

Re: hypothesis > accepted theory?

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On Jan 20, 1:56 pm, zion-lion <damianjohnbr...@xxxxxxxxxxxx> wrote:

over the past month, I have been thinking about the atom and even wrote a computer program in C++ to emulate a hydrogen/deuterium atom

what I have postulated is the layman's term for quantum mechanics I supposed that the particles of neutron, photon and electron moved around the atom in a certain shaped waveform

I have just started reading about the Schrodinger Equation, which fits

my layman hypothesis http://en.wikipedia.org/wiki/Schr%C3%B6dinger_equation

The Schroedinger Equation for the hydrogen atom was solved *exactly.* The form of the equation is identical to that of a wave equation for a central, $1/r^2$ field. There are no 'particles' moving around inside an atom. Neutrons don't exist for long. Photons move in straight lines under local conditions. Electrons bound into atoms and ions have no defineable position – only the energy of the electron is known, but it is known exactly.

The key to calculating orbitals for higher order species (ions, atoms, molecules) was the development of approximations: mathematical simplifications which will not introduce intractable errors in the results. In 1970 this step was taken with the NDDO approximation, which led to further improvements. <http://en.wikipedia.org/wiki/NDDO>

I'm sure this was all before you were born, so it must be old science you somehow never learned about.

I have spoken to academics about my hypothesis but they are not much help
it is not abstract like string theory, but includes linear wave-particle duality

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Their disinterest may be due to your outmoded paradigms.

I can program an atom and molecule emulator that drug firms can use to 'build' new drugs this is not a new phenomenon as there are already programs written for computational chemistry but mine will be available to anyone who wishes to use it, whether a chemistry student or a layman but also, the professors of chemistry will take note, along with nuclear physicists and the drug companies to line my pocket...

Forget it. Better programs are already out there.

"MNDO, or Modified Neglect of Differential Overlap is a semi-empirical method for the quantum calculation of molecular electronic structure in computational chemistry. It is based on the Neglect of Differential Diatomic Overlap integral approximation. Similarly, this method replaced the earlier MINDO method. It is part of the MOPAC program and was developed in the group of Michael Dewar. It is also part of the AMPAC, GAMESS (US), GAMESS (UK) and GAUSSIAN programs." from <http://en.wikipedia.org/wiki/MNDO>

These programs are already able to predict the bond lengths, bond angles, and force constants of small molecules based on s, p, d, and higher orbitals and hybrid orbitals to within the accuracy of experimental data. The challenge now for drug companies is calculating the conformations of biopolymers (proteins, RNA, DNA, etc.) and the processes that alter those conformations (i.e. "What makes the protein go 'bad' in VCJD?").

I think you need to go back to school. You are to the chemical physicist what NoEinstein is to the Relativistic Physics community. You are out of your league here.

You are roundly ignored by "the academics" because your questions and statements reveal more about your ignorance than about your knowledge.

And, FWIW, the "wave-particle duality" of light and electrons is an analytical artifact. Photons and electrons are neither waves nor particles. Depending on the analytical techniques used to study them they can *APPEAR* to be either. Mathematically they have more in common with Lorenzian four-tensors. Most non-mathematicians have trouble 'visualizing' such an abstraction as a four-tensor, but they feel a strong need to visualize things in order to better understand them. It is just that sometimes the mathematics of a four-tensor matches that of a particle in motion, and sometimes it matches that of a dynamic electromagnetic field ("wave"). It depends on whether the

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operator applied to the tensor to bring out the observable quantity
produces a scalar or another tensor.

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