BI-CRITICAL POINTS IN COMPRESSIBLE SOLIDS

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Outline

- Type II Phase Transition
  (*Larkin and Pikin, 1969*)
  - Coupling with deformation
  - Gibbs Free energy
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  - Spinodals
  - The Surface of Free Energy
  - Phase Diagrams
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Type II Phase Transition

Consider a type II Phase Transition at $T = T_c$. Generic Hamiltonian which leads to it, has the form

$$H(\{\eta_i\}) = \sum_i \left(\frac{a}{2}\eta_i^2 + \frac{b}{4}\eta_i^4 \right) + \sum_{ij} V_{ij}(\eta_i - \eta_j)^2 \tag{1}$$

The Helmholtz Free energy $F(T)$ at fixed volume V has a singularity

$$F(T) = F(T_c) - A|T - T_c|^{2-\alpha}, \quad \alpha > 0. \tag{2}$$

Elastic Deformation

Elastic deformation $\mathbf{u}(\mathbf{r})$ has the energy

$$H_{el} = \int d\mathbf{r} \left\{ \lambda \left(\frac{\partial u_\alpha}{\partial r_\alpha} \right)^2 + \mu \left(\frac{\partial u_\alpha}{\partial r_\beta} \right)^2 \right\} \tag{3}$$

Deformation also leads to a shift of critical temperature and parameter a in the Hamiltonian is replaced by

$$a \rightarrow a + q \, \frac{\partial \mathbf{u}}{\partial \mathbf{r}}$$

So,

$$H = \sum_i \left(\frac{a + q \text{ div } \mathbf{u}}{2} \eta_i^2 + \frac{b}{4} \eta_i^4 \right) + \sum_{ij} V_{ij} (\eta_i - \eta_j)^2. \tag{4}$$

Gibbs Free Energy

So, if we want to find now the Gibbs Free Energy $\Phi(T, \sigma_{\alpha\beta})$ at given stress $\hat{\sigma}$, the prescription is simple:

$$\Phi(T, \sigma_{\alpha\beta}) = -T \ln \int \prod_i d\eta_i d\mathbf{u}(\mathbf{r}_i) \exp\left[-\frac{H(\{\eta_i\}) + H_{el} - \sigma_{\alpha\beta} \sum_i \left(\partial u_\alpha / \partial r_i^\beta\right)}{T}\right] \tag{5}$$

For this purpose, represent

$$\frac{\partial u_\alpha(\mathbf{r})}{\partial r_\beta} = u_{\alpha\beta} + \frac{1}{N} \sum_{\mathbf{k}\neq 0} i k_\beta u_\alpha(\mathbf{k}) e^{i\mathbf{k}\mathbf{r}}$$

So, instead of integrations over $\mathbf{u}(\mathbf{r}_i)$ we can integrate over $\mathbf{u}(\mathbf{k})$ and $u_{\alpha\beta}$.

Partition Function

One can see that integration over transverse phonons $\mathbf{ku}(\mathbf{k}) = 0$ and the shear part of deformation tensor

$$u^{(s)}_{\alpha\beta} = u_{\alpha\beta} - \frac{\delta_{\alpha\beta}}{3}\; u_{\gamma\gamma}$$

are reduced to the Gaussian integration.

Integration over longitudinal phonons $\mathbf{ku}(\mathbf{k}) = ku$ results in appearance of the new term

$$\sim q^2 \sum_{\mathbf{k}\neq 0} \sum_{ij} \frac{\eta_i^2 \eta_j^2}{K_0 + 4\mu/3}\; e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)}$$

In order to add the missing term with $\mathbf{k} = 0$, make the substitution

$$u_{\alpha\alpha} = \frac{v}{K_0}\sqrt{\frac{3K_0 + 4\mu}{4\mu}} + \frac{1}{K_0}\left(1 - \sqrt{\frac{4\mu}{3K_0 + 4\mu}}\right) \sum_i \eta_i^2 - \frac{p}{K_0} \quad (6)$$

Partition Function

This results in

$$\Phi = \frac{p^2}{K_0} - T \ln \int dv \exp\left\{-\frac{1}{T}\left[\frac{3K_0+4\mu}{8\mu}\ v^2 + F\left(a + q\frac{v-p}{K_0}, b - \frac{3q^2}{3K_0+4\mu}\right)\right]\right\}$$

Macroscopic limit corresponds to the steepest descent in this integral. Therefore,

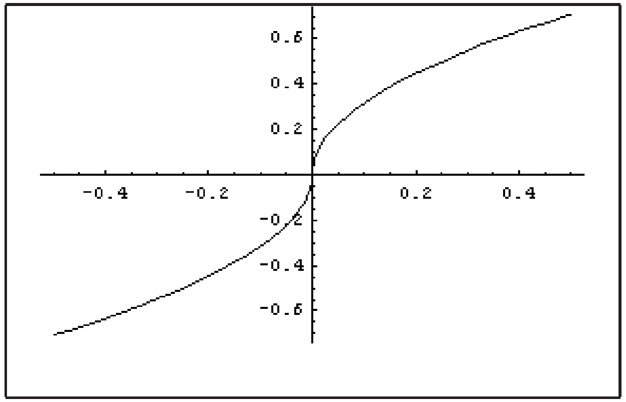
$$\Phi = \frac{p^2}{K_0} + \frac{3K_0+4\mu}{8\mu}\ v^2 + F\left(a + q\frac{v-p}{K_0}, b - \frac{3q^2}{3K_0+4\mu}\right)$$

$$\frac{\partial \Phi}{\partial v} = 0$$

Fold

since $F(a) \propto a^{2-\alpha}$, condition

$$\frac{\partial \Phi}{\partial v} = 0$$

can be presented graphically as 

LP

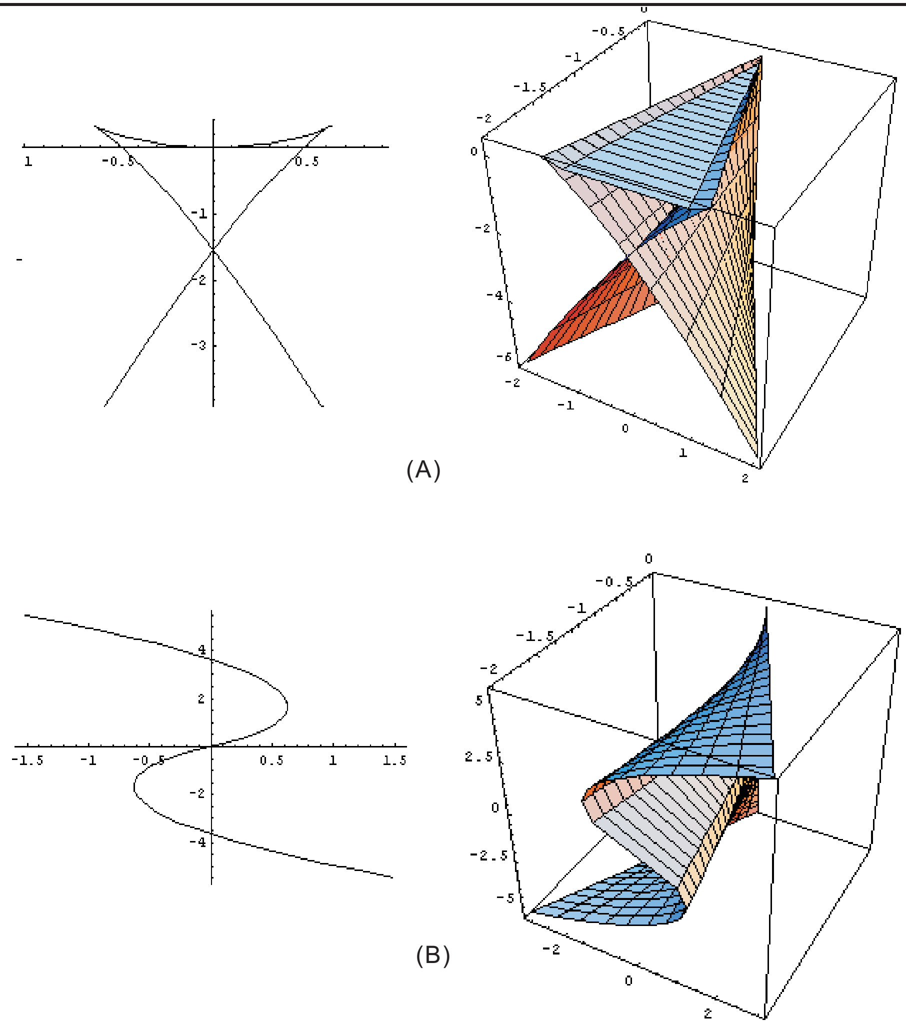
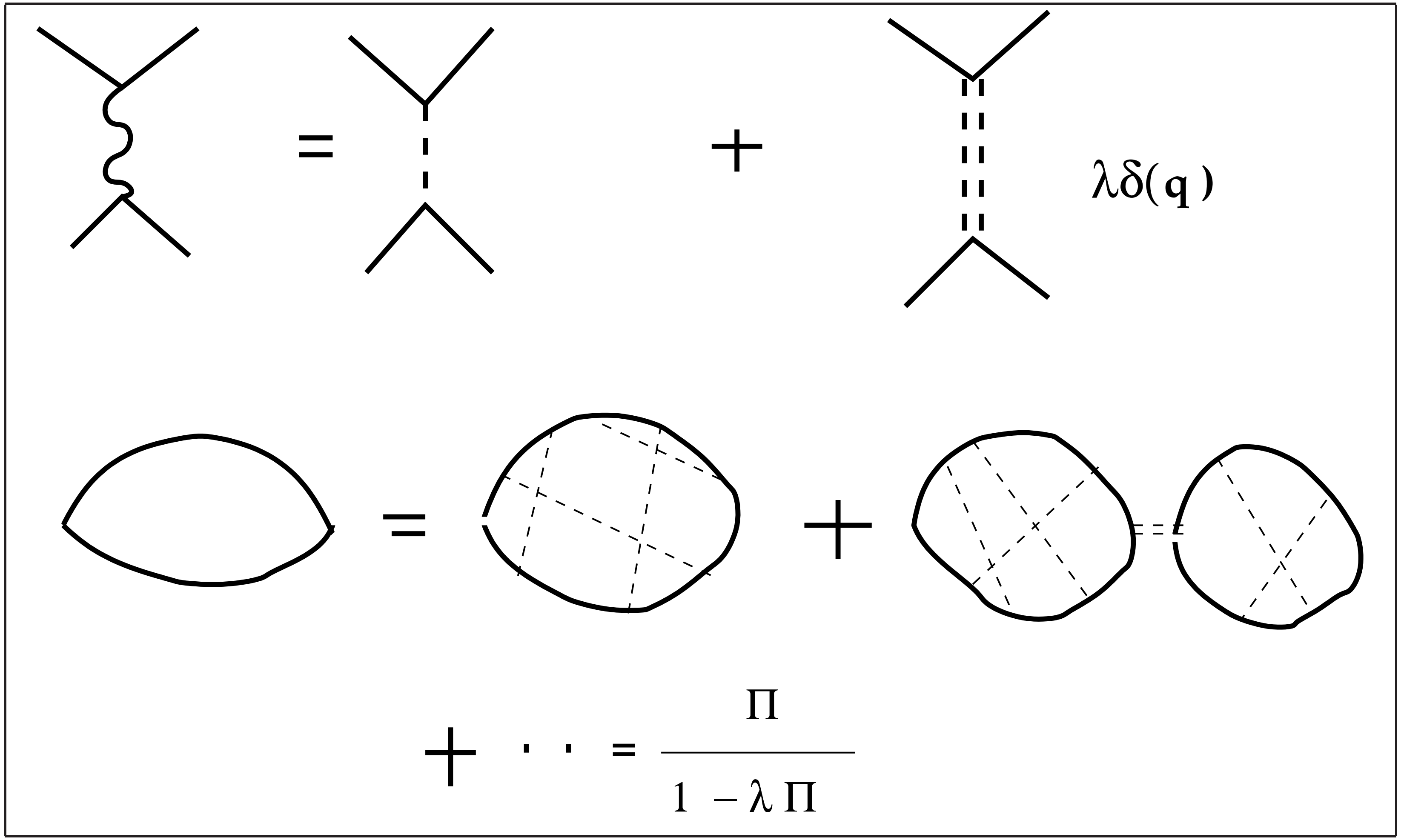
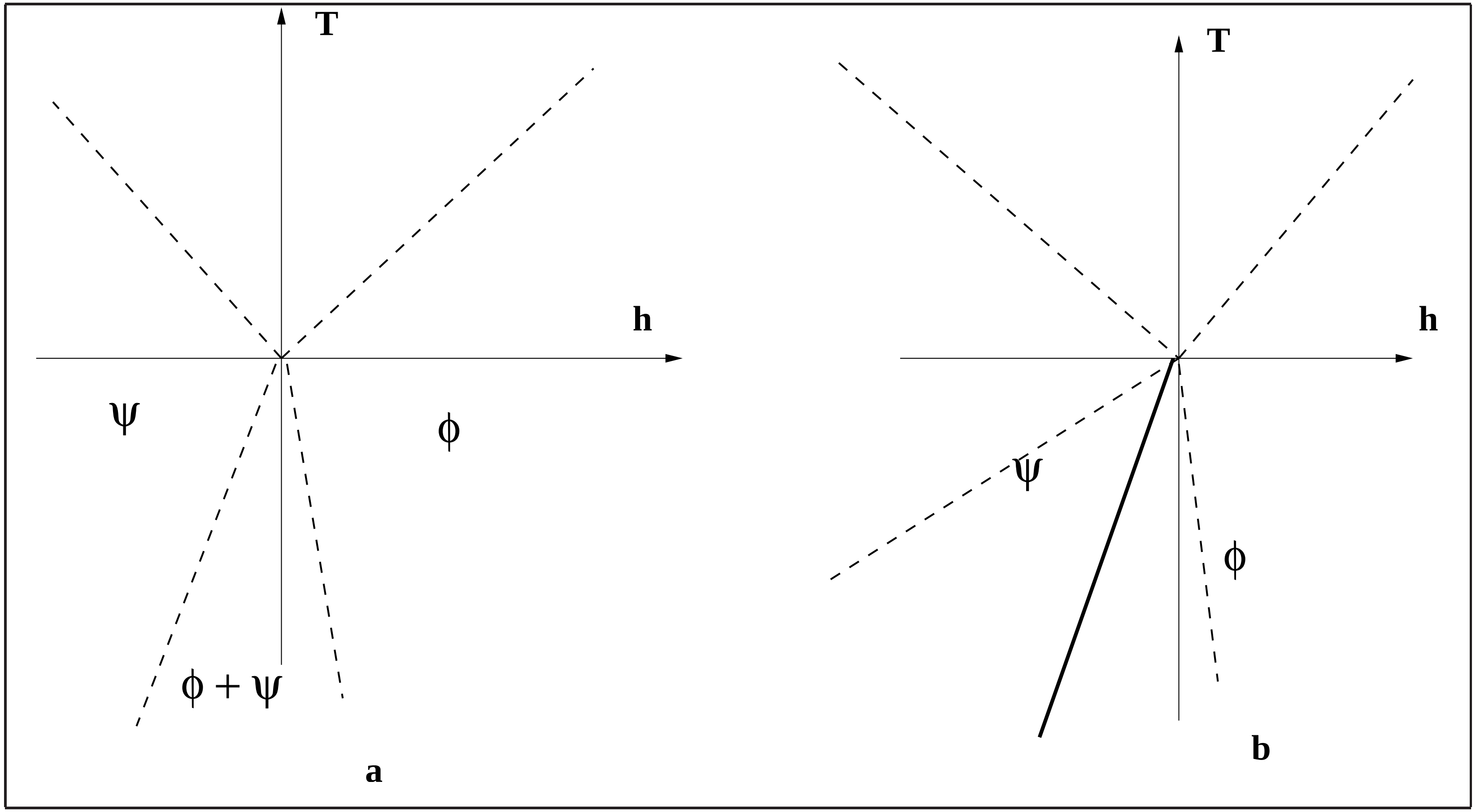


Figure 2

Alternative Explanation



Crossing. Mean Field



$$H = \sum_i \left[a\psi_i^2 + \alpha\phi_i^2 + b\psi_i^4 + \beta\phi_i^4 + \gamma\phi_i^2\psi_i^2 + .. \right]$$

Effect of compressibility

Assume the singularity

$$F(a,\alpha) \propto A|a|^{2-\xi} + B|\alpha|^{2-\zeta} + C|\alpha|^{1-\zeta}|a|^{1-\zeta}$$

Effect of elastic deformation

$$a \to a + q \ \mathrm{div}\mathbf{u}, \qquad \alpha \to \alpha + J \ \mathrm{div}\mathbf{u}$$

All this leads to

$$\Phi = -\frac{p^2}{K_0} + \frac{3K_0 + 4\mu}{8\mu} \ v^2 + F\left(a', \alpha', b', \beta', \gamma'\right)$$

$$\frac{\partial \Phi}{\partial v} = 0$$

where

$$a' = a + q\frac{v-p}{K_0}, \quad \alpha' = \alpha + J\frac{v-p}{K_0}, \quad b' = b - \frac{3q^2}{3K_0 + 4\mu}, \ldots$$

Projection

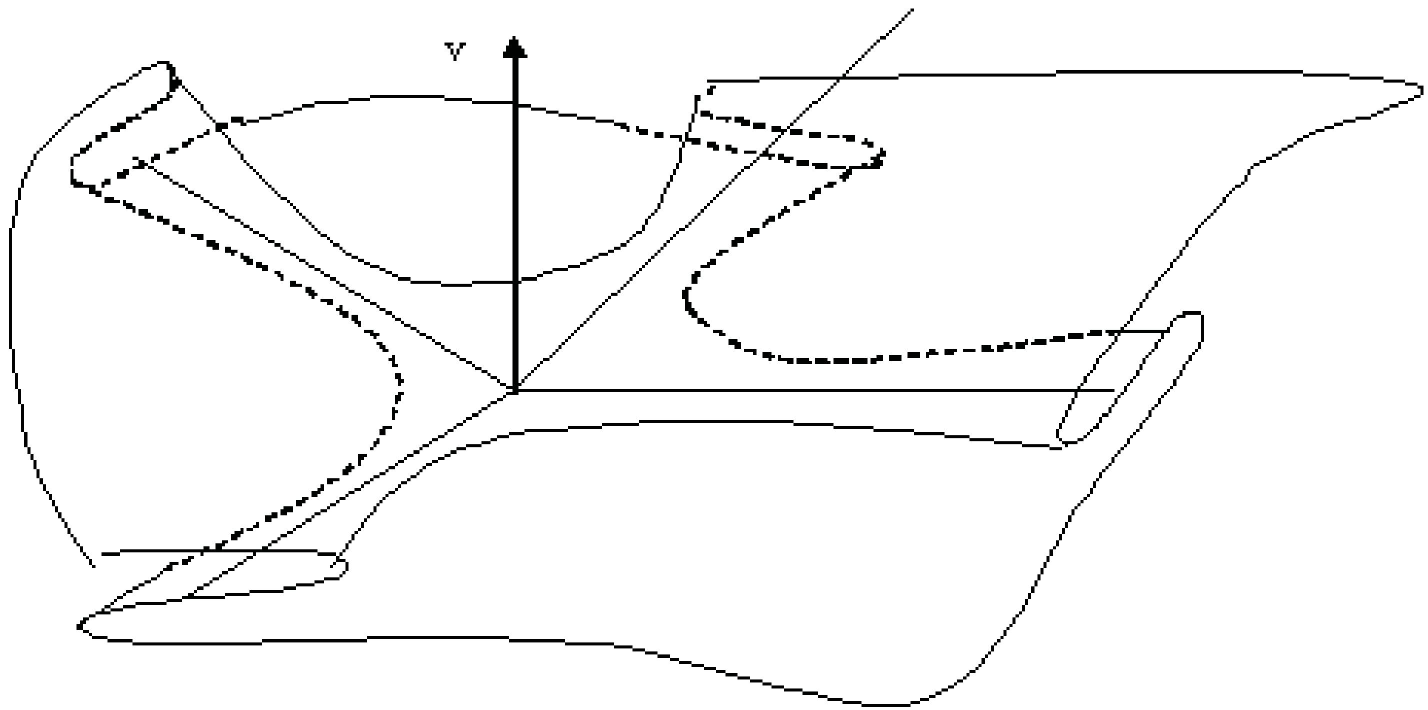
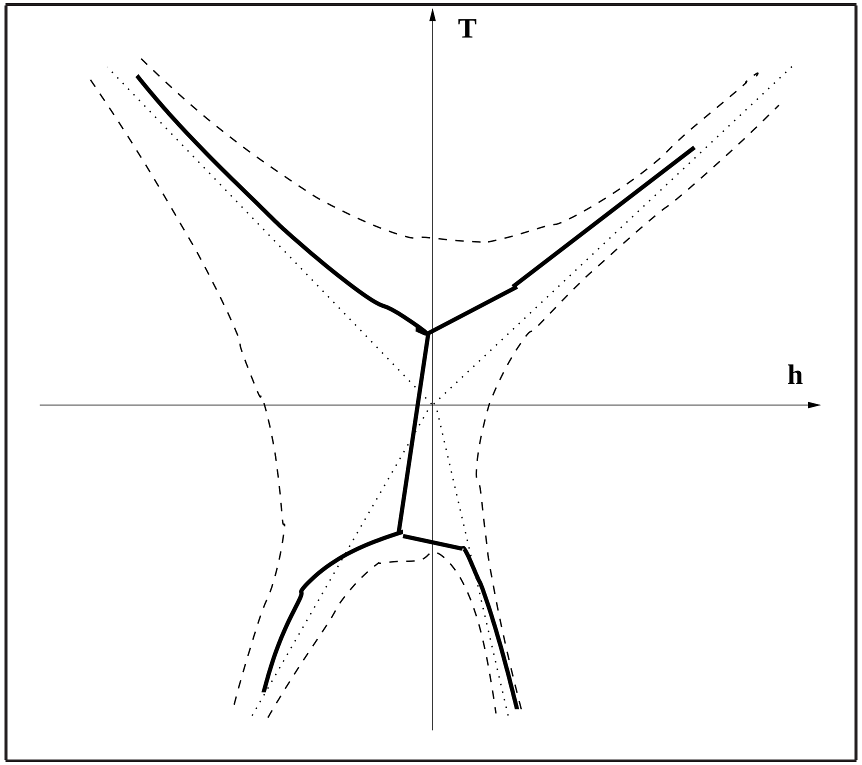
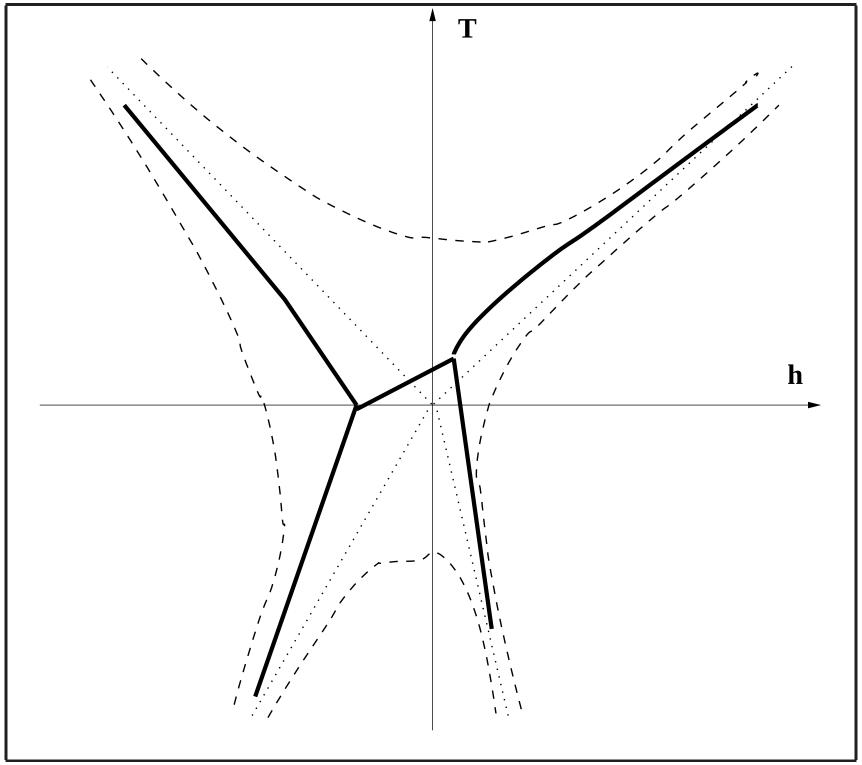


Figure 7

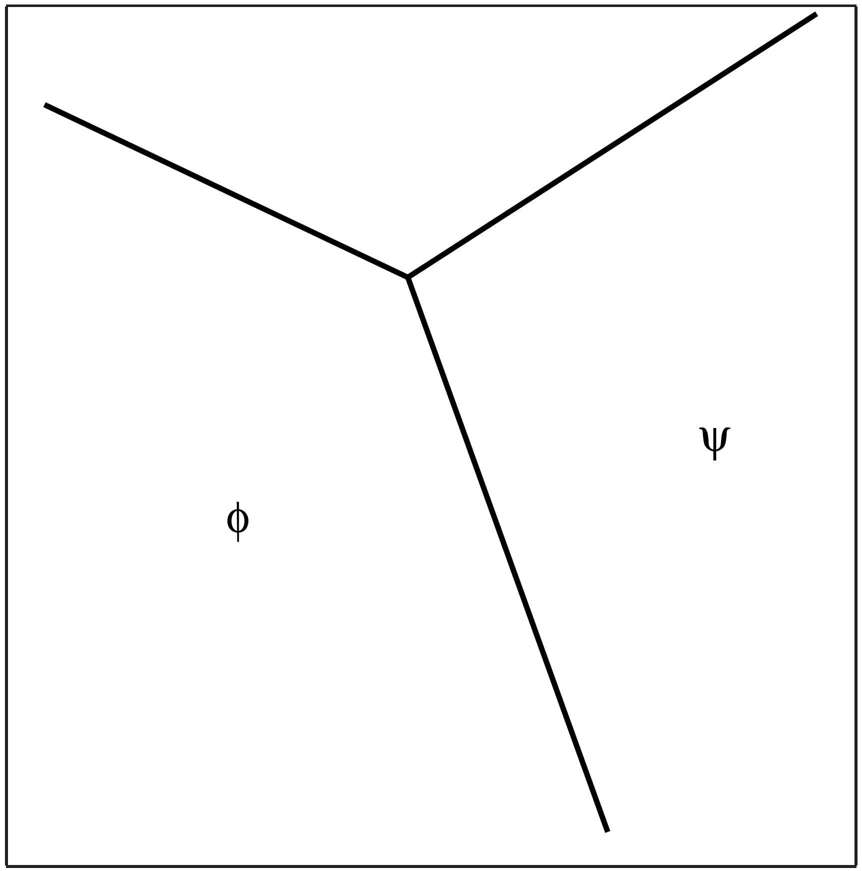
Phase Diagram



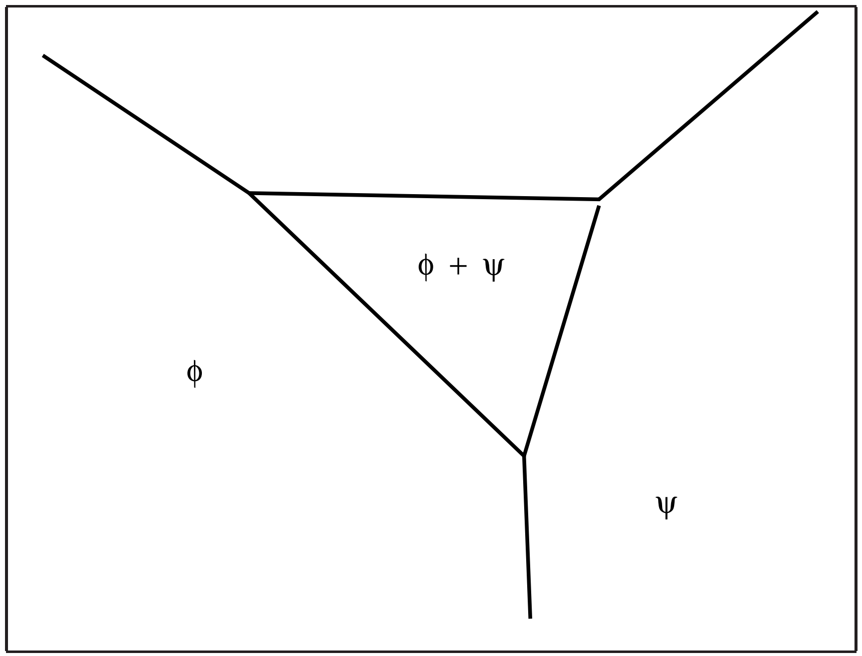
Phase Diagram



Phase Diagram



Phase Diagram



Summary