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Quantum Magnetism of Strongly Correlated Magnetic Atoms and Molecules

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Quantum Magnetism of Strongly Correlated Magnetic Atoms and Molecules

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Summary and Status of Effort

The electronic structure of magnetic lanthanide atoms and molecules are fascinating from a fundamental perspective. A submerged open 4f electron shell lies beneath a filled or closed 6s-shell. The relativistic nature of the active submerged electrons then gives the relevant features to the magnetic lanthanides. They have a large magnetic moment and a large electronic orbital angular momentum leading to anisotropies, i.e. orientation dependencies, in their mutual interactions. These anisotropies are crucial to proposals to use ultracold lanthanide atoms in spin-based quantum computers and the simulation of orbitronics, phenomena used in magnetic technologies. Anisotropic interactions can also help realize other exotic states of highly-correlated matter.

In the AFOSR supported research we developed successful theoretical models to study the interactions of the magnetic Dy, Er, and Tm lanthanide atoms in an external magnetic field as well as the non-magnetic Yb. For the magnetic lanthanides this allowed us to analyze hundreds of magnetic Feshbach resonances in their collisions. These resonances control three-atom recombination rates but were also used to convert an ultracold atomic gas into a gas of weakly-bound, highly-magnetic molecules. The magnetic moment of these molecules can be up to twice as large as those for its atoms.

In our study we paid attention to the long-range dispersion and magnetic interactions as well as short-range bonds in lanthanide molecules relying on advanced and efficient relativistic computations. Spin tensor analyses of the interactions allowed us to expand the interatomic forces in terms of a sum of spin-spin operators simplifying the tasks of future research. Seven tensor operators are necessary to describe the interactions. With this tensor description of the interactions and coupled-channels simulations we then evaluated the tightly-bound energetically lowest ro-vibrational energies of di-atomic Er_2 and Tm_2 and observed relatively simple but intriguing patterns in level diagrams. Weakly-bound, near threshold diatomic levels formed overlapping, uncoupled chaotic series that when combined are randomly distributed. We also showed that scattering of ultracold magnetic lanthanide atoms in a magnetic field is chaotic due to a combination of anisotropic interaction potentials and Zeeman coupling. In addition, we showed that lanthanide atoms are ideal candidates with which to study strong and unconventional quantum magnetism. We simulated time-dependent quantum magnetism of isolated pairs of ultracold spin-6 Er atoms placed in sites of a deep optical lattice. We focussed on the multichannel temporal spin evolution due to spin-dependent contact, anisotropic van der Waals, and dipolar forces. With a comparison to spin evolution of magnetic spin-3 Cr, we identified the leading mechanism, orbital anisotropy, that governs molecular spin dynamics among erbium atoms.

We also studied the formation of fermionic molecules from magneto-association of fermionic ^{173}Yb with fermionic ^6Li . We located magnetic Feshbach resonances for this system. It turned out that this system was also relevant for the understanding of three-body recombination near Feshbach resonances. We compared the process of three ultracold bosonic Er atoms to form weakly-bound Er_2 dimers and a hot Er atom with the equivalent process for two fermionic Yb atoms and a Li atom. The two processes have distinct energy dependences that could be experimentally distinguished.

Finally, our studies also touched upon charge transfer in ultracold atomic neutral-ion systems. Our theoretical analysis suggested the existence of reaction pathways when the optical lasers are present. We also modeled various dephasing and decoherence processes of trapped ultracold molecules prepared in superpositions of rotational states.

The research resulted in 28 publications in peer-reviewed journals and 17 invited talks at national and international conferences and colloquiums for the reported period.

Accomplishments

New ways of looking at the interactions between lanthanide atoms

Ultracold atomic physics is now poised to enter a new regime, where far-more complex atomic species can be cooled and studied. Magnetic lanthanide atoms with their large magnetic moment and large orbital momentum are extreme examples of such species. These atoms are located on a bottom row of the Periodic Table and together with the actinides belong to the group of rare-earth elements.

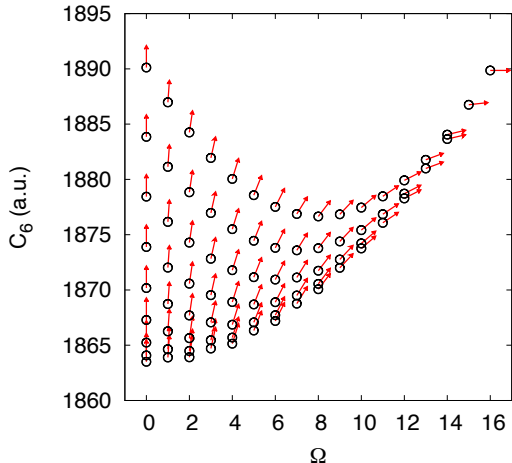


Figure 1: The gerade adiabatic C_6 coefficients in atomic units for the interaction between two ground state 5I_8 Dy atoms as functions of the projection Ω . The arrows on the graph symbolize the anisotropy or orientation-dependence of the interactions.

time. In fact, we realized that the number of the potentials with *gerade* symmetry is 49 for homonuclear Er_2 and 81 for Dy_2 . A similar number of *ungerade* states also exist. This can be compared to the single *gerade* potential for homonuclear alkali-metal dimers. Figure 1 shows the long-range van-der-Waals coefficients for *gerade* Dy_2 ground-state potentials as a function of Ω , the projection of the total electronic angular momentum on the interatomic axis. To generate potentials for all atom-atom separations we calculated the adiabatic electronic potential with maximal projection $\Omega = 16$ for Dy_2 and $\Omega = 12$ for Er_2 using a coupled-cluster method with single, double, and perturbative triple excitations (CCSD(T)) [8]. Splittings between the potential curves of other Ω states were found by assuming that they follow the splittings determined from the van der Waals potentials.

Further research relied on numerically solving coupled radial Schrödinger equations, *i.e.* coupled-channels models, to find scattering lengths and cross sections for ultracold bosonic Er and Dy collisions as well as to find weakly-bound bound states of the di-atoms in an external magnetic field with strength B . These models use atom-atom separation dependent couplings among the spins and angular-momenta in the collision. A representation in terms of such couplings is equivalent to that in terms of potential energy surfaces. Figure 2 shows a typical example of the scattering

Experimental breakthroughs in realizing quantum gases of atoms with large magnetic moments [1, 2, 3, 4] have opened a new scientific playground in which to study quantum magnetism at the interface between condensed matter and atomic physics. This research area relies on controllable and tunable long-range anisotropic interactions between atoms. Our research objective for the grant was the study of magnetic properties of ultra-cold highly-magnetic atoms and molecules. In particular, we focussed on interactions among open-4f-shell Dysprosium, Erbium, Thulium and metastable Ytterbium atoms as well as molecules formed from these atoms.

We studied the anisotropic interactions of lanthanide atoms in an external magnetic field and found magnetic Feshbach resonances in their collisions [5, 6]. Resonances control relaxation rates and can be used to convert an atomic gas into a gas of highly-magnetic Feshbach molecules [7]. We started by setting up the Hamiltonian of interatomic potentials for two ground-state lanthanide atoms, which was not known at the

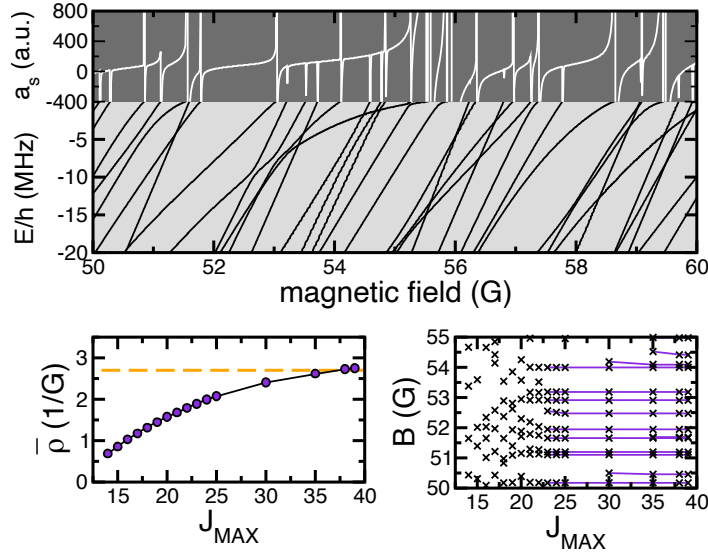


Figure 2: Top panel: Theoretical scattering length a_s in Bohr radii and near-threshold bound-state energies E for $^{168}\text{Er}(j = 6, m = -6) + ^{168}\text{Er}(j = 6, m = -6)$ as functions of magnetic field B . Here, h is Planck's constant. Bottom panels: Theoretical Feshbach-resonance density ρ as a function of $J_{\max}$ (purple circles) computed from resonance locations between 0 and 70 G. Convergence study of resonance locations (crosses) between 50 and 55 G as a function of $J_{\max}$.

length $a_s(B)$ and weakly-bound bound states for bosonic $^{168}\text{Er}(j = 6)$ atoms prepared in their energetically-lowest Zeeman level with spin-projection -6 as a function of B for only a small range of B of 10 G [9]. The sharp features in $a_s(B)$ are magnetic Fano-Feshbach resonances and we observe that whenever the scattering length approaches $\pm\infty$ the binding energy of one of the bound states approaches zero.

Quantum chaos in ultracold collisions of lanthanide atoms

In collaboration with experimental groups from the universities of Stuttgart and Innsbruck we demonstrated the existence of chaos-driven states in ultracold matter [9, 10]. The observed high density of Feshbach resonances of a few resonances per Gauss in Er and Dy collisions is without precedent in ultracold quantum gases. For comparison, the density of resonances in collisions of ultracold alkali-metal atoms is about two orders of magnitude smaller. The density and statistics of the Feshbach resonances in Er and Dy collisions are explained by our quantum-mechanical scattering calculations. The calculations find that the origin for the high level density lies in the anisotropy of the 50 or more potentials. Our results also revealed that the distribution of nearest-neighbor spacings (NNS) of resonance locations is chaotic consistent with Wigner-Dyson theory [11].

Furthermore, we studied the role of two types of anisotropies in the potentials on the NNS distribution of the weakly-bound molecular energy levels at $B = 0$. These two types of interactions correspond to a dispersion contribution $V_{\Delta C_6}(\vec{R}) \propto 1/R^6$ and a magnetic dipole-dipole contribution $V_{\text{MDD}}(\vec{R}) \propto 1/R^3$. We then expressed the total anisotropic interaction as $V_{\text{aniso}}(\vec{R}) = \lambda_{\Delta C_6} V_{\Delta C_6}(\vec{R}) + \lambda_{\text{MDD}} V_{\text{MDD}}(\vec{R})$, where $\lambda_{\Delta C_6}$ and λ_{MDD} are dimensionless strengths. Figure 3 shows bound state energies of $^{164}\text{Dy}_2$ within the last 3 GHz from two free dysprosium atoms as functions of λ_{MDD} and $\lambda_{\Delta C_6}$ with strengths from 0 to 1.2. The binding energies as functions of λ_{MDD} are regular. They look chaotic near $\lambda_{\Delta C_6} = 1$, corresponding to the physical dispersion strengths. We concluded that the large anisotropic *dispersion* interactions between lanthanide atoms gives rise to chaos.

Finally, we broadened the classification of chaotic behavior of weakly-bound magnetic lanthanide atoms by measuring the fractal dimension for large sets of molecular wavefunctions [12]. Our

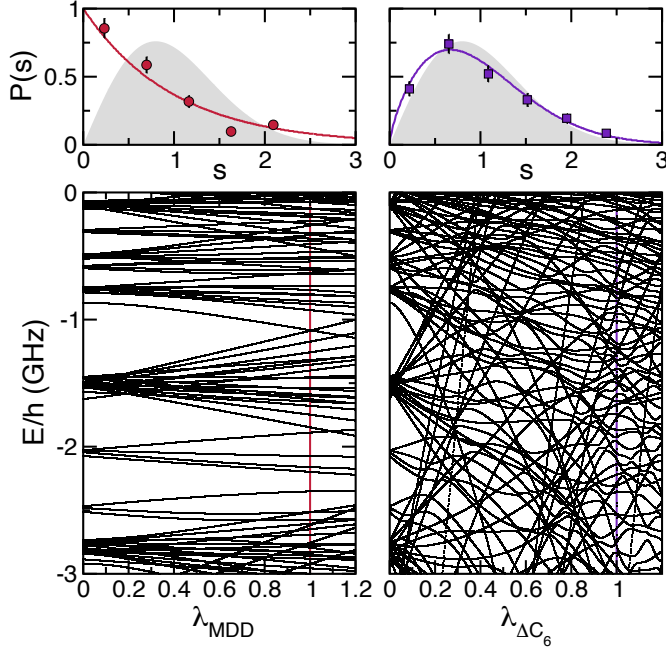


Figure 3: Anisotropy-induced chaos of near-threshold bound states of $^{164}\text{Dy}_2$ at $B = 0$. From left to right the two lower panels show bound-state energies as functions of the anisotropic magnetic dipole-dipole strength λ_{MDD} with $\lambda_{\Delta C_6} = 0$ and as functions of the anisotropic dispersion strength $\lambda_{\Delta C_6}$ with $\lambda_{\text{MDD}} = 0$, respectively. The two upper panels show scaled NNS distributions (markers and fitted curve) for $\lambda_{\text{MDD}} = 1, \lambda_{\Delta C_6} = 0$ and $\lambda_{\text{MDD}} = 0, \lambda_{\Delta C_6} = 1$, respectively. The grey area corresponds to the NNS distribution for a chaotic Wigner-Dyson distribution.

coupled-channels simulations revealed dynamic phase transitions in Dy_2 where partially localized states at small magnetic field turn into non-ergodic delocalized states by increasing the magnetic field strength to only a hundred Gauss. We explained the violation of ergodicity by strong coupling between near-threshold molecular states and the nearby continuum of free atoms. This analysis allowed us to obtain a detailed understanding of the crossover from Poisson to Wigner-Dyson statistics of level spacings in a magnetic field.

Orbital quantum magnetism in the spin dynamics of Er and Cr atoms

We have studied the time-dependent spin evolution and quantum magnetism of pairs of ultracold spin-6 ground-state erbium atoms placed in sites of a deep optical lattice and compared them with similar simulations of magnetism with pairs of spin-3 chromium atoms [13]. Spin evolution with chromium pairs in a single lattice site can be understood in terms of contact interactions with spin-dependent strengths. (A contact interaction is a potential that is proportional to a delta function located at zero atom-atom separation.) In contrast spin-6 erbium spin evolution required a *multi- or coupled-channel* description of the atom-atom interactions as both anisotropic van-der-Waals and magnetic dipole-dipole forces are important. Figure 4 shows the relevant electronic potentials of Cr_2 and Er_2 . In addition, the figure shows spin evolution for a pair of Cr atoms when both atoms are prepared in the $|3, -2\rangle$ Zeeman sublevel and for a pair of Er atoms when both atoms are prepared in the $|6, -5\rangle$ sublevel. Spin-dependent interactions then lead to population oscillations between states $|j, -j+1\rangle|j, -j+1\rangle$ and $|j, -j\rangle|j, -j+2\rangle$, where $j = 3$ or 6 for Cr and Er, respectively. We have assumed that the two species are confined in similar lattice potentials. Our simulations have allowed us to identify *orbital anisotropy* due to anisotropic van-der-Waals interactions as governing the spin evolution among erbium atoms. The role of an external magnetic field and the aspect ratio or geometry of the lattice-site trapping potential on the spin dynamics was also investigated.

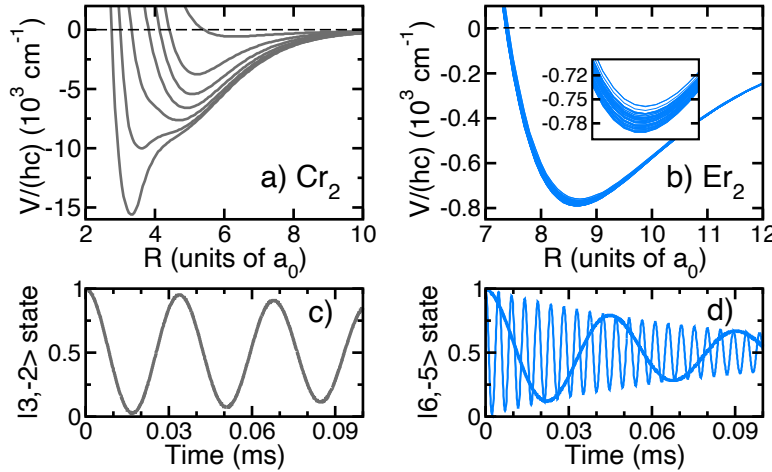


Figure 4: Ground-state potentials of Cr_2 and Er_2 and a comparison of their spin evolution. The fast and slow-oscillating curves in panel d) are for the full interaction potential and a potential that only includes the isotropic interactions, respectively. Damping is due to dephasing from interactions with atoms in neighboring lattice sites.

Relativistic calculations of Er_2 and Tm_2 electronic potential surfaces

We investigated the bond in homonuclear lanthanide molecules. We focus on the heavy magnetic Er_2 and Tm_2 dimers, which have atoms with open $4f^{12}$ and $4f^{13}$ shells, respectively, lying beneath a closed $6s^2$ shell. These molecules are chemically similar but have distinct physical properties. Electron motion in lanthanides is relativistic and spin-orbit coupling is strong. They, therefore, require the four-component Dirac equations to be used to describe their orbitals, which restricts the size of any many-electron configuration-interaction calculation. We performed relativistic configuration-interaction calculations of all Ω states as a function of interatomic separation R of the Er_2 and Tm_2 molecules using the DIRAC code [14]. The absolute ground state of Er has total electronic angular momentum of $j = 6$, that of Tm has $j = 7/2$. Energy splittings between the potential curves from $\Omega = 0$ to 12 for Er_2 and $\Omega = 0$ to 7 for Tm_2 were determined using direct relativistic configuration interaction (DIRRCI) calculations. The active space for the molecular systems was solely composed of molecular orbitals arising from excitations from the $4f$ atomic shells with the $6s$ orbitals kept doubly occupied. Keeping the $6s$ orbital frozen lead to reasonable memory requirements and computation times. The sole spin-stretched potential, i.e. $\Omega = 12$ for Er_2 and 7 for Tm_2 , were determined from separate coupled-cluster calculations with active $6s$ electrons and added to the splittings obtained by DIRRCI calculations.

Figures 5(a) and (c) show the *gerade* relativistic potential energy curves for Er_2 and Tm_2 as functions of internuclear separation near the equilibrium separation. There are 49 *gerade* potentials for Er_2 and 16 for Tm_2 . For the separations shown in the figure and, in fact, for larger separations the splittings are less than 10 % of the depth of the potentials relative to the dissociation energy. The figures for the *ungerade* states is qualitatively similar and reproduced in Supplemental Materials. There are 42 and 20 *ungerade* potentials for Er_2 and Tm_2 , respectively.

In addition, we performed a tensor decomposition of computed adiabatic potentials is to introduce PESs as weighted sums of individual coupling terms. It eradicates a complicated evaluation of non-adiabatic couplings between potentials as required, for example, for quantum dynamic simulations and determination of ro-vibrational structures of molecules. We believe that tensor format is essentially beneficial for our molecular systems with multiple adiabatic potentials in the ground configurations of Er_2 and Tm_2 (91 and 36, respectively). It turns out that the molecular elec-

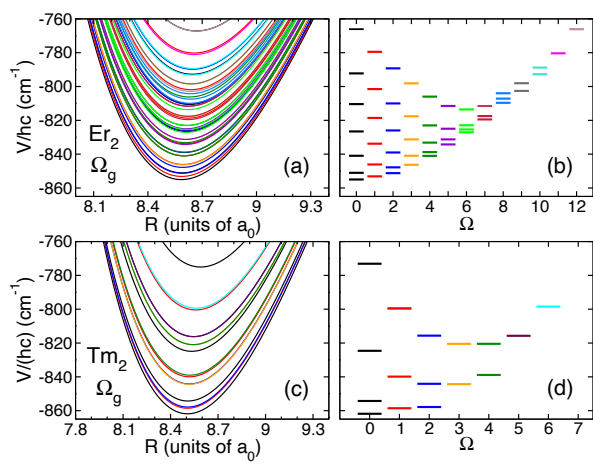


Figure 5: Relativistic $\Omega_g^\pm$ potential energy curves with *gerade* symmetry for Er_2 (panel a) and Tm_2 (panel c) as functions of internuclear separation R near the equilibrium separation as obtained from electronic structure calculations. All potentials approach zero energy for $R \rightarrow \infty$. Panels (b) and (d) show potential energies from panels (a) and (c) using the same line colors at the equilibrium separation as functions of projection quantum number Ω for Er_2 and Tm_2 , respectively. *Gerade* $\Omega = 0$ states are 0^+ states. Potentials of states with Ω and $-\Omega$ are degenerate.

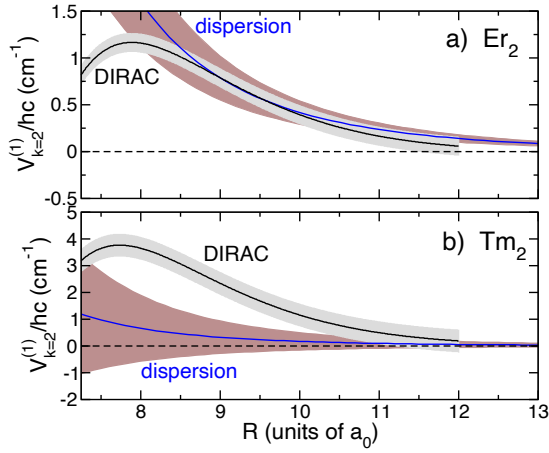


Figure 6: The fitted anisotropic spin-tensor strength $V_{k=2}^{(1)}(R)$ for Er_2 (panel a) and Tm_2 (panel b) as a function of R (black curve labeled DIRAC with gray one-standard-deviation uncertainty band). The strength is compared to the van-der-Waals dispersion potential $C_{k=2}^{(1)}/R^6$ (blue curve with brown one-standard-deviation uncertainty band).

tronic wavefunction to good approximation can be expressed as a product of ground-state atomic electron wavefunctions for all relevant interatomic separations. This also implies that the tensor representation of the potentials used in coupled-channels calculations is valid. The structure of the potentials as function of Ω has speed up our analysis to write the potential energy operator $V(\vec{R})$ as a sum of a small number of spherical-tensor operators. Specifically, we use the seven contributions $V(\vec{R}) = \sum_{i=1}^7 U^{(i)}(R) (C_k(\hat{R}) \cdot T_k^{(i)})$, where the rank k of spherical tensors $T_{kq}^{(i)}$ with components q is uniquely specified by index i .

The fitted $V_2^{(1)}(R)$ are shown in Fig. 6 as functions of R up to $12a_0$ for Er_2 and Tm_2 , respectively. The anisotropic strength is positive and at most a few times $hc \times 1 \text{ cm}^{-1}$ and approach zero for large R . These strengths are at least two orders of magnitude smaller than $V_0^{(1)}(R)$. This allow us to conclude that to good approximation the relativistic interactions between two identical Er or Tm atoms can be expressed in terms of two out of seven spin-tensors operators, one, $V_{k=0}^{(1)}(R)$, is spin independent while the other, $V_2^{(1)}(R)$, corresponds to an effective atomic quadrupole moment coupled to the mechanical rotation of the molecule.

Theoretical models of three-body recombination near Feshbach resonances

In our ongoing research collaboration with Dr. Gupta from the University of Washington, we study ultracold mixtures of lithium and ytterbium atoms with their extreme mass ratio or imbalance

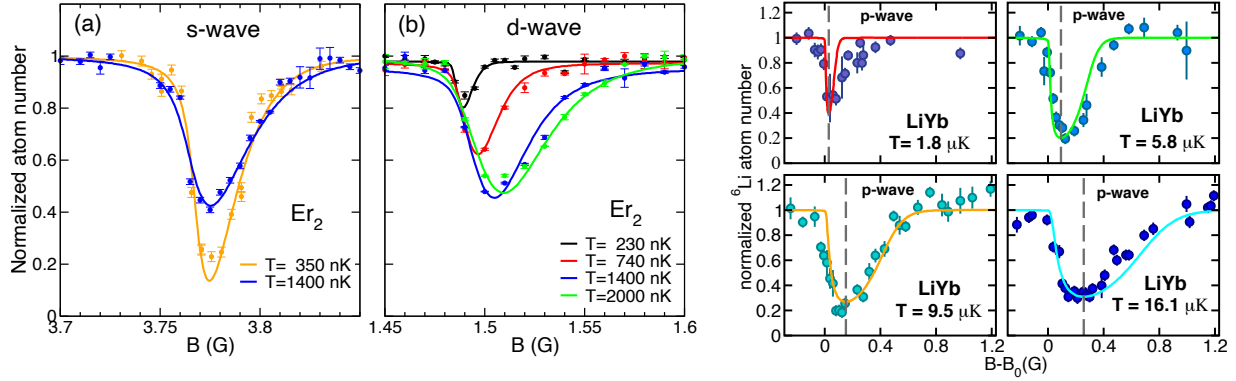


Figure 7: Panels show experimental (markers with error bars) and theoretical (solid curves) atom loss spectra as functions of magnetic field strength B for $^{164}\text{Er}_2$ and $^6\text{Li}^{173}\text{Yb}$. Atom loss is due to three-body recombination near Feshbach resonances and was investigated for temperatures between 350 nK to 16 μK . Theoretical curves were obtained from a model for recombination assuming a s -, p -, or d -wave three-body entrance channel as indicated in each panel.

of approximately 30 [15, 16, 17, 18, 19]. Quantum-degenerate mass-imbalanced mixtures are of interest for several reasons. They can be used to observe *fermionic* Efimov states [20, 21], to study Fermi-Fermi mixtures [22, 23], and to provide a platform for the simulation of the Kondo effect.

Recently, our joint efforts led to the first observation by atom loss of narrow magnetic Feshbach resonances in the fermionic mixture $^6\text{Li}+^{173}\text{Yb}$ [24]. Our calculations predicted the location and width of these resonances. They are narrow due to the weakness of atom-separation-dependent hyperfine interactions. We also reported on the temperature dependence of the resonance lines in conjunction with a theoretical model of resonant interspecies three-body recombination. As two of the three fermionic atoms in this process are identical, p -wave collisions and its corresponding Wigner-threshold behavior play a crucial role.

We compared the $^6\text{Li}+^{173}\text{Yb}$ results with atom loss data of bosonic ^{164}Er near narrow Feshbach resonances, a collaborative effort with groups from the Universities of Stuttgart and Innsbrück [9]. We found that the temperature dependence of atom loss by bosonic three-body recombination was either controlled by s - or d -wave collisions. Resonances with d -wave collisions have a surprisingly-strong temperature dependence. Figure 7 summarizes the experimental and theoretical data on atom loss as functions of magnetic field strength for colliding ^{164}Er atoms and $^6\text{Li}+^{173}\text{Yb}$ mixtures.

Personal

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- Prof. S. Kotochigova, PI, Physics Department of Temple University
- C. Makrides, graduate student (Ph.D. completed)
- Dr. Ming Li, research associate, Physics Department of Temple University
- Dr. J. Klos, Adjunct Professor, Physics Department of Temple University
- Dr. H. Li, Adjunct Professor, Physics Department of Temple University
- Chi Hong Yuen, graduate student (Ph.D. completed)

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 21. A. Green, J. Hui S. Toh, R. Roy, M. Li, S. Kotochigova, and S. Gupta, *Two-photon photoassociation spectroscopy of the $^2\Sigma^+$ YbLi molecular ground state*, Phys. Rev A **99**, 063416 (2019).
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 25. R. Bause, M. Li, A. Schindewolf, X-Y Chen, M. Duda, S. Kotochigova, I. Bloch, and X-Y Luo, *Tune-Out and Magic Wavelengths for Ground-State $^{23}\text{Na}^{40}\text{K}$ Molecules*, Phys. Rev. Lett. **125**, 023201 (2020).
 26. J. Kłos and S. Kotochigova, *Prospects for laser cooling of polyatomic molecules with increasing complexity*, Phys. Rev. Research **2**, 013384 (2020).

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27. B. K. Kendrick, H. Li, M. Li, S. Kotochigova, J. F. E. Croft, and N. Balakrishnan, *Non-adiabatic quantum interference effects and chaoticity in the ultracold $\text{Li} + \text{LiNa} \rightarrow \text{Li}_2 + \text{Na}$ reaction*, Phys. Chem. Chem. Phys. (2021), doi: 10.1039/d0cp05499b.
 28. T. Schuster, F. Flicker, M. Li, S. Kotochigova, J. E. Moore, J. Ye, and N. Y. Yao, *Realizing Hopf Insulators in Dipolar Spin Systems*, Phys. Rev. Lett. (2021) accepted for publication.

Invited Talks by PI

1. *Spin-dependent control of ultracold polar molecules in combined fields*, March 24, 2014, Max-Planck-Institute and LMU Colloquium, Munich, Germany.
2. *Long-range Universality and Chaos in Ultracold Collisions of the Highly Magnetic Atoms*, April 24, 2014, INT workshop, Seattle.
3. *Long-range Universality and Chaos in Ultracold Collisions of the Highly Magnetic Atoms*, April 24, 2014, INT workshop, Seattle, USA.
4. *Interaction anisotropy and chaos in collisions of ultracold highly-magnetic atoms* Colloquium at University of South Alabama, April 16th, 2015.
5. *Quantum chaos and quantum magnetism with ultracold magnetic atoms*, the workshop "Quantum Many-Body Systems Far From Equilibrium", 09-13 March 2015, Stellenbosch University, South Africa.
6. *Hybrid Molecular Quantum Systems*, International Workshop on Hybrid Quantum Systems, September 28-30, 2015, Hamburg, Germany.
7. *Interaction anisotropy and chaos in collisions of ultra-cold highly-magnetic atoms*, December 15-20, International conference Pacificchem2015, Honolulu, Hawaii.
8. *Quantum Chaos and Quantum Magnetism with Ultracold Lanthanide*, Colloquium at University of South California, March 28, 2016.
9. *Magnetism of chaotic high-spin lanthanides in the ultracold regime*, International Conference on Few-body Physics in Cold Atomic Gases, Beijing, China, April 14-17, 2016.
10. *Novel states of matter with ultracold magnetic lanthanides*, American Physical Society DAMOP meeting, Providence, RI, May 23-27, 2016.
11. *Magnetic lanthanide atoms in an optical lattice: Connecting a coherent multi-channel model to single-channel analytical approaches* International workshop on long-range interactions in the ultracold, Ercolano, Italy 6-9 September 2016.
12. *Conical Intersections in Chemical Reactions with Ultracold Molecules*, Workshop on Roaming and Cold Molecules, October 8-9, 2016, Emory University, Atlanta, Ga
13. *Three-Body Interactions with Magnetic Lanthanides*, KITP Workshop on Universality in Few-Body Systems, December 14, 2016. UCSB, CA
14. *Novel states of matter with ultracold magnetic lanthanides*, Colloquium of Physics Department, Temple University March 6, 2017, PA
15. *Scattering dynamics of ultracold magnetic lanthanides*, NIST Seminar, April 18, Gaithersburg, MD 2017.
16. *Molecules as reactive species at a collision energy close to absolute zero*, "Cold Molecules for Chemistry" symposium at the ACS Spring meeting, March 18-22, 2018, New Orleans, LA.
17. *Chemical Reactions with Ultracold Polar Molecules*, ITAMP International workshop "New frontiers in cold molecules", Cambridge, MA, May 21-23, 2019.

18. *Nonadiabatic Transitions via Conical Intersections in Ultracold Chemical Reactions*, 10th International Society of Theoretical Chemical Physics Tromso, Norway, 11-17 July 2019.
19. *Nonadiabatic Transitions via Conical Intersections at Ultracold Temperatures*, Joint Attosecond Annual Meeting, November 12-22, 2019, Arlington, VA.
20. *Quantum Chemistry with Ultracold Molecule*, Sanibel Symposium, February 18, 2020 St. Simons Island, GA.
21. *Chemical Reactivity and Nonadiabatic Coupling at Ultralow Temperatures*, United States Naval Academy, Colloquium, Annapolis January 30, 2020.
22. *Quantum-mechanical studies of interactions with ultracold atoms and molecules*, American Physical Society DAMOP meeting, June 1-5, 2020.

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