First experimental evidence of quantum monodromy

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Ohio State University physicists have obtained the first-ever experimental evidence of a particular quantum mechanical effect –- one that was theorized a decade ago.
The effect, called quantum monodromy* (Greek for "once around"), relates in part to the behavior of molecules based on their atomic structure and vibrational frequencies. A better understanding of quantum monodromy could have implications in astronomy, atmospheric science, and biology.

The physicists reported their results at the 60th International Symposium on Molecular Spectroscopy, held at Ohio State University .

In some molecules, the atomic bonds act like joints where the molecule can bend and rotate unusually far from their normal positions, like a human arm can bend or rotate at the elbow or shoulder, explained Manfred Winnewisser, adjunct professor of physics at Ohio State . The movement changes the shape of the molecule, and affects its vibrational and rotational energy as well as how it interacts with other molecules.

The water molecule, for instance, exhibits this behavior, and scientists suspect that the bending of that molecule might affect the function of water vapor in the atmosphere.

"In order to understand the absorption of solar radiation in the atmosphere, one has to understand the proper physics," Winnewisser said. "So an improved understanding of physics or chemistry or biology is actually the most important application of studies of monodromy."

To understand the movement of such molecules, scientists draw a graph, a kind of map of the molecule's energy. For molecules that exhibit quantum monodromy, the map looks like an upright cylinder with a bulge rising from the bottom, like the bottom of a wine or champagne bottle.

The top of the bulge is a critical point where the shape of the molecule changes, Winnewisser said.

To learn more about what happens at this "monodromy point," the Ohio State physicists studied the molecule cyanogen isothiocyanate (NCNCS). Its atoms fit together in a long chain that they hoped would exhibit the bending they wanted to see.

A special laboratory instrument enabled the test. Frank De Lucia, professor of physics at Ohio State, and his colleagues designed the instrument to utilize their FAst Scan Submillimeter Spectroscopy Technique (FASSST).

The technique offers a quick way for scientists to examine the spectrum of electromagnetic radiation absorbed by a molecule. Each molecule has its own one-of-a-kind spectral pattern, like lines in a bar code. FASSST takes a quick scan of a wide range of spectral wavelengths, so scientists can easily recognize the pattern of the molecule they are looking for.

In the case of the NCNCS molecule, Winnewisser and his colleagues used FASSST to record a series of spectral features, including the features corresponding to the energy of the molecule at the monodromy point.

Ivan Medvedev, a doctoral student in physics, and his colleagues, then used software he developed to reveal patterns in the spectrum. The open-source software, called Computer Aided Assignment of Asymmetric Rotor Spectra (CAAARS), is available for download from Medvedev's Web page (www.physics.ohio-state.edu/~medvedev/caaars.htm).

When they plotted the spectrum with CAAARS, the physicists could identify patterns that exactly matched patterns in the predicted spectrum for a molecule exhibiting quantum monodromy.

Other team members on this project included Brenda Winnewisser, also adjunct professor, and Markus Behnke, a postdoctoral researcher, both of the Ohio State Department of Physics, and Stephen Ross, professor of physics at the University of New Brunswick in Canada.

***Note:** More about quantum monodromy

Source: Ohio State University