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COMPLEX DIPOLAR MATTER

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14. ABSTRACT
A range of ultracold molecular problems were solved, leading to new opportunities for advanced material development and quantum simulators. These molecules include (1) the already quantum degenerate bi-alkali singlet sigma case potassium-rubidium (KRb) and related molecules; (2) opto-electrically trapped symmetric top molecules soon to reach quantum degeneracy and common in nature, like methyl fluoride (CH3F); and (3) the recently evaporatively cooled hydroxyl free radical (OH). Research achievements on this grant cycle include (A) a fundamental understanding of how strongly-interacting fermions pair to make molecules in the presence of a lattice; (B) experimental guidance and specific numerical predictions for five bi-alkali molecules being studied in labs around the world today, including potassium-rubidium; (C) a correction of phase diagrams for dipolar gases necessary to understand experimental measurements and build accurate quantum simulators; (C) a whole new area of quantum many body physics opened up in symmetric top molecules, involving e.g. exotic tunable XYZ magnetism and quantum liquid crystals; and (D) new high precision predictions for the spectra of the hydroxyl free radical absolutely necessary to reach quantum degeneracy.

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Lincoln D. Carr
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A range of ultracold molecular problems were solved, leading to new opportunities for advanced material development and quantum simulators. These molecules include (1) the already quantum degenerate bi-alkali singlet sigma case potassium-rubidium (KRb) and related molecules; (2) opto-electrically trapped symmetric top molecules soon to reach quantum degeneracy and common in nature, like methyl fluoride (CH3F); and (3) the recently evaporatively cooled hydroxyl free radical (OH). Research achievements on this grant cycle include (A) a fundamental understanding of how strongly-interacting fermions pair to make molecules in the presence of a lattice; (B) experimental guidance and specific numerical predictions for five bi-alkali molecules being studied in labs around the world today, including potassium-rubidium; (C) a correction of phase diagrams for dipolar gases necessary to understand experimental measurements and build accurate quantum simulators; (C) a whole new area of quantum many body physics opened up in symmetric top molecules, involving e.g. exotic tunable XYZ magnetism and quantum liquid crystals; and (D) new high precision predictions for the spectra of the hydroxyl free radical absolutely necessary to reach quantum degeneracy. This work resulted in eight publications and papers under review in peer-reviewed journals. Synergistic activities included (i) organizing an extended program at the Kavli Institute of Theoretical Physics and Kavli symposia for the National Academy of Sciences; (ii) editing a special issue of the New Journal of Physics bringing ultracold molecule researchers from around the world together with a planned collection of over sixty publications; (iii) an edited series on cold atoms and molecules; and (iv) thirty-two invited seminars, sixteen directly on the topic of this grant.

My AFOSR grant began in August 2011. The basic timeline of activities over the last three years are as follows. In 2011-2012 I was on sabbatical on a Humboldt fellowship at the University of Heidelberg, hosted by Matthias Weidemueller, a prominent experimentalist in ultracold molecules. I gave about 20 invited talks and set up research connections and collaborations with many places, perhaps most importantly Durham, which has just gotten a few thousand RbCs molecules to the ground state approaching quantum degeneracy, along with Innsbruck. In 2012-2013 I hired two post-docs on this grant, Kenji Maeda and Michael Wall; the latter went on to win the APS Metropolis Award for his PhD work done in 2008-2012 in my group, the top thesis award for computational physics. In Spring 2013 I organized a 10 week program on ultracold molecules at the Kavli Institute for Theoretical Physics (KITP). In 2013-2014 Dr. Maeda continued to work with me, supported by this grant, and we opened up a totally new field of quantum many body physics, building towards a recent successful renewal of our grant program with AFOSR. During this final period I also hosted visiting scientists from India, the UK, Israel, and Spain. In particular, Mr. Arya Dhar, now a post-doc with Paivi Torma at U. Aalto in Finland, was one of three graduate students in all of India to win an APS fellowship to come work in the US.

Key <u>research results</u> from 2011-2014 include the following.

1. We solved the basic problem of how fermions pair to make a molecule in optical lattices near unitarity, in a PRL/PRA pair in 2012/2013. There we developed the *Fermi Resonance Hamiltonian*. Many people tried this problem and got it wrong in PRLs etc. (including me back in 2005). I consider the Fermi Resonance Hamiltonian the first landmark result of the grant. The

key is to diagonalize the two-body problem in the lattice, to form a sort of two-body band structure for the molecules. Pairing of atoms to make a molecule in a Feshbach resonance is an important first step towards ground state quantum degenerate diatomic molecules, before STIRAP, and it's important to get it right.

2. In 2011/2012 we developed and solved the Molecular Hubbard Hamilitonian for 5 different singlet sigma molecular species providing specific guidance to experimentalists for realizing different many-body models. Calculations in this paper came out of my sabbatical in Heidelberg, and in many cases were personally requested by leading researchers, including my host Matthias Weidemueller in Heidelberg, Hans-Christoph Naegerl at Innsbruck, Simon Cornish at Durham, and Wolfgang Ketterle at MIT. An important aspect of our approach is to treat specific molecules in full detail. Other theorists have tended to create generic models. We have made a point to stay very close to experiments and make specific numerical predictions that can be directly tested.

3. In 2012/2013 we showed that effective interactions between dipoles in optical lattices are not really inverse cubic, and made new predictions for phase diagrams. This really changes what experimentalists actually measure when they are creating these quantum simulators. Such results apply to electric and magnetic dipoles both. The main reason for the deviation from inverse cube interaction energy are the quantum fluctuations in Wannier tails due to the optical lattice.

4. Inspired by new experimental results presented at the KITP in March 2013 on Stark cooling and opto-electrical trapping, we obtained the first many-body description of symmetric top molecules, demonstrating significant advantages over singlet sigma molecules. Thus we provided guidance for next generation experiments using different cooling technology. This work has continued up till now and is being pursued in the next grant cycle. The piece we did in 2013/2014 was to set up the many-body Hamiltonian and then show that we get e.g. unusual XYZ tunable magnetism. These kinds of models just can't be realized in singlet sigma molecules like KRb.

5. In keeping with the theme of new molecules past KRb and other singlet sigma cases, we turned to the hydroxyl free radical, OH. There we developed a high precision Hamiltonian bringing the spectral accuracy down to below 100 nK, which is absolutely necessary for any kind of effort towards quantum degeneracy. In the process we also made some significant corrections to higher temperature calculations used in the landmark Jun Ye paper demonstrating evaporative cooling of OH.

6. We performed extensive quantum entangled simulations on the dynamics of the long range Ising model, on quantum dephasing of singlet sigma molecules, and on the bilinear-biquadratic spin Hamiltonian. This work is still in progress but we expect it to result in papers over the next grant cycle. Several visiting researchers mentioned in my introductory paragraph participated in this work and are pursuing it now, building collaborations between our group and groups in the

US and Europe.

7. Finally, we produced new algorithmic developments for entangled quantum dynamical methods (matrix product states) absolutely necessary to make any progress on molecules, as of March 2014 available in our open source code; this latter work is so extensive that it is actually supported by a completely separate NSF PIF grant for open source code development. I emphasize that my AFOSR support involves no code development: it is all about the molecular and many-body physics, not computational physics. However, Dr. Maeda and a number of scientific visitors from Durham etc. were end-users of this development, so I feel it is important to mention here.

Key <u>synergistic activities</u> connected to my AFOSR funding in 2011-2014 include the following:

1. As mentioned in my intro summary, I organized a 10 week program and conference at the KITP entitled ``Fundamental Science and Applications of Ultra-cold Polar Molecules'' and ``New Science with Ultracold Molecules,'' respectively, with Roman Krems, Paul Julienne, and Susanne Yelin, which took place in spring 2013. The program had 78 participants and the conference had 105. The latter had the largest poster session in memory from the last decade at KITP, with over 50 posters.

2. I was the guest editor, with Jun Ye, for a focus issue of the New Journal of Physics (NJP) on Cold and Ultracold Molecules, which appeared in May of 2009. We had 40 separate contributions, including my own work on quantum entangled dynamical studies of ultracold molecules (using a preliminary version of the Molecular Hubbard Hamiltonian, not the full one we use now and supported by AFOSR). We wrote a review with David Demille and Roman Krems, which has ~350 citations and 10000+ downloads (NJP provides the latter metric). The four of us are now editing a second NJP Focus Issue for 2014-2015, ``New Frontiers in Cold Molecules Research.'' We have over 60 promised submissions for this Focus Issue. The development of this new focus issue happened in the AFOSR 2011-2014 grant cycle.

3. From 2011-2014 I was Associate Editor at NJP. I will continue to serve as an associate editor and board member for the New Journal of Physics, where one of my duties is to suggest and guide focus issues, including those concerning molecules and quantum simulations.

4. I organized a Kavli Frontiers of Science Symposium at the National Academy of Sciences in August 2013, and have been organizing a follow-up symposium in South Korea in July 2015. This is an interdisciplinary conference in the sciences bringing together top young people across the US, and in this case pairing them with South Korean counterparts. South Korea is an important US ally and as part of my work with AFOSR I will continue to grow our scientific connections there. I presented my AFOSR work on molecules as part of this symposium, and the theme of the next one is frontiers of quantum mechanics, including ultracold physics.

5. I co-edited a series on ultracold atoms and molecules for World Scientific with Kai Bongs, Ana Maria Rey, Hui Zhai, and Kirk Madison (chief editor). This series is a continuing effort and grows

the field of ultracold molecules.

6. I gave 32 invited talks over the grant period. Of these, 16 were on ultracold molecules. Likewise my post-docs supported on this grant gave numerous invited talks, were awarded long-stay programs at KITP and Aspen, and are generally doing very well. Dr. Wall is now an NRC Fellow and Dr. Maeda continues for a third year on the grant renewal, at the Colorado School of Mines.

<u>Detailed publication list:</u>

1. M. L. Wall and L. D. Carr, "Microscopic model for Feshbach interacting fermions in an optical lattice with arbitrary scattering length and resonance width," Phys. Rev. Lett., v. 109, p. 055302 (2012)
2. M. L. Wall and Lincoln D. Carr, "Out of equilibrium dynamics with Matrix Product States," New J. Phys., v. 14, p. 125015 (2012)
3. M. L. Wall and Lincoln D. Carr, "Strongly interacting fermions in optical lattices," Phys. Rev. A, v. 87, p. 033601 (2013)
4. M. L. Wall, E. Bekaroglu and Lincoln D. Carr, "The Molecular Hubbard Hamiltonian: Field Regimes and Molecular Species," Phys. Rev. A, v. 88, p. 023605 (2013)
5. M. L. Wall and Lincoln D. Carr, "Dipole-dipole interactions in optical lattices do not follow an inverse cube power law," New J. Phys. v. 15, p. 123005 (2013)
6. M. L. Wall, Kenji Maeda, and Lincoln D. Carr, "Simulating quantum magnets with symmetric top molecules," Ann. Phys. (Berlin) v. 525, p. 845 (2013)
7. K. Maeda, M. L. Wall, and L. D. Carr, “Hyperfine structure of the hydroxyl free radical (OH) in electric and magnetic fields,” New J. Phys., under review (2014)
8. M. L. Wall, K. Maeda, L. D. Carr, "Realizing unconventional quantum magnetism with symmetric top molecules," New J. Phys., under review (2014)