Abstract Submitted
for the FWS16 Meeting of
The American Physical Society

Calculating Nuclear Magnetic Relaxation (NMR) Rates with Numerical Linked Cluster Expansions[1] NICHOLAS SHERMAN, RAJIV SINGH, University of California, Davis — Numerically calculating low frequency spectral weights and NMR relaxation rates for quantum spin models, beyond a regime where the quasi-particle picture is valid, remains a challenging task. We explore several ways of calculating these quantities using NLC. These include Moriyas Gaussian approximation, as well as extrapolation from multiple frequency moments of the dynamical structure factor or of the spectral-weight function. We have employed these techniques on several spin models, including the antiferromagnetic Heisenberg model on the Ladder, Kagome, and Square Bilayer. We have found that Moriyas Gaussian approximation provides a good first approximation for the NMR rates in all cases. However, we find that an extrapolation from multiple frequency moments can provide the most accurate calculations for the NMR rates. The challenge in the extrapolation method arises with the convergence of high frequency moments breaking down early in NLC, and so one must balance using a large number of moments and extrapolation with fewer parameters. We believe the method of extrapolation of multiple frequency moments can be a versatile computational tool for addressing NMR rates and other low frequency probes in quantum-spin and strongly-correlated electron systems.

[1]This work is supported by NSF grant number DMR 1306048.

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Date submitted: 06 Oct 2016 Electronic form version 1.4