Real-Space Treatment of Spin-Peierls Transitions: Gap Equation of the S = 1/2 Heisenberg Antiferromagnetic Chain ZOLTAN SOOS, SHARON BEWICK, Princeton University — The spin-Peierls transition at T_{SP} of s = 1/2 Heisenberg AF chains with linear spin-phonon (sp-ph) coupling is modeled by exact solution up to 18 spins. Spin correlations alter the gap relation between T_{SP} and the singlet-triplet gap, E_{ST}, from the free-fermion or mean-field (mf) result by 30%. Direct solution accounts for the spin-Peierls transition, magnetic susceptibility and magnetization of the prototypical TTF^+ (tetrathiafulvalene) spin chain in TTFCu(BDT). Strong sp-ph coupling is required for size convergence. Exact analysis of finite chains conserves total spin, while mf or bosonization approximations for spinless fermions in infinite chains only conserve the z component and have axial rather than spherical symmetry in spin space.

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