Abstract Submitted
for the DAMOP20 Meeting of
The American Physical Society

Relativistic studies of anisotropic properties in magnetic lanthanide erbium and thulium dimers[1] JACEK KLOS, EITE TIESINGA, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg MD 20899, MING LI, ALEXANDER PETROV, SVETLANA KOTOCHIGOVA, Temple University, Physics Department, Philadelphia, PA 19122 — The recent realization of quantum degenerate gases of magnetic atoms, cooled and trapped to sub-μK temperatures, is expected to stimulate studies of magnetic superfluid matter. Atom-atom interactions play a central role in the behavior of such matter. Here, we study the anisotropic interactions for two high-spin magnetic species: $j = 6$ erbium and $j = 7/2$ thulium. Non-relativistic coupled-cluster calculations are combined with fully-relativistic configuration-interaction calculations to determine the electronic potentials for homonuclear Er_2 and Tm_2 dissociating to ground-state atoms with their partially-filled f-electron shells. State-of-the-art non-relativistic coupled-cluster calculations determine the potential for the "stretched" electronic state with the largest electron spin and orbital angular-momentum projection quantum numbers, while relativistic configuration-interaction calculations give the splittings among the potentials. We find a complicated picture of 91 and 36 potentials characterizing the Er_2 and Tm_2 dimers, respectively. An analysis in terms of spin-spin Hamiltonians shows that the splittings are well described by an anisotropic dipolar coupling between the atomic angular momentum with the mechanical rotation of the atom pair.

[1]This work was supported by the AFOSR Grant No. FA9550-14-1-0321

Jacek Klos
National Institute of Standards and Technology

Date submitted: 02 Feb 2020 Electronic form version 1.4