

Random Copolymer Models

Lattices and Trajectories: A Symposium of Mathematical Chemistry in honour of Ray
Kapral and Stu Whittington, Fields Institute

May 31 - June 2, 2007

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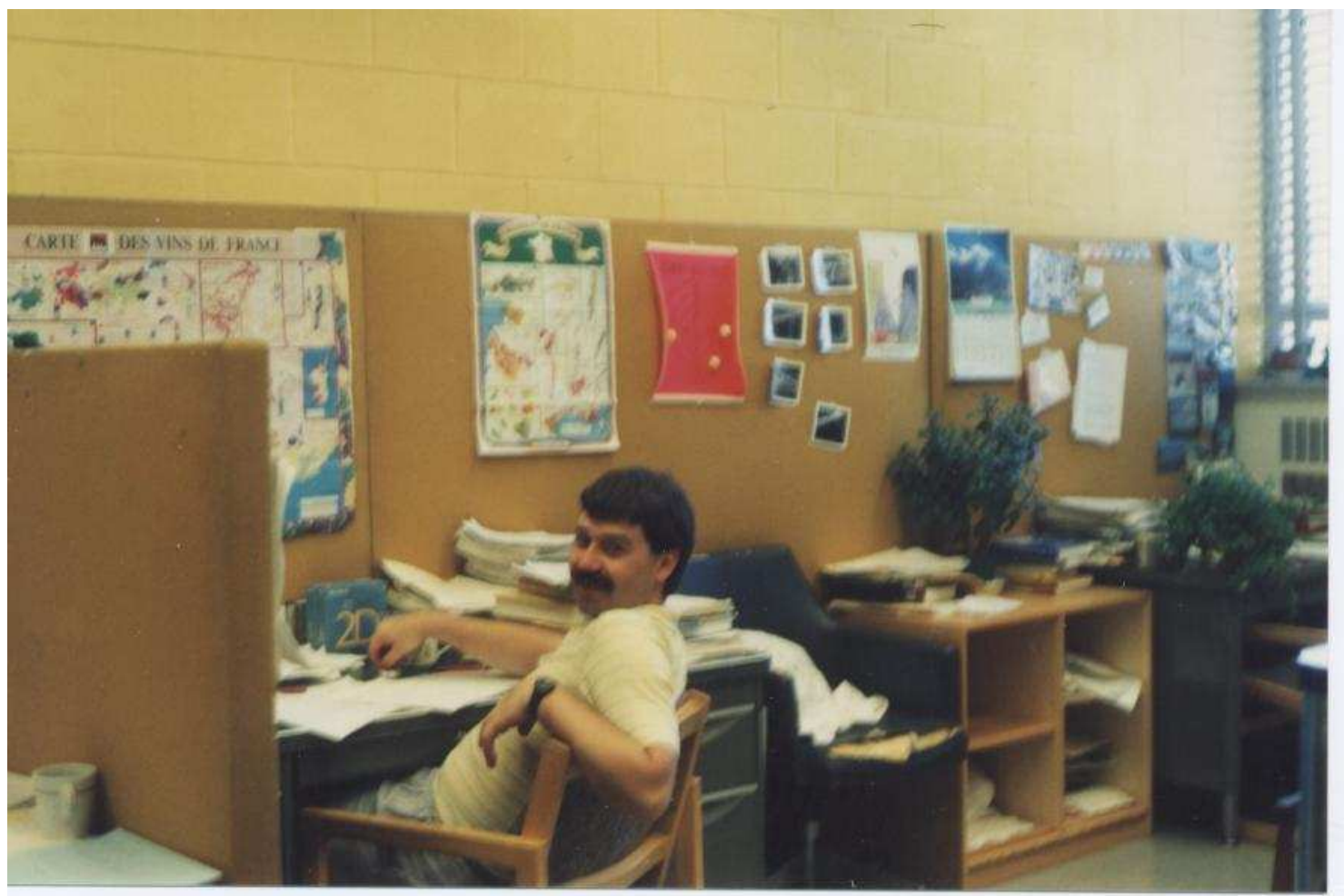
Acknowledgements:

NSERC of Canada ...

It was twenty years before this talk



10th Canadian Symposium on Theoretical Chemistry, Banff 1989

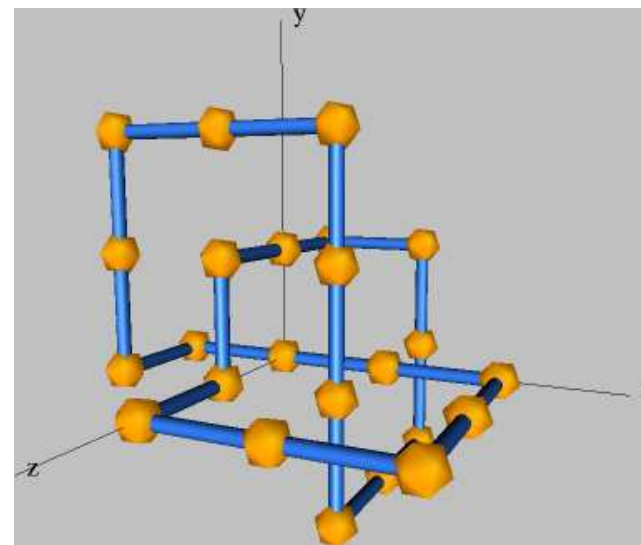


Ivan L'Heureux, Rm 402, Lash Miller circa 1987

Stu taught me about self-avoiding walk ...



MATH/CHEM/COMP 1991 - June 24-29, Dubrovnik



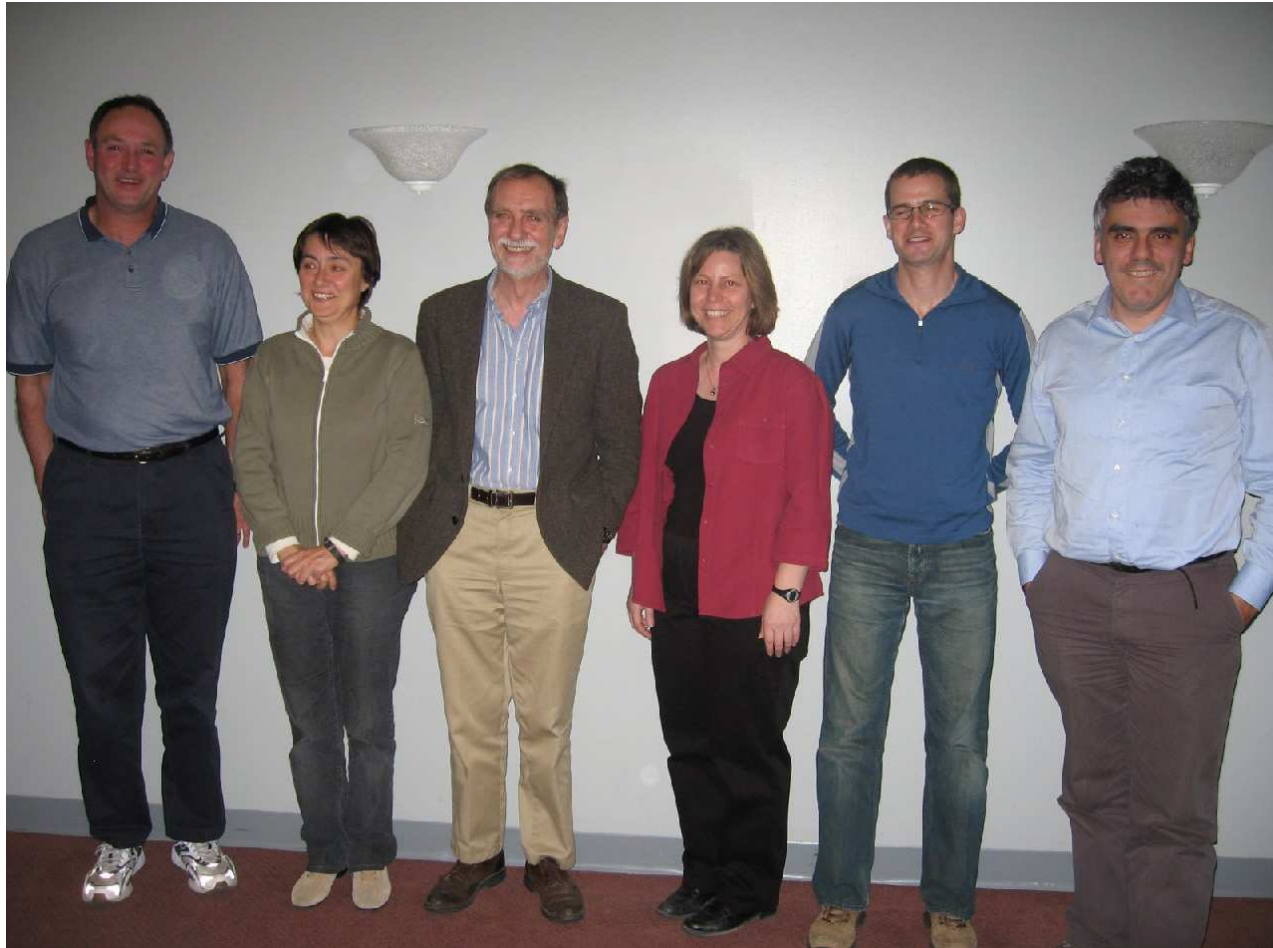
Self-avoiding polygon

CPTG always stays in style, and never fails to raise a smile ...



THANKS RAY, STU AND THE CHEMICAL PHYSICS THEORY GROUP

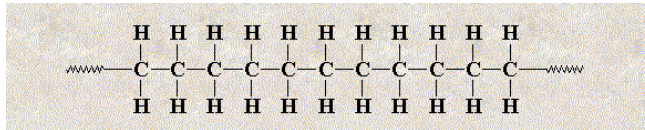
We're Stu's Self-Avoiding Walk Club Band



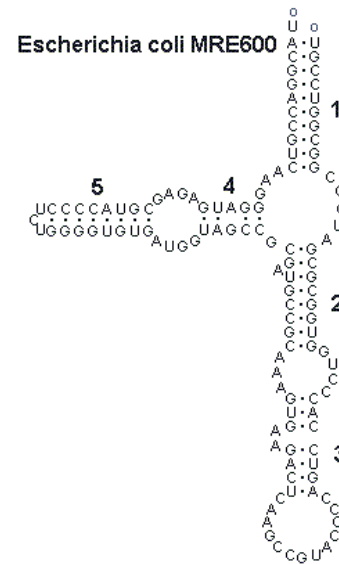
THANKS STU!

Introduction to Random Copolymers

Polymer: Large molecule made of repeated molecular units called *monomers*; if there is more than one type of monomer *Copolymer*



homopolymer - polyethylene

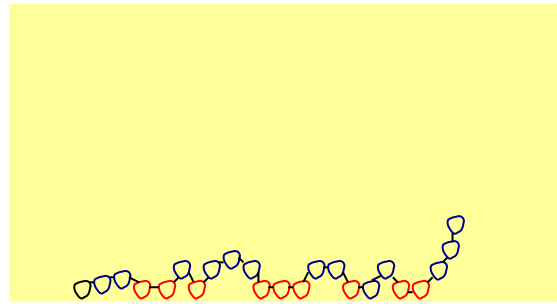


copolymer - RNA

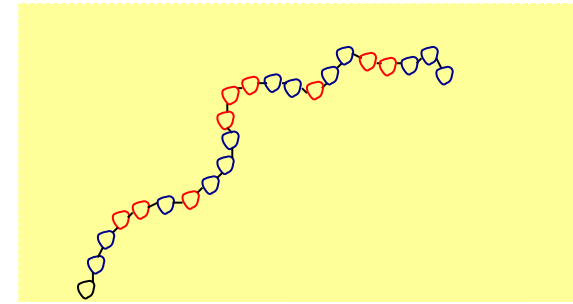
Random Copolymer: the sequence of monomers making up the polymer is determined by a random process

Random Copolymer Phase Transitions

Adsorption

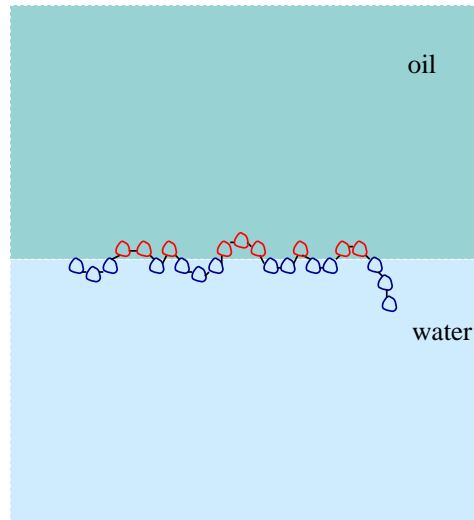


Low T - *Adsorbed*

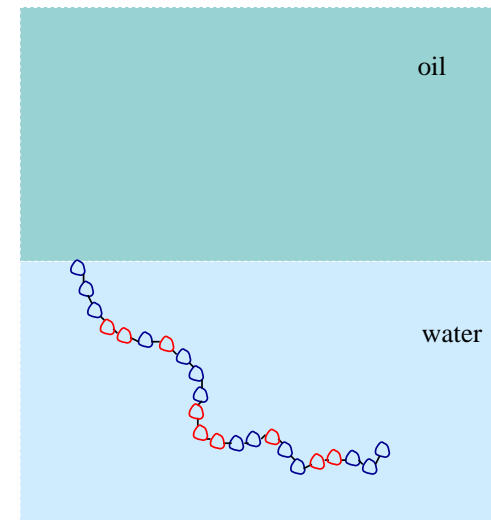


High T - *Desorbed*

Localization



Low T - *Localized*

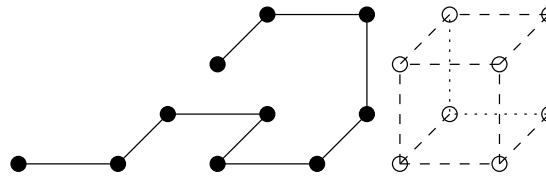


High T - *Delocalized*

Ingredients for Modelling a Random Copolymer System

A Model for the Polymer's Conformational Freedom:

Assume the polymer's conformation is represented by a self-avoiding walk on a lattice (e.g. \mathbb{Z}^3); dilute solution (hence polymer-polymer interactions can be ignored); assume at **equilibrium** and conformations of size n (number of monomers) with same energy are equally likely



A Model for the Comonomer Distribution:

Simplest Case: Two types of monomers A and B and the comonomer sequence is determined by a random

"colouring"	$\chi = \chi_1, \chi_2, \chi_3, \dots, \chi_n$	a sequence of i.i.d. r.v.'s such that
with prob. p	$\chi_i = 1$	indicating i th vertex monomer type A
with prob. $1 - p$	$\chi_i = 0$	indicating i th vertex monomer type B

$$\text{Prob}(\chi) = \pi(\chi) = p^{\sum_i \chi_i} (1 - p)^{n - \sum_i \chi_i}$$

System State: (χ, ω)

ω - n -step self-avoiding walk ; χ - a particular colouring.

Putting the Ingredients Together

Quenched Randomness: The sequence of monomers is determined by a random process but, once determined, it is then fixed.

Monomer sequence determined in or by the polymerization process; sequence can't then change without some chemical reaction occurring.

$$\rho^q(\omega, \chi) = \pi(\chi) \frac{e^{-\beta E(\omega|\chi)}}{Z_n(\beta|\chi)} \quad ; \quad Z_n(\beta|\chi) = \sum_{\omega} e^{-\beta E(\omega|\chi)} \quad ; \quad \beta = 1/k_B T$$

Quenched average free energy: $\bar{\kappa}_n(\beta) = n^{-1} \sum_{\chi} \pi(\chi) \log Z_n(\beta|\chi)$

Phase Transition: Corresponds to a point of non-analyticity of the limiting quenched average free energy $\bar{\kappa}(\beta) = \lim_{n \rightarrow \infty} \bar{\kappa}_n(\beta)$.

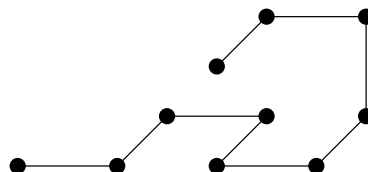
Annealed Randomness: The sequence of monomers is not fixed for a particular polymer molecular but rather changes randomly along with the polymer's conformation.

Not usually applicable to random copolymers but useful for approximations.

$$\rho^a(\omega, \chi) = \frac{\pi(\chi) e^{-\beta E(\omega|\chi)}}{\sum_{\chi} \pi(\chi) Z_n(\beta|\chi)}$$

Annealed average free energy: $\kappa_n^a(\beta) = n^{-1} \log \sum_{\chi} \pi(\chi) Z_n(\beta|\chi) \geq \bar{\kappa}_n(\beta)$

Properties of Self-avoiding Walks (SAWs)



c_n : the number of n -step SAWs starting at the origin

Square Lattice ($d = 2$): $c_1 = 4$, $c_2 = 12$, $c_3 = 36$, $c_4 = 3c_3 - 8 = 100$

$$c_{71} = 4190893020903935054619120005916 \sim 4 \times 10^{30} \ (d = 2)$$

Jensen www.ms.unimelb.edu.au/~iwan/saw/series/sqsaw.ser

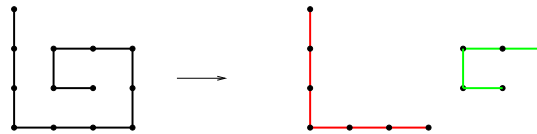
$$c_{30} = 270569905525454674614 \sim 2 \times 10^{20} \text{ (} d = 3 \text{)}$$

Clisby *et al* www.math.ubc.ca/~slade/se.pdf

Properties of Self-avoiding Walks (SAWs) Cont'd

$$d^n \leq c_n \leq 2d(2d-1)^{n-1}$$

Standard Subadditivity Argument



$$\boxed{c_{n+m} \leq c_n c_m \quad ; \quad c_n \geq 1} \quad \Rightarrow \quad \boxed{\lim_{n \rightarrow \infty} n^{-1} \log c_n \equiv \log \mu = \kappa_d}$$

(Hammersley Proc.Camb.Phil.Soc. **53** (1957), 642–5)

$$d \leq \mu \leq 2d - 1$$

$$\mu = 2.63815853031(3) \quad (d = 2) \qquad \mu = 4.684043(12) \quad (d = 3)$$

(Jensen JPA **36** (2003) 5731–45)

(Clisby *et al* (2007))

Homopolymer Adsorption of SAWs

$c_n(v)$: number of n -edge saws in \mathbb{Z}^d starting at origin and with v returns to the surface

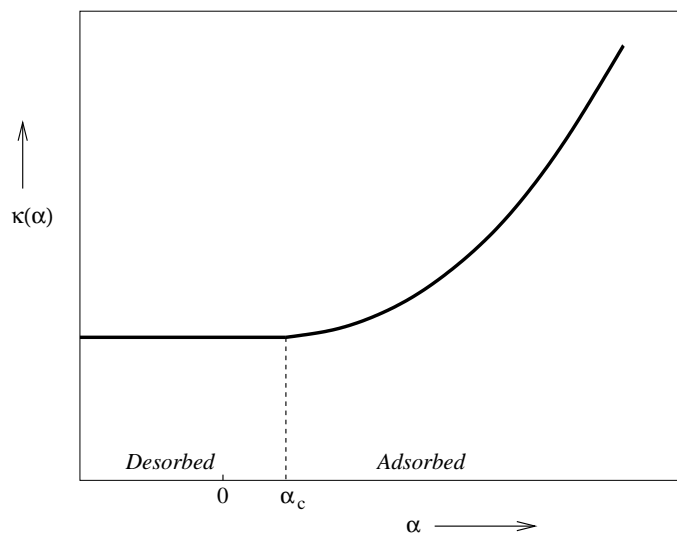
$$Z_n^{(d)}(\alpha) = \sum_{v=0}^n c_n(v) e^{\alpha v}$$

Hammersley, Torrie and Whittington (1982) JPA **15** 539

$$\boxed{\lim_{n \rightarrow \infty} n^{-1} \log Z_n(\alpha) \equiv \kappa(\alpha)} \text{ exists for all } \alpha \text{ and}$$

$$\max\{\kappa_d, \kappa_{d-1} + \alpha\} \leq \kappa(\alpha) \leq \max\{\kappa_d, \kappa_d + \alpha\}$$

\Rightarrow adsorption phase transition exists and $0 < \alpha_c \leq \kappa_d - \kappa_{d-1}$

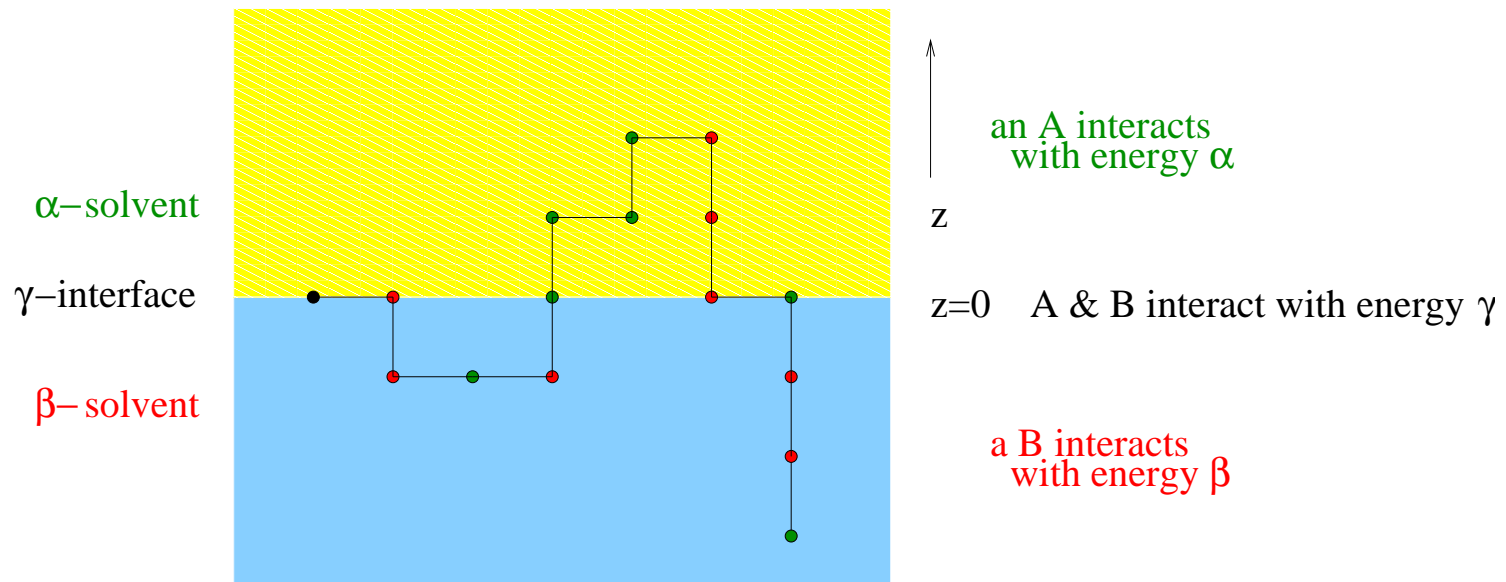


A Self-Avoiding Walk Model for Random Copolymer Localization

$c_n(v_A, v_B, w|\chi)$: given χ , number of SAWs starting at origin with

v_A A 's in $z > 0$, v_B B 's in $z < 0$, w vertices in $z = 0$.

Energy at Fixed χ :
$$-[1/(kT)]E(\omega|\chi) = \alpha v_A + \beta v_B + \gamma w$$



$w = 4$, $v_A = 3$ (green= $A=1$), $v_B = 4$ (red= $B=0$)

$\chi = 0, 0, 1, 0, 1, 1, 1, 1, 0, 0, 0, 1, 0, 0, 1$

Partition Function at Fixed χ :

$$Z_n(\alpha, \beta, \gamma|\chi) = \sum_{v_A, v_B, w} c_n(v_A, v_B, w|\chi) e^{\alpha v_A + \beta v_B + \gamma w}$$

Annealed average free energy:

$$\kappa_n^a(\alpha, \beta, \gamma) = n^{-1} \log \sum_{\chi} \pi(\chi) Z_n(\alpha, \beta, \gamma|\chi)$$

Intensive free energy at Fixed χ

$$\kappa_n(\alpha, \beta, \gamma|\chi) = n^{-1} \log Z_n(\alpha, \beta, \gamma|\chi)$$

Quenched average free energy:

$$\langle \kappa_n(\alpha, \beta, \gamma|\chi) \rangle = n^{-1} \sum_{\chi} \pi(\chi) \log Z_n(\alpha, \beta, \gamma|\chi) \leq \kappa_n^a(\alpha, \beta, \gamma)$$

$$\pi(\chi) = p^{\sum_i \chi_i} (1-p)^{n-\sum_i \chi_i}$$

Limiting Quenched average free energy:

$$\bar{\kappa}(\alpha, \beta, \gamma) = \lim_{n \rightarrow \infty} \langle \kappa_n(\alpha, \beta, \gamma|\chi) \rangle$$

Phase Transition: Corresponds to a point of non-analyticity of the limiting quenched average free energy $\bar{\kappa}(\alpha, \beta, \gamma)$.

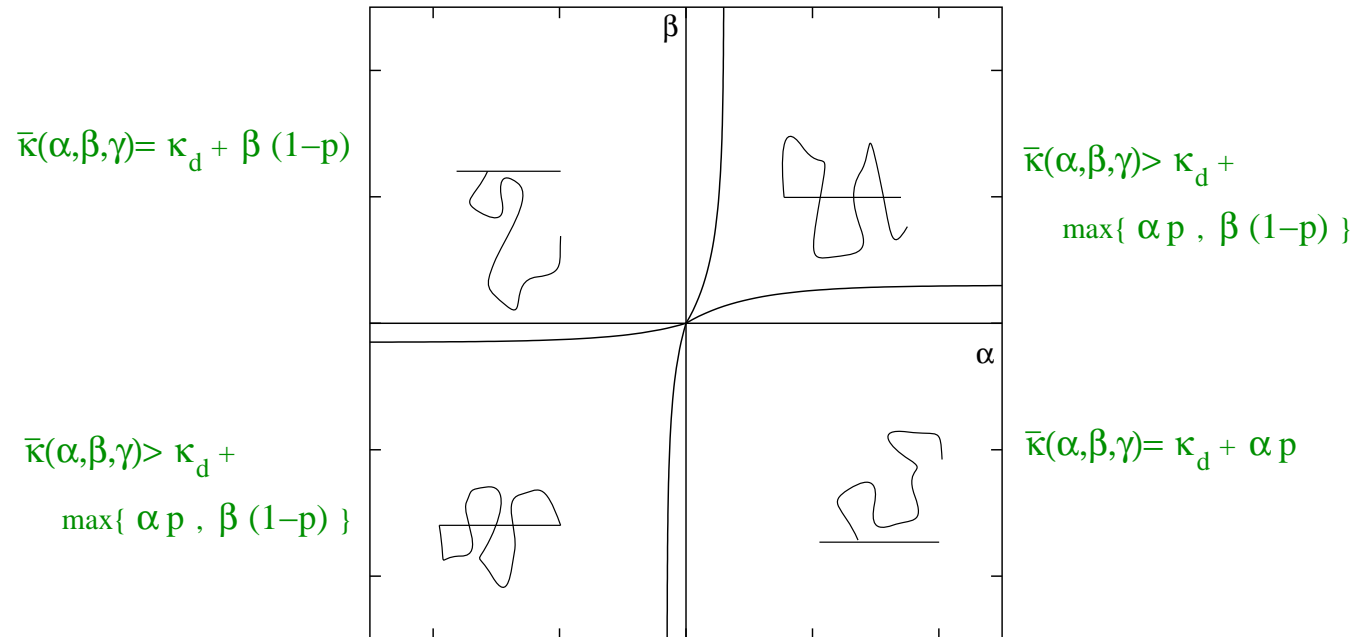
Some Rigorous Results for the SAW Model

The Limiting Quenched average free energy $\bar{\kappa}(\alpha, \beta, \gamma)$ exists and is convex, continuous, and non-decreasing (Martin *et al* JPA **33** (2000) 7903–18) and (Madras/Whittington JPA **36** (2003) 923–38).

$$Z_n(\alpha, \beta, \gamma | \chi) = \sum_{v_A, v_B, w} c_n(v_A, v_B, w | \chi) e^{\alpha v_A + \beta v_B + \gamma w}$$

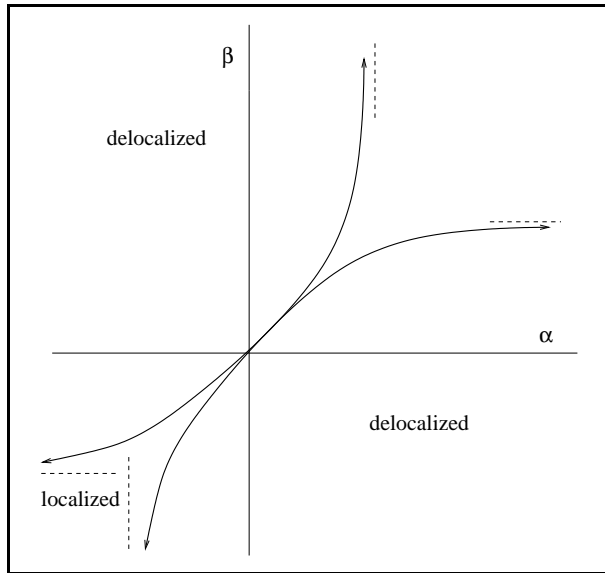
$$\Rightarrow \bar{\kappa}(0, 0, 0) = \lim_{n \rightarrow \infty} n^{-1} \log c_n = \kappa_d$$

Expected Phase Diagram for fixed $\gamma \leq 0$

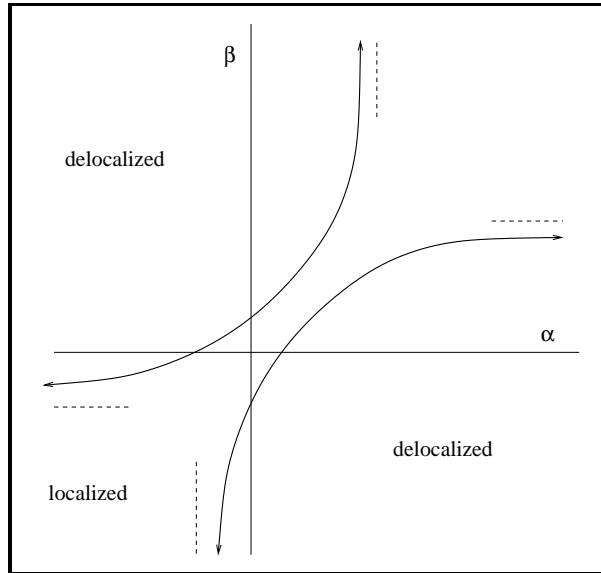


$p = 1/2$ (Martin *et al* JPA **33** (2000) 7903–18)

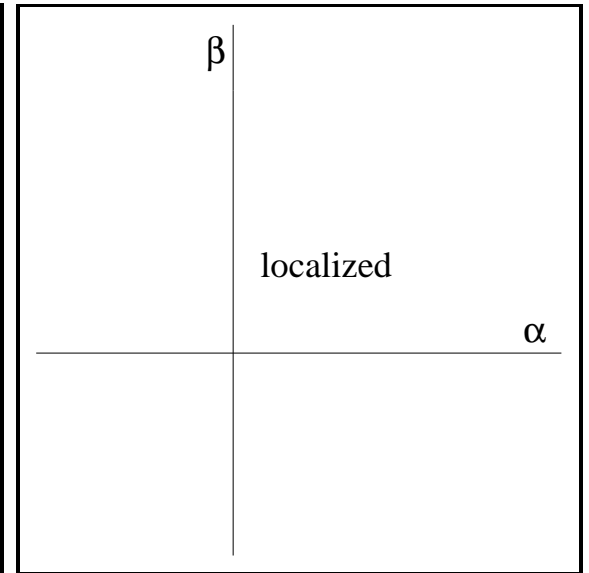
Further Results for fixed γ



$$\gamma \leq 0$$



$$\gamma > \gamma_1 \geq 0$$



$$\gamma > \gamma_3 \geq \gamma_2$$

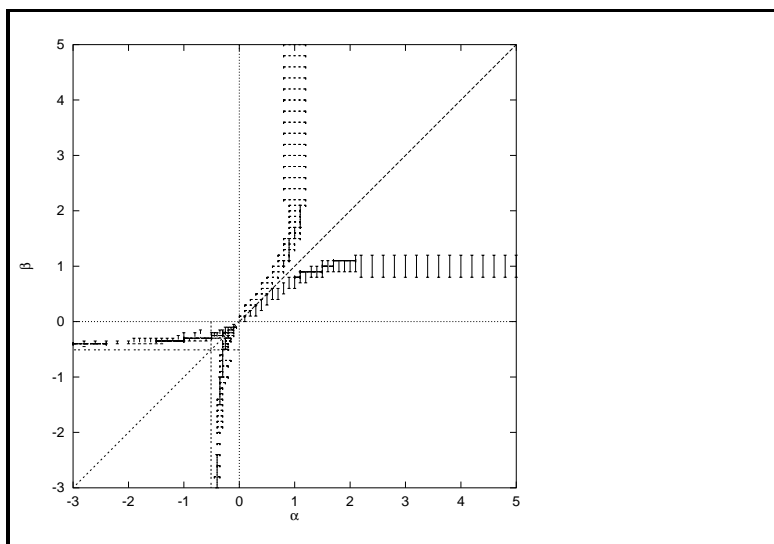
$$p = 1/2 \text{ (Madras/Whittington JPA } \mathbf{36} \text{ (2003) 923–38)}$$

γ_1 = adsorption critical point (homopolymer adsorption at a penetrable surface)

- conjectured that $\gamma_1 = 0$

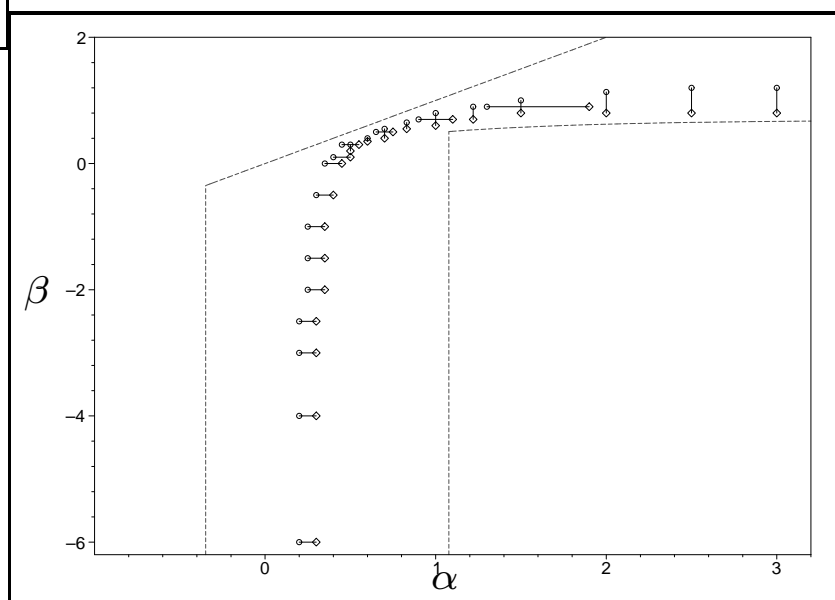
Exact Enumeration Analysis ($d = 3$, $p = 1/2$) supports $0 \leq \gamma_1 < 0.075$, $0.25 \leq \gamma_2 \leq 0.3$,

$1 \leq \gamma_3 \leq 1.1$ (James *et al* JPA **36** (2003) 11575–84)



$$\gamma = 0$$

(Martin *et al* JPA **33** (2000) 7903-18)



$$\gamma = 0.4$$

(James *et al* JPA **36** (2003) 11575-84)

Figure : Phase diagrams in (α, β) -plane from all states (ω, χ) up to $n = 20$ for $d = 3$ and $p = 1/2$.

Annealed Average Free Energy for Localization

The Annealed Average Free Energy for Localization.

$$\kappa_n^a(\alpha, \beta, \gamma) = n^{-1} \log \underbrace{\sum_{\chi} \sum_{\omega} p^{\sum_i \chi_i} (1-p)^{n-\sum_i \chi_i} e^{\alpha \sum_i \Delta_i^+(\omega) \chi_i + \beta \sum_i \Delta_i^-(\omega) (1-\chi_i) + \gamma \sum_i \Delta_i(\omega)}}_{\langle Z_n(\alpha, \beta, \gamma | \chi) \rangle}$$

$$\begin{aligned} \langle Z_n(\alpha, \beta, \gamma | \chi) \rangle &= \sum_{\omega} \prod_{i=1}^n e^{\gamma \Delta_i(\omega)} \left(\sum_{\chi_i=0}^1 p^{\chi_i} (1-p)^{1-\chi_i} e^{\alpha \Delta_i^+(\omega) \chi_i + \beta \Delta_i^-(\omega) (1-\chi_i)} \right) \\ &= \sum_{\omega} \prod_{i=1}^n e^{\gamma \Delta_i(\omega)} \left((1-p) e^{\beta \Delta_i^-(\omega)} + p e^{\alpha \Delta_i^+(\omega)} \right) \\ &= \sum_{v, v^+, v^-} c_n(v, v^+, v^-) e^{\gamma v} (1-p + p e^{\alpha})^{v^+} ((1-p) e^{\beta} + p)^{v^-} \end{aligned}$$

where $c_n(v, v^+, v^-)$ is the number of walks which have v returns to $z = 0$, v^+ vertices in $z > 0$ and v^- vertices in $z < 0$

Homopolymer Partition Function

The Morita Approximation (Constrained Annealing) for Localization

Recall: Quenched Average Free Energy

$$\bar{\kappa}_n(\alpha, \beta, \gamma) = n^{-1} \sum_{\chi} \pi(\chi) \log Z_n(\alpha, \beta, \gamma | \chi) = n^{-1} \langle \log Z_n(\alpha, \beta, \gamma | \chi) \rangle_{\pi}$$

Mazo (1963), Morita (1964), and Kuhn (1996) $\Rightarrow \bar{\kappa}_n(\alpha, \beta, \gamma)$ can be obtained as a solution to a variational problem involving a constrained annealed average free energy, i.e. the quenched average free energy can be obtained by

Minimizing: $n^{-1} \log Z^*(\alpha, \beta, \gamma, \lambda) = n^{-1} \log \langle Z_n(\alpha, \beta, \gamma | \chi) e^{\Lambda(\lambda | \chi)} \rangle_{\pi} \quad (***)$

with respect to *lagrange multipliers* $\lambda = \{\lambda_C, \emptyset \neq C \subseteq \{1, 2, \dots, n\} = [n]\}$, where the lagrange term

$$\Lambda(\lambda | \chi) = \sum_{C \subseteq [n]} \lambda_C \left[p^{|C|} - \prod_{i \in C} \chi_i \right].$$

The minimization ensures that for each subset C of vertices of the walk all the colouring constraints:

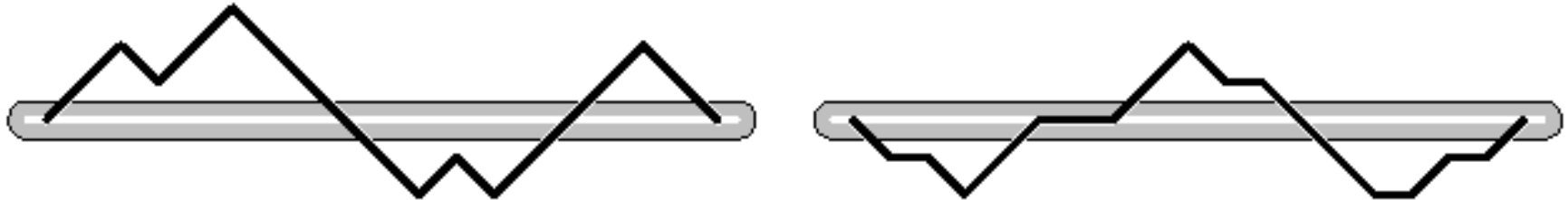
$$Prob(\text{all the walk vertices in } C \text{ are coloured } A) = \left\langle \prod_{i \in C} \chi_i \right\rangle_{\rho^q} = p^{|C|}$$

are satisfied, and hence all the correlations between walk vertex colourings have the correct distribution.

The Approximation: (Relax some constraints and minimize)

Solving $(***)$ with $\lambda_C = 0$ for some choices of C gives an UPPER BOUND on $\bar{\kappa}_n(\alpha, \beta, \gamma)$.

Directed Walk Models



Dyck path: a walk in two dimensions which starts at the origin and ends on the line $y = 0$, has no vertices with negative y -coordinate, and has steps only in the directions $(1, 1)$ and $(1, -1)$.

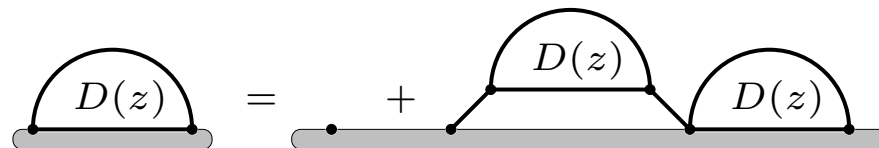
Motzkin path: like Dyck path but has three kinds of steps, $(1, 1)$, $(1, -1)$ and $(1, 0)$.

Bilateral Dyck path: like Dyck path but with vertices with negative y -coordinate allowed.

Bilateral Motzkin path: like Motzkin path but with vertices with negative y -coordinate allowed.

d_n : the number of n -step Dyck paths starting at the origin

$$D(z) = \sum_{n \geq 0} d_{2n} z^{2n} = D(z) = 1 + z^2 D(z)^2 = \frac{1 - \sqrt{1 - 4z^2}}{2z^2}$$

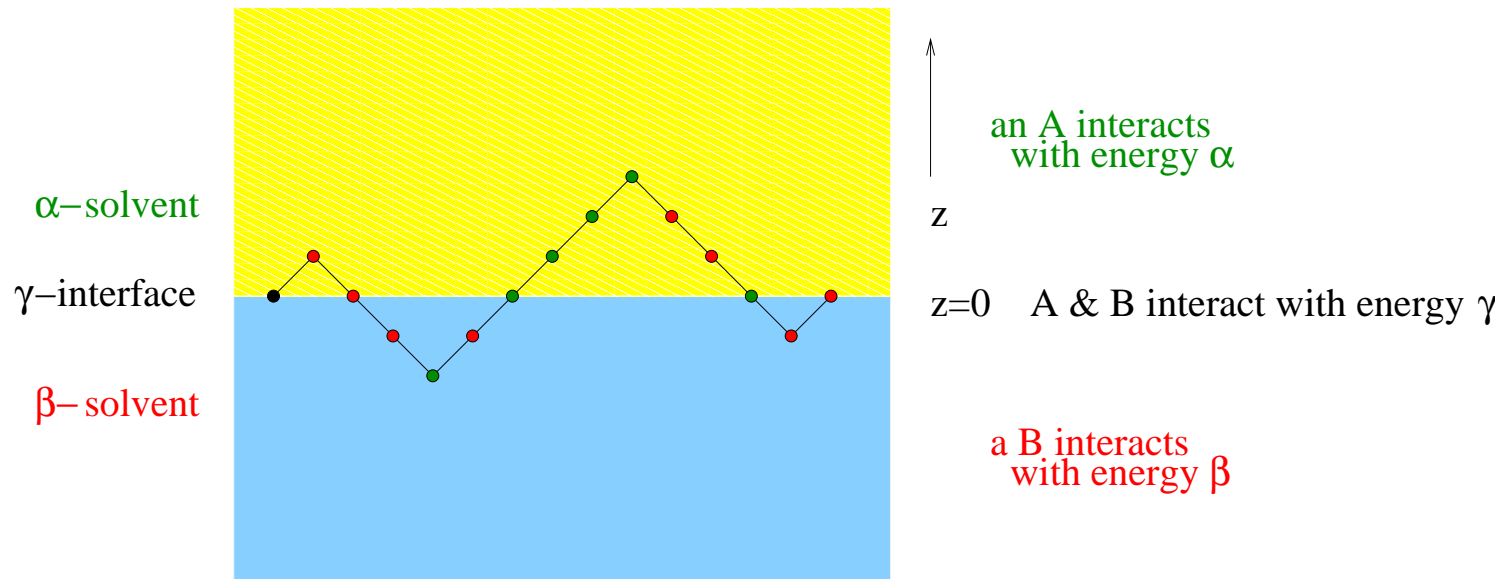


A Bilateral Dyck Path Model for Random Copolymer Localization

$c_n(v_A, v_B, w|\chi)$: given χ , number of n -edge Dyck paths starting at origin with

v_A A's in $z > 0$, v_B B's in $z < 0$, w vertices in $z = 0$.

Energy at Fixed χ : $-[1/(kT)]E(\omega|\chi) = \alpha v_A + \beta v_B + \gamma w$



$w = 4$, $v_A = 3$ (green=A=1), $v_B = 4$ (red=B=0)

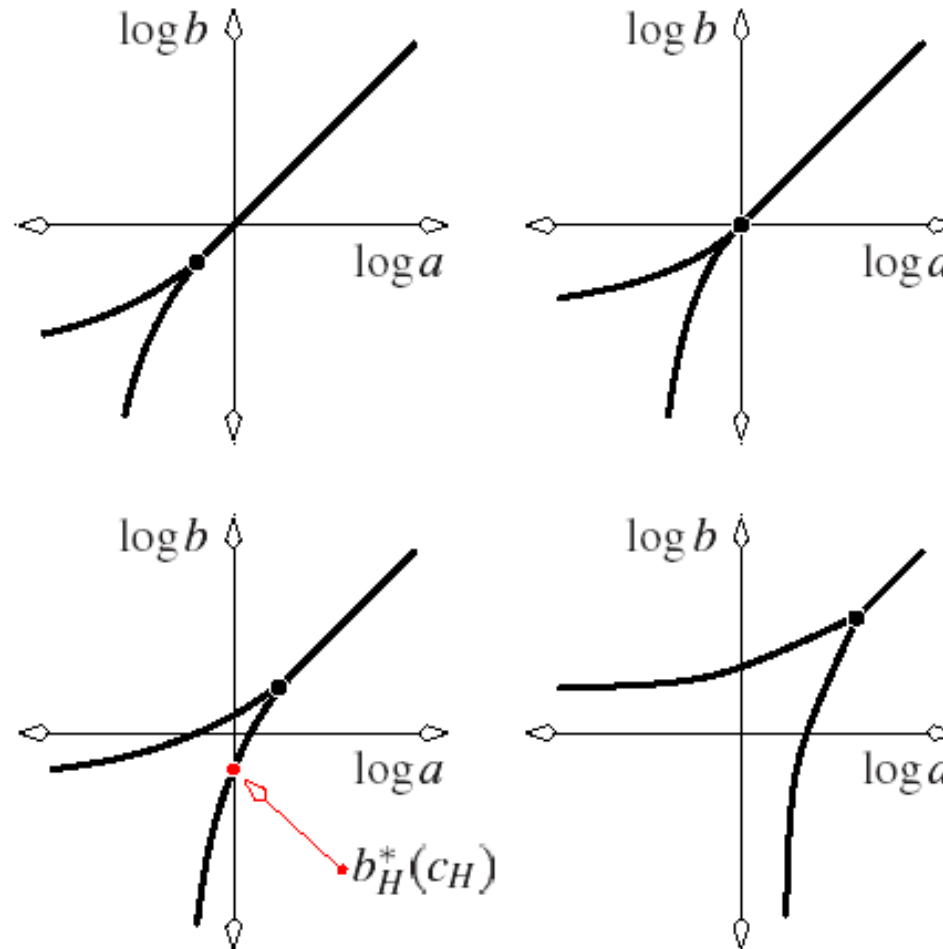
$\chi =$ 0,0,1,0,1,1,1,1,0,0,0,1,0,0,1

Morita Approximations for Bilateral Dyck Path Models of Localization

Annealed: $n^{-1} \log Z_n^a(\alpha, \beta, \gamma) = n^{-1} \log \sum_{\chi} \sum_{\omega} p^{\sum_i \chi_i} (1-p)^{n-\sum_i \chi_i} e^{\alpha v_A + \beta v_B + \gamma w}$

$$n^{-1} \log Z_n^a(\alpha, \beta, \gamma) \geq \langle \kappa_n(\alpha, \beta, \gamma | \chi) \rangle \text{ (Quenched Average Free Energy)}$$

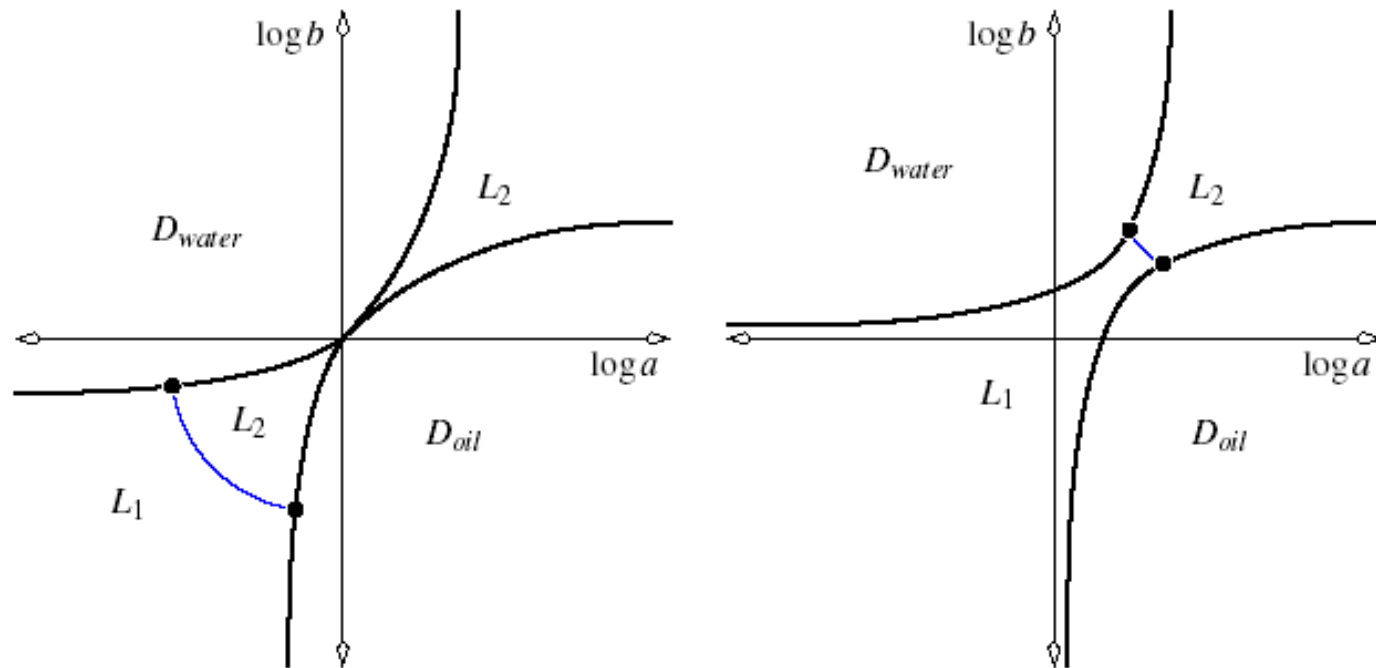
$p = 1/2$ Iliev *et al* JPA **38** (2005) 1209–1223



The First Moment Morita Approximation:

Constrain $\langle \sum_{i=1}^n \chi_i \rangle = np$

Minimize: $n^{-1} \log Z_n^{(1)}(\alpha, \beta, \gamma, \lambda) = n^{-1} \log \langle Z_N(\alpha, \beta, \gamma | \chi) e^{\lambda(\sum_{i=1}^n \chi_i - np)} \rangle_\pi$



For $p = 1/2$, on the left $\gamma < 0$ and on the right $\gamma > 0$. $\alpha = \log a$ and $\beta = \log b$. The delocalized phase boundary formula is independent of γ beyond the solid circle for $\gamma \geq 0$.

If higher order moment constraints are introduced can the “mixture” phase be eliminated?

Higher Order Morita Approximations:

Order σ Approximation: include only constraints involving non-overlapping correlations between neighbouring colours at most $\sigma - 1$ apart.

$$\underbrace{\chi_1, \chi_2, \dots, \chi_\sigma}_{\chi^{(1)}} \cdots \underbrace{\chi_{\sigma(i-1)+1}, \chi_{\sigma(i-1)+2}, \dots, \chi_{\sigma i}}_{\chi^{(i)}} \cdots \underbrace{\chi_{\sigma(n-1)+1}, \chi_{\sigma(n-1)+2}, \dots, \chi_{\sigma k}}_{\chi^{(k)}}$$

Given even $\sigma \geq 2$, consider randomly coloured bilateral Dyck paths of length $n = k\sigma$ ($k \geq 1$) and impose for each non-empty subset $C \subseteq \{1, 2, \dots, \sigma\} = [\sigma]$ the following set of constraints:

$$\sum_{i=1}^k \langle \prod_{j \in C} \chi_{\sigma(i-1)+j} \rangle = kp^{|C|}$$

so that

$$\Lambda(\lambda^{(\sigma)} | \chi) = \sum_{C \subseteq [\sigma]} \lambda_C \left[kp^{|C|} - \sum_{i=1}^k \prod_{j \in C} \chi_{\sigma(i-1)+j} \right]$$

Minimize:

$$F_{k\sigma}^{(\sigma)}(\alpha, \beta, \gamma, \lambda^{(\sigma)}) = (k\sigma)^{-1} \log \langle Z_{k\sigma}(\alpha, \beta, \gamma | \chi) e^{\Lambda(\lambda^{(\sigma)} | \chi)} \rangle_\pi$$

Higher Order Morita Approximations Continued:

Recall we want to **Minimize**:

$$F_{k\sigma}^{(\sigma)}(\alpha, \beta, \gamma, \lambda^{(\sigma)}) = (k\sigma)^{-1} \log \langle Z_{k\sigma}(\alpha, \beta, \gamma | \chi) e^{\Lambda(\lambda^{(\sigma)} | \chi)} \rangle_{\pi}$$

For the limiting Morita free energy we want

$$\kappa_{\sigma}^M(\alpha, \beta, \gamma) = \lim_{k \rightarrow \infty} (k\sigma)^{-1} \min_{\lambda^{(\sigma)}} \log \langle Z_{k\sigma}(\alpha, \beta, \gamma | \chi) e^{\Lambda(\lambda^{(\sigma)} | \chi)} \rangle$$

Define the grand canonical partition function (a.k.a. generating function)

$$G_{\sigma}(z, \alpha, \beta, \gamma, \lambda^{(\sigma)}) = \sum_{k=0}^{\infty} z^{k\sigma} \langle Z_{k\sigma}(\alpha, \beta, \gamma | \chi) e^{\Lambda(\lambda^{(\sigma)} | \chi)} \rangle$$

with radius of convergence r_G .

Define

$$\kappa_{\sigma, \lambda^{(\sigma)}}(\alpha, \beta, \gamma) = -\log r_G = \lim_{k \rightarrow \infty} (k\sigma)^{-1} \log \langle Z_{k\sigma}(\alpha, \beta, \gamma | \chi) e^{\Lambda(\lambda^{(\sigma)} | \chi)} \rangle.$$

$$\kappa_{\sigma}^U(\alpha, \beta, \gamma) = \min_{\lambda^{(\sigma)}} \kappa_{\sigma, \lambda^{(\sigma)}}(\alpha, \beta, \gamma) \geq \kappa_{\sigma}^M(\alpha, \beta, \gamma)$$

G_{σ} can be written in terms of a homopolymer generating function B_{σ} for bilateral Dyck paths which keeps track of the number of segments ω of the path that have the same sequence

$$s(\omega) = (\Delta_{2i-1}^-(\omega), \Delta_{2i}(\omega), i = 1, \dots, l).$$

Factorization can be used to solve for B_σ and obtain

$$r_B = \min\{|z_1|, |z_2|, \dots, |z_{\sigma+2}|\}$$

where z_1 and z_2 are square root singularities of B_σ corresponding to the delocalized above and delocalized below phases respectively. z_i 's are available for $\sigma = 2, 4$, otherwise involves solving a polynomial of degree greater than 5.

Note: $\kappa_\sigma^M(\alpha, \beta, \gamma) \leq \kappa_\sigma^U(\alpha, \beta, \gamma) = \min_\lambda \kappa_{\sigma,\lambda}(\alpha, \beta, \gamma) \leq \kappa_{\sigma,\lambda}(\alpha, \beta, \gamma, \lambda)$

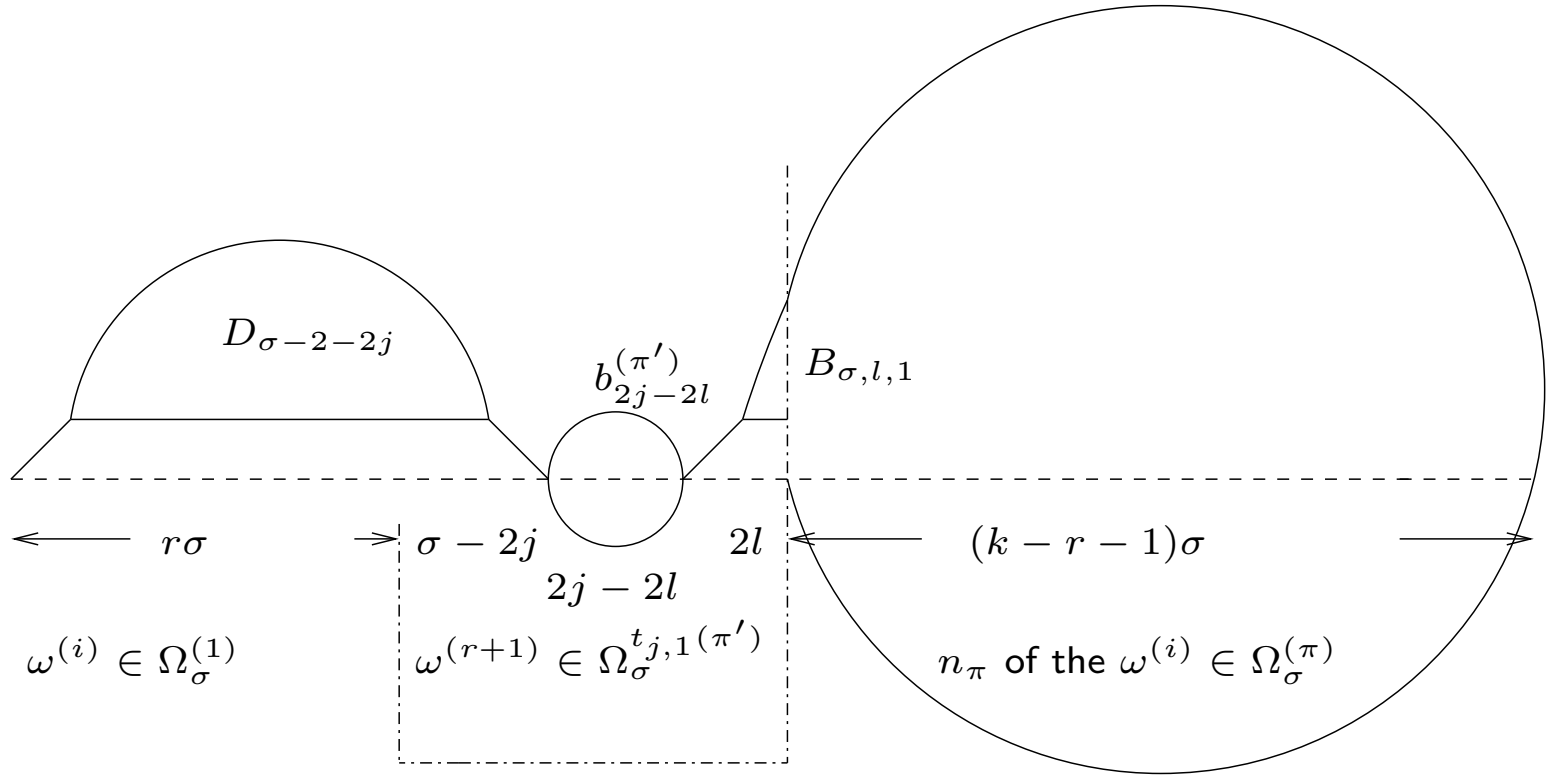


Figure : Schematic representation of factorization.

Mixture Phase

Delocalized Above: Morita free energy = Quenched average free energy = $\log 2 + \alpha p$

minimum is achieved at $\lambda = \lambda^{(A)} = (-\alpha|C|, C \subseteq [\sigma])$

Delocalized Below: Morita free energy = Quenched average free energy = $\log 2 + \beta(1 - p)$

minimum is achieved at $\lambda = \lambda^{(B)} = (-\beta(\sigma - |C|), C \subseteq [\sigma])$

and the delocalized (above) phase boundary can be determined from

$$\beta_c^A(\alpha, \gamma) = \sup\{\beta \mid \kappa_{\sigma, \lambda^{(A)}}(\alpha, \beta, \gamma) = \log 2 + \alpha p\}$$

By Caravenna & Giacomini (2005), this phase boundary will be the same as for the first moment Morita approximation ($\sigma = 1$).

For a given set of λ 's the mixture arises when the square root singularities are equal in magnitude, and they dominate any other singularities so that

$$\begin{aligned} \kappa_{\sigma, \lambda}(\alpha, \beta, \gamma) &= \log 2 + \frac{1}{\sigma} \left(- \sum_C \lambda_C p^{|C|} (1-p)^{\sigma-|C|} + \log \sum_C (pe^\alpha)^{|C|} (1-p)^{\sigma-|C|} e^{\lambda_C} \right) \\ &= \log 2 + \frac{1}{\sigma} \left(- \sum_C \lambda_C p^{|C|} (1-p)^{\sigma-|C|} + \log \sum_C p^{|C|} ((1-p)e^\beta)^{\sigma-|C|} e^{\lambda_C} \right). \end{aligned} \quad (1)$$

Note that the first right-hand side is the limiting average free energy associated with the set of Dyck paths which have all but their first and last vertex above the interface, and the second right-hand side is the limiting average free energy associated with the set of Dyck paths which have all but their first and last vertex below the interface.

One solution can be found: the *constrained limiting average mixture free energy*

$$\kappa_{mix,\sigma}(\alpha, \beta) = \log 2 + \frac{1}{\sigma} \sum_{m=0}^{\sigma} \binom{\sigma}{m} p^m (1-p)^{\sigma-m} \log(qe^{\alpha m} + (1-q)e^{\beta(\sigma-m)}) \quad (2)$$

where $q \in [0, 1]$ is the first solution in $[0, 1]$ to:

$$1 = \sum_{m=0}^{\sigma} \binom{\sigma}{m} p^m (1-p)^{\sigma-m} \frac{e^{\alpha m}}{qe^{\alpha m} + (1-q)e^{\beta(\sigma-m)}}. \quad (3)$$

Given any $\gamma < \gamma_L^{(U)} = -\log(1-p)$ and any $\alpha, \beta > 0$, our goal is to find a choice of σ such that $\kappa_{\sigma}^U(\alpha, \beta, \gamma) > \kappa_{mix,\sigma}(\alpha, \beta)$. To investigate this we consider a lower bound on $\kappa_{\sigma}^U(\alpha, \beta, \gamma)$ and determine σ such that the lower bound is greater than $\kappa_{mix,\sigma}(\alpha, \beta)$.

LOWER BOUND: We bound the Morita approximation below by a lower bound on the limiting quenched average free energy based on the fact that:

$$Z_{k\sigma}(\alpha, \beta, \gamma|\chi) \geq (Z_{\sigma}(\alpha, \beta, \gamma|\chi))^k$$

so that

$$\kappa_{\sigma}^U(\alpha, \beta, \gamma) \geq \sigma^{-1} \langle \log Z_{\sigma}(\alpha, \beta, \gamma|\chi) \rangle$$

For $\alpha = \beta$ sufficiently large and $\sigma \geq 12 \Rightarrow$

$$\sigma^{-1} \langle \log Z_{\sigma}(\alpha, \beta, \gamma|\chi) \rangle > \kappa_{mix,\sigma}(\alpha, \beta)$$

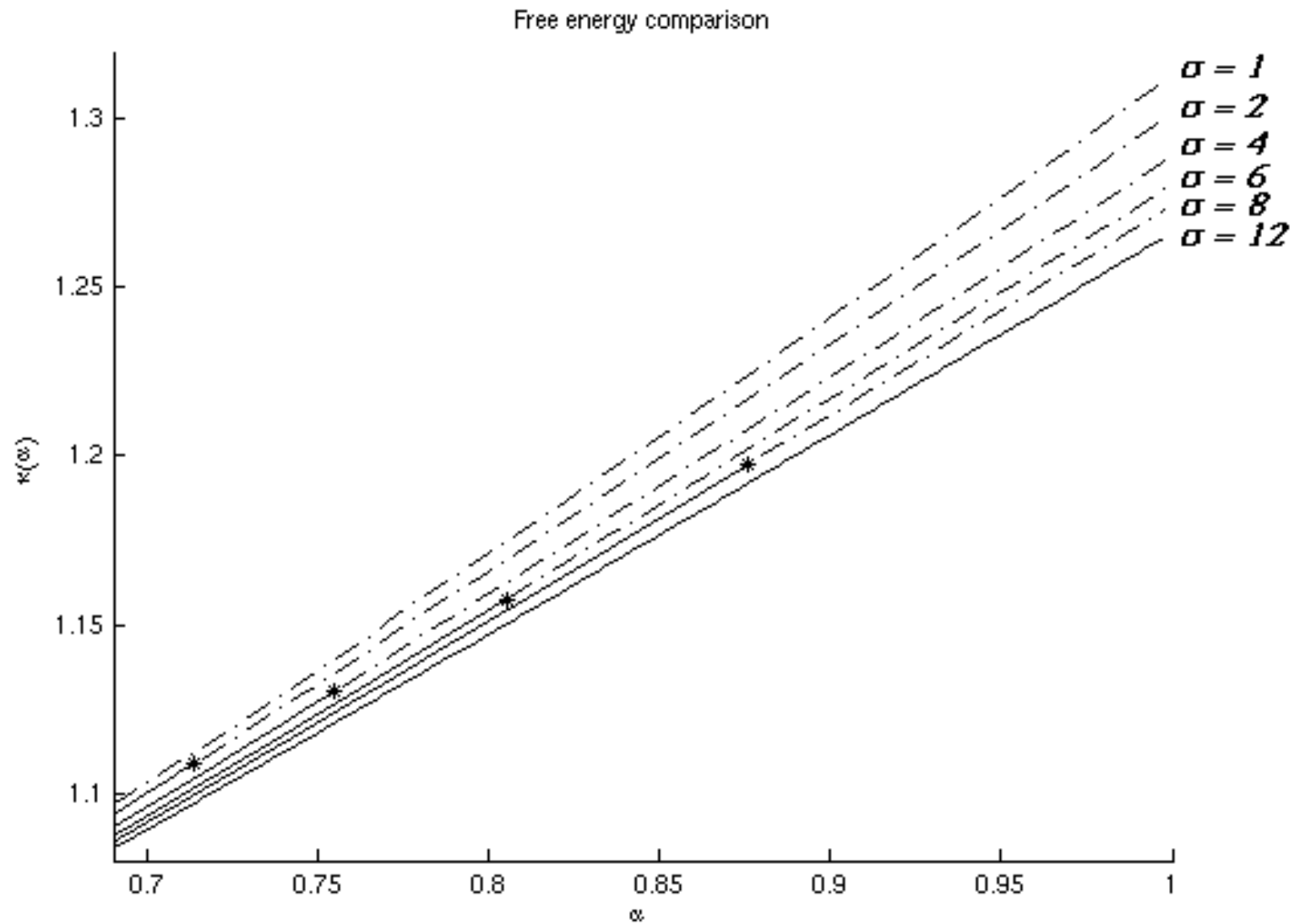
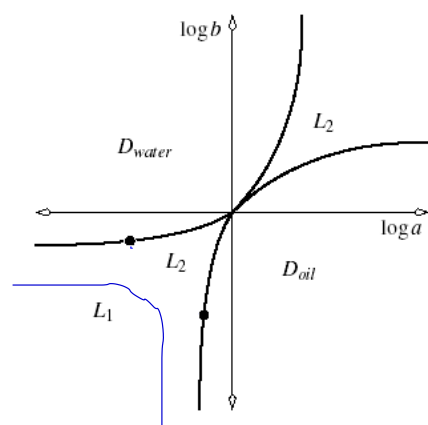
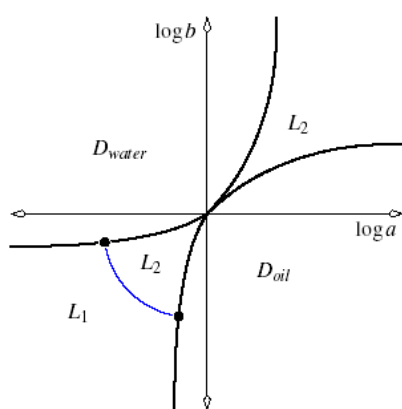


Figure : At $\gamma = \log(1.5)$ and $\alpha = \beta$, bounds on the limiting quenched average free energy for various choices of σ . Dotted curves correspond to bounds obtained from the mixture; solid curves correspond to bounds obtained using a pole.

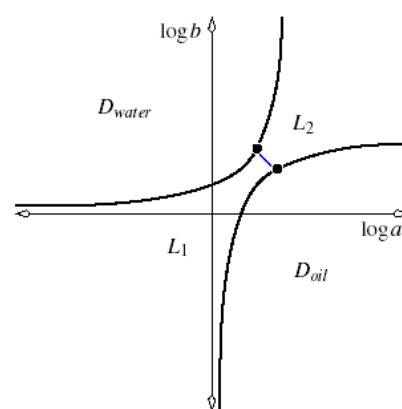
For $1 \leq \sigma < 12$:



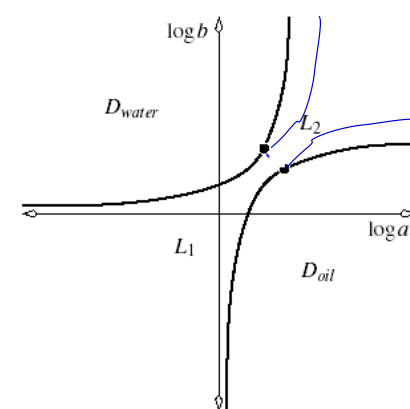
$$\gamma < \log(2/3)$$



$$\log(2/3) < \gamma < 0$$



$$0 < \gamma < \log 2$$



$$0 < \gamma < \log 2$$

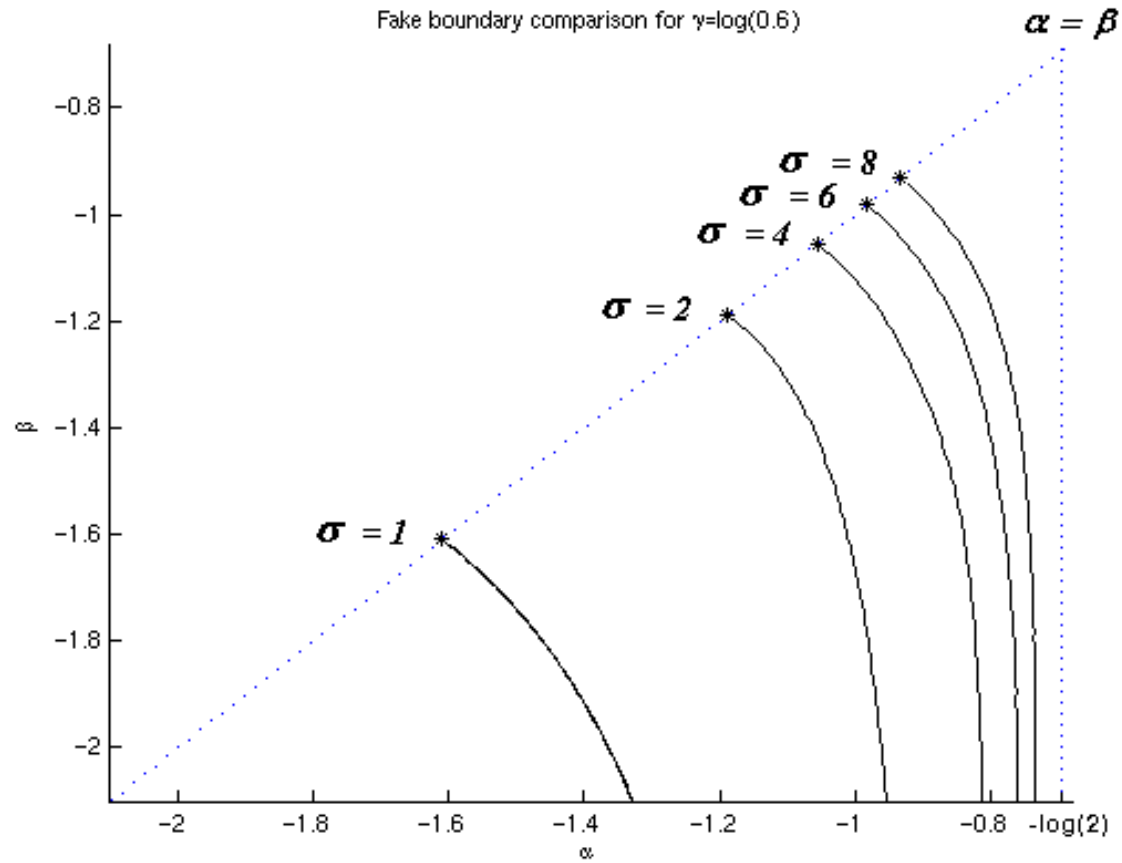


Figure : For $\gamma = \log(0.6)$, the phase boundary in the (α, β) -plane between the truly localized phase and the mixture phase is shown for various choices of σ .

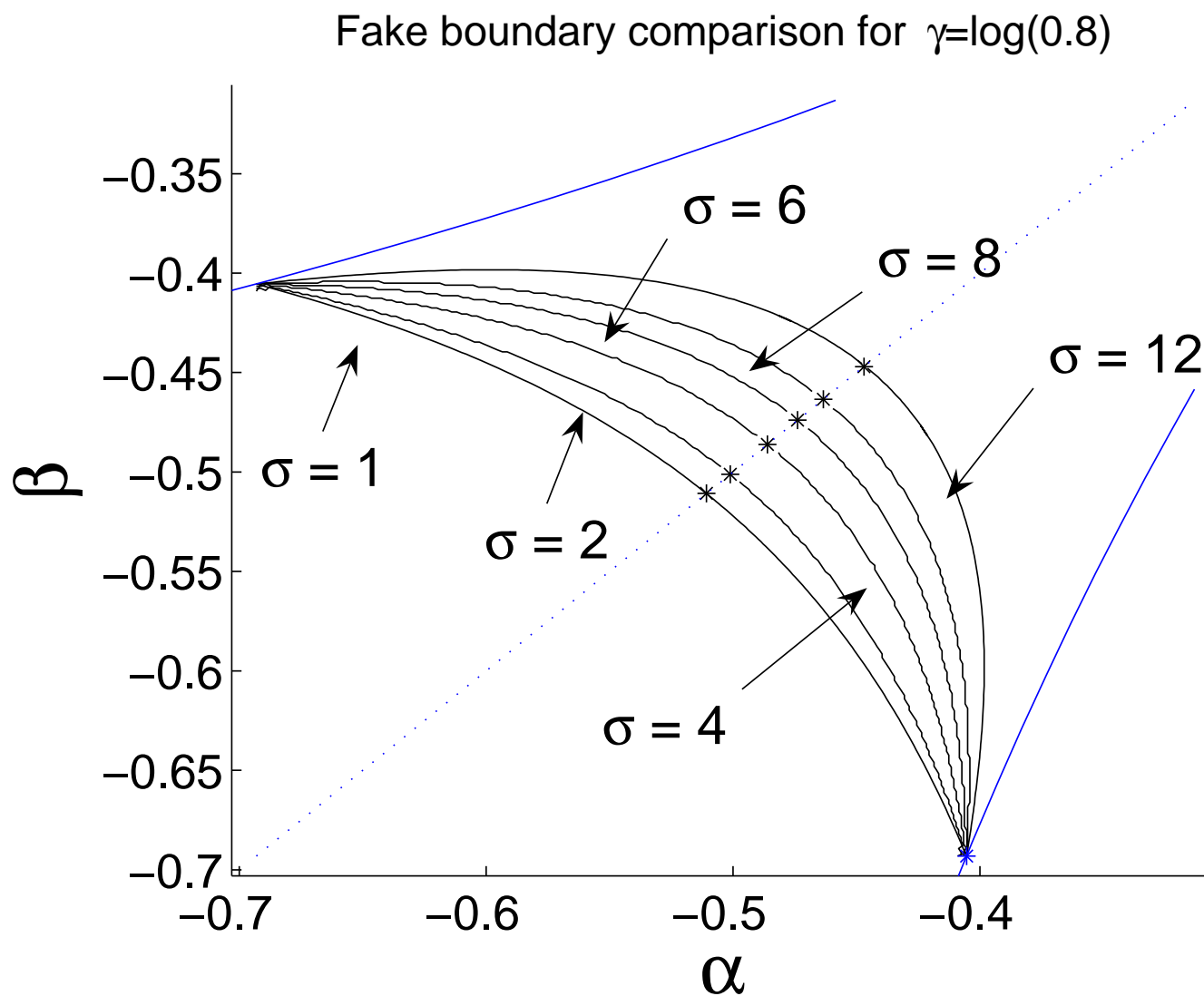


Figure : For $\gamma = \log(0.8)$, the phase boundary in the (α, β) –plane between the truly localized phase and the mixture phase is shown for various choices of σ .

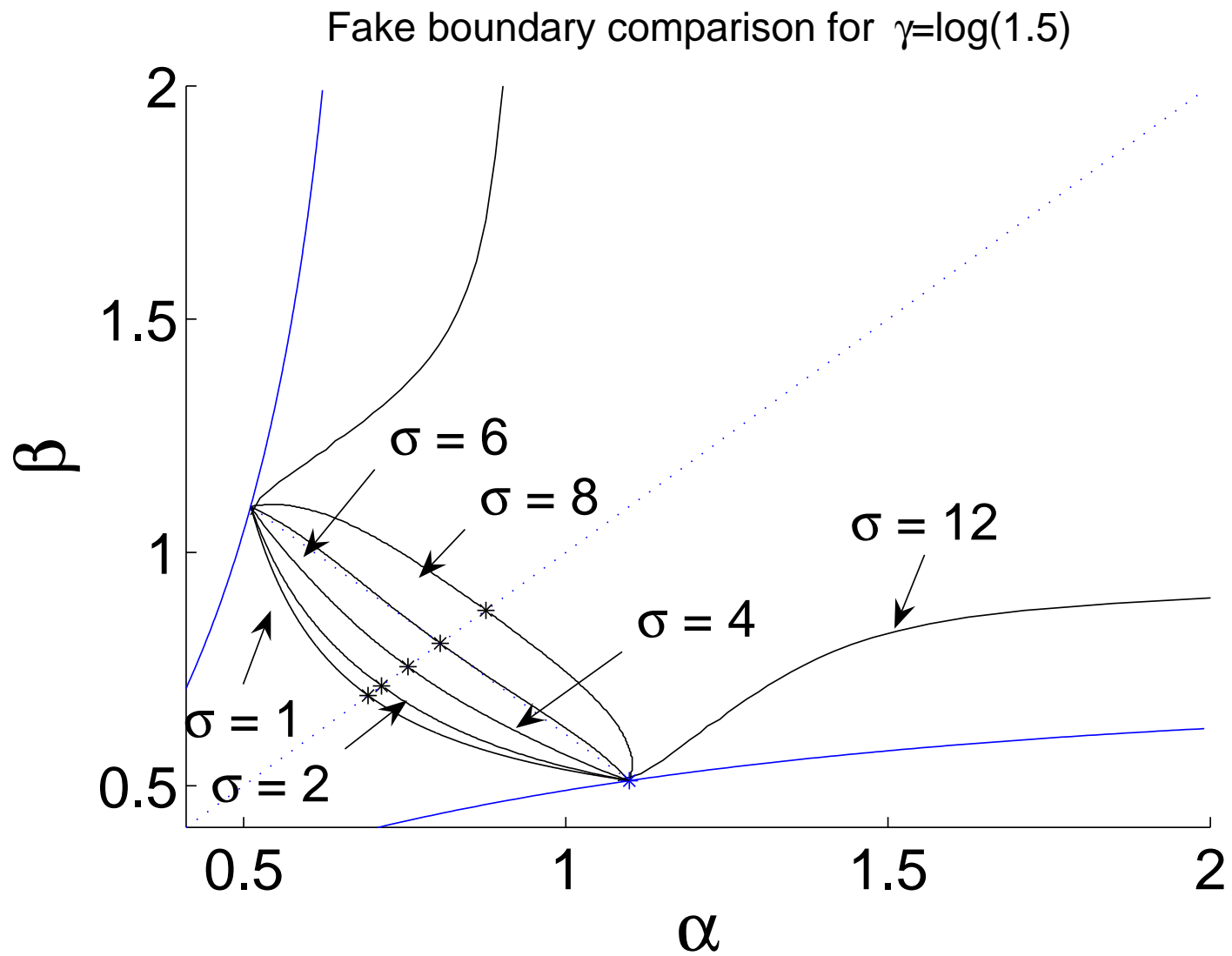


Figure : For $\gamma = \log(1.5)$, the phase boundary in the (α, β) –plane between the truly localized phase and the mixture phase is shown for $\sigma = 1, 2, 4, 6, 8, 12$.

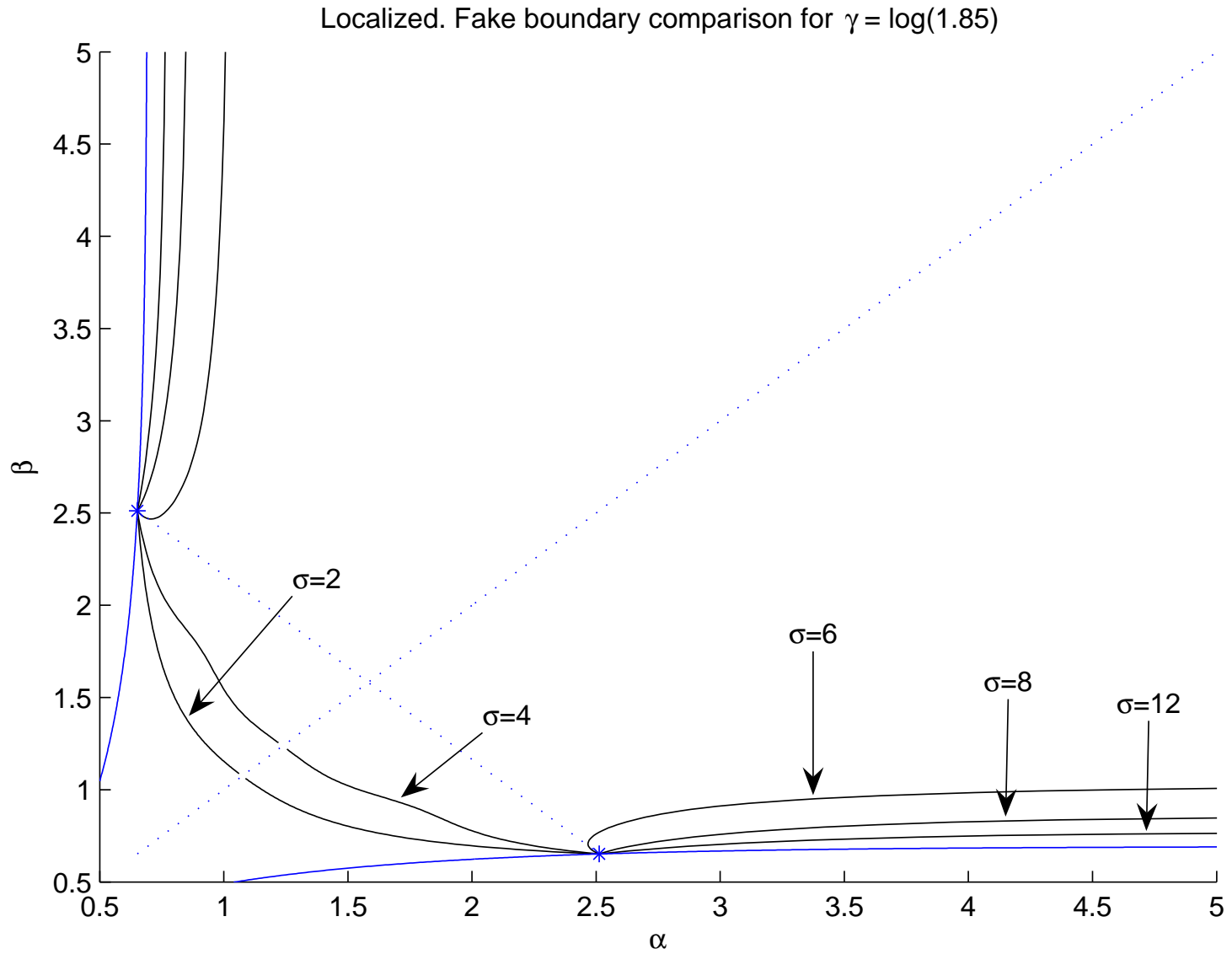


Figure : For $\gamma = \log(1.85)$, the phase boundary in the (α, β) -plane between the truly localized phase and the mixture phase is shown for $\sigma = 1, 2, 4, 6, 8, 12$.

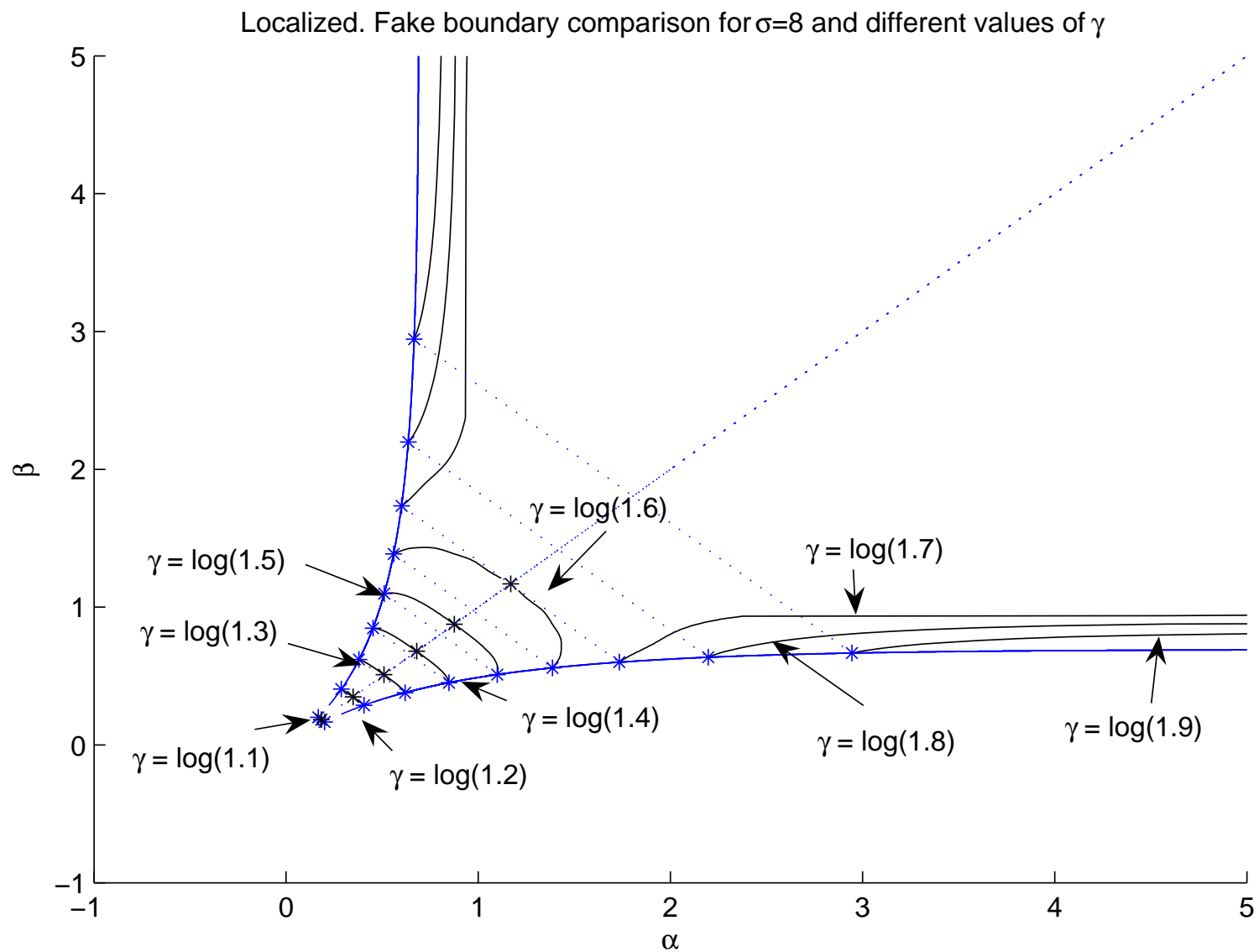


Figure : For $\sigma = 8$, the phase boundary in the (α, β) –plane between the truly localized phase and the mixture phase is shown for $\gamma = \log(1.1 + i(0.1)), i = 0, \dots, 8$. Blue line is $\beta = \log(1 - e^{-\alpha}/2) + \log 2$.