QFT CondM

ITEP Lattice

Simulation of lattice statistical models with defects: Critical Casimir Effect

Sergei Mostovoy, Oleg Pavlovsky

MSU & ITEP, Moscow, Russia

Critical Casimir Effect:

1. Motivation and historical remarks
    a. Casimir effect: Quantum and Critical
    b. Individual defect
    c. Casimir defect-defect interaction
2. Casimir effect and defect line
    a. Motivation
    b. Collapse of defect line
    c. Casimir self-energy of defect curves: Casimir "antigravity"
    d. Confinement on defect line
    e. Defect-antidefect pier creation
    f. Defect-defect and defect-antidefect interactions on the defect line
3. Conclusion

There are many parallels between the

Quantum Theory and **Classical Statistical Physics.**

Critical Casimir Effect is an example of such connection.

Critical Casimir Effect has numerous applications in

colloid physics,

material science,

nano-structure physics,

biophysics and biomedicine,

and many and many others …

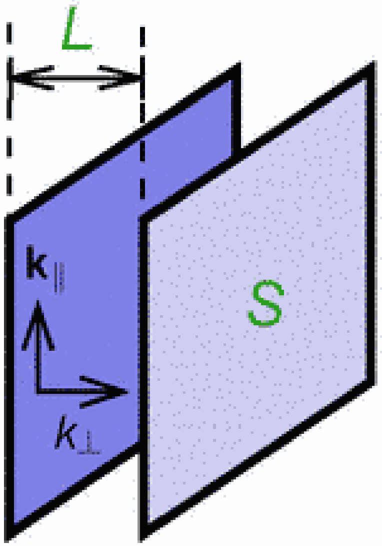
Casimir Effect:
short introduction

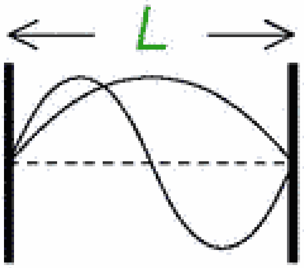
1) **Casimir Effect is macroscopic field theory effect**
2) **Casimir Effect is surface-like effect, surface forces are genereted.**
3) **Microscopic description of Casimir Effect - multipole expansion + relativism at long distance**

5) **At short distance Casimir forces becomes the composition of Van der Waals intermolecular forces.**

Casimir Effect: short introduction

Plates $\Rightarrow \mathbf{E}_{\parallel}, B_{\perp} = 0$, *Boundary conditions!*



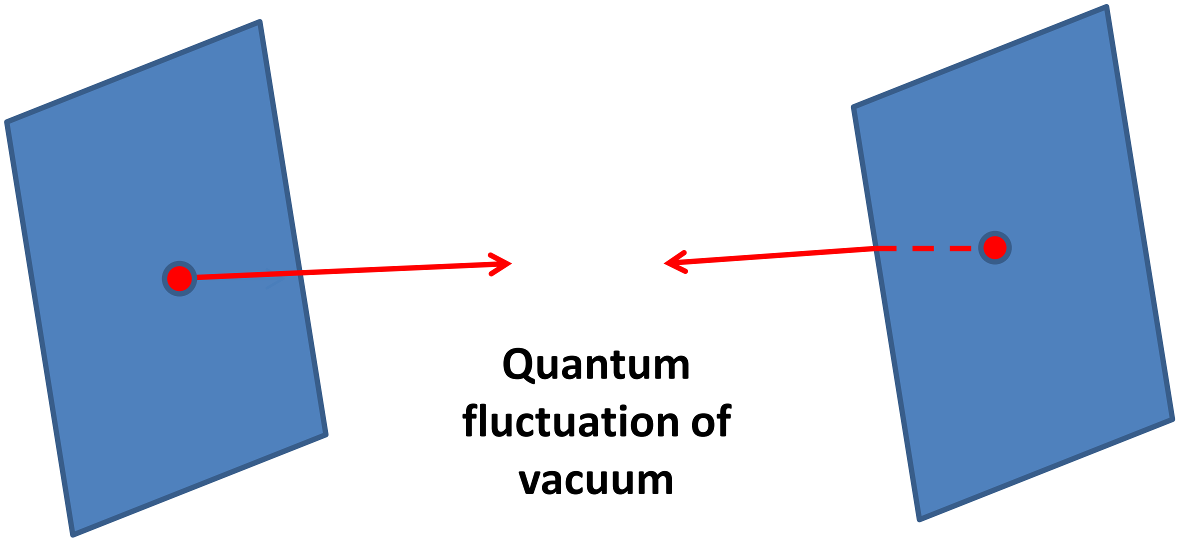


$\rightsquigarrow$ allowed *modes*: $k_{\perp} = \frac{\pi n}{L}, \quad n = 1, 2, \ldots$

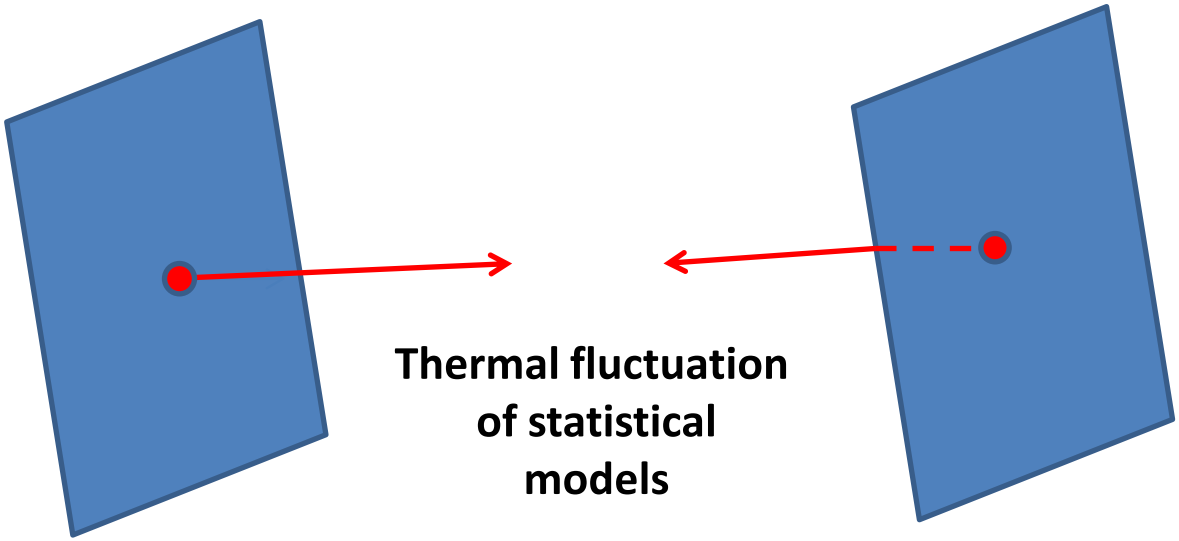
QED: $\mathcal{E} = \sum_{\text{modes}} \frac{1}{2} \hbar c |\mathbf{k}|_{\text{modes}}$ $\quad c$ = speed of light

$$\mathcal{E} = \mathcal{E}_{\text{bulk}} + \mathcal{E}_{\text{surf}}^{(L+R)} + S \frac{\hbar c}{L^3} \left[-\frac{\pi^2}{1440} + O((\kappa L)^{-2}) \right]$$

Critical Casimir Effect: Casimir Effect in statistical model



Critical Casimir Effect: Casimir Effect in statictical model

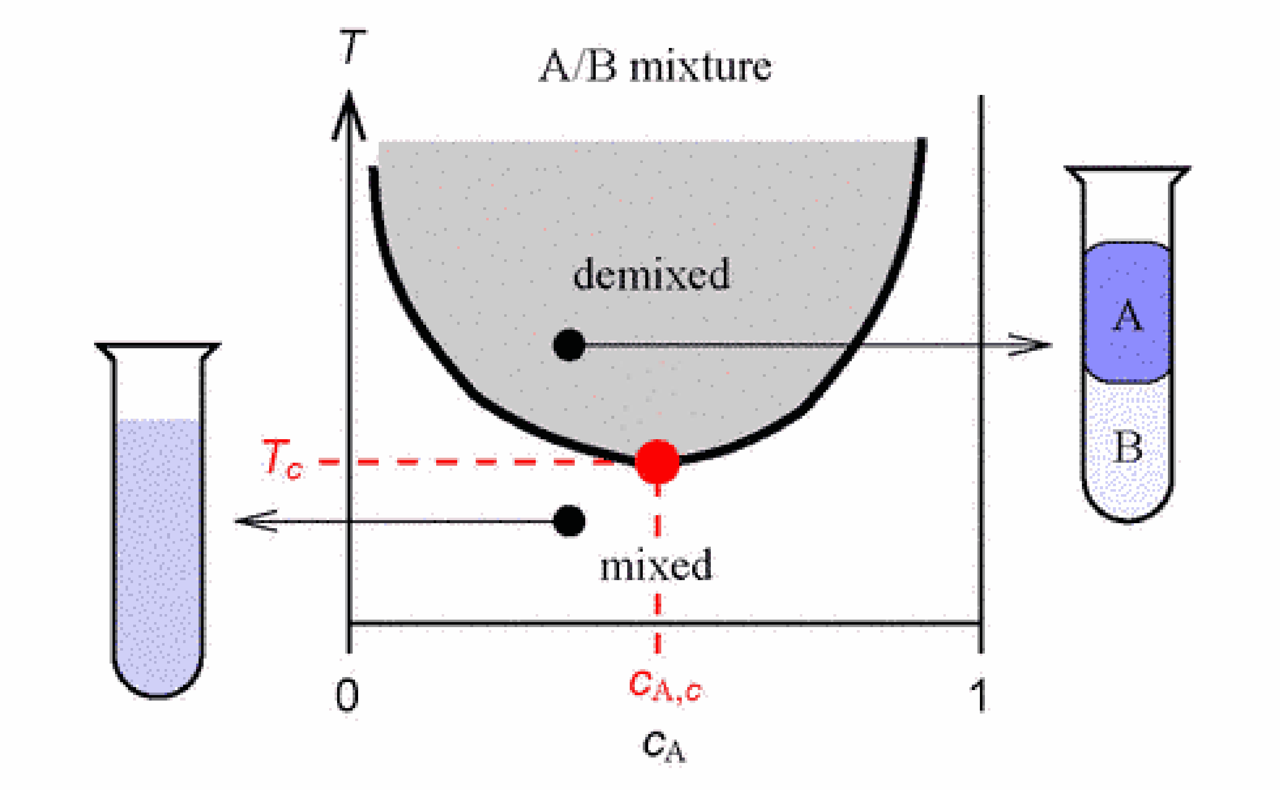


Thermal fluctuation of statistical models

M. E. Fisher, P.-G. de Gennes, C. R. Acad. Sci. Paris Ser. B **287** , 207 (1978).

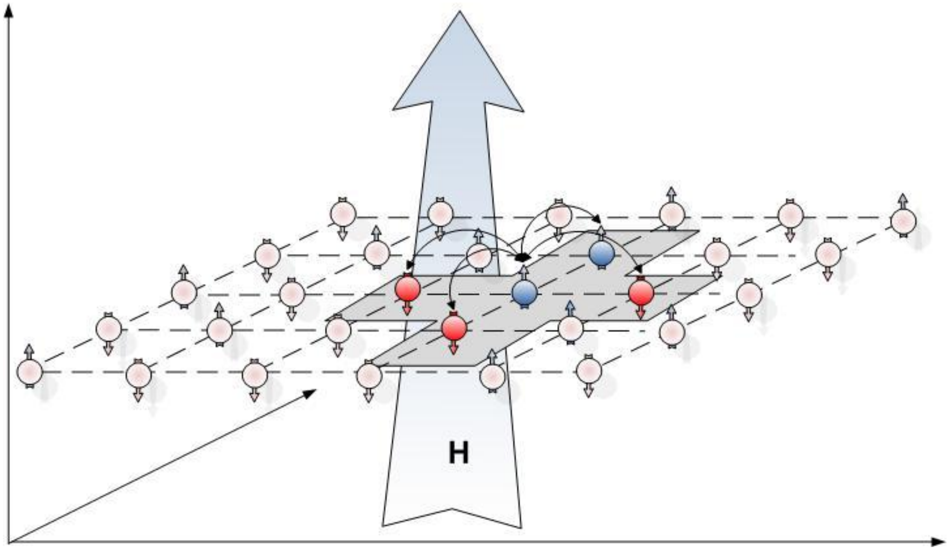
M. Krech, *The Casimir Effect in Critical Systems* (World Scientific, Singapore, 1994)

^{3}He – ^{4}He mixture



Crucial idea: we must study the **Binary Mixture Problem** on the example of suitable **Simple Model** which belongs to the same **class of Universality** that original system!

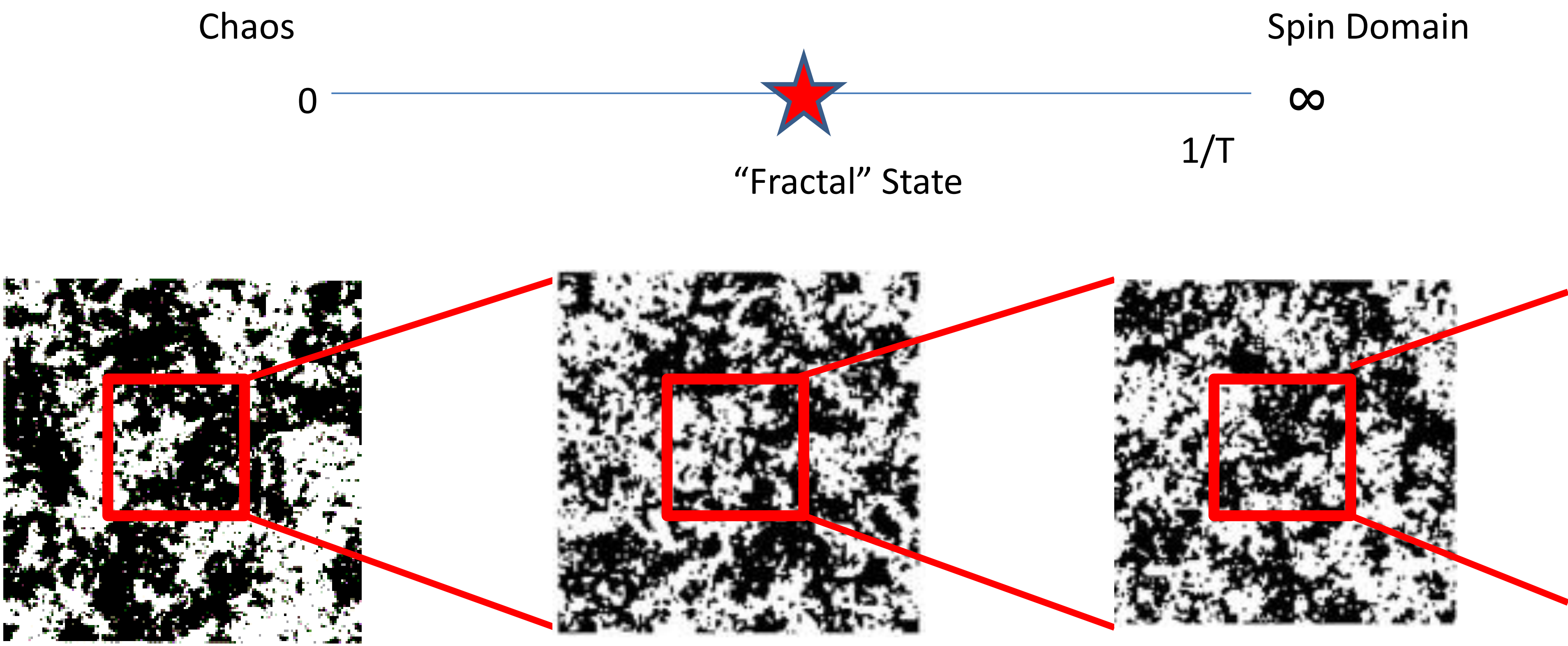
Conformal symmetry and phase transition: Ising model illustration



$$E(Conf) = -J \sum_{x,\mu} \sigma_x \sigma_{x+\mu} + H \sum_x \sigma_x ,$$

$$P(Conf) = \frac{1}{Z} e^{-\beta E(Conf)}$$

Scale invariance at “Fractal” State

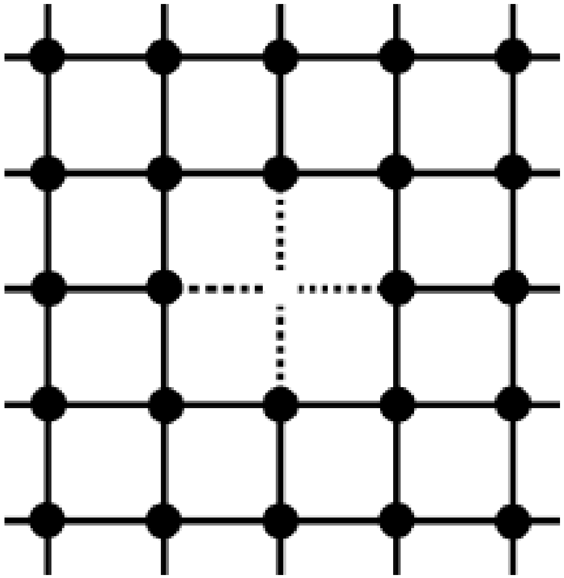


Scale invariance at “Fractal” State

“Fractal” State properties depend only from symmetry of the model.

So, if the model has , for example, defect which breaks **locally** symmetries, it leads to large **non-local** changing's in “Fractal” State at **Critical Point**.

Ising model with defect



$$E(Conf) = -\sum_{x,\mu} J_{x,x+\mu}\sigma_x\sigma_{x+\mu} + H\sum_x \sigma_x,$$

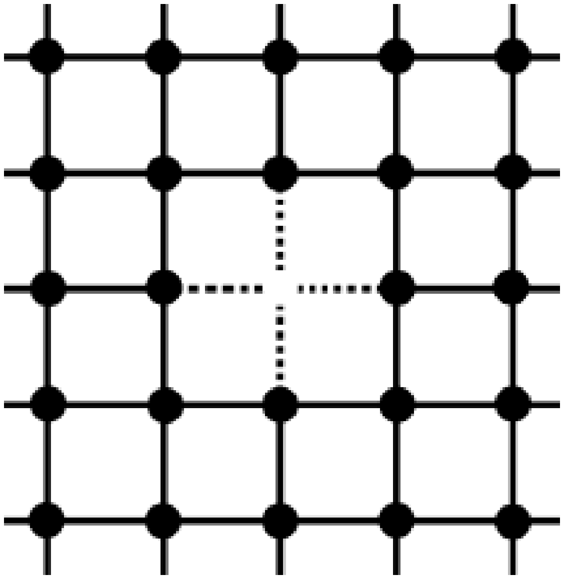
$$P(Conf) = \frac{1}{Z}e^{-\beta E(Conf)}, \qquad \varkappa = \beta J$$

Mass of defect:

$$m_d = E_d - E_0,$$

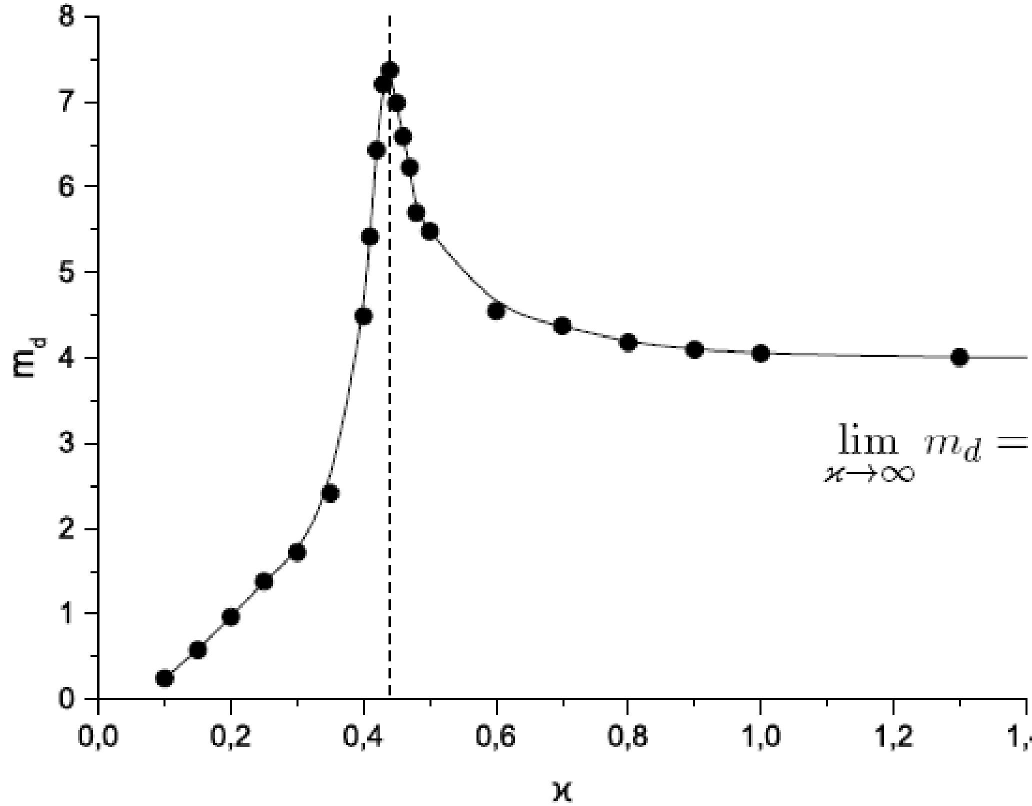
Subtraction procedure

MC of Ising model with defects



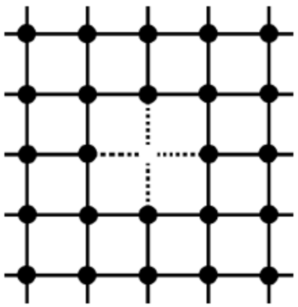
Mass of defect:

$$m_d = E_d - E_0,$$



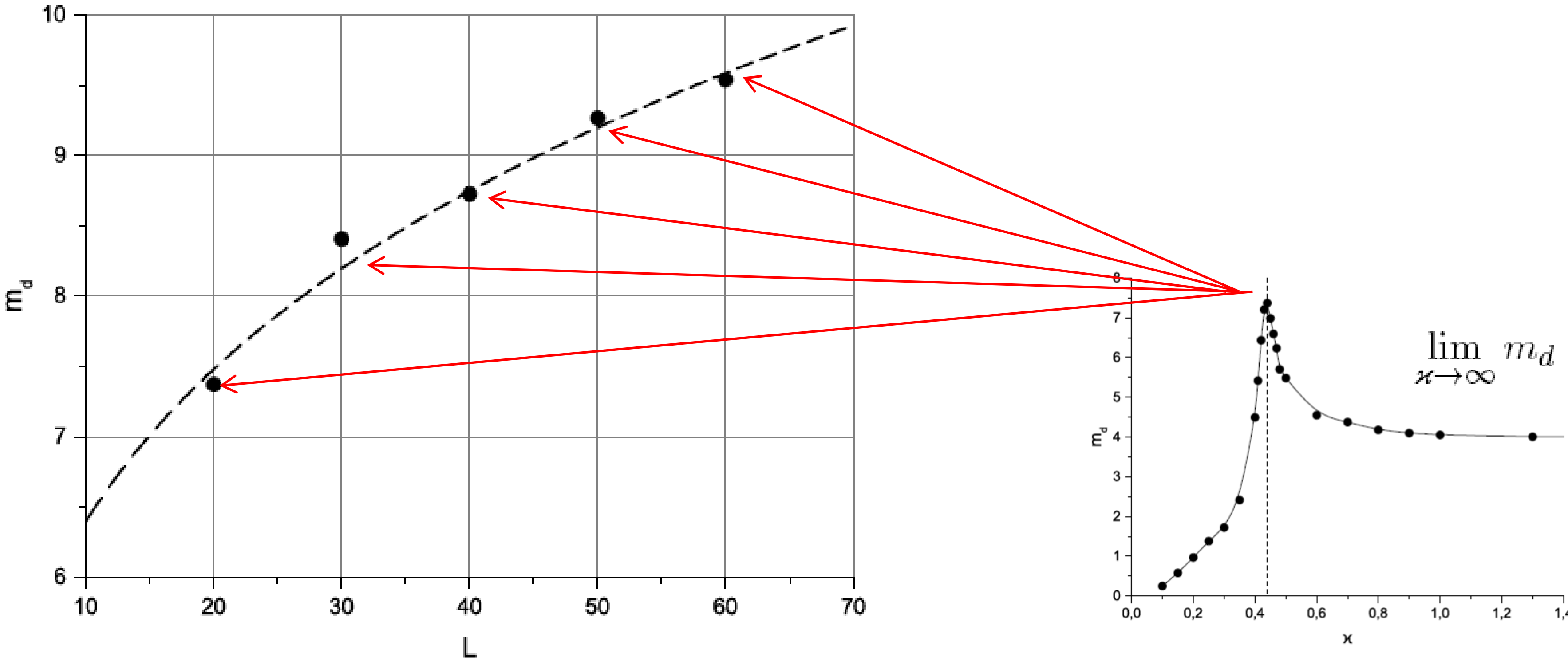
$$\lim_{\varkappa \to \infty} m_d = 4J.$$

Mass of defect: volume dependence



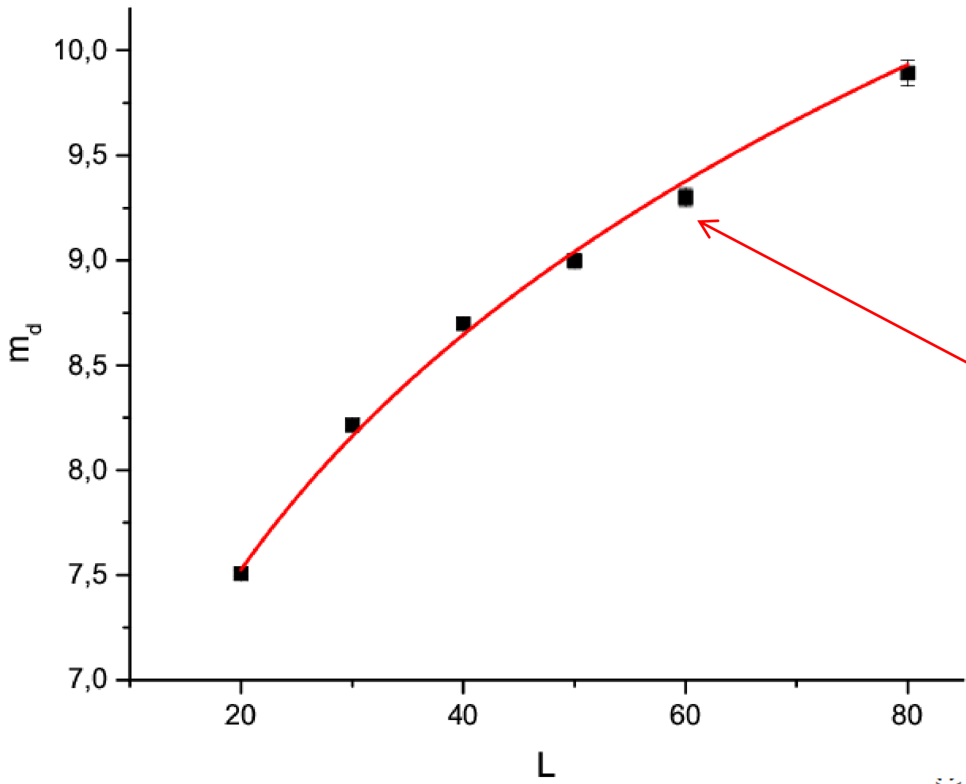
Масса дефекта:

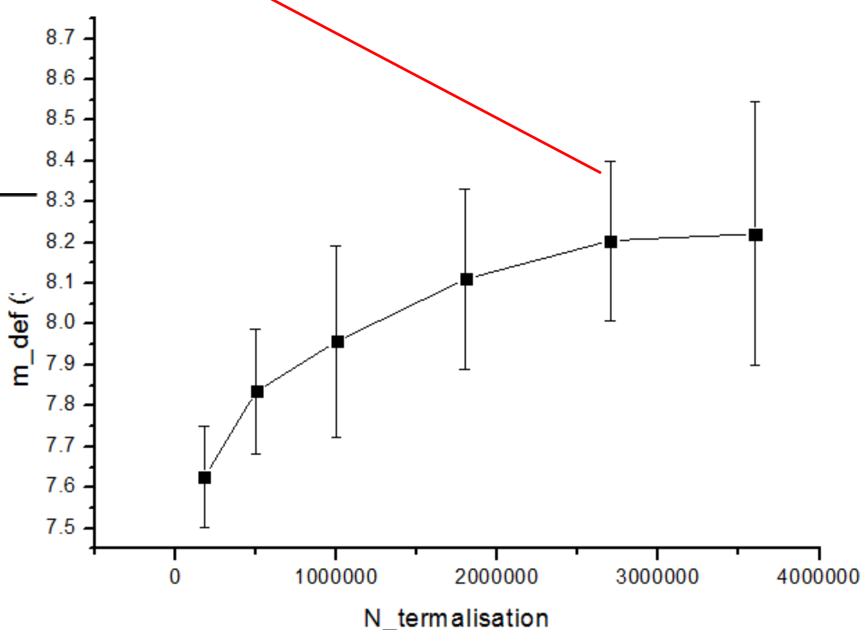
$$m_d = E_d - E_0,$$



$$\lim_{\varkappa \to \infty} m_d = 4J.$$

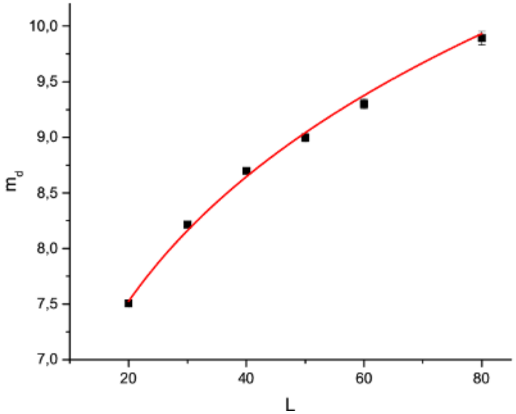
MC of defect mass: lattice volume dependence and thermalisation problems





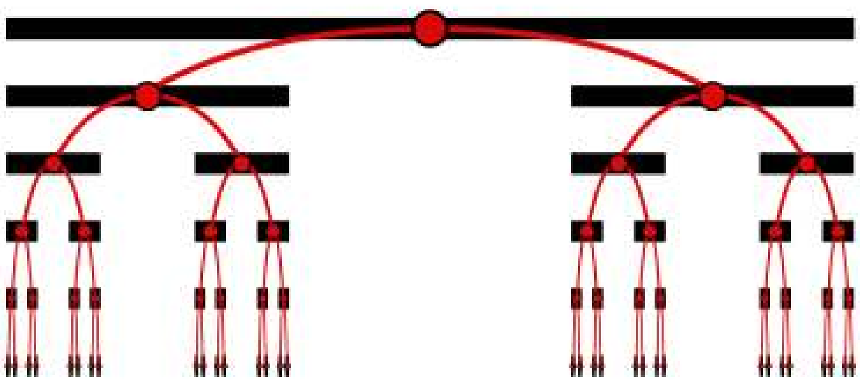
$$m_d^{\mathrm{cr}} = AL^n, \quad n \approx \frac{1}{5}$$

Defect in critical point: fractal dim object and Cantor set



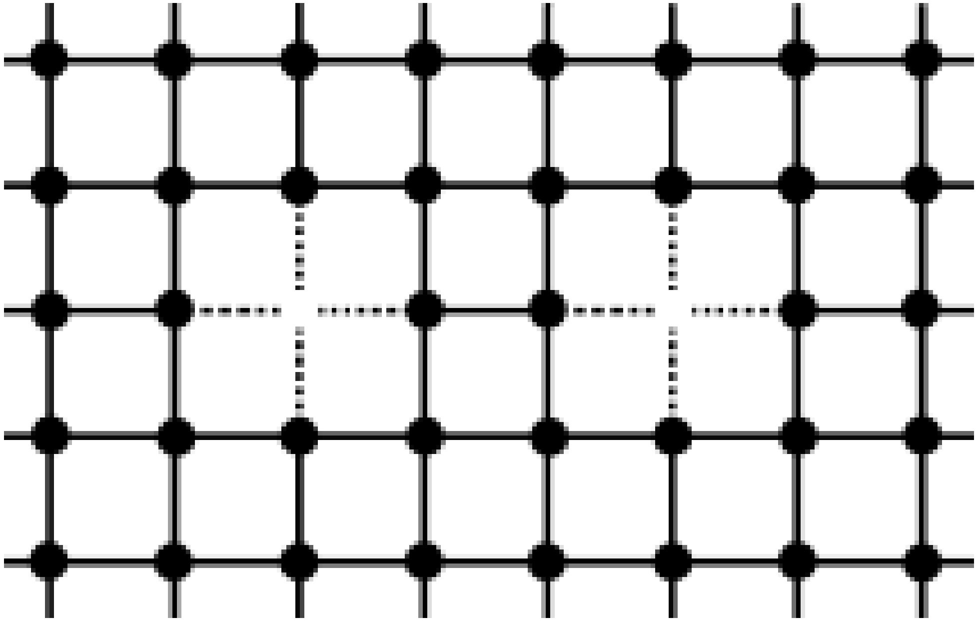
$$m_d^{\rm cr} = AL^n, \qquad n \approx \frac{1}{5}$$

Cantor set



Reflection in broken (fractal) mirror

Critical Casimir Forces between two defects



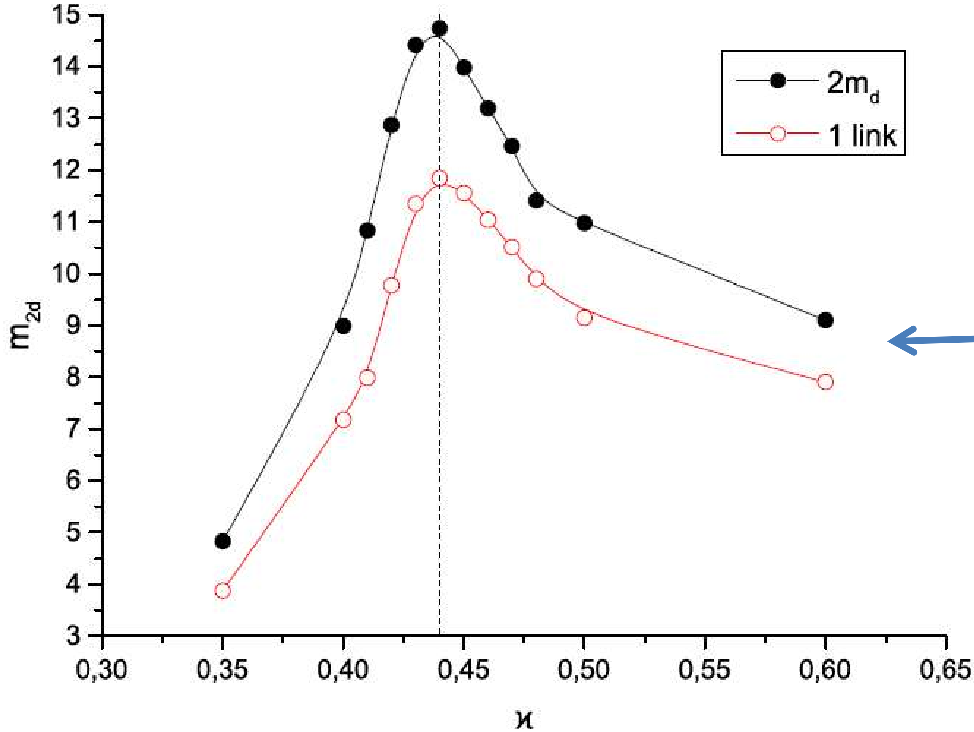
Two defects Bound Energy

$$E_{\text{int}} = E_{\text{tot}} - E_{L/2}$$

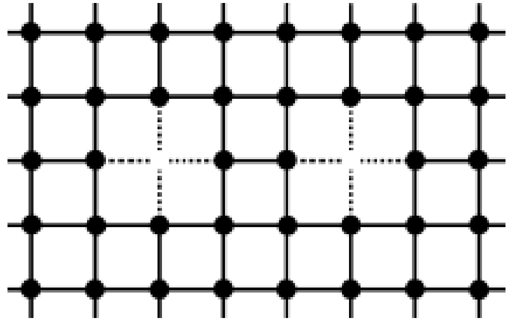
Subtraction procedure

Critical Casimir Forces between two defects

$$E_{\text{int}} = E_{\text{tot}} - E_{L/2}$$



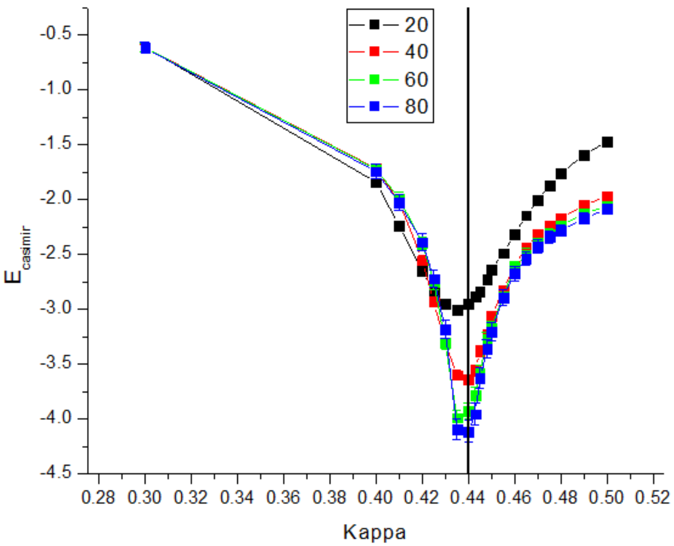
$m_{2d} < 2m_d$



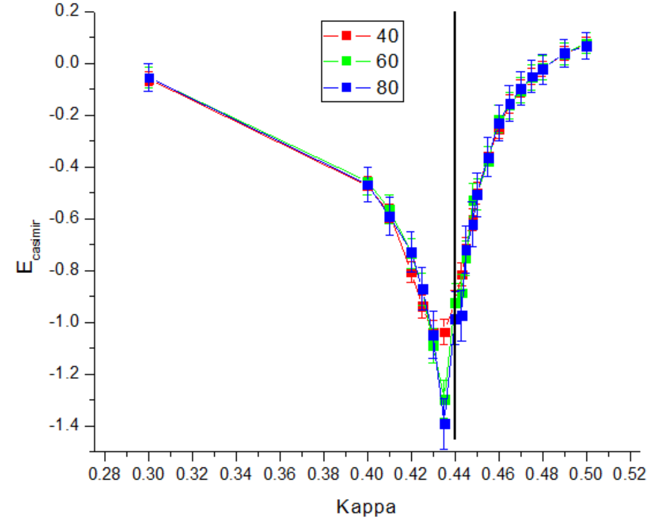
Critical Casimir Forces between two defects

$$E_{\mathrm{int}} = E_{\mathrm{tot}} - E_{L/2}$$

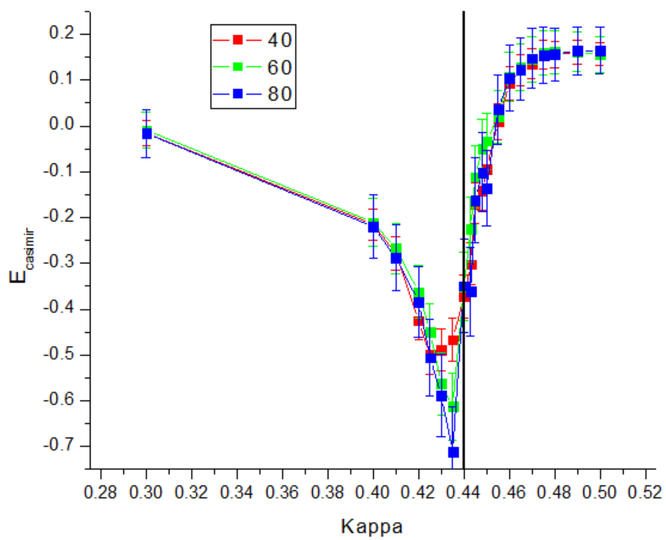
Dist. between def's = 1

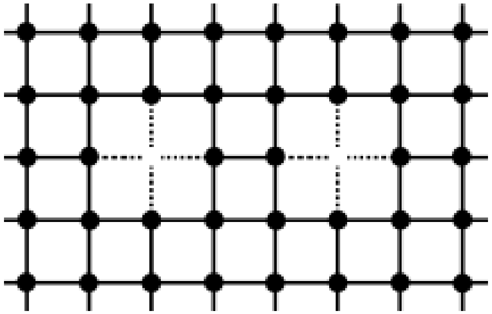


Dist. between def's = 2



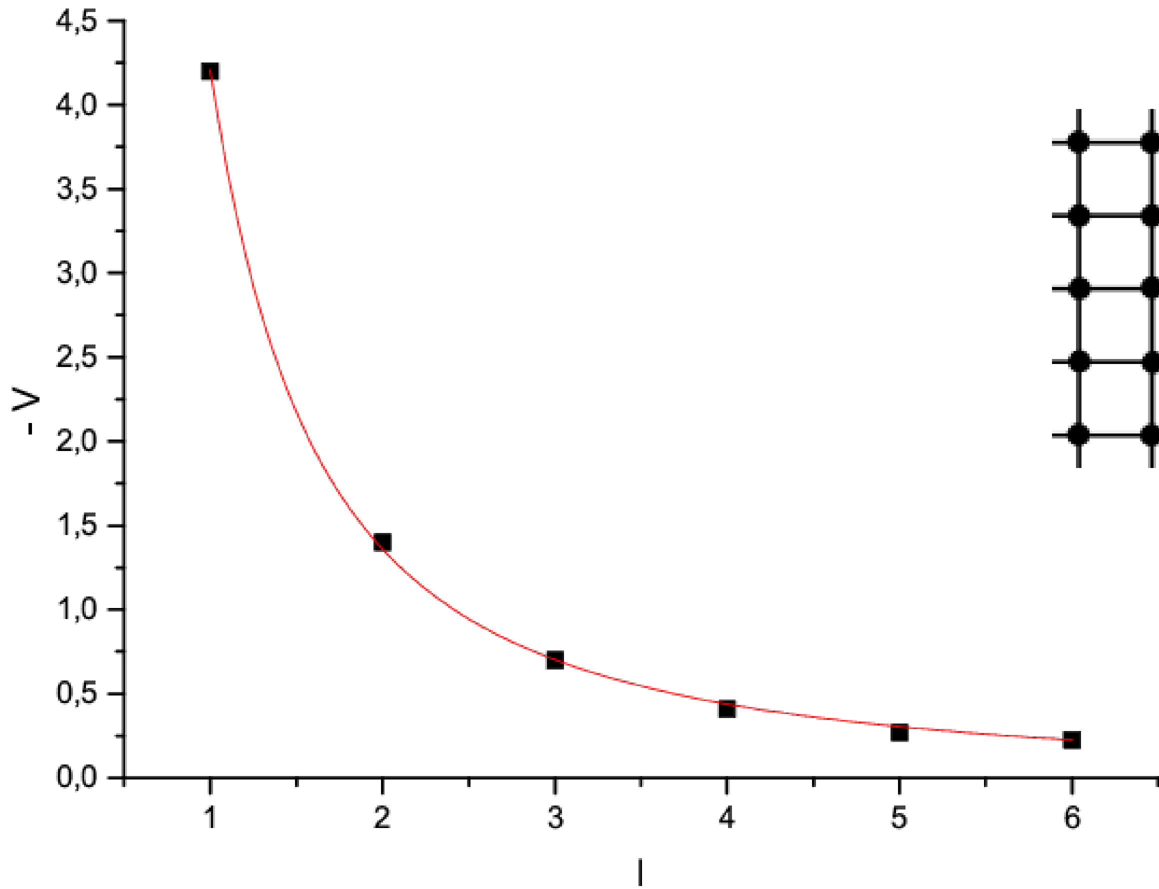
Dist. between def's = 3

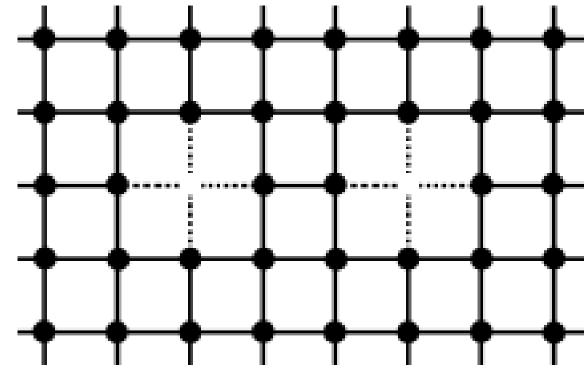




Critical Casimir Forces between two defects

$$E_{\text{int}} = E_{\text{tot}} - E_{L/2}$$

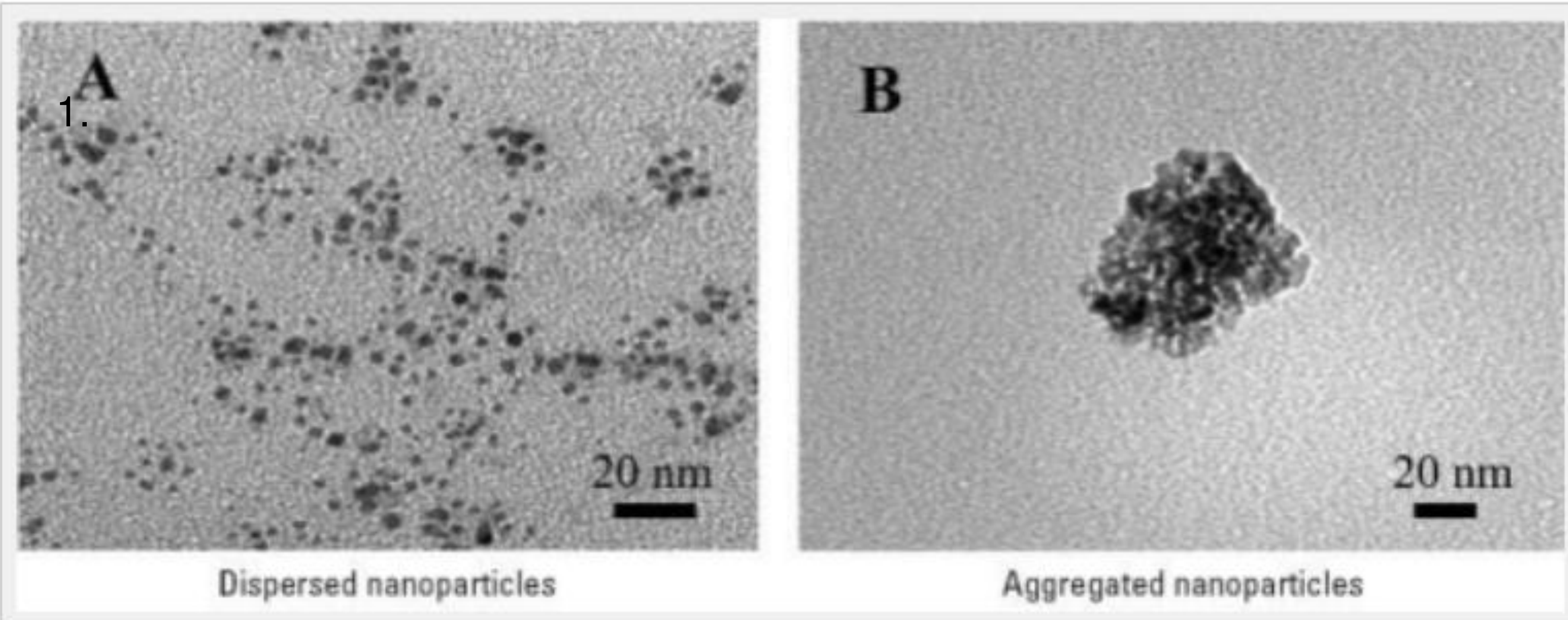


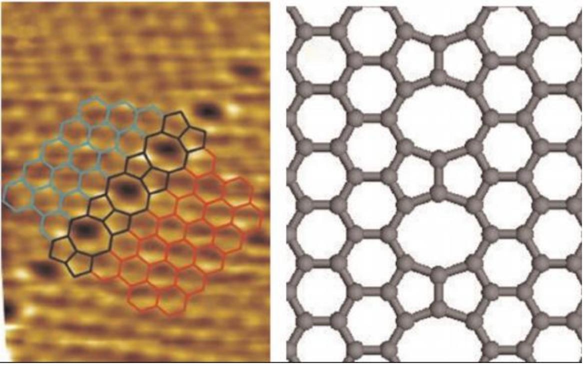


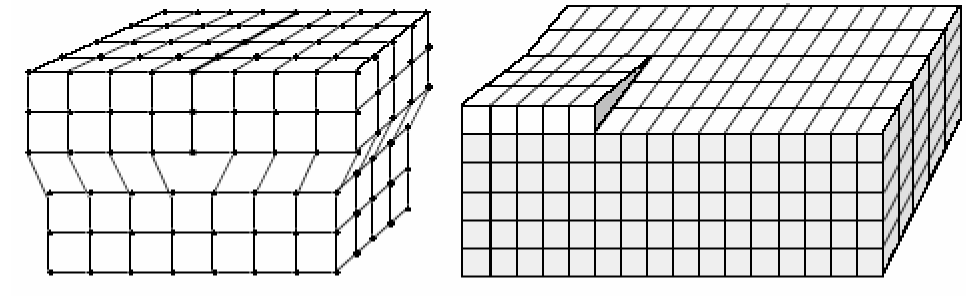
$$F(l) \sim \frac{1}{l^3}$$

P. Nowakowski, A. Maciolek, S. Dietrich,
Critical Casimir forces between defects in the 2D Ising model,
J. Phys. A: Mathematical and Theoretical, **49**, 48 (2016)

Defects aggregation







Critical Casimir Effect in defect lines

Critical Casimir Effect: BioPhysics Applications

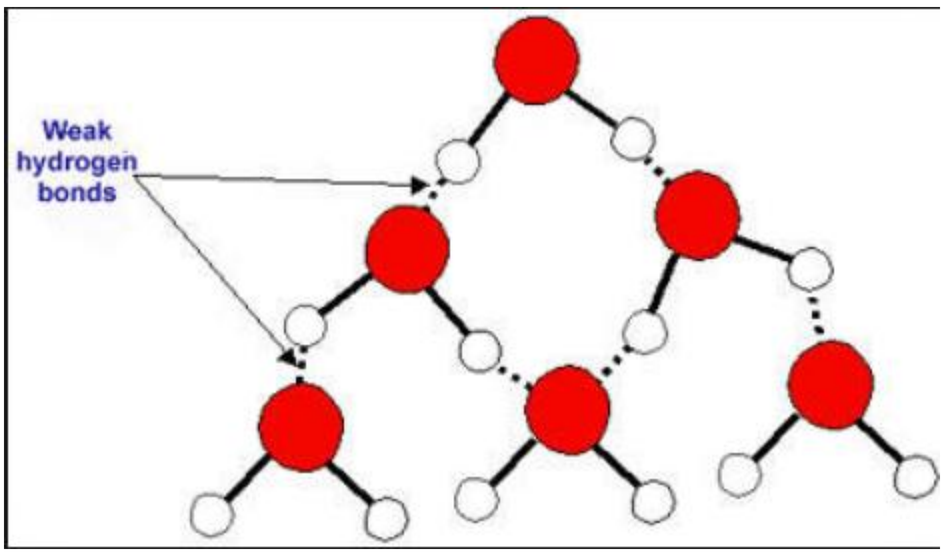
Biological processes in a medium of polarized molecules:

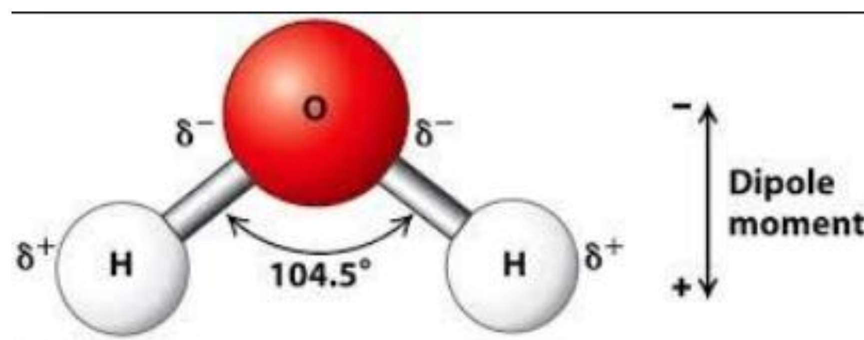
- Protein folding
- Cell membranes formation and lipid rafts
- Biological catalyst
- …

Critical Casimir Effect: BioMedical Application

1. Global protein structure formation

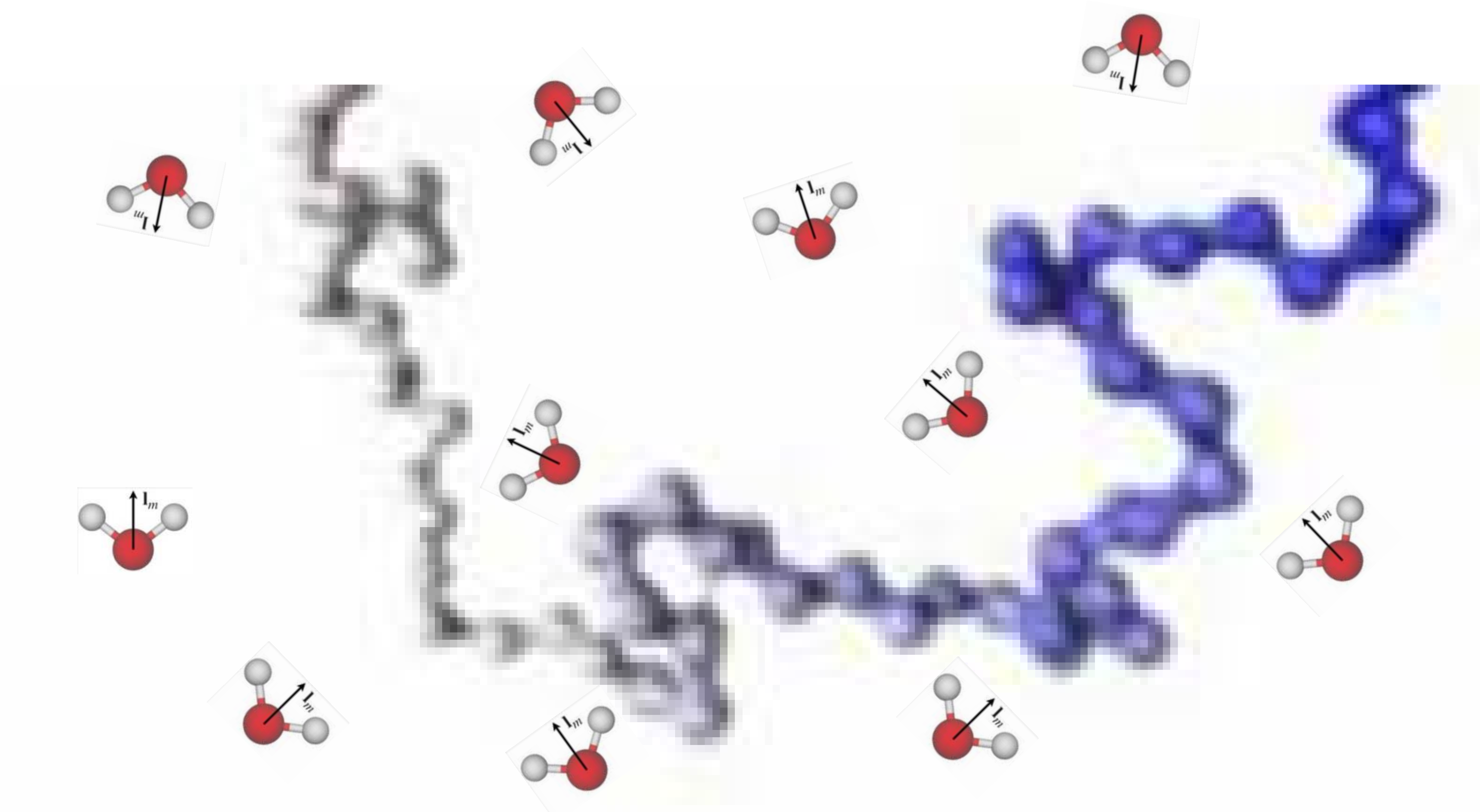
We have to take into account medium in which the protein folding is taken place.





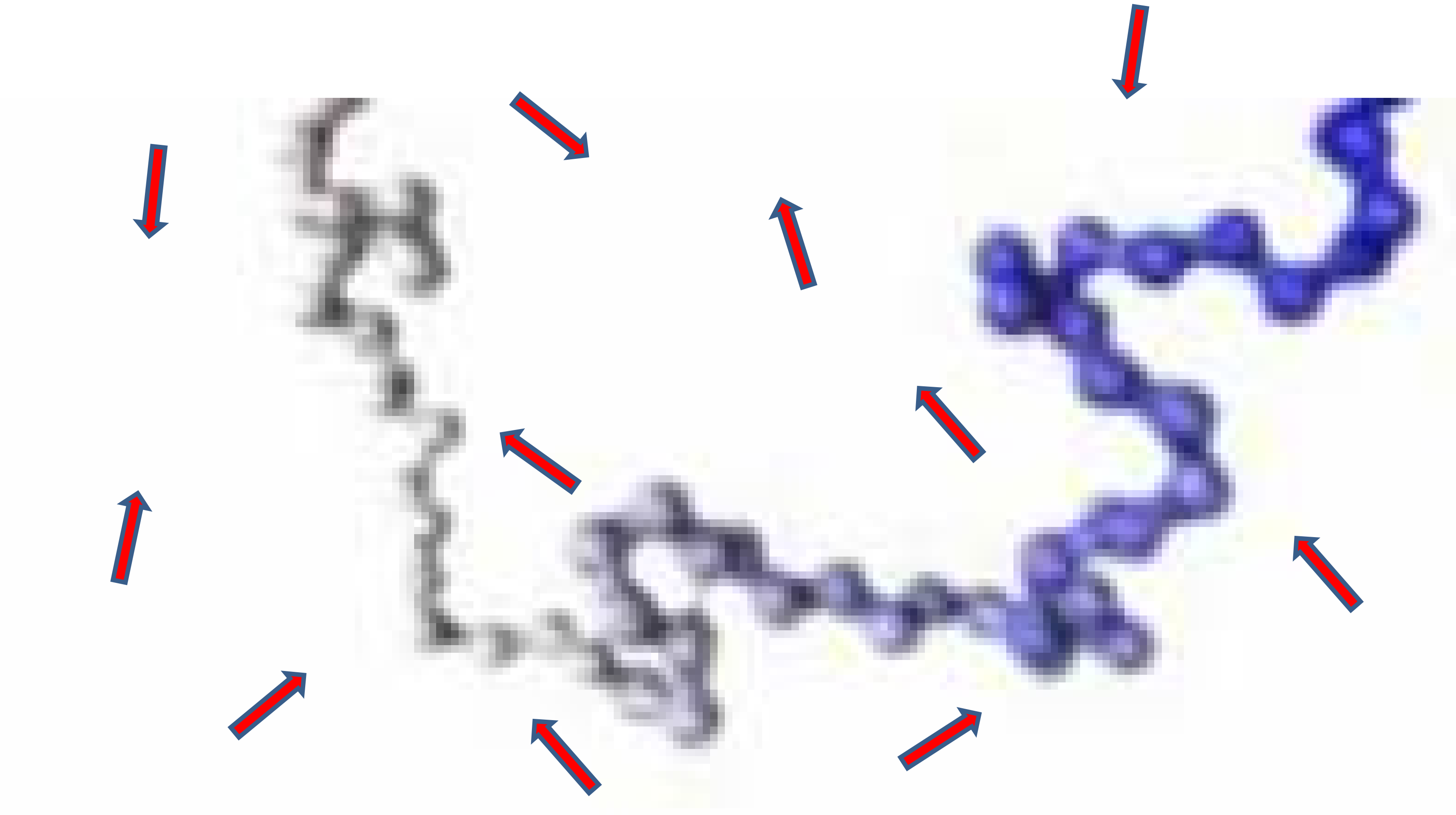
Critical Casimir Effect: BioMedical Application

1. Global protein structure formation



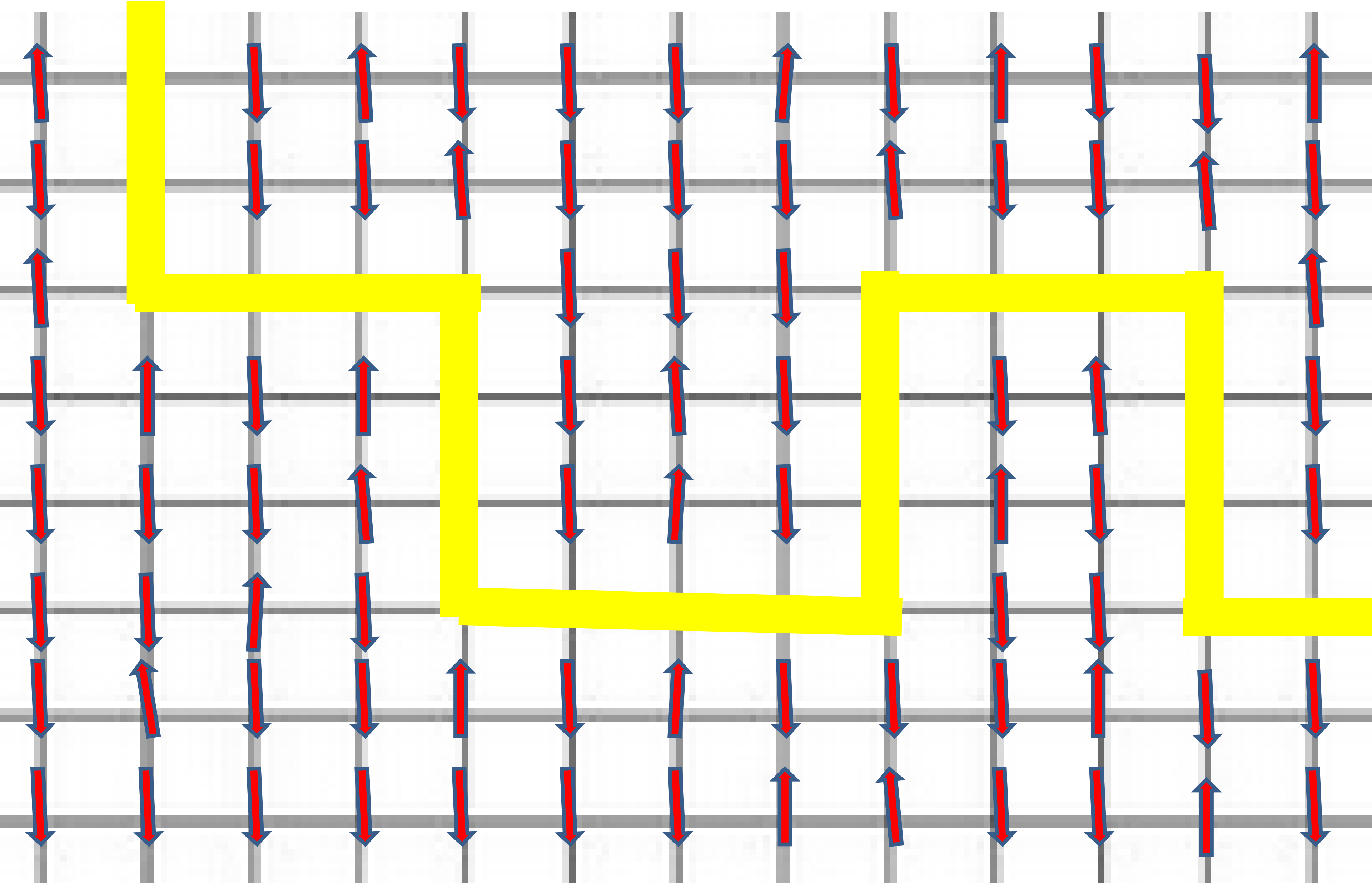
Critical Casimir Effect: BioMedical Application

1. Global protein structure formation

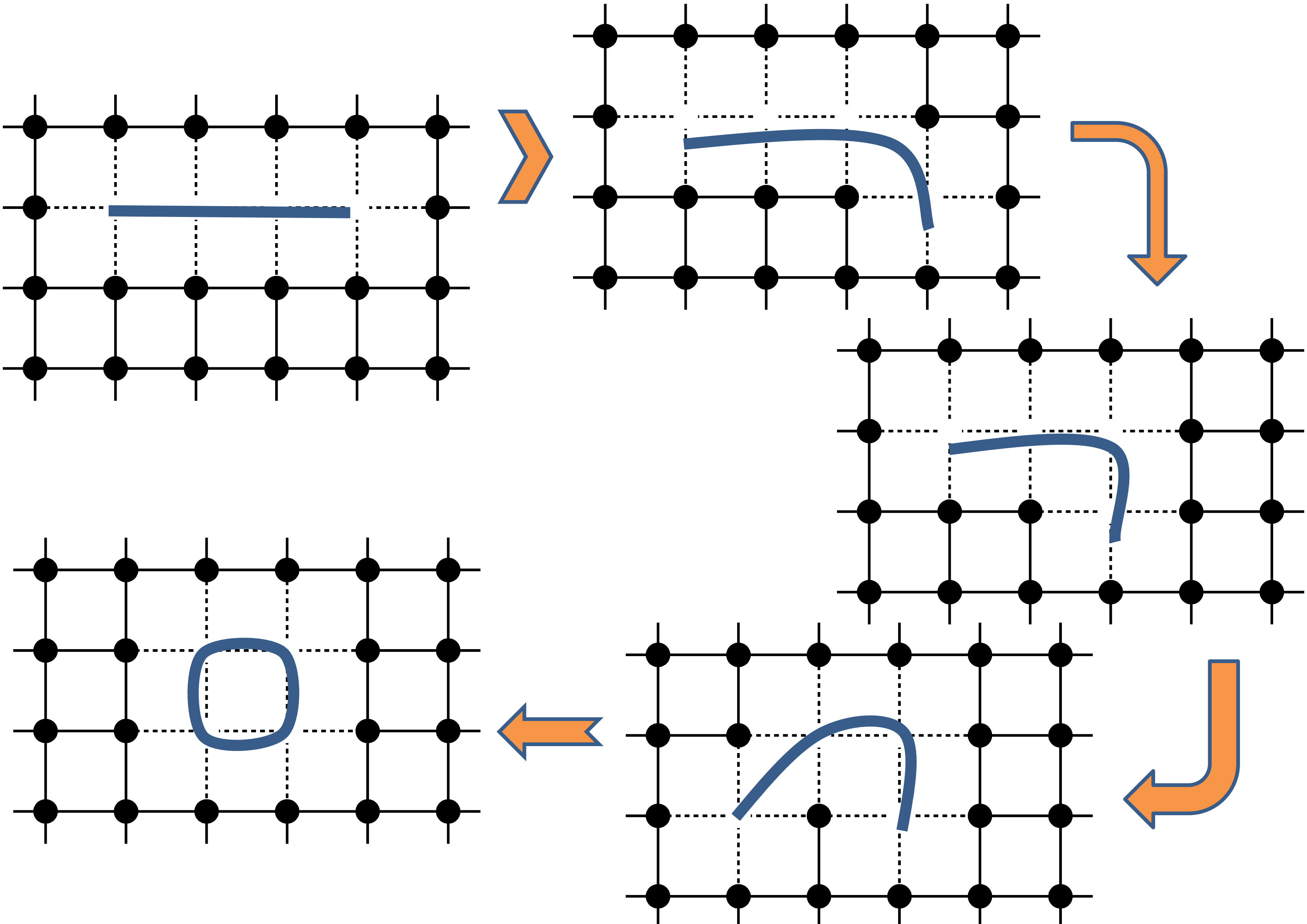


Critical Casimir Effect: BioMedical Application

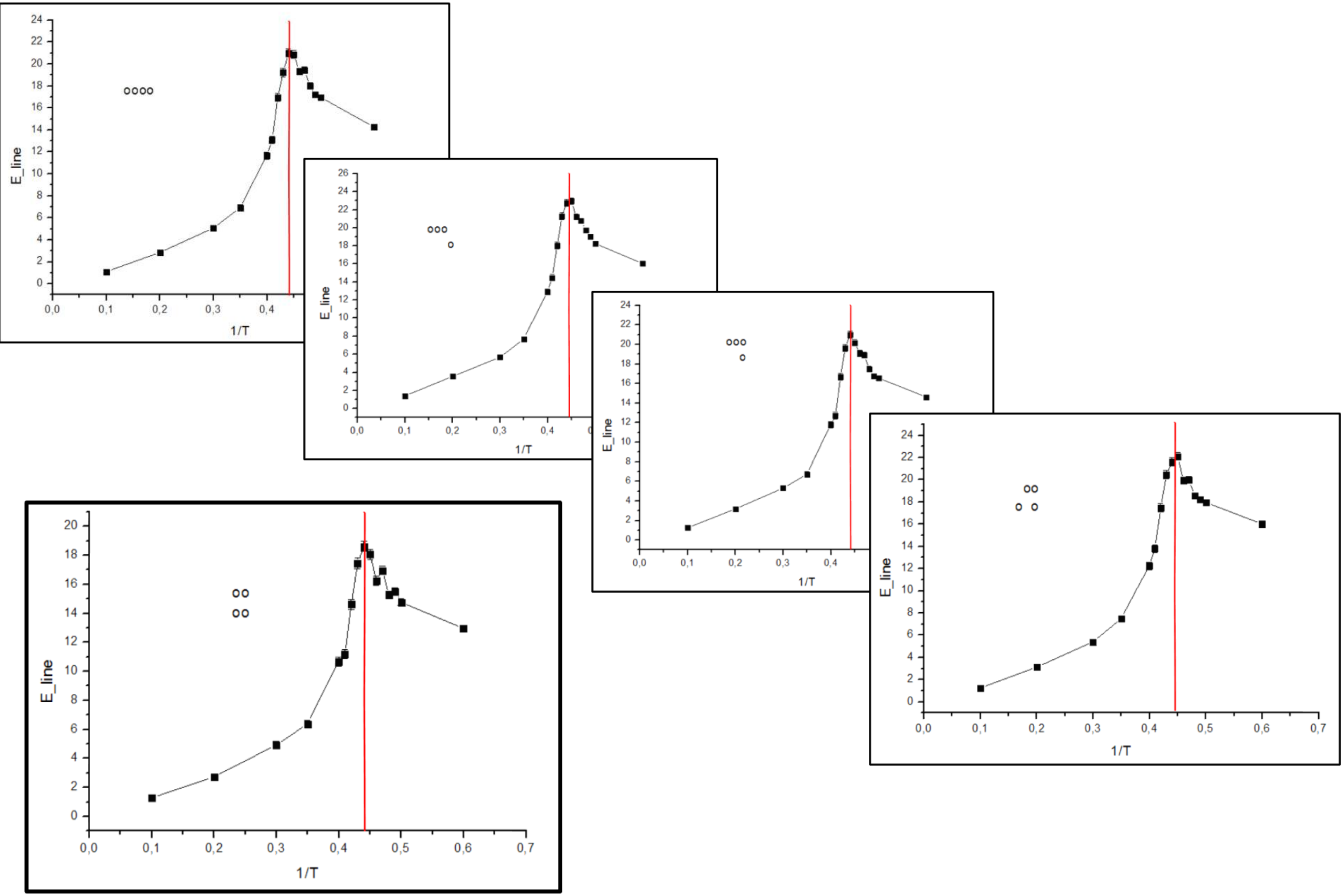
Discretization of the Model

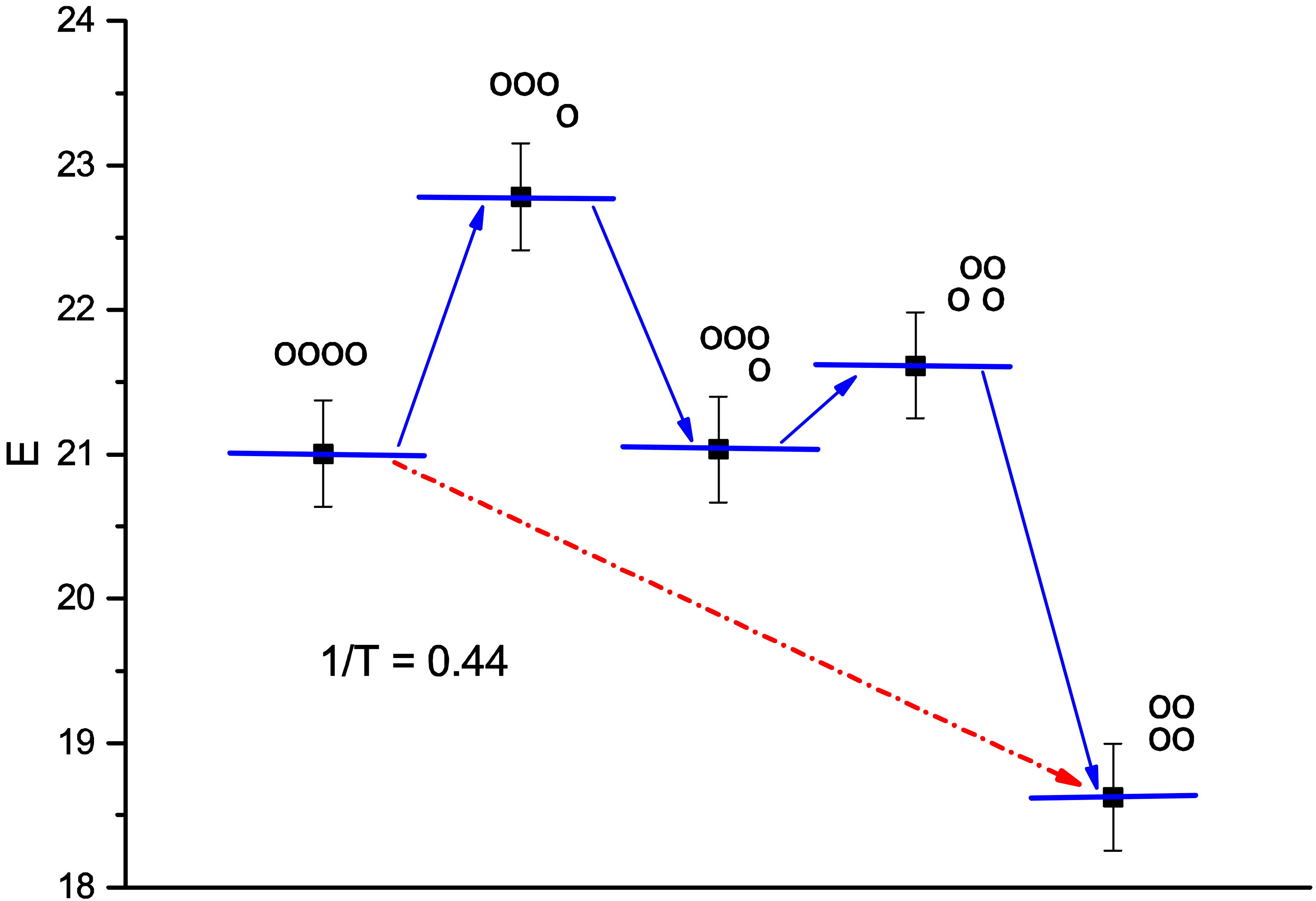


Simple example: collapse of 4 defects line

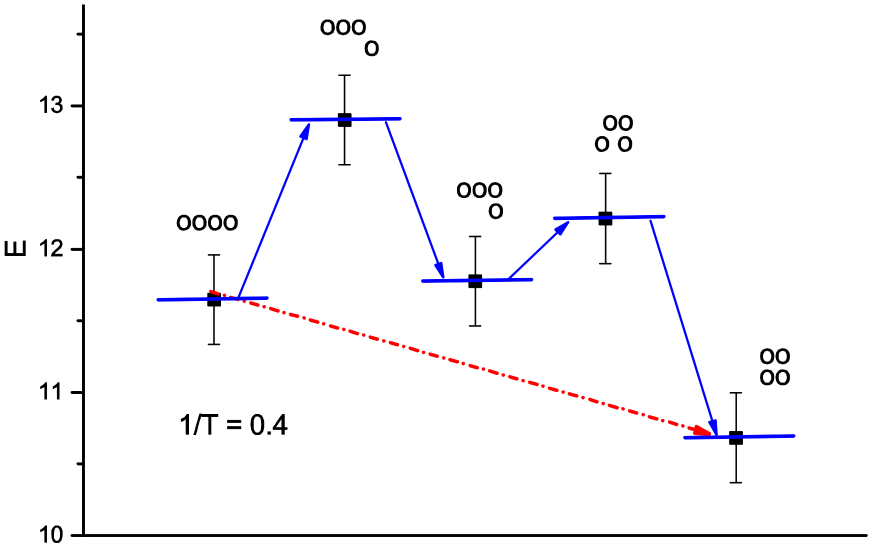


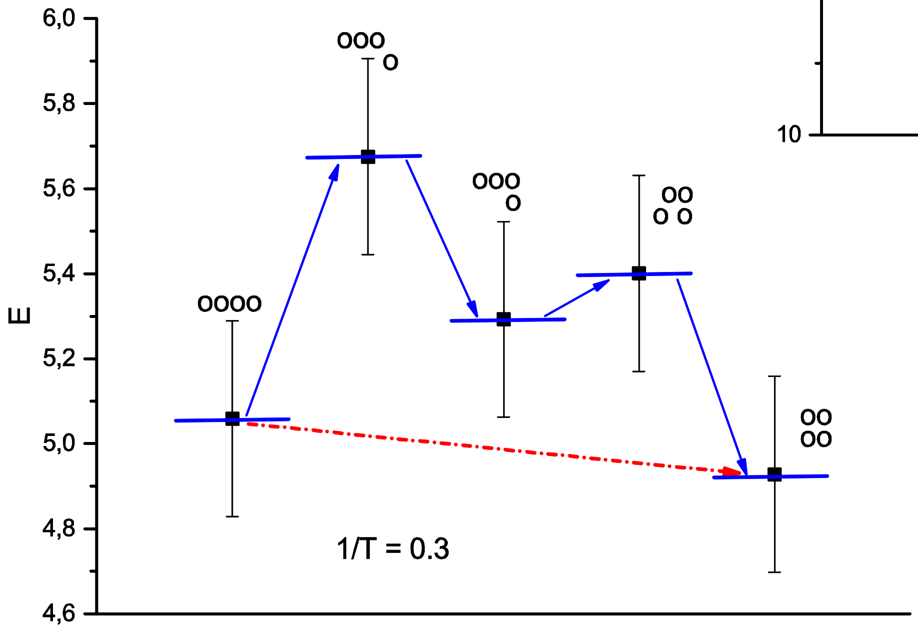
Defects aggregation - small line



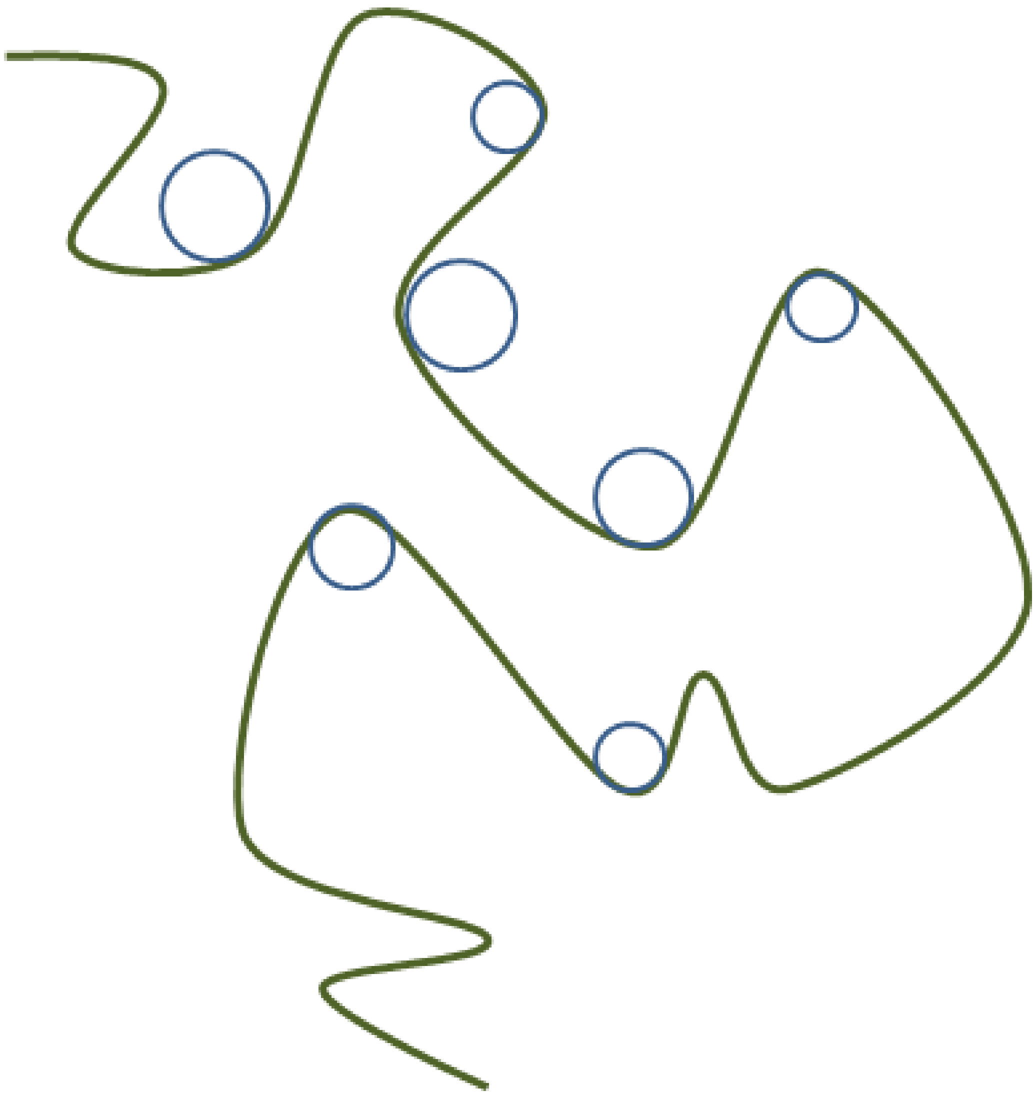

24
23
22
21
20
19
18
E
oooo
ooo
o
ooo
o
oo
o o
oo
oo
1/T = 0.44

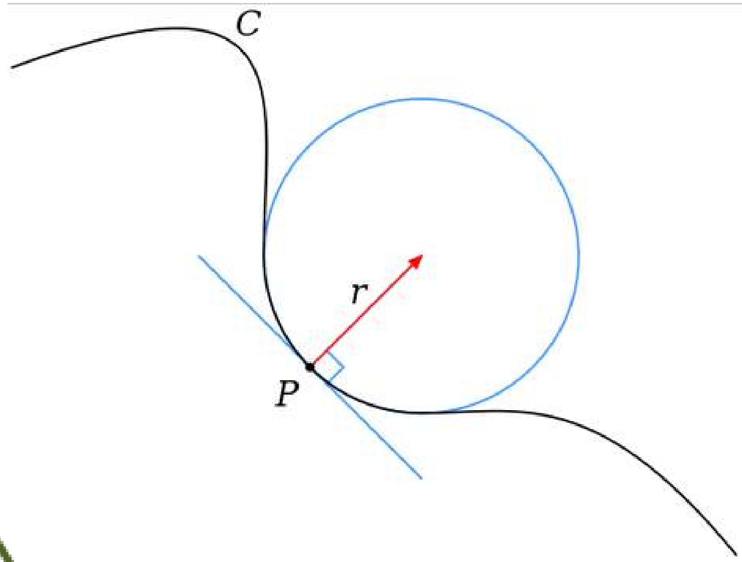
$1/T$	E
0.3	0.13
0.4	0.96
0.44	2.38

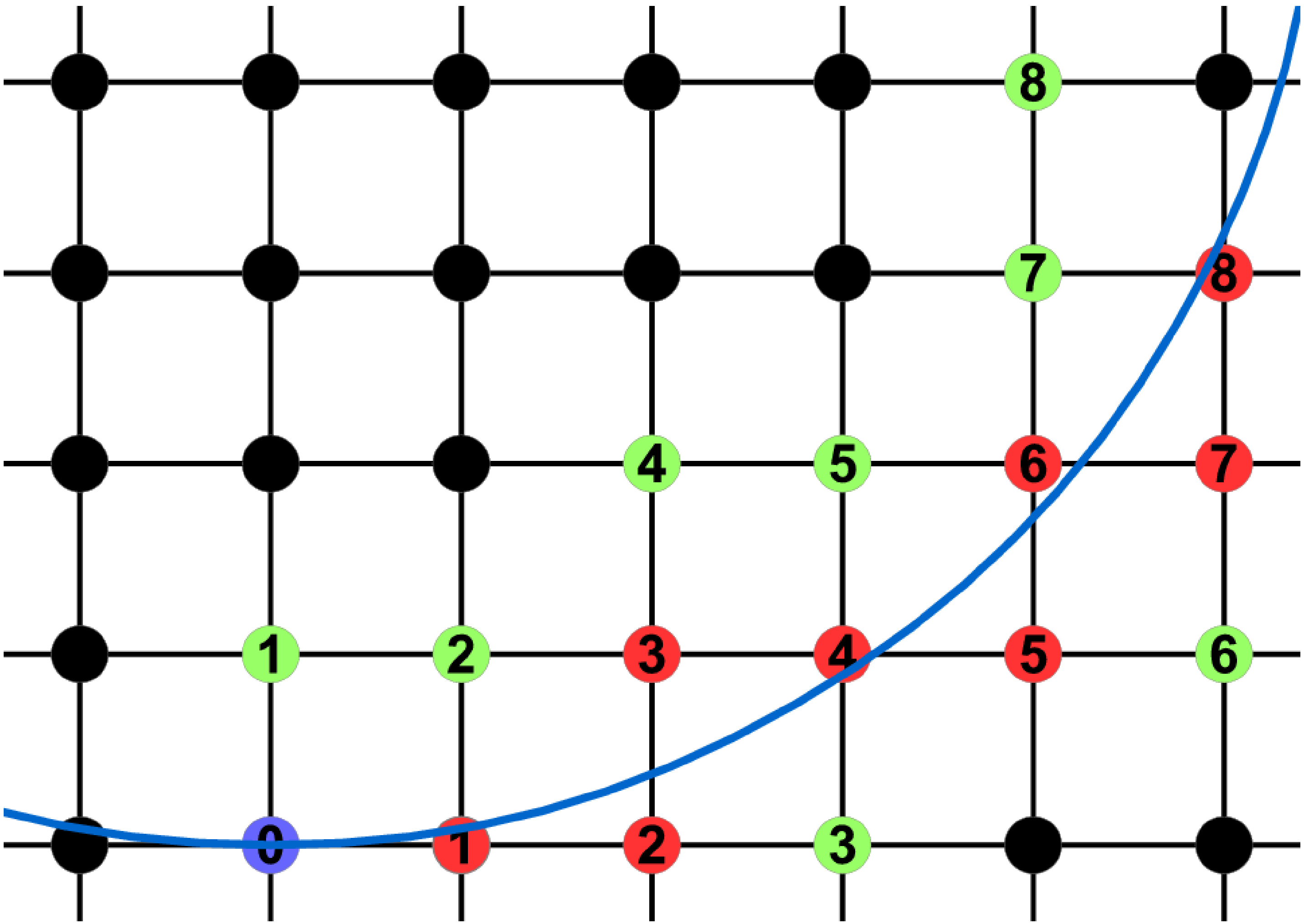


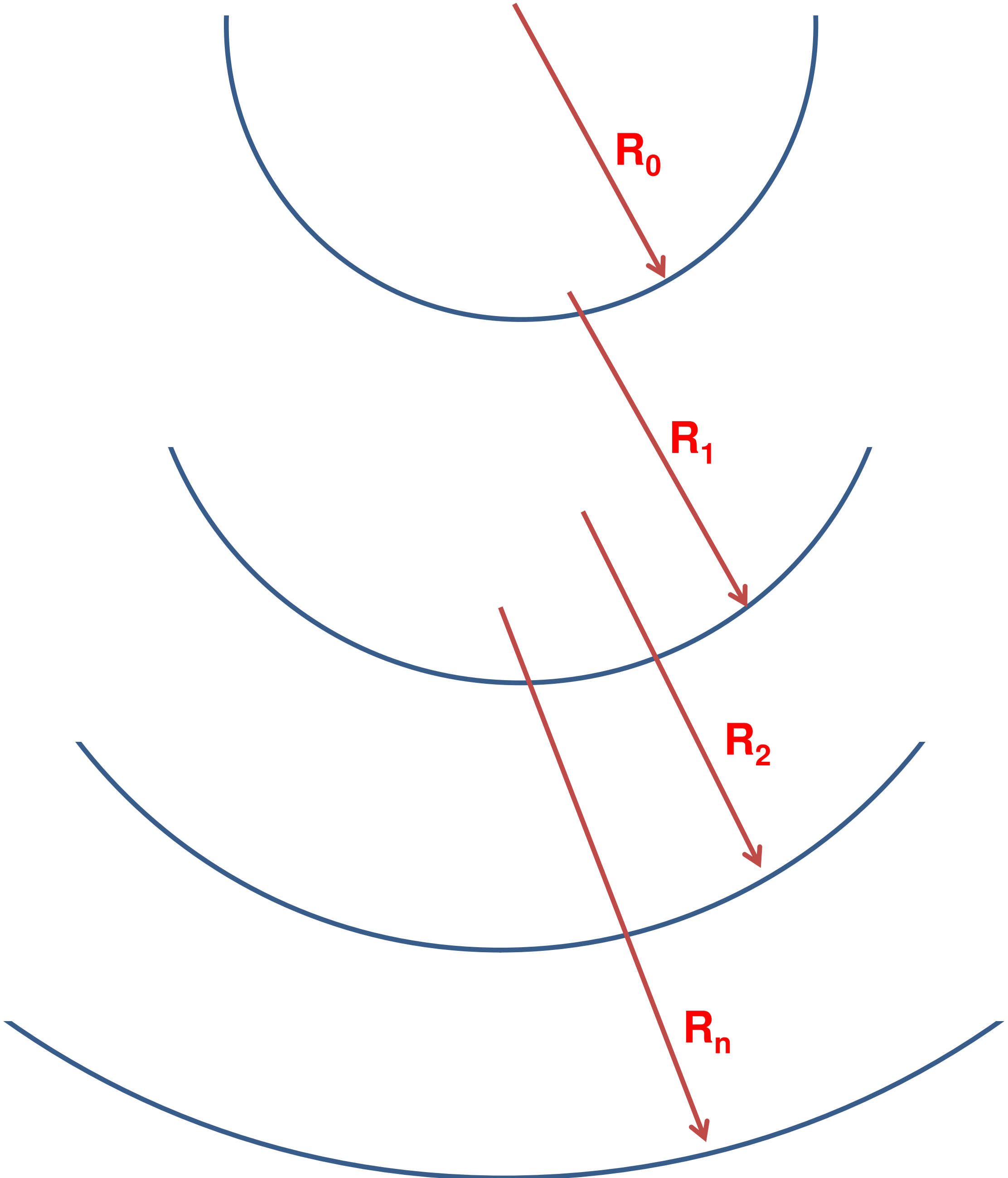


Elasticity of defect curves

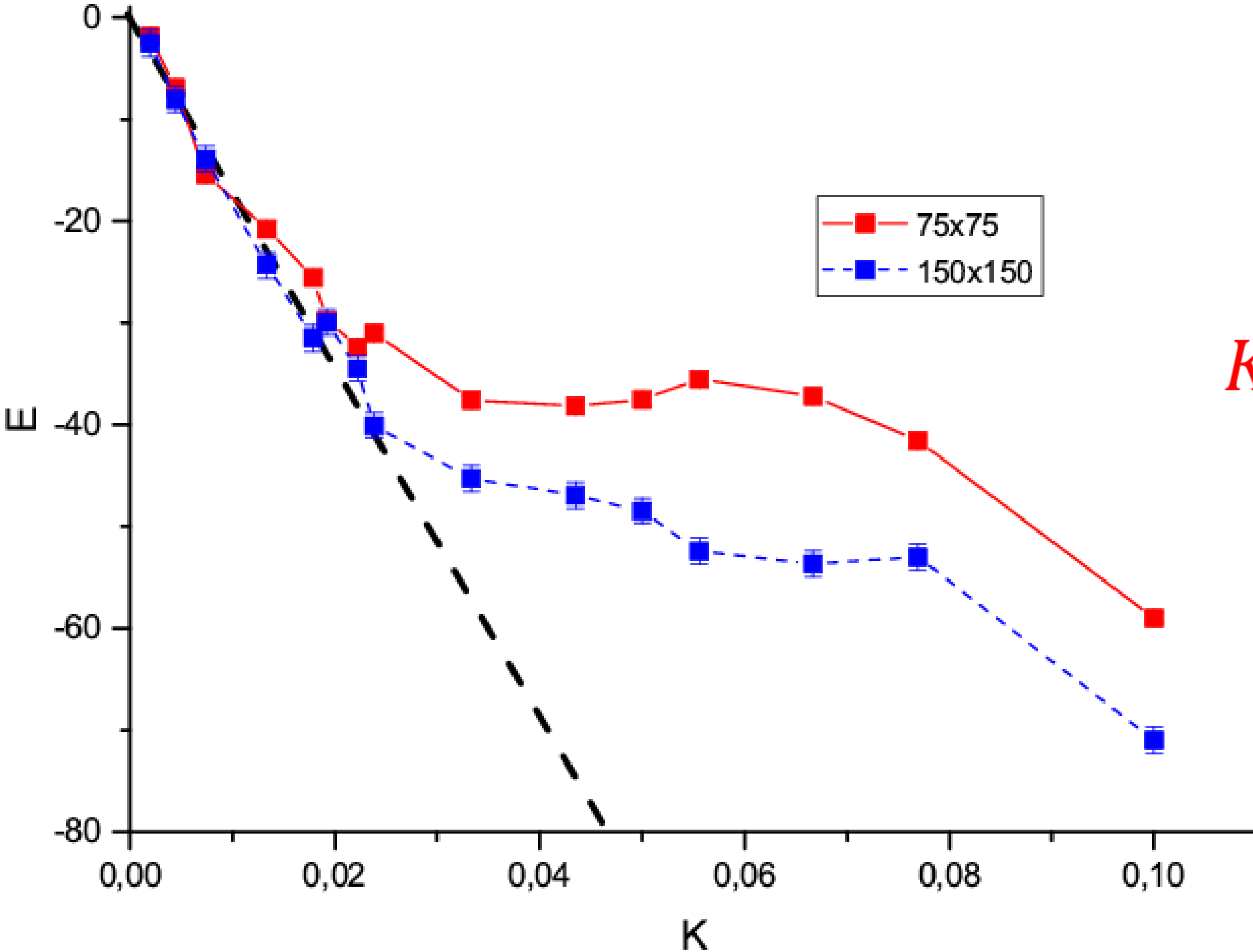




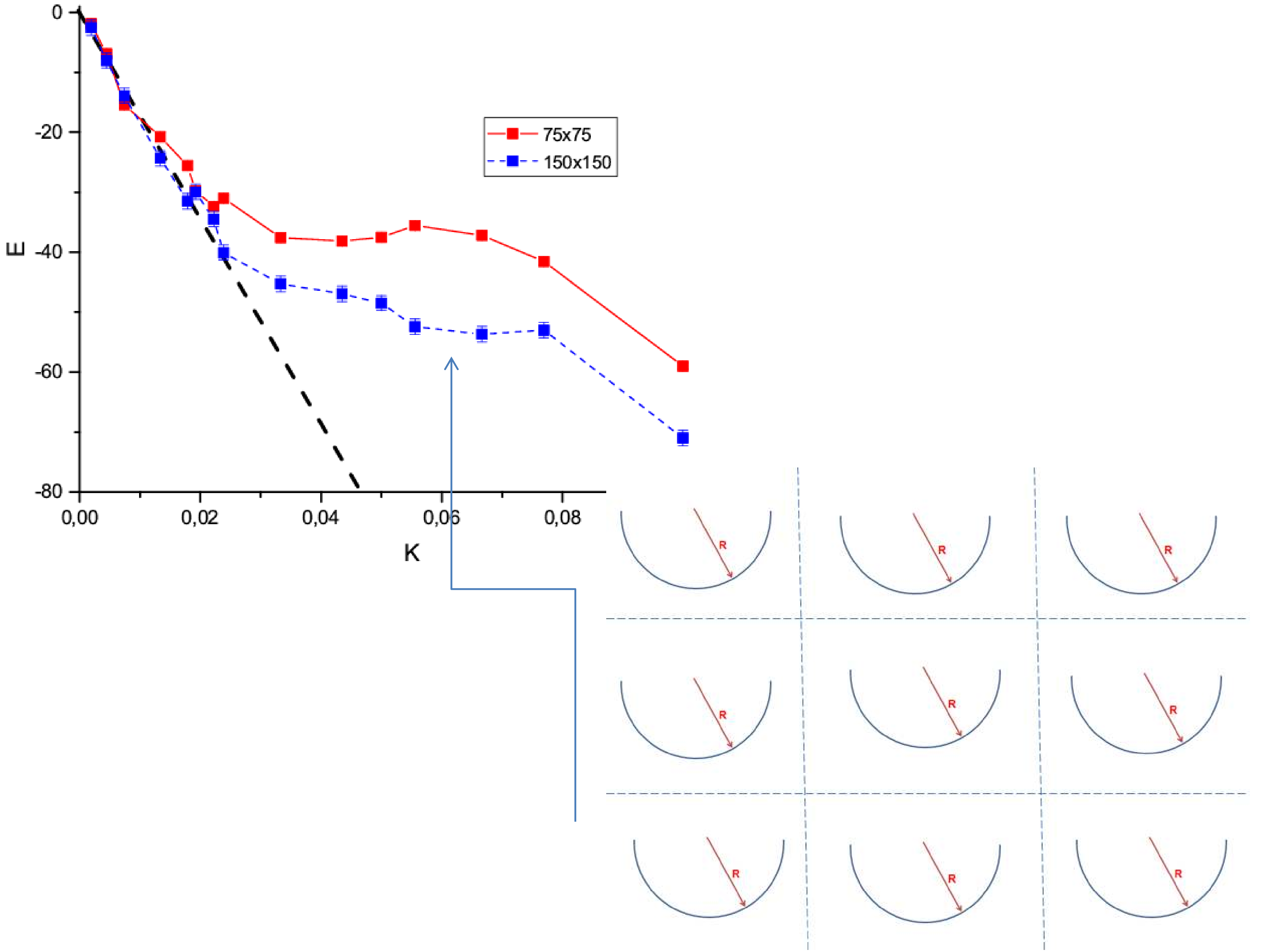

8
7
8
4
5
6
7
1
2
3
4
5
6
0
1
2
3



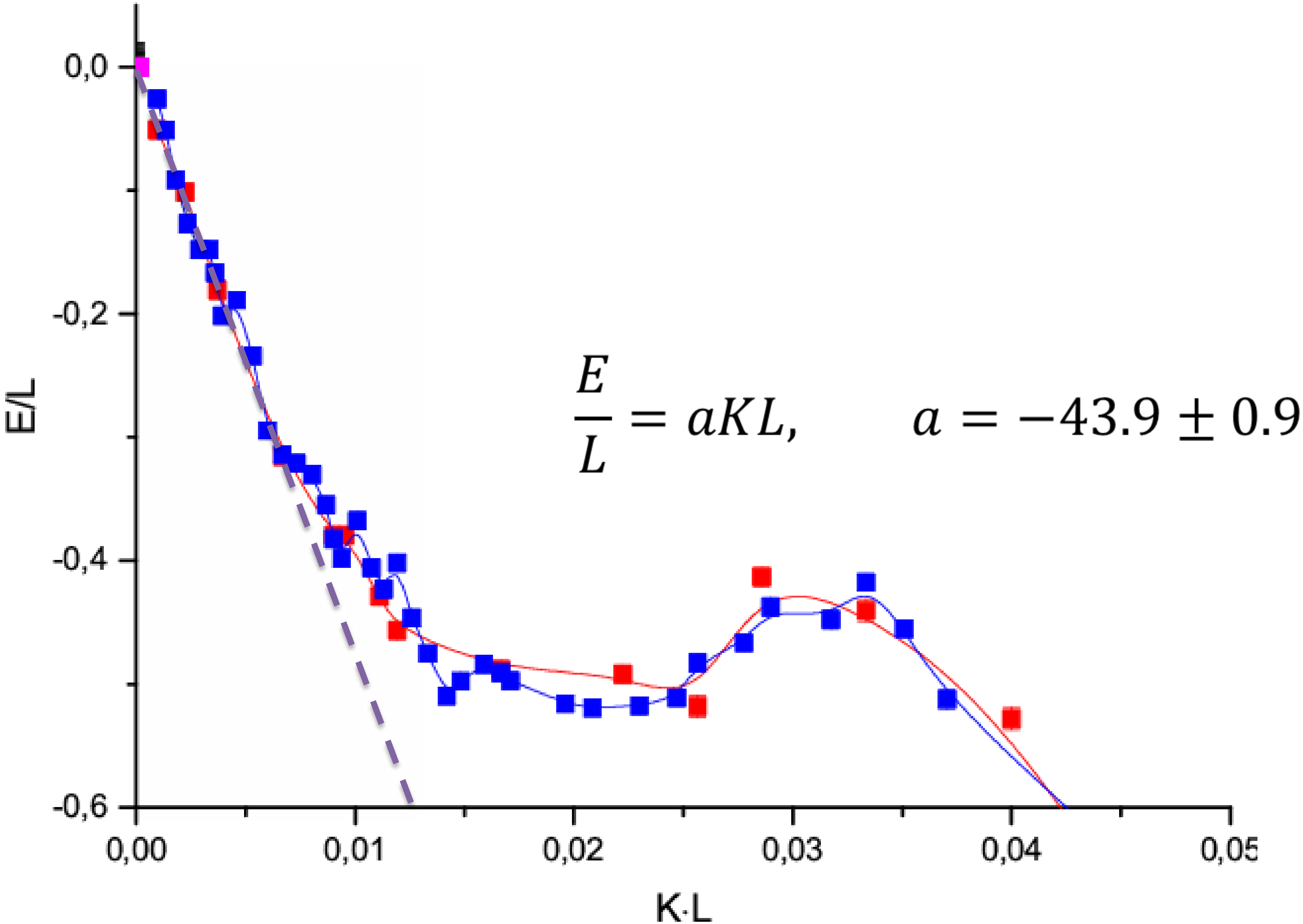
R0
R1
R2
Rn



$$K = \frac{1}{R}$$

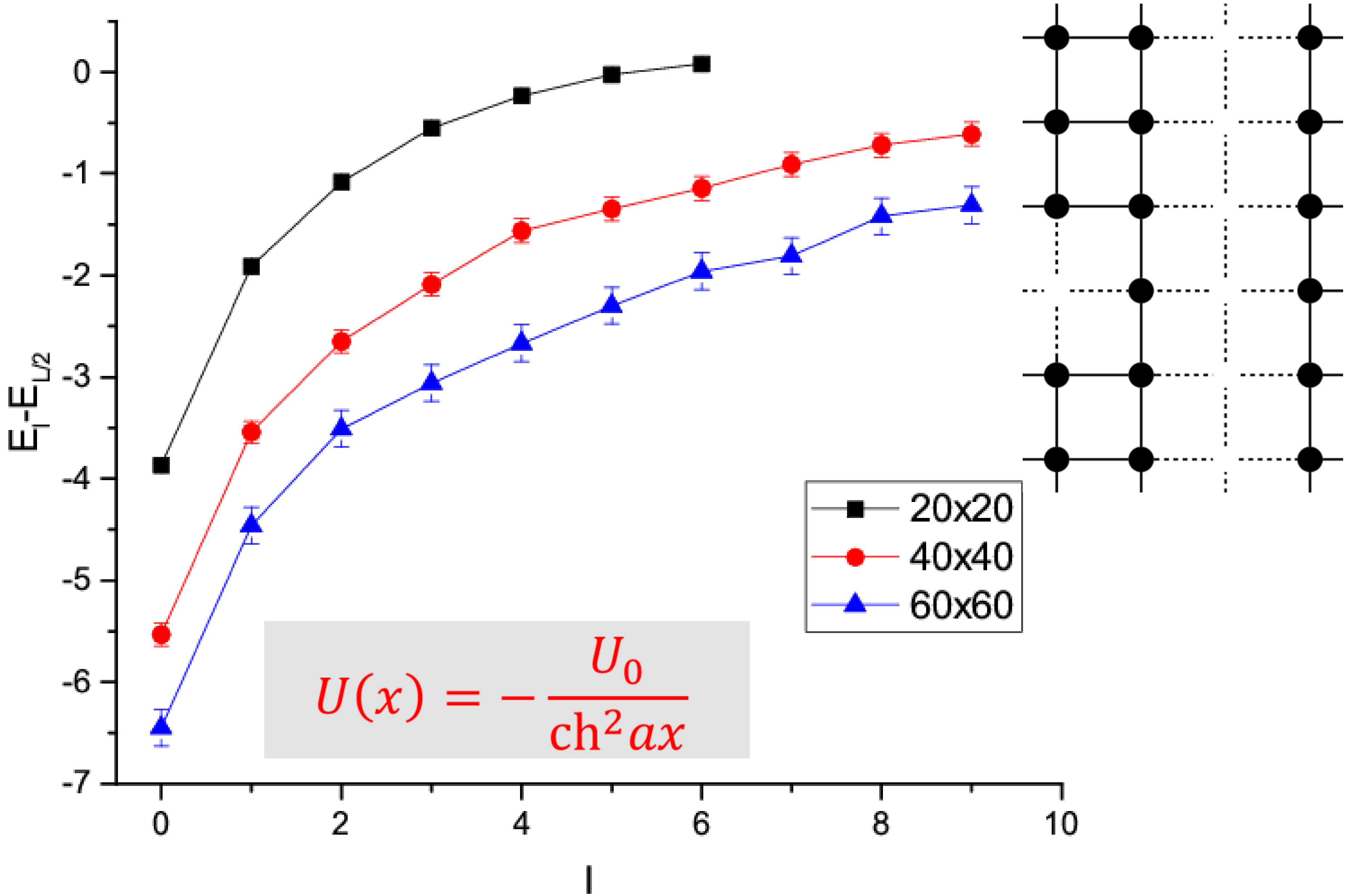


0
-20
-40
-60
-80
E
0,00
0,02
0,04
0,06
0,08
K
75x75
150x150
R



0,0
-0,2
-0,4
-0,6
E/L
0,00
0,01
0,02
0,03
0,04
0,05
K·L
$\frac{E}{L} = aKL, \qquad a = -43.9 \pm 0.9$

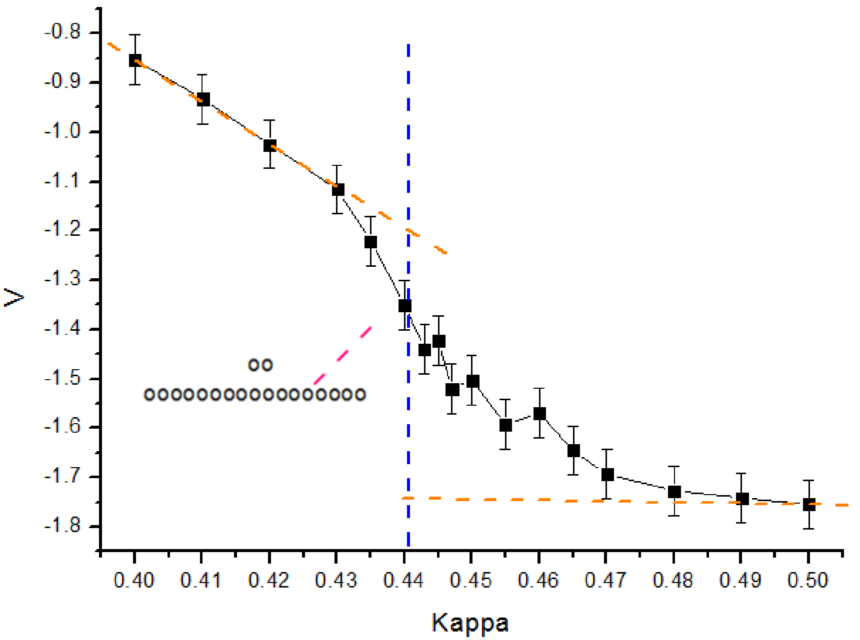
Defect Confinement on Defect line

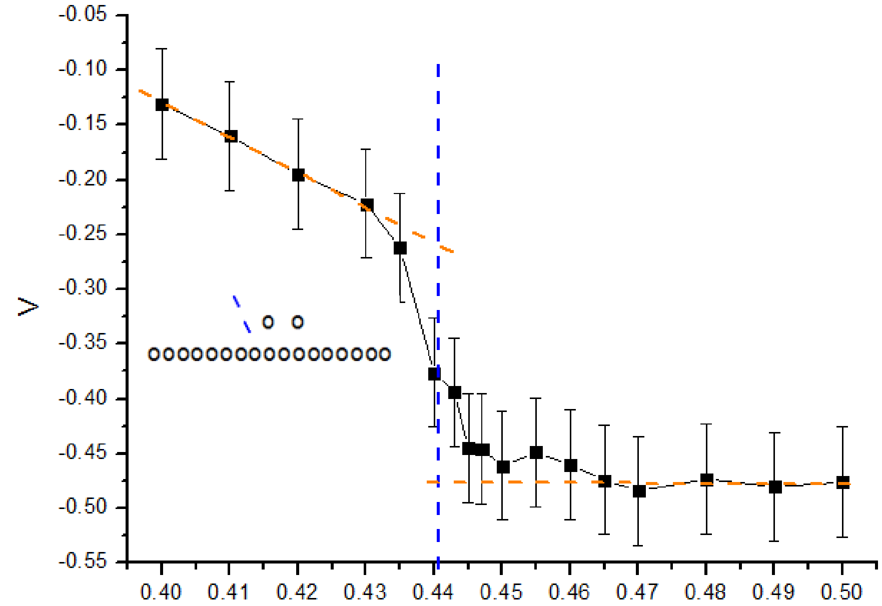


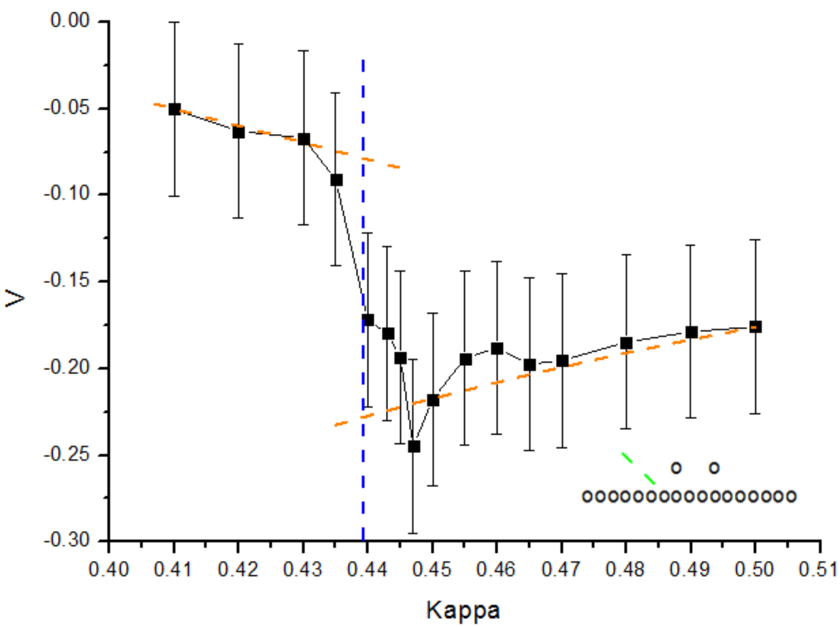
E_l-E_L/2
0
-1
-2
-3
-4
-5
-6
-7
0
2
4
6
8
10
l
20x20
40x40
60x60
$U(x) = -\frac{U_0}{\mathrm{ch}^2 ax}$

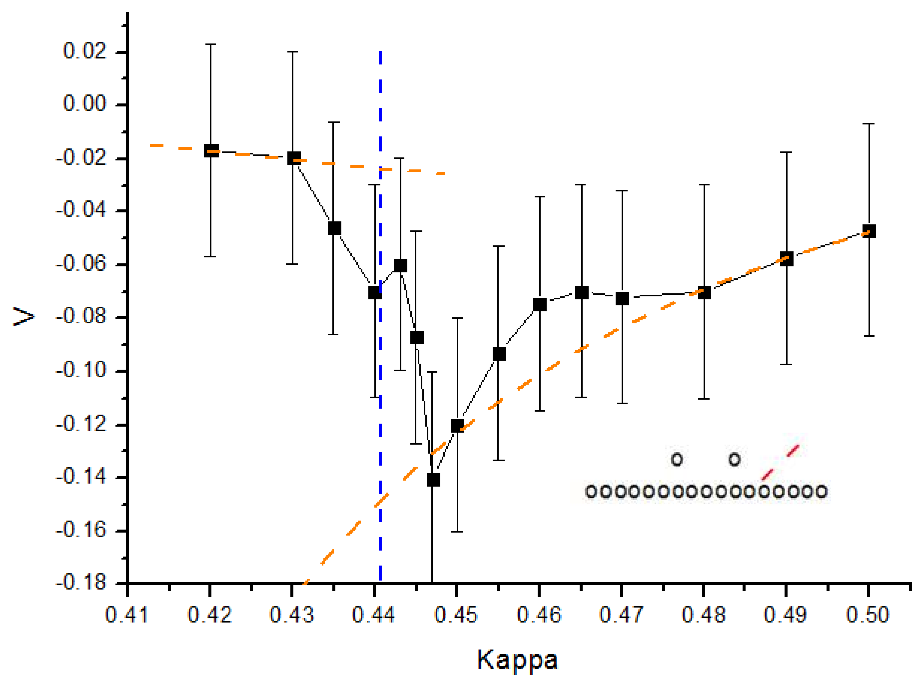
Two Defects on the defect line

Two defects on the defect line

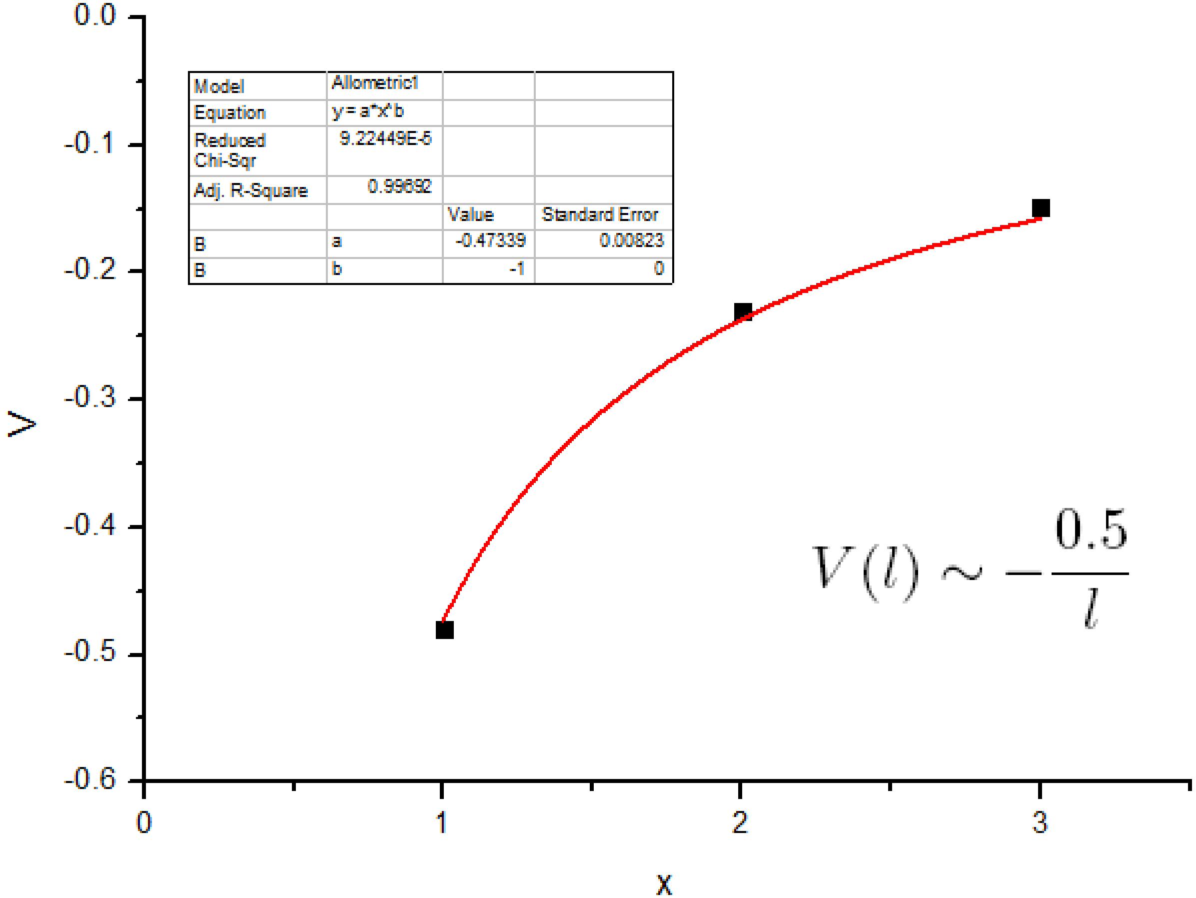








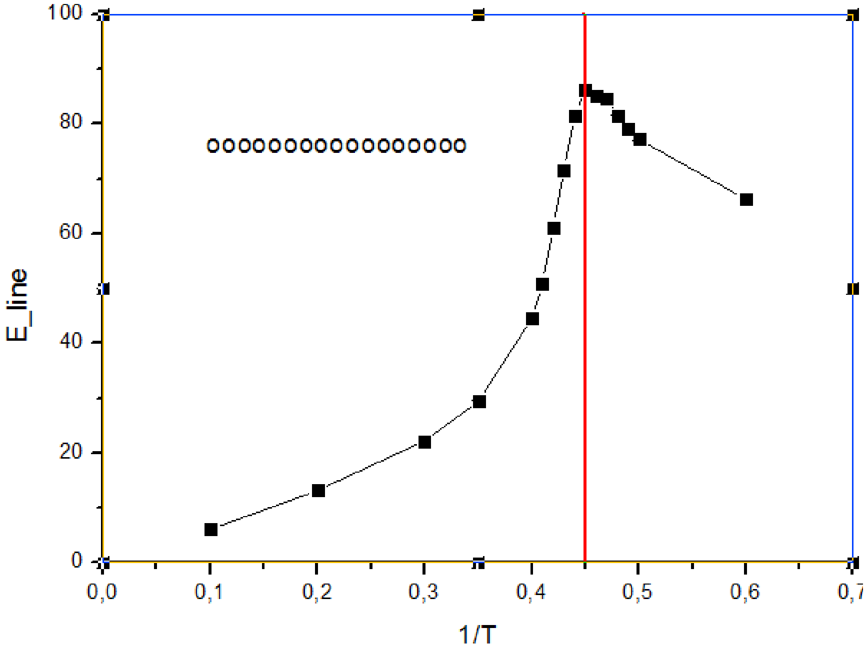
Two defects on the defect line
Interaction potential

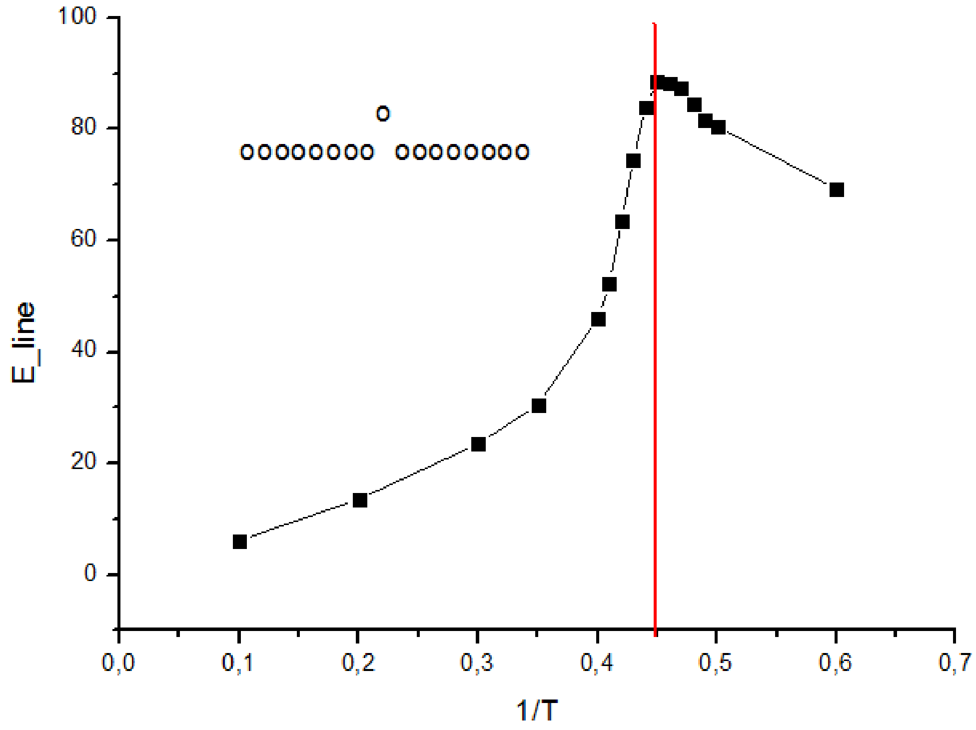


$$V(l) \sim -\frac{0.5}{l}$$

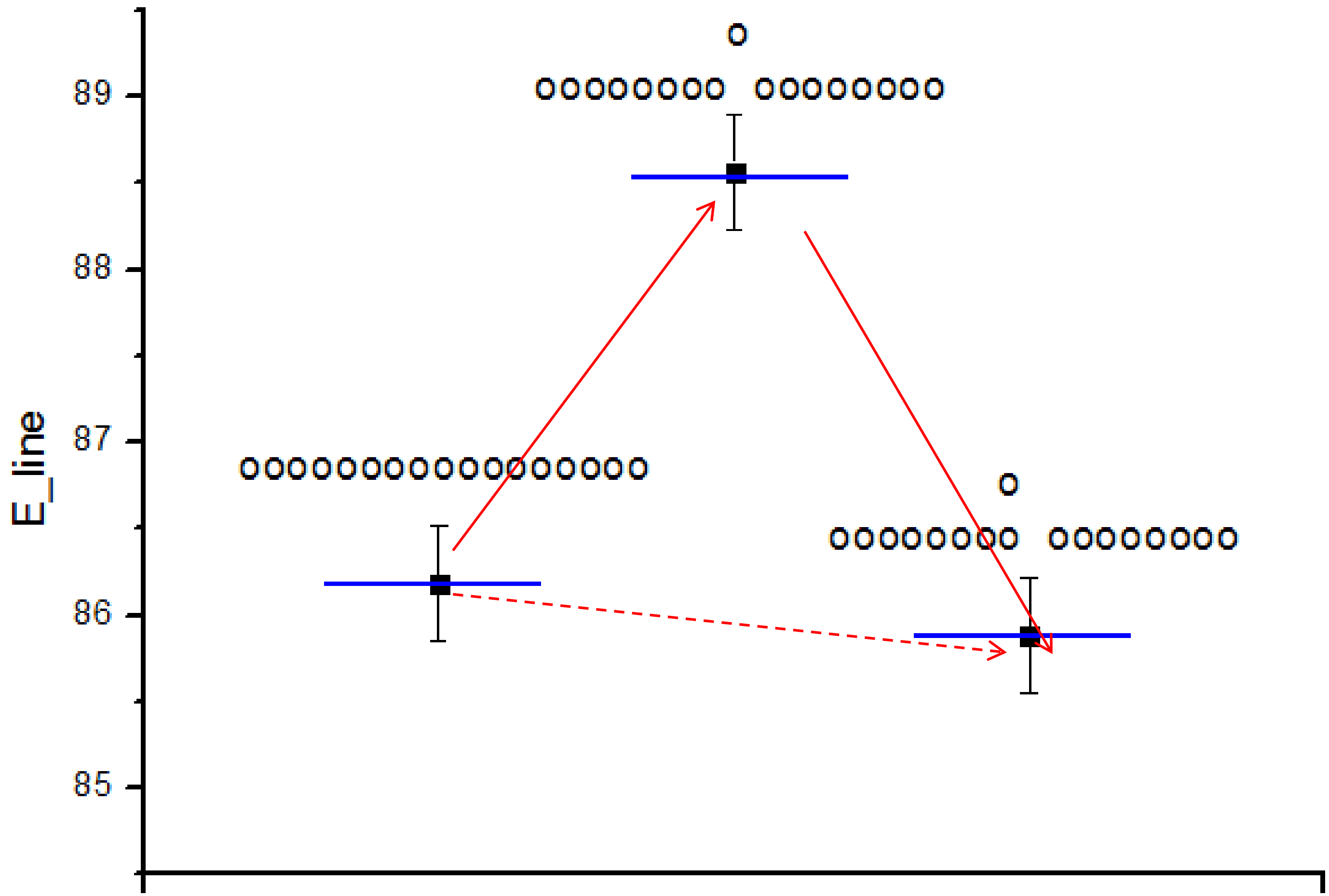
Defect – Anti-Defect pier creation

Defects aggregation - global line.
Def – AntiDef pier creation

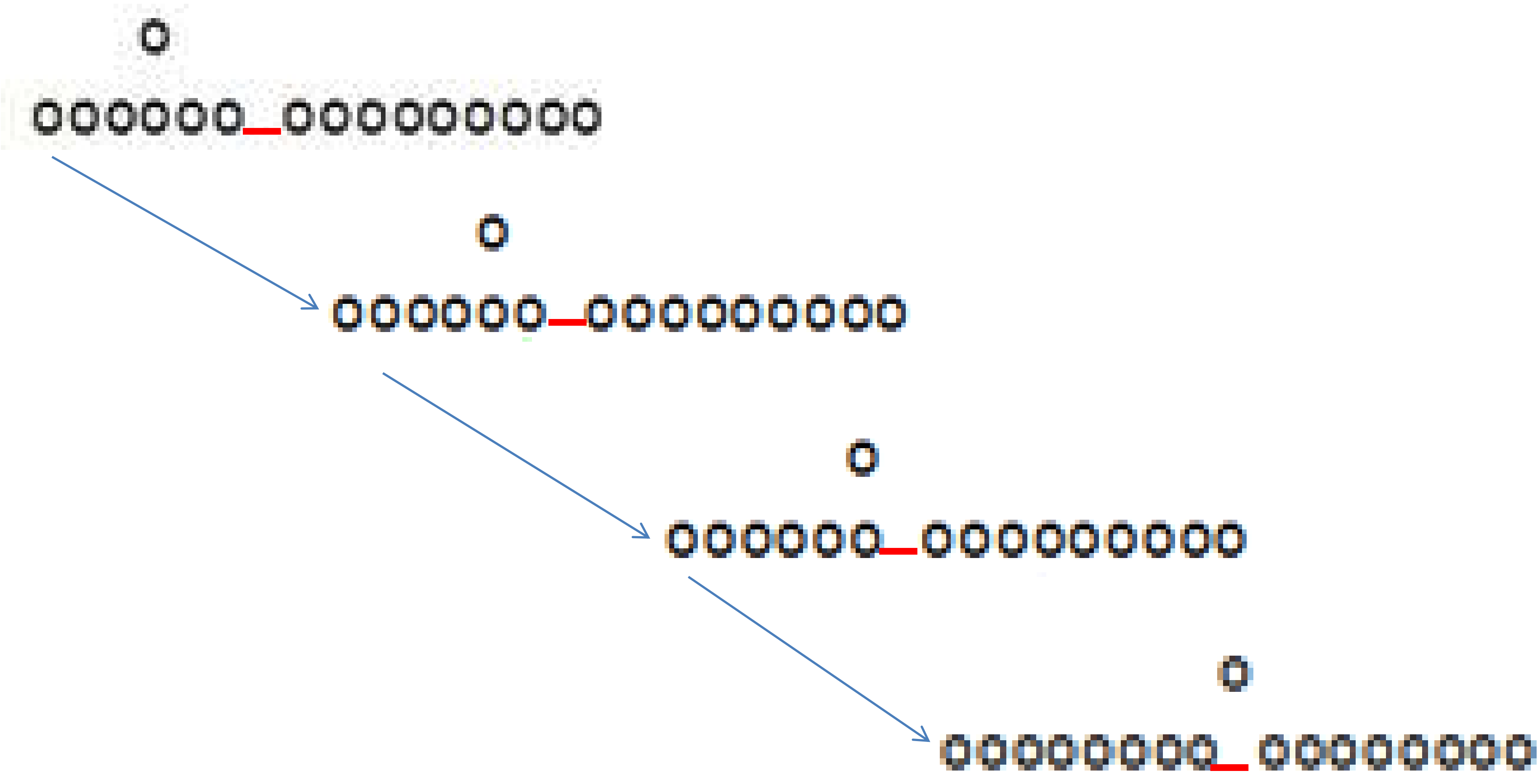




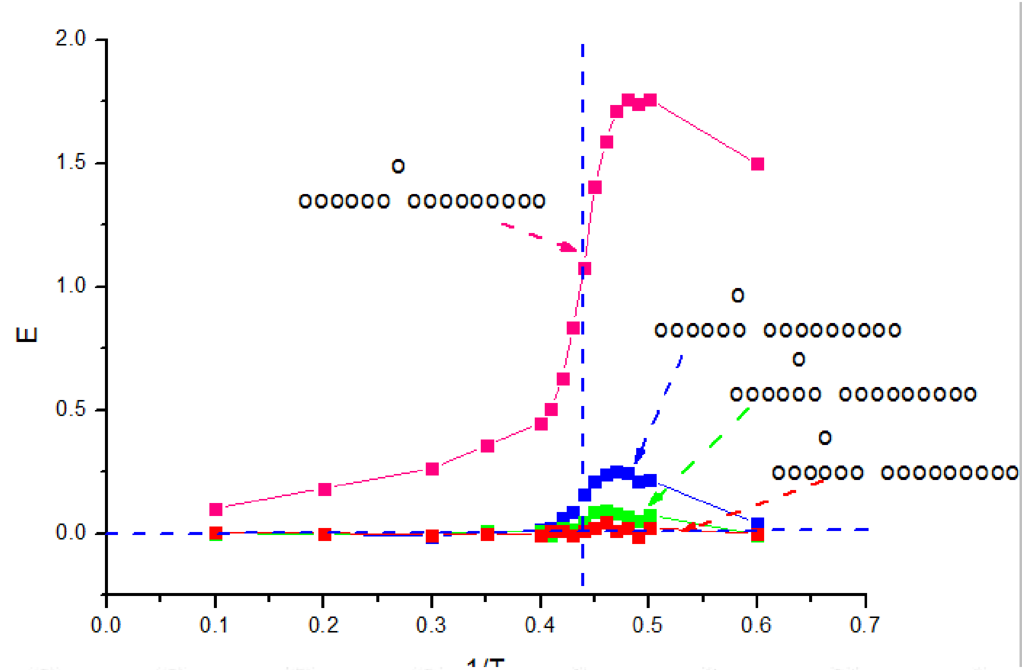
Defects aggregation - Def – AntiDef pier creation

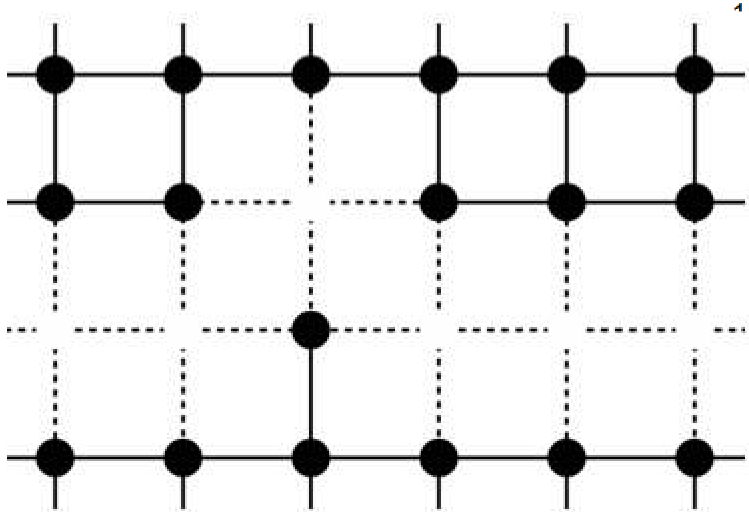


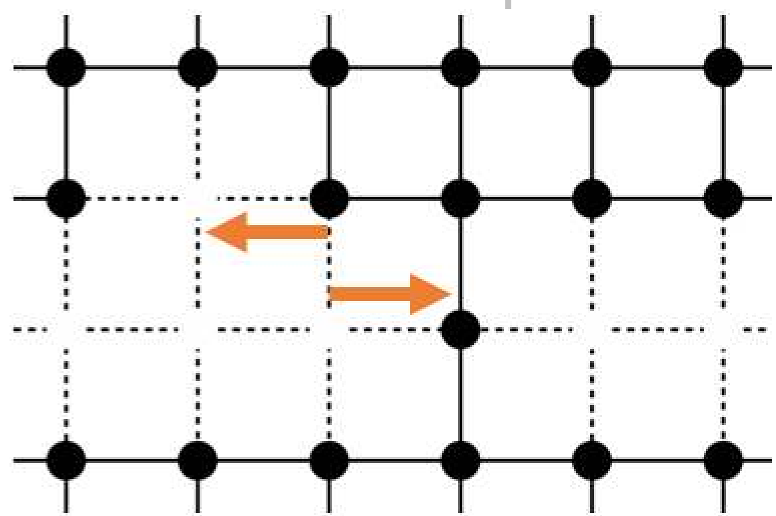
Defect – Anti-Defect intraction

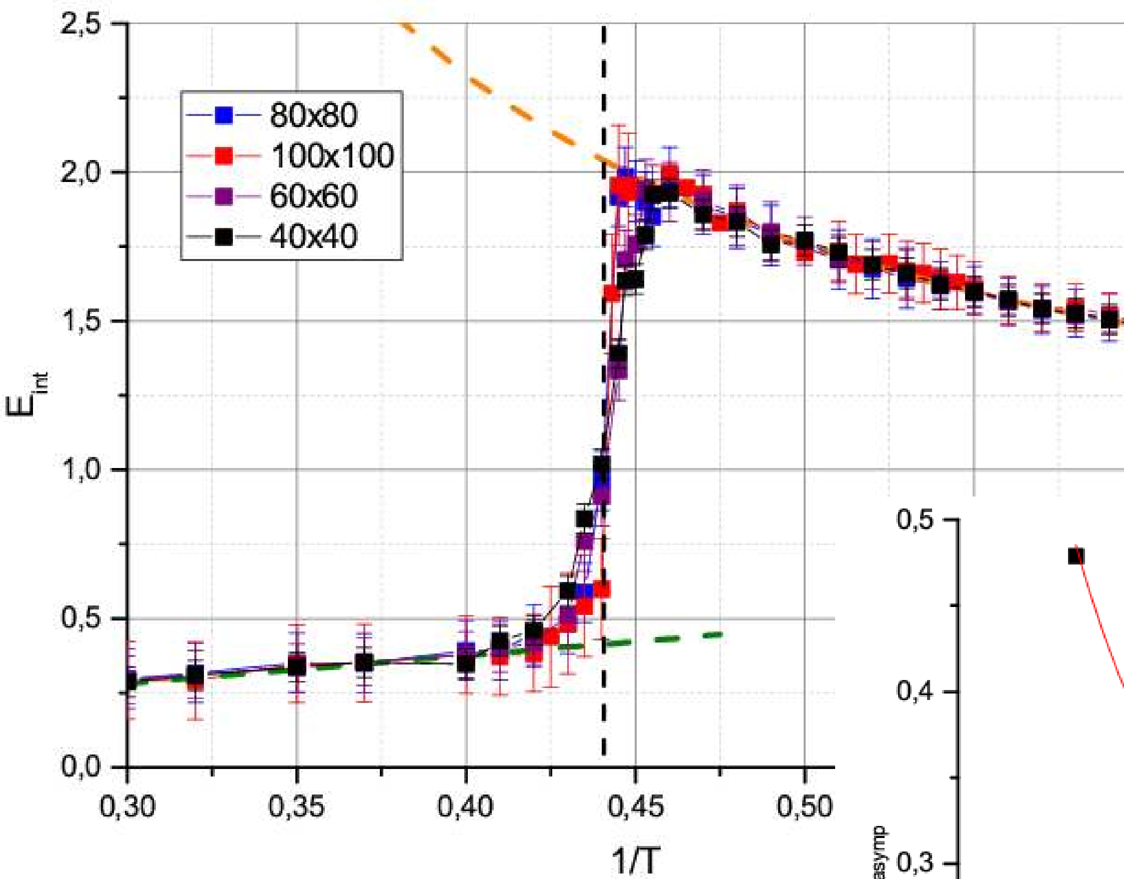


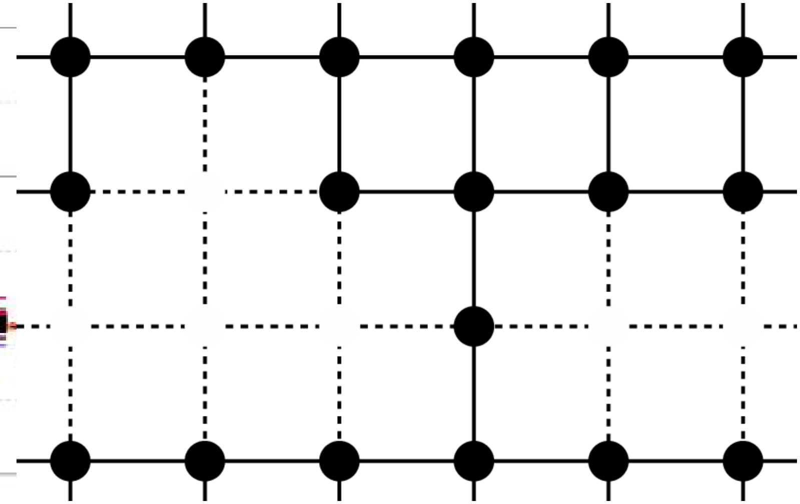
Def – AntiDef on the def line.
Repulsion

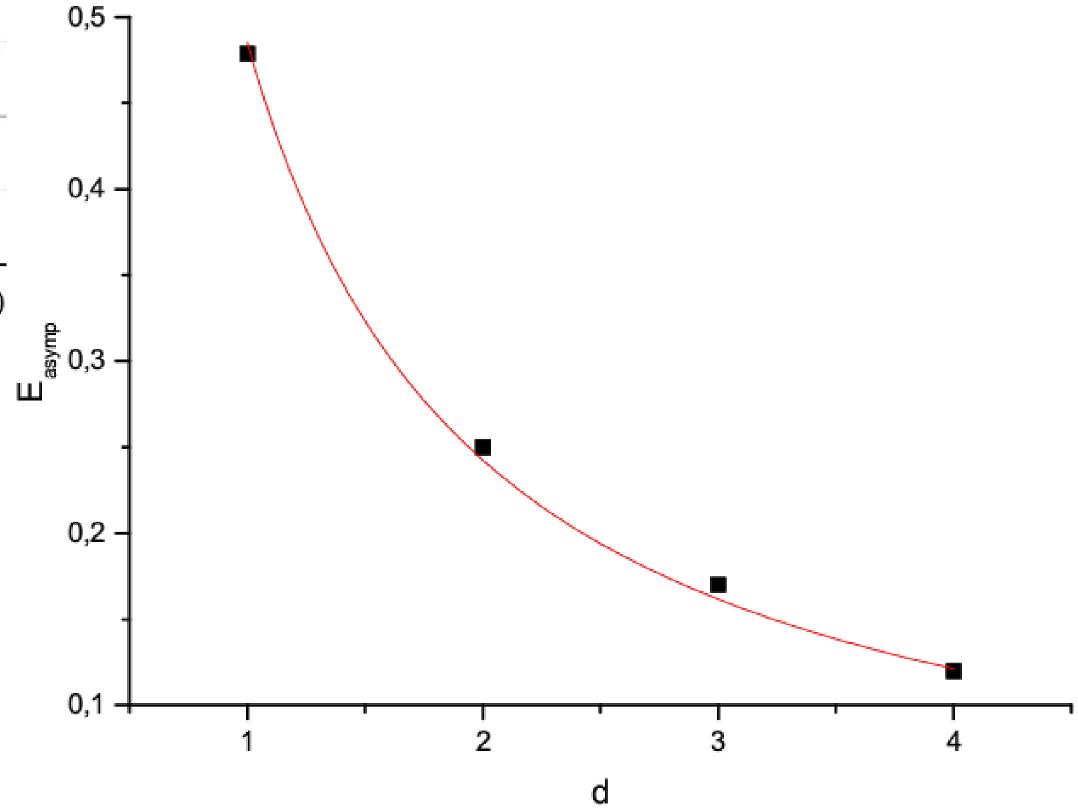












$$V(d) = ad^{-1},$$

$$a = 0.485 \pm 0.006$$

Conclusions:

1. The critical Casimir effect - a common phenomenon associated with the long-range correlations in stat. models at critical point, and as a result of long-range forces between defects.

2. The attraction of the Casimir interaction is not always destructive, it can lead to a collective phenomenon of self-organization.

3. Numerous applications in physics, chemistry, biology, economics, etc.