Anisotropy induced Feshbach resonances in a quantum dipolar gas of magnetic atoms

Alexander Petrov, Eite Tiesinga, and Svetlana Kotochigova

Department of Physics, Temple University, Philadelphia, Pennsylvania 19122 and National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, Gaithersburg, Maryland 20899, USA

We explore the anisotropic nature of Feshbach resonances in the collision between ultracold magnetic submerged-shell dysprosium atoms, which can only occur due to couplings to rotating bound states. This is in contrast to well-studied alkali-metal atom collisions, where most Feshbach resonances are hyperfine induced and due to rotation-less bound states. Our novel first-principle coupled-channel calculation of the collisions between open-4f-shell spin-polarized bosonic dysprosium reveals a striking correlation between the anisotropy due to magnetic dipole-dipole and electrostatic interactions and the Feshbach spectrum as a function of an external magnetic field. Over a 20 mT magnetic field range we predict about a dozen Feshbach resonances and show that the resonance locations are exquisitely sensitive to the dysprosium isotope.

PACS numbers: 03.65.Nk, 31.10.+z, 34.50.-s

A strongly interacting quantum gas of magnetic atoms, placed in an optical lattice, provides the opportunity to examine strongly correlated matter, creating a platform to explore exotic many-body phases known in solids, quantum ferrofluids, quantum liquid crystals, and superfluids [1][2]. Recent experimental advances [3][10] in trapping and cooling magnetic atoms pave the way towards these goals.

In general, interactions between magnetic atoms are orientationally dependent or anisotropic. At room temperature anisotropic interactions are much smaller than kinetic energies and other major interactions between atoms, therefore can be ignored. The situation is different for an ultracold gas of atoms with a large magnetic moment. It was, for example, demonstrated that the anisotropy due to magnetic dipole-dipole interactions between ultracold chromium atoms leads to an anisotropic deformation of a Bose Einstein condensate (BEC) [11]. Moreover, anisotropy plays a dominant role in collisional relaxation of ultracold atoms with large magnetic moments [5][1][12][15].

In this Letter we pursue ideas for using anisotropic magnetic and dispersion interactions to control collisions of ultracold magnetic atoms by using Feshbach resonances [16]. Resonances, shown schematically in Fig. 1, appear when the energy of “embedded” bound states cross the energy of the entrance channel or initial scattering state. The embedded state is a level of a potential crossing the energy of the entrance channel or initial scattering state. Their energy increases, indicated by arrows, with magnetic field and a resonance occurs when this energy equals the entrance-channel energy. Coupling with the entrance channel leads to a resonance.

Feshbach resonances make it possible to convert a weakly interacting gas of atoms into one that is strongly interacting and along the way promise to make available many of the collective many-body states mentioned above. Alternatively, interactions can be turned off all together to create an ideal Fermi or Bose gas, for which thermodynamic properties are known analytically. Feshbach resonances can also be used to create BECs of weakly-bound molecules [17], which can be optically stabilized to deeply-bound molecules [18]. For fermionic atoms the BCS-BEC phase transition [19] and universal many-body behavior of strongly interacting magnetic atoms can be studied via Feshbach resonances. Finally, three-body Efimov physics [20] can be explored.

![FIG. 1: (Color online) Potential energy curves for a $^{164}$Dy+$^{164}$Dy collision in an external magnetic field $B$ as a function of internuclear separation. The (red) dashed line with zero energy indicates the energy of the entrance channel. Two Feshbach resonances are schematically shown by (red) horizontal lines, which end at the classical outer turning point of a closed channel. Their energy increases, indicated by arrows, with magnetic field and a resonance occurs when this energy equals the entrance-channel energy. There are 91 diagonal potential matrix elements for channels $(j_1j_2)m_{j_1}m_{j_2}$ with $m_j+m_{j'}=-16$ and even $\ell \leq 10$. We use $B=50$ G. The curves are colored by their $m_j$ value, while for $m_j=-16$ curves their $\ell$ value is indicated. Here $1$ G=$0.1$ mT, $a_0=0.0529177$ nm is the Bohr radius, and $k=1.38065 \cdot 10^{-23}$ J/K is the Boltzmann constant.](image-url)
The most promising atoms to look for the effect of anisotropy on collisions are submerged-shell atoms, which have an electronic configuration with an unfilled inner shell shielded by a closed outer shell. In particular, we are interested in the rare-earth dysprosium (Dy) atom with a $^5\text{I}_s$ ground-state, a total angular momentum $j = 8$, and a large magnetic moment of $\approx 10\mu_B$, for which the electron spins of the inner $4f^{10}$ shell are aligned such that its orbital angular momentum is maximal and largely unquenched. Here $\mu_B$ is the Bohr magneton. As a result, Dy’s magnetic and electrostatic properties are highly anisotropic. A quantitative description of the collision between two dysprosium atoms is challenging. For example, our previous study [15] showed that there are 153 Born-Oppenheimer potentials that dissociate to the ground $^5\text{I}_s + ^5\text{I}_s$ state.

We present a first-principle coupled-channel model allowing us to calculate anisotropy-induced magnetic Feshbach-resonance spectra of bosonic Dy atoms. The model treats the Zeeman, magnetic dipole-dipole, and electrostatic isotropic and anisotropic dispersion interactions equally. Bosonic Dy isotopes have zero nuclear spin. Thus, there is no nuclear hyperfine structure and only Zeeman splittings remain. The weak quadrupole-quadrupole interaction [15] is included for completeness.

We already note that Feshbach resonances in rare-earth magnetic atoms are different in nature than those in alkali-metal atom collisions. As pointed out in Ref. [15] for a coupled-channel calculation there exists at most one channel with zero relative nuclear orbital angular momentum $\ell$, which for ultra-cold collisions is also the entrance channel. Consequently, resonances occur due to anisotropic coupling to bound states with non-zero $\ell$.

The focus of this Letter is on ultra-cold collisions of atoms prepared in the energetically-lowest Zeeman state $j = 8$ and projection $m = -8$. Inelastic exothermic atom-atom processes, where the spin projection of one or both of the atoms changes, are absent and, consequently, Feshbach resonances can be readily observed.

We start by setting up the Hamiltonian, interatomic potentials, and channel basis for two bosonic $^5\text{I}_s$ Dy atoms with zero nuclear spin. This Hamiltonian assuming a magnetic field $B$ along the $\hat{z}$ direction is

$$ H = \frac{\hbar^2}{2\mu_r} \frac{d^2}{dR^2} + \frac{\mu_b}{2\mu_r} R^2 + H_Z + V(\vec{R}, \tau), \quad (1) $$

where $\vec{R}$ describes the orientation of and separation between the two atoms. The first two terms are the radial kinetic and rotational energy operators, respectively. The Zeeman interaction is $H_Z = g_s\mu_B (j_{1z} + j_{2z}) B$ with $g_s = 1.24159$ the $g$-factor of Dy [21] and $j_{1z}, j_{2z}$ is the $z$ component of the angular momentum operator $\vec{j}_i$ of atom $i = 1, 2$. The electronic Hamiltonian, including nuclear repulsion, $V(\vec{R}, \tau)$ is anisotropic and $\tau$ labels the electronic variables. Finally, $\mu_r$ is the reduced mass and for $R \to \infty$ the interaction $V(\vec{R}, \tau) \to 0$.

Our coupled-channels calculations [22] are performed in the atomic basis $(|j_{12}\rangle|m_j, \ell m_\ell\rangle) \equiv |\ell m_\ell (\theta, \phi)\rangle(|j_{12}\rangle jm_\ell\rangle)$, where $|\ell m_\ell (\theta, \phi)\rangle$ is a spherical harmonic and angles $\theta$ and $\phi$ give the orientation of the internuclear axis relative to the magnetic field direction. In this basis the Zeeman and rotational interaction are diagonal with energies $g_{\mu B} \ell m_\ell B + \hbar \ell (\ell + 1)/(2\mu_r R^2)$. Coupling between the basis states is due to $V(\vec{R}, \tau)$ and will be discussed in detail below. Excited atomic states, for example those with $j_1 \neq 8$, are not included as their internal energy is sufficiently high that the effects of coupling to these states is negligible. The Hamiltonian $H$ conserves $M_{\text{tot}} = m_j + m_\ell$ and is invariant under the parity operation so that only even (odd) $\ell$ are coupled. For homonuclear collisions only basis states with even $j + \ell$ exist. Figure 1 shows an example of the long-range diagonal matrix elements in the atomic basis of the sum of the rotational, Zeeman, and electronic Hamiltonian. We have used $M_{\text{tot}} = -16$ and even $\ell \leq 10$. In fact, only the potentials dissociating to the six energetically-lowest Zeeman states are shown. The large number of potentials indicates the large number of resonances that, in principle, are possible.

Coupling between basis states is due to $V(\vec{R}, \tau)$. It is convenient to first evaluate this operator in a molecular basis with body-fixed projection quantum numbers defined with respect to the internuclear axis. We use the molecular basis $|(j_{12}\rangle j \Omega)\rangle$ with projection $\Omega$ of $\vec{j}$ along the internuclear axis. For Dy2 the matrix elements of $V(\vec{R}, \tau)$ conserve the projection $\Omega$ but not the length $j$. The eigenenergies of $V(\vec{R}, \tau)$ at each value of $R$ are the adiabatic (relativistic) Born-Oppenheimer potentials [23] [24]. Typically, these potentials $U_{\mu_\ell}\Omega_\sigma(R)$ are obtained from an electronic structure calculation and labeled by $\mu_\ell \Omega_\sigma(R)$, where $|\Omega\rangle$ is the absolute value of $\Omega$, $\sigma = g/u$ is the gerade/ungerade symmetry of the electronic wavefunction, and $n = 1, 2, \cdots$ labels curves of the same $|\Omega\rangle|\sigma\rangle/u$ in order of increasing energy. For bosonic Dy2 the 81 gerade states are superpositions of even $j$, while the 72 ungerade states are superpositions of odd $j$.

For $R > 2\ell_0$, beyond the Le Roy radius where the atomic electron clouds have negligible overlap, we assume that $V(\vec{R}, \tau) = 1/R^3$, the electric quadrupole-quadrupole, $V_{\text{QQ}}(\vec{R}) \propto 1/R^3$, and the van-der-Waals dispersion $V_{\text{disp}}(\vec{R}) \propto 1/R^6$ interaction. Reference [15] reported the matrix elements of the operator $V_{\text{disp}}(\vec{R})$ in the molecular basis and tabulated the adiabatic $C_{6\ell_n\ell_\sigma}$ dispersion coefficients obtained by diagonalizing $V_{\text{disp}}(\vec{R})$. Crucially, the eigenfunctions of $V_{\text{disp}}(\vec{R})$ are independent of $R$.

At shorter range coupling between basis states is more complex. Rather than determining all Born-Oppenheimer potentials, we have opted for the following approach. First, we calculate the single gerade potential $U_{16\ell_9}(\vec{R})$ with the maximal projection...
\[ \Omega = 16 \] using a coupled-cluster method with single, double, and perturbative triple excitations (CCSD(T)),

\[ \text{ECP28MWB pseudopotential and associated atomic } \]

double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).

\[ \text{ECP28MWB pseudopotential and associated atomic } \]
double, and perturbative triple excitations (CCSD(T)).
We stress that this behavior with increasing number of channels is unlike that observed in alkali-metal atom collisions [10] or even in collisions of strongly magnetic chromium atoms [27]. For these atoms resonances do not shift by more than a few Gauss when additional partial waves are added. Hence, resonances can be labeled by a partial wave quantum number. For dysprosium the anisotropic interactions are so strong that states with different partial waves are strongly mixed. We have also studied the effect of the uncertainty in the depth of the $\Omega = 16$ Born-Oppenheimer potential. The depth $D_c$ was changed by adding a localized correction to $U_{16g}(R)$ that does not modify its long-range potential. A depth change by no more than 10 cm$^{-1}$ changes its number of bound states by one. Changing the depth by smaller amounts changes the resonance spectrum non-trivially. For example resonance widths can be modified dramatically and rate coefficients with broad resonances that appear when $d$-wave channels are included can be observed.

The precise form of short-range potential and dispersion coefficients are not known. A few percent uncertainty is not unrealistic. For this Letter we have constructed potentials that lead to a positive $B = 0$ scattering length $a$ for $^{164}$Dy atoms in the $m = -8$ state. This choice is suggested by the recent observation of a Bose condensed gas of $^{164}$Dy atoms at nearly zero magnetic field. It thus possesses a positive scattering length at this field [8]. Moreover, we chose the scattering length to be approximately equal to the mean scattering length [28] for (fictitious) scattering of a van der Waals potential with a $C_6$ coefficient equal to the isotropic dispersion coefficient.

To further elucidate the effect of anisotropy, Fig. 4 shows the scattering length of $m = -8$ $^{164}$Dy collisions as a function of magnetic field for the bosonic isotopes $^{162}$Dy (top panel) and $^{160}$Dy (bottom panel). The magnetic state and number of included $\ell$ is as in Fig. 3.

FIG. 3: Scattering length of $m = -8$ $^{164}$Dy atoms as a function of magnetic field with and without the magnetic dipole-dipole or the anisotropic contribution of the dispersion interaction. The top panel shows the case when all interactions are included. At $B = 0$ the scattering length is $89a_0$. The middle and bottom panels are obtained when the dispersion and magnetic dipole-dipole anisotropy is set to zero, respectively. Even waves $\ell$ up to 10 are included.

FIG. 4: Scattering length as a function of magnetic field for the bosonic isotopes $^{162}$Dy (top panel) and $^{160}$Dy (bottom panel). The magnetic state and number of included $\ell$ is as in Fig. 3.

Conclusion. Applying a full coupled-channels calculation for ultracold atom-atom collisions, we have shown that the origin of Feshbach resonances in interactions between ultracold rare-earth atoms with large magnetic moments result from strong scattering anisotropies. Consequently, by tuning an applied magnetic field we predict that it will be possible to observe resonances and control collisions even for atoms with zero nuclear spin. This study is the first predictions of a Feshbach resonance spectrum for rare-earth atoms.

We have investigated the effects of different short-range and long-range anisotropic potentials as well as different...
isotopes on the scattering length of ultracold Dy atoms as a function of magnetic field strength. To optimize the potentials we must await experimental observations of resonances from multiple isotopic combinations.

ACKNOWLEDGMENTS

This work is supported by grants of the AFOSR grant No. FA 9550-11-1-0243 and NSF No. PHY-1005453.

* Corresponding author: skotoch@temple.edu
† Alternative address: St. Petersburg Nuclear Physics Institute, Gatchina, 188300; Department of Physics, St.Petersburg State University, 198904, Russia

[1] B. M. Fregoso and E. Fradkin, Phys. Rev. Lett. 103, 205301 (2009); B. M. Fregoso and E. Fradkin, Phys. Rev. B 81, 214443 (2010).
[2] B. M. Fregoso, K. Sun, E. Fradkin, and B. L. Lev, New J. Phys. 11, 103003 (2009).
[3] L. Santos and T. Pfau, Phys. Rev. Lett. 96, 190404 (2006).
[4] J. J. McClelland and J. L. Hanssen, Phys. Rev. Lett. 96, 143005 (2006).
[5] C. B. Connolly, Y. S. Au, S. C. Doret, W. Ketterle, and J. M. Doyle, Phys. Rev. A 81, 010702(R) (2010).
[6] Mei-Ju Lu, V. Singh, and J. D. Weinstein, Phys. Rev. A 79, 050702(R) (2009).
[7] M. Lu, S. H. Youn, and B. L. Lev, Phys. Rev. Lett. 104, 063001 (2010).
[8] M. Lu, N. Q. Burdick, S. H. Youn, and B. L. Lev, Phys. Rev. Lett. 107, 190401 (2011).
[9] D. Sukachev, A. Sokolov, K. Chebakov, A. Akimov, S. Kanorsky, N. Kolachevsky, and V. Sorokin, Phys. Rev. A 82, 011405(R) (2010).
[10] M. Lu, N. Q. Burdick, and B. L. Lev, arXiv:1202.4444v1 (2012).
[11] J. Stuhler, A. Griesmaier, T. Koch, M. Fattori, T. Pfau, S. Giovanazzi, P. Pedri, and L. Santos, Phys. Rev. Lett. 95, 150406 (2005).
[12] S. Hensler, J. Werner, A. Griesmaier, P. O. Schmidt, A. Görlich, T. Pfau, S. Giovanazzi, and K. Rzazewski, Appl. Phys. B 77, 765 (2003).
[13] C. I. Hancox, S. C. Doret, M. T. Hummon, L. Luo, and J. Doyle, Nature 431, 281 (2004).
[14] R. V. Kremes, G. C. Groenenboom, and A. Dalgarno, J. Chem. Phys. 108, 8941 (2004).
[15] S. Kotochigova and A. Petrov, Phys. Chem. Chem. Phys. 13, 19165 (2011).
[16] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Rev. Mod. Phys. 82, 1225 (2010).
[17] T. Köhler, K. Góral, and P.S. Julienne, Rev. Mod. Phys. 78, 1311 (2006).
[18] K.-K. Ni, S. Ospelkaus, M. H. G. de Miranda, A. Peér, B. Neyenhuis, J. J. Zirbel, S. Kotochigova, P. S. Julienne, D. S. Jin, and J. Ye, Science 322, 231 (2008).
[19] S. Giorgini, L.P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 80, 1215 (2008); I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
[20] T. Kraemer, M. Mark, P. Waldburger, J. G. Danzl, C. Chin, B. Engeser, A. D. Lange, P. Pilch, A. Jaakkola, H.-C. Nagerl, and R. Grimm, Nature 440, 315 (2006).
[21] Yu. Ralchenko, A.E. Kramida, J. Reader, and NIST ASD Team (2011). NIST Atomic Spectra Database. Available: [url to the website].
[22] A close-coupling calculation is a numerical method to find scattering solutions of a finite set of coupled radial Schrödinger equations.
[23] G. Herzberg, Spectra of Diatomic Molecules, (D. Van Nostrand Company, New York, 1950).
[24] H. Lefebvre-Brion and R. W. Field, Perturbations in the Spectra of Diatomic Molecules, (Academic Press, Inc, London, 1986).
[25] J. D. Watts, J. Gauss. and R. J. Bartlett, J. Chem. Phys. 98, 8718 (1993).
[26] R. Santra and C.H. Greene, Phys. Rev. A 67, 062713 (2003).
[27] J. Werner, A. Griesmaier, S. Hensler, J. Stuhler, T. Pfau, A. Simon, and E. Tiesinga, Phys. Rev. Lett. 94, 183201 (2005).
[28] G. F. Gribakin and V. V. Flambaum, Phys. Rev. A 48, 546 (1993).
[29] M. Kitagawa, K. Enomoto, K. Kasa, Y. Takahashi, R. Ciurylo, P. Naidon, and P. S. Julienne, Phys. Rev. A 77, 012719 (2008).
[30] E. Tiemann, H. Knöckel, P. Kowalczyk, W. Jastrzobski, A. Pashov, H. Salami, A. J. Ross, Phys. Rev. A 79, 042716 (2009).