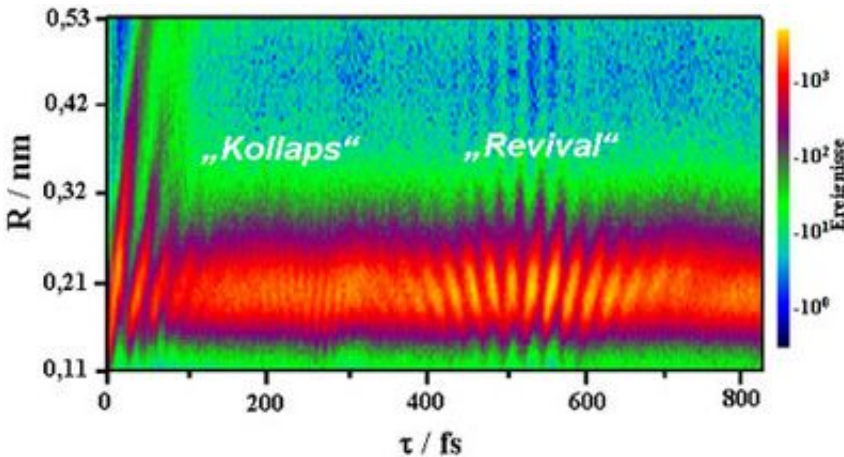


Molecular chords

November 16 2007



Researchers in Heidelberg visualised the development over time of molecular resonance (see related link [1]). The distance between the two nuclei (R) in the heavy hydrogen (deuterium) ion D_2^+ is plotted against the time. After approximately 100 femtoseconds, the wave packet, i.e. the location of the nuclei, starts to become hazy, after 400 femtoseconds there is a "revival" and the wave packet is put back together again. Image: Max Planck Institute for Nuclear Physics

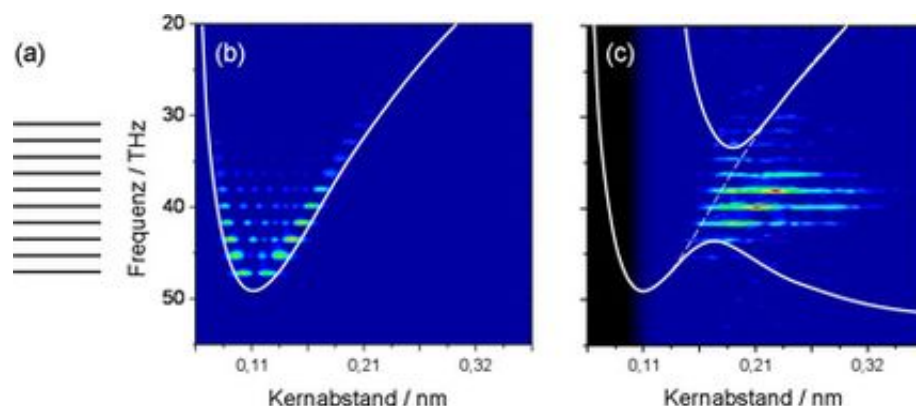
Max Planck researchers have for the first time analyzed the frequency of molecular resonance, in the same way as musicians analyze the notes of a chord. Their results have even been made audible.

In terms of physics, there is hardly any difference between the resonance in a molecule and a musical chord. Both are created when vibrations with different frequencies overlap. In music, it is the notes that make up

the chord. In molecules, these frequencies are also called quantum states.

Working with a theory group from Kansas State University, researchers from the Max Planck Institute for Nuclear Physics have for the first time determined the quantum states of a tiny hydrogen molecule. Instead of employing their faculty of hearing to do this, they needed ultrashort laser pulses lasting only a millionth of a billionth of second. They also made the molecular resonance audible to illustrate the results. These results mean that they are a step closer to being able to manipulate chemical reactions with laser pulses. (*Phys. Rev. Lett.*, 2007)

Waves from the sea never break on the shore with any consistency. Sometimes they are huge, and sometimes they hardly break at all. From time to time, no waves at all roll onto the shore, while at other times they arrive in rapid succession. This phenomenon is easy to explain. In the sea, many waves with different frequencies overlay each other. For example, large waves are triggered by earthquakes and small waves by the wind. Sometimes they cancel each other out, but sometimes it is equally possible that they reinforce each other.



The researchers broke the resonance of a deuterium molecular ion down into its frequencies. They showed which quantum states contribute to this and how laser fields affect the resonance. (a) Frequency spectrum of the quantum states which make up the molecular resonance. (b) Model calculation of the free resonance

(no laser field): the coloured strips represent the characteristic distribution of the inter-nuclear distance in the relevant quantum states. The white curve (potential curve) limits the amplitude of the vibration permitted for the molecule. The highest probabilities are at the possible maximum or minimum distances between the nuclei. This is because the atoms resonating against each other remain longest at their point of return which is where they are most likely to be found. (c) Experiment result: the probability distribution for the nuclei is shifted to the greater distances. Also, the laser field breaks the molecular bond in certain quantum states. The potential barrier opens here. The black background indicates where the laser pulse is not sufficiently sensitive. There is therefore no data from this area. Image: Max Planck Institute for Nuclear Physics

In principle, all types of vibration behave in the same way, whether it takes the form of sea waves, that is, vibrating water, or molecular resonance. Molecular resonance also usually consists of overlaid vibrations with different frequencies. The energy of these frequencies is equivalent to the energy which triggered the vibration.

"It has been known for a long time that unlike waves in water, the frequencies of molecular resonance cannot assume arbitrary values," says Bernold Feuerstein from the Max Planck Institute for Nuclear Physics. The frequencies of molecular resonance or their energies are "quantized". This is why physicists also refer to quantum states here. The acoustic example illustrates this: a musical chord is created when notes, that is, sound waves, with different frequencies overlay each other. As the notes are part of a scale, they only have certain frequencies. In exactly the same way, atoms in a molecule can only vibrate at certain frequencies which then overlay each other and finally create the complete molecular resonance.

A trained ear finds it easy to identify the individual notes in a chord. However, we are not equipped with an organ that will perceive

movement in the quantum world - the world of nanometer-sized molecules, atoms and electrons. Even a microscope cannot catch the movement of quanta. The scientists at the Max Planck Institute for Nuclear Physics in Heidelberg made use of a special aid. Together with the theory group working with Uwe Thumm at Kansas State University they have now analysed the resonance of a hydrogen molecule to reveal its quantum states.

The basis for this was that some time ago Max Planck researchers showed the resonance of the D_2^+ molecule (deuterium = heavy hydrogen) in extremely slow motion (fig. 1). To do this, they used two ultrashort laser pulses in order to first trigger the extremely fast movement of the atomic nuclei and then to photograph it. The film [2] shows how the distances between the nuclei and the resonance pattern change over time. In principle, this is what a film of sea waves would look like as well. Sometimes the resonance of the nuclei is clearer, sometimes the wave pattern is blurred, depending on which of the overlaid frequencies cancels the other out or reinforces another.

Because each frequency contributes in a unique way to the wave pattern, scientists can determine them, in the same way as a musician recognizes the notes in a chord. To do this, the scientists use a mathematical method, the Fourier transformation, which, like a "virtual ear", breaks a vibration down into its frequencies. In this way they put the data from the development over time of the molecule resonance through a Fourier transformation. "This allowed us to determine the quantum states of molecular resonance exactly for the first time," says Bernold Feuerstein.

The first result is a step ladder (spectrum) of the frequencies, that is, the quantum states, which make up molecular resonance (fig. 2a). To remain with the acoustic analogy: the notes of the chord. "What is remarkable is that we obtained such clear and unambiguous results for the quantum states," says Feuerstein.

When the researchers from Heidelberg had filmed the resonance with laser pulses, they had determined not only the frequency, but also the distances between the vibrating deuterium nuclei. They combined the information on the inter-nuclear distances with the frequencies in a diagram (fig. 2b,c); the results show that each frequency, that is each quantum state, is responsible for a characteristic distribution of the inter-nuclear distance.

In order to investigate how the laser pulses affect the resonance, the researchers prepared another model calculation which assumed uninterrupted resonance.

In the model calculation, the resonance amplitude is limited by a potential. The potential of the molecule depends primarily on the strength of the molecular bond. Depending on which quantum states have contributed to the molecular resonance, only certain amplitude can be reached. The potential can be illustrated by a bowl in which a marble rolls back and forth. The more forcefully the marble is pushed, that is, the more energy there is in the system, the greater the deflection of the marble. How great the deflection of the marble can be depends on the potential of the bowl, that is, how steep it is.

The potential of the resonance evens out with higher energies, as less and less energy needs to be used to make the atoms resonate further apart. At some point, the nuclei pull apart. This can be compared to a bowl which becomes less steep towards the top. If the ball is pushed with sufficient force, it will fly out of the bowl.

In a real experimental situation, the laser pulses have a significant effect on the resonance. At certain frequencies, a "window" opens outwards in the potential barrier. The molecular bond is broken. In these quantum states, the laser pulse which triggers the resonance increases the probability that the molecule will break up and the nuclei fly apart.

When that happened in an experiment, the second laser pulse either did not find any more nuclei or filmed them just as they flew apart. The characteristic distribution of the nuclei is therefore shifted to larger distances. That the molecule breaks up is, in principle, a simple chemical reaction triggered by the light field. To use the analogy with the marbles in the bowl: in this case there is a hole in the bowl. At a certain probability, the marble rolls directly into the hole and flies out of the bowl.

"It is interesting to see in which quantum states the laser field affects the resonance and how much it changes it," explains Bernold Feuerstein.

"With a weaker laser field, the window in the potential barrier would only open in higher quantum states." From this the researchers can conclude how certain laser fields affect chemical reactions and which quantum states contribute to a certain reaction. "The method can generally be applied to other quantum systems and also to more complex molecules," says Feuerstein. "We hope that this information will allow us to use laser fields for deliberate manipulation of enzyme activity."

By way of illustration, the researchers converted the resonance into an acoustic signal (sound waves) and made it audible, making the resonance into a musical chord. Variations in the loudness of the sound signals (beat) reflect the distance between the atomic nuclei resonating against each other. The audible beats are created by overlaying different pitches (frequencies), that is, the quantum states which make up the molecular resonance.

Related links:

[1] A leading edge camera for molecules:

www.physorg.com/news82211420.html

[2] Audio-visual example (approx. 10 MB):

www.mpg.de/video/FilmundAudio-KdM.wmv

Citation: B. Feuerstein, Th. Ergler, A. Rudenko, K. Zrost, C. D. Schröter, R. Moshammer, J. Ullrich, T. Niederhausen, and U. Thumm, Complete Characterization of Molecular Dynamics in Ultrashort Laser Fields, *Phys. Rev. Lett.* 99, 153002 (2007)

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