

Using a quantum phase transition to efficiently produce heteronuclear molecules

An atomic Bose–Fermi mixture was driven through a quantum phase transition by varying an applied magnetic field to tune the interspecies interactions. This approach enabled the efficient generation of sodium–potassium molecules in the quantum degenerate regime.

This is a summary of:

Duda, M. et al. Transition from a polaronic condensate to a degenerate Fermi gas of heteronuclear molecules. *Nat. Phys.* <https://doi.org/10.1038/s41567-023-01948-1> (2023).

Publisher's note

Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Published online: 13 February 2023

The challenge

Binding atoms into molecules is a basic chemical process, which in its simplest form leads to the formation of molecules composed of two atoms. Near absolute zero atoms exhibit collective behaviour; therefore, molecule production becomes very complicated owing to quantum effects and multiple collision processes, especially when the sample contains a mixture of bosonic and fermionic atoms. Below a critical temperature, bosonic atoms form a Bose–Einstein condensate (BEC), which has a much higher density than fermionic atoms. Near a Feshbach resonance the interaction strength between bosons and fermions can be tuned by varying the strength of an applied magnetic field, enabling the formation of weakly-bound Feshbach molecules. However, as Feshbach molecules form, the large density of the bosons leads to a severe loss of particles from the trap owing to collisions between the excess bosons and the newly formed molecules¹. This particle loss has hindered the quest to create a molecular Fermi gas in the quantum degenerate regime. Additionally, it is still under debate how a mixture of a BEC and an atomic Fermi gas can be converted into a Fermi gas of Feshbach molecules by tuning the interspecies interactions using a Feshbach resonance.

The solution

We prepared a sample with matched boson and fermion densities by using a species-dependent dipole trap. Confining both species with lasers tuned to a similar trapping frequency leads to a fermion density that is much lower than that of the bosons owing to the Pauli repulsion between the fermions. Therefore, we developed a trapping mechanism for fermionic potassium (K) and bosonic sodium (Na) using a laser that is tuned close to the frequency of an atomic transition of K, enhancing the confinement of the fermions and resulting in matched fermion and boson densities.

With the challenge of density-matching solved, we then explored the effect of tuning the strength of the Bose–Fermi attraction. Starting at low interaction strengths where the bosons and fermions decouple and form a BEC and a Fermi sea, we slowly increased the Bose–Fermi attraction without heating the sample. As the attraction strength increases, the fraction of bosons in the BEC decreases and the bosons bind to the fermions, forming heteronuclear

molecules (Fig. 1a). Eventually, the BEC is entirely depleted, and nearly all the bosons are associated into molecules.

The interpretation

Theoretical calculations^{2,3} predict that at absolute zero there exists a quantum phase transition (QPT) from a polaronic superfluid, in which a Fermi gas coexists with a BEC, to a molecular Fermi gas where the BEC has been depleted and all bosons are bound into molecules (Fig. 1b). Our observations of the depletion of the BEC and the simultaneous molecule formation suggest that the system was driven through the associated phase transition at finite temperature. Our results thus reveal signatures of the underlying QPT and demonstrate that driving the system through this transition enables the efficient production of molecules. Although the system heats up as it is driven through the transition, remarkably the system remains quantum-degenerate enough that after it has been cycled from the polaronic phase to the molecular phase and back the BEC can still be partially restored.

The order of this QPT is currently unknown and further investigations into whether order parameters, such as the fraction of bosons within the BEC, vanish continuously or by a sharp jump are the next natural step to characterize the transition. This challenge could be tackled using box-trap potentials, in which both particle densities are nearly homogeneous across the trapping region, to prevent varying density profiles smearing out sharp transitions. Furthermore, such a setting will enable a better understanding of the complex dynamics of Bose–Fermi mixtures close to the transition point.

Having created an ultracold sample of Feshbach molecules, we were then able to transfer these molecules to their rotational, vibrational, and electronic ground states, thereby creating a large collection of degenerate ground-state molecules. By exploiting the large phase-space density of the ground-state molecules we further cooled the sample into the deeply degenerate regime using so-called microwave shielding⁴. This development is an important step towards quantum simulations of strongly correlated dipolar quantum systems that contain molecules.

Jonas von Milczewski & Marcel Duda
Max Planck Institute for Quantum Optics,
Garching, Germany.

EXPERT OPINION

"The novel feature of this study is that it is conducted in a regime in which both components of the mixture are substantially degenerate, as opposed to one of them being in a non-degenerate impurity limit.

This regime has been experimentally challenging to explore because of interspecies loss due to the typically large condensate density in a trapped mixture." **An anonymous reviewer.**

FIGURE

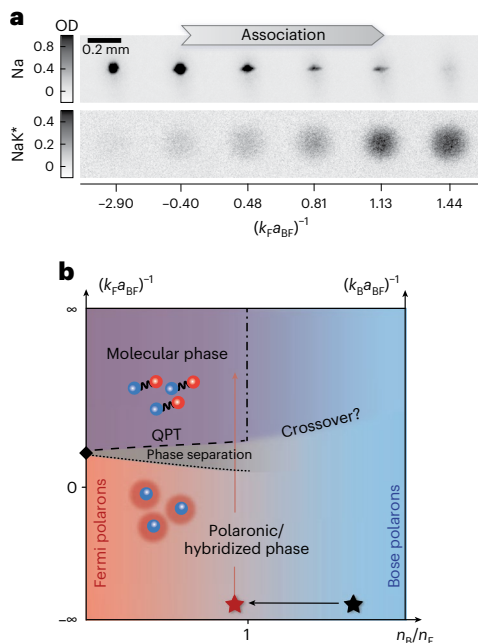


Fig. 1 | Signatures of a phase transition. **a**, Time-of-flight absorption images showing the optical density (OD) of Na atoms and Feshbach molecules (NaK*) as the strength of the Bose-Fermi coupling is increased (left to right). The images show the depletion of the BEC (top) and the simultaneous formation of a Fermi sea of NaK* molecules (bottom). **b**, Schematic phase diagram of degenerate Bose-Fermi mixtures as a function of the ratio of the boson and fermion densities (n_B/n_F) and the dimensionless interaction strength $(k_F a_{BF})^{-1}$, where k_F is the wave vector of the majority species and a_{BF} is the boson-fermion scattering length. The red arrow indicates the explored path from a polaronic condensate to a molecular Fermi gas. © 2023, Duda, M. et al., CC BY 4.0.

BEHIND THE PAPER

Our team has engaged in a decade-long quest to achieve quantum degeneracy in polar molecules. After various strategies for efficient molecule production were unsuccessful, we began to doubt whether it was possible to make a degenerate Fermi gas of NaK ground-state molecules given that previous studies suggest that bosons and fermions cannot be efficiently associated into molecules owing to a limited phase-space overlap⁵. One evening in December 2020 we inserted a final beam for density-matching the mixture. Initially, we did not see

any improvement, confirming that maybe the molecule association could never be efficient. However, we then noticed that a beam dump was blocking a critical beam. After removing the beam dump, at 5 am, we saw the first indication of the efficient production of Feshbach molecules: the molecule number had increased by a factor of three, and the deduced temperature of Feshbach molecules was well below the Fermi temperature. **M.D.**

REFERENCES

1. Zirbel, J. J. et al. Collisional stability of fermionic Feshbach molecules. *Phys. Rev. Lett.* **100**, 143201 (2008). **This article studies various collisional loss processes of Feshbach molecules.**
2. Ludwig, D., Floerchinger, S., Moroz, S. & Wetterich, C. Quantum phase transition in Bose-Fermi mixtures. *Phys. Rev. A* **84**, 033629 (2011). **This article studies the phase diagram of strongly coupled Bose-Fermi mixtures.**
3. Guidini, A., Bertaina, G., Galli, D. E. & Pieri, P. Condensed phase of Bose-Fermi mixtures with a pairing interaction. *Phys. Rev. A* **91**, 023603 (2015). **A theoretical study of the depletion of the condensate fraction.**
4. Schindewolf, A. et al. Evaporation of microwave-shielded polar molecules to quantum degeneracy. *Nature* **607**, 677 (2022). **This article studies evaporative cooling of molecules using microwave shielding.**
5. Zirbel, J. J. et al. Heteronuclear molecules in an optical dipole trap. *Phys. Rev. A* **78**, 013416 (2008). **This article studies the formation of heteronuclear Feshbach molecules in Bose-Fermi mixtures.**

FROM THE EDITOR

"This work stood out to us because it reveals signatures of a quantum phase transition in atomic Bose-Fermi mixtures in a strongly correlated regime, which has been extremely challenging to explore so far. But what really intrigued us was that reaching such a regime and understanding the underlying physics enabled the high-efficiency generation of Feshbach molecules, which might be a key step towards quantum information-processing applications with ensembles of polar molecules." **Editorial Team, Nature Physics.**