# New method can model chemistry in extreme magnetic fields of white dwarfs

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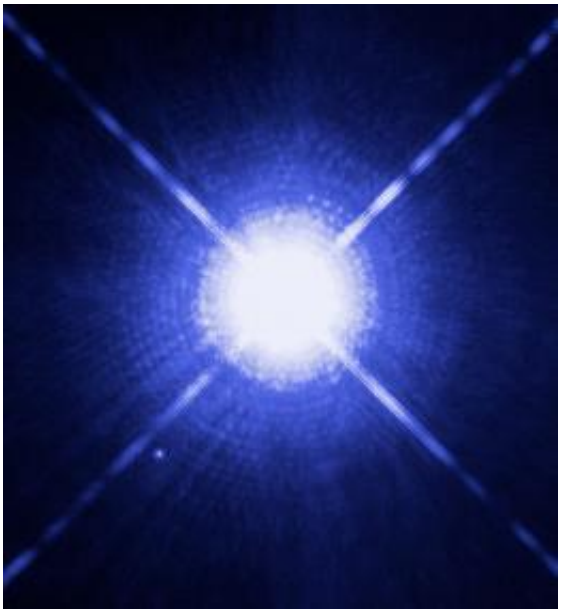

Image of Sirius A and Sirius B taken by the Hubble Space Telescope. Sirius B, which is a white dwarf, can be seen as a faint pinprick of light to the lower left of the much brighter Sirius A. Image: NASA, ESA

Most stars become white dwarfs when they reach the end of their stellar life cycle. Astrophysicists determine what elements are present in these collapsed stars by comparing spectra observed from space against either experimentally re-created spectra measured in laboratories on Earth or theoretical spectra generated using computer models based on quantum-chemical principles. Over time, they have found that white dwarfs not only contain elements like hydrogen and helium, but also oxygen, silicon,

phosphorous, carbon and carbon-containing compounds.

Approximately 10 to 20 percent of these white dwarfs exhibit strong magnetic fields.

"The strength of the magnetic field in some white dwarfs can reach up to 100,000 Tesla," said Stella Stopkowicz, a theoretical chemistry researcher at the Institute for Physical Chemistry at the University of Mainz in Germany.

In comparison, on Earth, the strongest magnetic fields that can be generated using nondestructive magnets are about 100 tesla. Therefore, studying the chemistry in such extreme conditions is only possible using theory and until now has not provided much insight to the spectra accompanying these white dwarfs. Stopkowicz and her colleague, Florian Hampe, describe their work modeling these systems this week in *The Journal of Chemical Physics*, from AIP Publishing.

"At these considerable field strengths, magnetic and Coulombic forces in the atom or molecule become equally important," Stopkowicz said. "The magnetic fields radically alter the electronic structure of atoms and molecules such that their chemistry under these conditions is to this day mostly unknown. This makes the interpretation of observational spectra challenging as they look very different from those obtained in Earth-like conditions. Exploring this problem became an important focus for our research."

"The first very accurate theoretical approach for examining the effect of a strong magnetic field on the electronic structure of atoms and molecules was the 'Full Configuration-Interaction' (FCI) method (also known as exact diagonalization). Unfortunately, this methodology is only applicable for systems with very few electrons such as hydrogen, helium, lithium and beryllium," Stopkowicz said. "FCI is computationally too

expensive to examine larger atoms such as oxygen and molecules such as small hydrocarbons and their corresponding ions like CH+."

Stopkowicz and her colleagues have therefore concentrated on different methodologies that are more widely applicable, while still retaining the desired accuracy to deal with atoms and molecules in the presence of strong magnetic fields.

"Building on prior work that we have done in the field, we have adapted the 'Equation of Motion Coupled-Cluster (EOM-CC) method' that can be used to access the electronically excited states of atoms and molecules to deal with strong magnetic fields," Stopkowicz said. We then developed a computer program that incorporated this method to assist us in calculating excitation energies; this was an important step towards the prediction of spectra."

"In the next stage, we will implement transition dipole moments which will make it possible to calculate theoretical spectra for atoms in strong fields," Stopkowicz said. "Astrophysicists can compare these theoretical spectra to observational ones and interpret what kinds of atoms and molecules might be present in magnetic white dwarfs."

The work is also beneficial to two other fields of research.

First, it furthers the understanding of chemical changes in atoms and molecules under extreme conditions where magnetic forces counterbalance Coulombic forces. This is an important area of fundamental chemistry research where, for instance, new phenomena are encountered such as "Perpendicular Paramagnetic Bonding"—a novel type of chemical bond that does not occur on Earth.

Second, the accurate data obtained using this methodology may help in the development of better functionals for the calculation of magnetic

properties in density functional theory, a widely used method in computational chemistry.

"Our biggest challenge is the fact that we are examining something that was previously unexplored. This is also what makes this work so interesting," Stopkowicz said. "The results from the computations are often surprising and not necessarily intuitive. Whenever we obtain something new, we have to make sense of it."

Going forward, Stopkowicz and her colleagues will continue their work on the key components necessary to generate theoretical spectra for atoms and molecules in strong fields.

"There is still a lot of work to do," Stopkowicz said, "but our vision is to contribute to the larger scientific effort to unveil the composition and chemistry of magnetic white dwarfs."

**More information:** Florian Hampe et al, Equation-of-motion coupled-cluster methods for atoms and molecules in strong magnetic fields, *The Journal of Chemical Physics* (2017). DOI: 10.1063/1.4979624

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