复旦大学物理系 Colloquium

Time: 14:00, Tuesday, 2021.09.28

Location: Room C108, Jiangwan Physics Building

Determining the range of magnetic interactions from the relations between magnon eigenvalues at high-symmetry k points and Designing light-element materials with large effective spin-orbit coupling

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Abstract: Magnetic exchange interactions (MEIs) define networks of coupled magnetic moments and lead to a surprisingly rich variety of their magnetic properties. Typically MEIs can be estimated by fitting experimental results. But how many MEIs need to be included in the fitting process for a material is not clear a priori, which limits the quality of results obtained by these conventional methods. In this paper, based on linear spin-wave theory but without performing matrix diagonalization, we show that for a general quadratic spin Hamiltonian, there is a simple relation between the Fourier transform of MEIs and the sum of square of magnon energies (SSME). We further show that according to the real-space distance range within which MEIs are considered relevant, one can obtain the corresponding relationships between SSME in momentum space. We also develop a theoretical tool for tabulating the rule about SSME. By directly utilizing these characteristics and the experimental magnon energies at only a few high-symmetry k points in the Brillouin zone, one can obtain strong constraints about the range of exchange path beyond which MEIs can be safely neglected. Our methodology is also general applicable for other Hamiltonian with quadratic Fermi or Boson operators. Focus on 3d systems, we also demonstrate that the interplay between crystal symmetry and electron correlation can dramatically enhance the SOC effect in certain partial occupied orbital multiplets, through the self-consistently reinforced orbital polarization as a pivot. We then provide design principles and comprehensive databases, in which we list all the Wyckoff positions and site symmetries, in all two-dimensional (2D) and three-dimensional (3D) crystals that potentially have such enhanced SOC effect.

主讲人简介: 万贤纲，南京大学物理学院教授，1990年至2000年在南京大学学习，获得学士、硕士、博士学位。2001起在南京大学历任讲师，副教授，2010年任教授。主要学术成绩为：提出了新型拓扑量子态—Weyl半金属,该工作入选美国物理学会PRB期刊创刊50年“里程碑”(MILESTONE)文章，评语是：提出了一种新的量子物质状态外尔半金属；发展了一套计算磁性相互作用的方法并确定多个复杂体系的基态磁构型；基于原子绝缘体基组发展了高效判断拓扑性能的理论方法，并用其对无机材料数据库里面所有非磁材料的拓扑特性进行了分类。