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：

Computatoinal Techniques for Accelerating the GW Calculation

邀请人：周爱辉 研究员

报告时间：**2013** 年 **9** 月 **10** 日（周二）

上午 **10:00-11:00**

报告地点：科技综合楼三层 **311**

计算数学所报告厅

Abstract:

One way to study the effects of electron excitation (e.g.photoemission) is to use the Green's function formalism of a many-body perturbation theory. In this approach, the effect of excitation is described in terms of quasi-particle energies (eigenvalues) of a single-particle Hamiltonian that contains a self-energy term used to properly describe the many-body excitation effects. These quasi-particle energies form the poles of a Green's function that describes the probability amplitude to detect an electron (or hole) at a spatial location and certain time when an electron (or hole) has been added to the system at another location and time. The exact form of the self-energy is unknown. A widely used technique to approximate the self-energy is to express it as the product of an one-particle Green's function (G) and a screened Coulomb operator (W) in the time domain. The construction of such an approximation is extremely computational demanding. We will describe a number of techniques for reducing the computational cost for a full-frequency GW calcuation.

欢迎大家参加！