CECAM/Psik Workshop Scientific Report

Workshop: **Correlated Electron Physics beyond the Hubbard Model**

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Location: University of Bremen, Germany,
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I. State-of-the-Art Summary

Realistic modeling of materials with strong electron correlations presents one of the central challenges in condensed matter theory to date and hold promises for novel materials developments in the domains from materials for energy applications to novel high temperature superconductors and topological states of matter.

On the theory side, the Hubbard model is one of the central models to understand various aspects of strongly correlated electrons. However, links between the Hubbard model and real materials can be ambiguous and the Hubbard model can even qualitatively fail to describing real materials whenever non-local interactions are not efficiently screened.

Various theoretical approaches from quantum physics and chemistry communities including Quantum Monte Carlo approaches, coupled cluster theories, Configuration interaction expansions, embedding theories, extensions of dynamical mean field theory, as well as renormalization group approaches and diagrammatic perturbation theory have been put forward to address strong electron correlations in presence of non-local interactions. However, our understanding of the electronic structure of these systems is still rather limited as regards electronic phase diagrams, excitation spectra, and excited state dynamics - both on the pure model side and particularly when it comes to modelling real materials.

The development of next-generation realistic many-body computational tools which are fast, reliable, and able to describe non-trivial quantum states of real materials requires clarification how non-local interactions affect the electronic properties of correlated electron systems. The workshop aimed to foster a clear understanding of merits and shortcomings of different simulation methods currently under development by bringing together the respective scientific communities from physics and chemistry and set the stage for developing novel simulation tools for real materials featuring correlated electrons.

II. Scientific content, main outcome of key presentations, selected discussions

The program consisted of 26 invited talks of 40 minutes (30+10) each, one poster session presenting 29 posters and three round table discussions of 45 minutes each. In addition, many social events (reception and conference dinner) allowed for informal exchange. The invited talks were given by well-established scientists from the different theoretical communities, which acted as platform for interesting cross-/interdisciplinary discussions. The invited talks were followed by a poster session where the young researcher participants showed their scientific work and exchanged ideas with each other and the present experts in the field. The organization was very compact with the participants accommodated in the same hotel fostering exchange and discussion also outside the meeting room.

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The general and central issue standing out in this conference was how to advance the field in order to achieve reliable predictions of properties of materials hosting strong electronic correlations. The conference gathered experts in a diverse collection of methods suitable to tackle this task, which was the foundation for lively discussions about both fundamental issues of the field and technical details of novel methods. On the one side, experts in methods designed for low energy methods presented and explained details of their respective advances, e.g., in dual approaches (Erik van Loon, Alexander Lichtenstein), different Monte Carlo approaches (James LeBlanc, Lucas Wagner, Stefan Wessel, Boris Svistunov, Nikolay Prokofiev, Sandro Sorella), renormalization theories (Sabine Andergassen, Chan-Wen Tsai), and variational approaches (Ryotaro Arita, George Booth, Malte Schüler). On the other hand, methods designed to tackle realistic materials including long-ranged interactions from the beginning were presented, like GW based methods and extensions thereof (Phillip Werner, Johannes Lischner, Silke Biermann, Ferdi Aryasetiawan, Mark van Schilfgaarde), and density functional based methods (Matteo Cococionni). Finally, we had experts in the field of downfolding methods (i.e., the task to excerpt low energy models from a high-energy manifold based on ab-initio methods) talking about the subtleties and advances in this field (Malte Rösner, Carsten Honerkamp). Multiple speakers took the opportunity to present applications of this zoo of methods to real materials (André-Marie Tremblay, Andy Millis, Silke Biermann, Ferdi Aryasetiawan).

The round table discussions reveled following issues: First, to assess the multitude of available methods applicable to model systems, a common benchmark is very much desirable. Often these methods are rather complementary and are best applied to different regimes. Here, a benchmark on common grounds against numerical exact results from, e.g., diagrammatic Monte Carlo simulations for a non particle-hole symmetric, slightly doped one-band model with local interactions on the order of the bandwidth and additionally non-local interactions is highly desired and would highlight if certain approximations, for instance the locality of the self-energy or the neglect of vertex corrections to non-local properties, hold. In a second step, it is unclear how this ultimately relates to real materials: due to the complexity of real materials, a numerical benchmark will not be possible in at least the next few years. Here it was brought up, if and to which extent experiments are a useful benchmark for methods only applied to model systems. One suggestion are artificially engineered ad-atom systems closely resembling model systems. Besides

experimental verification, the importance of comparing results from complimentary methods was brought up.

Another important topic in the discussions were different downfolding techniques and their reliability. Here, the advances of the constrained functional renormalization group theory approach, sheds light on the applicability of computationally more lightweight and therefor more often used constrained random phase approximation. However, it is unclear how these findings apply to real materials. It is now planned to perform a benchmark for a simple realistic material, i.e., graphene.

III. Assessment of the results and impact on future direction of the field.

The unambiguous theoretical description of correlated states of matter is still a major tackle. This workshop has shown that the field is advancing in all areas: i) a more accurate description of model systems including non-local interactions by diagrammatic and cluster extensions of dynamical mean-field theory as well as sophisticated Quantum Monte Carlo methos, ii) a better ab-initio description of weakly correlated materials and those in symmetry broken states, iii) a better understanding of downfolding procedures. In order to achieve actual progress in describing real materials in all parameter regimes, it is mandatory to combine and even further advance these approaches. The main results and impact of this workshop was to settle on open points (how important are non-local corrections, how accurate are current downfolding schemes, what is an appropriate benchmark) and share the respective advances in the field. It was decided to perform various benchmarks across complementary methods and models. This shows the importance of such workshops, where the respective experts of the field come together for open and productive discussions.

IV. Infrastructure requirements to make advances in the field

As discussed above, the advancement of theories of the operation of strongly correlated electron systems requires the development of novel theories and codes which can i) deal with the complexity given by electronic correlations in model systems, ii) treat realistic materials which include many bands, not all of which may host correlation effects, and iii) combine ab-initio and model approaches in an optimal way. The development of such theories and the resulting computer software will benefit the broad community of theoretical researchers, but also have important impacts on experimental studies. Here, the interplay with experimental researchers is crucial to provide excellent data sets which can serve as benchmarking and ultimately lead to a fruitful interplay between theoretical predictions and experiment. However, to achieve this, a continued investment is required, as method and code development usually occur on a longer time scale compared to the study of applications. This also requires the training of masters and PhD students not only in physics, but also in computer programming (including parallelization of software) and use of high-performance computing resources. Here, networks like Psi_k and coordinated research programs bringing modelling experts together have proven extremely useful.

V. Impact to address the need of industry in driving economic growth

Our workshop contributes to the potential development of technologies based the unique properties of materials hosting strong electronic correlations. This may have a number of societal and economic benefits, especially in terms of:

- The advent of superconducting materials with record high critical temperatures, leading to cheaper energy transfer and lower cost for cooling electromagnets based on superconducting materials.
- Novel switching devices utilizing the large susceptibilities in correlated materials, e.g., Mott metal-insulator transition.
- Using properties of materials with colossal magnetoresistance as memory devices.

In general, the study of strongly correlated materials is very much basic research, such that direct applications cannot be foreseen to full extent at this point. However, it is at the heart of science, that basic research pays off in one way or the other way. Especially the development of new methods and training of students has a strong indirect economic and societal impact.

Community needs

Discuss the needs of the community in terms of computational infrastructure (e.g. existing codes, use of HPC resources), networking (e.g. outreach to other communities including experimentalists), event organization (e.g. should a series of CECAM workshops on this topic be considered and if so why?)

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and codes which can i) deal with the complexity given by electronic correlations in model systems, ii) treat realistic materials which include many bands, not all of which may host correlation effects, and iii) combine ab-initio and model approaches in an optimal way. The development of such theories and the resulting computer software will benefit the broad community of theoretical researchers, but also have important impacts on experimental studies. Here, the interplay with experimental researchers is crucial to provide excellent data sets which can serve as benchmarking and ultimately lead to a fruitful interplay between theoretical predictions and experiment. However, to achieve this, a continued investment is required, as method and code development usually occur on a longer time scale compared to the study of applications. This also requires the training of masters and PhD students not only in physics, but also in computer programming (including parallelization of software) and use of high-performance computing resources. We have to work cross disciplinary to tackle correlated electrons (benchmarking; gaining predictive power) which requires networking and collaborations. Here, networks like Psi_k and coordinated research programs bringing modelling experts together have proven extremely useful.

Funding

Summarize typical funding channels and identify possible new sources in upcoming calls e.g. Horizon 2020, national funding schemes. Was the possibility of joint research proposals discussed during the meeting?

We could discuss a new collaborative initiative (DACH project by DFG, FWF and SNF) for modelling systems with strong non-local correlation phenomena including topological effects. Additionally, we could strengthen and foster collaboration between researchers from European based projects and the US based Simons Collaboration.

Will these developments bring societal benefits?

Discuss potential societal benefits of the research topic of the workshop. For example, summarize economic benefits, through the use of our methods by industry; societal benefits such as sustainability; health benefits such as novel drug design. If possible reference funding opportunities related to these benefits.

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February 21th 2019

The Organizers