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Computing with Molecules: A New Type of Quantum Molecular Computation



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COMPUTING WITH MOLECULES A new type of quantum molecular computation

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The computation concept, as used in computers, is basically derived from the *quantum measurement process*. Actually one "measures" two "states" of the silicon atoms, labeled 0 & 1.

In this context the classic theory is elaborated with Dirac's formalism, in which the "state" of the system is represented by a special vector, $|a\rangle$ in a N-dimensional complex space. An operator \hat{A} in this space is defined as: $|b\rangle = \hat{A}|a\rangle$, i.e. the operator "action" is to obtain from the "state" $|a\rangle$ the "state" $|b\rangle$.

The magnitude of the vector is obtained as: $\hat{A}|a_i\rangle = a_i|a_i\rangle$, where $|a_i\rangle$ are called eigenvectors and a_i - eigenvalues of the \hat{A} -operator. When the \hat{A} -operators belong to the Hermitian class they are called *observables* and their respective eigenvalues are susceptible to experimental determination (the 3rd postulate of quantum theory).

Using this formalism Rosen¹ suggested back in '960 that biological molecules, in some well defined experimental conditions, may function as "quantum measuring systems". He developed a mathematical model, in which a chemical reaction is represented as $[\Sigma A_i \rightarrow \text{products}]$, where the A_i -symbol stands for the A_i - chemical species and has the significance of a "state vector" (for the respective species). Assuming that the complete set of observables associated with A_i is given, a formal proof shows that the ensemble may be considered a "measuring apparatus". In a generalization Rosen² predicted this type of "measurement" in the primary genetic mechanisms of the epoch. A few decades later modern genetics revealed experimental results confirming the theoretical models, from which the

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¹ Rosen, R. **Bull.Math.Biophys. 22,** 227 (1960)

² Rosen, R. Bull.Math.Biophys. 23, 393 (1961)

subsequent use of biological components to perform computing operation ensued.

Back in the '70, based on these ideas, I suggested a "biological spectroscopy"³, assuming that the protein enzyme molecule (E) may function as a "quantum measuring system", recording some of the eigenvalues in the enzyme substrate (S) *observables* set. The main experimental result derived from this theoretical model is represented by a "perturbation" induced in chemical molecules (that may function as enzymic substrates) by irradiation with λ =546 nm and detected by kinetics modifications of enzyme reactions. These modifications were unexpected, i.e. a wave-like dependence of the kinetics on *the substrate irradiation times* is recorded, and not, as classically predicted, a linear dependence on *the energy* provided by the irradiation process. Since the visible light is not absorbed by these molecules, no excited states induced by electrons transitions is allowed. Hence, the possibility that we encounter here a new type of "state" electrically neutral, is strongly suggested.

Molecular Coherence induced by visible light

The detection of a possible molecular coherence, with *macroscopic exhibition and the ability to maintain long coherence times*, by the "quantum measuring systems" of biological molecule, predicted theoretically back in the '60-'70, was observed empirically in a series of experiments using enzymes & cellular preparations of the epoch.

For a review of the theoretical aspects concerning quantum properties of biological molecules see S.Comorosan⁴. For a review of the experimental models used in a variety of biological set-ups see S.Comorosan⁵.

The first physicist to put the discussion on solid physical ground was Fröhlich⁶, who predicted long range coherence in the action of enzymes, demonstrated subsequently in our experiments with visible light irradiated enzymic substrates. Fröhlich developed a series of theoretical models much

³ Comorosan, S. Int.J.Quantum Chem, Quantum Biol.Symp. 1, 221 (1974)

⁴ Comorosan, S. Biological Observables, in **Progress in Theoretical Biology**, R.Rosen Editor, Academic Press, 1976

⁵ Comorosan, S. A novel interaction of light with matter, **Journal of Biological Physics**, **17**, 151, 1990

⁶ Fröhlich, H. Long range coherence and the action of enzymes. **Nature, 228,** 1093 (1970)

discussed in the epoch⁷, with emphasize on the quantum macroscopic behavior in biological systems.

In physics "coherence" refers generally to the fact that oscillations at different places beat time with one another.

We refer here to the "quantum coherence" concept in Penrose⁸ meaning, the circumstances when large number of particles can collectively cooperate in a single quantum state that remains essentially unentangled with its environment.

Which is the situation in our visible light irradiated crystals.

Quantum phenomena with macroscopic exhibition was a long debated subject between '70-2000 at Löwdin's Miami Quantum Biology Symposia. Recently, the noted mathematician Penrose⁹ put the concept of quantum macroscopic coherence on solid theoretical grounds. It is observed that the "quantum" concept, as introduced here, refers to an "energetic" state of a molecule, different from the quantum realm of subatomic "excited" particles, and the laws governing them.

Experimental Evidence

The results presented in this section represent rates of enzymic reactions obtained with substrates in their ground state (i.e. non-irradiated), labeled as 0, and with substrates irradiation with visible light, λ =546 nm labeled as 1. Crystalline substrates were dissolved in bidistilled water and very thin solid layers were obtained by vacuum evaporation of 0.02 ml solution.

Irradiations were performed with a high-pressure Hg-lamp, for 0.5 sec. at an illumination of 7.10³ Lx.

Physical Stability & Memory Effect of irradiated molecules

The *molecular coherence* induced in the layers of irradiated crystals is very stable and retains its "structure memory" when subjected to other perturbations. When inactivated to the ground state, the same layer may

⁷ Fröhlich, H. General theory of coherent excitation in **Nonlinear Electrodynamics**, Plenum Press, New York (1984)

⁸ Penrose, R. Shadows of the Mind, Oxford University Press (1995)

⁹ Penrose, R. The road to reality, a guide to the laws of Universe, Alfred Knopf Ed. (2004)

acquire another stable coherence, which may again be inactivated to the ground state.

Successive irradiations	Value attached to reaction rate
Ground state molecular layer	$0^{\mathrm{v}}_{1\mathrm{v}^*}$
8- sec irradiated molecular layer	$1 - 2_{s}$ $1^{v*} - 2_{s}$
20- sec. irradiated molecular layer	$1^{v^{*}}_{-2s}$
Ground state molecular layer	0^{v}
8- sec. irradiated molecular layer	1^{v*}_{-8s}
20- sec. irradiated molecular layer	$1^{v^*}{8s}$
Ground state molecular layer	$0^{ m v}$

Decoherence by an Absorbed Frequency

During our experiments with enzymic irradiated substrates, it was observed that frequencies outside the common visible domain (UV or red), which are *absorbed* by molecules, will destroy instantaneously the "state" of molecular coherence induced by an irradiation with visible light (λ =546 nm), since they produce electronic transitions that will interfere with it.

Irradiation-frequency (nm)	Value attached to reaction rate
546	1
Successively 650	0

The relevancy of these results for a possible *molecular chip*, that is the 0-1 bit and the on (green) /off (red) gate, are straightforward.

Multiple Molecular Coherence States

During our experiments with enzymic irradiated substrates it was observed that each frequency of the visible domain induce a *specific molecular coherence state*.

The biggest effect on the enzyme kinetics is obtained by substrates irradiated with green (λ =546 nm) light. The blue & yellow domain induce smaller kinetics effects and the red domain (when molecules start to absorb) has no more influence.

Irradiation wavelength (nm)	Value attached to reaction rate (%)
546 (green)	100
405 (blue)	50
485 (blue)	60
577 (yellow)	75
650 (red)	0

Physical Comments

Let us stress here a clear distinction between 2 different phenomena in this phenomenology: the *physics* one, responsible for the inducement of different molecular perturbations, in the solid state, and the *biological* one, responsible for their detection in *solutions*. From the biological type of technology, some important physical characteristics of the irradiated crystals may be inferred.

1. The molecules *do not absorb* in the visible light range, the energy of this domain does not induce electronic transitions, that occur only in the UV and low visible spectra. Hence, we are left here with a new-type of electrically neutral "molecular perturbation".

2. The "quantum coherence" concept, as used here, represents the circumstances when large number of particles can collectively cooperate in a single quantum state, essentially unentangled with its environment. In this meaning a chemical molecule (i.e. a collection of large number of atoms) may be regarded as a specific energetic 3 D-profile (modern physico-chemistry provides now for some simple molecules such 3 D-profiles) in a "state" of quantum coherence (as defined above), which, stabilized by the collective cooperation of its elements, realizes the classic chemical ground state, unentangled with its environment. We may label this energetic "state" (profile) the 0-element of the bit. When a "perturbation" is now induced in this ground state collective coherence, through our visible light irradiation, the lattice energy spectrum is altered by the internal phonon wind and a new 3 D-energetic profile is realized. We may label this new energetic "state" the 1-element of the bit.

3. From the biological type of technology it may also be observed that *each time* of irradiation induces in the crystals a *specific molecular coherence state*. Moreover, *each frequency*, between the visible 400-600 nm range will induce in molecules *other* well defined specific molecular coherence states.

This means that, by variation of a simple frequency, coupled with a simultaneously irradiation with different times of different frequencies, on a microchip, one may generate a huge number of bits, increasing dramatically the computation power.

Molecular Quantum Computation. A possibility?

The techniques on which quantum computers are based stem from the molecular-magnetic-resonance (NMR) phenomenon, known to chemists since long ago & largely used in modern medical investigation.

Nuclear spin will line up with an externally applied magnetic field in a parallel manner (generating the "1" state of the qubit) or alternatively in an antiparallel one (generating the "0" state of the qubit). By varying the electromagnetic fields, spin can be made to flip between states and redirected at will. Laser pulses may affect the electronic states and evolve the initial superpositions into many different ones.

A desktop quantum computer with laser pulses to trigger superposition of atoms inside a liquid filled tube, with pole pieces, magnets and iron ore to ensure complete isolation is already available. The isolation request (unentangled with environment) limits technically, at present, the number of qubits at ~ 10 .

Molecular coherences, an alternative. From the biological type of technology it is observed that molecular coherences are *continuously induced* under the irradiation with visible light. Macroscopic stability of the respective coherence is observed only when the external "perturbation" stops. During the irradiation process a dynamics of the molecular quantum realm takes place, generating the superposition of a huge number of "energetic profiles", under permanent change. The analogy with nuclear spins under the effect of an externally applied EM-field is straightforward. Appropriate laser pulses may evolve, and manipulate, from a thin molecular film, under continuous irradiation with λ =546 nm an infinite number of coherent energetic states, instantaneously present in the respective quantum molecular realm. This theoretical set-up, realistic within modern

nanotechnological advance, may be considered in my opinion an alternative to the entanglement problems encountered in the atomic quantum realm.

Comments:

The experimental results presented in this paper may have a clear technological impact. The theoretical model, built around the concept of "molecular coherence" may open new perspective for the already suggested "unconventional computation".

There is a trend, rather significant, in the IT-domain, to work with & get inspiration from biological systems. An entirely new scientific discipline, *natural computation*, is emerging, advancing new concepts & techniques that go beyond the Turing model.

In this context my concept of "molecular coherence" may have some relevance.

Cellular metabolic pathways abound in exogenic chemical reactions that may change the energetic cellular medium, creating conditions for molecular energetic profile variations. The classic case of breaking ATP (adenosine- 3phosphate) high-energy bonds is a good example.

My old biological results indicate that accelerations of enzyme reactions occur at well defined irradiation times that induce specific energetic profile variations in the respective substrates. In an elaborated study on substrate irradiation times for enzymes involved in the metabolic sequences of glycolysis, gluconeogenesis, Krebs cycle and connected reactions¹⁰, it was observed that the specific irradiation times (that will induce specific molecular coherences) from this complex metabolic network realize a clear *control mechanism*, backed by a precise calculation. A hybrid-type of biological-physical-mathematical concepts and techniques are involved here. This is precisely the type of hybridization I would predict as a new trend for the IT-domains.

¹⁰ Comorosan, S. et al. *Physiol.Chem.* & *Physics*, 3, 103 (1971)