物性研究所セミナー

標題：理論セミナー：Learning the constitutive relation of polymeric flows with memory
日時：2021 年 2 月 12 日(金)　午後 4 時～午後 5 時
場所：On Zoom
講師：John MOLINA
所属：京都大学　大学院工学研究科
要旨：

While our knowledge of Polymer Physics has greatly evolved over the past century, the complex rheology of non-Newtonian fluids remains an open area of research. In particular, we have yet to fully understand the coupling between the microscopic dynamics of the entangled polymer chains and the macroscopic flow properties of the polymer melt. Multi-scale simulations (MSS), which simultaneously couple both micro and macro degrees of freedom, have been developed to address this issue, but their computational cost has limited them to simple flows and small system sizes. In this talk, we will present a learning strategy capable of inferring the constitutive relation for the stress of polymeric flows with memory. The learned constitutive relation can then be used within macro-scale flow simulations, allowing us to update the stresses in the fluid in a manner which satisfies the dynamics of the underlying microscopic model.

We assume that the constitutive relations can be expressed in differential form, as a function of the velocity gradient and stress, but no assumptions are made on their functional form. The required training data is obtained from stress trajectories generated during microscopic polymer simulations. This data is then used within a Gaussian Process (GP) regression scheme, in order to infer the most likely constitutive equation. We tested the method on a simple microscopic model (non-interacting Hookean dumbbells) and successfully recovered the exact constitutive relation (i.e., the Maxwell model). The resulting macroscopic flow simulations give the same level of accuracy as MSS at a small fraction of the cost. This opens the door for establishing a bottom-up design framework for polymeric materials. Finally, we will discuss extensions needed to learn the constitutive relation of more complex microscopic polymer models (i.e. the Doi-Takimoto Slip-Link model of entangled polymer melts) as well as applications to other Soft Matter systems (e.g., colloidal dispersions or cellular tissues).

Ref.

Seryo N, Sato T, Molina JJ, and Taniguchi T, Physical Review Research 02, 033107 (2020)
Seryo N, Molina JJ, and Taniguchi T, Nihon Reoroji Gakkaishi (J Soc. Rheol. Jpn.), in press (2021)

標題：理論インフォーマルセミナー：Magnetization plateaus of two-dimensional geometrically frustrated quantum spin systems from the one-dimensional perspective.
日時：2021 年 2 月 17 日(水)　午後 4 時～午後 5 時
場所：On Zoom
講師：Dr. Shunsuke C. Furuya
所属：Ibaraki University
要旨：

The Lieb-Schultz-Mattis theorem has recently drawn a renewed interest from theoretical physicists for its close connection to anomalies of quantum field theories. The U(1) flux-insertion argument is advantageous to discuss the

Lieb-Schultz-Mattis theorem. It provides a simple method to investigate the Lieb-Schultz-Mattis theorem in quantum spin systems on magnetization plateaus, the well-known Oshikawa-Yamanaka-Affleck condition.In this presentation, we first discuss an inspiring example of the flux insertion argument in quantum spin systems on the checkerboard lattice. The simple flux insertion argument with the periodic or the tilted boundary condition fails to forbid the unique gapped ground state. This failure originates from the fact that we need to impose an extra symmetry to exclude the possibility of the unique gapped ground state from the checkerboard-lattice quantum spin systems. We show how to incorporate the extra symmetry and the flux insertion argument.Next, we move on to kagome-lattice antiferromagnets. We give our attention to the 1/3 magnetization plateau of kagome antiferromagnets, where the Oshikawa-Yamanaka-Affleck condition admits the unique gapped ground state. We discuss the 1/3 magnetization plateau of a spin-1/2 three-leg spin tube based on an anomaly of SU(3) Wess-Zumino-Witten theory and relate it to the 1/3 plateau of the kagome antiferromagnet.

標題：理論セミナー：Sparse sampling approach to efficient ab initio and many-body calculations at finite temperature

日時：2021 年 2 月 19 日(金)　午後 4 時～午後 5 時

場所：On Zoom

講師：Assist. Prof. Hiroshi Shinaoka

所属：埼玉大学

要旨：

Efficient ab initio calculations of correlated materials at finite temperatures require compact representations of the Green's functions both in imaginary time and in Matsubara frequency. We have recently proposed a general procedure [1] which generates sparse sampling points in time and frequency from compact orthogonal basis representations, such as Chebyshev polynomials and intermediate representation (IR) basis functions [2]. These sampling points accurately resolve the information contained in the Green's function, and efficient transforms between different representations are formulated with minimal loss of information.

In this talk, we introduce compact orthogonal basis representations with a peculiar focus on the IR basis. As a demonstration, we apply the sparse sampling scheme to diagrammatic GW and second-order Green's function theory calculations of a hydrogen chain of noble gas atoms and of a silicon crystal. Furthermore, we demonstrate its efficiency in Migdal-Eliashberg calculations considering the retardation effect in phonon-mediated superconductors [3]. Finally, we will briefly discuss the extensions of the sparse sampling approach to two-particle quantities [4].

[1] J. Li, M. Wallerberger, N. Chikano, C.-N. Ye, E. Gull, HS, PRB 101, 035144 (2020).

[2] HS, J. Otsuki, M. Ohzeki, K. Yoshimi, PRB 96, 035147 (2017).

[3] T. Wang, T. Nomoto, Y. Nomura, HS, J. Otsuki, T. Koretsune, R. Arita, PRB 102, 134503 (2020).

[4] M. Wallerberger*, HS*, A. Kauch, arXiv:2012.05557

標題：理論セミナー：Impact of anisotropic interactions on cubic Eg quadrupole orders

日時：2021 年 2 月 24 日(水)　午後４時～午後５時

場所：On Zoom

講師：Kazumasa HATTORI

所属：Tokyo Metropolitan University

要旨：

Multipole degrees of freedom and their orders in strongly correlated electron systems have attracted growing interest in recent years. In several cubic Pr-based f-electron systems with two f electrons per a Pr ion, it is reported that they possess non-Kramers doublet crystalline-electric field ground state with Eg quadrupole and Txyz type octuple moments. They show various quadrupole orders, non-Fermi liquids, superconductivity, and many interesting low temperature properties [1].

In this study, we analyze a model with non-Heisenberg (non-XY type) anisotropic interactions present in the real quadrupole systems. We find that their effects are drastic and even qualitative changes emerge in their ordered phases. In this talk, first we show results of mean-field analysis for interacting quadrupole moments in a cubic fcc lattice [2]. We demonstrate that novel partial ordered states at high temperature are generally realized rather than a simple quadrupole order with a single wave number. In the second part, we analyze a “double transition” observed in PrV2Al20, which is expected to be triggered by the ferro Txyz octuploe order [3]. We propose a simple scenario for the double transition when the anisotropic quadrupole interactions in addition to simple octupole-octupole one are taken into account [4]. The magnetic-field vs temperature phase diagrams are also examined and several field-induced phases are proposed for the field directions [001], [110], and [111].

[1] T. Onimaru and H. Kusunose, J. Phys. Soc. Jan. 85, 082002 (2016).

[2] H. Tsunetsugu, T. Ishitobi, and KH, arXiv.2102.06346.

[3] A. Sakai et al., unpublished; A. S. Patri et al., Nat. Comm. 10, 4092 (2019).

[4] T. Ishitobi and KH, unpublished.