Bifurcation Analysis of a mildly repulsive model for biaxial phases

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Pavia, 14th April 2005

Summary

Mean-field model for $\gamma = 0$

Phase diagram and order parameters

Reference model parameters domain

Conjugated phase diagram

Extension to a mildly repulsive model

Bifurcation analysis

Phase diagram for the repulsive case

Biaxials' model

$$\mathbf{q} := \mathbf{m}\otimes\mathbf{m} - \frac{1}{3}\mathbf{I}, \quad \mathbf{b} := \mathbf{e}\otimes\mathbf{e} - \mathbf{e}_\perp\otimes\mathbf{e}_\perp$$

$$V = -U_0\left\{\mathbf{q}\cdot\mathbf{q}' + \gamma(\mathbf{q}\cdot\mathbf{b}' + \mathbf{b}\cdot\mathbf{q}') + \lambda\mathbf{b}\cdot\mathbf{b}'\right\}$$

$U_0 > 0$ and λ, γ model parameters

$$\mathbf{Q} = S(\boldsymbol{e}_z\otimes\boldsymbol{e}_z - \frac{1}{3}\mathbf{I}) + T(\boldsymbol{e}_x\otimes\boldsymbol{e}_x - \boldsymbol{e}_y\otimes\boldsymbol{e}_y)$$

$$\mathbf{B} = S'(\boldsymbol{e}_z\otimes\boldsymbol{e}_z - \frac{1}{3}\mathbf{I}) + T'(\boldsymbol{e}_x\otimes\boldsymbol{e}_x - \boldsymbol{e}_y\otimes\boldsymbol{e}_y)$$

pseudo-potential

$$U = -U_0(\mathbf{q}\cdot\mathbf{Q} + \lambda\mathbf{b}\cdot\mathbf{B})$$

Mean-field equations

partition and distribution functions

$$Z(\mathbf{Q},\mathbf{B},\beta,\lambda)=\int_{\mathbb{T}}\exp\left(\beta\left(\mathbf{Q}\cdot\mathbf{q}+\lambda\mathbf{B}\cdot\mathbf{b}\right)\right)$$

$$f=\frac{1}{Z}\exp\left[\beta(\mathbf{q}\cdot\mathbf{Q}+\lambda\mathbf{b}\cdot\mathbf{B})\right]$$

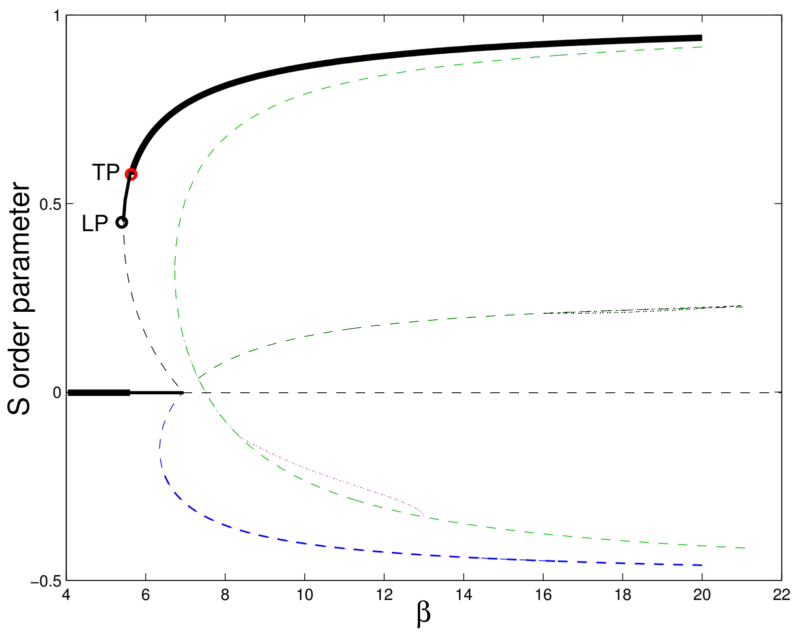
$$\mathbb{T}:=\mathbb{S}^2\times\mathbb{S}^1,\quad \beta:=\frac{U_0}{k_B t}$$

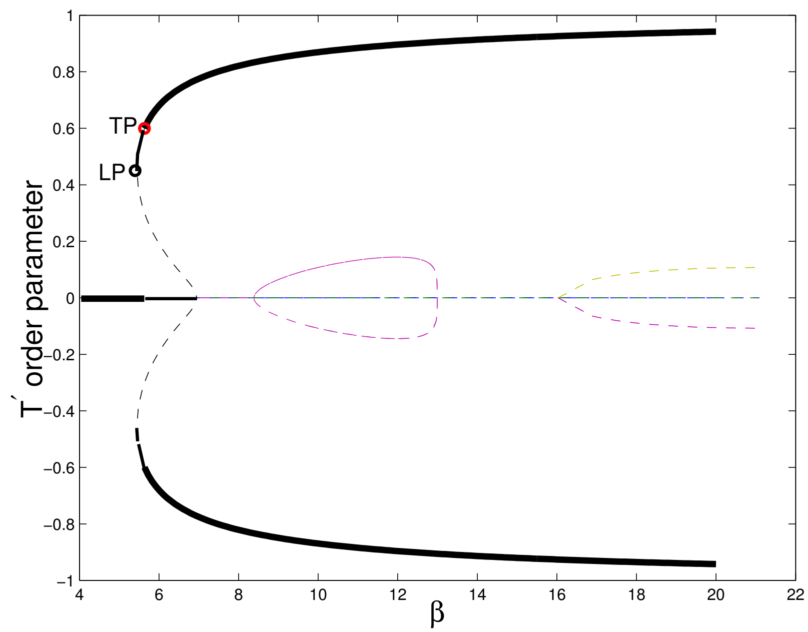
k_B Boltzmann constant and t absolute temperature

$$\mathbf{Q}=\langle\mathbf{q}\rangle=\int_{\mathbb{T}}f\mathbf{q}\qquad \mathbf{B}=\langle\mathbf{b}\rangle=\int_{\mathbb{T}}f\mathbf{b}$$

$$\mathcal{F}(\mathbf{Q},\mathbf{B},\beta,\lambda)=U_0\left\{\frac{1}{2}\mathbf{Q}\cdot\mathbf{Q}+\frac{\lambda}{2}\mathbf{B}\cdot\mathbf{B}-\frac{1}{\beta}\ln\left(\frac{Z(\mathbf{Q},\mathbf{B},\beta,\lambda)}{8\pi^2}\right)\right\},$$

$\lambda = 0.36$

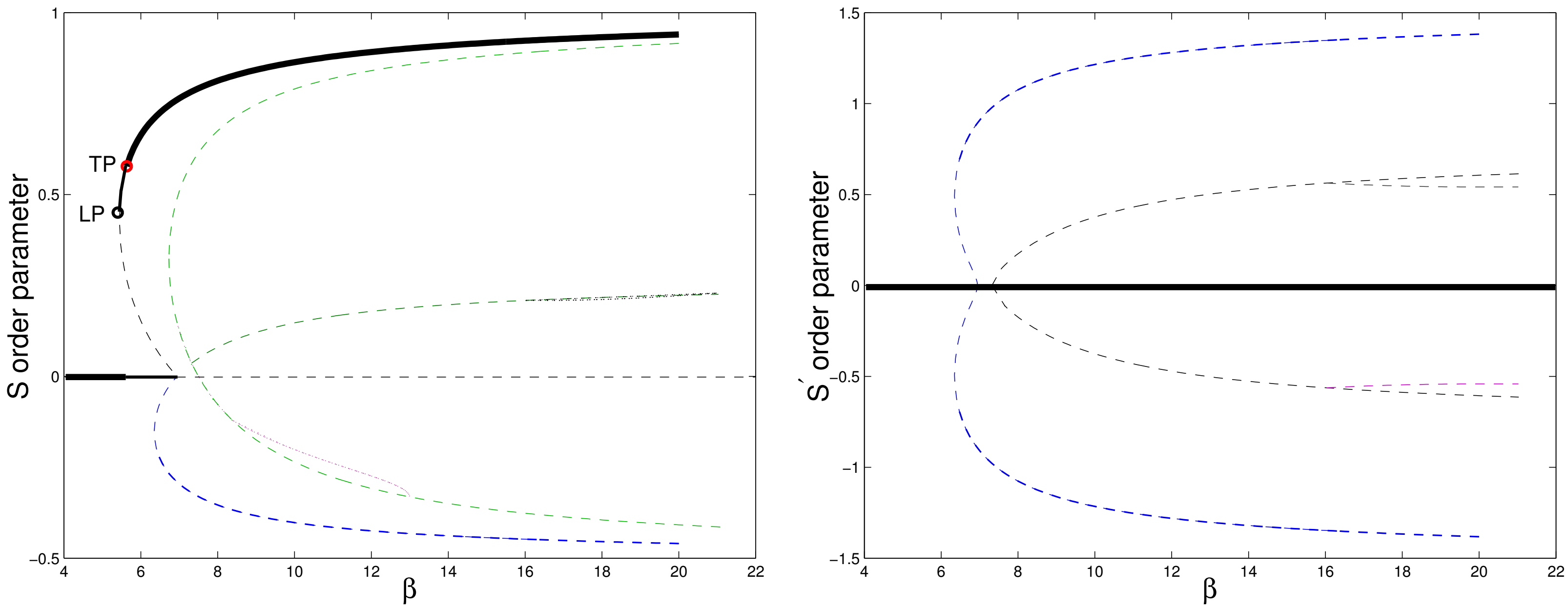




dominant stable biaxial states $(S, 0, 0, T')$

$$\mathbf{Q} = S(\mathbf{e}_z \otimes \mathbf{e}_z - \frac{1}{3}\mathbf{I}) \qquad \mathbf{B} = T'(\mathbf{e}_x \otimes \mathbf{e}_x - \mathbf{e}_y \otimes \mathbf{e}_y)$$

$\lambda = 0.36$

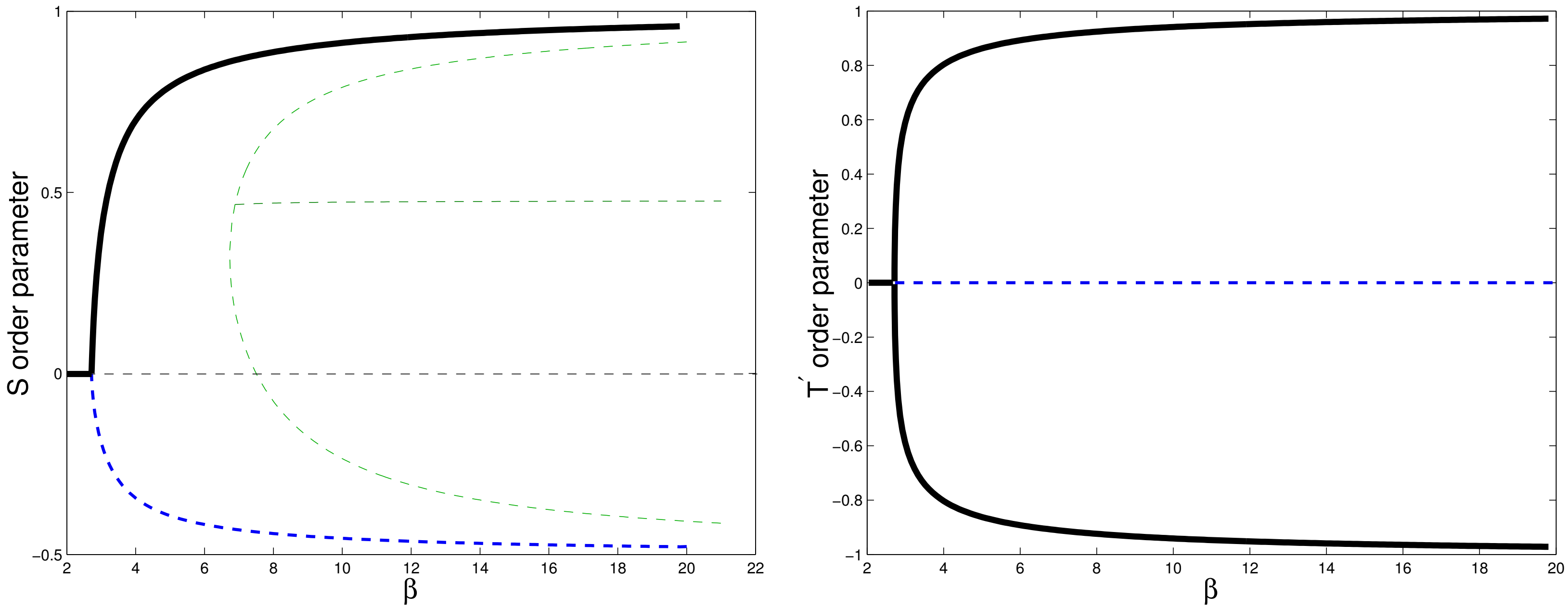


unstable uniaxial states with a greater value of free energy $(S, 0, S', 0)$

$$\mathbf{Q} = -S(\mathbf{e}_y \otimes \mathbf{e}_y - \frac{1}{3}\mathbf{I}) \qquad \mathbf{B} = -S'(\mathbf{e}_y \otimes \mathbf{e}_y - \frac{1}{3}\mathbf{I})$$

$$\mathbf{Q} = -S(\mathbf{e}_x \otimes \mathbf{e}_x - \frac{1}{3}\mathbf{I}) \qquad \mathbf{B} = -S'(\mathbf{e}_x \otimes \mathbf{e}_x - \frac{1}{3}\mathbf{I})$$

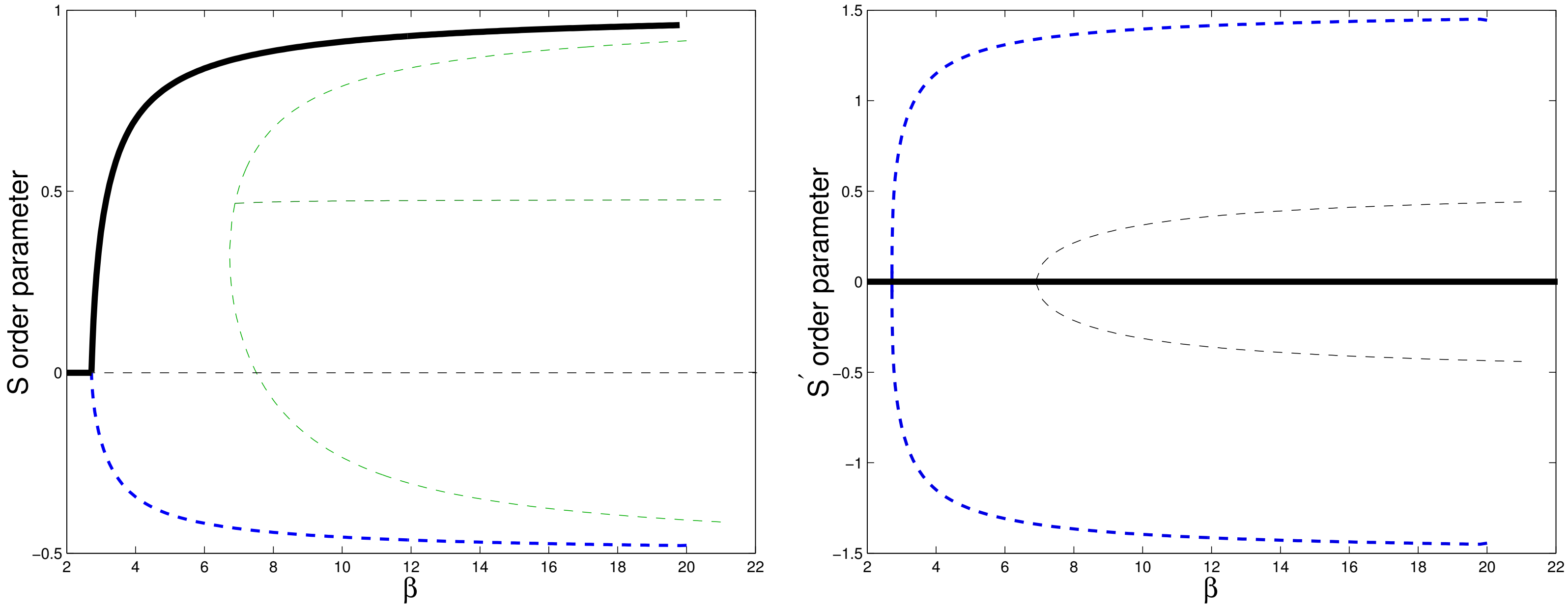
$\lambda = 0.92$



dominant stable biaxial states $(S, 0, 0, T')$

$$\mathbf{Q} = S(\mathbf{e}_z \otimes \mathbf{e}_z - \frac{1}{3}\mathbf{I}) \qquad \mathbf{B} = T'(\mathbf{e}_x \otimes \mathbf{e}_x - \mathbf{e}_y \otimes \mathbf{e}_y)$$

$\lambda = 0.92$

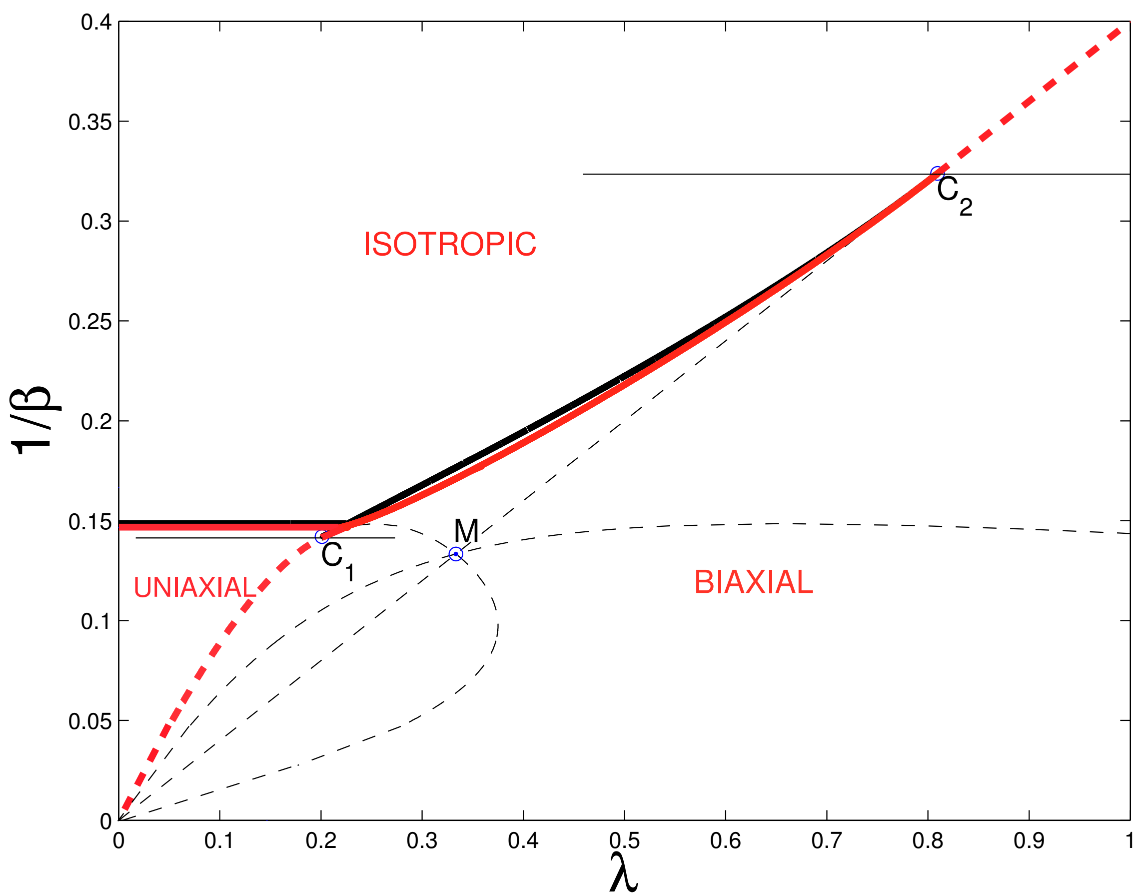


unstable uniaxial states with a greater value of free energy $(S, 0, S', 0)$

$$\mathbf{Q} = -S(\mathbf{e}_y \otimes \mathbf{e}_y - \frac{1}{3}\mathbf{I}) \qquad \mathbf{B} = -S'(\mathbf{e}_y \otimes \mathbf{e}_y - \frac{1}{3}\mathbf{I})$$

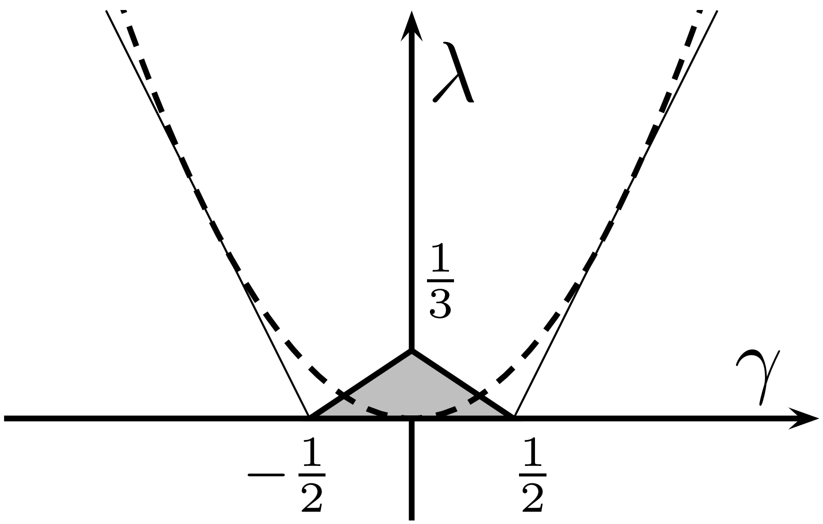
$$\mathbf{Q} = -S(\mathbf{e}_x \otimes \mathbf{e}_x - \frac{1}{3}\mathbf{I}) \qquad \mathbf{B} = -S'(\mathbf{e}_x \otimes \mathbf{e}_x - \frac{1}{3}\mathbf{I})$$

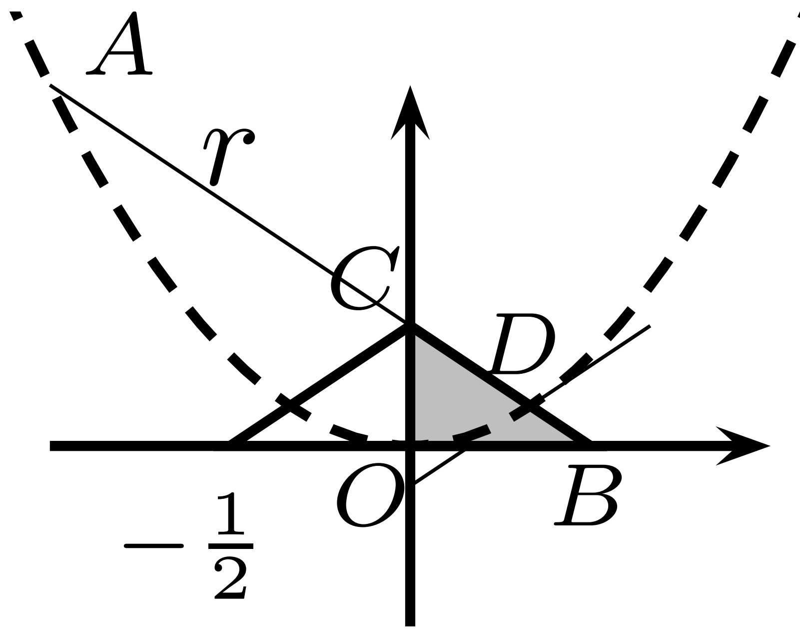
Phase Diagram and Tricritical points



Durand, Sonnet, Virga (2003) De Matteis, Romano ,Virga (2004)

Reference triangle





$$D\left(\frac{1}{3},\frac{1}{9}\right),\quad B\left(\frac{1}{2},0\right),\quad C\left(0,\frac{1}{3}\right),\quad A\left(-1,1\right)$$

$$r : 2\gamma + 3\lambda - 1 = 0$$

Model: $2\gamma = 1 - 3\lambda$

$$\mathbf{q}^* := \mathbf{e} \otimes \mathbf{e} - \frac{1}{3}\mathbf{I}, \quad \mathbf{b}^* := \mathbf{m} \otimes \mathbf{m} - \mathbf{e}_\perp \otimes \mathbf{e}_\perp$$

$$V = -U_0 \left\{ \left(\frac{9\lambda - 1}{2} \right) \mathbf{q}^* \cdot \mathbf{q}^{*\prime} + \left(\frac{1-\lambda}{2} \right) \mathbf{b}^* \cdot \mathbf{b}^{*\prime} \right\}$$

$$V^* = -U_0 \left(\frac{9\lambda - 1}{2} \right) \left\{ \mathbf{q}^* \cdot \mathbf{q}^{*\prime} + \lambda^* \mathbf{b}^* \cdot \mathbf{b}^{*\prime} \right\}$$

which is equivalent to $\gamma = 0$ model by transforming the model parameter and β as follows

$$\beta^* = \beta \left(\frac{9\lambda - 1}{2} \right), \quad \lambda^* = \frac{1-\lambda}{9\lambda - 1}$$

$$\left[\frac{1}{9}, 1 \right] \mapsto [0, \infty], \left[\frac{1}{9}, \frac{1}{3} \right] \mapsto \left[\frac{1}{3}, \infty \right] i.e. \overline{DA} \mapsto \overline{OP_\infty}, \overline{CD} \mapsto \overline{CP_\infty}$$

$$P_\infty (0, \infty)$$

Order parameters

$$\mathbf{Q}^* = S^*(\boldsymbol{e}_z \otimes \boldsymbol{e}_z - \frac{1}{3}\mathbf{I}) + T^*(\boldsymbol{e}_x \otimes \boldsymbol{e}_x - \boldsymbol{e}_y \otimes \boldsymbol{e}_y)$$

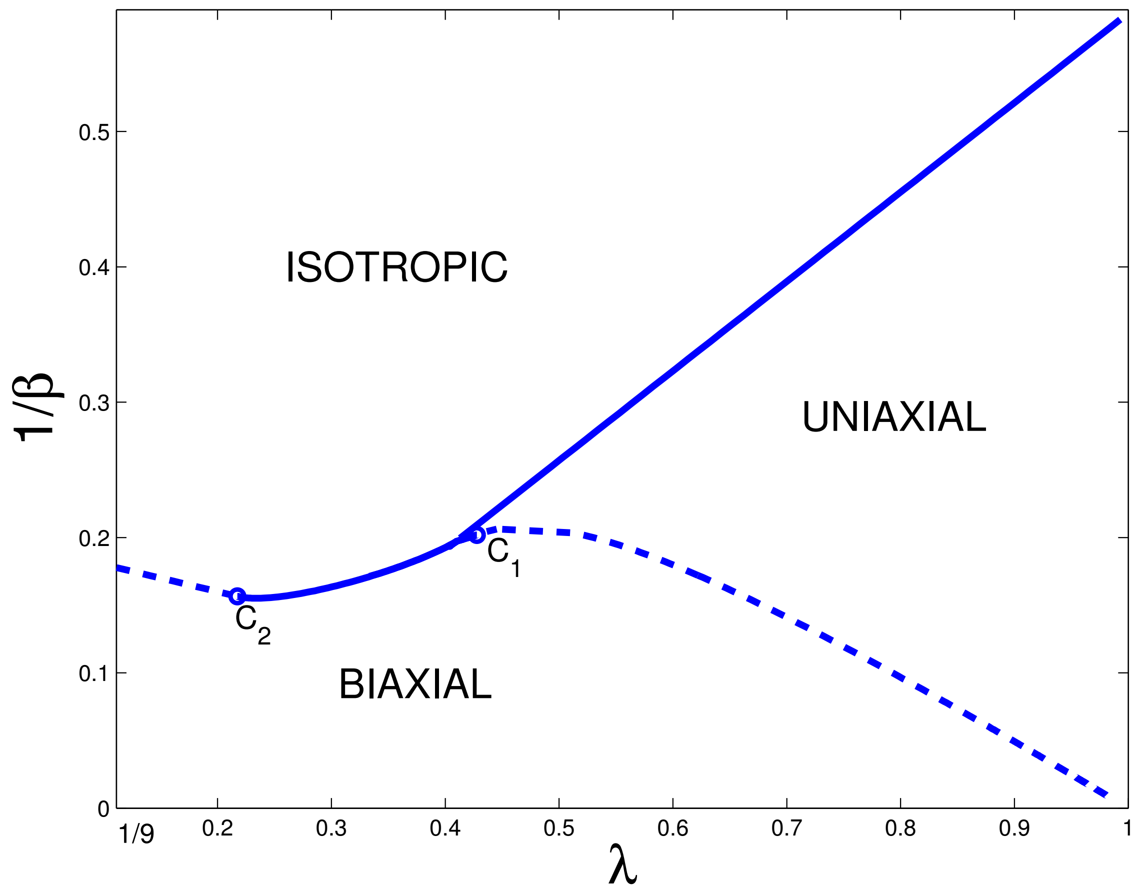
$$\mathbf{B}^* = S'^*(\boldsymbol{e}_z \otimes \boldsymbol{e}_z - \frac{1}{3}\mathbf{I}) + T'^*(\boldsymbol{e}_x \otimes \boldsymbol{e}_x - \boldsymbol{e}_y \otimes \boldsymbol{e}_y)$$

with the following corrispondence on the order parameters

$$S = \frac{S'^* - S^*}{2}, \quad T = \frac{T'^* - T^*}{2},$$

$$S' = \frac{S'^* + 3S^*}{2}, \quad T' = \frac{T'^* + 3T^*}{2}$$

Conjugated phase diagram



$$2\gamma = 1 - 3\lambda \quad \frac{1}{9} \leq \lambda \leq 1$$

We can rewrite the model in the following way

$$V_\mu = -U_0 \left(\frac{1-\lambda}{2}\right) \left\{ \mathbf{b}^* \cdot \mathbf{b}^{*\prime} - \mu \mathbf{q}^* \cdot \mathbf{q}^{*\prime} \right\}$$

$$\mu = \frac{1-9\lambda}{1-\lambda}, \quad \beta_\mu = \beta \left(\frac{1-\lambda}{2}\right)$$

$$\lambda \in \left[0, \frac{1}{9}\right] \Leftrightarrow \mu \in [0,1] \Leftrightarrow \overline{BD}$$

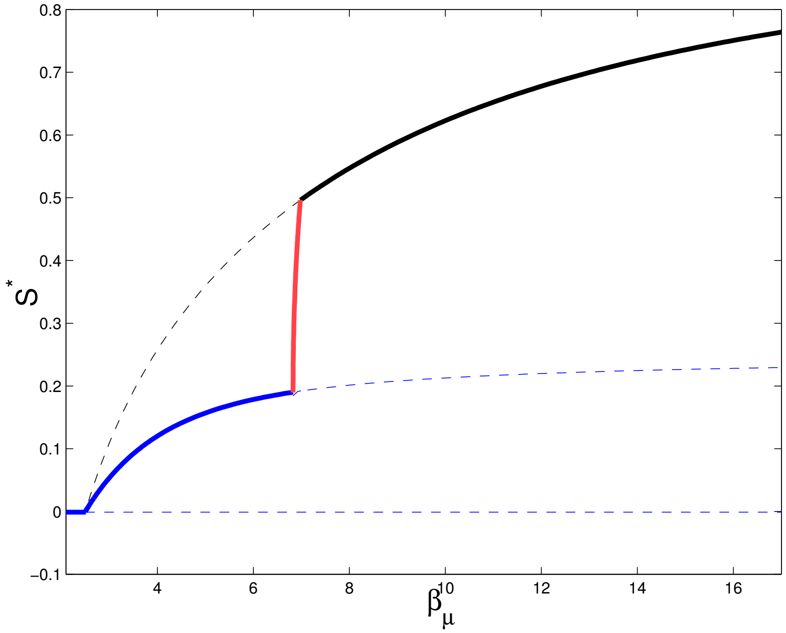
mean-field

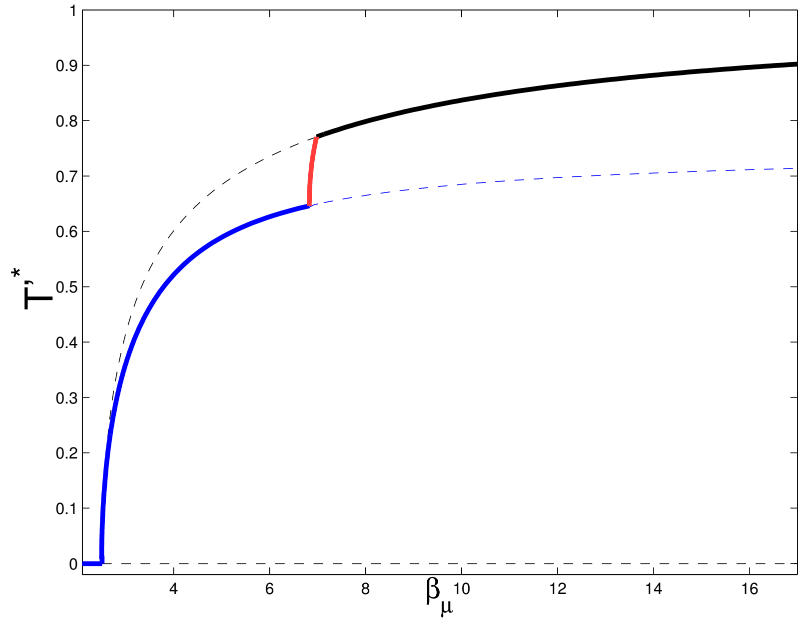
$$f_\mu = \frac{1}{Z_\mu} \exp\left(\beta_\mu \left(\mathbf{B}^* \cdot \mathbf{b}^* - \mu \mathbf{Q}^* \cdot \mathbf{q}^*\right)\right)$$

$$Z_\mu := \int_{\mathbb{T}} \exp\left(\beta_\mu \left(\mathbf{B}^* \cdot \mathbf{b}^* - \mu \mathbf{Q}^* \cdot \mathbf{q}^*\right)\right)$$

$$\mathbf{Q}^* = \langle \mathbf{q}^* \rangle = \int_{\mathbb{T}} f_\mu \mathbf{q}^* \qquad \mathbf{B}^* = \langle \mathbf{b}^* \rangle = \int_{\mathbb{T}} f_\mu \mathbf{b}^*$$

$$\mu = 0.7$$

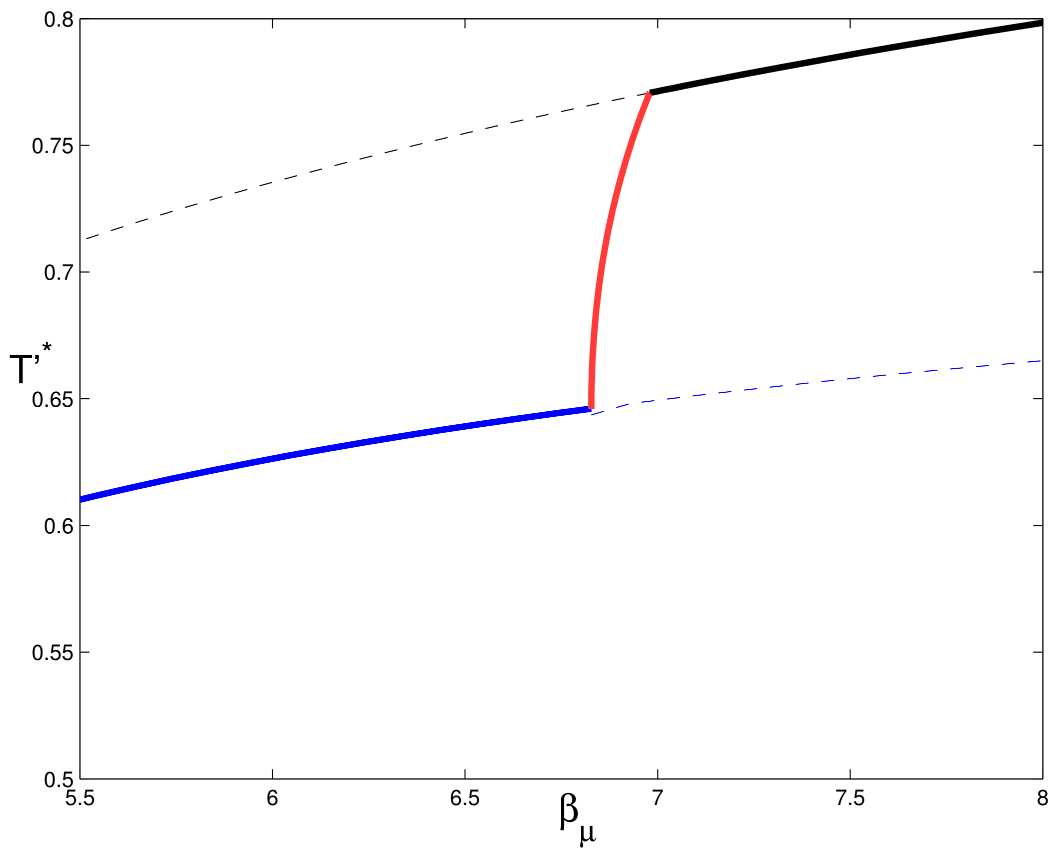




$$\mathbf{Q}^* = S^*(\mathbf{e}_z \otimes \mathbf{e}_z - \frac{1}{3}\mathbf{I}) \quad \mathbf{B}^* = T'^*(\mathbf{e}_x \otimes \mathbf{e}_x - \mathbf{e}_y \otimes \mathbf{e}_y) \Leftrightarrow T^* = S'^* = 0$$

$$\mathbf{Q}^* = -2S^*(\mathbf{e}_x \otimes \mathbf{e}_x - \frac{1}{3}\mathbf{I}) \quad \mathbf{B}^* = -2S'^*(\mathbf{e}_x \otimes \mathbf{e}_x - \frac{1}{3}\mathbf{I}) \Leftrightarrow$$

$$S^* = -T^*, S'^* = -T'^*$$



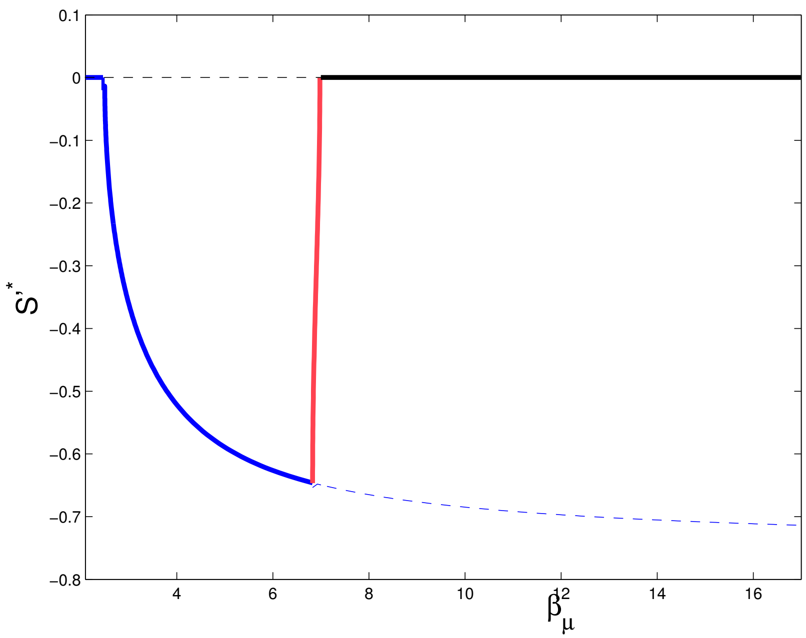
T'*
0.8
0.75
0.7
0.65
0.6
0.55
0.5
5.5
6
6.5
7
7.5
8
β μ

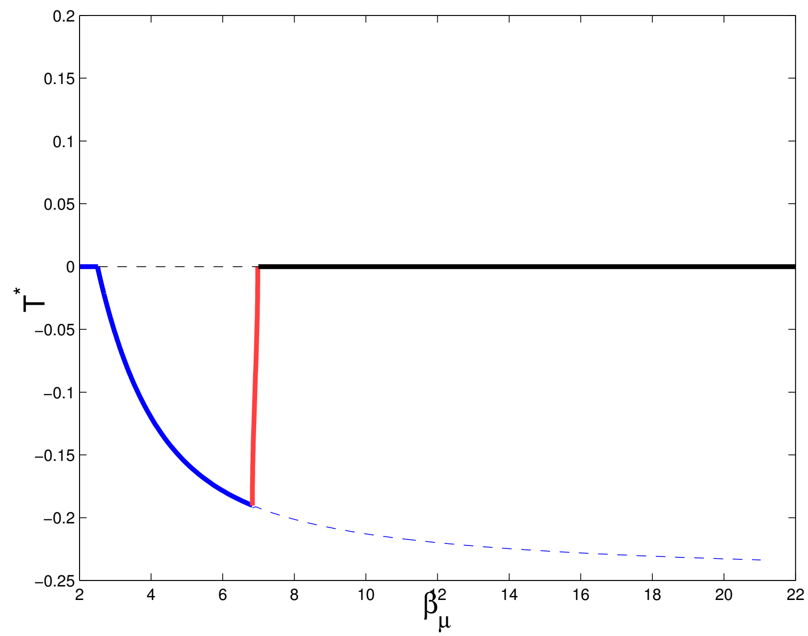
$$\mu = 0.7$$

$$\mathbf{Q}^* = S^*(\mathbf{e}_z \otimes \mathbf{e}_z - \frac{1}{3}\mathbf{I}) \quad \mathbf{B}^* = T'^*(\mathbf{e}_x \otimes \mathbf{e}_x - \mathbf{e}_y \otimes \mathbf{e}_y) \Leftrightarrow T^* = S'^* = 0$$

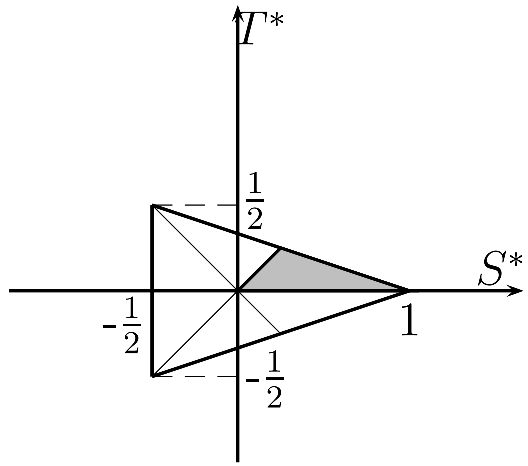
$$\mathbf{Q}^* = -2S^*(\mathbf{e}_x \otimes \mathbf{e}_x - \frac{1}{3}\mathbf{I}) \quad \mathbf{B}^* = -2S'^*(\mathbf{e}_x \otimes \mathbf{e}_x - \frac{1}{3}\mathbf{I}) \Leftrightarrow$$

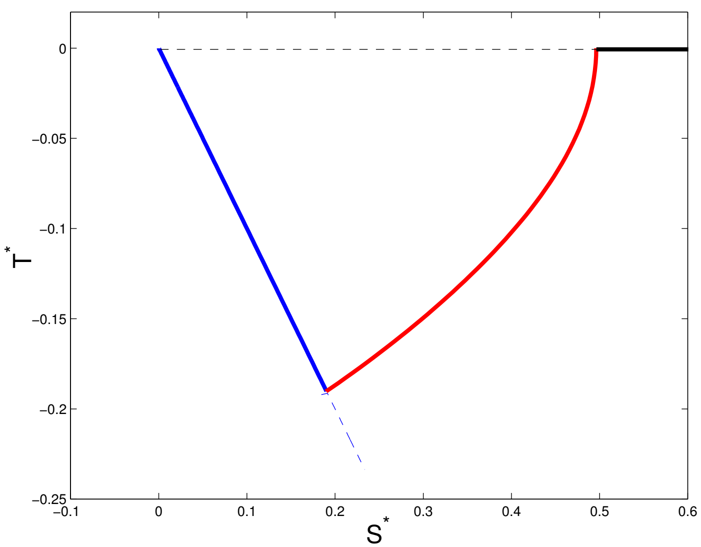
$$S^* = -T^*, S'^* = -T'^*$$

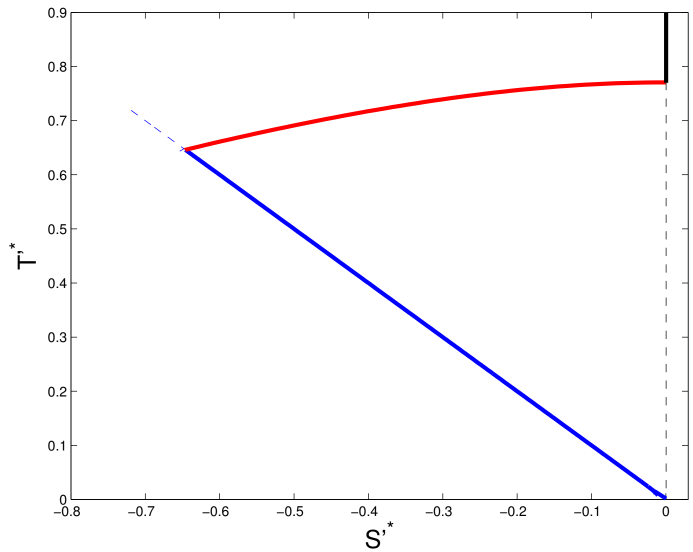




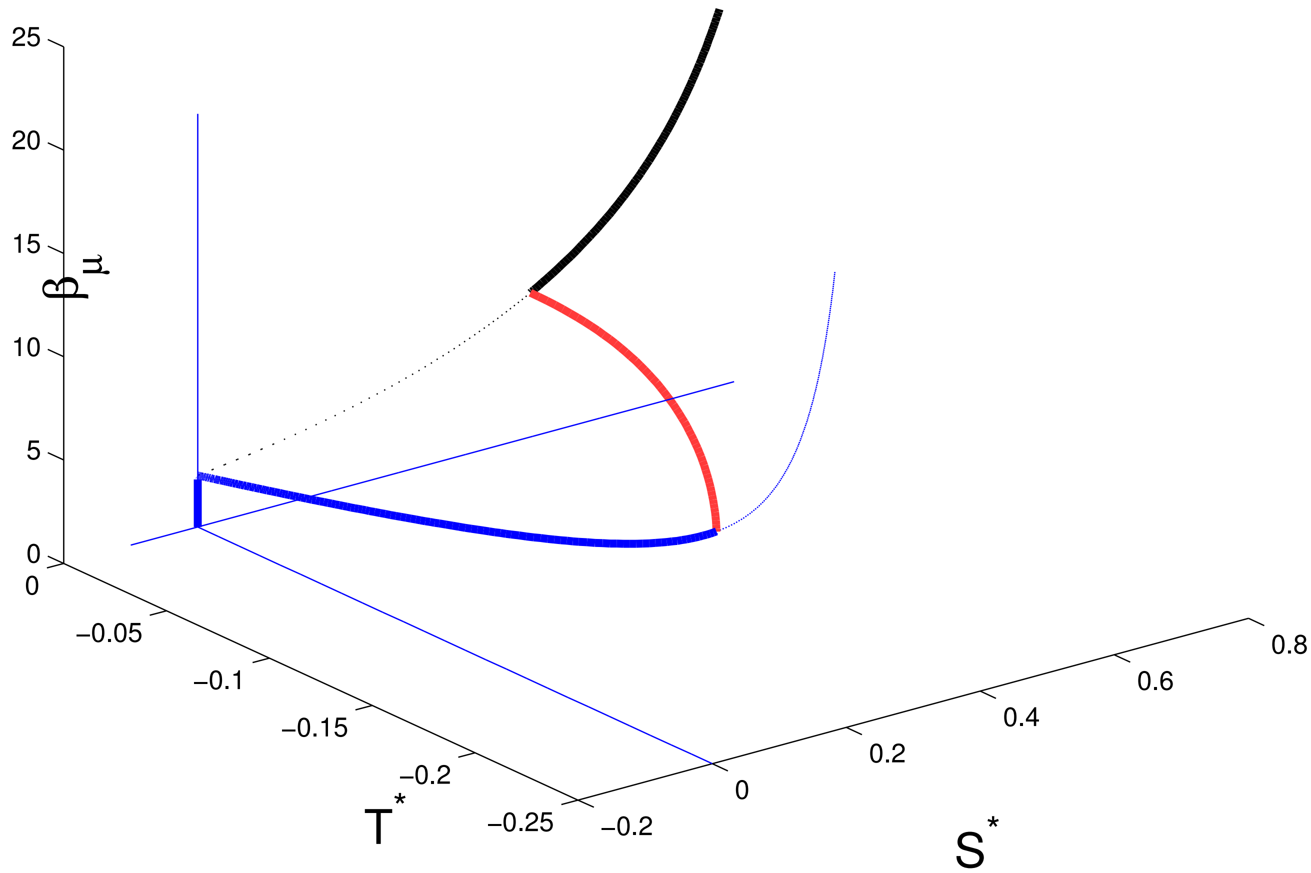
Representation in the order parameters space for $\mu = 0.7$





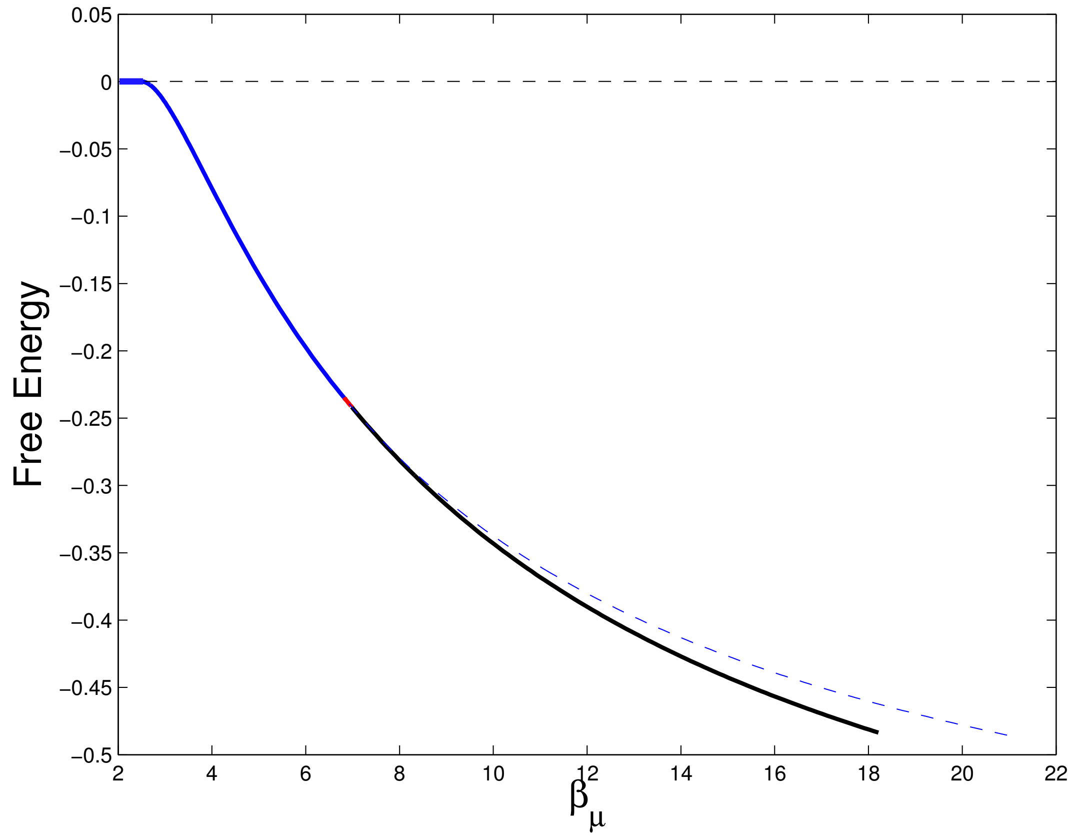


3D representation

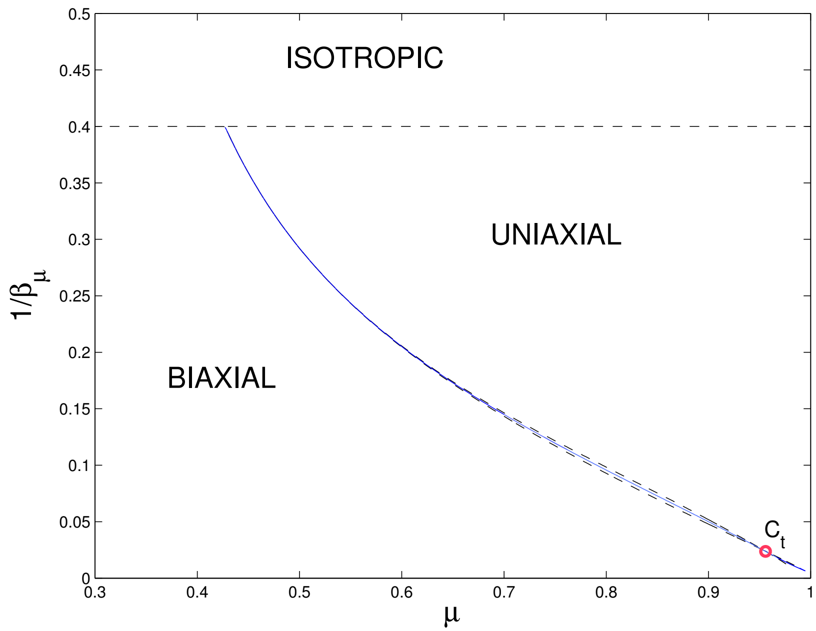


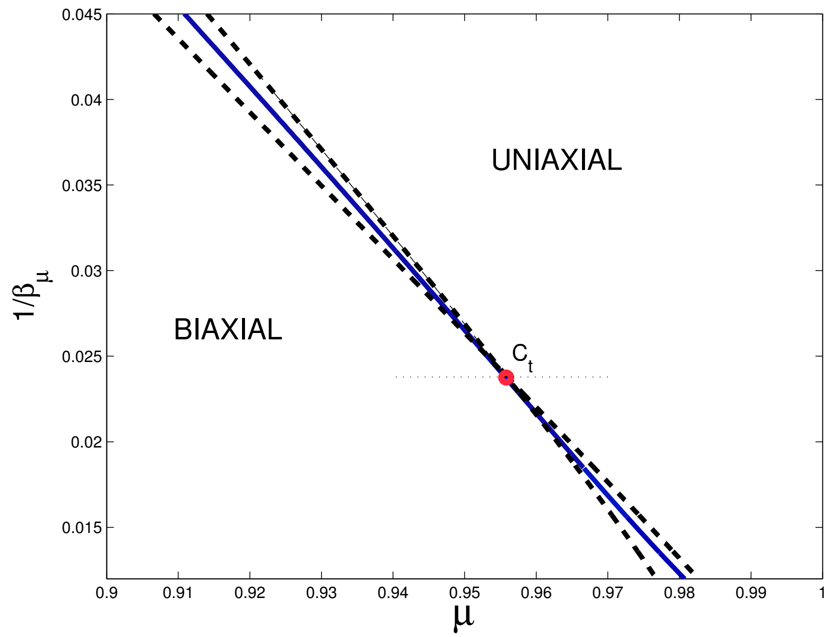
$$\mu = 0.7$$

$$\mathcal{F}_\mu = \left\{ \frac{1}{3} S'^2 + T'^2 - \frac{\mu}{3} S^2 - \mu T^2 - \frac{1}{\beta_\mu} \log \frac{Z_\mu}{8\pi^2} \right\}$$



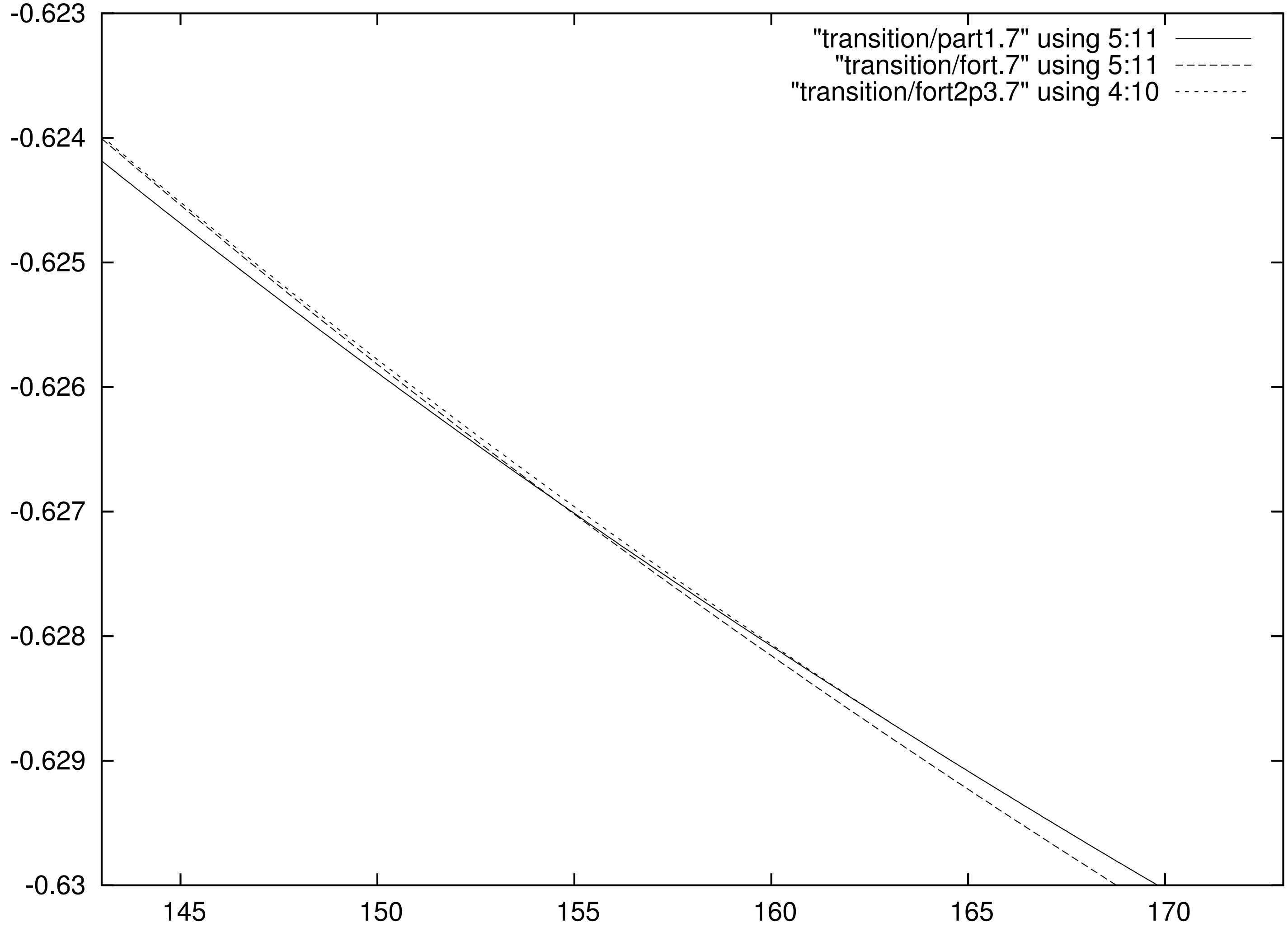
Bifurcation points' path



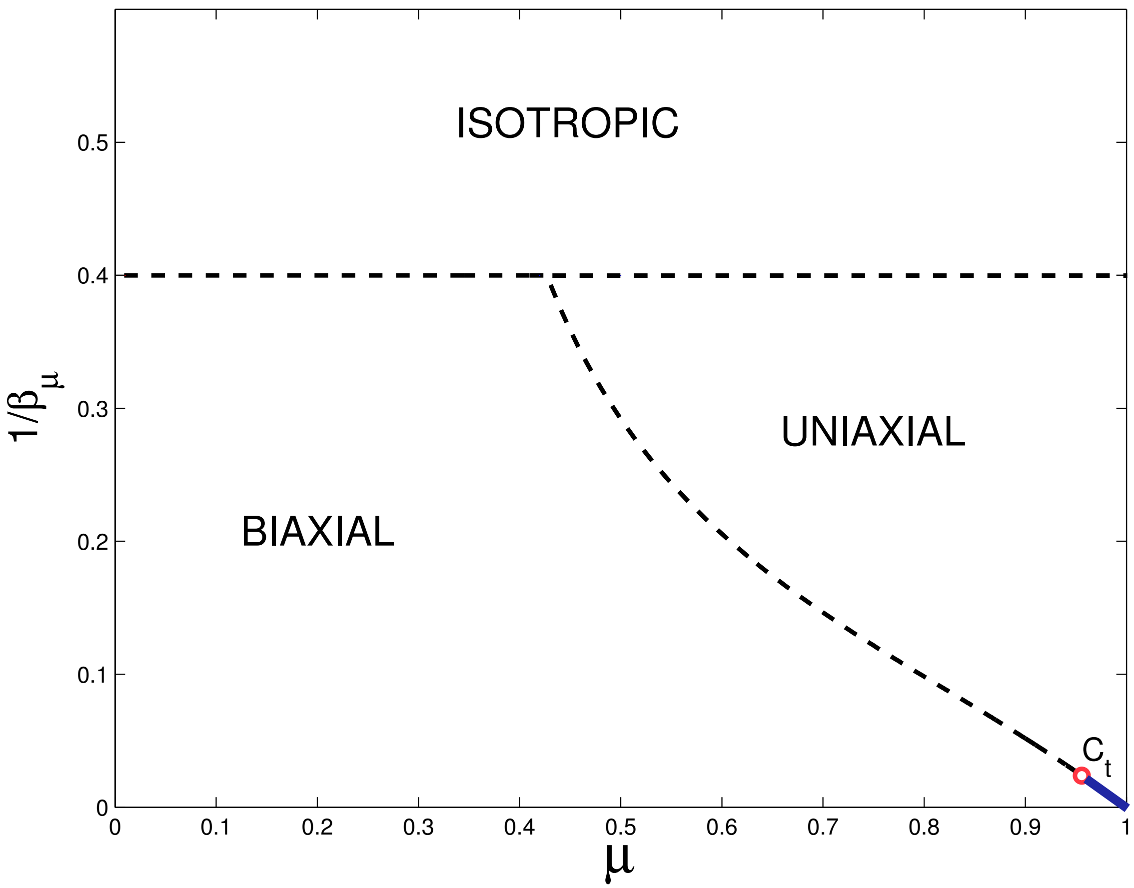


$$C_t\,(0.958, 0.023)$$

$\mu = 0.989 > \mu_t$ Free energy at the transition point

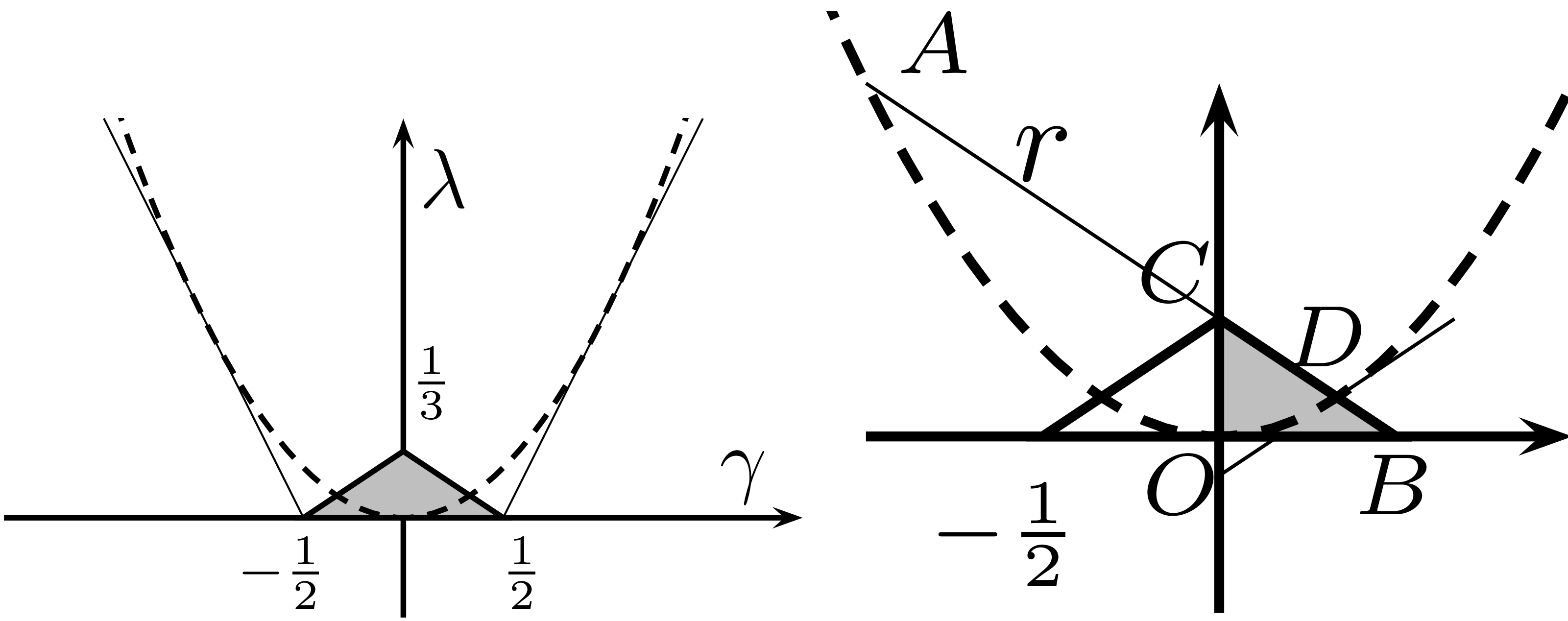


μ−model phase diagram



$$\mu \in [0,1] \Leftrightarrow \overline{BD}$$

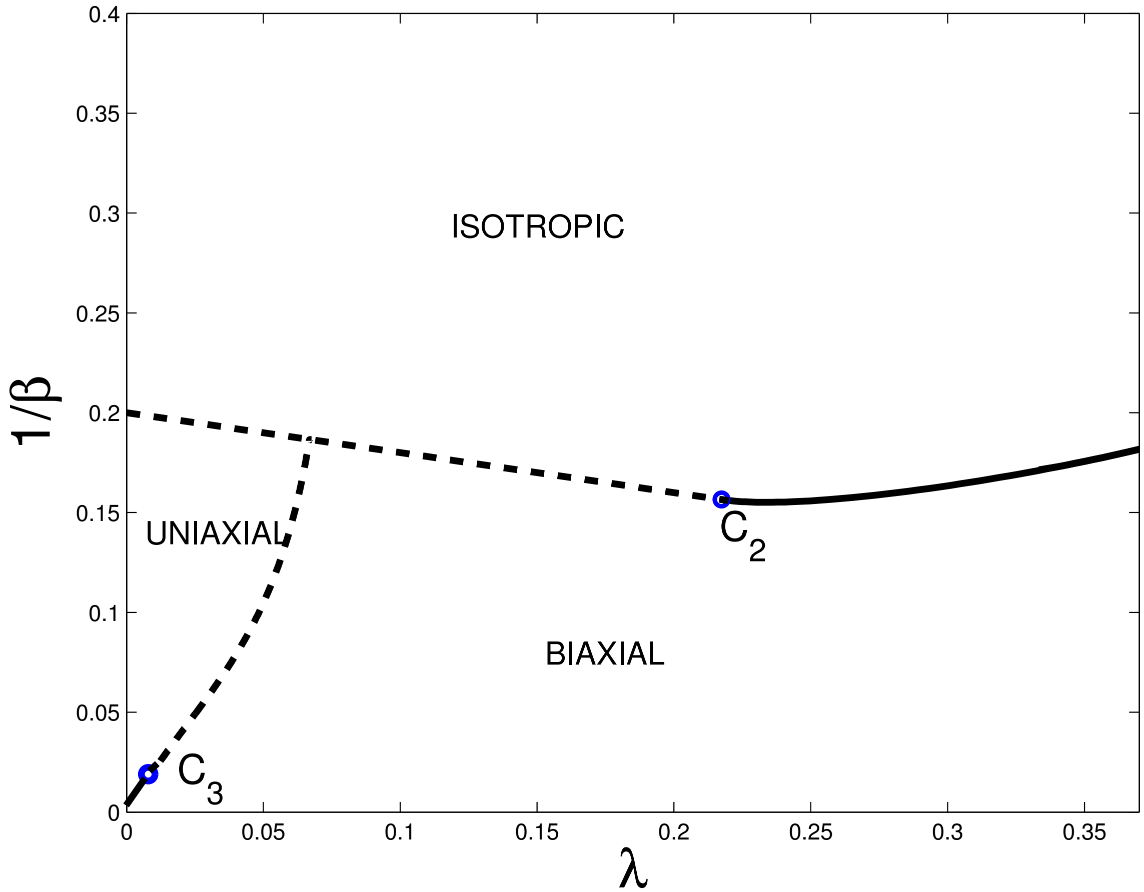
Reference triangle



$$D\left(\frac{1}{3},\frac{1}{9}\right),\quad B\left(\frac{1}{2},0\right),\quad C\left(0,\frac{1}{3}\right),\quad A\,(-1,1)$$

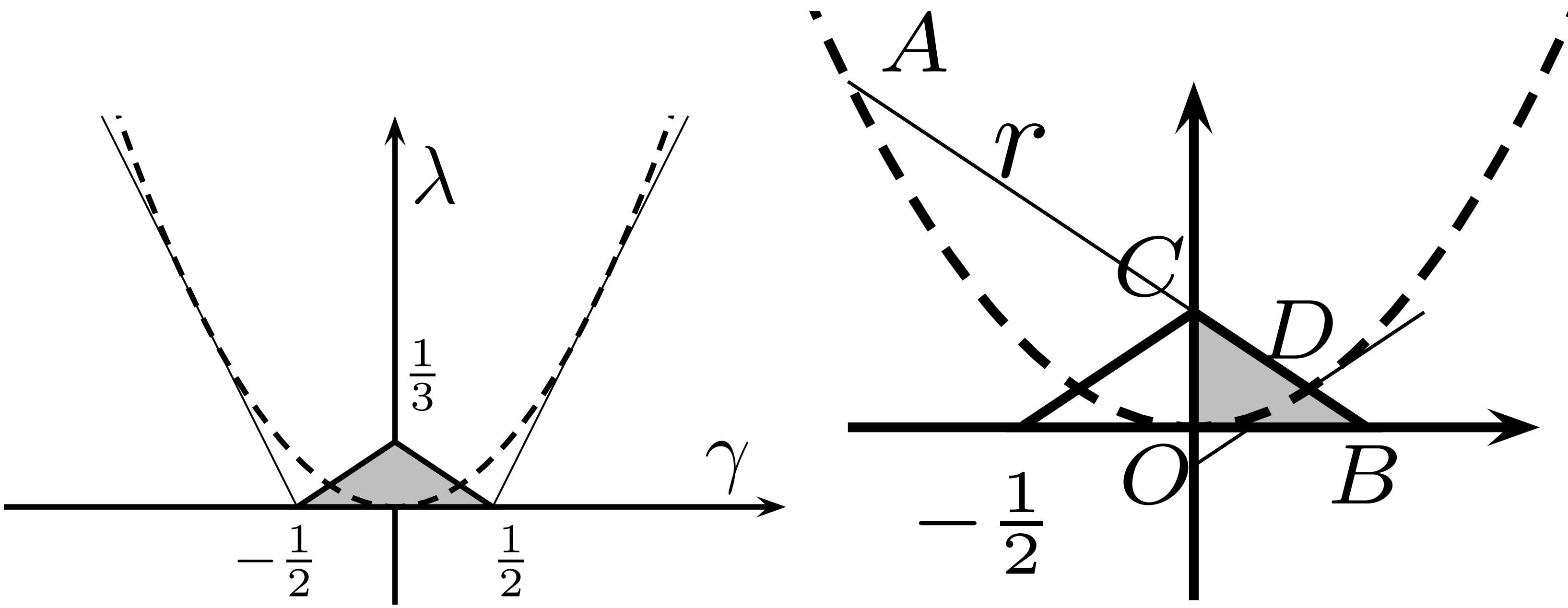
$$r : 2\gamma + 3\lambda - 1 = 0$$

Complete Phase diagram



$$2\gamma = 1 - 3\lambda \quad 0 \leq \lambda \leq \frac{1}{3} \Leftrightarrow \overline{CB}$$

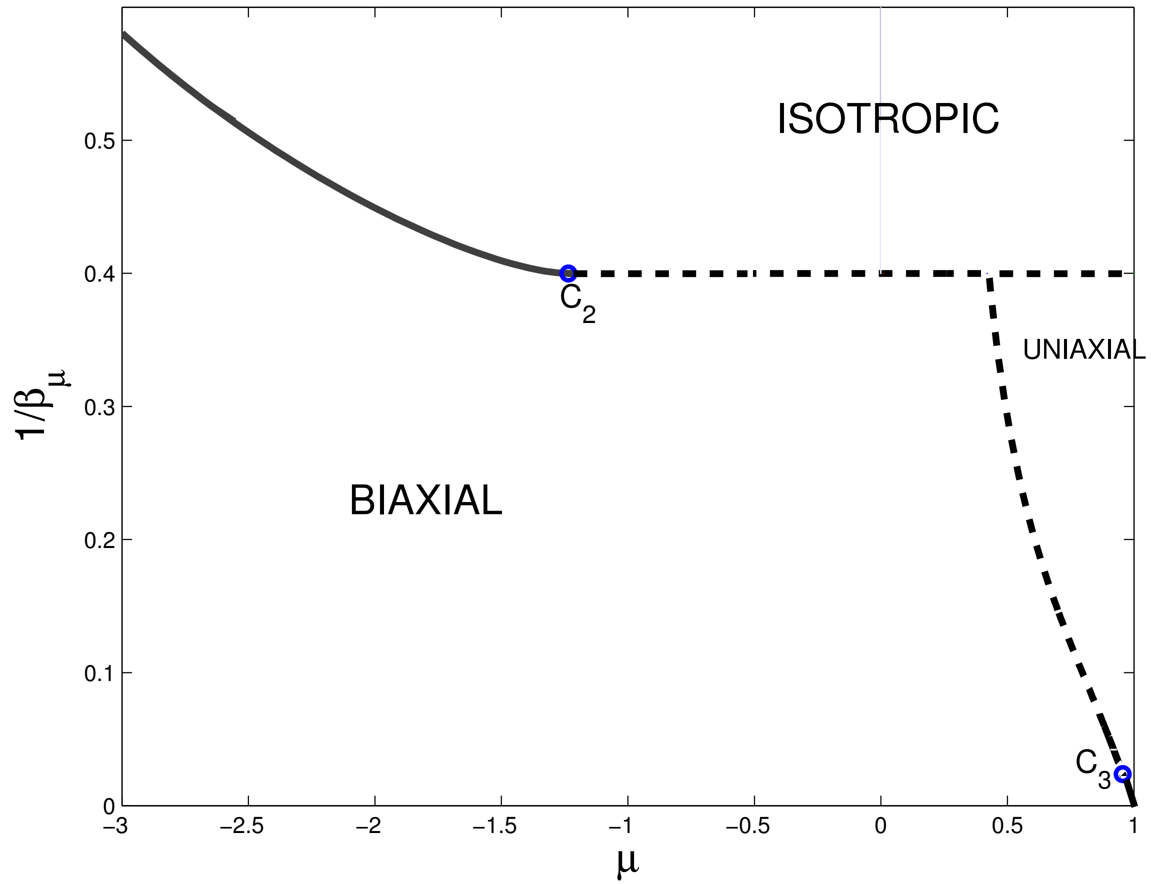
Reference triangle



$$D\left(\frac{1}{3},\frac{1}{9}\right),\quad B\left(\frac{1}{2},0\right),\quad C\left(0,\frac{1}{3}\right),\quad A\left(-1,1\right)$$

$$r : 2\gamma + 3\lambda - 1 = 0$$

Complete Phase diagram: μ−version



Future work

- Bifurcation Analysis inside the reference triangle to identify the generic topology of the phase diagram and to analyse its convergence to $\gamma = 0-$model and $2\gamma = 1 - 3\lambda-$model.
- Numerical continuation of the tricritical points C_2 and C_3

.... and finally I would thank

- my advisor Prof. E. Virga
- Prof. Gartland, Prof. Durand and Prof. S. Romano, Dr. Riccardo Rosso and Dr. Fulvio Bisi for very helpfull conversations