北京大学量子材料科学中心
International Center for Quantum Materials, PKU

Weekly Seminar

NORG帮助免除在DFT+DMFT电子结构计算中的负符号问题

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Time: 4:00pm, Nov. 18, 2020 (Wednesday)

时间: 2020年11月18日 （周三）下午4:00

Venue: Room W563, Physics building, Peking University

地点: 北京大学物理楼，西563会议室

Abstract

There are many novel quantum phenomena in strongly correlated electronic materials. How to understand and characterize them has always been one of the central topics in condensed matter physics. The DFT+DMFT electronic structure calculation method is considered to be the most powerful and promising method for studying strongly correlated electronic materials, which combines the first-principles electronic structure calculation based on the density functional theory (DFT) and the dynamical mean field theory (DMFT). Nevertheless, the DFT+DMFT calculation method now suffers the sign problem with its quantum Monte Carlo impurity solver, which seriously hinders the development and application of DFT+DMFT. On the other hand, the quantum renormalization group (RG) procedure is one of the most important and accurate approaches for studying interacting many-electron correlated systems, upon which we propose a new concept in the framework of natural orbitals so that we can generalize the RG into general orbital space, namely natural orbitals renormalization group (NORG). We show that the NORG takes a polynomial rather than exponential computational cost in the number of electron bath sites to solve the low-energy states of a quantum impurity model. Moreover, the NORG can work on a quantum impurity model with any lattice topological structure. Actually, the effectiveness of the NORG is basically irrespective of a model's topological structure. Thus, the NORG is naturally appropriate for studying quantum cluster-impurity model. This makes the NORG be a natural impurity solver to dynamical mean field theory.

About the speaker

卢仲毅，中国人民大学物理系教授，主要从事凝聚态物质的电子结构研究和计算方法发展，在铁基超导和量子多体理论等研究方面取得了一批有原创性的成果：提出了铁基超导的反铁磁超交换作用机理，正确预言了母体的反铁磁半金属特性，确认了FeTe和$K_2Fe_3Se_4$的反铁磁长程序及电子结构；明确了铁磁金属层中量子阱态的共振隧穿等输运性质；提出了自然轨道重正化群方法，并应用于多自由度的量子杂质系统研究；用多体场论方法研究了几种自旋链系统的奇异特性。2007年获国家杰出青年基金资助，2012年聘为教育部长江学者特聘教授，2015年获教育部自然科学一等奖，同年获中国物理学会叶企孙物理奖，2019年获得国家自然科学奖二等奖。