THE UNIVERSITY OF CHICAGO

Departments of Computer Science, Mathematics, Statistics, and the Computation Institute

SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

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Decay Properties of Matrix Functions, with Applications to $O(N)$ Methods in Electronic Structure and Beyond

THURSDAY, March 6, 2014, at 4:30 PM

Eckhart 133, 5734 S. University Avenue

ABSTRACT

Motivated by applications in quantum chemistry and solid state physics, we apply general results from approximation theory and matrix analysis to the study of the decay properties of functions of large and sparse Hermitian matrices. Our theory leads to a rigorous proof of the exponential off-diagonal decay of the density matrix for arbitrary gapped systems (insulators) at zero electronic temperature, thus providing a firm theoretical foundation for the development of $O(N)$ methods in electronic structure calculations for non-metallic systems, The theory also covers the case of metallic systems at positive temperatures. Extensions of the theory and additional applications will be briefly discussed.

This is joint work with Paola Boito (University of Limoges).

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