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：

Recent Progress in Numerical Methods for Many-Body Wigner Quantum Dynamics

邀请人：　曹礼群研究员

报告时间：**2017** 年 **11** 月 **17** 日**(**周五**)**

下午 **15:00--17:00**

报告地点：　数学院南楼七层

714 会议室

报告摘要：

The Wigner function has provided an equivalent and convenient way to render quantum mechanics in phase space. It allows one to express

macroscopically measurable quantities, such as currents and heat fluxes, in statistical forms as usually does in classical statistical mechanics, thereby facilitating its applications in nanoelectronics, quantum optics and etc. Distinct from the Schrödinger equation, the most appealing feature of the Wigner equation, which governs the dynamics of the Wigner function, is that it shares many analogies to the classical mechanism and simply reduces to the classical counterpart when the reduced Planck constant vanishes. Despite the theoretical advantages, numerical resolutions for the Wigner equation is notoriously difficult and remains one of the most challenging problems in computational physics, mainly because of the high dimensionality and nonlocal pseudo-differential operator. On one hand, the commonly used finite difference methods fail to capture the highly oscillatory structure accurately. On the other hand, all existing stochastic algorithms, including the affinity-based Wigner Monte Carlo and signed particle Wigner Monte Carlo methods, have been confined to at most 4D phase space. Few results have been reported for higher dimensional simulations. My group has made substantial progress in both aspects.

(1) We completed the design and implementation of a highly accurate numerical scheme for the Wigner quantum dynamics in 4D phase space. Our algorithm combines an efficient conservative

semi-Lagrangian scheme in the temporal-spatial space with an accurate spectral element method in the momentum space. With it, the Wigner function for a one-dimensional Helium-like system was clearly shown for the first time.

(2) We explored the inherent relation between the Wigner equation and a stochastic branching random walk model. With an auxiliary function, we can cast the Wigner equation into a renewal-type integral equation and prove that its solution is equivalent to the first moment of a stochastic branching random walk. In order to realize an efficient, reliable and integrated particle-based scheme to capture complicated quantum features in phase space, we utilized the probabilistic interpretation of the Wigner equation, efficient Monte Carlo strategies and non-parameter density estimation techniques.

It should be noted that all proposed numerical schemes fully exploit the mathematical structure of the Wigner equation. Our target is an efficient simulator for analyzing some fundamental issues in many-body quantum mechanics, such as the nuclear quantum effect and dynamical correlation.

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