Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Calculating the density of states in disordered systems using free probability[1] JIAHAO CHEN, ERIC HONTZ, MATTHEW WELBORN, JEREMY MOIX, TROY VAN VOORHIS, Department of Chemistry, Massachusetts Institute of Technology, ALBERTO SUÁREZ, Departamento de Ingenieria Informatica, Escuela Politecnica Superior, Universidad Autonoma de Madrid, Ciudad Universitaria de Cantoblanco, RAMIS MOVASSAGH, ALAN EDELMAN, Department of Mathematics, Massachusetts Institute of Technology — We approximate the density of states in disordered systems by decomposing the Hamiltonian into two random matrices and constructing their free convolution. The error in this approximation is determined using asymptotic moment expansions. Each moment can be decomposed into contributions from specific joint moments of the random matrices; each of which has a combinatorial interpretation as the weighted sum of returning trajectories. We show how the error, like the free convolution itself, can be calculated without explicit diagonalization of the Hamiltonian. We apply our theory to Hamiltonians for one-dimensional tight binding models with Gaussian and semicircular site disorder. We find that the particular choice of decomposition crucially determines the accuracy of the resultant density of states. From a partitioning of the Hamiltonian into diagonal and off-diagonal components, free convolution produces an approximate density of states which is correct to the eighth moment. This allows us to explain the accuracy of mean field theories such as the coherent potential approximation, as well as the results of isotropic entanglement theory.

[1]Funded by NSF SOLAR NSF Grant No. 1035400

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Date submitted: 21 Dec 2011 Electronic form version 1.4