Bounds for directed walk models of random copolymer localization

Random Polymers

June 18-22, 2007

EURANDOM, Eindhoven, The Netherlands

Chris Soteros

Department of Mathematics and Statistics

University of Saskatchewan

Collaborators:

Stu Whittington, Department of Chemistry, Univ. of Toronto

Juan Alvarez, Math & Stats, Univ. of Sask.

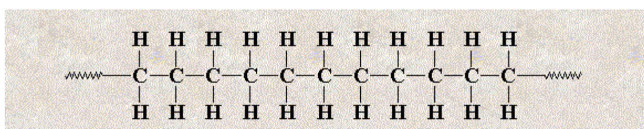
Enzo Orlandini, Dipartimento di Fisica & Sezione CNR-INFM, Univ. di Padova

Acknowledgements:

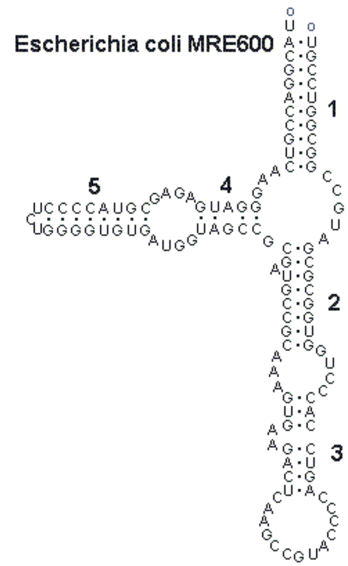
NSERC of Canada

Introduction to Random Copolymers

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



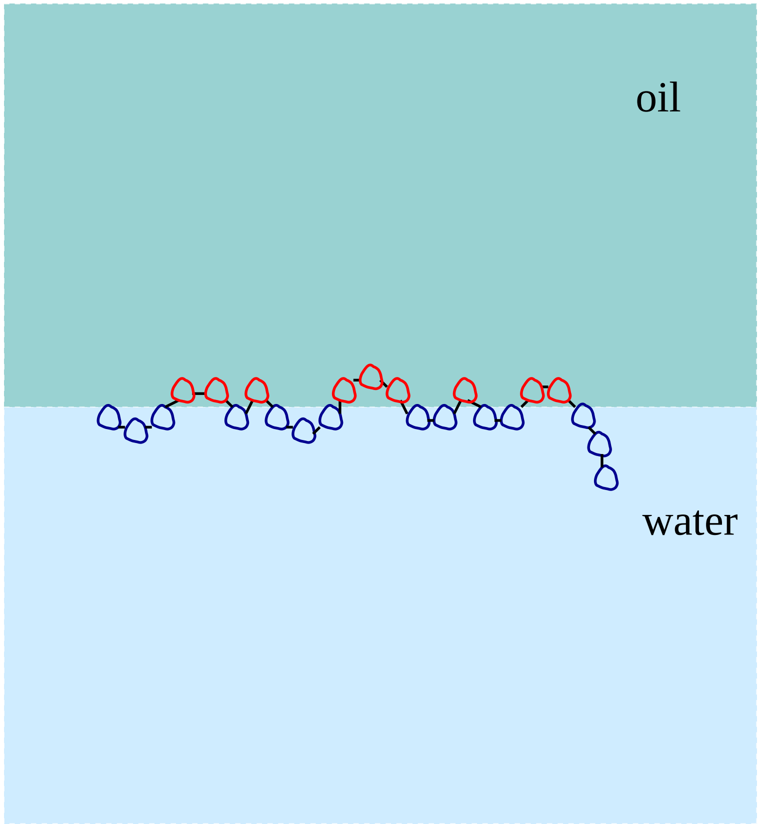
homopolymer - polyethylene



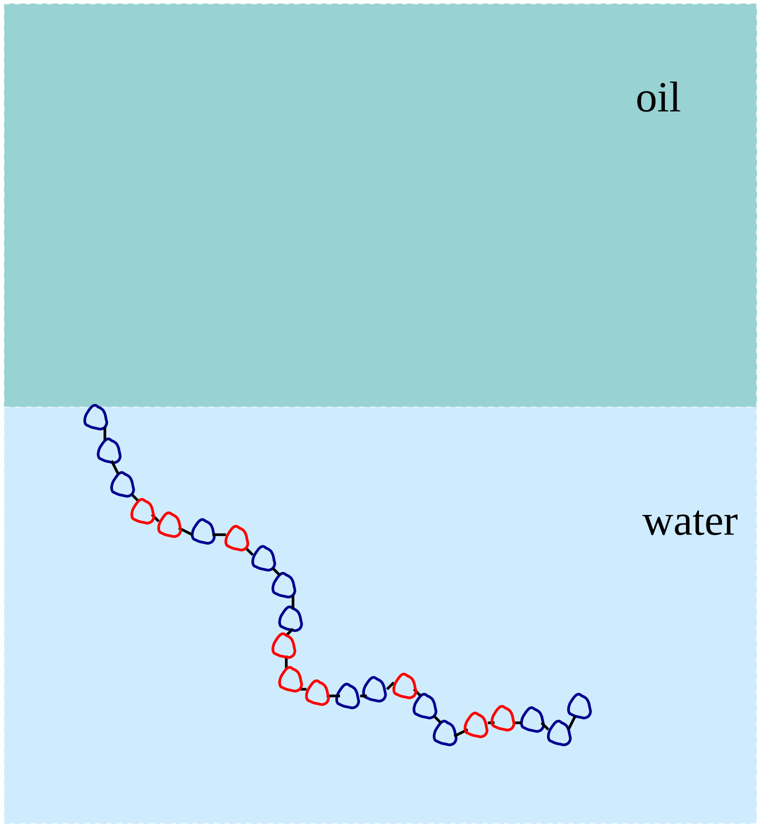
copolymer - RNA

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

Random Copolymer Localization Phase Transition



Low T - *Localized*



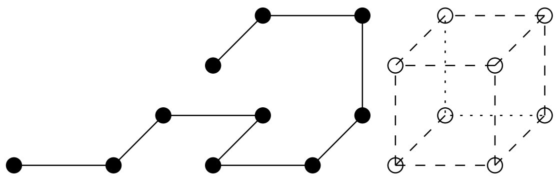
High T - *Delocalized*

Experimental Evidence: Phipps J S, Richardson R M, Cosgrove T and Eaglesham A 1993 Neutron reflection studies of copolymers at the hexane/water interface *Langmuir* **9** 3530-3537

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"	$\chi = \chi_1, \chi_2, \chi_3, ..., \chi_n$	a sequence of i.i.d. r.v.'s such that
with prob. p	$\chi_i = 1$	indicating ith vertex monomer type A
with prob. $1-p$	$\chi_i = 0$	indicating ith 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 $\bar{\kappa}(\beta) = \lim_{n\to\infty}\bar{\kappa}_n(\beta)$.

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.

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

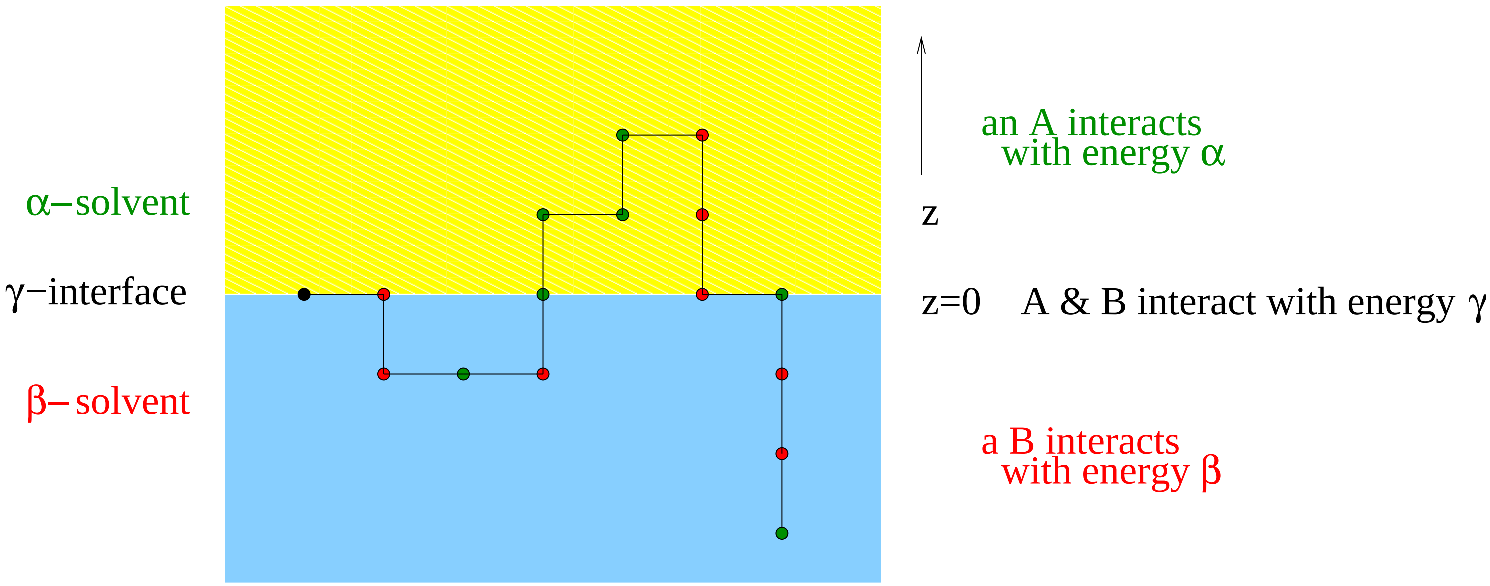
Annealed average free energy: $\kappa_n^a(\beta) = n^{-1}\log\sum_\chi \pi(\chi)Z_n(\beta|\chi) \geq \bar{\kappa}_n(\beta)$

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:

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

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

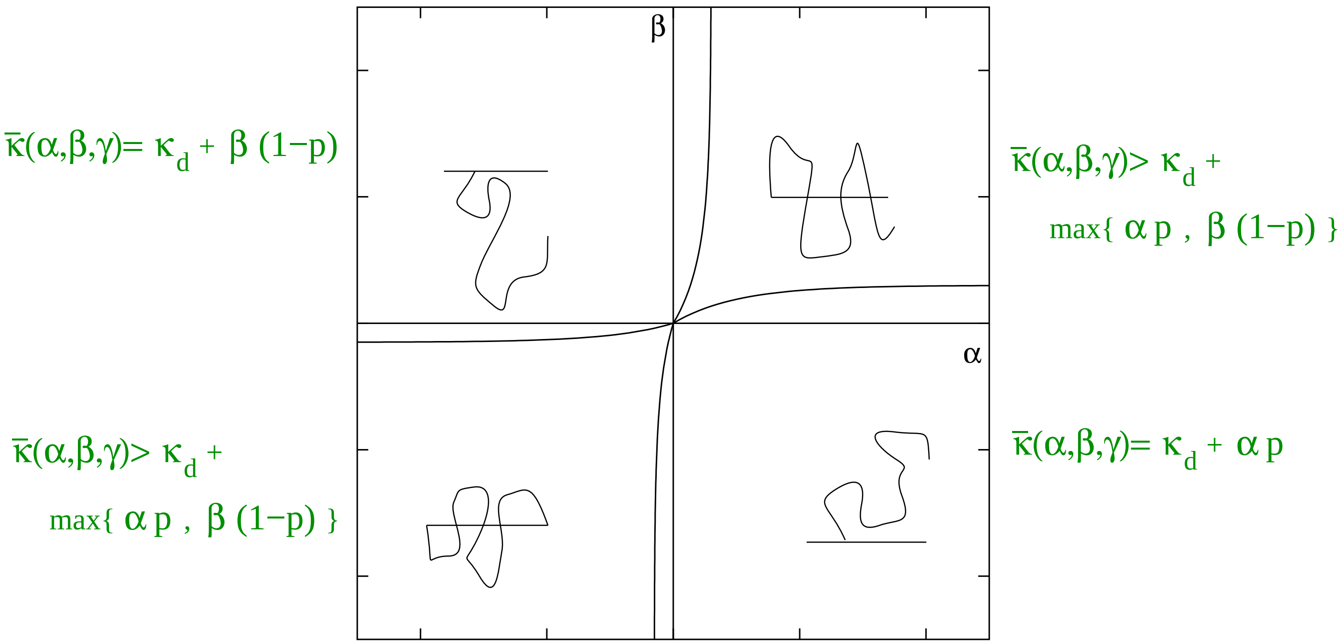
Some Rigorous Results for the SAW Model

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).

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

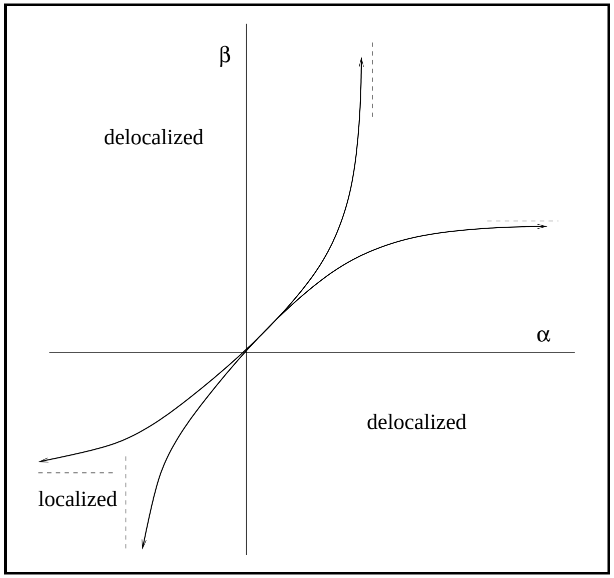
$\Rightarrow \bar{\kappa}(0,0,0) = \lim_{n\to\infty} n^{-1} \log c_n = \kappa_d$

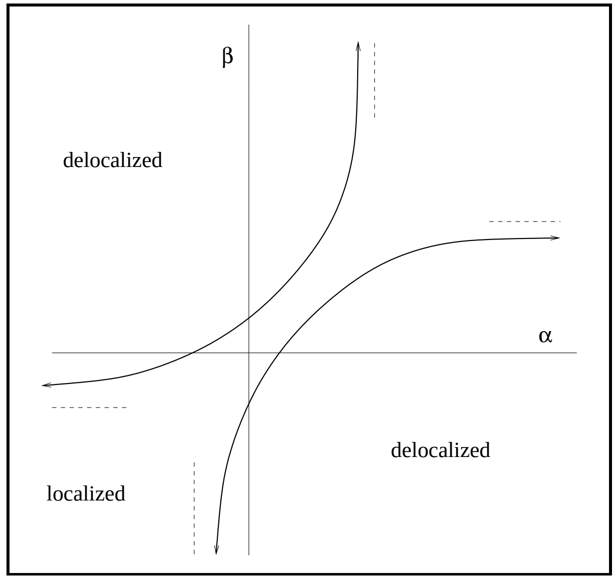
Expected Phase Diagram for fixed $\gamma \le 0$

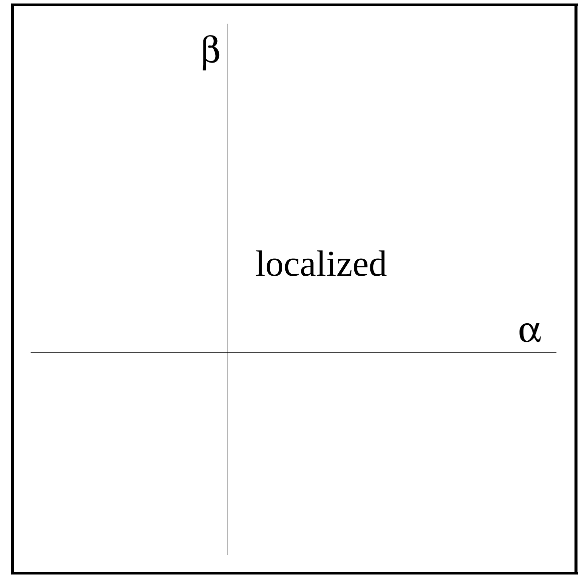


$p = 1/2$ (Martin *et al* JPA **33** (2000) 7903–18)

Further Results for fixed γ





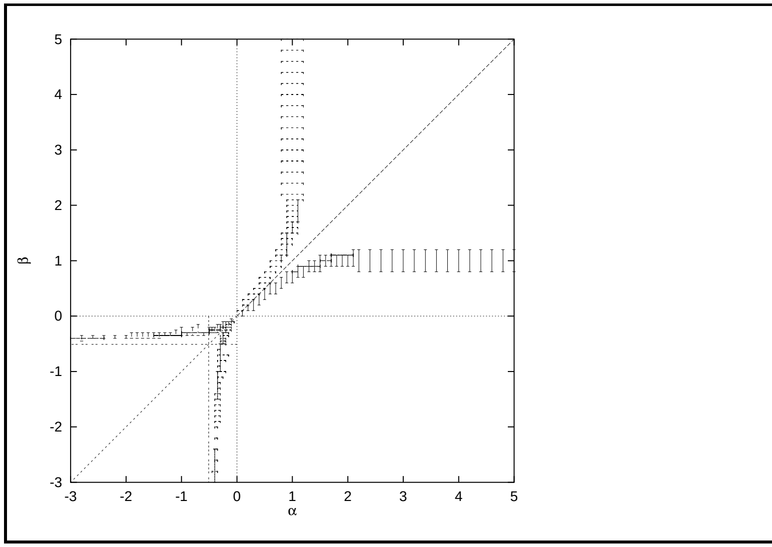


$\gamma \leq 0$ $\quad$ $\gamma > \gamma_1 \geq 0$ $\quad$ $\gamma > \gamma_3 \geq \gamma_2$

$p = 1/2$ (Madras/Whittington JPA **36** (2003) 923–38)

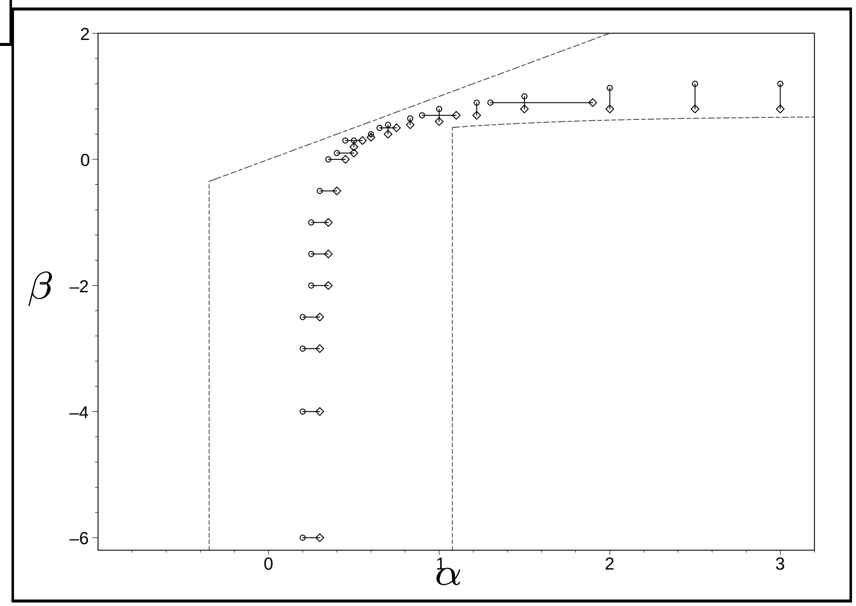
γ_1 = adsorption critical point (homopolymer adsorption at a penetrable surface)
- conjectured that $\gamma_1 = 0$

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)

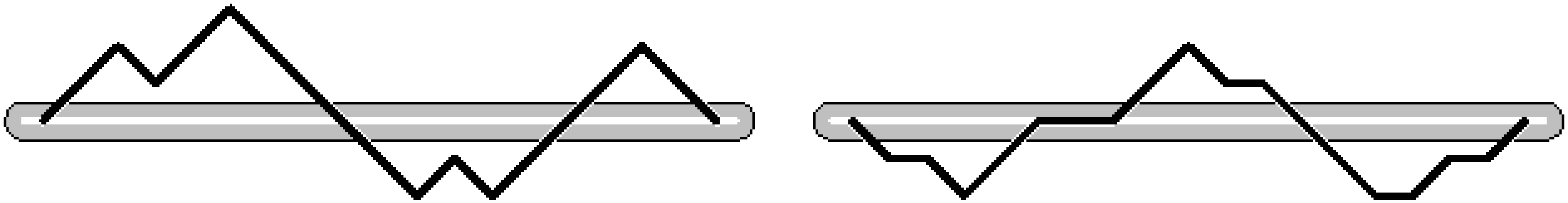


$\gamma = 0.4$

(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 $p = 1/2$.

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 $(1,-1)$.

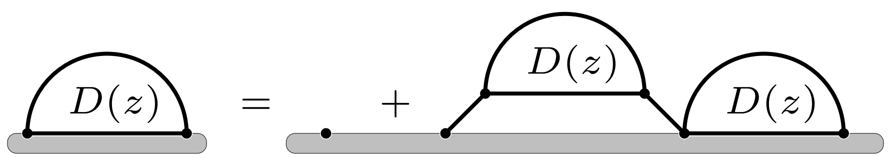
Motzkin path: like Dyck path but has three kinds of steps, $(1,1)$, $(1,-1)$ and $(1,0)$.

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

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

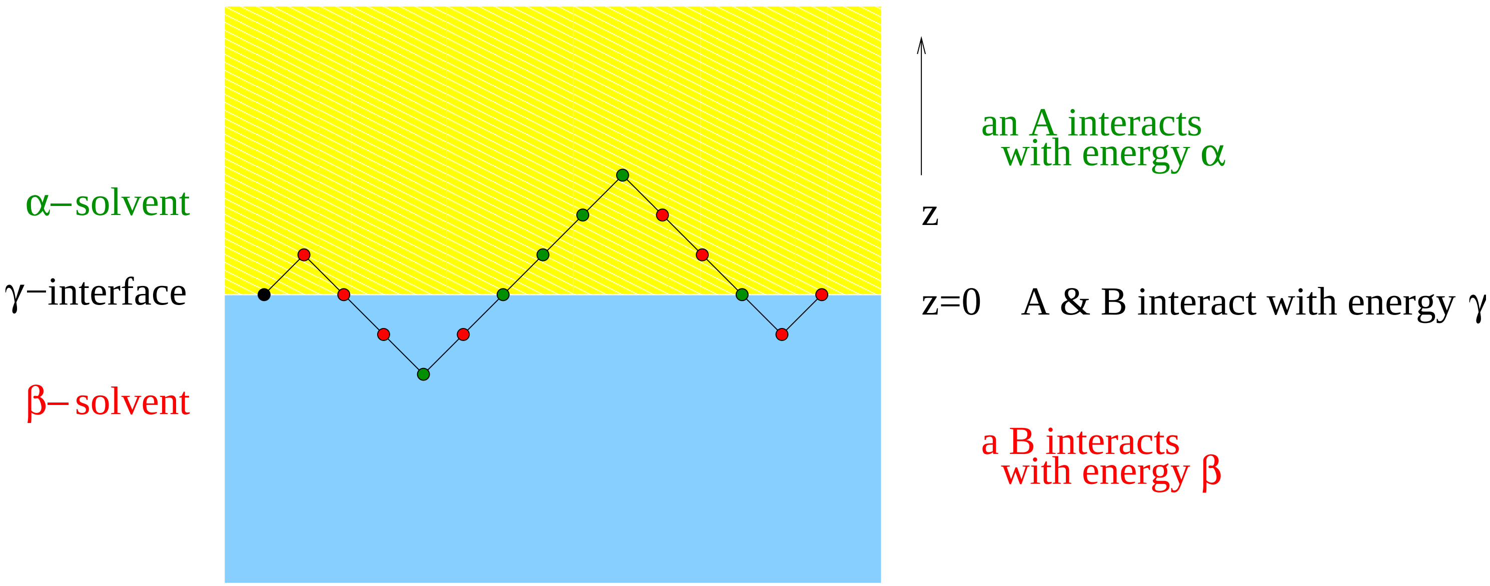


A Bilateral Dyck Path Model for Random Copolymer Localization

$c_n(v_A, v_B, w|\chi)$: 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)

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

Annealed Average Free Energy for Localization

The Annealed Average Free Energy for Localization.

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

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

$$= \sum_{\omega}\prod_{i=1}^{n} e^{\gamma\Delta_i(\omega)}\left((1-p)e^{\beta\Delta_i^-(\omega)} + pe^{\alpha\Delta_i^+(\omega)}\right)$$

$$= \sum_{v,v^+,v^-} c_n(v,v^+,v^-)e^{\gamma v}(1-p+pe^{\alpha})^{v^+}((1-p)e^{\beta}+p)^{v^-}$$

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 $z<0$

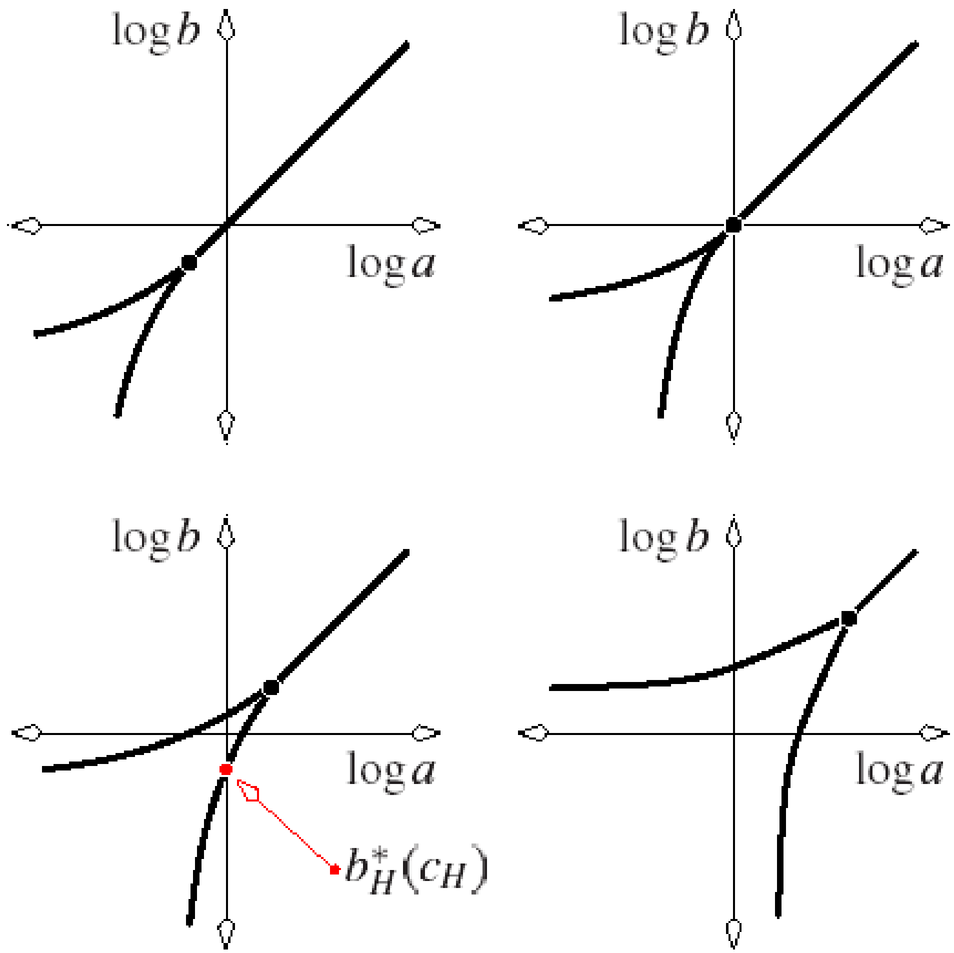
Homopolymer Partition Function

Annealing for Bilateral Dyck Path Localization

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

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

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



The Morita Approximation (Constrained Annealing) for Localization

Recall: Quenched Average Free Energy

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

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:

$$n^{-1} \log Z^*(\alpha, \beta, \gamma, \lambda) = n^{-1} \log \sum_{\chi} \pi(\chi) Z_n(\alpha, \beta, \gamma | \chi) e^{\Lambda(\lambda|\chi)} \qquad (***)$$

with respect to *lagrange multipliers* $\lambda = \{\lambda_C, C \subseteq \{1, 2, ..., n\} = [n]\}$, 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:

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

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

The Approximation:

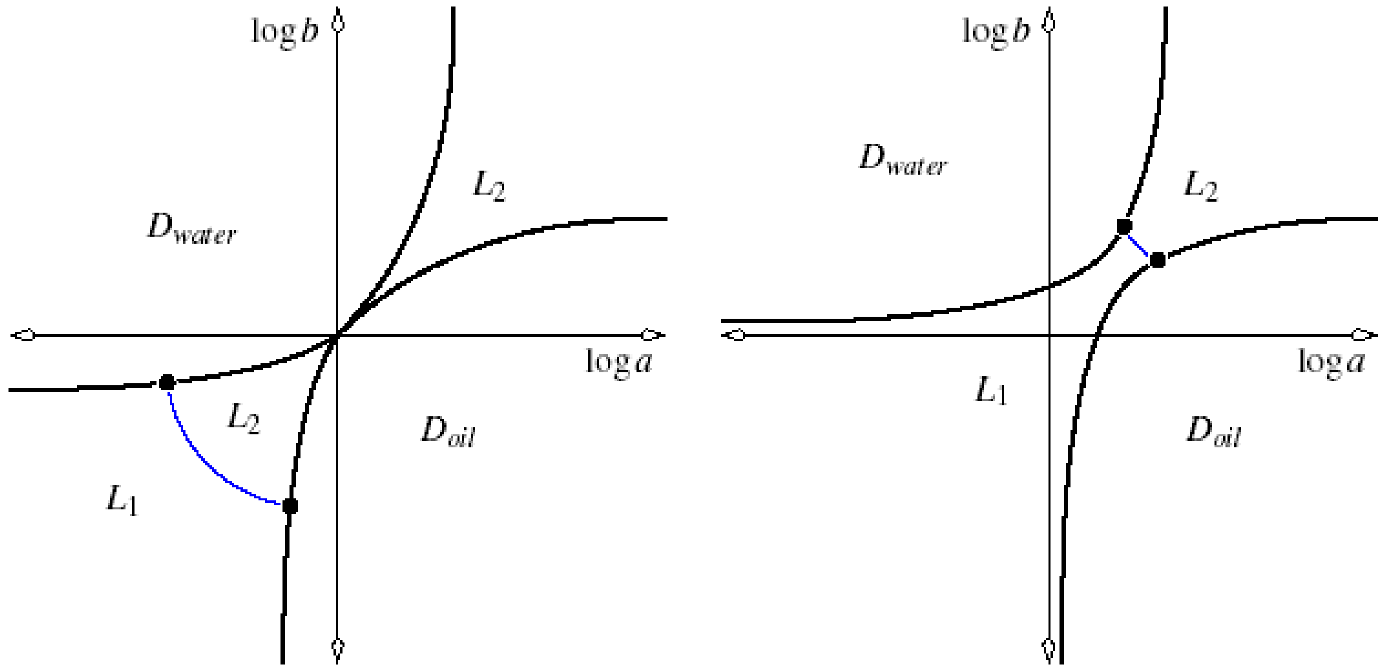
Solving $(***)$ with $\lambda_C = 0$ for some choices of C gives an UPPER BOUND on $\bar{\kappa}_n(\alpha, \beta, \gamma)$.

UPPER BOUNDS : Morita for Bilateral Dyck Path Localization

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?

Note: Caravenna and Giacomin (2005) ElectronCommProbab 10 179-89 $\Rightarrow$ deloc phase bounds don't change.

Higher Order Morita Approximations:

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

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

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 $C \subseteq \{1, 2, \ldots, \sigma\} = [\sigma]$ 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

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

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

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

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

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

Factorization can be used to solve for B_σ and obtain

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

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

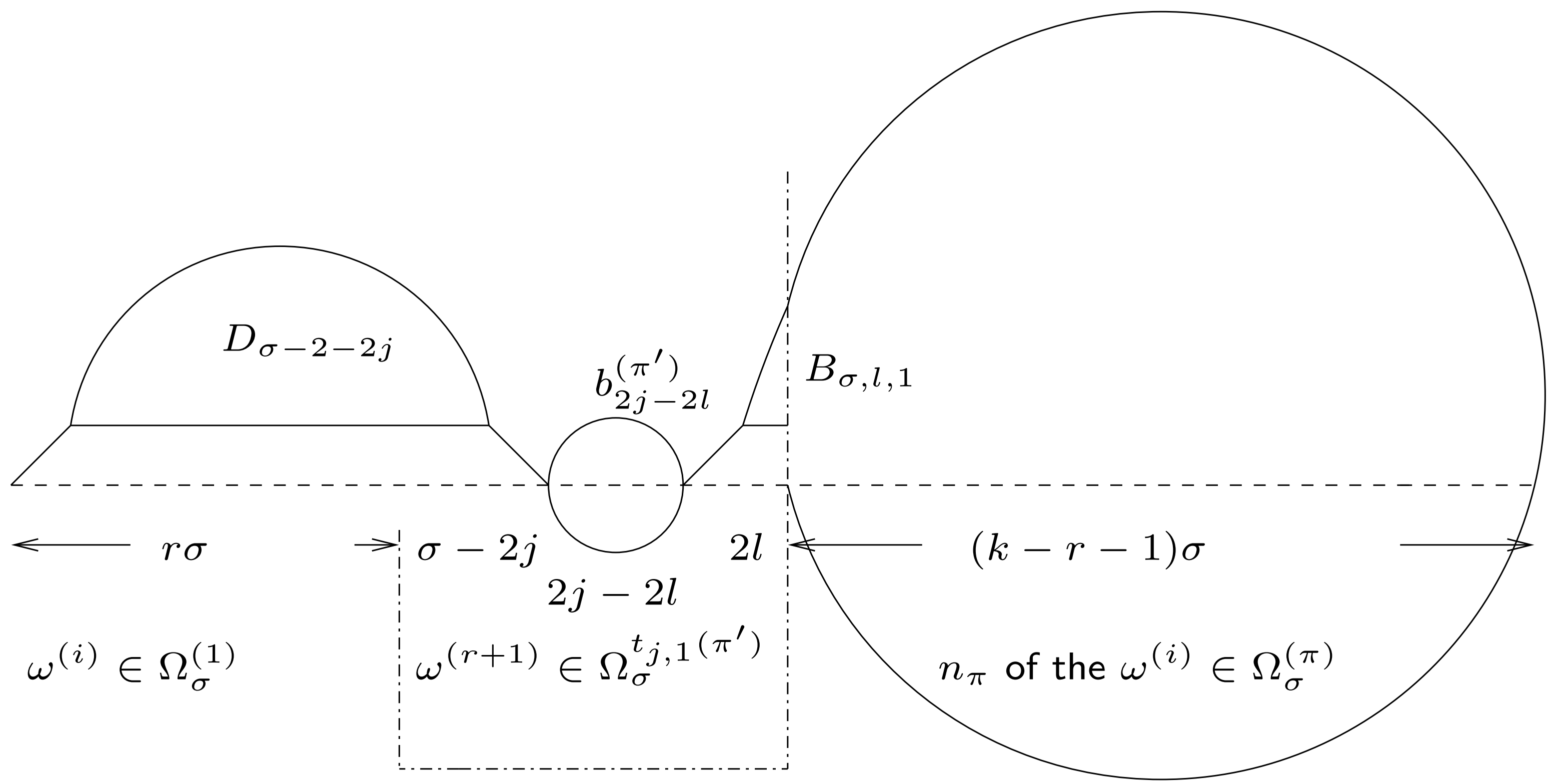


Figure : Schematic representation of factorization.

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

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

By Caravenna & Giacomin (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

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

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*

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

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

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

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 $\sigma \geq 12 \Rightarrow$

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

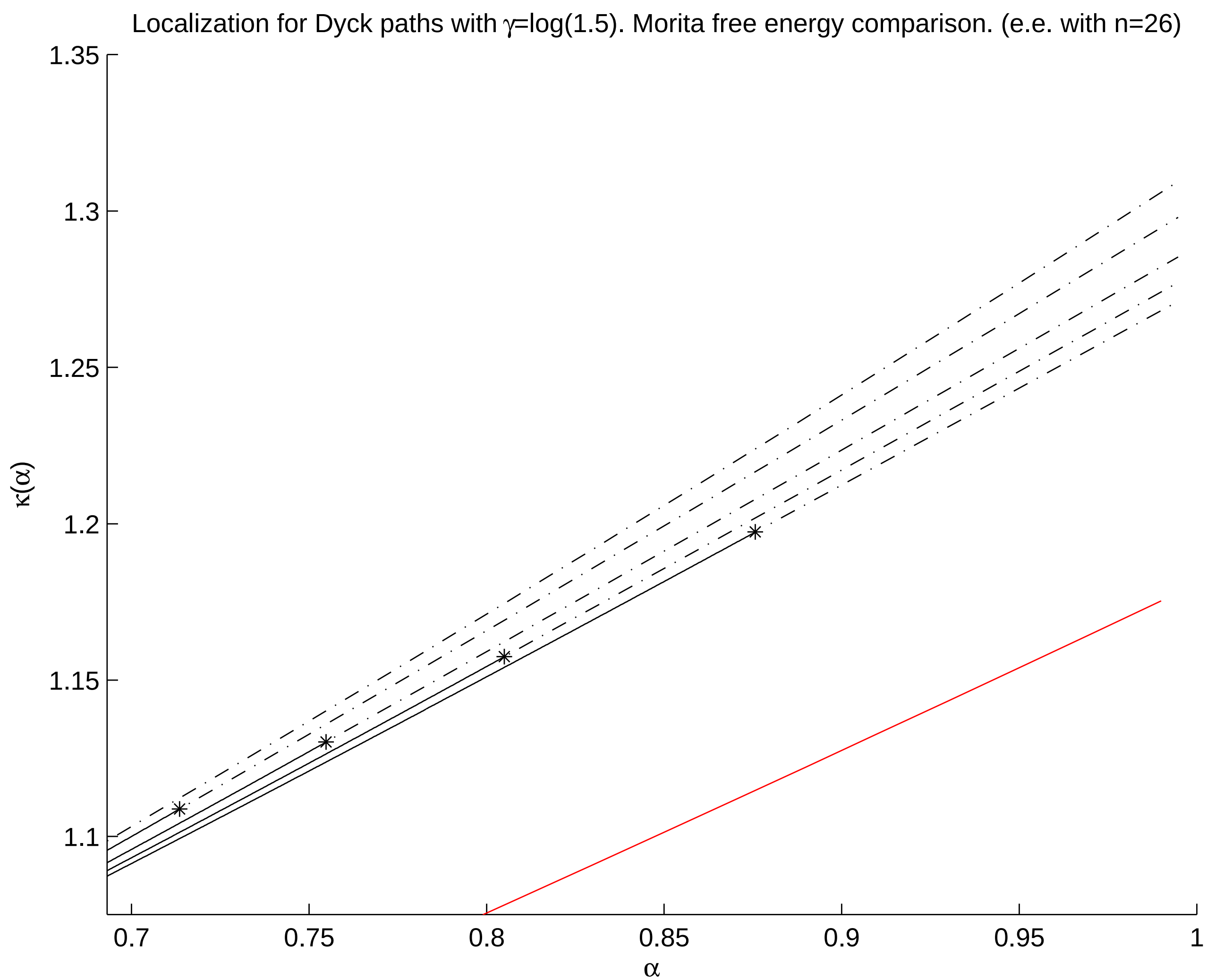
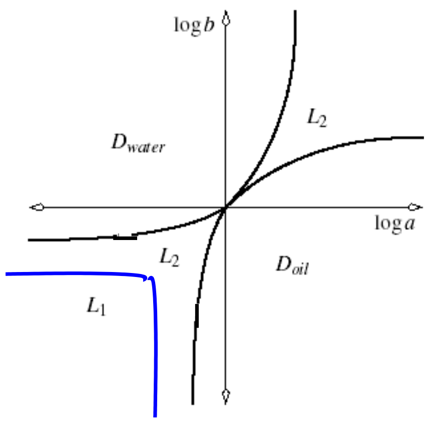
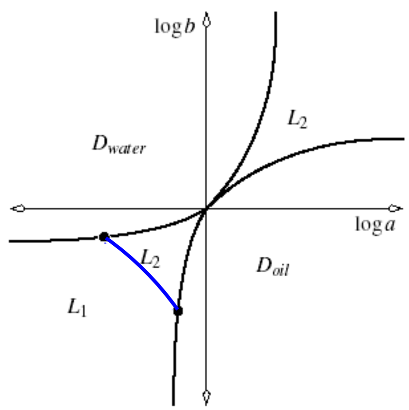


Figure : At $\gamma = \log(1.5)$ and $\alpha = \beta$, bounds on the limiting quenched average free energy for various choices of σ. Dotted curves correspond to bounds obtained from the mixture; solid curves correspond to bounds obtained using a pole.

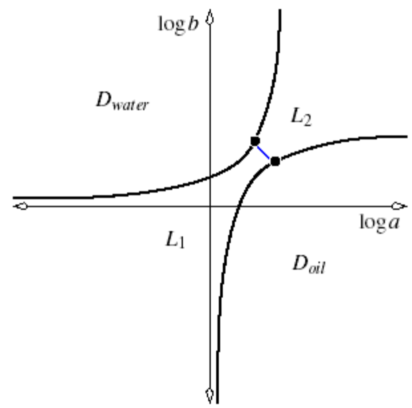
For $1 \leq \sigma < 12$:



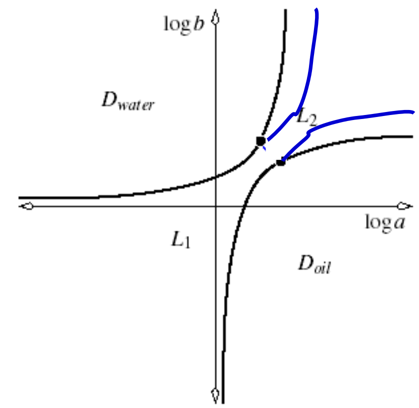
$\gamma < \log(2/3)$



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



$0 < \gamma < \log 2$



$0 < \gamma < \log 2$

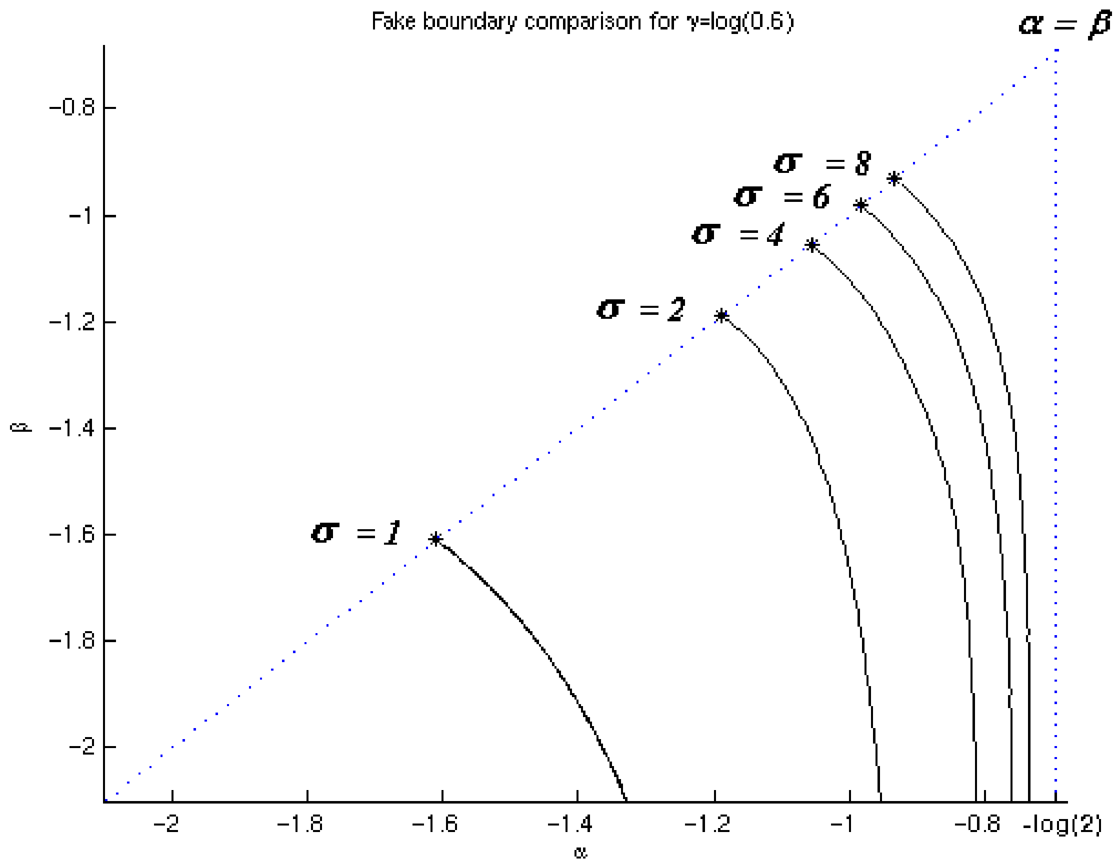


Figure : For $\gamma = \log(0.6)$, the phase boundary in the $(\alpha, \beta)-$plane between the truly localized phase and the mixture phase is shown for various choices of σ.

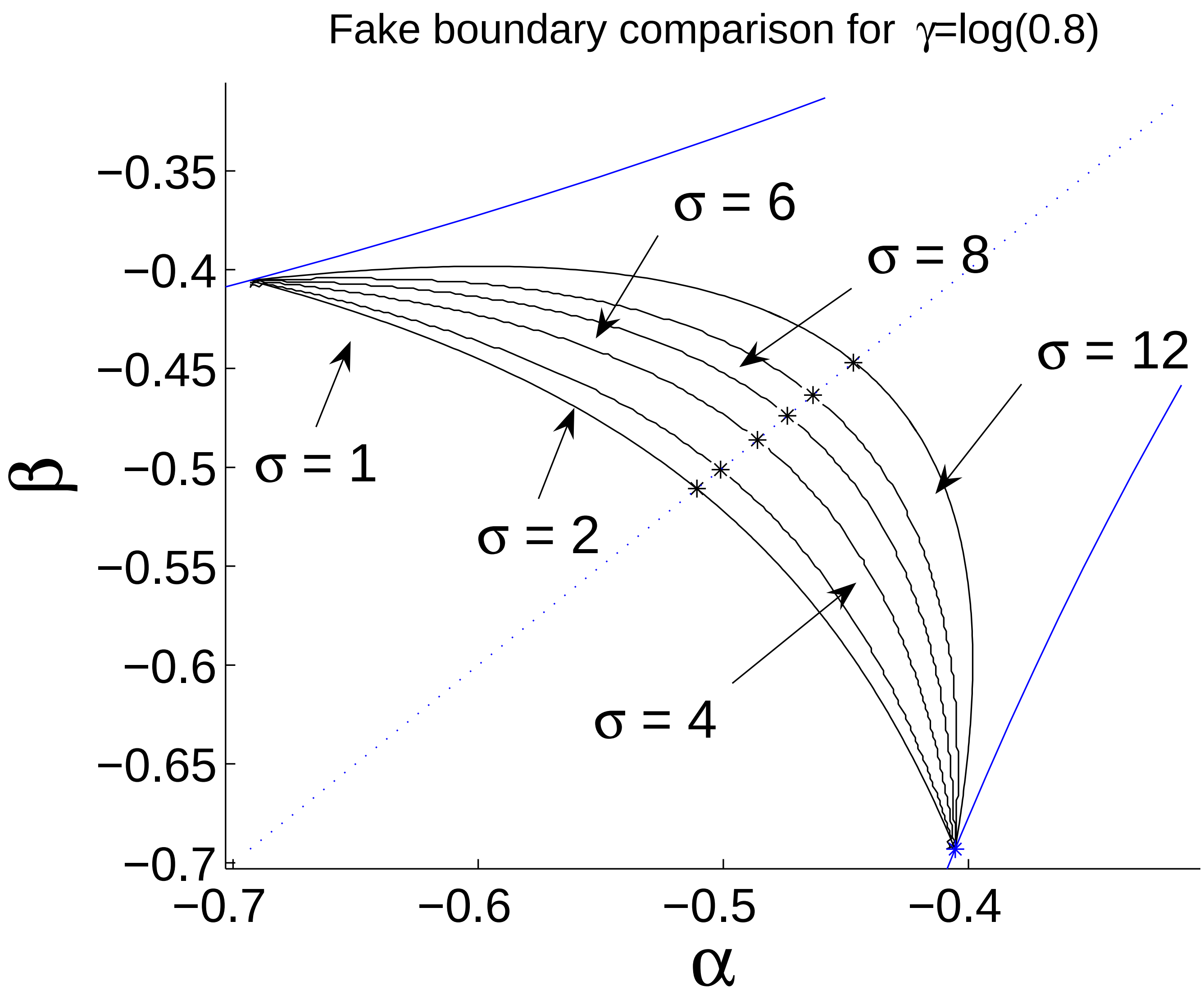


Figure : For $\gamma = \log(0.8)$, the phase boundary in the $(\alpha, \beta)-$plane between the truly localized phase and the mixture phase is shown for various choices of σ.

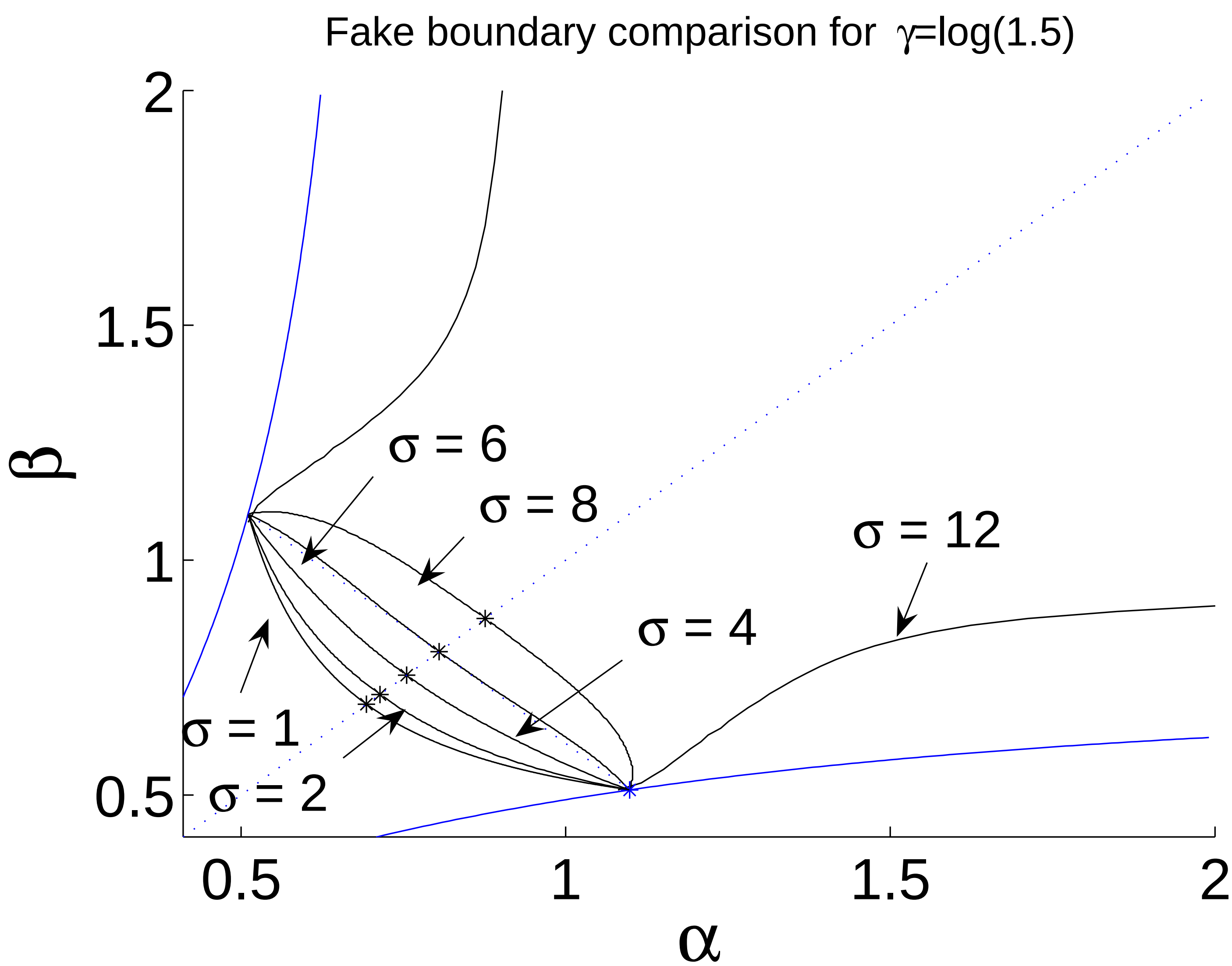


Figure : For $\gamma = \log(1.5)$, the phase boundary in the $(\alpha, \beta)-$plane between the truly localized phase and the mixture phase is shown for $\sigma = 1, 2, 4, 6, 8, 12$.

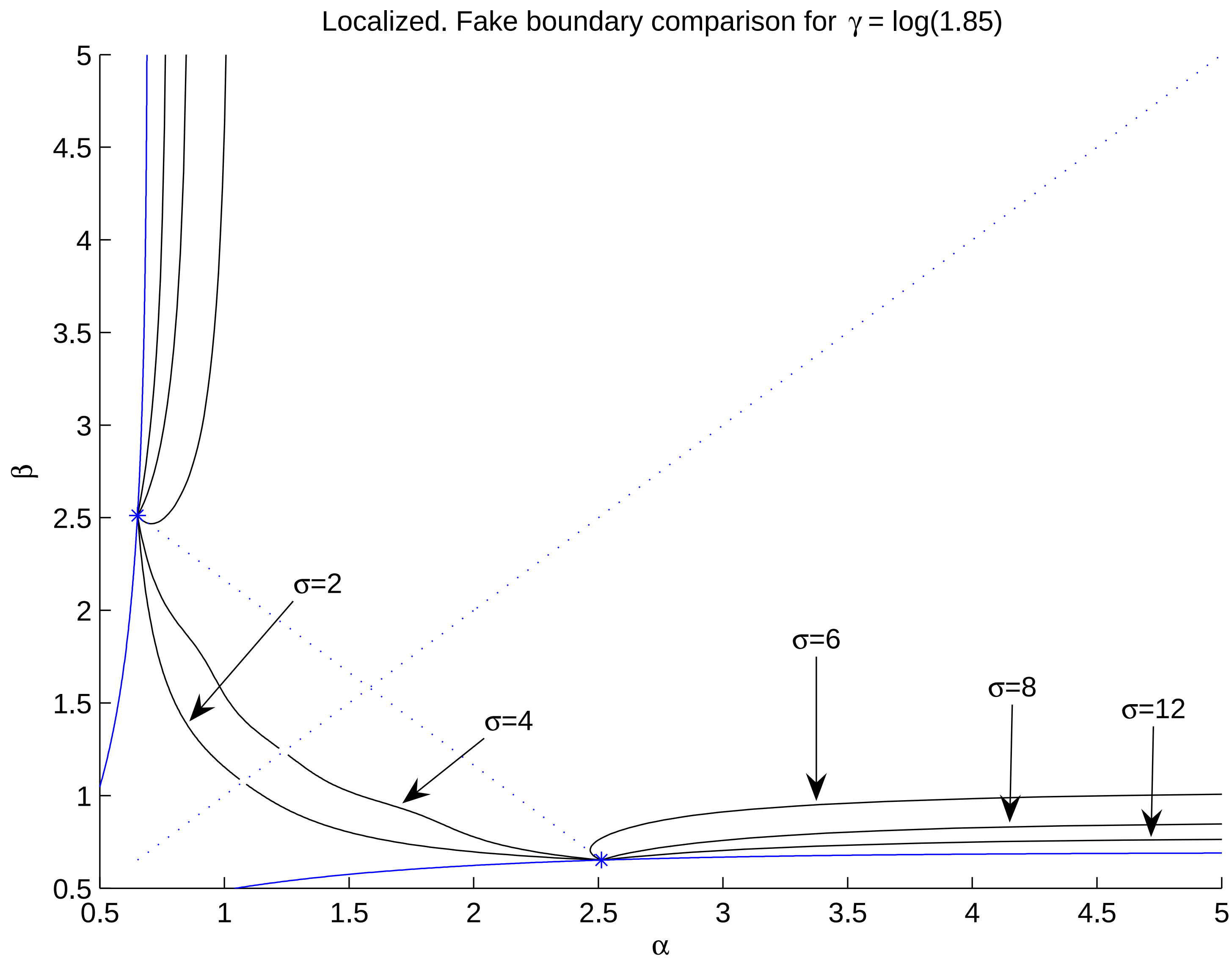


Figure : For $\gamma = \log(1.85)$, the phase boundary in the $(\alpha, \beta)-$plane between the truly localized phase and the mixture phase is shown for $\sigma = 1, 2, 4, 6, 8, 12$.

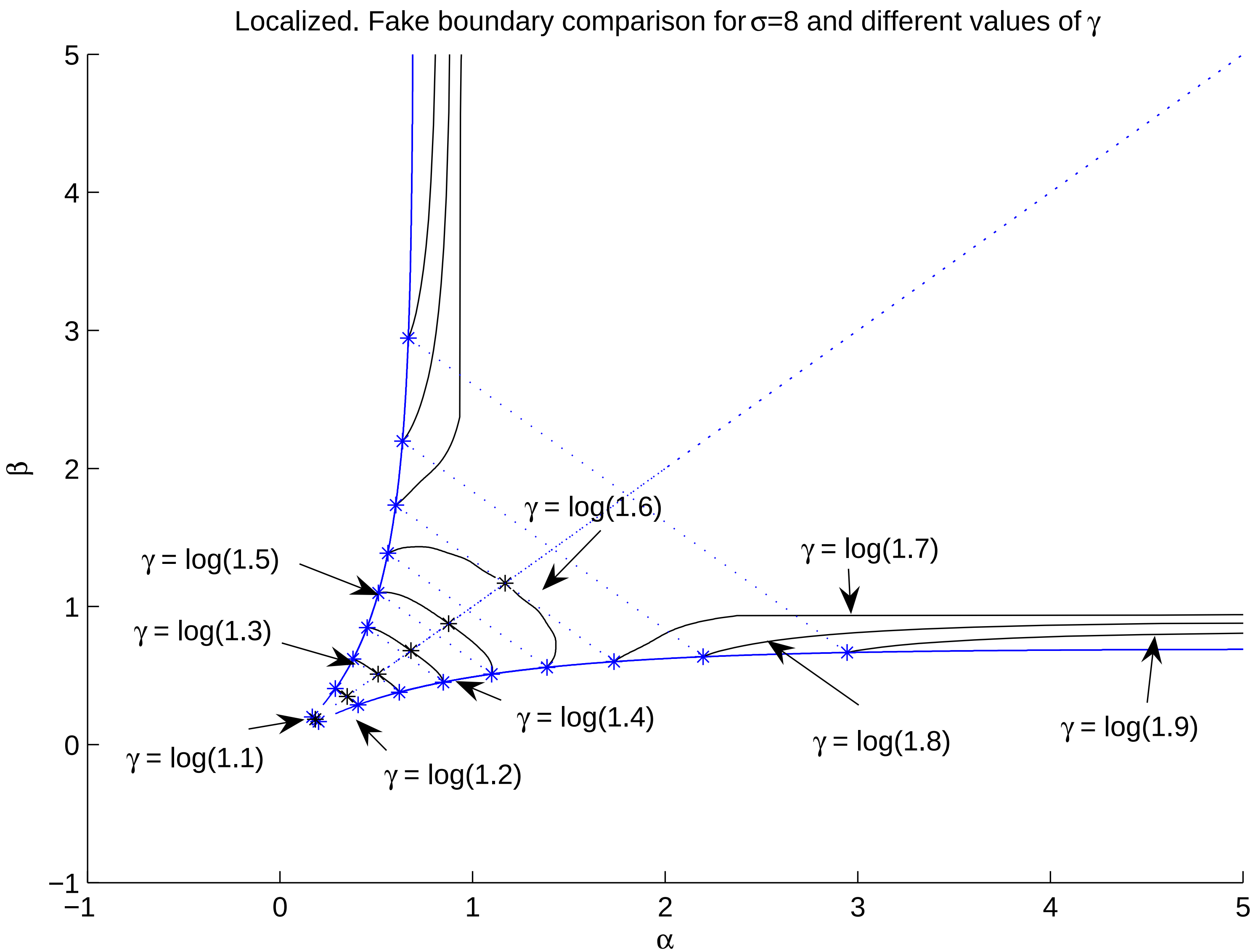


Figure : For $\sigma = 8$, the phase boundary in the $(\alpha, \beta)-$plane between the truly localized phase and the mixture phase is shown for $\gamma = \log(1.1 + i(0.1)), i = 0, ..., 8$. Blue line is $\beta = \log(1 - e^{-\alpha}/2) + \log 2$.

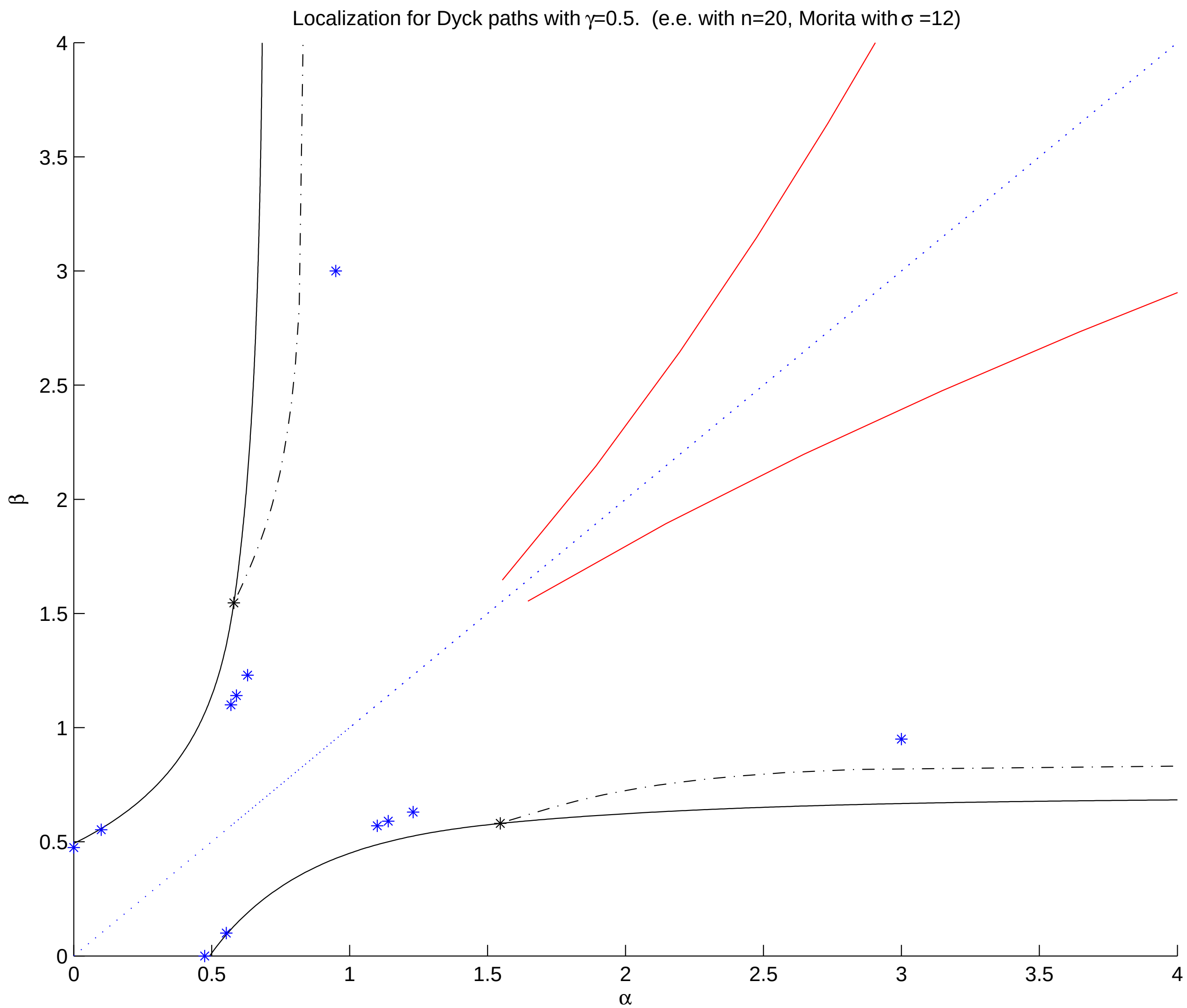


Figure : For $\gamma = 0.5$, some bounds on the phase boundary and monte carlo estimates.

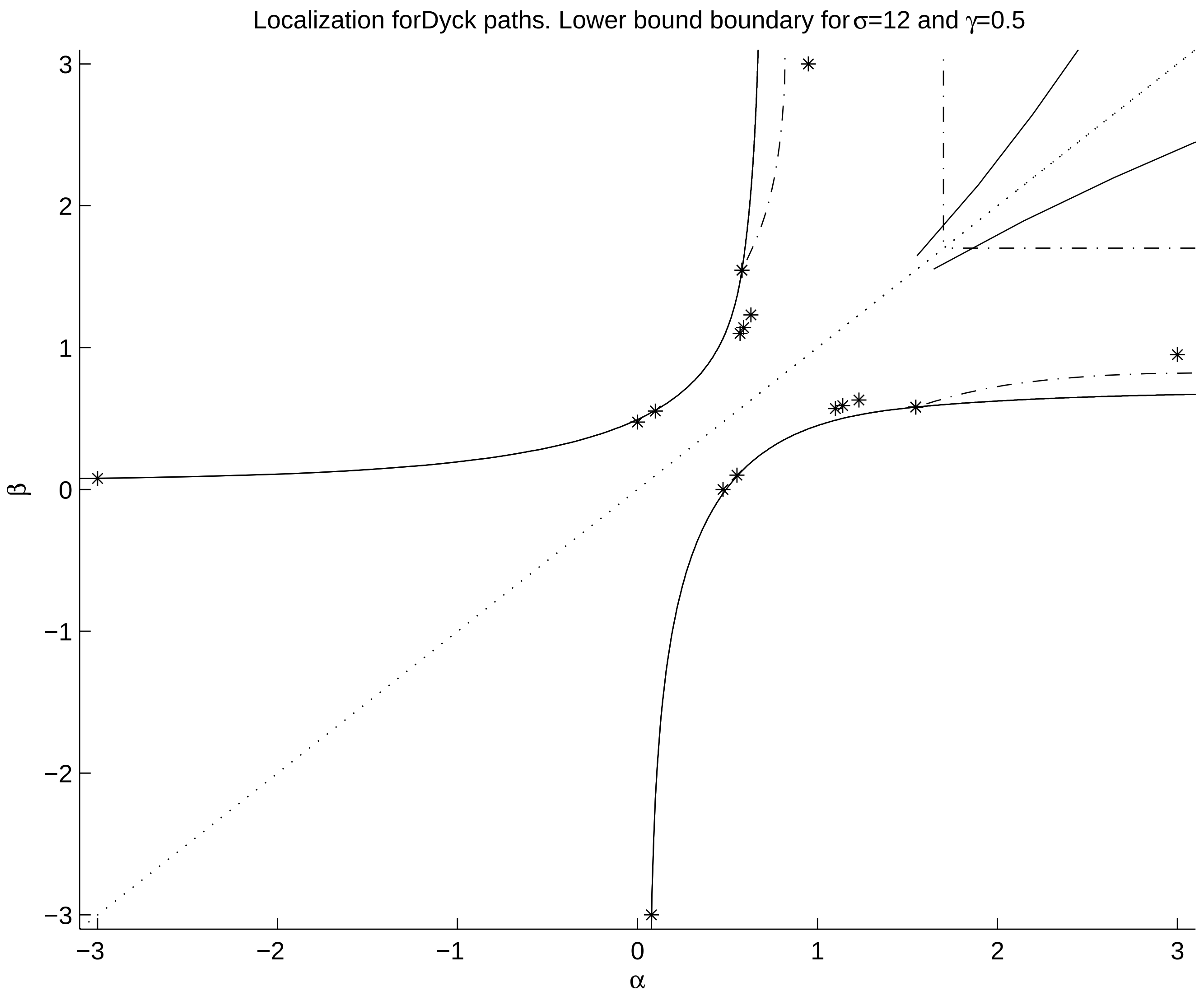


Figure : For $\gamma = 0.5$, some bounds on the phase boundary and monte carlo estimates.

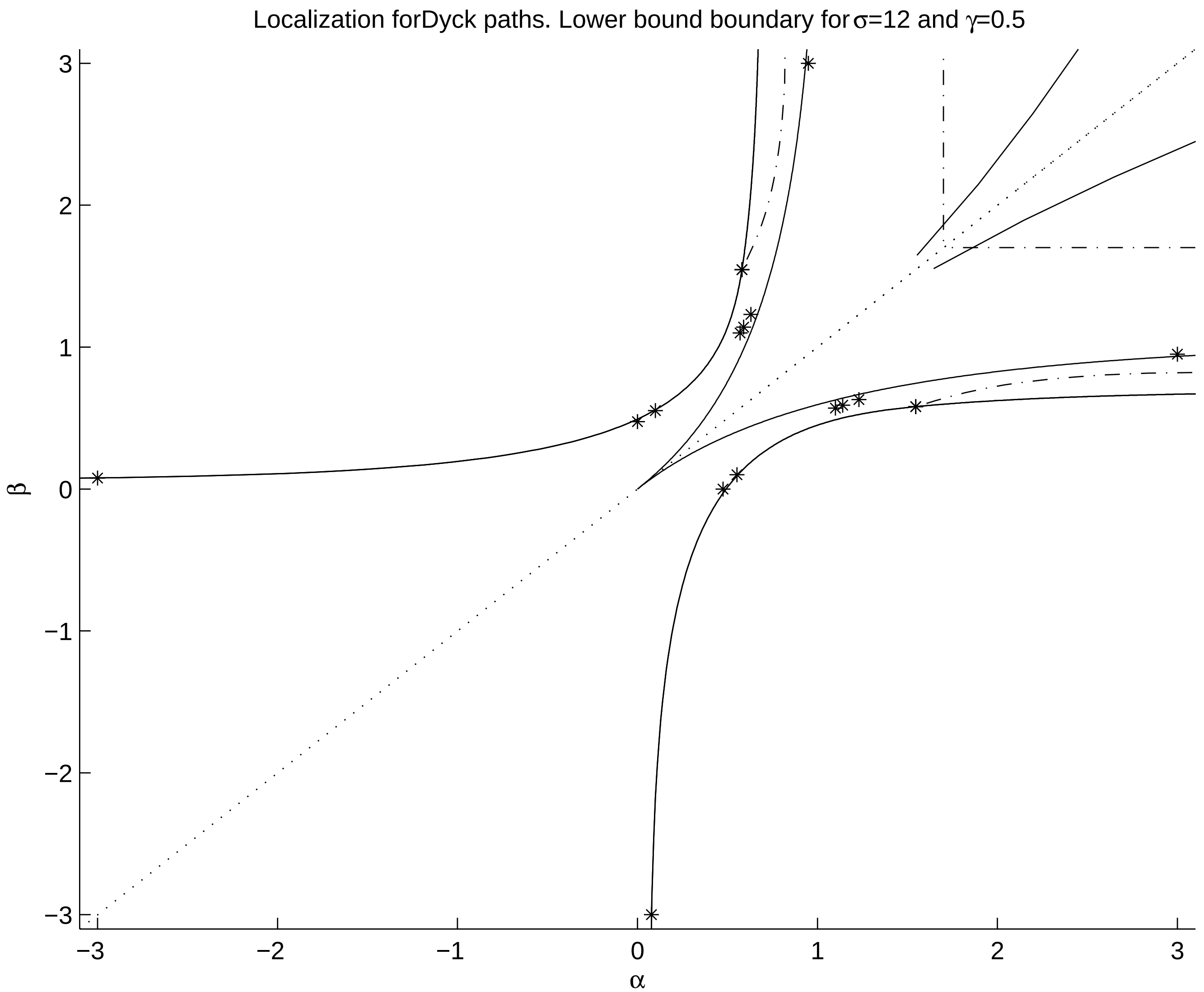


Figure : For $\gamma = 0.5$, Bodineau and Giacomin (2004) JSP 117 801-18 lower bound $\Rightarrow \beta_c \leq (3/2)\log(2 - e^{-2\alpha/3})$.

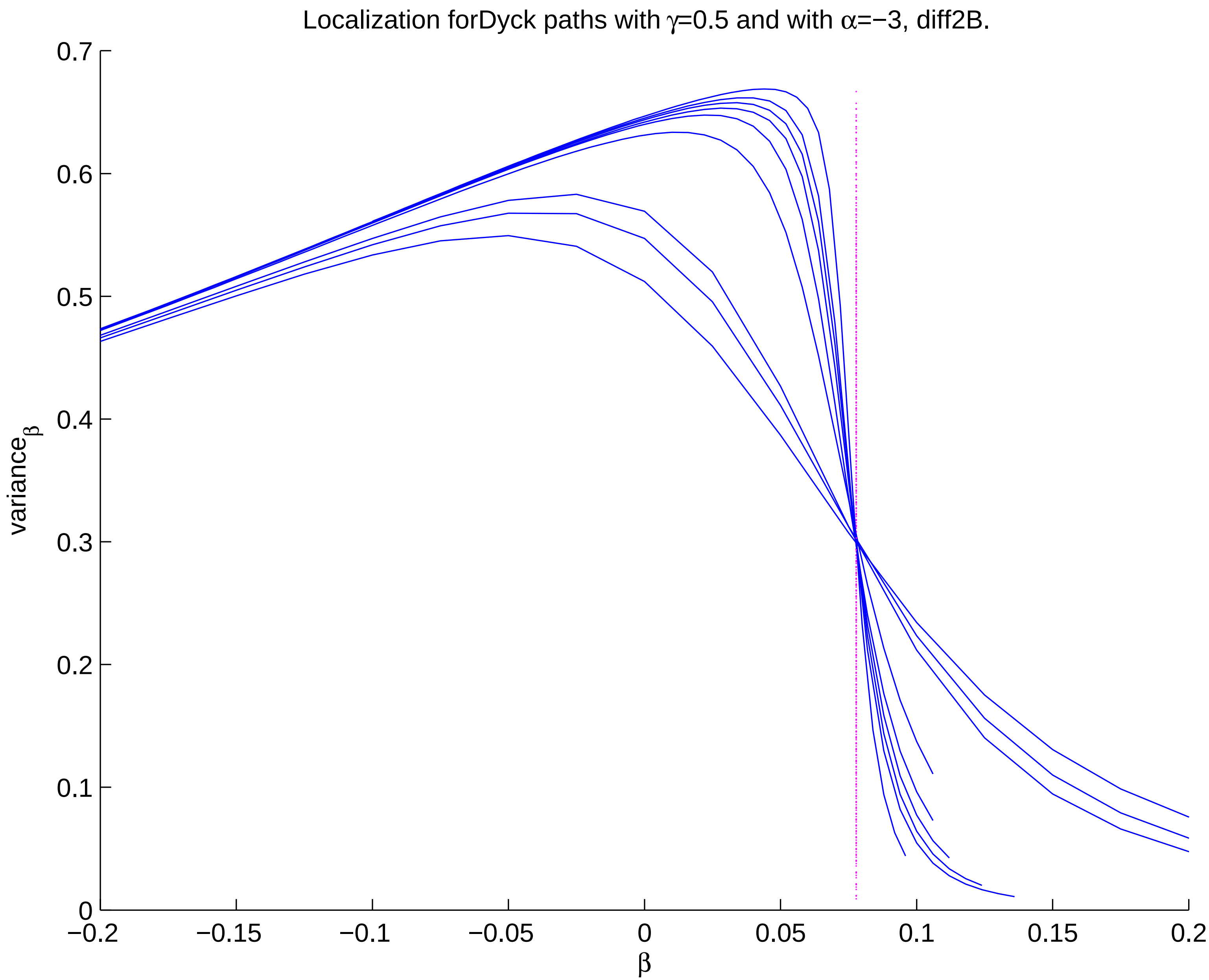


Figure : For $\gamma = 0.5, \alpha = -3$, the variance of the number of B's below, $\mathrm{var}(\mathrm{v_B})$.

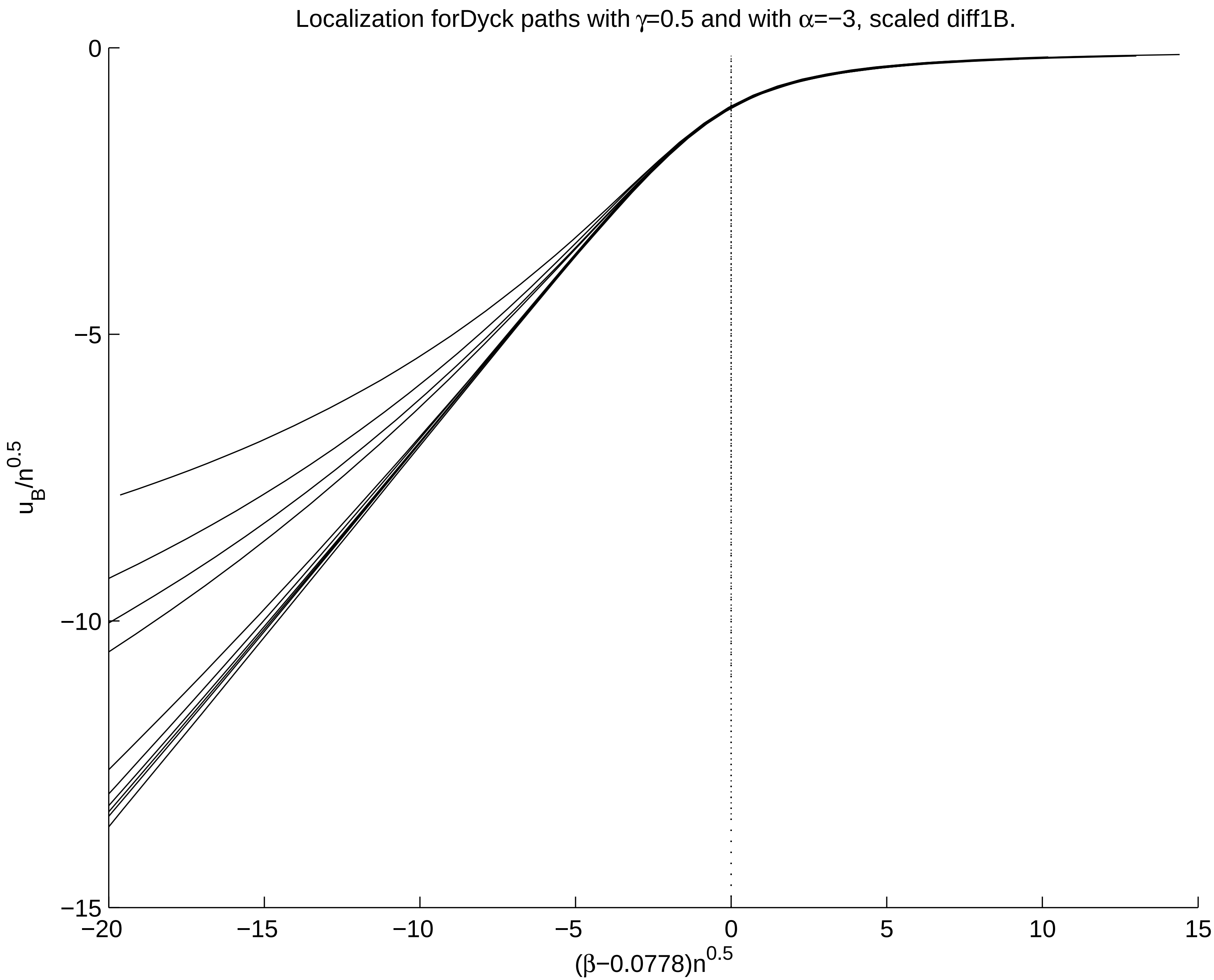


Figure : For $\gamma = 0.5, \alpha = -3$, the scaled "energy".

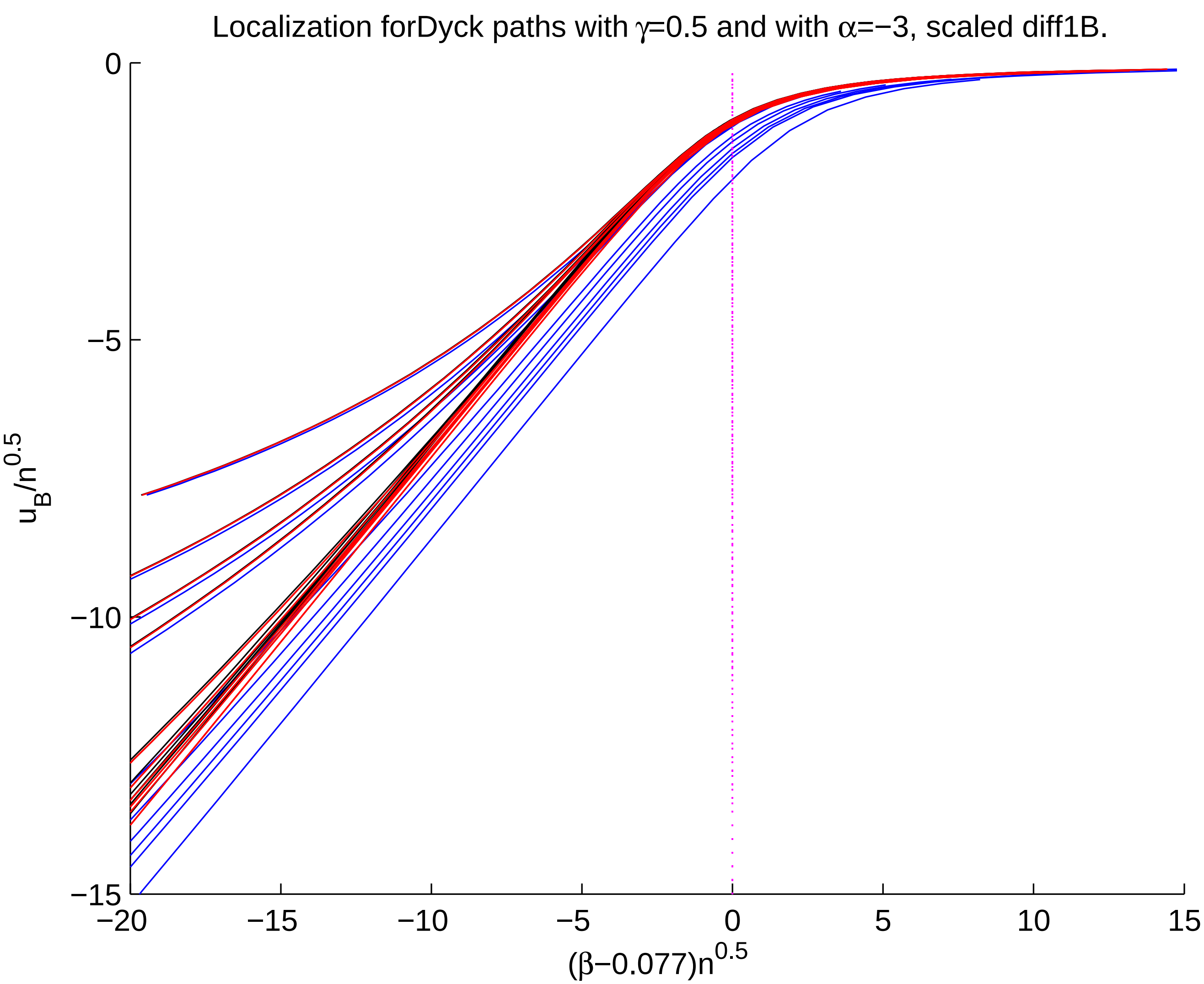


Figure : For $\gamma = 0.5, \alpha = -3$, different choices for scaling function $\beta_c = 0.077$(red), 0.07(blue), 0.078(black).

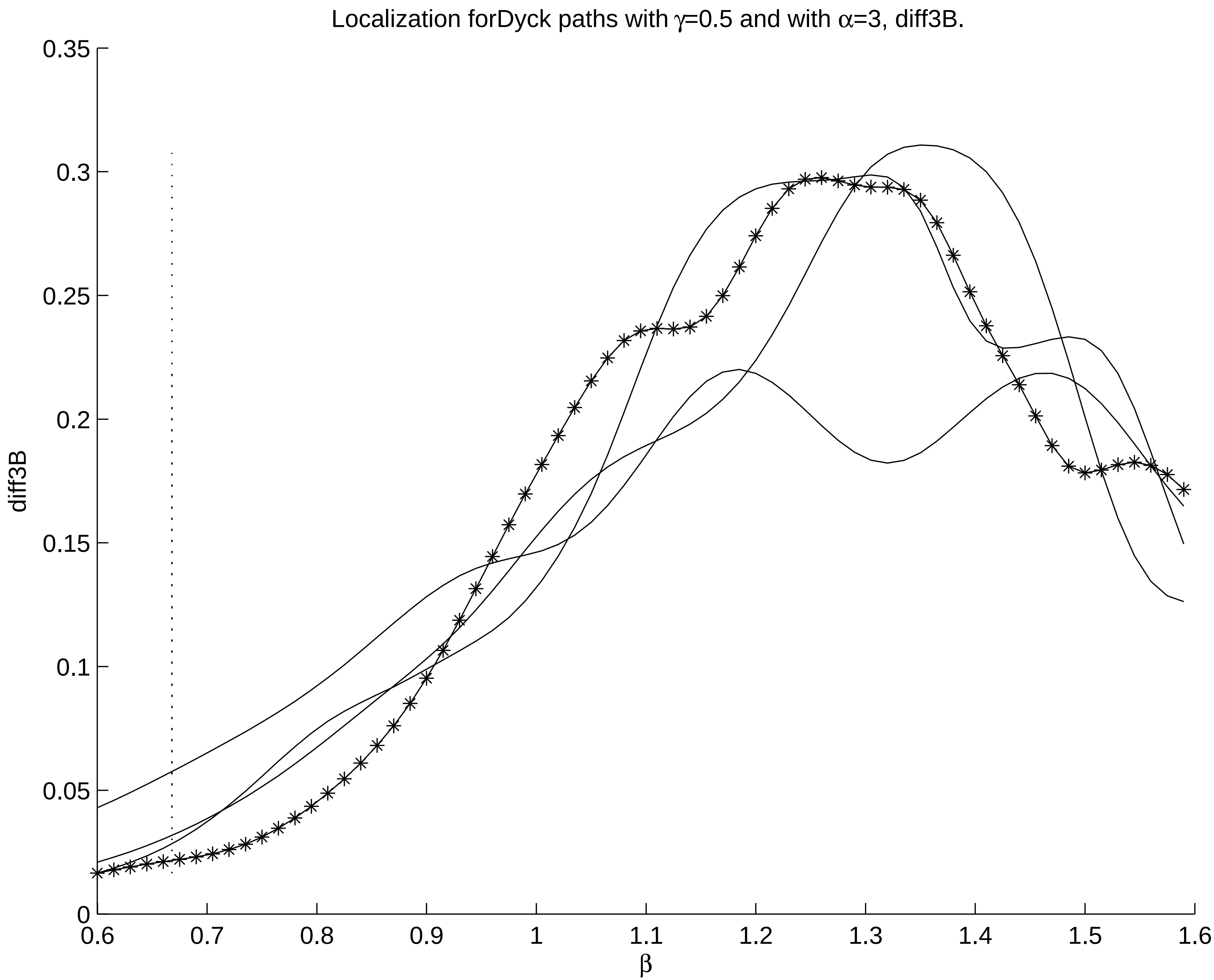


Figure : For $\gamma = 0.5, \alpha = 3$, the 3rd deriv w.r.t. β for $n = 500, 1000, 1500, 2000$.

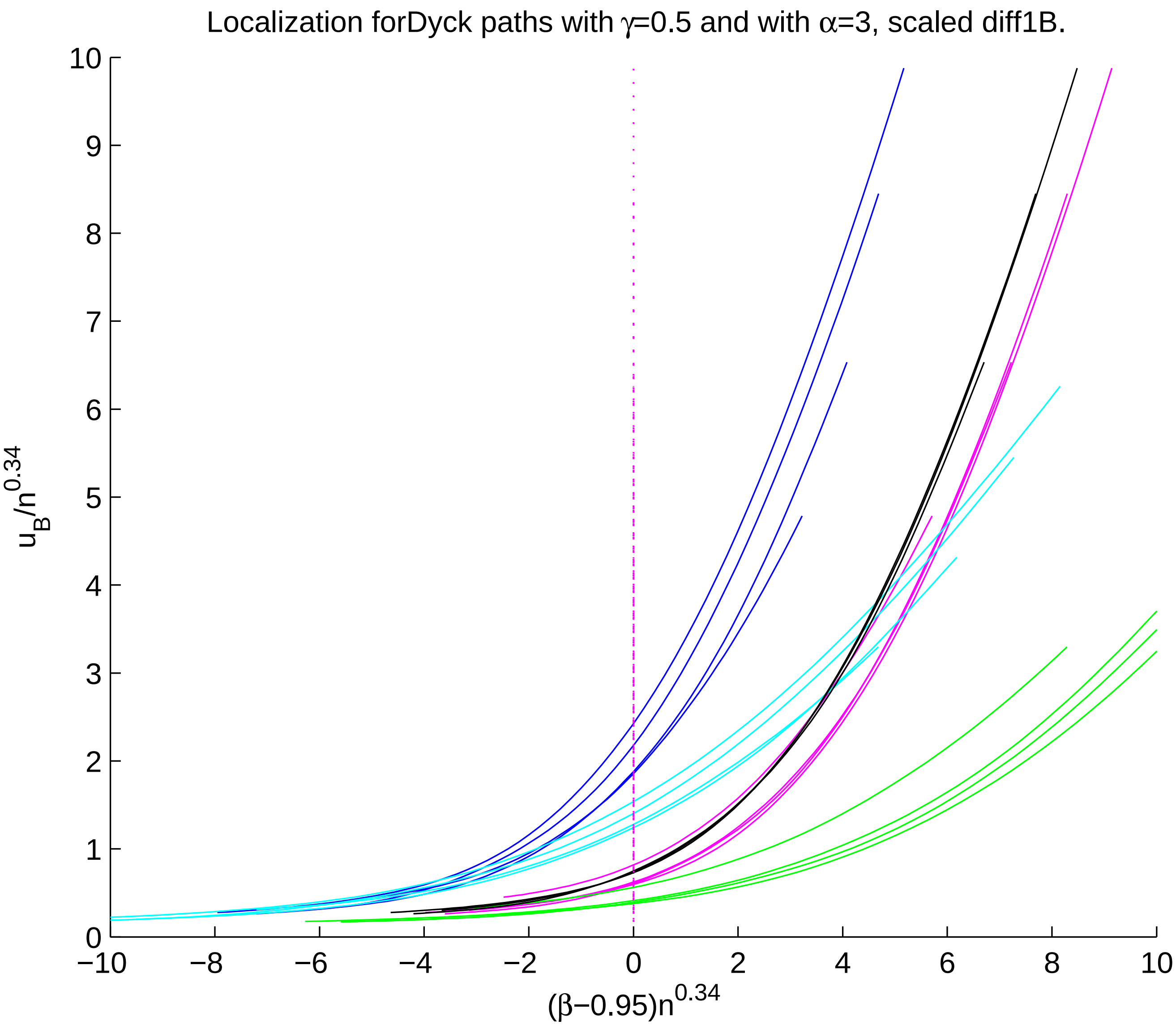


Figure : For $\gamma = 0.5, \alpha = 3$, different choices for scaling function (ϕ, β_c) = (0.34,0.9) (magenta), (0.34,1.2) (blue), (0.34,0.95) (black), (0.4,0.9) (green), (0.4,1.2) (turq).

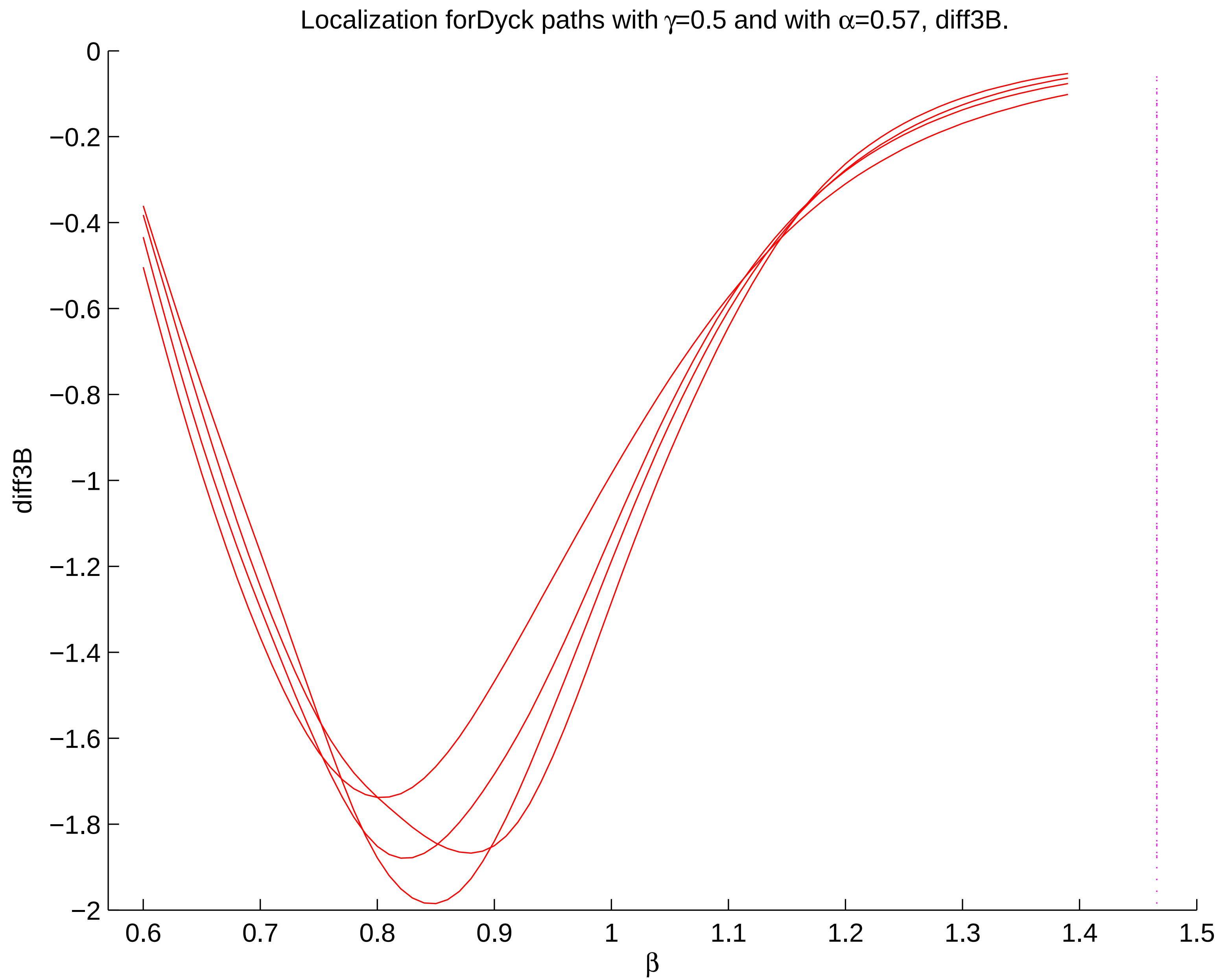


Figure : For $\gamma = 0.5, \alpha = 0.57$, the 3rd deriv w.r.t. β.

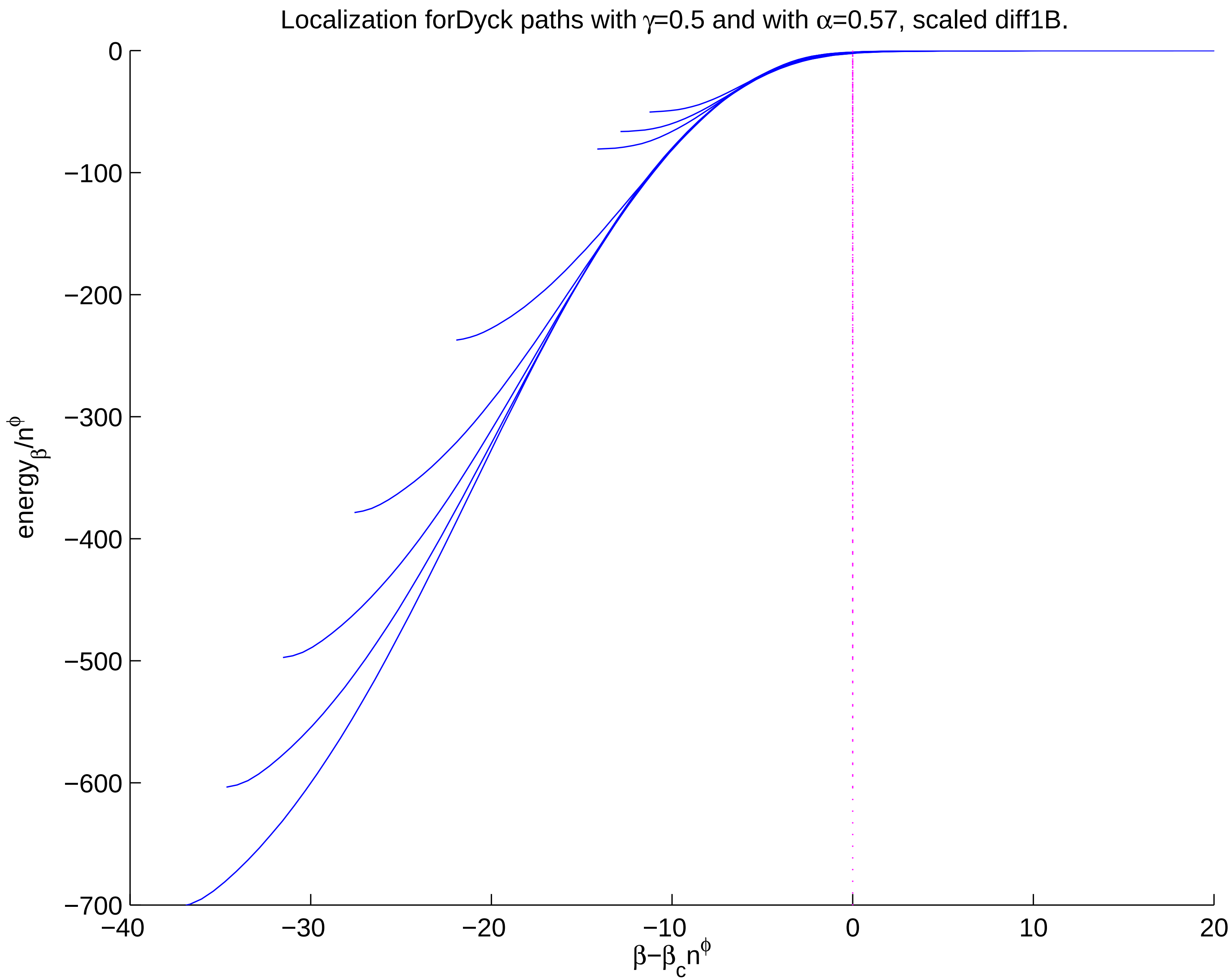


Figure : For $\gamma = 0.5, \alpha = 0.57$, the scaled "energy" with $\phi = 0.37$ and $\beta_c = 1.1$.

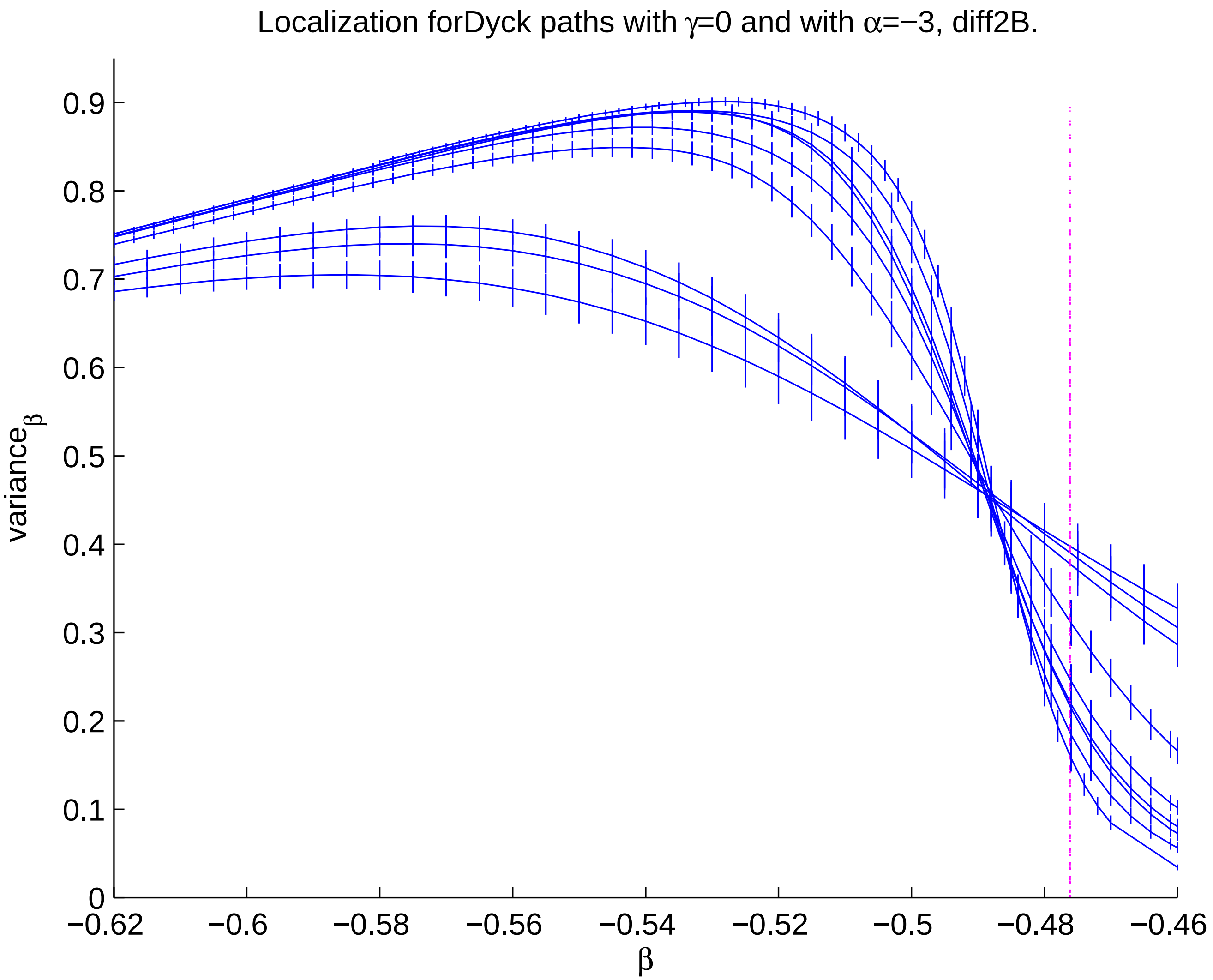


Figure : For $\gamma = 0.0, \alpha = -3$, the variance of the number of B's below, $\mathrm{varv_b}$.

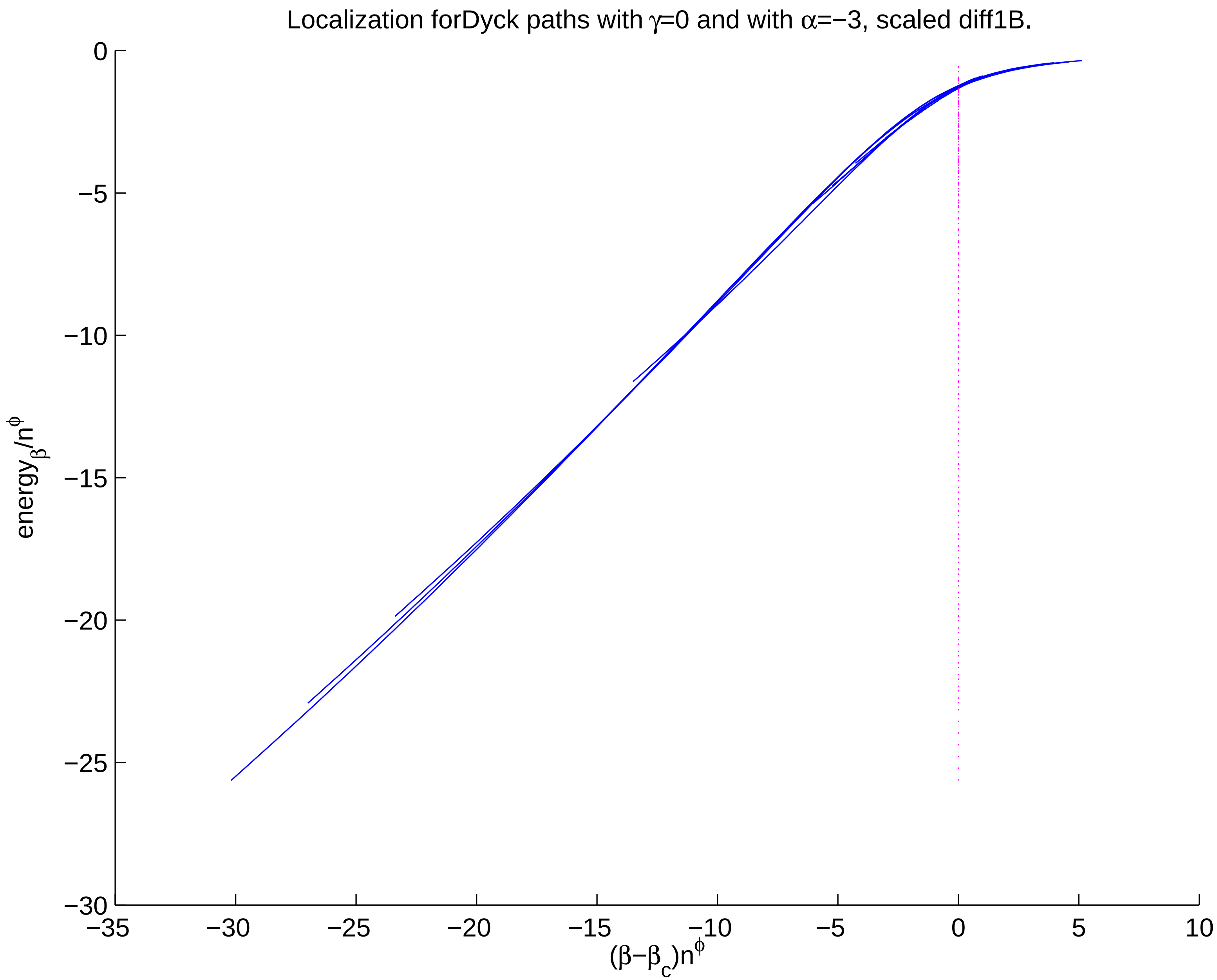


Figure : For $\gamma = 0.0, \alpha = -3$, the scaled "energy".