Geometrical Aspects of the Multicritical Phase Diagrams for the Blume-Emery-Griffiths Model

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Abstract

A Ruppeiner metric is defined on a 2D phase space of dipolar (M) and quadrupolar (Q) order parameters for the spin-1 mean-field Blume-Emery-Griffiths model. Then, an expression for the Ricci scalar (R) is derived and temperature/crystal field variations of R are presented using four different phase diagram topologies introduced by Hosten and Berker (1991). Its behaviour near the continuous/discontinuous phase transition temperatures as well as the multicritical points is investigated. Besides the study of R along the phase equilibria we have located the R=0 boundary lines in the multicritical phase diagrams.

Model Hamiltonian [1-5]

\[ H = -J \sum_{\langle i,j \rangle} S_i S_j - K \sum_i S_i^4 - D \sum_i S_i^2 \]

Spin variable : \( S_i = -1, 0, +1 \)

Nearest-neighbour spins : \( < 0 > \)

Dipole-dipole interaction energy : \( J \)

Quadrupole-quadrupole interaction energy : \( K \)

Crystal field or single-ion anisotropy : \( D \)


\[ \mu(M, Q) = -\frac{1}{2} M^2 + \frac{1}{2} Q^2 \]

Lattice coordination number : \( z \)

Number of spins : \( N \)

Magnetisation per lattice site : \( M = \langle S_i \rangle \)

Quadrupolar moment : \( Q = \langle S_i^4 \rangle \)

Reduced quantities : \( r = M / z \), \( D / Dz \)

Reduced temperature : \( \theta = kT / j \)

Temperature : \( T \)

Boltzmann constant : \( k \)

Entropy : \( S = k \ln \Omega \)

\[ \Omega = (2M)_r (2Q)_r (2D)_r (2k)_r (2k)_r (2k)_r (2k)_r (2k)_r (2k)_r \]

Self-Consistent Equations [5]

Equilibrium conditions : \( \frac{\partial H}{\partial M} = 0 \), \( \frac{\partial H}{\partial Q} = 0 \)

Self-consistent equations:

\[ M = \exp \left[ \frac{\partial H}{\partial M} \right] \]

\[ Q = \exp \left[ \frac{\partial H}{\partial Q} \right] \]

Geometrical Aspects of the Multicritical Phase Diagrams

Various thermodynamic coordinates:

\( \chi = (1, 2, \ldots, n) \)

Definition of a metric in a n-dimensional thermodynamic state space of coordinates:

\( d\chi^i = G_{ij} d\chi^j \)

Metric tensor elements (Ruppeiner Metric):

\( G_{ij} = \delta_{ij} - \beta \delta_{ij} \phi \)

Thermodynamic potential per site:

\( \phi = \phi_0 \)

Derivative with respect to the coordinates:

\( \beta = \beta_0 \phi \)

Inverse temperature:

\( \beta = 1/\kappa \phi \)

Christoffel symbols:

\( \Gamma^i_{jk} = \frac{1}{2} \left( \partial_k G_{ij} + \partial_j G_{ik} - \partial_i G_{jk} \right) \)

Inverse of metric tensor:

\( G^{ij} \)

Ricci tensor:

\( R_{ij} = \partial_k \Gamma^k_{ij} - \partial_j \Gamma^k_{ik} + \Gamma^k_{ij} \Gamma^l_{kl} - \Gamma^k_{ik} \Gamma^l_{jl} \)

Curvature tensor:

\( R_{ijkl} \) as well known as thermodynamic curvature:

\( \rho = G^{ij} R_{ij} \)

A two-dimensional manifold is chosen with:

\( \{ (\chi^3, \chi^4) ; (M, Q) \} \)

We have found Ricci scalar as:

\( R = \rho / \kappa \phi \)

References