北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Seminar

Cluster Diagrammatic Monte Carlo Method for Interacting Electrons

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Time: 10:00am, Nov. 27, 2018 (Tuesday)

时间：2018年11月27日 （周二）上午10:00

Venue: Room W563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

We introduce a simple yet highly efficient Monte Carlo algorithm (Cluster Diagrammatic Monte Carlo, CDMC) to sum high order Feynman diagrams for generic interacting electrons. The method samples Feynman diagrams in terms of sign-cancelled groups rather than individual diagrams, which massively suppresses the sign problem. In this talk, we show that combining this method with a variational approach results in a powerful and accurate solver to the generic solid state problem, in which a macroscopic number of electrons interact by the long range Coulomb repulsion. We apply the solver to the quintessential problem of solid state, the uniform electron gas (UEG), which is at the heart of the density functional theory (DFT) success in describing real materials, yet it has not been adequately solved for over 90 years. Our method allows us to calculate the momentum-frequency resolved spin response functions for the first time, and to improve on the precision of the charge response function. The accuracy of both response functions is sufficiently high, so as to uncover previously missed fine structure in these responses. This method can be straightforwardly applied to a large number of moderately interacting electron systems in the thermodynamic limit, including realistic models of metallic and semiconducting solids.

References:

K Chen and K Haule, Feynman's solution of the quintessential problem in solid state physics, arXiv:1809.04651.

About the speaker

Dr. Kun Chen is currently a Simons Postdoc Fellow at Rutgers University. His research interests include to combine the field-theoretic approach and controlled numerical methods to explore emergent phenomena in strongly correlated quantum matters. Recently, he has been working on a new numerical scheme which generalizes the field-theoretic renormalization group method with a diagrammatic Monte Carlo algorithm. This scheme provides a systematic approach to explore and calculate effective field theories in interacting fermionic and bosonic systems.