



復旦大學
FUDAN UNIVERSITY

Applied Math
Ph.D. Seminar

A Structure-Preserving LOBPCG Algorithm for the Bethe–Salpeter Eigenvalue Problem

Speaker: Xinyu Shan (Fudan University)

Time: 2026-06-11, 16:10 to 17:00

Location: Rm 1801, Guanghai East Tower

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Abstract: The Bethe–Salpeter eigenvalue problem is a structured eigenvalue problem arising in many-body physics. In practice, a few smallest positive eigenvalues and the corresponding eigenvectors need to be computed. This problem can be solved by the LOBPCG algorithm, either in its classical form or in an indefinite variant. While the indefinite LOBPCG algorithm is computationally more efficient, it may encounter convergence stagnation as rounding errors propagate. To address this issue, we propose a strategy combining the improved Hetmaniuk–Lehoucq trick with conditional reorthogonalization to enhance the numerical stability. Furthermore, we introduce an adaptive mechanism that automatically switches from the more efficient C_n -inner product to the more robust Ω -inner product upon detecting convergence stagnation. Numerical experiments demonstrate that the proposed algorithm can efficiently and accurately compute the desired eigenpairs. Since the symplectic eigenvalue problem for symmetric positive definite matrices can be transformed to the Bethe–Salpeter eigenvalue problem, our algorithm can naturally be adopted as a symplectic eigensolver.