E–mail: victor_tokarev@protonmail.com

On Applicability of Rotational Band Approximation

V. V. Tokarev

V. N. Karazin Kharkiv National University, Faculty of Chemistry, 4 Svobody Sq., 61022 Kharkiv, Ukraine

Rotational band approximation (RBA) is valid for quantum antiferromagnetic Heisenberg model on finite bipartite lattices. It assumes that for lower energy levels $E_{min}(S) \approx cS(S+1)$. It's known that increasing number of lattice unit cells or introducing geometric frustration deteriorate this approximation, but it's not well understood how critical number of elementary cells or frustration strength depends on lattice structure.

Usage of eigendecomposition of exchange parameter matrix J allows us to write Heisenberg Hamiltonian in the following form

$$H = \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \mathbf{S}_j = \sum_{l=1}^{n} \lambda_l \sum_{\langle i,j \rangle} v_{li} v_{lj} \mathbf{S}_i \mathbf{S}_j, \tag{1}$$

where λ_l and $\mathbf{v}_l$ are eigenvalue and corresponding eigenvector of J.

We show that for d-regular bipartite expander graphs (namely bipartite double covers of strongly regular graphs) of any size RBA is valid at least for ground state energy E_0 in second order of perturbation theory in spectral parameter $\delta = \lambda_2/d$, where λ_1 is second largest eigenvalue of J.

For this type of lattices energy of ground and lower excited states of antiferromagnetic Heisenberg model with $S = const$ is accurately predicted by spin wave theory. We use the fact that spin wave energy and wavefunctions can be expressed as functions of $\lambda_l, \mathbf{v}_l$ and that eigenvectors $\mathbf{v}_l$ have definite lattice symmetry to perturbatively study influence of uniform frustration $J \to J + \alpha(J - dI)$ and approximate critical value of frustration parameter α_c that corresponds to quantum phase transition.