Topical: Quantum Atomic Matter Near Novel Two-Dimensional Materials in Microgravity

Primary Author:

Valeri N. Kotov
Valeri.Kotov@uvm.edu
802.656.4548

Department of Physics and Materials Science Program, University of Vermont, Burlington, VT 05405

Co-Authors:

Adrian Del Maestro	Department of Physics and Astronomy, Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, TN
Naceur Gaaloul	Institute for Quantum Optics, Leibniz University of Hanover, Germany
Robert J. Thompson	Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA
Christopher Herdman	Department of Physics, Middlebury College, Middlebury VT
Nicholas P. Bigelow	Department of Physics and Astronomy, The Institute of Optics, University of Rochester, Rochester, NY

A portion of this research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration.

1 Introduction & Relevance to NASA's Mission

Novel two-dimensional (2D) atomically flat materials, such as graphene and transition-metal dichalcogenides, exhibit unconventional Dirac electronic spectra. propose to effectively engineer their interactions with cold atoms in microgravity, leading to a synergy between complex electronic and atomic collective quantum phases and phenomena. Dirac materials, which range from semimetals to semiconductors, form a unique class of two-dimensional solids where electrons effectively have relativistic-like dispersion (massless or massive under certain conditions), with details that are strongly material- and environment-dependent [1–5]. This makes them susceptible to manipulation and quantum engineering via changes in their electronic properties by application of strain, doping with carriers, adjustment of their dielectric environment, etc. Consequently the interaction of atoms with such materials, namely the van der Waals / Casimir-Polder interaction, can be predicted with great accuracy, and effectively manipulated, leading to the potential observation of novel physical effects. The exploitation of these effects in furtherance of NASA's

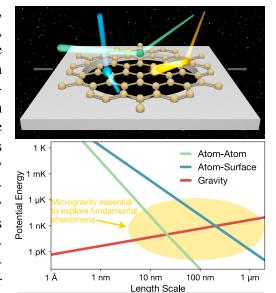


Figure 1: Atoms near surfaces in microgravity. A schematic showing the tunability of 2D materials (top) and a comparison of the energy and length scales where interaction effects between atoms and surface compete with gravity.

fundamental physics mission could result in revolutionary technologies in the fields of energy harvesting, quantum information, atomic sensors, custom film coatings, and materials design.

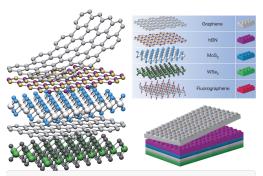


Figure 2: Two-dimensional crystals beyond graphene. A great variety of two-dimensional materials with diverse properties, ranging from Dirac semimetals to massive Dirac insulators with strong spin-orbit interactions, provide fantastic opportunities for new quantum states of electronic and atomic matter. These materials can also be assembled layer by layer to form van der Waals heterostructures (adapted from [2]).

We propose that this novel paradigm can be explored through four integrated research directions: (1) Quantum reflection of atoms; (2) Trapped Bose-Einstein Condensates near 2D Materials; (3) Exotic Low Dimensional Quantum Phases; and (4) Third Sound and Pattern Formation in Superfuid He Films. To expose the underlying emergent quantum behavior, the competing interactions and length scales involved (see Fig. 1) directly necessitate the microgravity environment of the current and future Cold Atom Laboratory (CAL) missions on the International Space Station. CAL has already achieved great success in producing trapped Bose-Einstein condensates (BECs) in microgravity [6] and we aim to chart a groundbreaking new direction for the planned BEC-CAL (Bose-Einstein Condensate Cold Atom Laboratory) mission [7] and well beyond, as envisaged by the NASA Fundamental Physics Program. Our decadal vision is to:



Leverage ground and future NASA space-based missions in microgravity for the discovery and engineering of fundamental and exotic physical phenomena at the interface of atomic matter and two-dimensional quantum materials.

The main driver of unconventional physics is the van der Waals (VDW) / Casimir-Polder (CP) interaction between neutral atoms and 2D Dirac materials [8]. Here, the unique nature of electron motion causes this interaction to have a well-defined crossover, at the scale of several hundred nanometers, between the non-relativistic (VDW) and the relativistic, vacuum fluctuation (Casimir) components. Therefore our proposal offers a unique, materials-based way to study these weak dispersion forces which are of fundamental importance in Nature (see Fig. 1 where ultracold coherent atoms are released at low momenta near a tunable atomically flat surface), with an impact akin to previous groundbreaking studies on the effects of microgravity on critical phenomena [9].

2 Quantum Reflection of Atoms

One of the most fundamental quantum phenomena with no classical analogue is above-barrier Quantum Reflection (QR). Scattering of atoms off VDW/CP potential tails [10] can provide an extremely sensitive probe of the strength of these fundamental interactions. QR has been studied previously for bulk materials, for example by using BECs [11] or narrow ultracold atomic beams. The OR in these experiments saturated below unity due to atomic interaction effects driven by collective excitations of the quantum gas during the reflection. In order to benefit from the unique low atomic velocities achievable with BECs [12], a release from a shallow trap of few Hz in necessary. Such traps are, however, heavily distorted by the gravity pull on Earth. A unique feature of 2D materials, acting as atomic mirrors, is that accurate theoretical predictions can be made for the VDW interactions and from there the QR, for a variety of materials with different levels of functionalization (i.e. under different external factors such as strain (Fig. 3), carrier density, etc.). At very low atomic velocities the quantum reflection tends to the maximum value of unity, and the material surface acts as a perfect atomic mirror. The atom-surface interactions can be accurately measured as

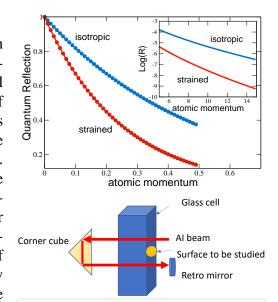


Figure 3: Probing fundamental forces near surfaces. Top: Quantum reflection coefficient for Na atoms near pristine and (uniaxially) strained graphene at low atomic momenta (velocities), in units of inverse VDW length [8]. The inset shows the high momentum part. Bottom: atomic interferometry (AI) set-up for precision measurement of phase shifts induced by atom-surface interactions (see text).

a phase shift in an atom interferometer. Here, a cold atomic sample with a small drift velocity parallel to a surface is interrogated by four $\pi/4$ pulses such that one branch of the AI can spend long times in the vicinity of a surface of interest (Fig. 3). These quantum sensors, as planned for BECCAL for example, become extremely sensitive when the drift times are stretched to several seconds as made possible by a microgravity operation.

The phenomenon of Quantum Reflection is highly sensitive to the electronic motion in atomically thin materials providing a route to study atom reflection from pristine, suspended materials as well as functionalized 2D materials in microgravity.

3 Trapped BECs near 2D Materials as Ultrasensitive Force Sensors

The study of trapped BECs near material surfaces offers another opportunity to utilize the unique capabilities of BECCAL and a microgravity environment for the manipulation and thus precision measurement of the VDW / Casimir force. The cold atom trapping potential is modified due to the attractive force of the material atoms which can result in a noticeable change in the BEC condensate's center of mass oscillation frequency [13] which is protected from gravitational sagging effects (see Fig. 4). Advances in atom-on-chip techniques [14, 15], and in particular the utilization of 2D materials such as graphene, will make it possible to place the BEC even closer to the material (of order hundreds of nanometers), without suffering any losses and maintaining high atom lifetimes. Experiments in microgravity can produce ultra-coherent condensates [6] necessary to push the boundaries of quantum force measurement.

The predictive power of theory for trapped BECs near 2D quantum materials is very high, as the relevant potential changes can be calculated with great accuracy for a variety of materials (an example is provided in Fig. 4).

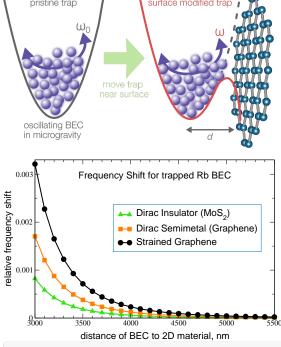


Figure 4: Bose-Einstein Condensates near 2D surfaces. Top: Schematic diagram of confined BEC near material showing the modification of the trapping potential. Bottom: Calculated relative change of the frequency of center of mass oscillations, $(\omega_0 - \omega)/\omega_0$, for different 2D materials, versus distance to the surface. (unpublished calculations by the authors)

Theoretically-predicted frequency changes of BECs near 2D Dirac materials in microgravity show extraordinary sensitivity to material parameters and therefore this set-up can be used as a powerful and ultrasensitive probe of the nature and strength of VDW / Casimir interactions.

4 Exotic Low Dimensional Quantum Phases

Strong many-body interactions in condensed matter and atomic physics can result in the appearance of complex collective states of matter, such as superconducting (charged) and superfluid (neutral) phases that can flow without resistance as well as correlated insulators without classical analogues. Under the right conditions, brought about by changes in parameters such as the electron density, lattice structure, application of pressure, etc., quantum phase transitions can take place between correlated states with different symmetries at zero temperature.

Such exotic phases are more likely to appear in lower (two or one) spatial dimension due to a reduction in the number of local classical constraints, however engineering them is a challenge due to the inherent fragility of macroscopic quantum wavefunctions, enhanced fluctuations, and competition with competing classical energy scales (e.g. gravity). We propose:

The adsorption of light atoms on free-standing highly tunable atomically flat surfaces in microgravity will provide a route to the creation, observation, and engineering of novel quantum phases of matter.

Here, VDW interactions again play a leading role, and control the thickness of the adsorbed film, as well as the 2-body interaction between atoms [8, 16]. Unlike the oft-studied case of ultra-cold lattice gases, the scale (and even sign!) of the 2-body interaction can be tuned in proximity to the 2D material opening up the ability to freely explore phase diagrams in a real materials platform (see Fig. 5). The realization of atomically flat superfluid phases offers the possibility to explore new coherent quantum phenomena, with applications in quantum information science, quantum sensing, and the construction of high precision quantum interference devices [17] able to aid in navigation in the absence of a local GPS system that will be essential for future planetary exploration missions.

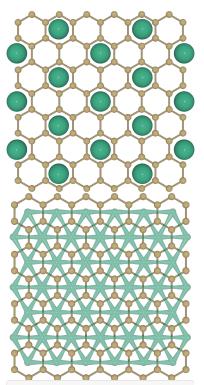


Figure 5: Quantum many-body adsorbed phases. Top: correlated insulator; Bottom: superfluid.

5 Third Sound in Superfluid Films and Emergent Pattern Formation

On the surface of thin superfluid helium films (below T_{λ}) the propagation of waves with a quantum origin, usually called third sound, is possible Most importantly, [19]. the restoring force which makes such a wave possible is the effective VD-W/CP ("disjoining pressure" [20]) between the substrate - film - vacuum boundary. In the context of 2D materials used as sub-

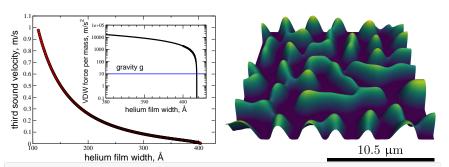


Figure 6: Manipulating thin superfulid films in microgravity. Left: Third sound velocity variation with superfluid 4 He film width on graphene, ($T \ll T_\lambda$, unpublished calculations by the authors). Inset shows the effective VDW force responsible for the wave, relative to earth's gravity. Microgravity is essential to tune to the zero velocity limit. Right: "Spinodal de-wetting pattern" [18], a variation of the film width exhibiting a characteristic wavelength, above T_λ ; the finite temperature manifestation of this critical phenomenon.

strates for superfluid films, such a configuration can display a unique type of "quantum critical" surface (i.e. effectively zero temperature) phenomenon. As illustrated in Fig. 6, using graphene as an example, and due to the fact that atomically thin materials are generically weak adsorbers (as they are 2D!), the velocity of third sound shows a very significant variation as a function of film

thickness and could even vanish at a critical value. Such criticality can be a very important addition to other types of critical phenomena studied in microgravity [9], and future missions focused on this effect would be able probe quantum fluid dynamics and quantum turbulence in a regime with a tunable velocity. At the critical film thickness, gravity would begin to directly compete with the VDW/CP interaction and thus being able to fully arrest the surface waves crucially relies on a microgravity environment.

If the temperature is raised above T_{λ} at that critical thickness, the helium will undergo a classical phase transition to a viscous fluid, and a characteristic spinodal de-wetting pattern develops. Here, large height variations (that can penetrate all the way to the 2D surface, see Fig. 6) can occur with a characteristic wavelength that is material and coating dependent. Therefore we propose that:

The study of third sound wave propagation, driven by VDW / Casimir-Polder forces, for superfluid films on graphene provides a previously-unexplored path to detect surface critical phenomena. Varying temperature from the quantum critical, low temperature $T\ll T_\lambda$ regime to normal liquid, $T>T_\lambda$, results in complex, spinodal-type ("de-wetting") surface pattern formation which is of fundamental as well as potentially technological importance.

Once the conditions under which the instability forms are fully understood, the phenomena could be dynamically driven by manipulating an externally accessible knob (e.g. strain, electric gating) in a constructive fashion enhancing the effect. This could lead to the ability to release films on surfaces *on demand* in a fully reproducible manner, which could be exploited to keep important energy generating solar materials free of dust, enhancing both their capabilities and lifetimes.

6 Outlook: Beyond Conventional Materials Science → Functional Intelligent Materials

The phenomena discussed in this white paper are in principle possible within the present level of our theoretical understanding and current NASA technologies. Looking beyond the horizon:

In the future the above effects can be further "designed" and engineered, in the following sense. Given the wide variety of currently known 2D materials, it is potentially feasible to construct materials, using artificial intelligence [21] with specific properties, optimized in such a way that their interaction with atoms has the desired strength for a given desired functionality. This could provide unprecedented control over the fundamental van der Waals / Casimir-Polder force, never previously achieved in a theoretical or laboratory setting. The NASA fundamental physics program can play a decisive role in this process through its unique ability to provide an accessible microgravity laboratory able to probe the quantum effects of atoms near 2D materials. Interesting opportunities in this regard are of course the planned bilateral mission BECCAL but also other multi-user facilities in simulated microgravity such as the Einstein Elevator in Hanover, Germany (see white paper "Earth-based platforms for microgravity research on ultra-cold atom devices for space applications").

Reference Cited

- [1] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim. "The electronic properties of graphene." Rev. Mod. Phys. **81**, 109 (2009). http://link.aps.org/doi/10.1103/RevModPhys.81.109
- [2] A. K. Geim and I. V. Grigorieva. "Van der Waals heterostructures." Nature **499**, 419 (2013). https://doi.org/10.1038/nature12385
- [3] S. Manzeli, D. Ovchinnikov, D. Pasquier, O. V. Yazyev, and A. Kis. "2D transition metal dichalcogenides." Nature Reviews Materials 2 (2017). https://doi.org/10.1038/natrevmats.2017.33
- [4] B. Amorim, A. Cortijo, F. de Juan, A. Grushin, F. Guinea, A. Gutiérrez-Rubio, H. Ochoa, V. Parente, R. Roldán, P. San-Jose, J. Schiefele, M. Sturla, and M. Vozmediano. "Novel effects of strains in graphene and other two dimensional materials." Physics Reports 617, 1 (2016). https://www.sciencedirect.com/science/article/pii/S0370157315005402
- [5] V. N. Kotov, B. Uchoa, V. M. Pereira, F. Guinea, and A. H. Castro Neto. "Electron-electron interactions in graphene: Current status and perspectives." Rev. Mod. Phys. 84, 1067 (2012). https://link.aps.org/doi/10.1103/RevModPhys.84.1067
- [6] D. C. Aveline, J. R. Williams, E. R. Elliott, C. Dutenhoffer, J. R. Kellogg, J. M. Kohel, N. E. Lay, K. Oudrhiri, R. F. Shotwell, N. Yu, and R. J. Thompson. "Observation of Bose–Einstein condensates in an Earth-orbiting research lab." Nature 582, 193 (2020). https://doi.org/10.1038/s41586-020-2346-1
- [7] K. Frye, S. Abend, W. Bartosch, A. Bawamia, D. Becker, H. Blume, C. Braxmaier, S.-W. Chiow, M. A. Efremov, W. Ertmer, et al. "The Bose-Einstein condensate and cold atom laboratory." EPJ Quantum Technology 8 (2021). http://dx.doi.org/10.1140/epjqt/s40507-020-00090-8
- [8] N. S. Nichols, A. Del Maestro, C. Wexler, and V. N. Kotov. "Adsorption by design: Tuning atom-graphene van der Waals interactions via mechanical strain." Phys. Rev. B 93, 205412 (2016). http://journals.aps.org/prb/abstract/10.1103/PhysRevB.93.205412
- [9] M. Barmatz, I. Hahn, J. A. Lipa, and R. V. Duncan. "Critical phenomena in microgravity: Past, present, and future." Rev. Mod. Phys. **79**, 1 (2007). https://link.aps.org/doi/10.1103/RevModPhys.79.1
- [10] H. Friedrich, G. Jacoby, and C. G. Meister. "Quantum reflection by Casimir van der Waals potential tails." Phys. Rev. A 65, 032902 (2002). http://link.aps.org/doi/10.1103/PhysRevA.65.032902
- [11] T. A. Pasquini, M. Saba, G.-B. Jo, Y. Shin, W. Ketterle, D. E. Pritchard, T. A. Savas, and N. Mulders. "Low Velocity Quantum Reflection of Bose-Einstein Condensates." Phys. Rev. Lett. 97, 093201 (2006).
 - https://link.aps.org/doi/10.1103/PhysRevLett.97.093201
- [12] C. Deppner, W. Herr, M. Cornelius, P. Stromberger, T. Sternke, C. Grzeschik, A. Grote, J. Rudolph, S. Herrmann, M. Krutzik, et al. "Collective-mode enhanced matter-wave optics." Physical Review Letters 127, 100401 (2021). https://link.aps.org/doi/10.1103/PhysRevLett.127.100401
- [13] D. M. Harber, J. M. Obrecht, J. M. McGuirk, and E. A. Cornell. "Measurement of the Casimir-Polder force through center-of-mass oscillations of a Bose-Einstein condensate." Phys. Rev. A **72**, 033610 (2005).
 - http://link.aps.org/doi/10.1103/PhysRevA.72.033610

- [14] M. Keil, O. Amit, S. Zhou, D. Groswasser, Y. Japha, and R. Folman. "Fifteen years of cold matter on the atom chip: promise, realizations, and prospects." Journal of Modern Optics 63, 1840 (2016). https://doi.org/10.1080/09500340.2016.1178820
- [15] K. Wongcharoenbhorn et al. "Using graphene conductors to enhance the functionality of atom-chips." arXiv:2105.01907 (2021). http://arxiv.org/abs/2105.01907
- [16] J. Yu, E. Lauricella, M. Elsayed, K. Shepherd, N. S. Nichols, T. Lombardi, S. W. Kim, C. Wexler, J. M. Vanegas, T. Lakoba, V. N. Kotov, and A. Del Maestro. "Two-dimensional Bose-Hubbard model for helium on graphene." Phys. Rev. B 103, 235414 (2021). https://link.aps.org/doi/10.1103/PhysRevB.103.235414
- [17] Y. Sato and R. Packard. "Superfluid helium interferometers." Phys. Today **65**, 316 (2012). https://doi.org/10.1063/pt.3.1749
- [18] J. M. Vanegas, D. Peterson, T. I. Lakoba, and V. N. Kotov. "Spinodal de-wetting of light liquids on graphene." arXiv:2103.01978 (2021). http://arxiv.org/abs/arXiv:2103.01978
- [19] C. W. F. Everitt, K. R. Atkins, and A. Denenstein. "Third Sound in Liquid Helium Films." Phys. Rev. 136, A1494 (1964). https://link.aps.org/doi/10.1103/PhysRev.136.A1494
- [20] S. Sengupta, N. S. Nichols, A. Del Maestro, and V. N. Kotov. "Theory of Liquid Film Growth and Wetting Instabilities on Graphene." Phys. Rev. Lett. 120, 236802 (2018). https://link.aps.org/doi/10.1103/PhysRevLett.120.236802
- [21] G. Carleo, I. Cirac, K. Cranmer, L. Daudet, M. Schuld, N. Tishby, L. Vogt-Maranto, and L. Zdeborová. "Machine learning and the physical sciences." Rev. Mod. Phys. **91**, 045002 (2019). https://link.aps.org/doi/10.1103/RevModPhys.91.045002