Using musical chords to analyze and illustrate hydrogen molecule's response to laser pulses

January 31 2008

For Kansas State University physics professor Uwe Thumm, confirmation of a theory about the behavior of small molecules became music to his ears -- literally. He and colleagues in Heidelberg, Germany, have shown how a hydrogen molecule responds to laser pulses by using the changing musical chord created by the molecule's vibrational motion.

Thumm is a member of K-State's J.R. Macdonald Laboratory, where he is among several researchers who work on the properties and behavior of atoms and small molecules.

For decades, researchers had used the Macdonald Laboratory to make atoms and molecules collide with particles. Thumm said much of what scientists know about atoms and molecules is based on such collision experiments. To predict and explain what happens in these collisions, a large group of experimental physicists works closely with Thumm and two other theorists. The theorists use computers, make models and crunch numbers with the hope of producing results that are compatible with what experiments show.

Thanks to improvements in laser technology, around 1999 the Macdonald Laboratory researchers realized that they could transfer a lot of their expertise in atomic collisions to study in detail what happens when atoms and molecules get irradiated by very intense laser light. The new laser systems in the laboratory offer some advantages over the big particle accelerators, Thumm said. The laser pulses offer more control and can be made so short that the researchers now routinely observe the motion of nuclei inside small molecules in time. In addition, the laser pulses' peak intensity is enormous and would equal all of the sun's light focused onto a small spot of the size of a postage stamp or smaller.

Motivated by these opportunities, Thumm and his colleagues became curious about figuring out what would happen if the smallest and simplest molecule, hydrogen, were exposed to such ultra short and intense laser pulses. Together with his postdoctoral collaborator Bernold Feuerstein, Thumm developed a model and did calculations to determine how laser pulses influence the motion of the two protons in the hydrogen molecule.

"The short answer is that the laser pulse either makes the molecules vibrate more violently or blows them apart," Thumm said. He said this wasn't surprising because in the hydrogen molecule, two protons are connected by two electrons that function like a spring. When hit with the laser pulses, the protons oscillate back and forth.

Although this model may be easy to imagine on a large scale, Thumm said particles behave differently at the quantum level. This means that determining the locations of these oscillating protons isn't easy. Thumm described determining the protons' movements after being hit with the laser like what happens if you drop a marble in a bathtub. Looking at the circular ripples of water in the center of the tub, it's pretty easy to tell where the marble was dropped in. But when those ripples bounce off the sides of the tub, the wave pattern changes shape, and it becomes harder to tell where the marble was dropped. The wave gets delocalized. Thumm said the same thing happens to the protons not in a matter of seconds, but in a matter of femtoseconds -- that's a billionth of a millionth of a second. After about 60 femtoseconds, it's impossible to tell where the protons are.

"You quickly loose track of what the distance between the two protons is," Thumm said." All you can say is that they have a certain likelihood of being at a certain distance. This is in agreement with the bathtub experiment: Seconds after the marble was dropped, you can't tell where exactly it plunged in."

But things work differently at the quantum level, and the researchers were surprised that about 600 femtoseconds after being hit with the laser, the distance between the protons again becomes well defined. "We call this a revival of the original motion of the protons," Thumm said. "It's not going to happen in the bathtub, but it happens at the quantum level."

Thumm and Feuerstein published their theoretical prediction in 2003. Thumm said that they were pleasantly surprised when experiments at the Max-Planck Institute in Heidelberg, Germany, in 2006 confirmed the revival described in their model. "The agreement between the new experiments and our model was almost perfect and exceeded our expectations," Thumm said.

Feuerstein had since moved to Heidelberg, where he and his group of researchers continued to collaborate with Thumm's group at K-State. Excited about the success of their model, they began to analyze the molecule's vibrational motion by breaking it down into its various frequencies. Each frequency being like a note in a chord, the frequencies told researchers how the protons were behaving. However, the frequency of these molecular vibrations is way above the audible range. The two researchers share an interest in music and had collaborated musically before. So when it came time to illustrate the revival, they decided the best way to do it was to scale the frequencies down to 1,000 Hertz, which is in the range at which the human ear hears best. "This way you can listen to the vibrations and hear the revival. In the same way sound is analyzed and decomposed, we decomposed the vibration with regard to the frequencies," Thumm said. Their result, a changing musical chord coupled with a movie illustrating the protons' vibrations can be heard and viewed at http://www.mpg.de/video/FilmundoAudio-KdM.wmv

Thumm said researchers hope to be able to do the same thing for more complex molecules like water or methane. Just as a C Major chord sounds different from a d minor chord, Thumm said other molecules also would have their own unique sound. Thumm and Feuerstein's most recent work was first published last fall in the *Physical Review Letters*. Their research was supported by the National Science Foundation, the U.S. Department of Energy and the Max-Planck Society. Thumm said such basic research supports the long-term goal of applying lasers to steer chemical reactions. The hope is to largely increase the efficiency of chemical reactions by enhancing desired reaction pathways with lasers, he said.

Source: Kansas State University

Citation: Using musical chords to analyze and illustrate hydrogen molecule's response to laser pulses (2008, January 31) retrieved 24 April 2024 from https://phys.org/news/2008-01-musical-chords-hydrogen-molecule-response.html