Magnetic susceptibilities of rectangular Heisenberg $S=1/2$ antiferromagnets

TOM VALLEAU, ROB BUTCHER, BRIAN KEITH, CHRISTOPHER LANDEE, MARK TURNBULL, Clark University, ANDERS SANDVIK, Boston University — Rectangular antiferromagnets are two-dimensional systems with inequivalent exchange strengths $(J', J)$ along the two principle axes with $J' \equiv \alpha J, \alpha \leq 1$. They have an intermediate dimensionality that can vary continuously from 1D ($\alpha = 0$) to square 2D ($\alpha = 1$). There exist a number of physical realizations of rectangular antiferromagnets ($\text{CuPzBr}_2, \text{CuPzCl}_2, \text{CuPz(N}_3\text{)}_2$ where Pz = pyrazine) but there has been no previous mechanism for interpreting their susceptibilities in terms of two exchange parameters. We have simulated the susceptibility of the rectangular $S=1/2$ Heisenberg antiferromagnet using the stochastic series expansion quantum Monte Carlo method [1] and used the results to interpret our experimental data. For example, copper pyrazine diazide, $\text{CuPz(N}_3\text{)}_2$, has a primary exchange of 15.5 K and an anisotropy parameter $\alpha = 0.4$. The stronger exchange is due to the superexchange pathway through the pyrazine molecule and the weaker corresponds to the azide bridges. [1] A. Sandvik, PRB 59, R14157 (1999).