

New Math Technique Improves Atomic Property Predictions to Historic Accuracy

NIST



By combining advanced mathematics with high-performance computing, scientists at the National Institute of Standards and Technology (NIST) and Indiana University (IU) have developed a tool that allowed them to calculate a fundamental property of most atoms on the periodic table to historic accuracy — reducing error by a factor of a thousand in many cases. The technique also could be used to determine a host of other atomic properties important in fields like nuclear medicine and astrophysics.

NIST's James Sims and IU's Stanley Hagstrom have calculated the base energy levels for the four electrons in the element beryllium, an accomplishment that has required nearly an entire career's effort on Sims' part. Precise determination of the base energy — crucial for determining the amount necessary to raise an atom from its base energy level to any level higher — has great intrinsic value for fundamental atomic research, but the team's technique has implications far broader than for a single element.

Sims says the technique allowed the calculation of excitation states with eight-decimal accuracy, resulting in a remarkably smooth curve that they expected theoretically but were not sure they would attain in practice. For the vast majority of the elements in the periodic table, the calculated results are a thousand times more accurate than previous values. The results, according to Sims, suggest their method could enable computation of other atomic properties — electron affinity and ionization potential, for example — that are important for nuclear medicine, astrophysics and other fields of atomic research. A form of cancer treatment now under development called boron neutron capture therapy may benefit from these calculations, he says.

Their method is the culmination of decades of effort aimed at using quantum mechanics to predict base energy levels from first principles. Sims first proposed in the late 1960s that such a quantum approach could be possible, but the complex calculations involved were beyond the reach of the world's best computers. Only in 2006, after the advent of parallel computing — linking many computers together as a unified cluster — were he and Hagstrom able to create workable algorithms for calculating the energies for a two-electron hydrogen molecule more accurately than could be done experimentally. Then, in 2010, they improved the algorithms to bring lithium's three electrons within reach.

Beryllium's four electrons proved a new hurdle, but perhaps the last significant one. Much of the difficulty stems from the fact that mutual repulsion among the electrons, combined with their attraction for the nucleus, creates a complex set of interacting forces that are at least time-consuming, if not practically impossible, to calculate. The complexity grows with the addition of each new electron, but the team found a mathematical approach that can reduce an atom's electron cloud to a group of problems, none of which are more complex than solving a four-electron system.

Calling their approach a shortcut would be in some ways a misnomer. Where the calculation for lithium required a cluster of 32 parallel processors, beryllium required 256, and even then, the cluster needed to operate at extremely high efficiency for days. But the payoff was that they could calculate the energies for all four-electron ground states—meaning not only all of the elements in beryllium's column on the periodic table, each of which has four electrons in its outer shell, but also for all other elements in ionized states that have four electrons, such as boron with one electron missing, carbon missing two, and so forth, on up to the as-yet-unnamed element 113.

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