Long-term Overseas Dispatch report

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Overview:

- Research topic: Floquet DFT investigation
- Research group: Prof. Kieron Burke's group
- Location: University of California, Irvine
- Duration: 2019/1/14 $\sim$ 2019/3/14

Research Background

Electronic structure computation methods have become a common standard for studying material properties under arbitrary conditions, with the density functional theory (DFT) methods playing a central role due to their innate efficiency for calculating large systems. Despite its long history, there are still fields in which to expand the DFT formalism, among which the combination Floquet theory with DFT is one of them. This combination would enable us to describe the time-periodic environments, such as a continuous laser irradiation, much more efficiently than the more general time-dependent DFT (TDDFT) formalism. This extension has been the main research focus of the trip, with the supervision of Prof. Kieron Burke who contributed to proving the incompatibility of this combination.

Another main goal for this research trip was to get a proper understanding of the fundamental theories behind DFT from the leading developers of these theories. A common problem with DFT methods is that these are often misused in the application to real systems, and with the perspective of one of the main contributors to DFT, one can get ahead of this problem and know the reasons behind the common misinterpretations.

Summary of the dispatch

The two month research internship at Prof. Kieron Burke's group at University of California Irvine (UCI) has been a great learning experience both academically and culturally. Studying the development of DFT and working on its expansion to Floquet systems gave me a more thorough understanding of the various DFT variants than I would have expected. Culturally, the main objective of this internship was to experience the research environment outside of Japan and learn how other research groups operate differently, even when the topic of research is very closely related. Although the program was too short to finalize the formulation of a Floquet-DFT formalism, the research internship was still successful on all of the other points.

On the suggestion of Prof. Burke, I have attended the DFT class taught by him during that quarter on the ground-state DFT, the most basic DFT formulation. Although I wouldn't have considered revisiting this formalism, I am glad I took his advice. I have gained a different and

more thorough understanding of this basic method, and analysis methods used to investigate the functionals and the theory in general. With the group's focus on the development and understanding of the basic theoretical framework of DFT, I have gained a different perspective on the current DFT research, and the methods used to study and expand the DFT formalism. One example is the asymmetric Hubbard dimer toy model, which is used to evaluate the success of DFT approximations in the strongly correlated limit among other regimes.

As for the application of Floquet theory in DFT, it is still an ongoing project I am pursuing with the continuing guidance of Prof. Burke. During the research internship, we have attempted to combine Floquet theory with DFT beyond the previous formulations, and even though it has not proven to be successful yet, the source of the incompatibility thus far is itself useful for later formulations. During the visit the focus has been on finding a one-to-one correspondence between the external potential and electron density independent of the choice of Floquet states. While we have come up with a few methods to describe the Floquet states uniquely, which is otherwise one of the main problem of working with Floquet systems and has been the main source of incompatibility in the previous formulations of Floquet DFT, the one-to-one correspondence is still not properly proven. We have since changed our attention to the TDDFT formalism, which seems to hold some clues over the compatibility of Floquet theory and DFT, and hopefully we can finalize this project and write a paper on the whole problem.

Finally, regarding the general experience of researching at Prof. Burke's group, it has been very useful experience to have had, both for the prospective of pursuing a research career in America, and having an oversight on how the leading research groups operate. The common theme has been that in America there is more focus on the individuals, and while it is a common observation most people make, experiencing first-hand the effects of this organization method is incomparable. One example is the weekly individual meeting between the professor and each member of the group, which also takes up a whole day for the professor. While at first it could feel daunting to have worthwhile results to present every week, it does help steer the research in the proper direction early on. The group meetings, organization of the research group, the member's research presentation, and various other things are all organized differently from my current research group either for the better or worse. I am looking forward to incorporating the experiences gained during this internship into my current and future research environment.

Acknowledgment

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