New method improves modeling of electrons' motions in complex molecules

March 11 2011, By Steve Koppes

(PhysOrg.com) -- David Mazziotti has significantly improved a quantum computational method that he introduced in 2004 for efficiently modeling the electrons in atoms and molecules.

Although in principle quantum mechanics can describe the properties of molecules and materials in which the electrons' motions are strongly correlated, in practice such computations are formidable. Molecules can have from 10 to hundreds or thousands of electrons, and the computational cost of modeling molecules increases exponentially with the number of strongly correlated electrons.

Mazziotti, an associate professor in chemistry at the University of Chicago, has been developing a new approach in which any molecule's energies and properties can be computed as a function of just two of the molecule's many electrons. Such a strategy provides accurate approximations for strongly correlated electrons without an exponential computational scaling. In the Feb. 25 issue of *Physical Review Letters*, Mazziotti announced a newly improved method that is at least 10 to 20 times faster than previous methods.

Mazziotti's original approach already has been applied to studies of aromatic rings, which are employed in computer displays, and of the energy-transfer process that enables fireflies to glow in the dark.

"The present advance will enable treatment of larger molecules and materials with strongly correlated electrons," he said.

In the *Physical Review Letters* article, Mazziotti applied this method to the metal-insulator transition of metallic hydrogen, which forms under the intense pressure found at the cores of Jupiter and Saturn. Computing the electronic properties of a dissociating chain of 50 hydrogen atoms during this transition would require 10 octillion (10^{28}) variables from traditional quantum solutions, while the world's largest supercomputers can treat approximately a billion (10^{9}) variables. The two-electron approach, however, requires only 9.4 million variables and 3.9 million constraints.

The algorithm in Mazziotti's method is a member of a special family of algorithms known to mathematicians as semidefinite programming. The advance in the Physical Review Letters article also has applications in engineering, computer science, statistics, finance, and economics.

"Remarkably, behind seemingly unrelated phenomena, there lies a common mathematical thread," Mazziotti said.

In Mazziotti's method, the energy of a molecule with many electrons is minimized as a function of two electrons, which are constrained to represent all of the electrons.

"In the same fashion, in finance, one might be optimizing profit over a set that is constrained to represent a certain amount of money or a given inventory of products," he explained. "Both problems require a search — or optimization —of a quantity subject to real-world constraints. In finance these constraints will follow from the laws of business while in chemistry they will follow from the laws of quantum mechanics."

More information: "Large-Scale Semidefinite Programming for Many-Electron Quantum Mechanics," David A. Mazziotti, *Physical Review Letters*, Vol. 108, No. 8, Feb. 25, 2011.

Provided by University of Chicago