数学与系统科学研究院

计算数学所系列学术报告

报告人：**Prof. Chao Yang**

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报告题目：

Green's Function Method for Electron Excitation

邀请人：　周爱辉 研究员

报告时间：

2014 年 **11** 月 **20** 日（周四） 上午 **9:00-11:00**
2014 年 **11** 月 **25** 日（周二） 上午 **9:00-11:00**
2014 年 **11** 月 **27** 日（周四） 上午 **9:00-11:00**

报告地点：　数学院南楼七层 **702** 会议室

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 frequency representation 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 the Green's function (denoted by G) to be determined and a screened Coulomb operator (denoted by W) in the time domain. The construction of such an approximation is extremely computational demanding.

In this talk, we will begin with the derivation of the Dyson's equation that defines the quasi-particle eigenvalue problem from the many-body perturbation theory. Topics to be covered include: Lehmann representation, Wick's theorem, Hedin's equation etc. We will then discuss a number of techniques for improving the efficiency and accuracy of the self-energy calculation in the GW framework. Topics include the derivation of the Coulomb-hole and screened exchange (COHSEX) and exchang and correlation (XCOR) expressions of the self energy, the random phase approximation of the independent particle irreducible polarizability, dielectric function, linear response and Sternheimer equation, contour deformation for self energy integration.

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