Algorithm Advance Produces Quantum Calculation Record

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Two theoreticians from the National Institute of Standards and Technology and Indiana University have published the most accurate values yet for fundamental atomic properties of a molecule -- values calculated from theory alone.

In a recent paper,* James Sims of NIST and Stanley Hagstrom of IU announced a new high-precision calculation of the energy required to pull apart the two atoms in a hydrogen molecule (H_2). Accurate to 1 part in 100 billion, these are the most accurate energy values ever obtained for a molecule of that size, 100 times better than the best previous calculated value or the best experimental value. Their results are intrinsically interesting to astronomers studying galactic clouds of hydrogen, and to anyone else doing precision hydrogen spectroscopy, but the methods they used are perhaps equally important.

The calculation requires solving an approximation of the Schrödinger equation, one of the central equations of quantum mechanics. It can be approximated as the sum of an infinite number of terms, each additional term contributing a bit more to the accuracy of the result. For all but the simplest systems or a relative handful of terms, however, the calculation rapidly becomes impossibly complex. While very precise calculations have been done for systems of just three components such as helium (a nucleus and two electrons), Sims and Hagstrom are the first to reach this level of precision for H_2 with two nuclei and two electrons. Their calculations were carried out to 7,034 terms.

To make the problem computationally practical, Sims and Hagstrom merged two earlier algorithms for these calculations—one which has advantages in ease of calculation, and one which more rapidly achieves accurate results—into a hybrid with some of the advantages of both. They also developed improved computer code for a key computational bottleneck (high-precision solution of the large-scale generalized matrix eigenvalue problem) using parallel processing. The final calculations were run on a 147-processor parallel cluster at NIST over the course of a weekend—on a single processor it would have taken close to six months.

* J. Sims and S. Hagstrom. 2006. High precision variational calculations for the Born-Oppenheimer energies of the ground state of the hydrogen molecule. *The Journal of Chemical Physics*, 124, 094101 (published online on March 1).

Source: NIST