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 Hoston 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 boundry lines in the multicritical phase diagrams.

Model Hamiltonian [1-5]

$$\mathrm{H}\{S_i\} = -J\sum_{<ij>} S_i S_j - K\sum_{<ij>} S_i^2 S_j^2 - D\sum_i S_i^2$$

Spin variable :	$S_i = -1,\ 0,\ +1$
Nearest-neighbour spins :	$<ij>$
Dipole-dipole interaction energy :	J
Quadrupole-quadrupole interaction energy :	K
Cyrstal field or single-ion anisotropy :	D

Magnetic Gibbs Energy Functional [5]

$$\phi(M,Q) = \frac{G}{zJ} = -\frac{1}{2}NM^2 - \frac{1}{2}NrQ^2 + NdQ - \theta \ln\Omega(M,Q)$$

Lattice coordination number :	z
Number of spins :	N
Magnetisation per lattice site :	$M = \langle S_i \rangle$
Quadrupolar moment :	$Q = \langle S_i^2 \rangle$
Reduced quantities :	$r = K/zJ \qquad d = D/zJ$
Reduced temperature :	$\theta = kT/zJ$
Temperature :	T
Boltzmann constant :	k_B
Entropy :	$S_E = k_B \ln\Omega$

$$\ln\Omega(M,Q) = -N\left[\frac{1}{2}(Q+M)\ln\frac{1}{2}(Q+M) + \frac{1}{2}(Q-M)\ln\frac{1}{2}(Q-M) + (1-Q)\ln(1-Q)\right]$$

Self-Consistent Equations [5]

Equilibrium conditions : $\frac{\partial\phi}{\partial M} = 0 \qquad \frac{\partial\phi}{\partial Q} = 0$

Self-consistent equations :

$$M = \frac{2\sinh(M/\theta)}{\exp[(d-rQ)/\theta] + 2\cosh(M/\theta)}$$

$$Q = \frac{2\cosh(M/\theta)}{\exp[(d-rQ)/\theta] + 2\cosh(M/\theta)}$$

Geometrical Perspective [6]

Various thermodynamic coordinates :	$x^i\,(i = 1,2,\ldots,n)$
Definition of a metric in a *n*-dimensional thermodynamic state space of coordinates :	$ds^2 = G_{ij}dx^i dx^j$
Metric tensor elements (Ruppeiner Metric) :	$G_{ij} = -\beta\partial_i\partial_j\phi$
Thermodynamic potential per site :	$\phi = \Phi/N$
Derivative with respect to the coordinates :	$\partial_i = \partial/\partial x^i$
Inverse temperature :	$\beta = 1/k_B\theta$
Christoffel symbols :	$\Gamma^i_{jk} = \frac{1}{2}G^{il}\left(\partial_k G_{lj} + \partial_j G_{lk} - \partial_l G_{jk}\right)$
Inverse of metric tensor :	G^{il}
Ricci tensor :	$R^i_{jkl} = \partial_k\Gamma^i_{jl} - \partial_l\Gamma^i_{jk} + \Gamma^i_{mk}\Gamma^m_{jl} - \Gamma^i_{ml}\Gamma^m_{jk}$
Curvature tensor :	$R_{ij} = R^n_{inj}$
Ricci curvature scalar (also known as thermodynamic curvature) :	$R = G^{ij}R_{ij}$
A two-dimensional manifold is choosen with :	$(x^1, x^2) = (M,Q)$
We have found Ricci scalar as :	$R(M,Q) = -\frac{1}{2}\frac{A}{B^2}\theta^3$

$$A = Q(Qr - 2r + 2) + M^2 - \theta + r - 1$$

$$B = rQ^2(Q - \theta - 1) + rM^2(Q+1) + Q\theta(r+1) - \theta(M^2 + \theta)$$

Numerical Calculations on *R*

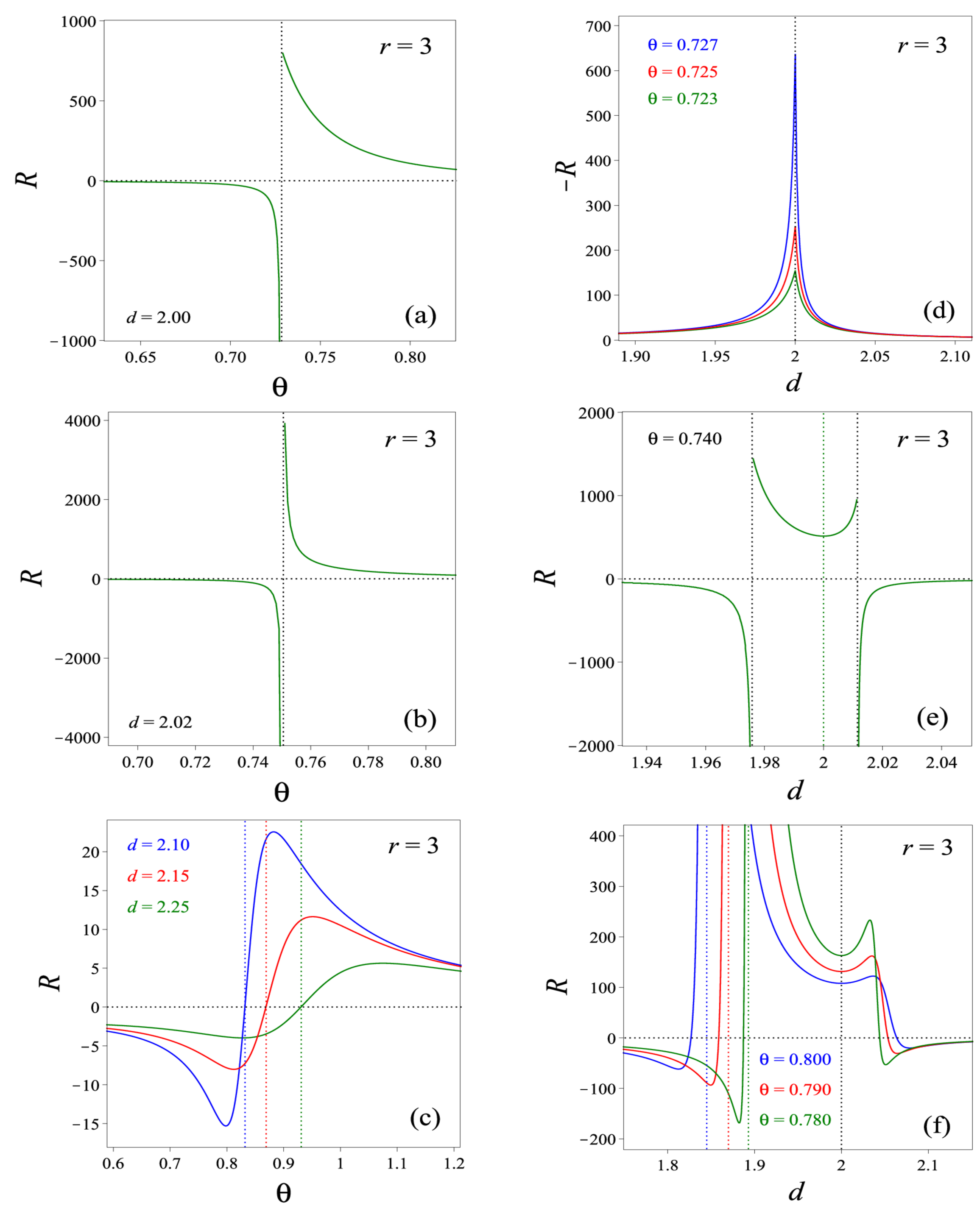

Fig. 1. *R vs.* reduced temperature and single-ion anisotropy for *r* = 3

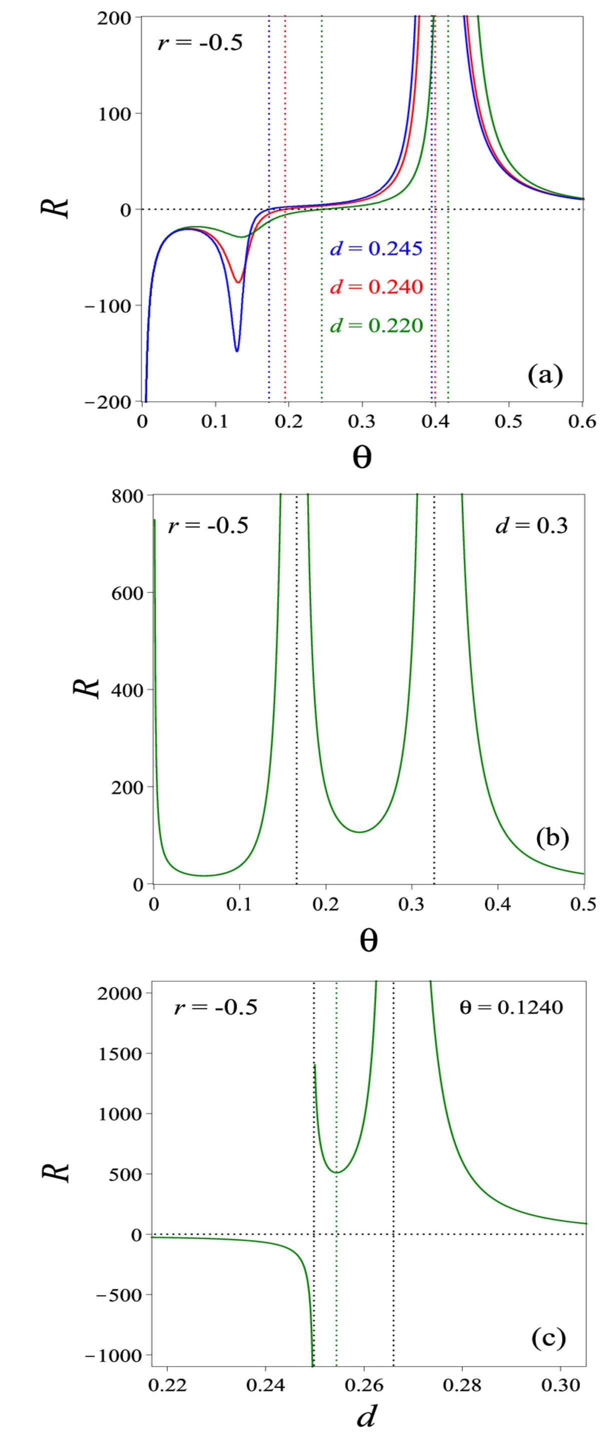

Fig. 2. Same as Fig. 1 but for *r* =-0.5

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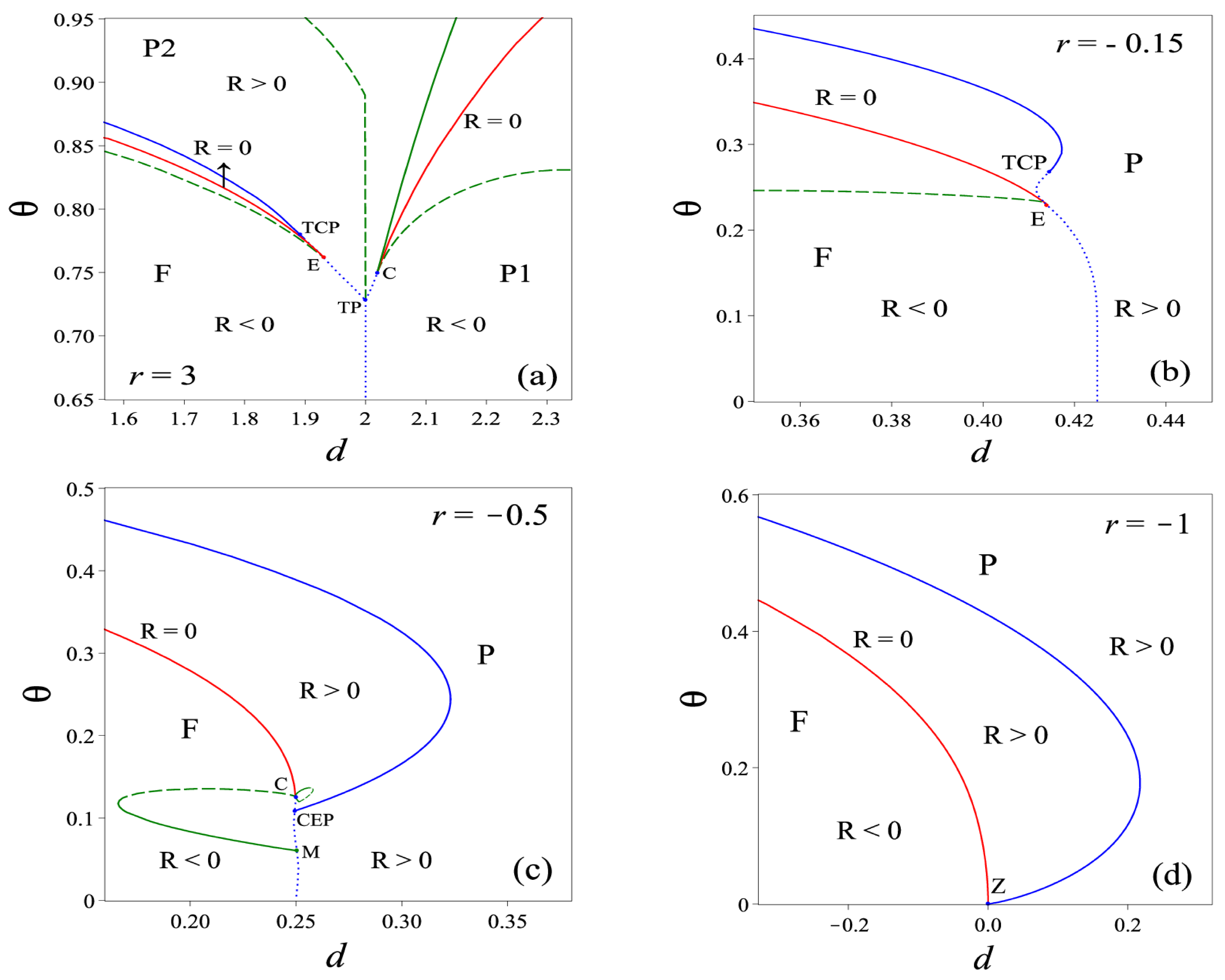

Fig. 3. Loci of the maxima (green solid curves) and minima (green dashed curves) of *R* with R=0 curve (red solid curves) for **(a)** *r* =3, **(b)** *r* =-0.15, **(c)** *r* =-0.5 and **(d)** *r* = -1.

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