

A Cellular Automaton Molecular Model based on Wave Equation: An Alternative to Cellular Automata QM

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Abstract

In a recent paper, it has been argued that QM can arise from classical cellular automata. This is a fresh approach started by some authors including Prof. Gerard 't Hooft. Nonetheless, in a previous paper, we have reviewed some inadequacies of Schrödinger equation, hence the entire wave mechanics. According to Shpenkov, the classical wave equation is able to derive a periodic table of elements -which is close to Mendeleev's periodic table-, and also other phenomena related to the structure of molecules. It is suggested that Shpenkov's interpretation of classical wave equation can complement Schrödinger equation. Therefore in this paper we will discuss how we can arrive to a cellular automaton molecular model starting from classical wave equation, as an alternative to cellular automata based QM.

Key Words: Schrödinger Equation, classical wave equation, George Shpenkov, periodic table, element, molecule, cellular automata, PDE, Maxwell-Dirac electromagnetic theory.

1. Introduction

In a series of recent papers, Elze wrote about possible re-interpretation of QM starting from classical automata principles.[15][16] This is surely a fresh approach to QM, started by some authors including Prof. Gerard 't Hooft. While his papers are indeed interesting, those neglect neglect the basic facts of inadequacies of spherical solution of Schrödinger's equation to say anything about the structure of molecules. It is a common fact, that the spherical solution of Schrödinger equation and its comparison with experimental data is hardly discussed properly in many quantum mechanics textbooks, with an excuse that it is too complicated.

According to Shpenkov, the classical wave equation is able to derive a periodic table of elements -which is close to Mendeleev's periodic table-, and also other phenomena related to the structure of molecules. It is suggested that Shpenkov's interpretation of classical wave equation can complement Schrödinger equation. Therefore in this paper we will discuss how we can arrive to a cellular automaton molecular model starting from classical wave equation, as an alternative to cellular automata based QM.

2. Schrödinger equation vs. classical wave equation (of sound)

George Shpenkov's work is based on [1]: (1) Dialectical philosophy and dialectical logic; (2) The postulate on the *wave nature* of all phenomena and objects in the Universe. He uses the classical wave equation is as follows:

$$\Delta\hat{\Psi} - \frac{1}{c^2} \frac{\partial^2\hat{\Psi}}{\partial t^2} = 0 \quad (1)$$

This equation is also known as the wave equation of sound or string vibration [18, 22].

George Shpenkov claims that classical wave equation is able to explain the following:

- a. Derive a periodic table of elements (slightly different from but close to the Mendeleev's periodic law) based on spherical solution of his standing wave equation [9];
- b. Give a dynamical model of elementary particles [8];
- c. Derive binding energy of deuterium, tritium, helium and carbon [10];
- d. Derive the atom background radiation of hydrogen which corresponds to the observed COBE/CMBR (Cosmic Microwave Background Radiation) [7];
- e. Derive the shell-nodal model of atoms and molecules [11];
- f. Explain anisotropy of graphene [12];
- g. Describe the shell-nodal picture of carbon and grapheme [13];
- h. Describe electron "orbitals";
- i. Describe electron "spin";
- j. Derive neutron magnetic moment;
- k. Derive proton magnetic moment;
- l. And other things [14].

Therefore, it seems that Shpenkov's wave model of particles and molecules may be a promising alternative to complement the standard quantum/wave mechanics.

George Shpenkov points out that there are several weaknesses associated with (spherical solution of) Schrödinger's equation:

- i. Its spherical solution is rarely discussed completely (especially in graduate or undergraduate quantum mechanics textbooks), perhaps because many physicists seem to feel obliged to hide from public that the spherical solution of Schrödinger's wave equation does not agree with any experiment.
- ii. Schrödinger equation is able only to arrive at hydrogen energy levels, and it has to be modified and simplified for other atoms. For example, physicists are forced to use an approximate approach called *Density Functional Theory* (DFT) in order to deal with N-body system.¹
- iii. The introduction of variable wave number k in Schrödinger equation, depending on electron coordinates, and the omission of the azimuth part of the wave function, were erroneous [6]. Schrödinger's variable wave number should be questioned, because the potential function cannot influence the wave speed or consequently the wave number.

¹ Anonymous, Density Functional Theory for Beginners. URL: http://newton.ex.ac.uk/research/qsystems/people/coomer/dft_intro.html (accessed at April 28th, 2014)

- iv. Introduction of the potential function V in the wave equation, which results in dependence of the wave number k on the Coulomb potential, *generates divergences* that do not have a physical justification. They are eliminated in an artificial way.[6, p.27]
- v. Modern physics erroneously interprets the meaning of polar-azimuthal functions in Schrödinger's equation, ascribing these functions to atomic "*electron orbitals*". [1, p.5]
- vi. Schrödinger arrived at a "correct" result of hydrogen energy levels using only a radial solution of his wave equation, with one major assumption: the two quantum numbers found in the solution of his wave equation were assumed to be the same with Bohr's quantum number [2].
- vii. Quantum mechanics solutions, in their modern form, contradict reality because on the basis of these solutions, the existence of crystal substances-spaces is not possible. [6, p.26]
- viii. Schrödinger's approach yields abstract phenomenological constructions, which do not reflect the real picture of the micro-world.[2]
- ix. Schrödinger himself in his 1926 paper apparently wanted to interpret his wave equation in terms of vibration of string [3][4]. This is why he did not accept Born's statistical interpretation of his wave equation until he died. Einstein and de Broglie also did not accept the statistical interpretation of quantum mechanics.
- x. The interpretation and the physical meaning of the Schrödinger's wave function was a problem for physicists, and it still remains so, although many researchers understand its conditional character [6].

In the initial variant, the Schrödinger equation (SE) has the following form [2]:

$$\Delta\Psi + \frac{2m}{\hbar^2} \left(W + \frac{e^2}{4\pi\epsilon_0 r} \right) \Psi = 0 \quad (2)$$

The wave function satisfying the wave equation (2) is represented as:

$$\Psi = R(r)\Theta(\theta)\Phi(\varphi)T(t) = \psi(r, \theta, \varphi)T(t) \quad (3)$$

Where $\psi(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi)$ is the complex amplitude of the wave function, because

$$\Phi_m(\varphi) = C_m e^{\pm im\varphi} \quad (4)$$

For standard method of separation of variables to solve spherical SE, see for example [20][21].

The Φ , Θ and T equations were known in the theory of wave fields. Hence these equations presented nothing new. Only the R was new. Its solution turned out to be *divergent*. However, Schrödinger together with H. Weyl (1885-1955), contrary to the logic of and all experience of theoretical physics, artificially cut off the divergent power series of the radial function $R(r)$ at a κ -th term. This allowed them to obtain the radial solutions, which, as a result of the cut off operation, actually were the fictitious solutions.[2]

Furthermore, it can be shown that the time-independent SE [20]:

$$\nabla\Psi + \frac{2m}{\hbar^2} (E - V)\Psi = 0, \quad (5)$$

Can be written in the form of standard wave equation [2]:

$$\nabla\Psi + k^2\Psi = 0, \quad (6)$$

Where

$$k = \pm\sqrt{\frac{2m}{\hbar^2}(E - V)}. \quad (7)$$

Or if we compare (6) and (2), then we have [2]:

$$k = \pm\sqrt{\frac{2m}{\hbar^2}\left(W + \frac{e^2}{4\pi\epsilon_0 r}\right)}. \quad (8)$$

This means that the wave number k in Schrödinger's radial wave equation is a quantity that *varies continuously in the radial direction*. Is it possible to imagine a field where the wave number, and hence the frequency, change from one point to another in the space of the field? Of course, it is not possible. Such wave objects do not exist in Nature.

3. Shpenkov's interpretation of classical wave equation

Now I will introduce the Shpenkov's interpretation of classical wave equation, which can be written simply as follows:

$$\nabla\Psi + \frac{\omega^2}{c^2}\Psi = 0, \quad (9)$$

Where the wave number $k = \frac{\omega}{c}$, is constant, instead of variable [6]. Here, ω denotes the fundamental carrying frequency of the wave field at the corresponding level of space, and c denotes the speed of light. In order to correct the faults of wave mechanics, it is necessary to write down the above wave equation, which meets the conditions: (a) the wave number is constant, and (b) the azimuth factor must be taken into consideration along with radial $R(r)$ and polar factor of the wave-function [6].

In this case, the differential equation for the radial factor $R(r)$ is:

$$\rho\frac{d^2R_l}{d^2\rho} + 2\rho\frac{dR_l}{d\rho} + [\rho - l(l+1)]R_l = 0 \quad (10)$$

Where $\rho = kr$ [6].

The value of the fundamental frequency ω determines only the absolute scale of all parameters at the corresponding level of space. At the atomic and subatomic levels, it is equal to: [6, p.27]

$$\omega_e = 1.86916197 \cdot 10^{18} s^{-1}. \quad (11)$$

The wave radius corresponding to (11) is:

$$\lambda_e = \frac{c}{\omega_e} = 1.603886998 \cdot 10^{-8} cm. \quad (12)$$

As we can see, λ_e is equal to one-half of mean value of the interatomic distance in crystals (in terms of the generally accepted atomic model); therefore it is not a random coincidence. [6, p.27]

The detailed analysis to find spherical solution of equation (9) is discussed in Shpenkov's other papers [9, 11].

Some consequences of the solution of the Shpenkov's interpretation of classical wave equation are [6]:

- a. As masses of atoms are multiple of the neutron mass (or hydrogen atom mass), following Haiüy's ideas makes it reasonable to suppose that any atom, like the elementary Haiüy's molecule, is the neutron (H-atom) molecule;
- b. Therefore, atoms should be considered as neutron (H-atom) quasispherical multiplicative molecules. The word 'multiplicative' means that particles, constituted of these elementary molecules, must be coupled by strong bonds, which we call multiplicative bonds.
- c. Potential polar-azimuthal nodes of spherical shells in stable atoms (nucleon molecules) contain by two coupled nucleons.
- d. Polar potential-kinetic nodes (not filled with nucleons in the most abundant and stable atoms) are ordered along the z axis of symmetry (in spherical coordinate system) of the atoms.
- e. Exchange (interaction) between completed nodes inside (strong) and outside (electromagnetic) of the atoms is realized by exchange charges of nucleon and electron on the fundamental frequency (11).
- f. It is possible to get this method yielding the actual picture of distribution of nodes-extremes, corresponding to Haiüy's elementary molecules.
- g. Principal azimuth nodes of the wave space of atoms are marked by ordinal numbers. These numbers coincide with the ordinal numbers of elements of Mendeleev's periodic table. The quantity of neutrons, localized in one node, is equal to or less than two.
- h. Arranging atoms with the same or similar structure of outer shells one under another, one arrives at the *periodic-nonperiodic law of spherical spaces* that constitutes periodic table, slightly differing from the conventional one of Mendeleev.

To be fair, Shpenkov may not be the first person who uses that the classical wave equation to study atoms and particles. There are at least two persons that I can recall here who appear to attempt similar thing: Randell L. Mills and Robert A. Close. Randell Mills calls his theory *Classical Quantum Mechanics*, while Robert Close calls his theory *The Classical Wave Theory of Matter*.

4. Correspondence between classical wave equation and quantum mechanics

a. Ward & Volkmer's derivation of Schrödinger equation from wave equation

My viewpoint is that there is connection between classical and quantum mechanics, see also [17][19]. Therefore it seems possible to find theoretical correspondence between classical electromagnetic wave equation and Schrödinger equation. Such a correspondence has been discussed by David Ward & Sabine Volkmer [23]. They give a simple derivation of the Schrödinger equation, which requires only knowledge of the electromagnetic wave equation and the basics of Einstein's special theory of relativity.

They begin with electromagnetic wave equation in one dimensional case:

$$\frac{\partial^2 E}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} = 0. \quad (13)$$

This equation is satisfied by plane wave solution:

$$E(x, t) = E_0 e^{i(kx - \omega t)}, \quad (14)$$

Where $k = \frac{2\pi}{\lambda}$ and $\omega = 2\pi\nu$ are the spatial and temporal frequencies, respectively. Substituting equation (14) into (13), then we obtain:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) E_0 e^{i(kx - \omega t)} = 0 \quad (15)$$

Or

$$\left(k^2 - \frac{\omega^2}{c^2} \right) E_0 e^{i(kx - \omega t)} = 0 \quad (16)$$

Solving the wave vector, we arrive at dispersion relation for light in free space: $k = \frac{\omega}{c}$. Note that this is similar to wave number k in equation (8).

Then, recall from Einstein and Compton that the energy of a photon is $\varepsilon = h\nu = \hbar\omega$ and the momentum of a photon is $p = \frac{h}{\lambda} = \hbar k$. We can rewrite equation (14) using these relations:

$$E(x, t) = E_0 e^{\frac{i}{\hbar}(px - \varepsilon t)}, \quad (17)$$

Substituting this equation into (13) we find:

$$-\frac{1}{\hbar^2} \left(p^2 - \frac{\varepsilon^2}{c^2} \right) E_0 e^{\frac{i}{\hbar}(px - \varepsilon t)} = 0 \quad (18)$$

Then we get an expression of relativistic total energy for a particle with zero rest mass:

$$\varepsilon^2 = p^2 c^2. \quad (19)$$

We now assume with de Broglie that frequency and energy, and wavelength and momentum, are related in the same way for classical particles as for photons, and consider a wave equation for non-zero rest mass particles. So we want to end up with:

$$\varepsilon^2 = p^2 c^2 + m^2 c^4. \quad (20)$$

Inserting this equation (20) into equation (18), it is straightforward from (15), that we get:

$$\left(\nabla^2 - \frac{m^2 c^2}{\hbar^2} \right) \Psi = \frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2} \quad (21)$$

which is the Klein-Gordon equation for a free particle [23]. Now we want to obtain Schrödinger equation, which is non-relativistic case of (21). The first step is to approximate $\varepsilon^2 = p^2 c^2 + m^2 c^4$, as follows:

$$\varepsilon = mc^2 \sqrt{1 + \frac{p^2}{m^2 c^2}} \approx mc^2 + \frac{p^2}{2m} \approx mc^2 + T. \quad (22)$$

After some approximation steps, then Ward & Volkmer obtained the Schrödinger equation:

$$-\frac{\hbar^2}{2m} \nabla^2 \phi = i\hbar \frac{\partial \phi}{\partial t}, \quad (23)$$

Where the non-relativistic wave function Φ is also constrained to the condition that it be normalizable to unit probability.

While we can conclude that there exists formal connection between classical wave equation and Schrödinger equation, but it still requires some assumptions and approximations. Therefore we can consider that Shpenkov's interpretation of classical wave equation is more realistic for atomic and molecular modeling.

b. Sound wave analogy with quantum mechanics

Hilbert and Batelaan [24] explores equivalence between the quantum system and the acoustic system. They find that the analytic solution to the quantum system exhibits level splitting as does the acoustic system. A simple physical system is discussed that mirrors the quantum mechanical infinite square well with a central delta well potential. They compare the acoustic resonances in a closed tube and the quantum mechanical eigen-frequencies of an infinite square well. They find that the acoustic displacement standing wave is:

$$\xi(x) = \xi_{\max} \sin\left(\frac{n\pi x}{2a}\right), \quad (24)$$

For the nth resonance. Equation (36) is the same shape as the quantum mechanical wave function. Their approach to find analogy between sound wave and quantum mechanics may be useful to be investigated further.

5. Two routes to cellular automata model of wave equation

a. Xin-She Yang & Y. Young's method

A plausible method to describe cellular automata model of wave equation is depicted in [27]. For the 1D linear wave equation, where c is the wave speed. The simplest central difference scheme leads to

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{(\Delta t)^2} = c^2 \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \quad (25)$$

Which after some steps, it can be written in generic form (by choosing $\Delta t = \Delta x = 1, t = n$) as follows:[27]

$$u_i^{t+1} + u_i^{t-1} = g(u^t), \quad (26)$$

which is reversible under certain conditions. This property comes from the reversibility of the wave equation because it is invariant under the transformation: $t \rightarrow -t$.

b. Randall O'Reilly's method

O'Reilly has shown that the coupled Maxwell-Dirac electrodynamic system can be implemented in an analog cellular-automaton operating within a 3D regular face-centered cubic lattice.[28] The result of this approach can be expressed in terms of a second order wave equation as follows:

$$s_i^{t+1} = s_i^t + \dot{s}_i^{t+1} \quad (27)$$

He concludes that the second order wave equation is arguably one of the simplest possible continuous-valued CA update equations that does anything physically interesting. Furthermore, he is able to show that all of electrodynamics can be built of elaborations of this one fundamental interaction. This seems like a compelling argument in favor of the idea that this kind of analog CA provides a particularly simple, elegant way of modelling fundamental physics.[28]

Concluding remarks

We have discussed some weaknesses of Schrödinger equation for description of atom and molecules. Then we discuss Shpenkov's wave model of atom and molecules based on classical wave equation. It is shown that his model is able to arrive at a periodic table of elements which is close to Mendeleev's periodic law. We also discuss a plausible cellular automaton molecular model based on classical wave equation, as an alternative to Cellular automaton QM.

While we emphasize that a wave equation should be able to model atom and molecule in realistic way, our view is that there can be possible correspondence between classical mechanics and

quantum mechanics. In this regards, cellular automata models may help to bring complexity modeling into molecular mechanics.

As it has been shown by O'Reilly that all of electrodynamics can be built of elaborations of this one fundamental interaction. This seems like a compelling argument in favor of the idea that this kind of analog CA based on wave equation provides a particularly simple, elegant way of modelling fundamental physics.

Further investigations in this direction are recommended, in particular using Shpenkov's interpretation of classical wave equation of sound.

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