronics, magnetoelectrical traps, and precision lasers. The semiconducting and superconducting qubits require the capability to engineer sub-hundred nanometre-structures using precision nano-fabrication tools, ultra-high vacuum systems, low noise and high-frequency electrical measurements down to a temperature a few milli-kelvin away from absolute-zero. On the physics side we require a deep understanding of quantum physics, atomic physics, superconducting and/or semiconducting circuits depending on the platform. While, for the technology development we are looking at a combination of expertise on the above-mentioned fields, most of which do not have much academic or industrial foot prints in India. To develop and sustain this field, as a Nation, we need to become self-reliant. Beyond a few qubits, the development of a quantum computer is not a pure academic/research scale job, we need our industries to step in, use their expertise and take the technology further. Currently most of the technology and equipment required for performing these job need to be imported. Being a sensitive technology restriction could be imposed by overseas suppliers. Building the human resource, technological know-how, basic infrastructure and maintaining a healthy scientific interaction with concerned industries is the key for us to succeed in this area.

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