**PROPOSAL WHITE PAPER Friday, July 20, 2016**

**FOA:** N00014-16-R-FO05

**Proposed title:**

*Universal quantum many-body computing with accelerated correlation enumerators* (uniqMBace)

**Proposer:** Mackillo Kira

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**Topic 6 (AFOSR):**

Revolutionary Advances in Computational Quantum Many Body Physics

**1. Identification of the research and issues**

Interacting many-body systems are ubiquitous in nature, and yet simulating those exhausts computation resources as the interactions create correlations with an exponentially increasing complexity among particles. Our team will tackle the core problem of equilibrium and non-equilibrium properties in strongly correlated systems by creating an *accelerated correlation-enumerator (ACE) framework*. We will optimally merge complementary ideas to deliver a new modular ACE that overcomes the exponential resource demands impeding universal quantum many-body computations. The universality of our framework will be demonstrated by explaining and predicting non-equilibrium transients as well as static correlations in experiments at the broad frontier of quantum and materials science, including coupling to the environment.

Our team will develop the first universal quantum many-body solver by integrating the most beneficial aspects of density-functional theory (DFT), phase-space methods such as truncated Wigner approximation (TWA) and its discrete generalizations (DTWA) [PRX **5**, 011022 (2015)][[1]](#footnote-1), quantum Monte Carlo (QMC), non-stochastic, full configuration interaction (FCI), and density-matrix renormalization group (DMRG) into our ACE. For example, by representing interacting fermionic problems in phase-space[arXiv 1604.08664], TWA dynamics will avoid the notorious *“sign problem”* of pure fermionic QMC. Similarly, our cluster-expansion (CE) approach [*Semiconductor Quantum Optics*, (Cambridge University Press, 2012)] defines an exact energy correlation functional [NJP **15**, 093040 (2013)] that is unknown in pure DFT. We will systematically benefit from such a synergy by developing rigorous benchmarking to optimize hybrid methods and by finding efficiently scalable and parallelizable algorithms to deliver a modular and open-source-ready ACE framework for next-generation supercomputers.

We will systematically improve our ACEs by applying them to analyze relevant experiments in atomic, molecular and optical (AMO) systems [NJP **17**, 065009 (2015), PRL. **114**, 045701 (2015), Nat. Comm. **6**, 6624 (2015)], nuclear-matter [Nature **512**, 378 (2014), Nat. Phys. **12**, 186 (2016)], quantum-chemistry [Chem. Sci. **7**, 1712 (2016)], nanodevice [PRL **114**, 116802 (2015)], solid-state [Nature **533**, 225 (2016)], and quantum information science [NJP **18**, 023023 (2016)]. We expect that our ACE simulations will revolutionize the understanding of several unresolved problems in quantum and materials science by developing strategies to best tackle the following four interconnected challenges: (i) Quantum information scales exponentially with particle number. (ii) Interactions scramble quantum information by creating entanglement/correlations among particles, yielding loss of information, i.e. dissipation, unless fully tracked. (iii) Correlations stem from the hierarchy problem that usually prevents exact solutions. (iv) As interactions generate correlations, computations must handle multiple time and length scales besides managing the exponential overhead in quantum information.

**2. Proposed technical approaches**

It is convenient to classify many-body approaches based on how they treat correlations: **Correlation-truncation (C-T)** approaches describe properties of low-rank correlations or observables by systematically truncating the hierarchy at a predefined level. Most non-stochastic methods such as coupled-clusters (CC), CE, and dimension-reduction (DR) approaches are C-Ts. **Correlation-upconversion (C-up**) schemes use either functionals or ensembles of low-rank correlation solutions to describe high-order correlations, as in done in DFT and TWA, respectively. **Correlation-downconversion (C-down)** methods compress exact information about high-rank clusters via direct diagonalization, iterations, or ensemble averaging of configurations as is done in FCI, DMRG, and QMC, respectively.

|  |  |
| --- | --- |
|  | **Figure 1:** Illustration of the simulation efficiency for a traditional (left) vs. a hybrid **A**ccelerated-**C**orrelation-**E**numerator (ACE, right) approach. Rigorous benchmarks will be carried out to determine the specific order at which the methods will be combined. |

Figure 1 (left) illustrates how “traditional” simulations droop at the expense of computational cost when using only a single C-T (blue), C-up (black), or C-down (red) approach, which has so far prevented mesoscale simulations of quantum effects. Nevertheless, each approach initially improves in accuracy very fast with only a little added numerical cost. We will develop ACEs by optimally interlacing the strengths of C-T, C-up, and C-down approaches to eliminate the efficiency droop (Fig. 1, right). As discussed above, already a CE-DFT combination improves the accuracy because the CE defines functionals exactly for the DFT while the DFT can provide an *ab initio* Hamiltonian for the CE. In the same way, QMC, DMRG, and FCI can improve the accuracy of truncations applied in the CE, DFT, DR, CC, and DTWA while feeding this improvement back will accelerate the hybrid C-T-up-down approach, with low costs. For example, DMRG and QMC can systematically include quantum correlations to TWA which is otherwise exact only for linear systems and for systems approaching the classical limit.

To accelerate the computations further, we will also introduce formal transformations to an excitation picture [Ann. Phys. **351**, 200 (2014)] which focuses the investigations only to the correlations among excited states. Since the number of excited states is typically massively lower than the total number of states, the numerical gain of a successfully introduced excitation picture is typically dramatic. One also can introduce efficient annealing protocols to drive systems very fast without transitions from uncorrelated to strongly correlated states[Anatoli, fill in] by using counter-diabatic drives in both real and imaginary time. Instead of stochastic QMC, we will also use quasi Monte-Carlo that samples ensembles based on number theory to improve convergence.

Our overall the goal is to systematically synthesize a universal ACE framework where many-body correlations are always solved with the most efficient combination of methods, at user-defined accuracy. For that, we will develop rigorous benchmarks and also explore the possibility to use machine-learning protocols [Chem. Sci., doi10.1039/C5SC04786B (2016)] to select the best combination of strategies for different length and time scales. To foster universal ACE solutions, we create ideas through six different topics (1) AMO systems, (2) nuclear matter, (3) numerical methodology, (4) quantum information, (5) quantum chemistry, and (6) semiconductor quantum optics. We will program the ACE modules by using openMP and openACC for flexible and efficient parallel computing and by extensively analyzing computational and mathematical structures [*Fast and Efficient Algorithms in Computational Electromagnetics,* (Artech House, Inc. Norwood, MA, 2001)] to develop numerical algorithms that maximally use current and future super-computing resources.

**3. Potential impact on DoD capabilities**

We expect that our ACEs will deliver the following capabilities for DoD:

* A universal ab initio framework with rigorous benchmarks for mesoscale quantum many-body computations with next-generation, high-performance computers.
* Foundations for a universal open-source interface to describe diverse mesoscale quantum phenomena covering both non-equilibrium dynamics and steady-state properties.
* Modelling of state-of-the-art experiments in quantum and materials science.

By combining these outcomes, we will be able to make the broadest possible impact on universal strongly correlated matter studies in regimes where other known methods have failed.

In the context of AMO, we expect to solve long-standing problems including long-range interactions and non-equilibrium effects in ion traps as well as quantum kinetics in strongly interacting Bose and Fermi gases including multi-particle interaction effects giving rise to Efimov physics, which is also relevant for nuclear matter. By including exact correlation functionals in DFT, we will be able to gain insight on the thermodynamics and quantum kinetics of generic systems ranging from nanodevices to neutron stars and supernovae explosions. The expected capability to tackle the dynamics of quantum coherences and entanglement with ACEs will help to promote mesoscale design of solid-state devices, including novel materials such as transition metal dichalcogenides, and the search for topological quasiparticles such as Majorana fermions, realized in hybrid semiconductor/superconductor systems, or new forms of stable particle clusters such as dropletons [Nature **506**, 471 (2014)]. We also expect that ACEs will create new insights to existing phenomena, such as fractional quantum Hall effect, and lead to discovery of emergent behavior mediated by light-matter interactions relevant in AMO, chemical reactions, nanostructures. This body of work could introduce storage and retrieval protocols that interface quantum-light states with complex many-body states. Moreover, the proposed application of ACEs for the optimization of annealing protocols can be useful for quantum information processing in a variety of platforms because decoherence processes could be mitigated by fast operation.

**4. Potential team and management plan**

Our team contains six principal investigators (PIs) covering a broad expertise in quantum many-body science: **(PI1) Alán Aspuru-Guzik (Harvard Univ.)** has innovated first-principles approaches to address a broad range of problems in quantum computation, quantum information, quantum chemistry, and biological systems. **(PI2) Wick Haxton (UC Berkeley)** has pioneered many-body theory (effective theories) in nuclear physics (as well as in atomic physics and condensed matter physics). **(PI3) Mackillo Kira (Proposer, Univ. Michigan)** has introduced the CE approach and excitation picture to efficiently describe semiconductor quantum optics and strongly interacting Bose gas. **(PI4) Eric Michielssen (Univ. Michigan)** has developed fast and efficient solvers for converting challenging mathematical formulations into efficiently scalable supercomputing. **(PI5) Anatoli Polkovnikov (Boston Univ.)** has discovered exact solutions for nonequilibrium dynamics of isolated quantum systems and counter-adiabatic methodology. **(PI6) Ana Maria Rey (JILA, Univ. Colorado)** has developed DTWA and CE methodologies to tackle the non-equilibrium quantum dynamics of long-range interacting systems relevant for AMO experiments.

Our team will have at least the following **external collaborators:** theory collaborations with **Morten Hjorth-Jensen (State Univ. Michigan**) who is an expert in CC, FCI, QMC computations in quantum dots and nuclear matter and **Michael Wall (JILA, Univ. Colorado)** who is an expert in DMRG computations. We also quantitatively analyze experiments measured by the following groups: **Steven Cundiff (Univ. Michigan)** has developed quantum-optical and multi-dimensional spectroscopy to access many-body correlation and ultrafast processes in solids and AMO systems. **John Bollinger (NIST, Boulder)** has pioneered a Penning trap set-up to form 2-D arrays of 30 to 300 ions with externally controllable interactions. **Rupert Huber (Univ. Regensburg, Germany)** leads the experimental development of strong-field, few-cycle, near-field, terahertz spectroscopy to drive and time resolve quantum kinetics of quasiparticles.

We will work roughly in 6-month-long cycles. At the beginning of each cycle, we will go over the realized breakthroughs and based on them, agree on the new challenges, objectives, and collaborative efforts between the subprojects. This will be done by finding common connections and mathematical structure, and by revising goals and rules for our modular ACE programming. Within each cycle, PI1-PI3, PI5, and PI6 will merge and develop ACEs to explore quantum many-body effects within their respective fields of expertise while PI4 will focus on converting mathematical formulations into accelerated HPC solutions. As results emerge, we will jointly integrate the physical and computational ideas to a universal quantum many-body solver that will be developed modularly from different ACE components and carefully benchmarked. The benchmarking will involve intensive and dynamically changing collaborations between all teams. As ACE solutions emerge, they will be complementarily tested by using them to quantitative analyze our collaborators’ experiments.

Since our team covers a very broad range of systems, each PI will supervise on average 1 student and 1 postdoc to develop new ACE ideas within their core topic area. To intensify the collaborations, we intend to have 3 postdocs who will work with two or more PIs to merge different approaches and insights to our ACE. We will establish a Wikipedia platform to jointly develop and share ideas and modular programs, and for documentation. As synergy emerges, the involved PIs and their groups will meet roughly biweekly over skype, besides the daily one-on-one communications. All PIs will participate in a monthly reporting and planning meetings via skype. Also a program for short-term visits will be established to further stimulate collaborations between the participants. The results of the teams will also be presented at conferences, (a trip per person per year is reserved for this purpose) and by publishing in high-rank/open-access journals.

**5. Summary of estimated costs**

The estimated annual budget is tabulated below including overheads (time investment of each PI indicated in [%], all sums including fringe benefits and indirect costs, if applicable):

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Item** | | **PI1[?%]** | **PI2[?%]** | **PI3**[50%] | **PI4[?%]** | **PI5[5%]** | **PI6**[25%] | **Central** |
| Students | $60,000 | | $60,000 | $60,000 | $60,000 | $55,000 | $60,000 | --- |
| Postdocs | $90,000 | | $90,000 | $90,000 | $90,000 | $100,000 | $90,000 | 3\*$90,000 |
| Summer salary | $25,000 | | $25,000 | $25,000 | $25,000 | $25,000 | --- | --- |
| HPC grants | $10,000 | | $10,000 | $10,000 | $10,000 | ---- | $10,000 | --- |
| PCs/upgrades | --- | | ---- | --- | --- | --- | --- | $20,000 |
| Conferences,  Internal meetings,  Short-term visits (STV) | 3\*$2000  =$6000  Confe­rences | | 3\*$2000  =$6000  Confe­rences | 3\*$2000  =$6000  Confe­rences | 3\*$2000  =$6000  Confe­rences | 3\*$2000  =$6000  Confe­rences | 3\*$2000  =$6000  Confe­rences | $76,000=  3\*$2000 (Conf.postdocs)  6\*$1500 (PIs)  24\*$1750(all)  $20,000 (STV) |
| Open-access  Publications | $3000 | | $3000 | $3000 | $3000 | $3000 | $3000 | --- |
| Sum | $194,000 | | $194,000 | $194,000 | $194,000 | $189,000 | $169,000 | $366,000 |

**Total budget = $1.5M/year**

* MURI with 8 postdocs and 6 students (3 postdocs are shared by multiple PIs).
* PIs meeting: allocate postdocs, PC, short-term visits from the central budget.
* Annual meeting includes expenses by 3 external members

**Curriculum vitae of PI1: Alán Aspuru-Guzik**

*Current position, title, and address:*

**Curriculum vitae of PI2: Wick Haxton**

*Current position, title, and address:*

Professor, Department of Physics, University of California, Berkeley 431 Old LeConte, MC-7300, Berkeley, CA

**Tel.** (510) 664-4321 **Fax:** (510) 486-4794

**Email:** [haxton@berkeley.edu](mailto:haxton@berkeley.edu)

*Education:*

* B.S. in Physics with Highest Honors, BS in Mathematics with Highest Honors, College Honors, University of California, Santa Cruz, 1967-71.
* M.S., Theoretical Physics, Stanford University, 1973.
* Ph.D., Theoretical Physics, Stanford University, 1976.

*Employment:*

* Postdoctoral Research Associate (1975–77), Institut fur Kernphysik der Universitat Mainz.
* Postdoctoral Staff Member and J.Robert Oppenheimer Fellow (1977–82), Los Alamos.
* Assistant Professor (1980–81), Purdue University.
* Staff Member (1982–85), Theoretical Division, Los Alamos National Laboratory (LANL).
* Associate Professor (1984–87), Professor (1987–2009), Univ. of Washington.
* Director (1991–2006), Senior Fellow (2006-9), Inst. for Nuclear Theory (INT), Univ. of Washington.
* Adjunct Professor Astronomy (1994–2009), University of Washington.
* Associate Senior Fellow (2009–present), Emeritus Professor (2009–present), INT, Univ. of Washington.
* Professor of Physics (2009–present), Univ. of California, Berkeley.
* Faculty Senior Scientist (2009–present), LBNL.

***Mentors:***

* Ph.D. Advisor (1974-1976): T. W. Donnelly, Stanford University
* Postdoctoral Advisors (1975-1982): D. Drechsel, U. Mainz; J. Ginocchio and P. Herczeg, T-Division. LANL

*Honors:*

Member, National Academy of Sciences, 1999-; Fellow, American Academy of Arts and Sciences, 1999-; Fellow, American Association for the Advancement of Science, 1988-; Inaugural Member, Washington State Academy of Sciences, 2008-; Fellow, American Physical Society, 1987-; Miller Fellow, UC Berkeley, 2000-2001; Bethe Lecturer, Cornell University, 2000-2001; Guggenheim Fellow,2000-2001; American Physical Society Hans Bethe Prize, 2004; Senior Humboldt Research Award, 2012; Phi Beta Kappa Visiting Scholar, 2012; Simons Foundation Fellow, 2016.

*Five selected publications relevant for this proposal:*

1. K.S. McElvain and W. C. Haxton, *Nuclear Physics without High-Momentum Potentials: Direct Construction of the Effective Interaction from Scattering Observables*, Submitted to Phys. Rev. Letts. (2016).
2. W. C. Haxton and D. J. Haxton, *Composite Fermions and the First-Landau-Level Fine Structure of the*

*Fractional Quantum Hall Effect,* Phys. Rev. B 93, 155138 (2016).

1. W. C. Haxton, *Form of the Effective Interaction in Harmonic-Oscillator-Based Effective Theory,* Phys.

Rev. C 77, 034005 (2008).

1. W. C. Haxton, K.Nollett, and K. Zurek, *Piecewise Moments Method: Generalized Lanczos Technique for Nuclear Response Surfaces,* Phys. Rev. C 72, 065501 (2005).
2. W. C. Haxton and T. Luu, *Perturbative Effective Theory in an Oscillator Basis?,* Phys. Rev. Lett. 89, 182503 (2002).

*Five other relevant publications:*

1. W. C.Haxton. Neutrino Physics: What Makes the Sun Shine. Nature 512, 378 (2014).
2. A. L. Fitzpatrick, W. C. Haxton. E. Katz, N. Lubbers, and Y. Xu, *The Effective Theory of Dark Matter Detection,* JCAP 02, 004 (2013).
3. W. C. Haxton. R. G. H. Robertson, and A. M. Serenelli, Solar Neutrinos: Status and Prospects, Ann. Rev. Astron. and Astrophys. 51, 21(2013).
4. E. G. Adelberger et al. Solar fusion cross sections II. Rev. Mod. Phys. 83, 195 (2011).
5. P. Banerjee, W. C. Haxton, and Y.-Z. Qian. A Long, Cold, Early r-process? Neutrino-driven Nucleo-synthesis in Supernova He shells Revisted. Phys. Rev. Lett. 106, 201104 (2011).

***Synergistic Activities:***

* Selected American Physical Society Service: APS Executive Board Member 2011-13; 2014-15; Board of Directors, 2015- Division Councilor, Nuclear Physics, 2010-; Chair, Division of Astrophysics, 1996; Chair, Division of Nuclear Physics, 1993.
* Selected National Academy of Sciences/National Research Council Service: Chair, Physics Section, 2013-2016; Chair, Nuclear Physics Panel, 2004-8 and 2012; Physics Section Representative, Class Membership Committee, 2010-16; Member, Board on Physics and Astronomy
* Current Editorial Activities: Editor, Physics Letters B, 1995-, Editorial Board Member, Annual Review of Nuclear Part. Sci., 2007-2008; Associate Editor, 2009-
* Recent Conference and School Organization: CIPANP 2015, Aspen, June 2015 (co-chair), TAUP2013: 13th Workshop on Astroparticle and Underground Physics, Asilomar, Sept. 2013 (chair), Recent Workshop Organization (at Institute for Nuclear Theory, Seattle), Neutrino Astrophysics and Fundamental Properties, Summer 2015; Workshop on Nuclear Aspects of Dark Matter Searches, Dec. 8-12, 2014; Nuclei and Fundamental Symmetries, Summer 2013.

***Current Collaborators:***

Baha Balantekin (U. Wisconsin); J. Beller (Darmstadt); A. L. Fitzpatrick (Boston U); D. J. Haxton (Berkeley); A. Heger (Monash); B. R. Holstein (U. Massachusetts); E. Katz (Boston U.); X. Ji (Jiao Tong U); C. Pena-Garay (U. Valencia);Y.-Z. Qian (Minnesota); R. G. H. Robertson (U. Washington); A. Schwenk (Darmstadt); A. Serenelli (U. Barcelona).

***Students and Postdoctoral Associates:***

**Postdocs:** Matt Kistler (Stanford); Ken Shen (Berkeley); Andre Walker-Loud (LBNL); Sergey Syritsyn (Stony Brook), Projjwal Banerjee (Minnesota), Amy Nicholson (current), Austin Harris (current). **Total: 7**

**Students:** Satoru Inoue (S. Carolina); Cory Schillaci (Data Science); Ken McElvain (current); Nikhil Anand (Johns Hopkins), Raymond Co (Berkeley). **Total: 5**

***Current and Pending Support (as annual direct costs)*:**

* **DOE**: *“Nuclear Physics and Astrophysics Theory at UC Berkeley.”* PI. $580K, 7/1/16-6/30/19.
* **DOE SciDAC*:*** *“A Multi-Scale Approach to Nuclear Structure/Reactions: Forming the Computational Bridge between LQCD and Nuclear Structure.”* PI. $3.54M, 8/1/12-7/31/17.
* **Sather Foundation:** *“Advanced Computational Methods for the Quantum Mechanical Many-Body Problem in Physics and Chemistry.”* PI. $25K, 7/1/15-12/31/16.
* **LBNL LDRD Grant:** *“Fundamental Interactions and Astrophysics*.” PI. $480K, 8/1/14-7/31/17.
* **DOE:** *“Lawrence Berkeley Lab Nuclear Theory Group.”* Co-PI. $1.885M, 10/1/2015-9/30/2016.
* **Simons Foundation:** *“Topics in Effective Theory and Neutrino Astrophysics.”* PI. $150K, 7/16-6/17.
* **DOE:** *“Nuclear Theory for Double Beta Decay and Fundamental Symmetries.”* Co-PI. $160K (Berkeley subcontract), 1/1/16-12/31/20.
* **NSF:** *“Network for Neutrinos, Nuclear Astrophysics, Symmetries.” PI. $2.398M 9/16-8/21 (pending)*

**Curriculum vitae of PI3 (Proposer): MACKILLO KIRA**

*Current position, title, and address:*

Visiting Professor, Professor (from Sept. 1st, 2016) Electrical Engineering and Computer Science, University of Michigan, 3116 ERB 1, 2200 Bonisteel Blvd. Ann Arbor, MI 48109-2099

**Tel.** (734) 763-4878, **FAX** (734)763-4876

**Email:** [mackkira@umich.edu](mailto:mackkira@umich.edu)

*Education:*

* Physics MSc, Helsinki University of Technology (HUT, Current name Aalto University), Finland, 1992
* Ph.D. Physics, Helsinki University of Technology (HUT, Current name Aalto University), Finland, 1996

*Employment:*

* Research Assistant (1990–1992) Low Temperature Laboratory, HUT, Finland; Physics.
* Research Assistant (1992–1993) Dep. of Applied Physics,Univ. of Jyväskylä, Finland; Physics.
* Research Assistant (1992–1995) Research Institute for Theoretical Physics, Univ. of Helsinki, Finland; Physics
* Postdoctoral Fellow (1996–1998): Department of Physics, Philipps Univ. of Marburg, Germany; Physics
* Research Associate (1999–2002): Department of Physics, Royal Institute of Technology, Sweden; Physics
* Assistant Professor (2002–2006): Department of Physics, Philipps Univ. of Marburg, Germany; Physics
* Professor (W2, 2006–2016): Department of Physics, Philipps Univ. of Marburg, Germany; Physics
* Professor (2016-present): Electrical Engineering and Computer Science, University of Michigan; Physics

***Mentors:***

* Ph.D. Advisor: Stig Stenholm (1993–1995), Univ. of Helsinki, Finland
* Postdoctoral Advisor: Stephan W. Koch (1995–1998) , Philipps Univ. of Marburg, Germany

*Honors:*

APS Fellow, American Physical Society, 2015; C-PHOM Visiting Professor, Univ. Michigan, 2015; Visiting Professor, Aalto University, Finland 2012; JILA visiting fellow, JILA, NIST/University of Colorado, 2007; Academy Research Fellow, Academy of Finland 2002; Marie Curié Fellow, Commission of European Union, 1996; Graduation Award, Helsinki University of Technology (HUT), Finland, 1996; Postgraduate Fellowship, Univ. of Jyväskylä, Finland, 1993; Graduation award, Helsinki University of Technology (HUT), Finland, 1992.

*Five selected publications relevant for this proposal:*

1. T. Maag, A. Bayer, S. Baierl, M. Hohenleutner, T. Korn, C. Schüller, D. Schuh, D. Bougeard, C. Lange, R. Huber, M. Mootz, J. E. Sipe, S. W. Koch, and M. Kira, *Coherent cyclotron motion beyond Kohn's theorem*, Nat. Phys. 12, 119 (2016).
2. F. Langer, M. Hohenleutner, C. Schmid, C. Poellmann, P. Nagler, T. Korn, C. Schüller, M. S. Sherwin, U. Huttner, J. T. Steiner, S. W. Koch, M. Kira, and R. Huber, *Lightwave-driven quasiparticle collisions on a sub-cycle timescale*, Nature 533, 225 (2016).
3. M. Kira, *Excitation picture of an interacting Bose gas*, Ann. Phys. 351, 200-249 (2014).
4. A.E.Almand-Hunter, H. Li, S.T. Cundiff, M. Mootz, M. Kira, and S.W. Koch, *Quantum droplets of electrons and holes*, Nature 506, 471 (2014).
5. M. Kira and S.W. Koch, *Many-body correlations and excitonic effects in semiconductor spectroscopy*, Prog. Quantum Electron. 30, 155 (2006).

***Five other relevant publications:***

1. M. Hohenleutner, F. Langer, O. Schubert, M. Knorr, U. Huttner, S.W. Koch, M. Kira, and R. Huber, *Real-time observation of interfering crystal electrons in high-harmonic generation*, Nature 523, 572 (2015).
2. M. Kira, *Coherent quantum depletion of an interacting atom condensate*, Nat. Comm. 6, 6624 (2015).
3. M. Kira, *Hyperbolic Bloch equations: atom-cluster kinetics of an interacting Bose gas*, Ann. Phys. 356, 185 (2015).
4. M. Mootz, M. Kira, and S.W. Koch, *Pair-excitation energetics of highly correlated many-body states*, New J. Phys. 15, 093040 (2013).
5. M. Kira, S.W. Koch, R.P. Smith, A.E. Hunter, and S.T. Cundiff, *Quantum spectroscopy with Schrödinger-cat states*, Nat. Phys. 7, 799 (2011).

***Synergistic Activities:***

* Referee for several international journals.
* Mentor of undergraduate, and graduate students; and postdocs.
* Organizer and member of the advisory board of various national and international workshops and conferences.
* Presented a number of talks to general audiences and public lectures.
* Co-author and coordinator of Wikipedia pages on semiconductor quantum optics, semiconductor Bloch and luminescence equations, semiconductor laser theory, cluster-expansion approach etc.

***Current Collaborators:***

Manfred Bayer (Univ. Dortmund, Germany), Sangam Chatterjee (Univ. Giessen, Germany), Steven Cundiff (Univ. Michigan), Manfred Helm (Helmholtz-Zentrum Dresden-Rossendorf, Germany), Rupert Huber (Univ. Regensburg, Germany), Martin Koch (Univ. Marburg, Germany), Stephan W. Koch (Univ. Marburg, Germany), Junichiro Kono (Rice University), , Franz Kärtner (DESY, Germany), Yun-Shik Lee (Univ. Oregon), Frank Heggman (Univ. Alberta), Theodore Norris (Univ. Michigan), Daniel Sanches-Portal (Centro de Física de Materiales, Spain), Harald Schneider (Helmholtz-Zentrum Dresden-Rossendorf, Germany), John Sipe (Univ. Toronto), Mark Sherwin (UC Santa Barbara), Duncan Steel (Univ. Michigan), Ilkka Tittonen (Aalto University, Finland).

***Students and Postdoctoral Associates (2009–2015):***

**Postdocs:** Christian Berger,Christoph Böttge, Daniel Golde, Peter Hawkins, Martin Mootz,Lukas Schneebeli,

Johannes Steiner, Osmo Vänskä. **Total: 8**

**Graduate students:** Christian Berger, Gunnar Berghäuser, Christoph Böttge, Bennjamin Breddermann,

Daniel Golde, Ulrich Huttner, Martin Mootz, Andrea Klettke, OsmoVäskä. **Total: 9**

**Undergraduate students:** Thomas Ahlich, Christian Berger, Simon Bode, Markus Borsch, Benjamin Breddermann, Dominik Breddermann, Alexander Bronn, Jakob Geipel, Onno Hansen-Goos, Ulrich Huttner, Martin Mootz,

Ralf Riedinger, Andre Rinn, Johannes Schurer. **Total: 14**

***Current and Pending Support (as annual direct costs)*:**

Since I will move from Marburg (Germany) to the Univ. Michigan, I am starting my US funding. At the moment, I have the following German funding from Deutsche Forschungsgemeinschaft (DFG) whose funding is typically defined in terms of number of positions:

* **DFG:** co-PI within SFB 1083 "Struktur und Dynamik innerer Grenzflächen", my project ”Microscopic Theory of Optical Excitations in Interface-Dominated Material Systems”, funding for one PhD student 2015-18.
* **DFG:** PI in “Quantum‐optical spectroscopy of semiconductor nanostructures”, funding for one PhD student 2015-18.
* **DFG:** Co-PI in “SOLids in Strong Terahertz and Infrared CE-phase-stable waveforms (SOLISTICE)” within DFG Priority Programme 1840 “Quantum Dynamics in Tailored Intense Fields”, funding for two PhD students 2015-18.

**Curriculum vitae of PI4: Eric Michielssen**

*Current position, title, and address:*

**Curriculum vitae of PI5: Anatoli Polkovnikov**

*Current position, title, and address:*

Professor, Boston University, Physics Department, 590 Commonwealth Ave., Boston, MA 02215.

Tel. (*617) 358-4393*

Email:[*asp@bu.edu*](mailto:asp@bu.edu)

*Education:*

* Physics BSc & MSc, St. Petersburg State Technical University, 1998
* PhD in Theoretical Physics, Yale University, 2003

*Employment:*

* Research Assistant (1998–1999), A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia; Physics.
* Research Assistant (1999–2003), Yale University; Physics.
* Postdoctoral Fellow (2003-2005), Department of Physics, Harvard University; Physics.
* Assistant Professor (2005-2011), Department of Physics, Boston University; Physics.
* Associate Professor (2011-2015), Department of Physics, Boston University; Physics.
* Professor of Physics (2016-present), Department of Physics, Boston University; Physics.

***Mentors:***

* Ph.D. Advisor: Subir Sachdev (1999-2003), Yale University.
* Postdoctoral Advisor: Mikhail Lukin (2003–2005) ITAMP, Harvard University

*Honors:*

Simons Fellowship in Theoretical Physics, 2012; Sloan Research Fellowship, 2009; US AFOSR Young Investigator Program Award, 2006; G. Soros Fellowship, 1996, 1998.

*Five selected publications relevant for this proposal:*

1. A. Polkovnikov, *Phase space representation of quantum dynamics*, Ann. Phys. 325, 1790 (2010).
2. S. M. Davidson, D. Sels, V. Kasper, A. Polkovnikov, *Phase Space Approach to Dynamics of Interacting Fermions*, arXiv:1604.08664 (2016).
3. C.-W. Liu, A. Polkovnikov, A. W. Sandvik, *Quantum versus classical annealing: insights from scaling theory and results for spin glasses on 3-regular graphs*, Phys. Rev. Lett. 114, 147203 (2015)
4. S. Davidson, A. Polkovnikov, SU(3) *semiclassical representation of quantum dynamics of interacting spins*, Phys. Rev. Lett. 114, 045701 (2015)
5. D. Sels, and A. Polkovnikov, *Minimizing irreversible losses in quantum systems by local counter-diabatic driving*, arXiv:1607.XXXX (2016).

***Five other relevant publications:***

1. A. Polkovnikov, *Universal adiabatic dynamics across a quantum critical point*, Phys. Rev. B 72, 161201(R) (2005).
2. L. D'Alessio, Y. Kafri, A. Polkovnikov, M. Rigol, *From Quantum Chaos and Eigenstate Thermalization to Statistical Mechanics and Thermodynamics*, arXiv:1509.06411, Adv. in Phys. (2016)
3. A. Polkovnikov, K. Sengupta, A. Silva, M. Vengalattore, *Colloquium: Nonequilibrium dynamics of closed interacting quantum systems*, Rev. Mod. Phys. 83, 863 (2011).
4. M. Heyl, A. Polkovnikov, S. Kehrein, *Dynamical Quantum Phase Transitions in the Transverse Field Ising Model*, Phys. Rev. Lett. 110, 135704 (2013).
5. M. Bukov, L. D'Alessio, A. Polkovnikov, *Universal High-Frequency Behavior of Periodically Driven Systems: from Dynamical Stabilization to Floquet Engineering*, Adv. in Phys. 64, 139 (2015).

***Synergistic Activities:***

* Referee for several international journals.
* Add stuff.

***Current Collaborators*** (excluding students, postdocs):

R. Barnett (Imperial College), J. Dalibard (ENS), E. Dalla Torre (Bar Ilan), E. Demler (Harvard), V. Gritsev (Amsterdam), D. Huse (Princeton), Y. Kafri (Technion), E. Katz (BU), S. Kehrein (Gottingen), K. Lehnert (JILA), F. Marquardt (Erlangen), J. Martinis (UCSB), L. Mathey (Hamburg), P. Mehta (BU), V. Oganesyan (CUNY), D. Podolsky (Technion), M. Rigol (PennState), A. Sandvik (BU), L. Santos (Yeshiva), A. Silva (SISSA, ICTP), M. Ueda (Tokyo), M. Vengalattore (Cornell).

***Students and Postdoctoral Associates (2009–2015):***

**Postdocs:** Dries Sels\*, M. Tomka\*, L. D’Alessio (current), M. Kolodrubetz, I. Danshita, R. Barankov. **Total: 6**

**Graduate students:** L. D’Alessio, C. De Grandi, R. Hipolito, T. Souza\*, M. Bukov\*, S. Davidson\*, S. Vajna\* (U of Budapest), P. Grisins (U. of Viena), T. Ikeda (U. of Tokyo), C. Neuenhahn (LMU, Munich). **Total: 11**

***Current and Pending Support (as annual direct costs)*:**

Add if applicable.

**Curriculum vitae of PI6: ANA MARIA REY**

*Current position, title, and address:*

JILA Fellow and Research Assistant Professor, Department of Physics, University of Colorado Boulder

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*Education:*

* Physics BSc, Universidad de los Andes, Bogotá, Colombia 1999
* Ph.D. Physics, University of Maryland, College Park, MD 2004

*Employment:*

* Research Assistant (2004–2005) NIST-Gaithersburg; Physics.
* Postdoctoral Fellow (2005–2008): ITAMP, Harvard-Smithsonian Center for Astrophysics; Physics.
* Associate JILA Fellow (2008–2012), JILA, University of Colorado, Boulder.
* JILA Fellow (2012–present), JILA, University of Colorado, Boulder.

***Mentors:***

* Ph.D. Advisor: Charles W. Clark (2000–2004) NIST, University of Maryland
* Postdoctoral Advisor: Charles W. Clark (2000–2004) NIST, University of Maryland
* Postdoctoral Advisor: Mikhail Lukin (2005–2008) ITAMP, Harvard University

*Honors:*

APS Fellow, American Physical Society, 2015; National Hispanic Scientist of the Year, 2014; Maria Goeppert Mayer Award, 2014; Presidential Early Career Award for Scientists and Engineers, December 2013; MacArthur Fellow, September 2013; Great Minds in STEM, “Most Promising Scientist award”, October 2013; CSWP Woman Physicist of the Month Award, June 2012; Fundacion Alejandro Angel Escobar, Exact, Physical and Natural Sciences Prize, September 2007; Postdoctoral fellowship, ITAMP 2005–2008; Atomic, Molecular, and Optical Physics Outstanding Doctoral Thesis Award (DAMOP thesis prize), American Physical Society, 2005; Cooperative Fellowship NIST/Chemical Physics (UMD), 2002–2004; Departmental Fellowship, University of Maryland, 2000–2002.

*Five selected publications relevant for this proposal:*

1. J. Schachenmayer, A. Pikovski, and A. M. Rey, “Many-body quantum spin dynamics with Monte Carlo trajectories on a discrete phase space,” *Phys. Rev. X*, 5, 011022 (2015).
2. K. R A. Hazzard, B. Gadway, M. Foss-Feig, B. Yan, S. A. Moses, S. A. , J. P. Covey, N.Y. Yao, M. D. Lukin, J. Ye, D. S. Jin,and A. M. Rey, “Many-Body Dynamics of Dipolar Molecules in an Optical Lattice,” *Phys. Rev. Lett.*, 113(19), 195302 (2014).
3. J. G. Bohnet, B. C. Sawyer, Joseph W. Britton, Michael L. Wall, Ana Maria Rey, Michael Foss-Feig, John J. Bollinger,” Quantum spin dynamics and entanglement generation with hundreds of trapped ions”, Science 352, 1297 (2016).
4. J. Schachenmayer, A. Pikovski, and A. M. Rey, “Dynamics of correlations in two-dimensional spin models with long-range interactions: A phase-space Monte-Carlo study,” *New J. Phys.*, 17, 065009 (2015).
5. K. R. A. Hazzard, M. van den Worm, M. Foss-Feig, S. R. Manmana, E. G. Dalla Torre, T. Pfau, M. Kastner, and A. M. Rey, “Quantum correlations and entanglement in far-from-equilibrium spin systems,” Phys. Rev. A, 90(6), 063622 (2014).

***Five other relevant publications:***

1. D. Dylewsky, J. K. Freericks, M. L. Wall, A. M. Rey, and M. Foss-Feig, “Nonperturbative calculation of phonon effects on spin squeezing,” *Phys. Rev. A,* 93, 013415 (2016).
2. X. Zhang, M. Bishof, S. L Bromley, C. V. Kraus, M. S. Safronova, P. Zoller, A. M. Rey, and J. Ye, “Spectroscopic observation of SU(N)-symmetric interactions in Sr orbital magnetism,” *Science*, 345, 1467 (2014).
3. M. J. Martin, M. Bishof, M. D. Swallows, X. Zhang, C. Benko, J. von-Stecher, A. V. Gorshkov, A. M. Rey, and J. Ye, “A quantum many-body spin system in an optical lattice clock,” *Science*, 341, 632 (2013).
4. A. V. Gorshkov, M. Hermele, V. Gurarie, C. Xu, P. S. Julienne, J. Ye, P. Zoller, E. Demler, M. D. Lukin, and A. M. Rey*, “*Two-orbital su(n) magnetism with ultracold alkaline-earth atoms,” *Nature Physics*, 6, 289 (2010).
5. B. Yan, S. A. Moses, B. Gadway, J. P. Covey, K. R. A. Hazzard, A. M. Rey, D. S. Jin, and J. Ye, “Observation of dipolar spin-exchange interactions with lattice-confined polar molecules,” *Nature*, **501**, 521 (2013).

***Synergistic Activities:***

* Referee for several international journals.
* Involved in the physics undergraduate education at the University of Colorado.
* Mentor of high-school, undergraduate, and graduate students; and postdocs.
* Organizer and member of the advisory board of various national and international workshops and conferences.
* Presented a number of talks to general audiences and public lectures.

***Current Collaborators:***

John Bollinger (NIST), Charles. W. Clark (NIST and University of Maryland, JQI), Andrew Daley (University of Strathclyde), Eugene Demler (Harvard University), Alexey Gorshkov (NIST and University of Maryland, JQI), Victor Gurarie ( University of Colorado), Kaden Hazzard (Rice University), Michael Hermele ( University of Colorado), Murray Holland (JILA, University of Colorado), Michael Kastner (National Institute for Theoretical Physics, South Africa), Andrew Ludlow (NIST), Mikhail Lukin (Harvard University), Chris Oates (NIST), Tilman Pfau (Stuttgart University), Anatoli Polkovnikov (Boston University), Leo Radzihovsky (University of Colorado), Mariana Safronova (University of Delaware), Florian Schreck (University of Amsterdam), James Thompson (JILA, University of Colorado, NIST), Jun Ye (JILA, NIST, University of Colorado), Susanne Yelin (University of Connecticut), Peter Zoller (Universität Innsbruck).

***Students and Postdoctoral Associates (2009–2015):***

**Postdocs:** Gang Chen, Martin Gärttner, Kaden Hazzard, Leonid Isaev, Salvador Manmana, Alex Pirovski, Arghavan Safavi-Naini, Óscar Leonardo Acevedo Pabón, Johannes Schachenmayer, Sergey Syzranov, Javier Von Stecher, & Michael Wall. **Total: 12**

**Graduate students:** Peiru He, Andrew Koller, Shuming Li, Michael Foss-Feig, Chester Rubbo, & Bihui Zhu. **Total: 6**

**Undergraduate students:** Trent Fridey. **Total: 1**

***Current and Pending Support (as annual direct costs)*:**

**ARO** “Exploring New States of Matter with Ultracold Polar Molecules,” $50.9 K/yr; 09/01/12–08/31/16

**AFOSR** “Alkaline Earth Atoms as Quantum Simulators of Many-body Hamiltonians,” $111.9 K/yr; 03/01/13–02/28/18

**AFOSR-MURI** “Advanced Quantum Materials—A New Frontier for Ultracold Atoms,” $53.8 K/yr ; 02/15/14–02/14/19

**NSF-PFC** JILA Atomic, Molecular and Optical Physics Frontier Center, $49.5 K/yr; 08/15/11–07/31/17.

**NSF-PIF** “Dynamics of Entanglement in Dissipative Many-body Systems,” (with M. Holland and V. Gurarie) $22.8 K (yr. 1); $23.9 K (yr. 2), 13.9K (yr. 3) for this investigator, 08/01/15**–**07/31/18

**DARPA** (Pending) “Extreme Sensing Using Collective Quantum Physics,” (with J. Thompson, J. Ye and M. Holland)~ $100 K/yr for this investigator, 01/01/17**–** 12/31/2021

Curriculum Vitae of External Collaborators: John J. Bollinger

Curriculum Vitae of External Collaborators: Steven Cundiff

Curriculum Vitae of External Collaborators: Rupert Huber

Curriculum Vitae of External Collaborators: Morten Hjorth-Jensen

Curriculum Vitae of External Collaborators: Michael Wall

Identification of any Organizational Conflict(s) of Interest (if any):

None

Identification of anticipated human or animal subject research

None

1. Recent contributions of our team to quantum many-body investigations are referenced. [↑](#footnote-ref-1)