**青年学术论坛邀请报告**

报告人： 邵美悦 博士

单位：美国劳伦斯伯克利国家实验室

时间：11月21日（周二）上午9：30-10：30

邀请人： 朱升峰

地点：闵行数学楼102室

题目： Recent progress on the Bethe--Salpeter eigenvalue problem

摘要 : In electronic structure calculations, excited state properties of molecules and solids can be obtained by solving the Bethe--Salpeter equation (BSE). Discretization of the BSE leads to a structured non-Hermitian dense eigenvalue problem with a special 2-by-2 block structure. In principle all excitation energies are of interest. We first present a structure preserving algorithm that computes all eigenpairs of the BSE Hamiltonian. In some circumstances instead of computing each individual excitation energy, we need to estimate the optical absorption spectrum, which is a frequency dependent matrix functional and is measurable in optical absorption experiments. We propose a structure preserving Lanczos procedure to quickly compute the optical absorption spectrum. A recently developed technique of generalized averaged Gauss quadrature is also adopted to accelerate the convergence of the Lanczos algorithm.

报告人简介: 邵美悦分别于2006年和2009年获复旦大学学士和硕士学位，2009年-2012年在瑞典Umea University大学计算机系获Ph.Lic.，2012年-2014年在瑞士洛桑联邦理工学院(Ecole Polytechnique Federale de Lausanne)获博士学位。2014年起在美国劳伦斯伯克利国家实验室做博士后研究。2017年11月晋升为美国劳伦斯伯克利国家实验室的项目科学家。

