



復旦大學
FUDAN UNIVERSITY

Applied Math
Ph.D. Seminar

Solving many-electron Schrödinger equation with ACE

Speaker: Dexuan Zhou

(Beijing Normal University)

Time: 2024-03-21, 16:10 to 17:00

Location: Rm 1801, Guanghua East Tower

Advisor: Huajie Chen

(Beijing Normal University)

Abstract: In this talk, we'll explore the parameterization of many-electron wave functions with ACE and computation of ground state for atom and molecule systems using the Variational Monte Carlo method, the novelty of our method lies in (i) a convenient and accurate linear polynomial expansion; (ii) a hierarchical structure that applies naturally to a multigrid variation; and (iii) possible revealing the correlation of the system by increasing the body-order.