# Biomolecular Quantum Computation

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In terms of leveraging the total power of quantum computing, the prevalent current (2020) model of designing quantum computation devices to follow the von Neuman model of abstraction is highly unlikely to be making full use of the full range of computational assistance possible at the atomic and molecular level. This is particularly the case for molecular modeling, in using computational models that more directly leverage the quantum effects of one set of molecules to estimate the behavior of some other set of molecules would remove the bottleneck of insisting that modeling first be converted to the virtual binary or digital format of quantum von Neuman machines. It is argued that even though this possibility of "fighting molecular quantum dynamics with molecular quantum dynamics" was recognized by early quantum computing founders such as Yuri Manin and Richard Feynman, the idea was quickly overlooked in favor of the more computer-compatible model that later developed into qubits and qubit processing.

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**[NEW]** Biomolecular quantum computation

## I. BIOLOGICAL MOLECULES AS NATURAL QUANTUM PROCESSORS

In 1980 one of the earliest proposers of quantum computing, Yuri Manin, arrived at his version of the idea by postulating that biological molecules routinely use superpositions of virtual automata to achieve near-classical levels of reliability when selecting desirable reaction pathways. [1]

The nascent but richly promising field of quantum computational chemistry [2] proposes to leverage recent innovations in quantum computing to deal with the same issue that Manin noted, which is that even simple molecules leverage quantum mechanics in ways that are prohibitively costly to model with conventional computers. Feynman also addressed this issue [3] when he suggested his own variant of quantum computing, which might best be described as fighting fire with fire. His idea was to use the quantum features of particle and molecular systems to model the intractable quantum behaviors of a much broader range of similar phenomena, thus creating a universal quantum simulator.

## II. USING DIVERSE MOLECULES AS PARTS OF QUANTUM-CHEMISTRY COMPUTERS

If simple molecules and diverse scales of condensed atomic matter are difficult to model computationally due to their inclusion of what amounts to naturally occurring quantum computing, this presents the possibility that with sufficient understanding and calibration these same molecules and condensed matter phenomena could be used as custom components in chemistry-focused quantum computers. Such components would provide situation-specific modeling capabilities in much the same way that graphics accelerators speed processing in general purpose computers. This approach would amount to a generalization of Feynman's idea, since in both cases the overall goal would be to model roughly similar chemical systems more efficiently.

## III. A CLOSER LOOK AT MANIN'S MODEL

Forty years ago in the introduction to his 1980 book *Computable and Uncomputable*, [4] Yuri Manin provided a strikingly prescient description of the necessity of some form of "demonic" information processing to implement DNA replication using the protein machinery of cells:

"Replication of the double helix of a bacterial chromosome



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involves the uncoiling of about 300,000 turns accompanied by an intricate set of highly specific chemical reactions…" [1]

FIG. 1. shows an updated example of the mechanical complexity of the cellular DNA replication process.

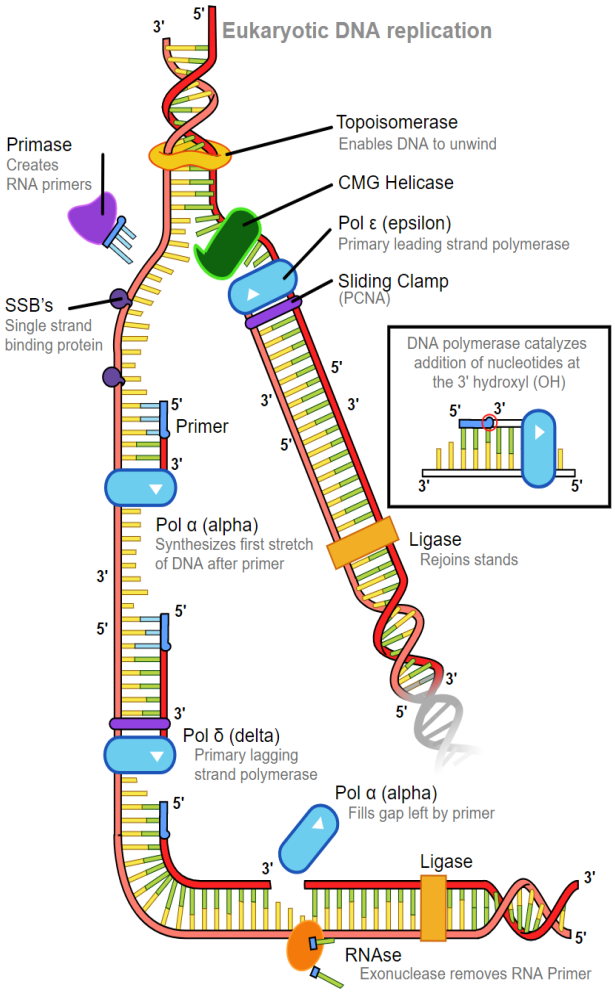


FIG. 1. The mechanical complexity of DNA replication in eukaryotic (non-bacterial) cells. Pages 14-15 of the Introduction to Yuri Manin's *Computable and Uncomputable* include a figure showing the mechanical complexity of bacterial double helix replication. This 2 July 2019 CC0 1.0 public domain image uses research information acquired in the four decades since his book.

Manin was struck in particular by the similarity of the replication process to the design of a Turing machine. At the same time, he recognized clearly there is something deeply incorrect about this seemingly straightforward comparison of large-scale and molecular-scale versions of a Turing machine. The problem in Manin's perspective around the fact that molecules are so close to the quantum mechanical threshold that classical-scale assumptions of nearly perfect reproducibility of critical process steps — which it should be noted are by no means trivial to make sufficiently reliable even at the full classical level — are instead replaced by a complex phase space of barriers and attractors that are inherently probabilistic in nature:

"A classical continuously evolving system governed by differential equations can imitate a discrete automaton only if its phase space is extremely elaborate: it must include many stability domains, or attractors, separated by low energy barriers. The input of a program creates a labyrinthine system of passages in these barriers creating a path for a trajectory that approximates the discrete process of computation."

It is at this point that Manin was inspired to postulate that the way biological systems achieve spectacularly reliable Turing-machine-like operation in such seemingly inherently quantum-uncertain machines was to apply the same principles of least-action superposition seen in path integrals to the quantum superposition of *Turing machines* implied by a quantum-level version of such a machine:

"…Perhaps, for a better understanding of this phenomenon, we need a mathematical theory of quantum automata… In particular… a quantum system… can be considered… as a state of various virtual classical automata… Then the model of evolution is the unitary rotation in a finite dimensional Hilbert space, and the decomposition of the system into its virtual parts corresponds to the tensor product decomposition of the state space (quantum entanglement)."

Along with Paul Benioff's much more detailed 1980 proposal of Hamiltonian-based quantum mechanical computers, [5] as well as Feynman's 1982 universal quantum emulator paper, [3] Manin is often quoted as one of the early inspirations for quantum computing, due almost entirely to this short description added almost as an afterthought to the introduction to his book. However, of these three founders of quantum computing, only Manin seems to have recognized fully the roles that quantum coherency and entanglement must play in guiding the processes of common biomolecules.

Manin was furthermore struck by the phenomenal thermodynamic efficiency of any such guiding quantum process in biomolecules, since the *classical* execution of large clouds of Turing machines would be prohibitively costly in terms of energy, if it could be done at all. He quoted the thermodynamic efficiency assessments of R. P. Poplavskii [6] to argue that the energy efficiency with which biomolecules accomplish their tasks flatly contradicts the naïve assumption that such behaviors can be understood classically. Manin noted for example that "… a computer must be extremely *unstable* [in the sense that] a change in one bit of input generally leads to a totally different computation … [yet] … as a physical evolution must be very *stable*. … [These] requirements … doomed the development of mechanical computers."

Unfortunately, Manin's insightful demonic molecular interpretation of quantum computing — that is, his idea that molecular machines achieve classically inaccessible levels of process path efficiency by virtue of residing at the boundary between classical mechanics and quantum coherence — was subsequently lost in the rush to make the

quantum world look more like the familiar digital computing world. This in turn led to subtle but critical change in subsequent decades on how to design useful quantum computing devices.

In Manin's original inspiration, it was the Turing *machines* that were virtual, and thus subject to the coercive effects of path reinforcement. However, attempting to build devices that rely on superpositions at the device level would restrict them in size to the molecular scale, where a quantum superposition of many virtual devices remains plausible and accessible. The superposition model cannot be translated to classical Turing machines, which are too large to enable device-level superpositions of states in any experimentally or computationally meaning fashion.

Unfortunately, and due in part to the fact that the needed prerequisite technologies for atomic-level manipulation and construction did not exist in the 1980s and 1990s, this implicit analysis and discarding of the molecular option for building useful quantum computing devices was made at such an instinctive that it was never made explicit. The option of designing molecular sized quantum computers does not appear ever to have been considered seriously beyond its introduction by Manin in 1980.

What took its place was a strikingly different strategy of designing quantum computers as *classical* devices that incorporate and leverage *quantum* threads of computation. The same barriers and attractors which Manin described as necessary to keep molecular computations on track were replaced classical equivalents that were no longer were subject to quantum state superposition. The quantum part was instead constrained to states moving through an overall design that was full classical. Since the simplest possible state within a classical computer is a two-state *bit*, this strategy of extreme quantum minimization led a bit in time to the concept of *quantum bits*, or *qubits*. [7] [8]

While much easier to understand and model than the concept of entire *devices* entering into a superposition of stated, qubits unfortunately do not easily lend themselves to demonic molecular computing. The situation is akin to why computer bits do not easily lend themselves to performing rapid but low-resolution analog computing. [9] Defining quantum computing entirely in terms of qubits forces delicate phase spaces to be elaborated first into imitating the complex and highly dynamic classical structure of a von Neumann digital computer. By the time this massive complexity barrier has been overcome — if it can be overcome at all — there is precious little coherency left to deal with the problems for which such devices were originally designed.

Given the intriguing insights made decades ago by folks such as Manin and Poplavskii, it is an interesting question whether the concept of demonic molecular computing — that is, of quantum computing through the construction of calculating machines whose atomic components are small enough to use quantum coherence as the ultimate lubricating oil — fully qualifies as "new" physics. Such machines, which include the zetta-size sets of protein molecules that keep every human alive, must after all still follow Hamiltonians, obey path integrals, and evolve through unitary rotation in Hilbert spaces of large but finite dimensions. However, given how history has unfolded since that time, it is probably safe to say that demonic molecular computing is an intriguing and potentially research-rich example of both overlooked and underexploited physics.

Work such as that by Gábor Vattay *et al* [10] on how diverse biomolecules seem nonetheless to leverage the same unique electron conductance mechanism, one that can be found only at the transition between insulators and disordered metallic conductors, may hint at a more general rule for how to access demonic information processing. The rule amounts to a quantum elaboration of David Christian's "Goldilocks Principle": In any system at any scale, expect the most interesting modes of behavior and complexity to emerge at the boundaries between boredom and chaos. [11] For biomolecules this edge appears to be where the kinematics and dynamics of the highly constrained, machine-like classical interpretations of the molecules touch upon the coherent near-infinities of their quantum interpretations.

## IV. DISCUSSION

The potential power of demonic molecular computing has profound implications for everyday life, since for example protein folding in general and the specific case of COVID-19 protein structures are good examples of tasks where, as Feynman suggested, the only truly effective path forward when facing the computational implications of quantum entanglement is to fight demons with demons. Classically structured computing methods, which ironically include qubit-based strategies that require von Neumann elaboration of their phase spaces, remain largely inadequate for such tasks.

The bottom line is that we need to entice the information demons of the quantum biological world to work for us in a more direct fashion. Exploring the boundaries between classical and quantum kinematics and dynamics, in particular by applying the Quantum Goldilocks Principle both to molecular-scale structures and to larger-scale but still quantum-touching devices, may provide a good starting point for embarking on such a quest.

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