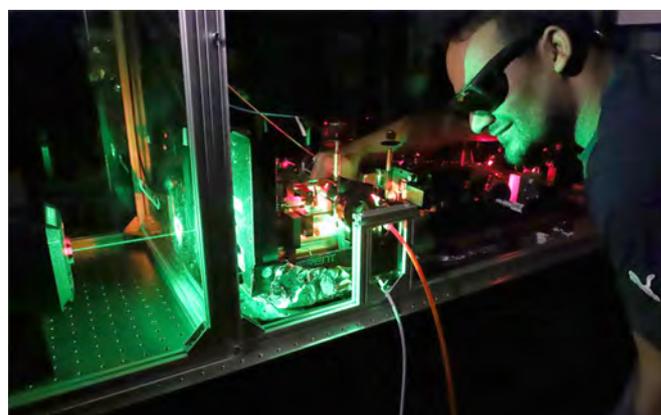


Simplified Steps to Make Ultracold Molecules Lay Path to Study Fundamental Physics

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Researchers at the Centre for Quantum Technologies (CQT), National University of Singapore, have found a simple and effective way to coax pairs of disparate atoms toward their coldest molecular state. The creation of such ultracold polar molecules is the groundwork for experiments in quantum simulation and fundamental physics.

The work by Principal Investigator Kai Dieckmann and his team is described in the paper, “Singlet Pathway to the Ground State of Ultracold Polar Molecules”, published in the April 2020 issue of *Physical Review Letters*. The paper was co-authored by Dieckmann along with current and former group members Yang Anbang, Sofia Bosti, Sunil Kumar, Sambit Pal, Mark Lam, Ieva Čepaitė and Andrew Laugharn [1].

“What we’re doing is control of the quantum world in a bottom up approach,” says Dieckmann. “With molecules, we have degrees of freedom that are vibrational and rotational. Our work has shown a wonderful way of controlling these modes,” Dieckmann states. In the lab, the team traps clouds of lithium (Li) and potassium (K)

atoms, cooling them with help from rubidium atoms (Rb). Molecules form when Li and K pair up, with each experimental run making up to 10,000 such molecules.

Due to the atoms’ different sizes, these molecules have a large electric dipole moment. This creates interesting possibilities to control and use the molecules because they interact strongly over large distances.

For example, molecules could host information in quantum computing applications. As quantum bits, they could be controlled by lasers shining onto each molecule. Their long-range interactions mean that molecules could be widely spaced for easier addressing, while still interacting in the ways required to implement logic gates. Compared to other groups around the world working with dipolar molecules, as of now, Dieckmann’s choice of atoms offers the largest possible dipole moment that has been produced.

Researchers want these molecules in their lowest-energy state to begin experiments. To get to that lowest-energy

state, normally all the energy levels of the molecules must be known, then lasers are used to drive steps between those levels. Finding the energy levels involves both intensive calculations and experimental searches. In the case of Li-K molecules, it was difficult to find a ladder of energy levels similar to those used for other dipolar molecules. Consequently, a new and promising route was proposed.

The route to the ground state

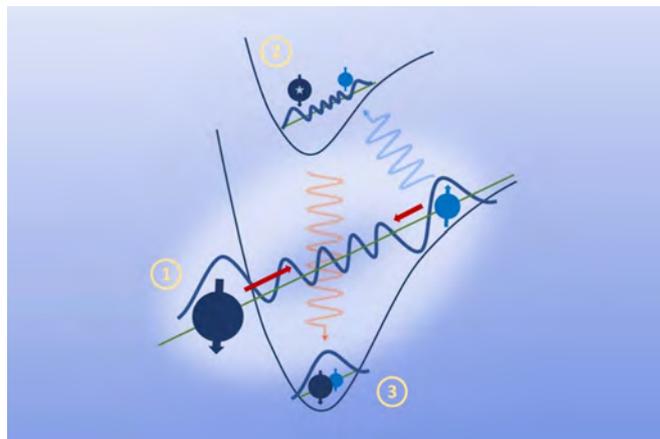
The typical path to the ground state involves both singlet states and triplet states of the molecules, which differ in the orientation of the atoms' quantum spins. Dieckmann and his team realized that they could instead make all of their steps between singlet states. "With the new pathway, we use molecular states that are easier to understand and model, known as stretched singlet states. That simplifies the spectroscopy and bypasses heavy molecular structure calculations. It gives us an ideal three-level system. It's a really clean and robust method," Dieckmann explains.

The method could be applied to other molecules too, says Dieckmann, who has presented the findings to other groups in the field. In the current paper, the team performed a detailed analysis to verify that the method would work and be feasible for other molecular species.

One laboratory tool that helped the researchers with details of the new method was a vintage laser. The team purchased a refurbished dye laser that was originally manufactured in the 1980s. The group added a few modern components to obtain stable operation at high output power.

Dye lasers are no longer common because they are bulky and fiddly to operate compared to modern diode lasers, but they have the advantage of offering high power light over a vast tunable range of frequencies. The vintage dye laser helped the researchers search for the frequencies that would most effectively drive their molecules' transitions.

"Doing spectroscopy can be very time-consuming. It is a bit like fishing in the dark. Although we calculated the energies of the ground states with existing literature, the uncertainties were much larger than the linewidths, making the states hard to find," explains Anbang. He suggested an approach to search through the molecules' vibrational modes (denoted by quantum number v) to



find the ground state. "I proposed to start from ground state $v=3$, searching from $v=2, 1, 0$, step by step, instead of directly searching for $v=0$ ground state. By doing this, we learned that our calculated energies have an offset around 3GHz from the experimental values. It accelerates our 'searching for $v=0$ ' process."

The team has now identified all the energy levels that make a ladder to move the molecules to the ground state. Putting the molecules in the ground state is the next challenge. The researchers will use a technique known as Stimulated Raman Adiabatic Passage (STIRAP) with two lasers stabilized to the same cavity. They can now retire the dye laser and, using stable diode lasers, will continue their work.

"The route to the ground state provides us with a robust platform," says Sofia Botsi, a PhD candidate who is working on the project. Once they have molecules in the ground state, the researchers will begin experiments in fundamental physics. A first goal is to perform quantum simulations based on the dipolar interaction to search for unusual properties of quantum materials. In particular, they are interested in a prediction that the eigenstate thermalization hypothesis will break down in a disordered dipolar lattice system. Dipolar molecules offer many avenues for further work. In the future, the researchers may look at using molecules for chemistry at ultracold temperatures, testing gravity at short scales or for applications such as clocks and quantum computing.

References

- [1] Yang Anbang, Sofia Botsi, Sunil Kumar, Sambit B. Pal, Mark M. Lam, Ieva Čepaitė, Andrew Laugharn, and Kai Dieckmann. "Singlet pathway to the ground state of ultracold polar molecules." *Physical Review Letters* 124, no. 13 (2020): 133203.