Weekly Seminar

Solving multiorbital dynamical mean-field theory using natural orbitals renormalization group

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Time: 3:00 pm, Nov. 2, 2022 (Wednesday)

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Abstract

We have proposed the natural orbitals renormalization group (NORG) as an efficient numerical method for solving zero-temperature properties of multisite and multiorbital quantum impurity systems. Here, we implement the NORG as an impurity solver for dynamical mean-field theory (DMFT). In comparison with the exact diagonalization method, the NORG method can treat much more bath sites in an impurity model to which the DMFT maps a lattice model and can find accurate zero-temperature Matsubara and low-frequency retarded Green's functions. We demonstrate the effectiveness of this method on a two-orbital Hubbard model on the Bethe lattice and find successfully the orbital selective Mott transition with a Kondo resonance peak in the wide band and two holon-doublon bound state excitation peaks in the narrow band.

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。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奖一等奖，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。