(Incepted 7 October 2020; Published 22 October 2020; ob1; Tweaked 2021-07-11.15:53)

==== Posted at APS 2020-10-07 ~16:00, Copied 2020-10-08.11:25 ====

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1. Broader leveraging of molecular quantum mechanics

Terry Bollinger

Posted Wednesday, October 7, 2020 at 4 PM

Topic: Using diverse molecules as parts of quantum-chemistry computers

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.

The discussion topic I would like to suggest is this:

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, is it possible 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. Such uses 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.

(Incepted 7 October 2020; Published 22 October 2020; ob1; Tweaked 2021-07-11.15:53)

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==== Background: Posted Friday, August 14, 2020 at *Physics Today* ====

First posted at a ***Physics Today*** at discussion site url:
https://physicstoday.scitation.org/doi/10.1063/PT.3.4546#comment-5030797608

Terry Bollinger
Friday, August 14, 2020 4:43 PM

Forty years ago in the introduction to his 1980 book *Computable and Uncomputable*, Yuri Manin provided a strikingly prescient description of the necessity of "demonic" information processing at the biomolecular level:

"Replication of the double helix of a bacterial chromosome involves the uncoiling of about 300,000 turns accompanied by an intricate set of highly specific chemical reactions … Perhaps, for a better

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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, as well as Feynman's 1982 universal quantum emulator paper, Manin is often quoted as one of the early inspirations for quantum computing. However, only Manin seems to have recognized fully the roles that quantum coherency and entanglement play in the information manipulations of ordinary biomolecules. Manin quoted the thermodynamic efficiency assessments of R. P. Poplavskii to argue that the astonishing 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 demonic molecular interpretation of quantum computing — his idea that molecular machines achieve almost unimaginable efficiency by residing right 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. Qubits do not easily lend themselves to demonic molecular computing for much the same reason that computer bits do not easily lend themselves to rapid (but low-resolution) analog computation. Defining quantum computing entirely in terms of qubits forces delicate phase spaces to be elaborated first towards imitating the complex and (in terms of information) 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* 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

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"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. 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.

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.