数学与系统科学研究院

计算数学所定期学术报告

报告人：**Associate Prof. Tiao Lu**

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报告题目：

High-order Quantum Moment Models of Density Functional Theory

邀请人：　邸亚娜 副研究员

报告时间：2013 年 5 月 23 日（周四）

下午 16：00~17：00

（15：30~16：00 茶歇）

报告地点：　科技综合楼三层 311

计算数学所报告厅

Abstract：

We derived a series of high-order quantum moment models of the Wigner equation in (Cai, Fan, Li, Lu and Wang, J. Math. Phys., 2012). In this talk, I will discuss about how to extended this work to density function theory (DFT). The most popular implement of DFT is the Kohn-Sham equation, which transforms a many-particle interacting system into a fictitious non-interacting one-particle system. The Kohn-Sham equation is a non-linear Schr\"odinger equation, and the corresponding Wigner equation can be derived as an alternative implementation of DFT. We derived quantum hydrodynamic models of the Wigner equation by moment closure following in (Cai, Fan, Li, Lu and Wang, J. Math. Phys., 2012). The derived quantum hydrodynamic models are globally hyperbolic thus locally wellposed. The contribution of the Kohn-Sham potential is turned into a nonlinear source term of the hyperbolic moment system. This work provides a new possible way to solve DFT problems.

参考文献：

Z.-N. Cai, Y.-W. Fan, R. Li, T. Lu and W.-Q. Yao, *Quantum Hydrodynamic Model of Density Functional Theory*, Journal of Mathematical Chemistry, DOI: 10.1007/s10910-013-0176-1.
http://www.springerlink.com/openurl.asp?genre=article&id=doi:10.1007/s10910-013-0176-1

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