数学与系统科学研究院

计算数学所学术报告

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报告题目：

Numerical Integration for ab initio self energy calculations within the GW approximation

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报告时间：**2014** 年 **10** 月 **22** 日（周三）

下午 **16:00-17:00**

报告地点：　　数学院南楼七层 **702** 会议室

Abstract:

In the Green's function formalism of many-body perturbation theory, the excitation of the material is described in terms of quasi-particle energies of a single-particle Hamiltonian that contains a self energy term. Within the GW approximation of the self energy, due to the presence of singularities in the integrand for the convolution of a Green's function with a screened Coulomb potential on the real axis, the numerical convolution must be carried out with care. We present a numerical integration scheme for evaluating this convolution. Both theoretical analysis and numerical examples show that this scheme is more reliable and accurate than the standard quadrature rules such as the trapezoidal rule.

This is a joint work with Chao Yang, Lin Lin, Lex Kemper, Jack Deslippe, Jeffrey Neaton's group, and Steven Louie's group.

欢迎大家参加！