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Quantum Monte Carlo Gap Analysis of Neel-VBS Phase Transition HIDEMARO SUWA, ANDERS SANDVIK, Department of Physics, Boston University — We have developed a generalized moment method for calculating excitation gaps in finite-temperature and ground-state projector quantum Monte Carlo simulations. We show analytically that this estimator is unbiased in the low-temperature or long-projection-length limit. Not only the first gap but also the second gap for each quantum number can be calculated without any systematic errors. As a demonstration, we have applied this approach to the Neel–valence-bond-solid transition of the two-dimensional J-Q spin model. The transition point was successfully obtained from the singlet-triplet level crossing. Interestingly, the size-scaling of the crossing point is the same as in the one-dimensional case ($1/L^2$, L being the system length).

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