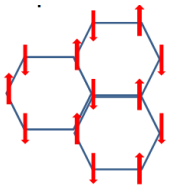
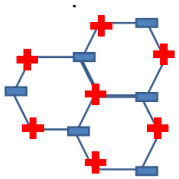
Применение методов решеточной КТП к задачам физики графена, к исследованию эффекта Казимира, а также к задачам квантовой механики многих тел.

Олег Павловский
(Физический факультет МГУ имени М.В. Ломоносова)

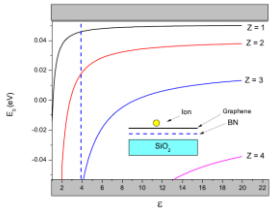
Основные темы

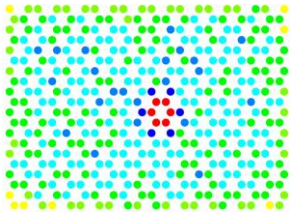
Фазовые явления в ТП моделях графена





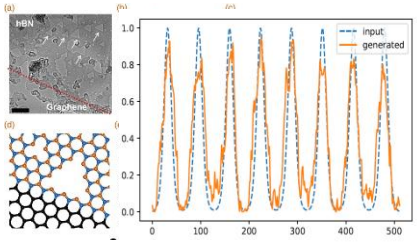
Критический заряд в графене

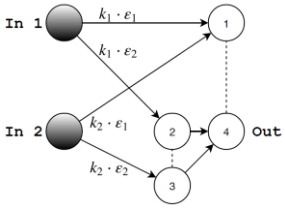




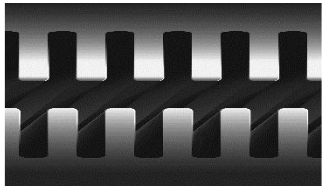
Решеточные методы КТП и методы Монте-Карло

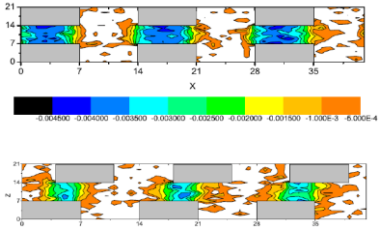
Искусственные нейронные сети на основе двойных дефектов



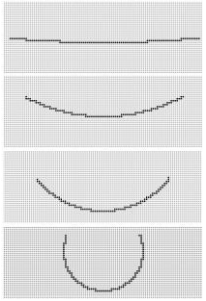


Энергия Казимира в решеточной КТП





Критическое силы Казимира между дефектами

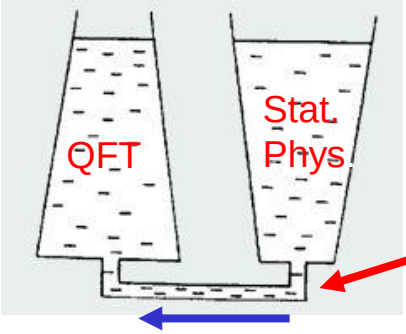


«Мир» теоретико-полевые моделей в физике конденсированного состояния вещества: немного истории…

Вычисления в физической точке в физике адронов

Киральные фермионы

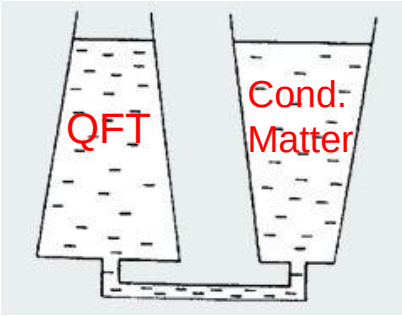
Решеточная квантовая теория (поля)



Квантовая теория в формализме континуального интеграла в евклидовом времени

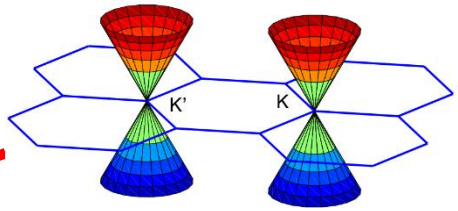
Больцмановская статистическая модель

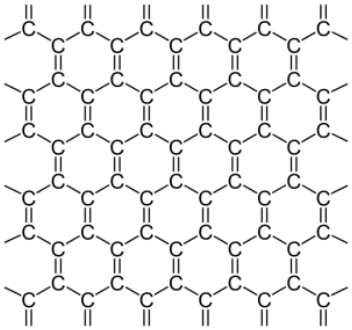
«Мир» теоретико-полевые моделей в физике конденсированного состояния вещества: время платить долги



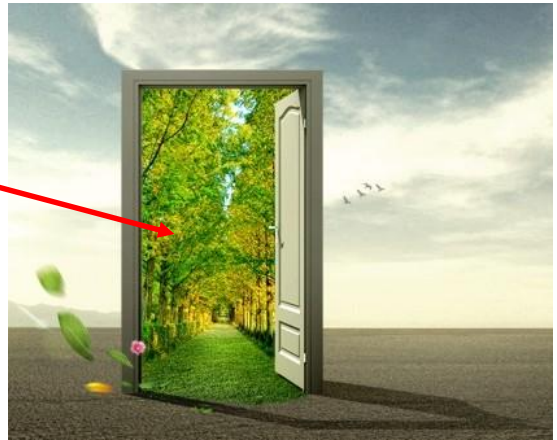
Киральные фермионы

Физика полуметаллов: Графен





Теоретико-полевые модели графена



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[3] Новосёлов А.А., Павловский О.В. Расчёт критических явлений в графене. // Ядерная физика и инжиниринг – 2017 – Т.8(2) – С. 29-32.

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ках эффективной теории поля. // Письма в "Журнал экспериментальной
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[10] Novoselov A.A., Pavlovsky O.V., Ulybyshev M.V. Monte-carlo calculations for some problems of quantum mechanics.// Physics of Atomic Nuclei – 2012 – Vol.75 – P.1119–1122.

[11] Pavlovsky O.V., Ulybyshev M.V. Monte-carlo calculation of the lateral casimir forces between rectangular gratings within the formalism of lattice quantum field theory // International Journal of Modern Physics A – 2011 – Vol.26 – P. 2743–2756. Cite: 12

[12] Pavlovsky O.V., Ulybyshev M.V. Casimir energy calculations for chern-simons surfaces and dielectric plates within the formalism of lattice quantum field theory.// Physics of Particles and Nuclei Letters – 2010 – Vol.7 – P.345–348.

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[14] Pavlovsky O.V., Ulybyshev M.V. Casimir energy calculations within the formalism of the noncompact lattice QED.// International Journal of Modern Physics A – 2010 – Vol.25 P. 2457–2473, 2010. Cite: 10

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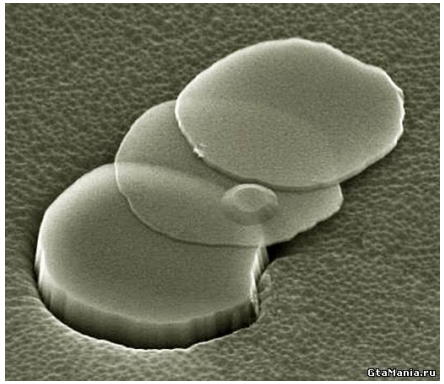
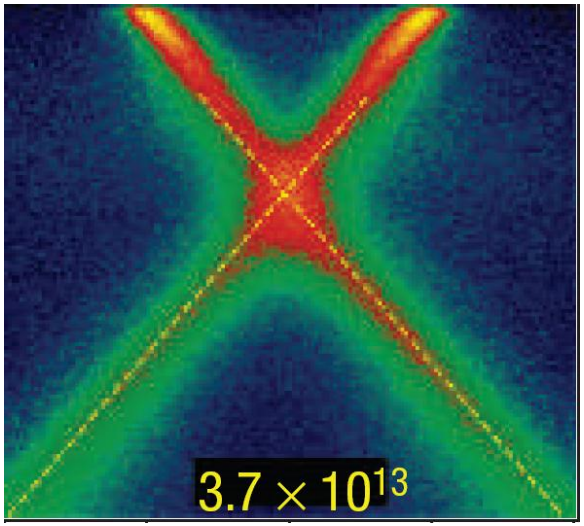
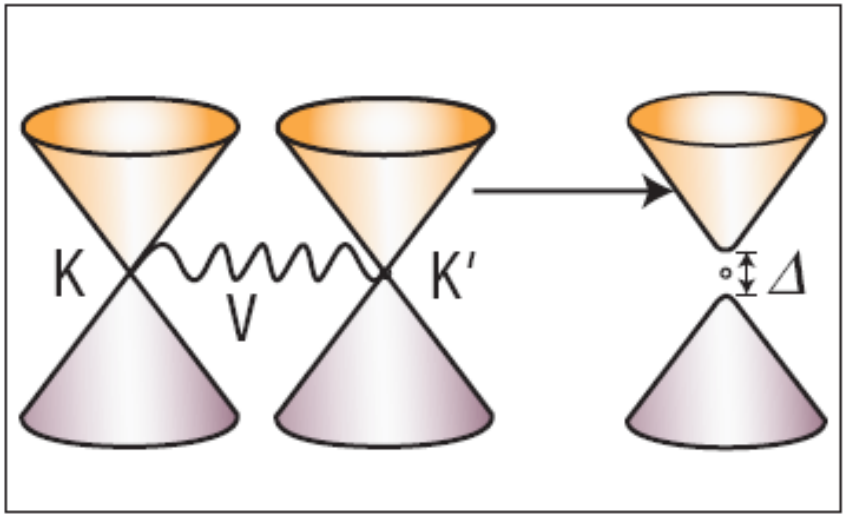
Темы исследований

Фазовые явления
в
графене

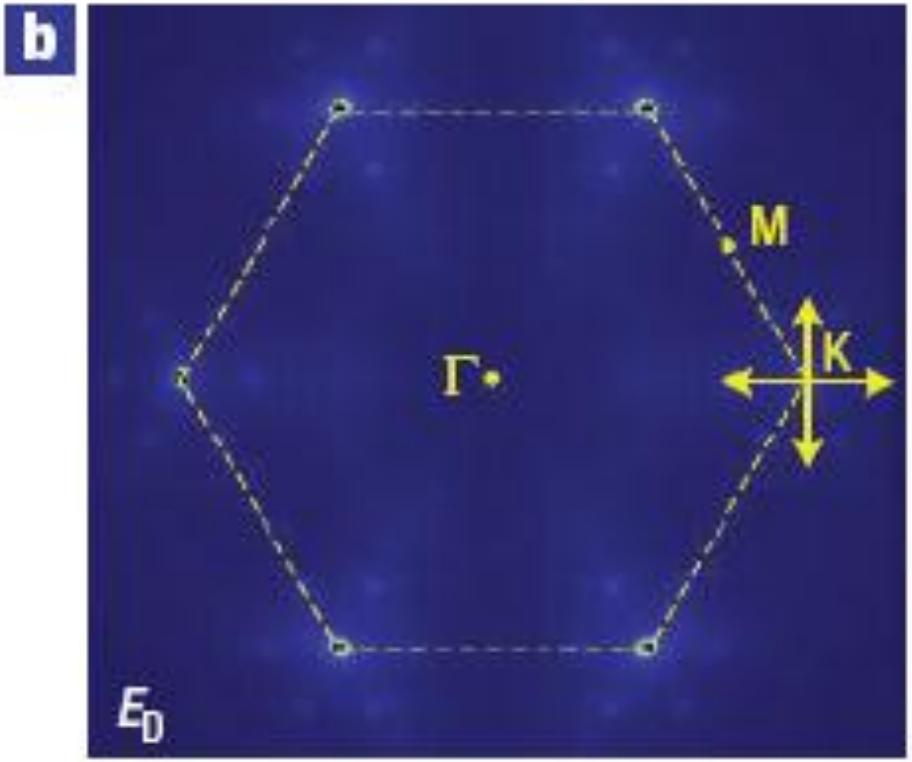
Графен: фазовый переход изолятор-проводник

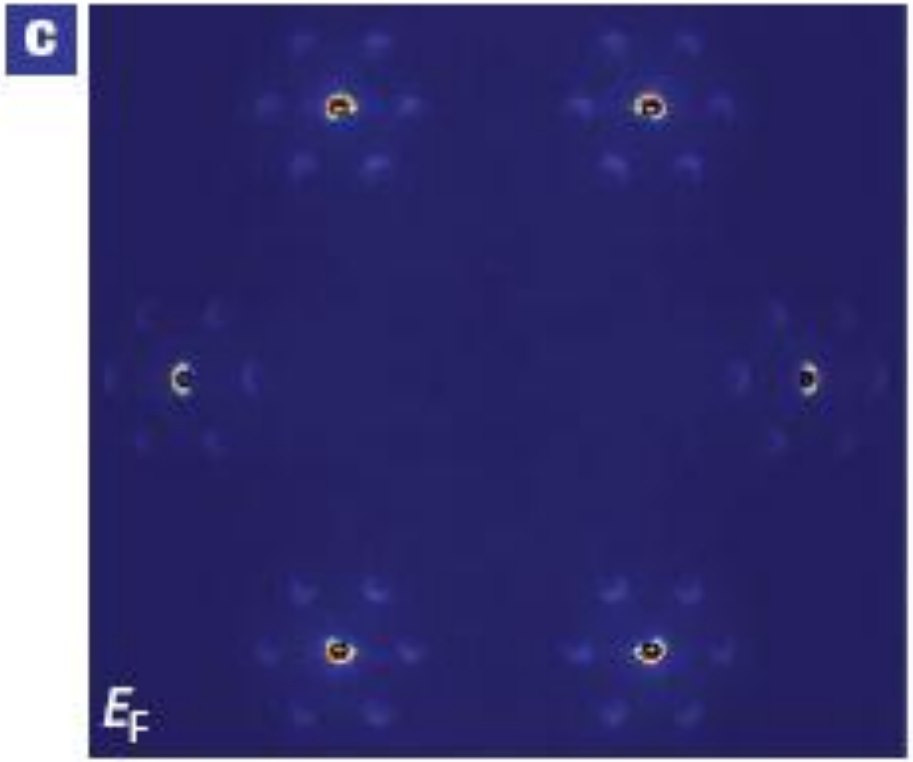






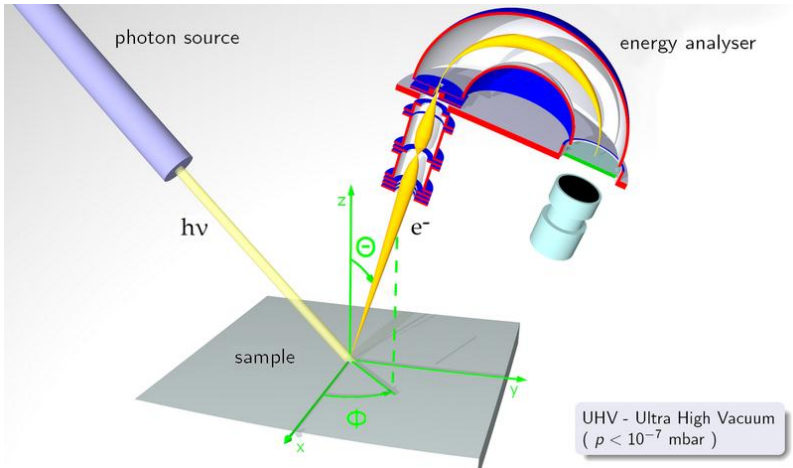
Графен: что видно в эксперименте



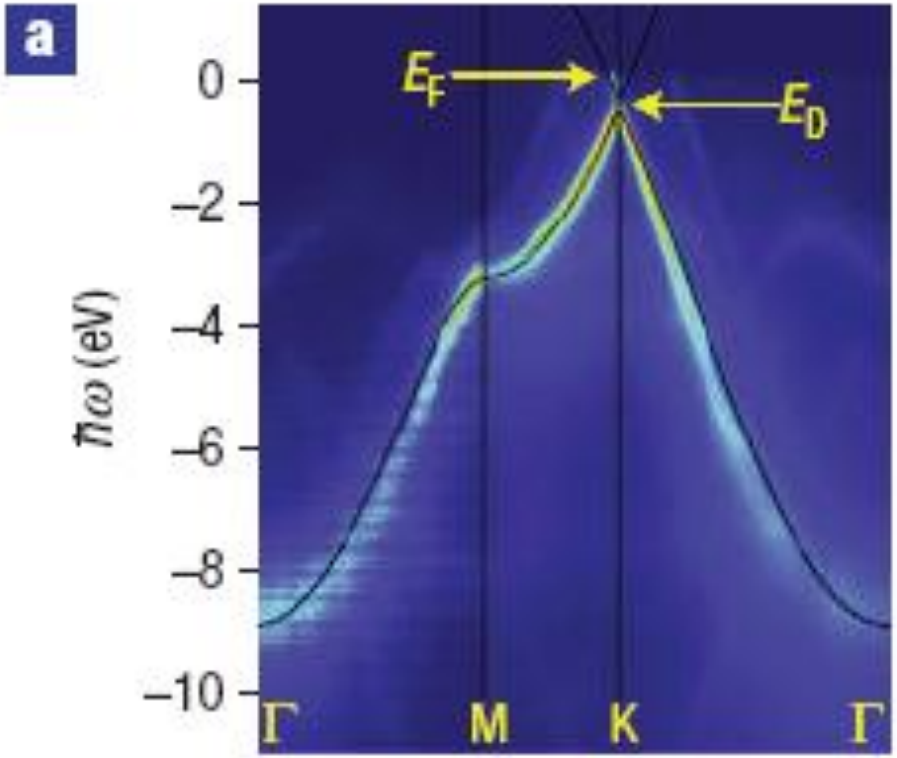


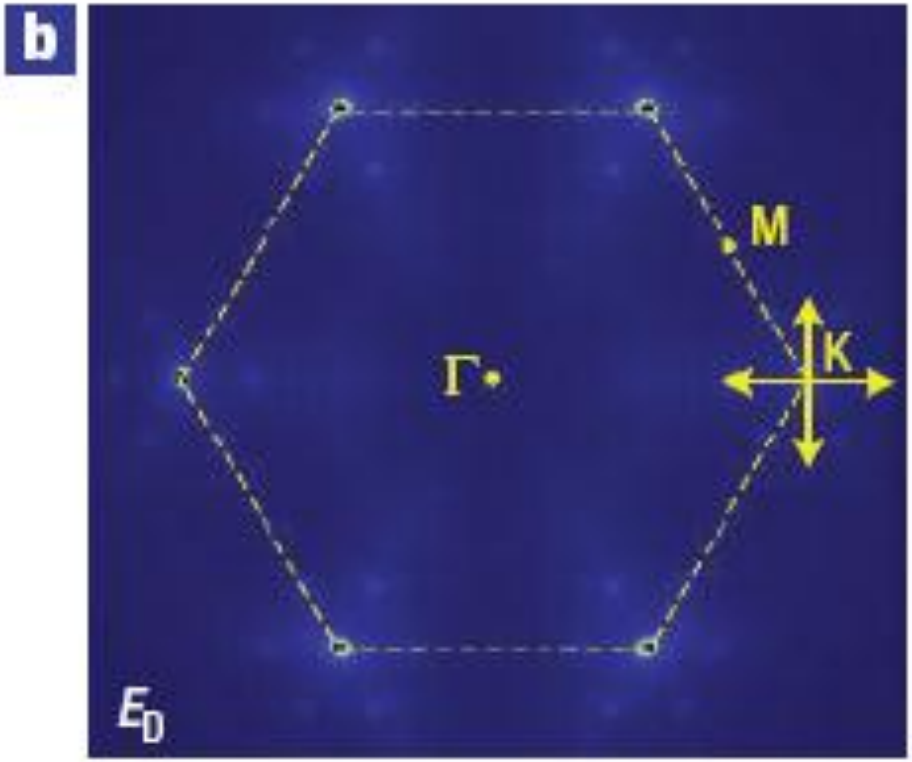
Получено методами Angle-resolved photoemission spectroscopy

$$k_{i\perp} = \frac{1}{\hbar}\sqrt{2m(E_f \cos^2\theta + V_0)}$$



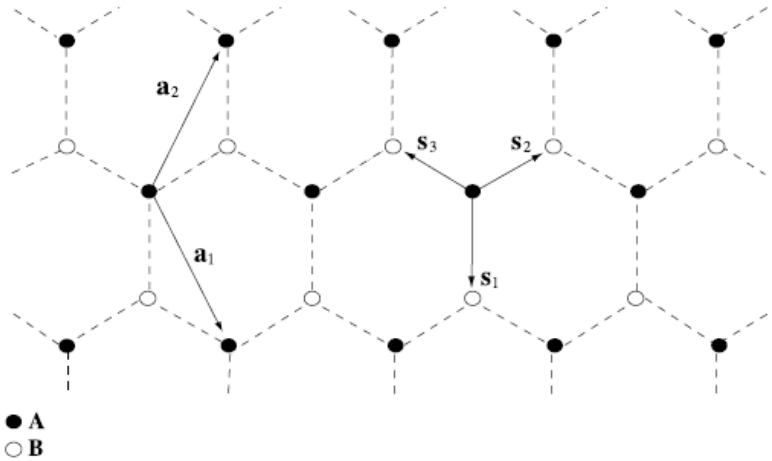
Графен: что видно в эксперименте





Модели электронных явлений в графене
Иерархия моделей

Tight-binding model

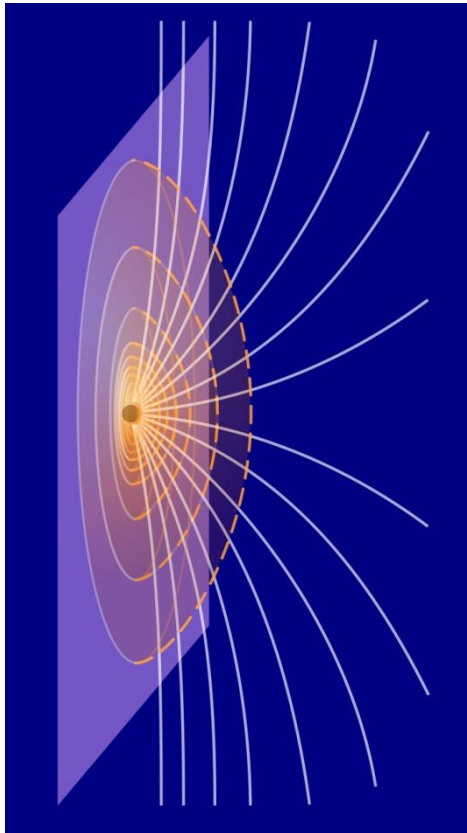


$$H = \sum_{\vec{A},i} \left(t\ b^\dagger_{\vec{A}+\vec{s}_i} a_{\vec{A}} + t^*\ a^\dagger_{\vec{A}} b_{\vec{A}+\vec{s}_i} \right) \quad + \quad \ldots$$

Теоретико-полевая модель графена

$$S = -\sum_{a=1}^{N} \int dt d^2x (\bar{\psi}_a \gamma^0 \partial_0 \psi_a + v \bar{\psi}_a \gamma^j \partial_i \psi_a + i A_0 \bar{\psi}_a \gamma^0 \psi_a)$$

$$+ \frac{1}{2g^2} \int dt d^3x (\partial_i A_0)^2 .$$



Природа сильной связи в системе: перемасштабирование полей!

$$\alpha_g \simeq 300\alpha \ > 1\ !$$

Антиферромагнитный конденсат в эффективной полевой модели графена

* **Смотрели следующую решеточную теорию:**

$$S_E^g[\theta_0] = \frac{\beta}{2}\sum_{\boldsymbol{n}}\left[\sum_{i=1}^{3}(\theta_{0,\boldsymbol{n}} - \theta_{0,\boldsymbol{n}+\boldsymbol{e}_i})^2\right], \qquad \beta \equiv v/g^2$$

$$S_E^f[\bar{\chi}, \chi, U_0] = -\sum_{\boldsymbol{m},\boldsymbol{n}} \bar{\chi}_{\boldsymbol{m}} D_{\boldsymbol{m},\boldsymbol{n}}[U_0]\chi_{\boldsymbol{n}}, \qquad U_0 = \exp(i\theta_0)$$

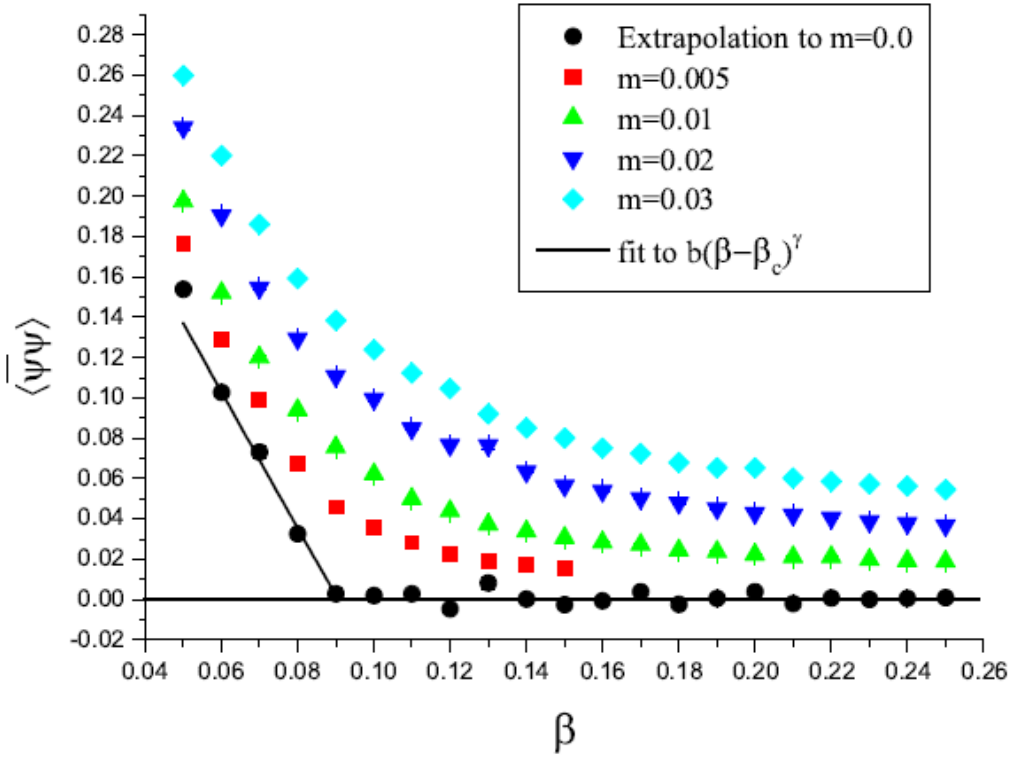
$$D_{\boldsymbol{m},\boldsymbol{n}}[U_0] = \frac{1}{2}[\delta_{\boldsymbol{m}+\boldsymbol{e}_0,\boldsymbol{n}} U_{0,\boldsymbol{m}} - \delta_{\boldsymbol{m}-\boldsymbol{e}_0,\boldsymbol{n}} U_{0,\boldsymbol{n}}^\dagger] + \frac{1}{2}\sum_i \eta_{i,\boldsymbol{m}}[\delta_{\boldsymbol{m}+\boldsymbol{e}_i,\boldsymbol{n}} - \delta_{\boldsymbol{m}-\boldsymbol{e}_i,\boldsymbol{n}}] + m_0\delta_{\boldsymbol{m},\boldsymbol{n}},$$

$$\eta_{1,\boldsymbol{n}} = (-1)^{n_0} \quad \text{and} \quad \eta_{2,\boldsymbol{n}} = (-1)^{n_0+n_1}.$$

* **Исследовали величину R:**

$$\sigma \equiv \langle \bar{\psi}_b \psi_b \rangle,$$

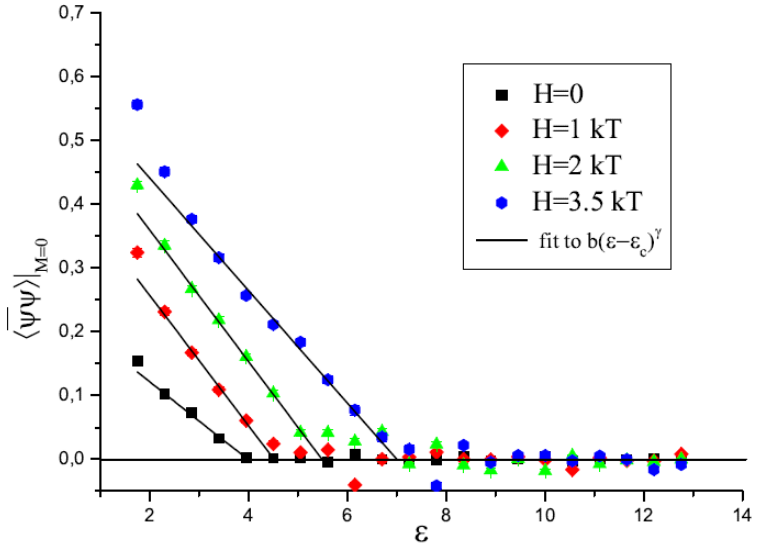
Результаты численного анализа антиферромагнитного конденсата

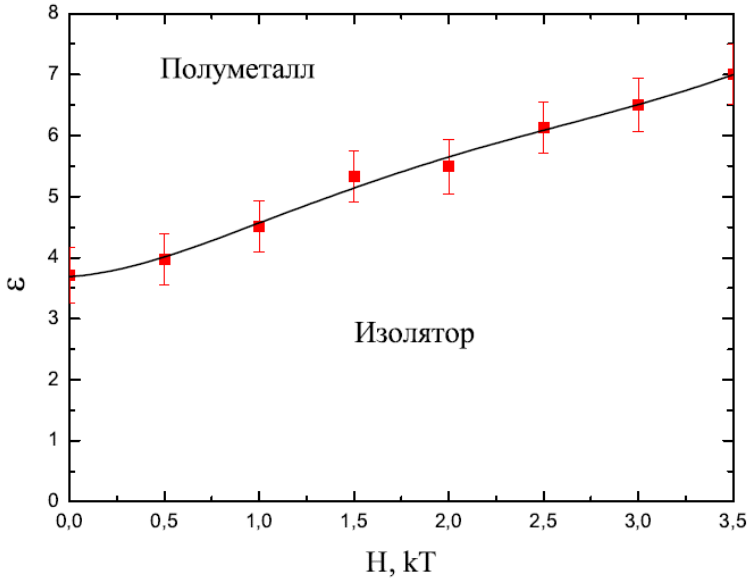


$$\langle \bar{\psi}\psi \rangle \sim (\beta_c - \beta)^\gamma \text{ с } \beta_c = 0.0908 \pm 0.0018 \text{ и } \gamma = 1.0 \pm 0.16.$$

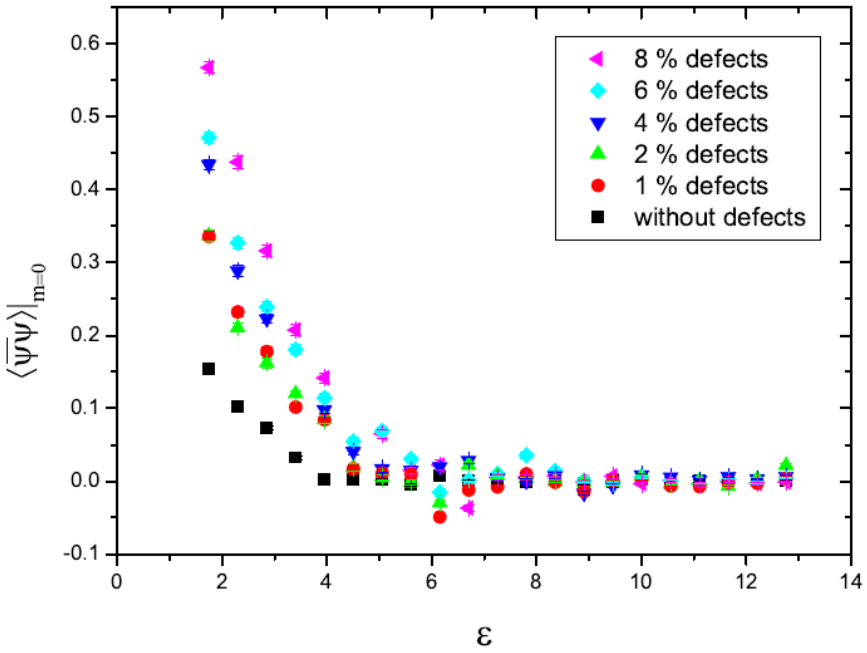
$$\beta \equiv \frac{1}{g^2} = \frac{v_F}{4\pi e^2}\,\frac{\epsilon + 1}{2},$$

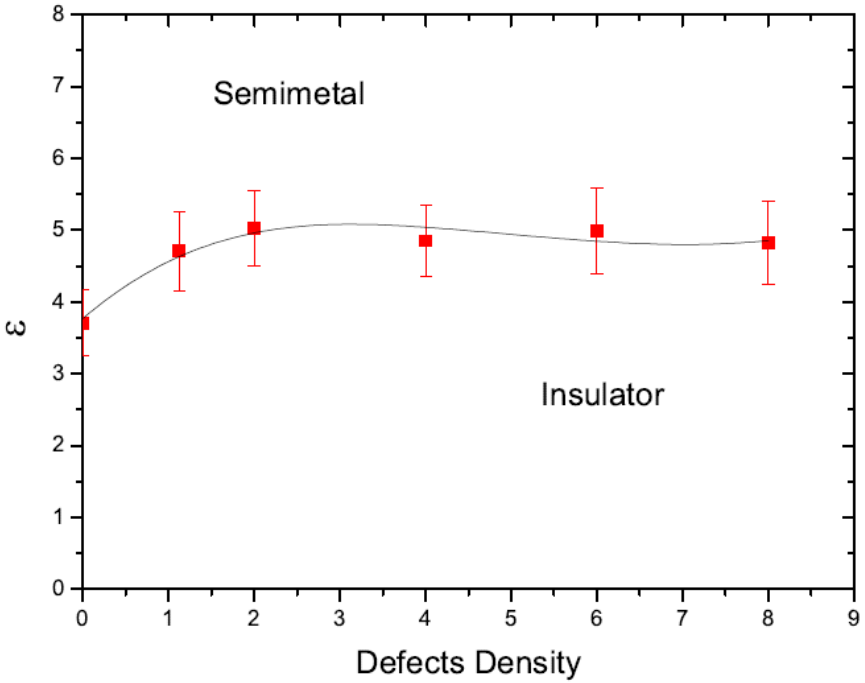
Результаты численного анализа антиферромагнитного конденсата





Результаты численного анализа антиферромагнитного конденсата



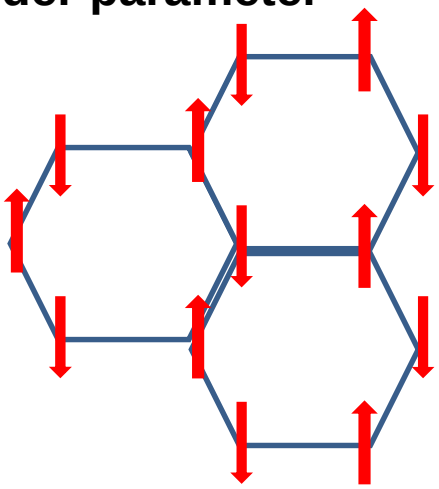


Конденсаты в графене: микроскопическая картина

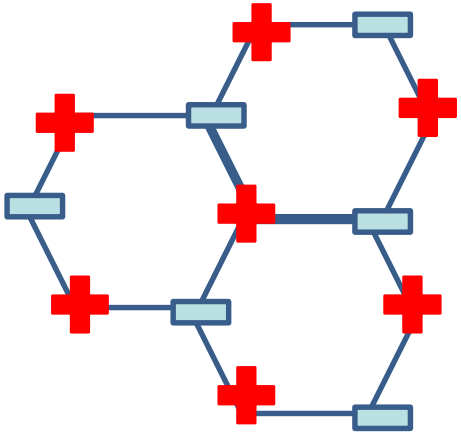
Transport properties of Graphene

Phase transition phenomena in Graphene

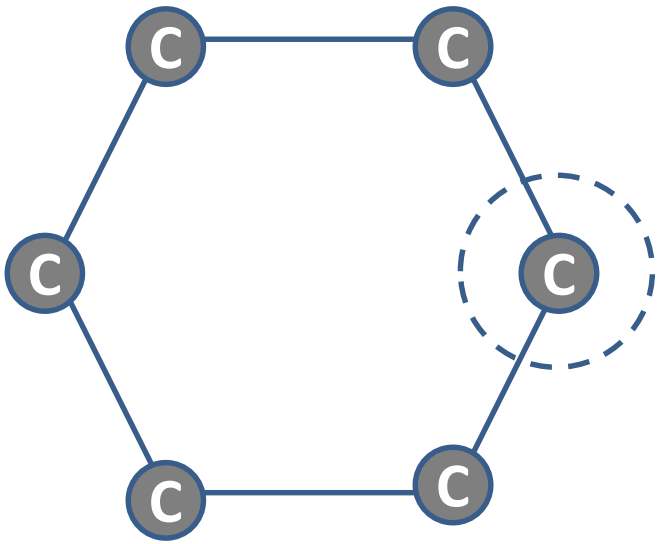
Anti-ferromagnetic order parameter



Anti-ferroelectric order parameter



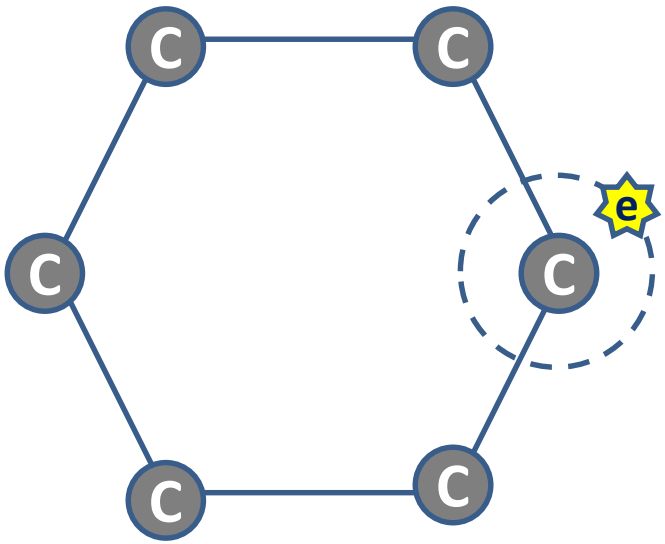
Electron / hole excitations



Charge of this site
=
Charge of C (+1)
+
Charge π-orbital electrons (0)
=
+1

This is HOLE state!

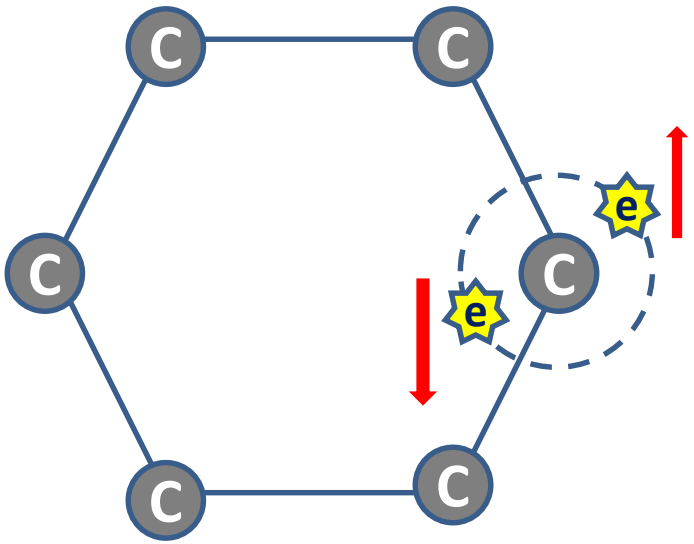
Electron / hole excitations



Charge of this site
=
Charge of C (+1)
+
Charge π-orbital electrons (-1)
=
0

These are Neutrality states!

Electron / hole excitations

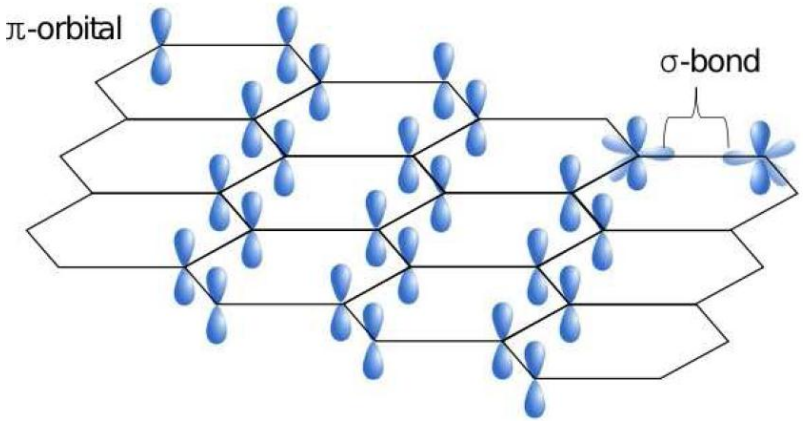


Charge of this site
=
Charge of C (+1)
+
Charge π-orbital electrons (-2)
=
-1

This is Electron state!

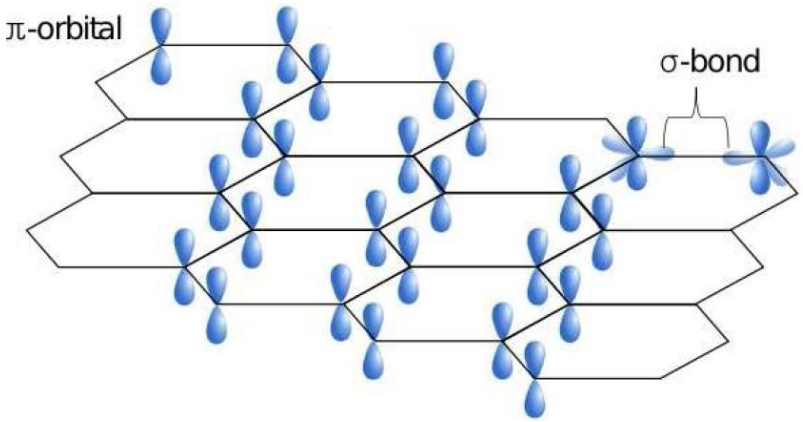
Tight-binding lattice Hamiltonian of Graphene

$$H = H_\kappa + H_h + H_c$$



Tight-binding coupling lattice Hamiltonian of Graphene

$$H = H_\kappa + H_h + H_c$$

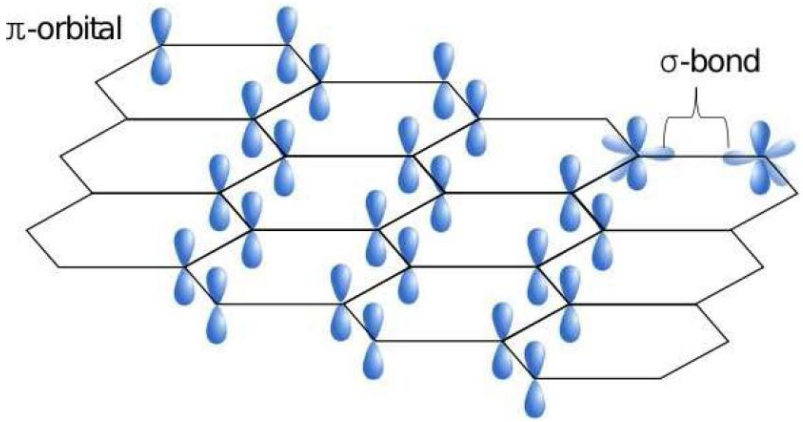


1) Hopping term:

$$H_\kappa = \kappa \sum_{x,\mu,\sigma} \left(\psi^\dagger_{\sigma,x+\mu} \psi_{\sigma,x} + \psi^\dagger_{\sigma,x} \psi_{\sigma,x+\mu} \right)$$

Tight-binding lattice Hamiltonian of Graphene

$$H = H_\kappa + H_h + H_c$$

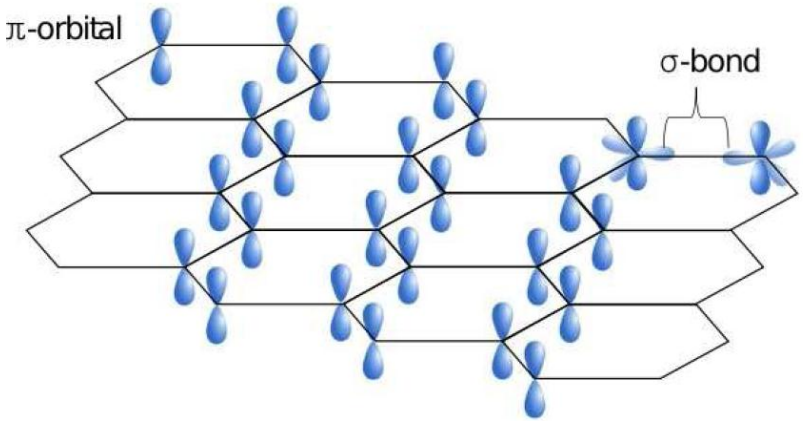


2) On-site interaction term:

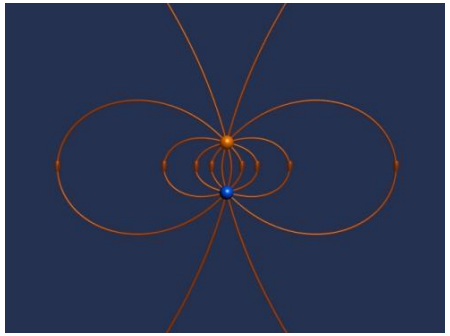
$$H_h = \sum_x q_x \; V_{x,x} \; q_x$$

Tight-binding lattice Hamiltonian of Graphene

$$H = H_\kappa + H_h + H_c$$



3) Coulomb interaction term:



$$H_c = \sum_{x \neq x'} q_x V_{x,x'} q'_x.$$

$$V_{x,x'} = \frac{\alpha}{|x - x'|}$$

Creation / annihilation operators

$$\begin{cases} a^\dagger = \psi_\uparrow^\dagger \\ a = \psi_\uparrow, \end{cases}$$

Creation / annihilation operators for "electron"

$$\begin{cases} b^\dagger = \psi_\downarrow \\ b = \psi_\downarrow^\dagger \end{cases}$$

Creation / annihilation operators for "hole"

$$\begin{aligned} \hat{q}_x &= 1 - \psi_{\uparrow,x}^\dagger \psi_{\uparrow,x} - \psi_{\downarrow,x}^\dagger \psi_{\downarrow,x} \\ &= 1 - a^\dagger a - b b^\dagger = b^\dagger b - a^\dagger a \end{aligned}$$

Basic vectors

$|\ \downarrow\ \cdot\rangle$ **"Vacuum" state**

$|\ \uparrow\downarrow\rangle$ **"Electron" state**

$|\ \uparrow\ \cdot\rangle$ **"Electron + hole" state**

$|\ \cdot\ \cdot\rangle$ **"Hole" state**

$$a^\dagger a|\downarrow\ \cdot\rangle = a^\dagger a|\cdot\ \cdot\rangle = b^\dagger b|\downarrow\ \cdot\rangle = b^\dagger b = |\downarrow\uparrow\rangle = 0\,,$$

$$a^\dagger a|\cdot\ \uparrow\rangle = b^\dagger b|\cdot\ \uparrow\rangle = 1 * |\cdot\ \uparrow\rangle\,,$$

$$a^\dagger a|\downarrow\uparrow\rangle = 1 * |\downarrow\uparrow\rangle; \qquad b^\dagger b|\cdot\ \cdot\rangle = 1 * |\cdot\ \cdot\rangle\,.$$

Occupation numbers formalism

$$a_x^\dagger a_x|\,\rangle = m_x|\,\rangle; \qquad b^\dagger b|\,\rangle = n_x|\,\rangle$$

$$n_x,\, m_x = 0, 1.$$

$$\boxed{q_x = n_x - m_x.}$$

$\lvert\ \downarrow\ \cdot\rangle$	q = 0
$\lvert\ \uparrow\downarrow\rangle$	q = 1
$\lvert\ \uparrow\ \cdot\rangle$	q = 0
$\lvert\ \cdot\ \cdot\rangle$	q = -1

$$\boxed{|S\rangle = |\{n_x\}\{m_x\}\rangle}$$

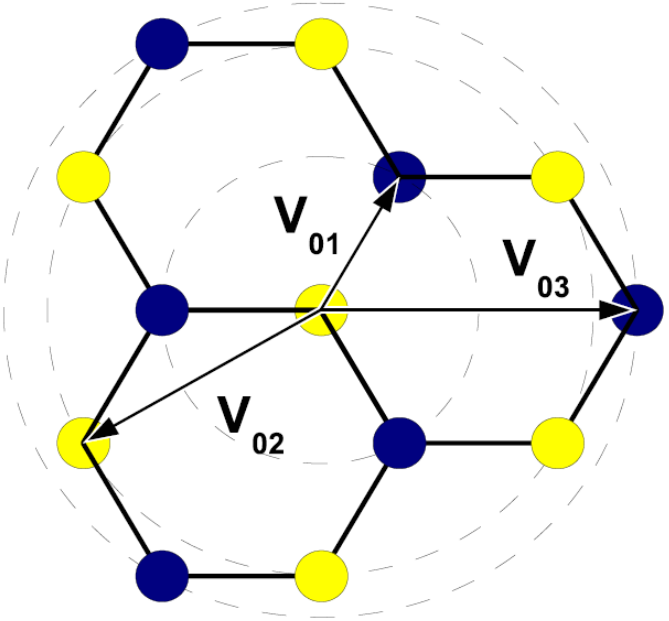
Role of the Terms in Hamiltonian of Graphene

$$H = H_\kappa + H_h + H_c$$

$$H_\kappa = \kappa \sum_{x,\mu,\sigma} \left(\psi^\dagger_{\sigma,x+\mu} \psi_{\sigma,x} + \psi^\dagger_{\sigma,x} \psi_{\sigma,x+\mu} \right) \qquad \kappa = 2.8 \text{ eV}$$

$$H_h = \sum_x q_x \; V_{x,x} \; q_x \qquad V(x,x) = 9.3 \text{ eV}$$

$$H_c = \sum_{x \neq x'} q_x V_{x,x'} q'_x. \qquad V(0,1) = 5.5 \text{ eV}$$



$$H = H_\kappa + H_h + H_c$$

Monte-Carlo "calculus"

$$\langle \hat{O} \rangle = \frac{1}{\mathcal{Z}} \operatorname{Tr} \left(\hat{O} \, \mathrm{e}^{-\beta \hat{H}} \right).$$

$$\mathcal{Z} = \operatorname{Tr} \mathrm{e}^{-\beta \hat{H}}$$

$$\hat{H} = \hat{H}_{(2)} + \hat{H}_{(4)} = \sum_{x,y,\sigma,\sigma'} t_{xy\sigma\sigma'} \hat{c}^{\dagger}_{x\sigma} \hat{c}_{y\sigma'} + \sum_{x,y,\sigma,\sigma'} U_{xy\sigma\sigma'} \hat{n}_{x\sigma} \hat{n}_{y\sigma'},$$

$$\hat{n}_{x\sigma} = \hat{c}^{\dagger}_{x\sigma} \hat{c}_{x\sigma}$$

$$\operatorname{Tr} \, \mathrm{e}^{-\beta \hat{H}} \approx \operatorname{Tr} \left(\mathrm{e}^{-\delta \hat{H}_{(2)}} \, \mathrm{e}^{-\delta \hat{H}_{(4)}} \, \mathrm{e}^{-\delta \hat{H}_{(2)}} \, \mathrm{e}^{-\delta \hat{H}_{(4)}} \ldots \right).$$

Метод Хаббарда-Стратановича

$$\mathrm{Tr}\ \mathrm{e}^{-\beta\hat{H}} \approx \mathrm{Tr}\left(\mathrm{e}^{-\delta\hat{H}_{(2)}}\ \mathrm{e}^{-\delta\hat{H}_{(4)}}\ \mathrm{e}^{-\delta\hat{H}_{(2)}}\ \mathrm{e}^{-\delta\hat{H}_{(4)}}\ \ldots\right).$$

$$\exp\left(-\frac{\delta}{2}\sum_{x,y}U_{x,y}\hat{n}_x\hat{n}_y\right) \cong$$

$$\cong \int D\phi_x \exp\left(-\frac{1}{2\delta}\sum_{x,y}\phi_x U^{-1}_{xy}\phi_y\right)\ \exp\left(i\sum_x \phi_x\hat{n}_x\right),$$

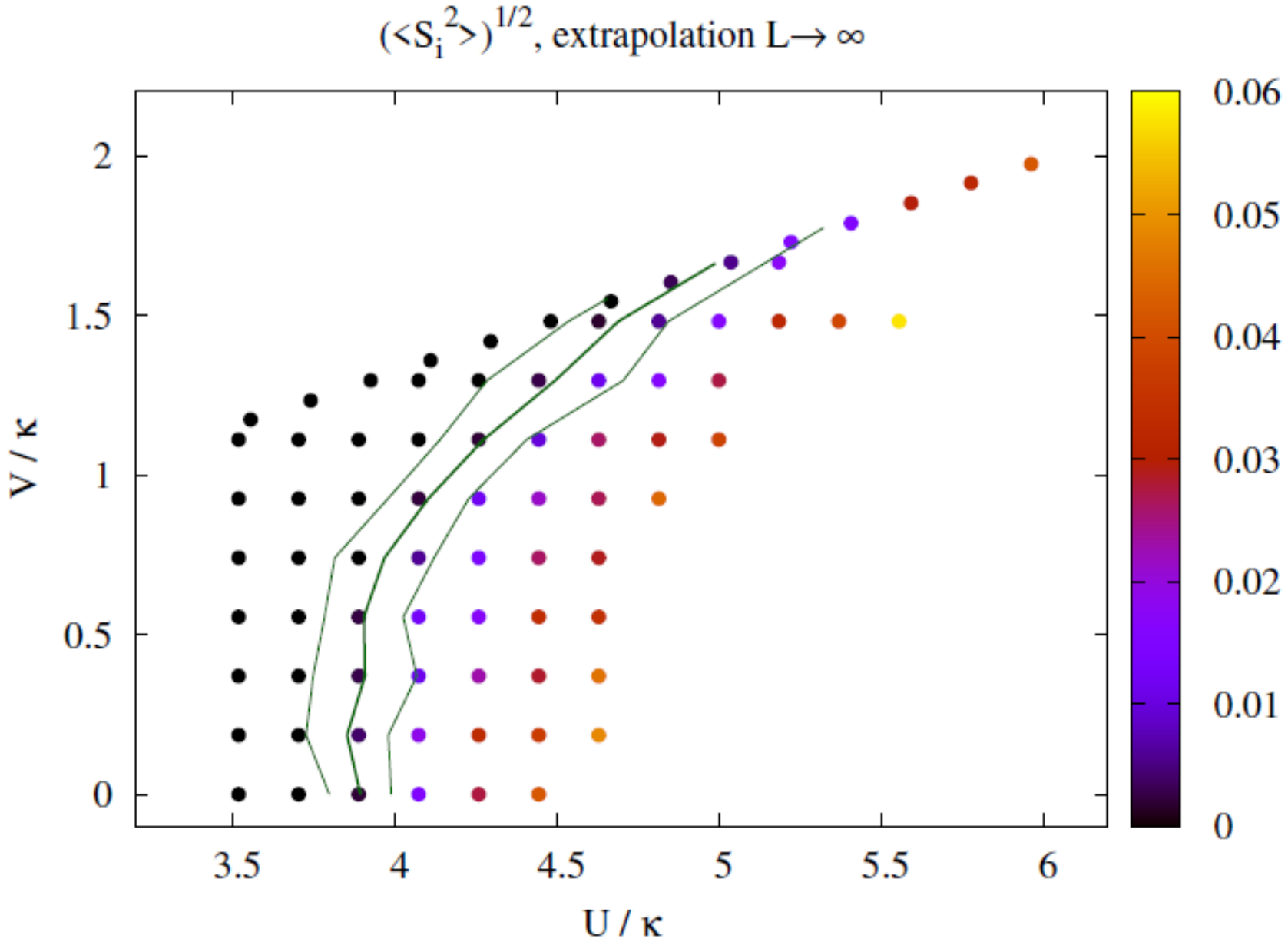
$$\exp\left(\frac{\delta}{2}\sum_{x,y}U_{x,y}\hat{n}_x\hat{n}_y\right) \cong$$

$$\cong \int D\phi_x \exp\left(-\frac{1}{2\delta}\sum_{x,y}\phi_x U^{-1}_{xy}\phi_y\right)\ \exp\left(\sum_x \phi_x\hat{n}_x\right).$$

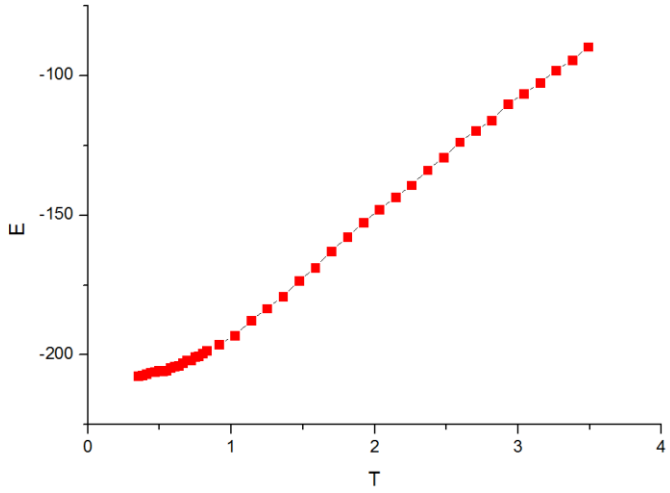
$$\mathcal{Z}_c = \int \mathcal{D}\phi_{x,t}\chi_{x,t}\exp^{-S_\alpha}\det M_{\mathrm{el}}\det M_h,$$

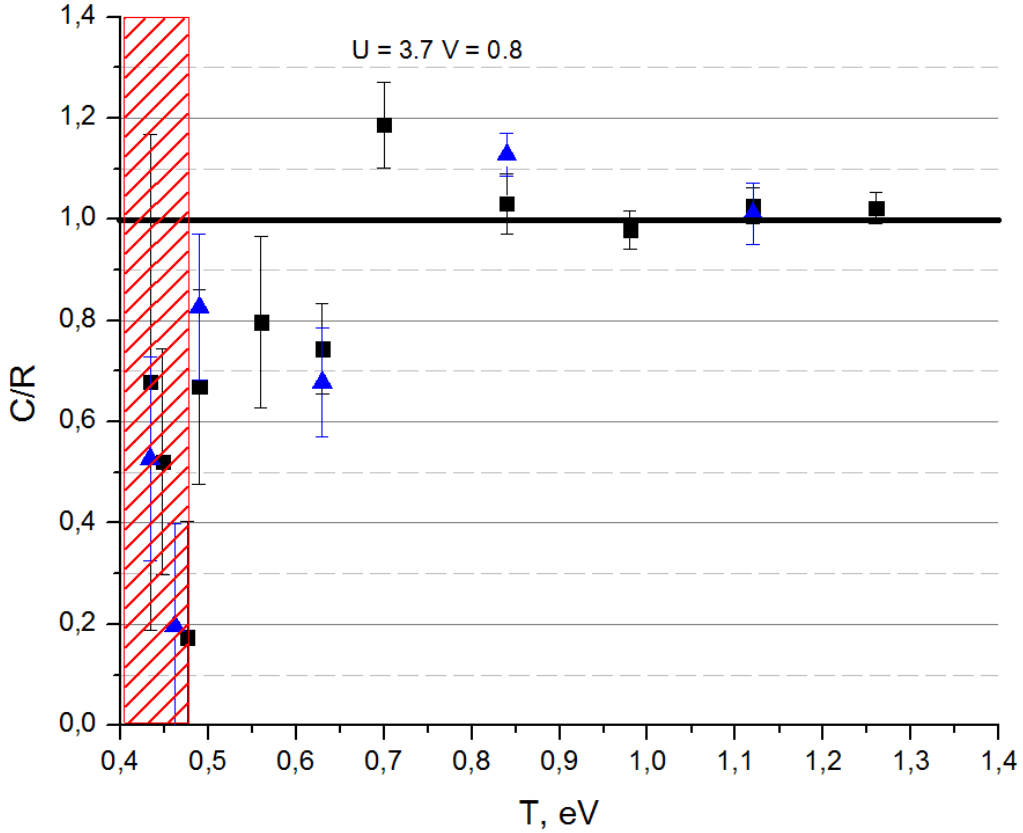
$$S_\alpha(\phi_{x,t},\chi_{x,t}) = \sum_{x,t}\frac{\phi^2_{x,t}}{2\alpha\delta U} + \sum_{x,t}\frac{(\chi_{x,t}-(1-\alpha)\delta U)^2}{2(1-\alpha)\delta U},$$

Результаты

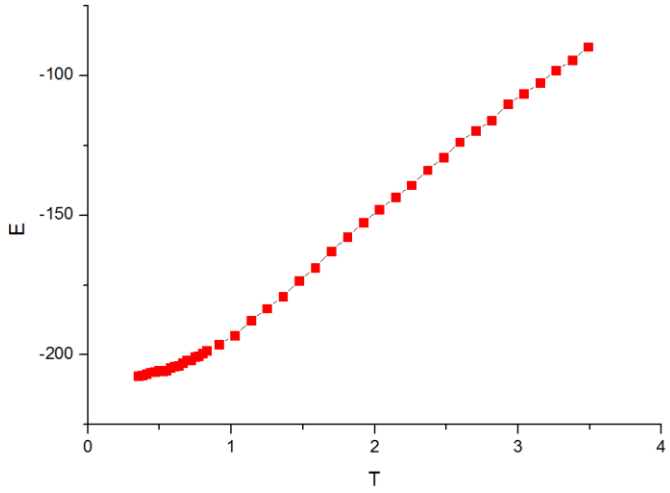

$(\langle S_i^2 \rangle)^{1/2}$, extrapolation $L \to \infty$
V / κ
U / κ
0
0.5
1
1.5
2
3.5
4
4.5
5
5.5
6
0.06
0.05
0.04
0.03
0.02
0.01
0

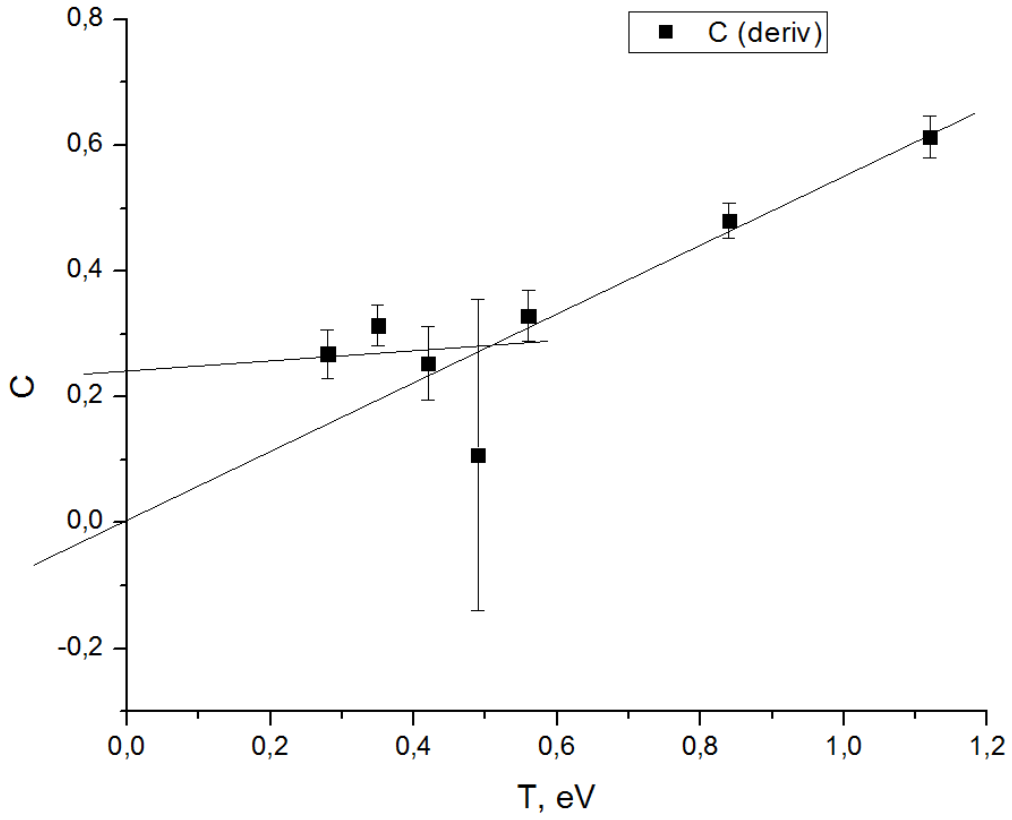
Результаты


-100
-150
-200
E
0
1
2
3
4
T

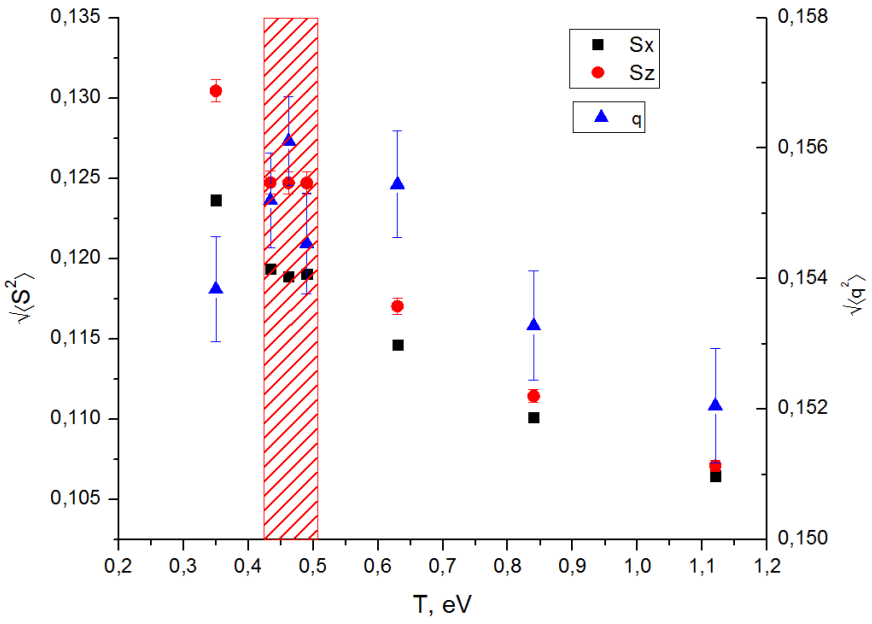

U = 3.7 V = 0.8
1,4
1,2
1,0
0,8
0,6
0,4
0,2
0,0
C/R
0,4
0,5
0,6
0,7
0,8
0,9
1,0
1,1
1,2
1,3
1,4
T, eV

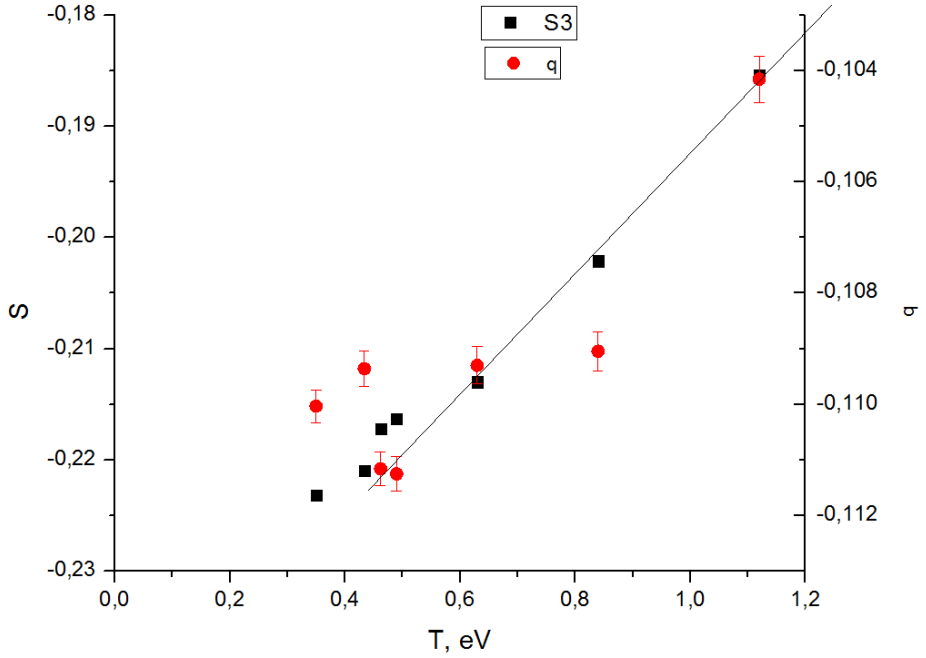
Результаты


-100
-150
-200
E
0
1
2
3
4
T

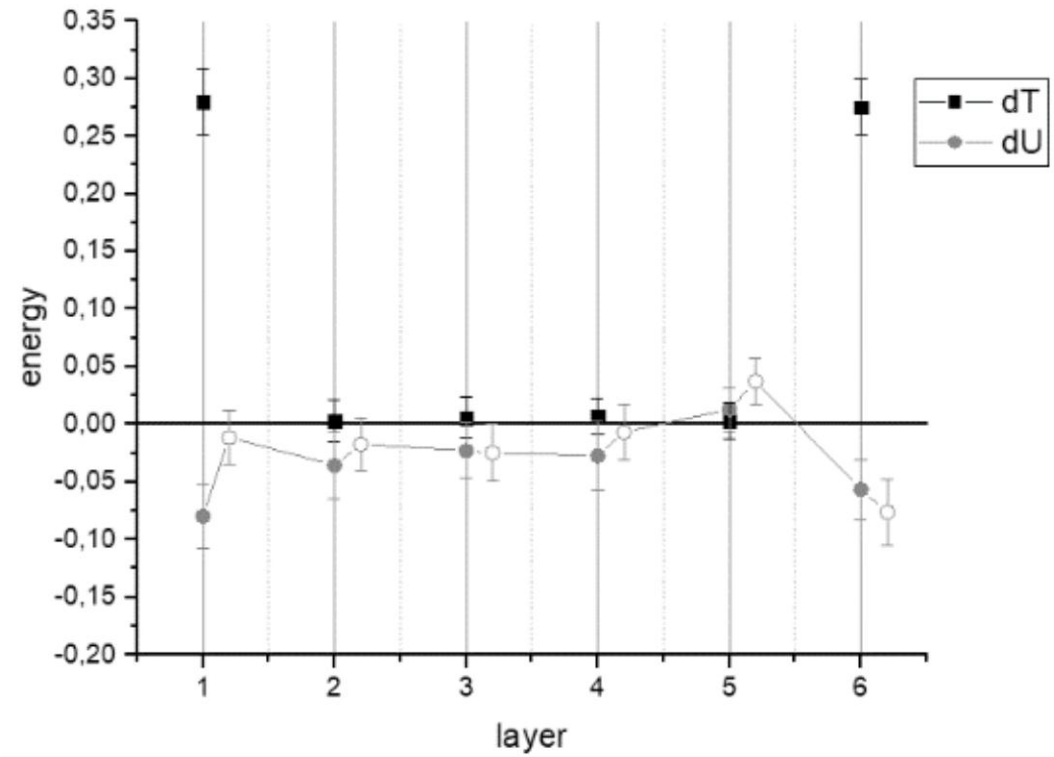

C (deriv)
0,8
0,6
0,4
0,2
0,0
-0,2
C
0,0
0,2
0,4
0,6
0,8
1,0
1,2
T, eV

Результаты


Sx
Sz
q
0,135
0,130
0,125
0,120
0,115
0,110
0,105
0,158
0,156
0,154
0,152
0,150
0,2
0,3
0,4
0,5
0,6
0,7
0,8
0,9
1,0
1,1
1,2
T, eV


S3
q
-0,18
-0,19
-0,20
-0,21
-0,22
-0,23
S
-0,104
-0,106
-0,108
-0,110
-0,112
q
0,0
0,2
0,4
0,6
0,8
1,0
1,2
T, eV

Результаты


0,35
0,30
0,25
0,20
0,15
0,10
0,05
0,00
-0,05
-0,10
-0,15
-0,20
energy
1
2
3
4
5
6
layer
dT
dU

Role of the Terms in Hamiltonian of Graphene

$$H = H_\kappa + H_h + H_c$$

$$H_\kappa = \kappa \sum_{x,\mu,\sigma} \left(\psi^\dagger_{\sigma,x+\mu} \psi_{\sigma,x} + \psi^\dagger_{\sigma,x} \psi_{\sigma,x+\mu} \right) \qquad \kappa = 2.8 \text{ eV}$$

$$H_h = \sum_x q_x \; V_{x,x} \; q_x \qquad V(x,x) = 9.3 \text{ eV}$$

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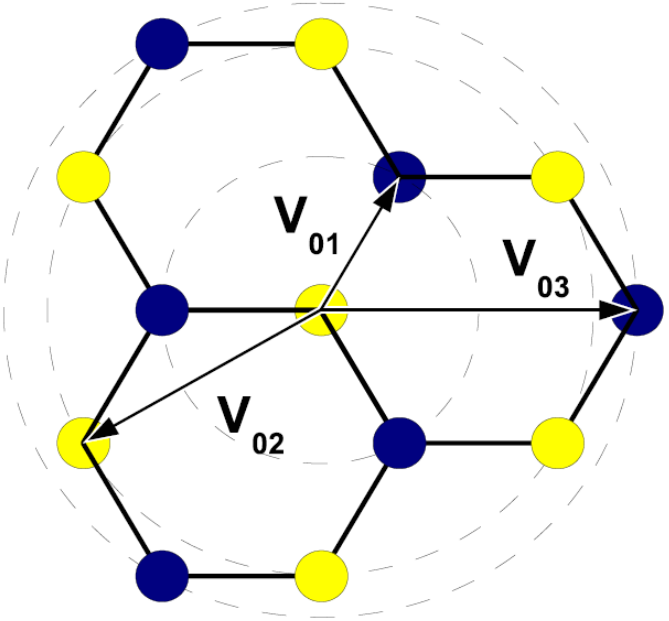


$$H = \cancel{H_\kappa} + H_h + H_c$$

First order Hamiltonian of Graphene in terms of occupation numbers

$$Z = \sum_{\{n\}\{m\}} e^{-\frac{1}{T}H(\{n\}\{m\})} =$$

$$= \exp\left\{-\frac{1}{T}\left(\sum_x V_{xx}(n_x - m_x)^2 + \right.\right.$$

$$\left.\left. + \sum_{x<y} V_{xy}(n_x - m_x)(n_y - m_y)\right)\right\}$$

$$\langle O \rangle = \frac{1}{Z} \sum_{\{n\}\{m\}} O \exp\left\{-\frac{1}{2T}\left(\sum_x V_{xx}(n_x - m_x)^2 + \right.\right.$$

$$\left.\left. + \sum_{x \neq y} V_{xy}(n_x - m_x)(n_y - m_y)\right)\right\}$$

First order Hamiltonian of Graphene in terms of electric charges

$$|\{q_x\}\rangle$$

$$\left\langle \hat{O} \right\rangle = \frac{\sum_{\{q_x\}} O(\{q_x\}) \exp^{-\beta H(\{q_x\})} \prod_x (1 + \delta_{q_x,0})}{Tr\left(\exp^{-\beta H(\{q_x\})}\right)}$$

$$H(\{q_x\}) = \frac{1}{2}\left(\sum_x V_{xx}(q_x)^2 + \sum_{x \neq y} V_{xy}(q_x)(q_y)\right)$$

q = 1

q = 0

q = - 1

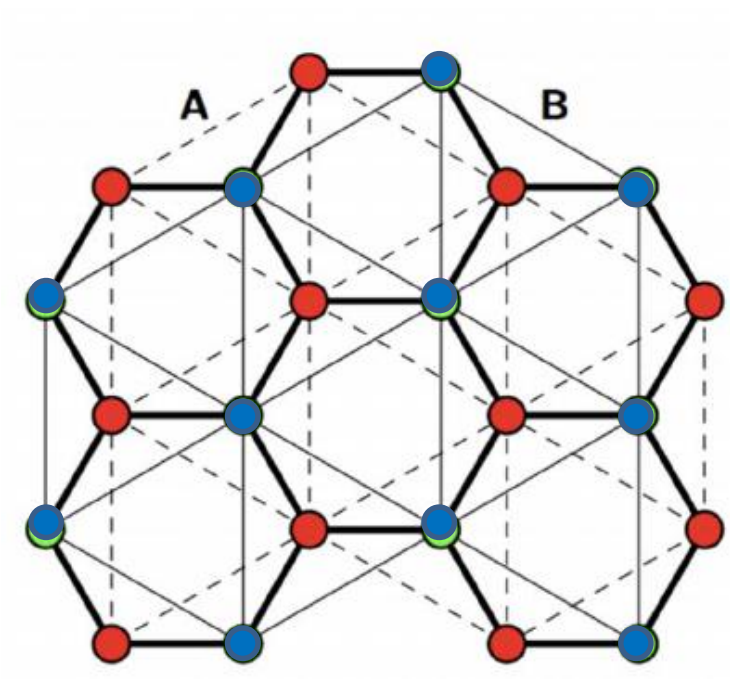
Chiral Domain Vacuum or Neutrality point Vacuum

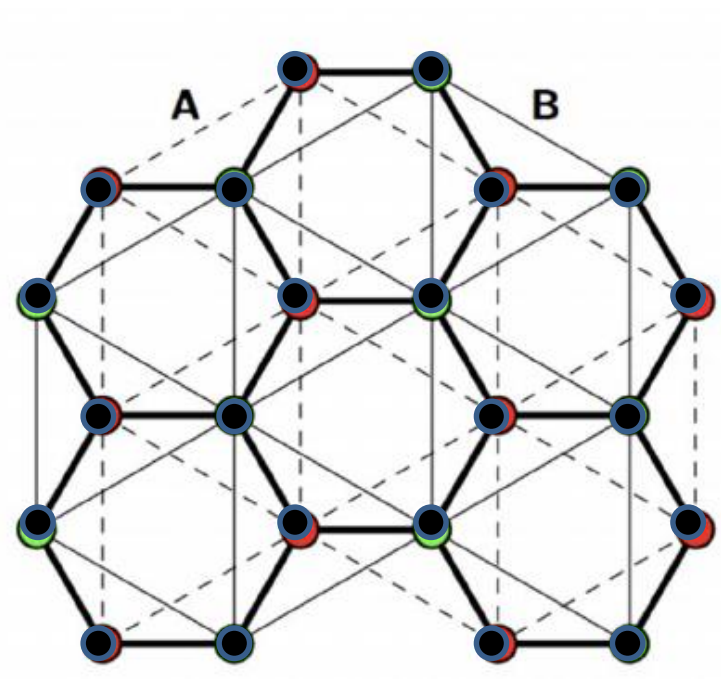
$H_h > H_c$

$H_h > H_c$

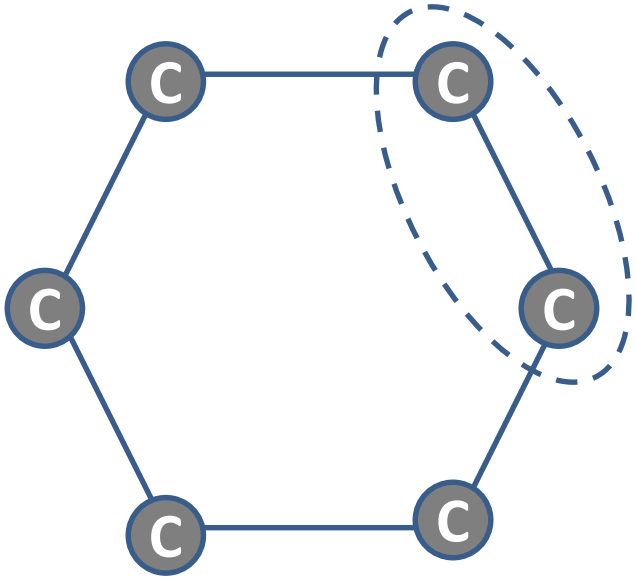
Chiral domain

Neutrality point





Simple model



Interaction ONLY between
neighboring sites

$$Z = \sum_{\{q_x\}} \exp^{-\beta H(\{q_x\})}$$

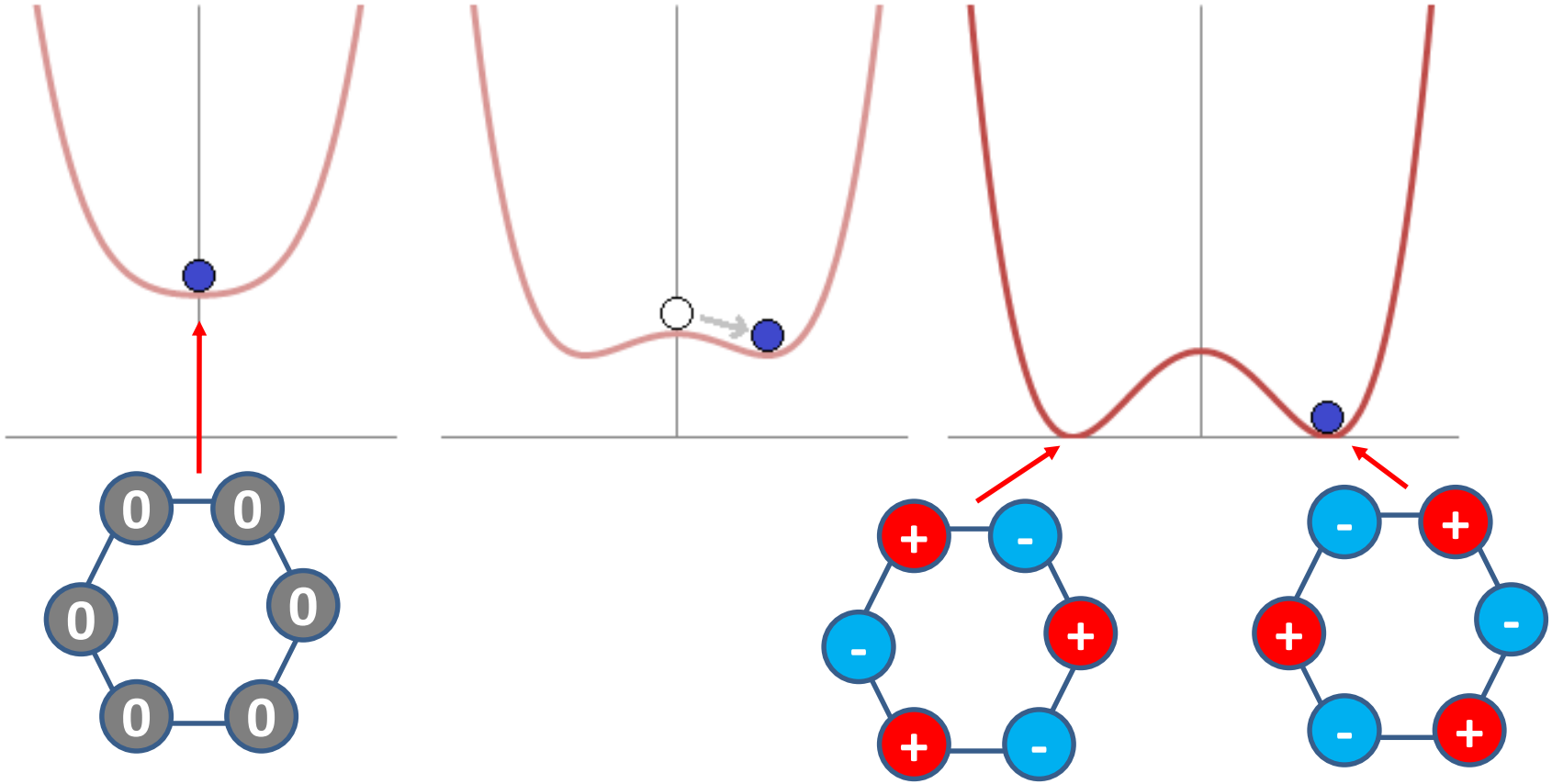
$$H(\{q_x\}) = \frac{1}{2}\left(V_{00}\sum_{x} q_x^2 + V_{01}\sum_{x,\mu} q_x q_{x+\rho_b}\right)$$

Simple model: Ground state

$$H(\{q_x\}) = \frac{1}{2}\left(V_{00}\sum_x q_x^2 + V_{01}\sum_{x,\mu} q_x q_{x+\rho_b}\right)$$

$V_{00} \gg V_{01}$

$V_{00} \ll V_{01}$



Critical value of on-site interaction

$$Z = \sum_{\{q_x\}} \exp^{-\beta H(\{q_x\})}$$

$$H(\{q_x\}) = \frac{1}{2}\left(V_{00}\sum_{x} q_x^2 + V_{01}\sum_{x,\mu} q_x q_{x+\rho_b}\right)$$

If temperature → 0

$$\begin{cases} V_{00} \gg V_{01} & \text{Neutrality point} \\ V_{00} \ll V_{01} & \text{Chiral domain} \end{cases}$$

Critical V_{00} → $2\cdot(V_{00}/2) - 3\cdot V_{01} = 0.$

V_{00}^{c} = **16.5 eV**

Paradox of Anti-ferroelectricity of Graphene

Theoretical prediction for anti-ferroelectiric phase transition

$$V_{00}^{c} = 16.5 \text{ eV}$$

On-site interaction in free Graphene (T.O. Wehling arXiv: 1101.4007)

$$V_{00} = 9.5 \text{ eV}$$

Free Graphene is anti-ferroelectiric ?!

Monte-Carlo Studding of Graphene

In framework of occupation number formalism

Graphene is a statistical model

$$Z = \sum_{\{q_x\}} \exp^{-\beta H(\{q_x\})}$$

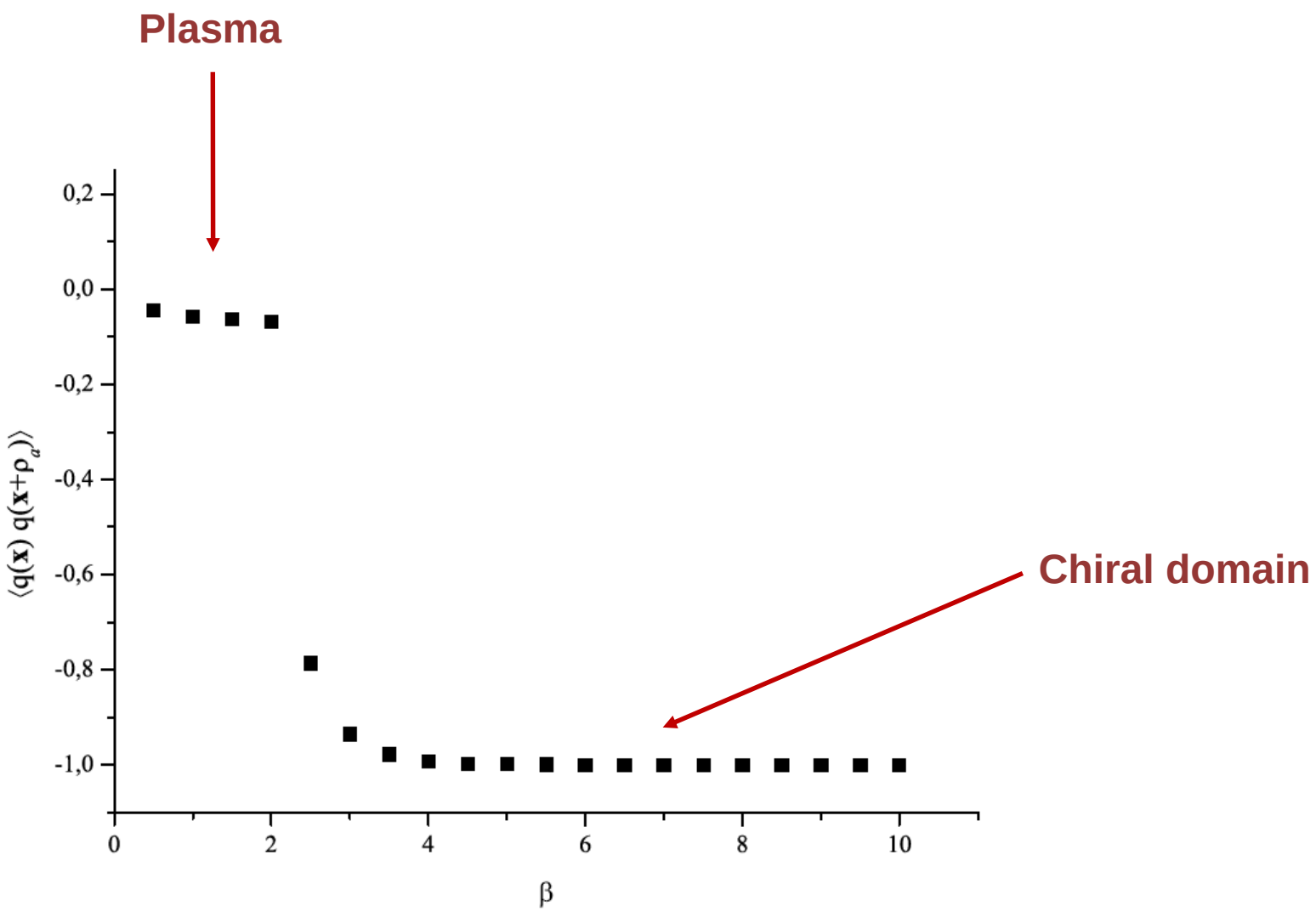
$$H(\{q_x\}) = \frac{1}{2}\left(V_{00}\sum_{x} q_x^2 + V_{01}\sum_{x,\mu} q_x q_{x+\rho_b}\right)$$

$$\langle O \rangle = \langle q_x q_{x+\mu} \rangle$$

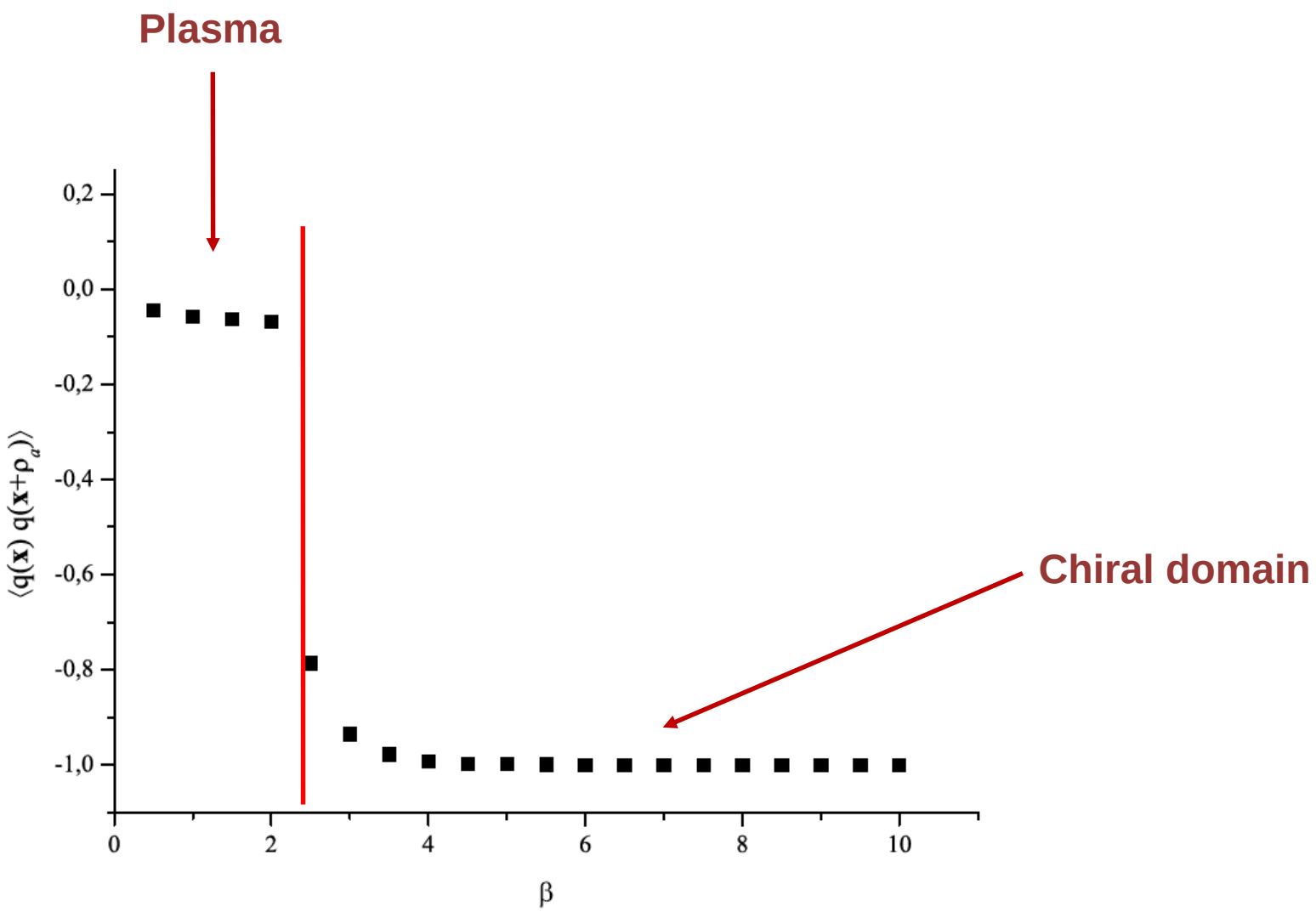
-1 for domain

0 for plasma

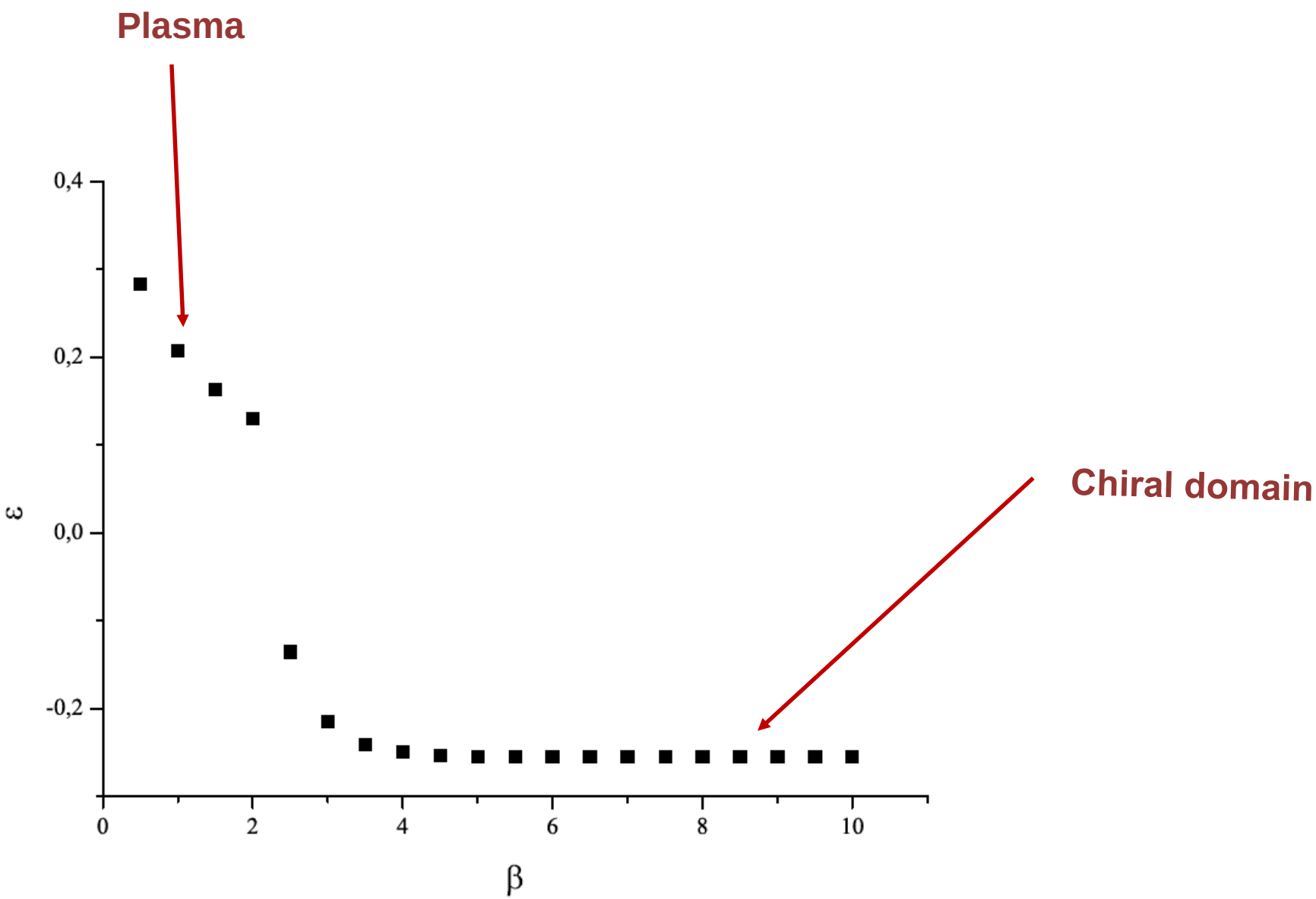
Results of Monte-Carlo calculations



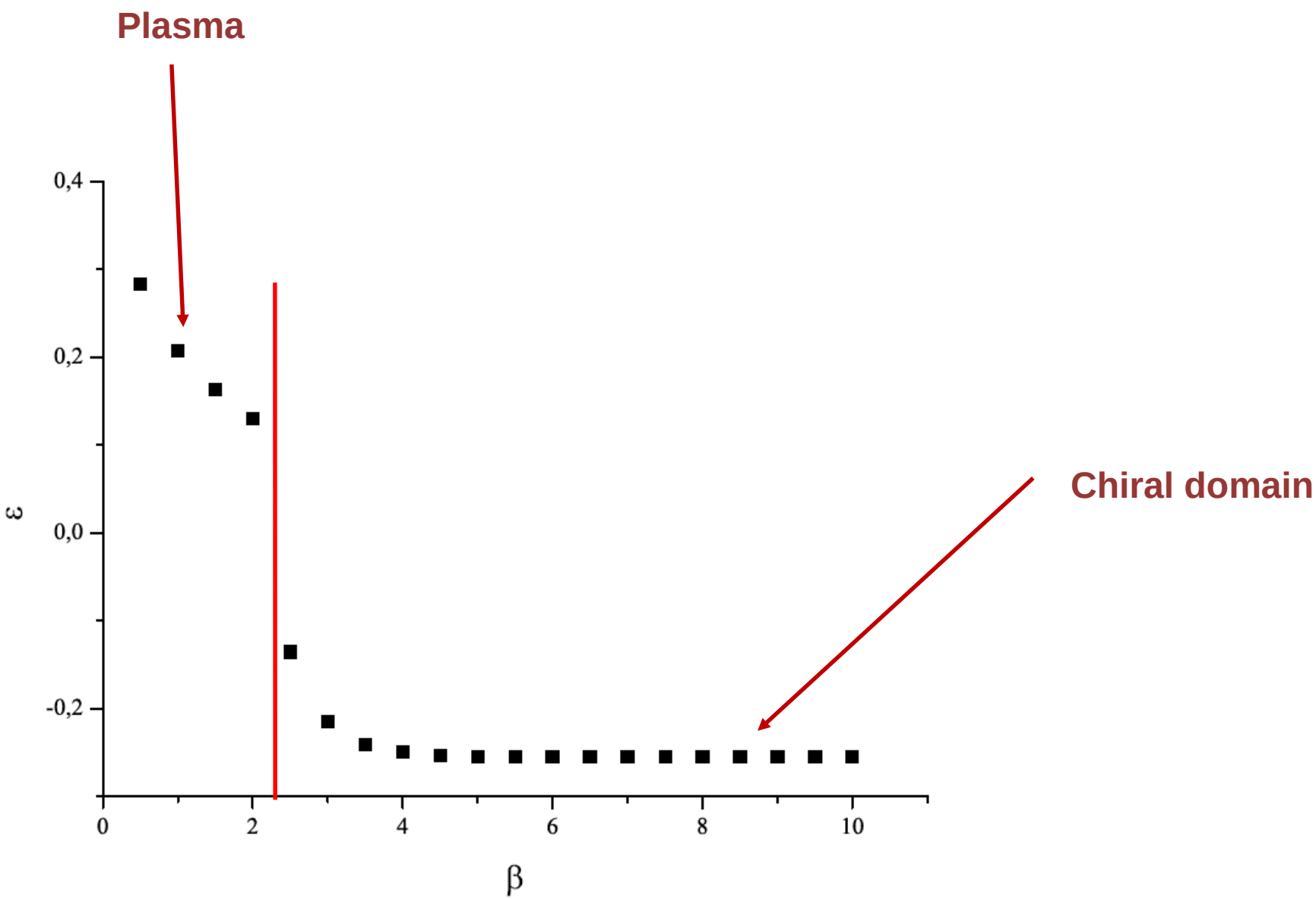
Results of Monte-Carlo calculations



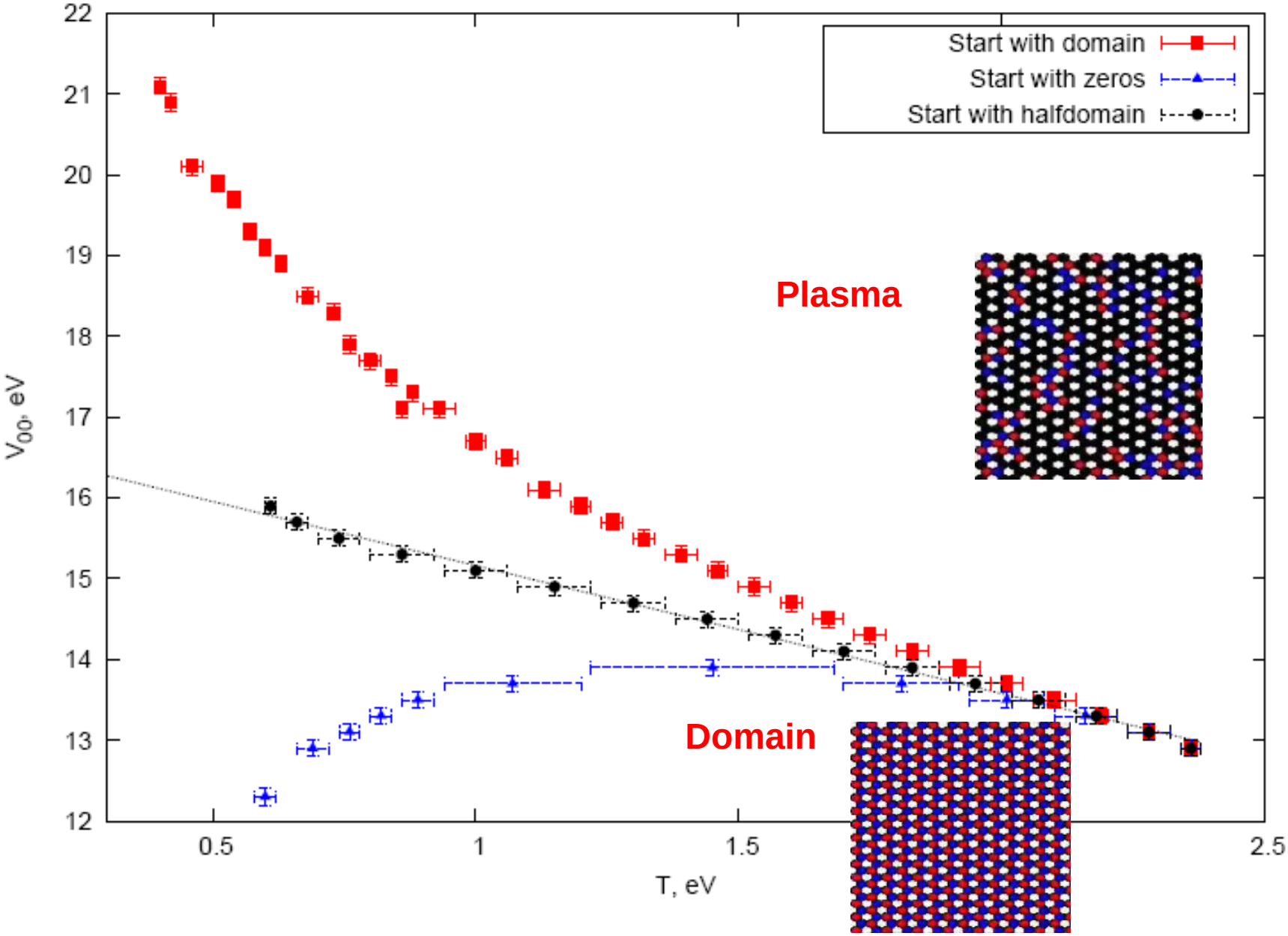
Results of Monte-Carlo calculations



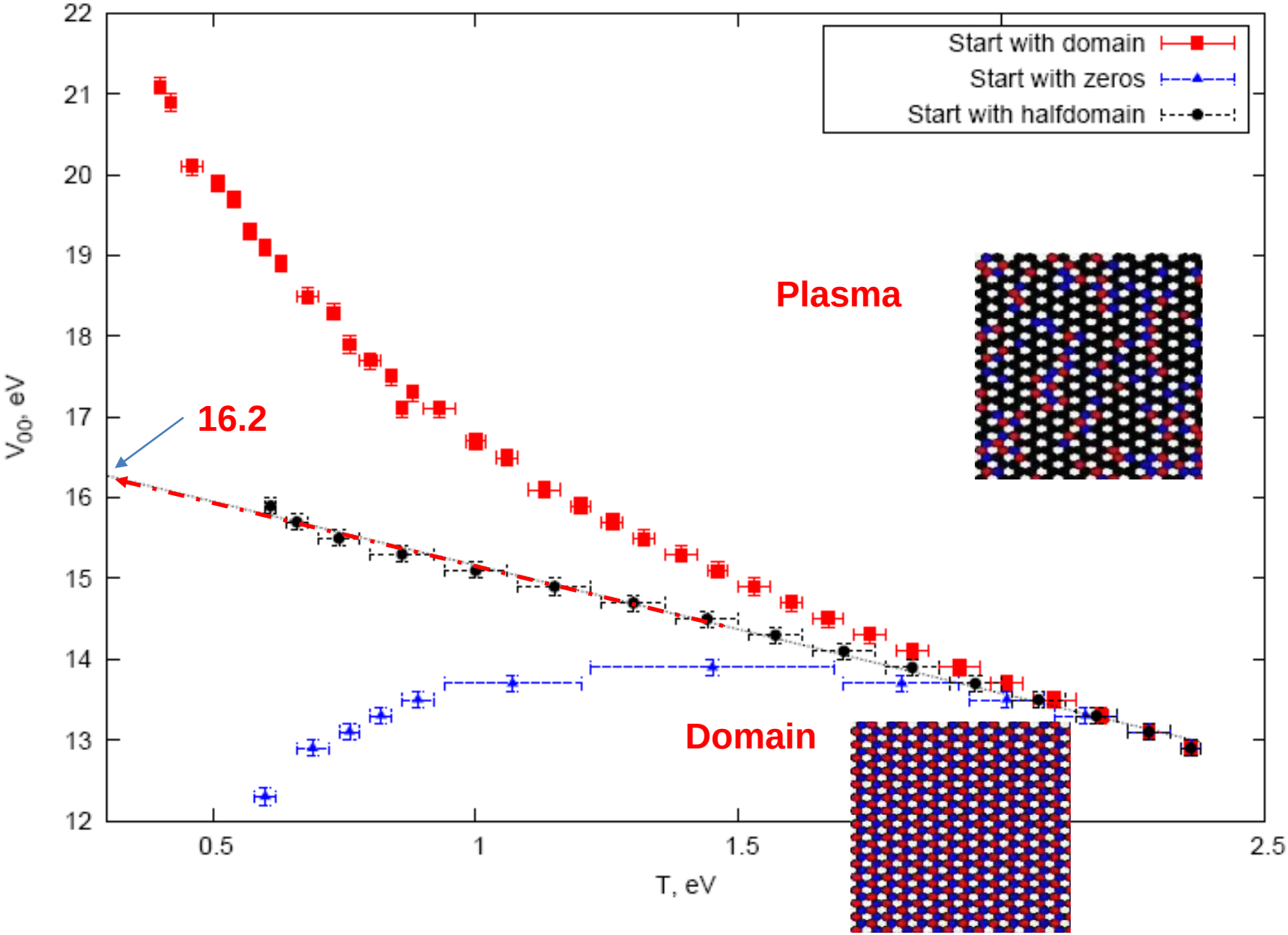
Results of Monte-Carlo calculations



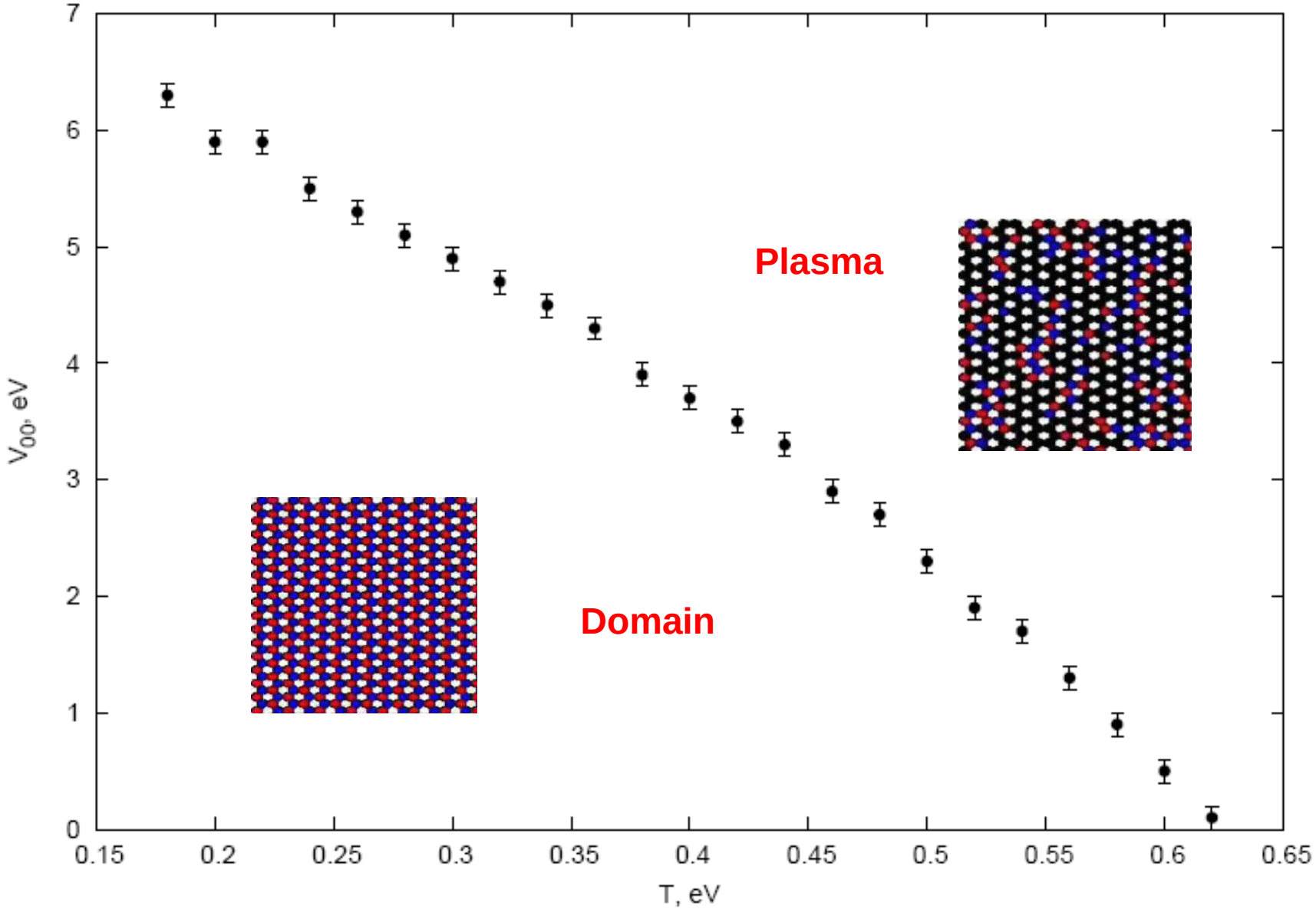
Results of Monte-Carlo calculations: 1st radius



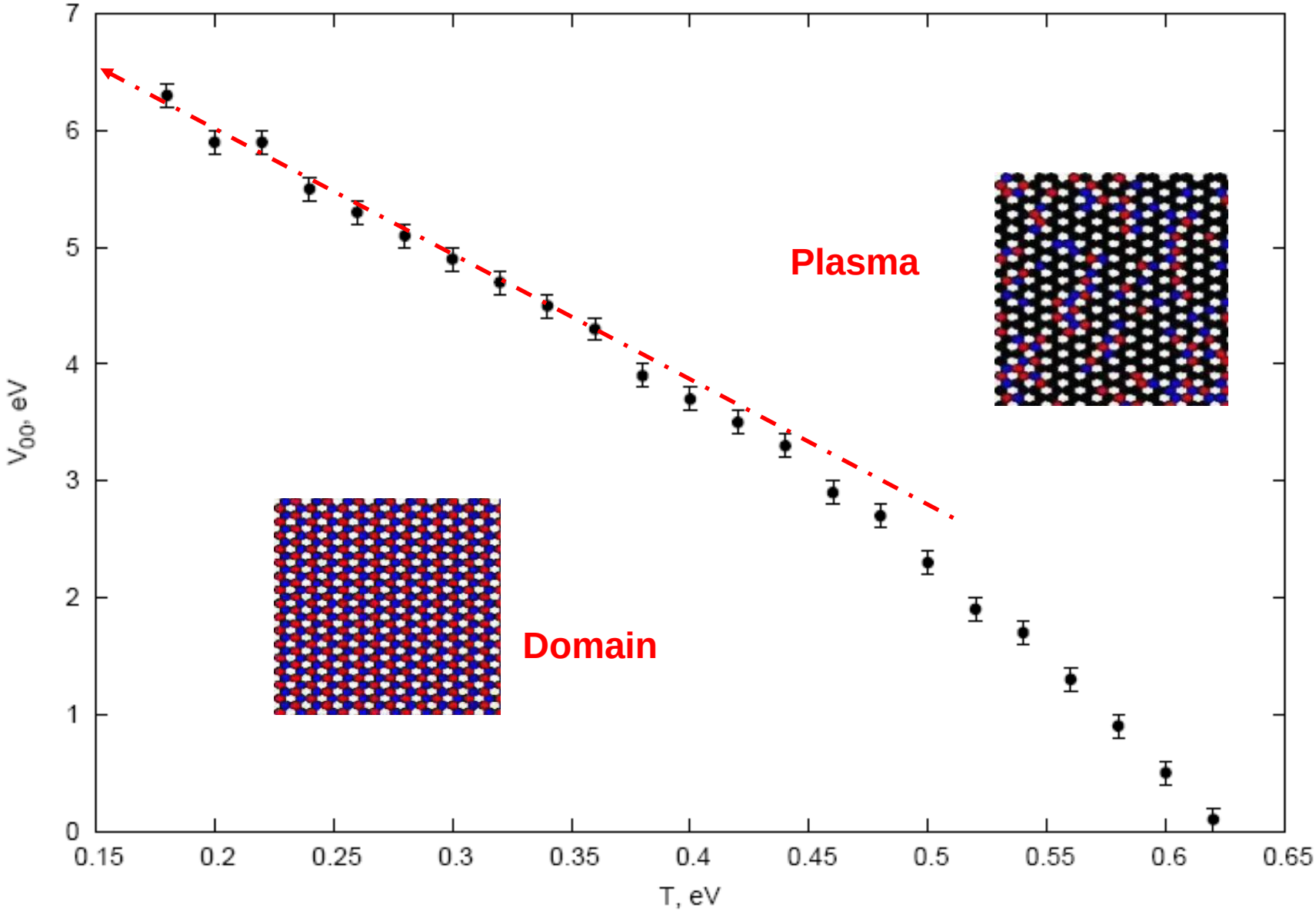
Results of Monte-Carlo calculations: 1st radius



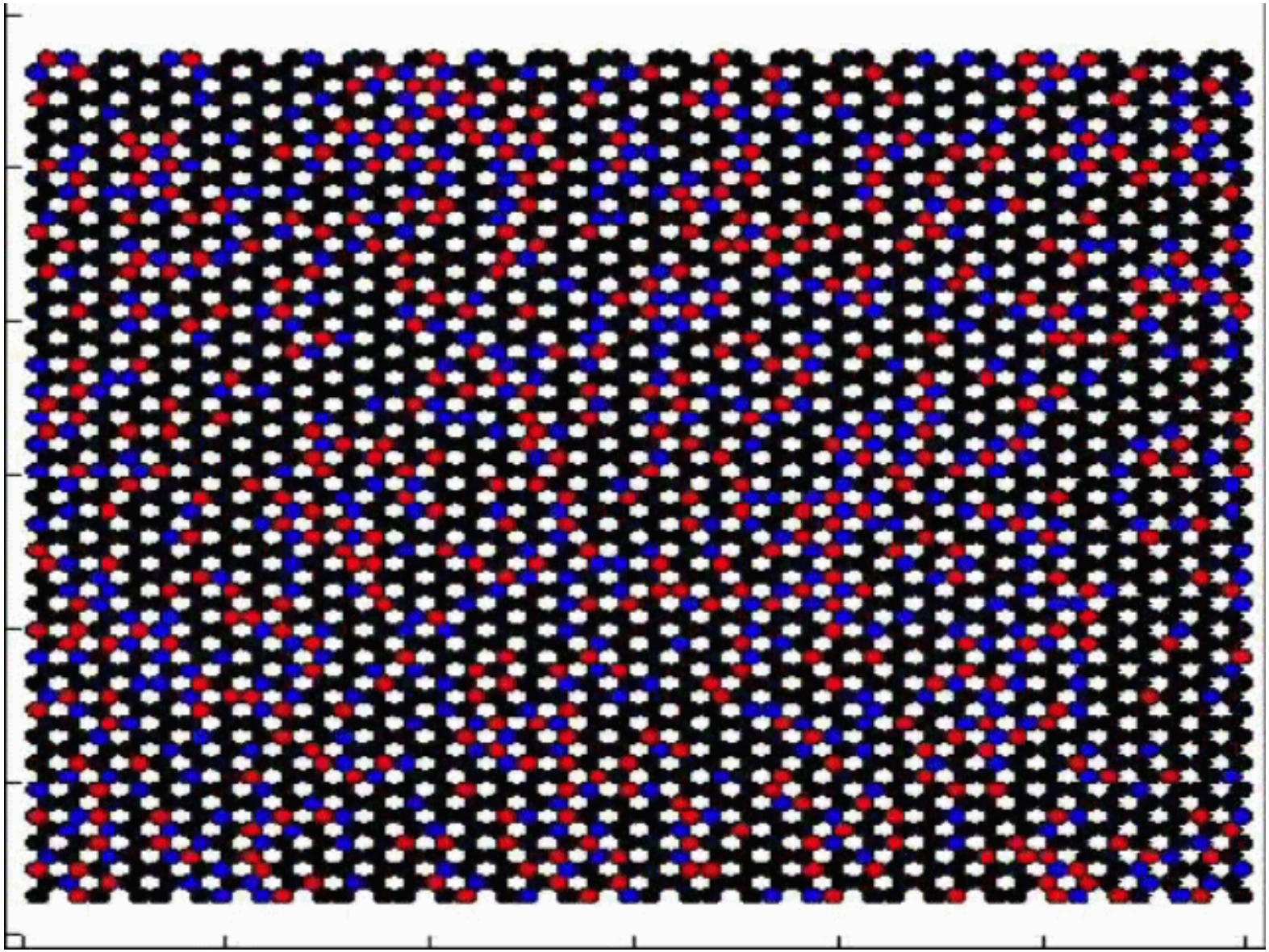
Results of Monte-Carlo calculations: all radius



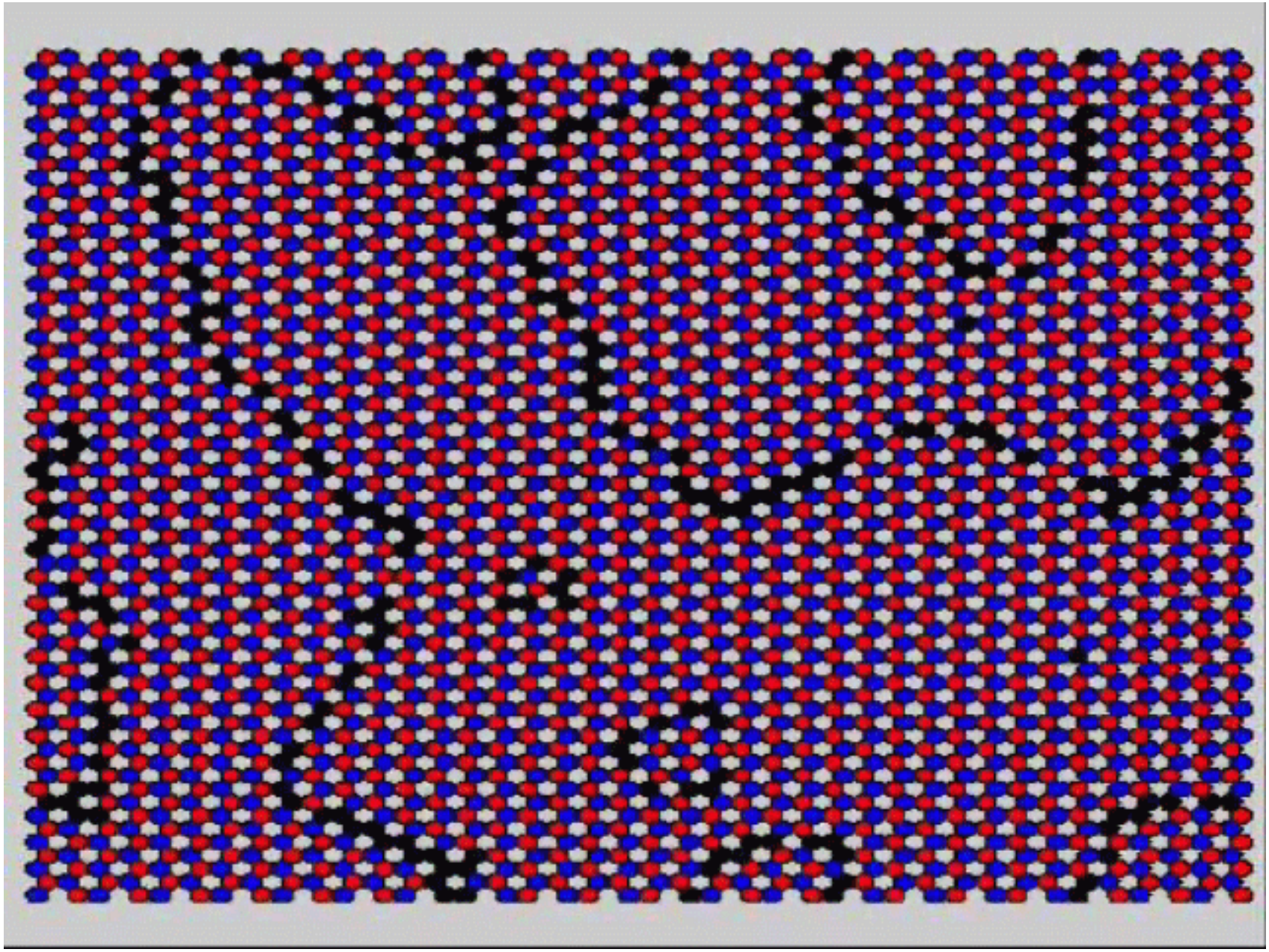
Results of Monte-Carlo calculations: all radii



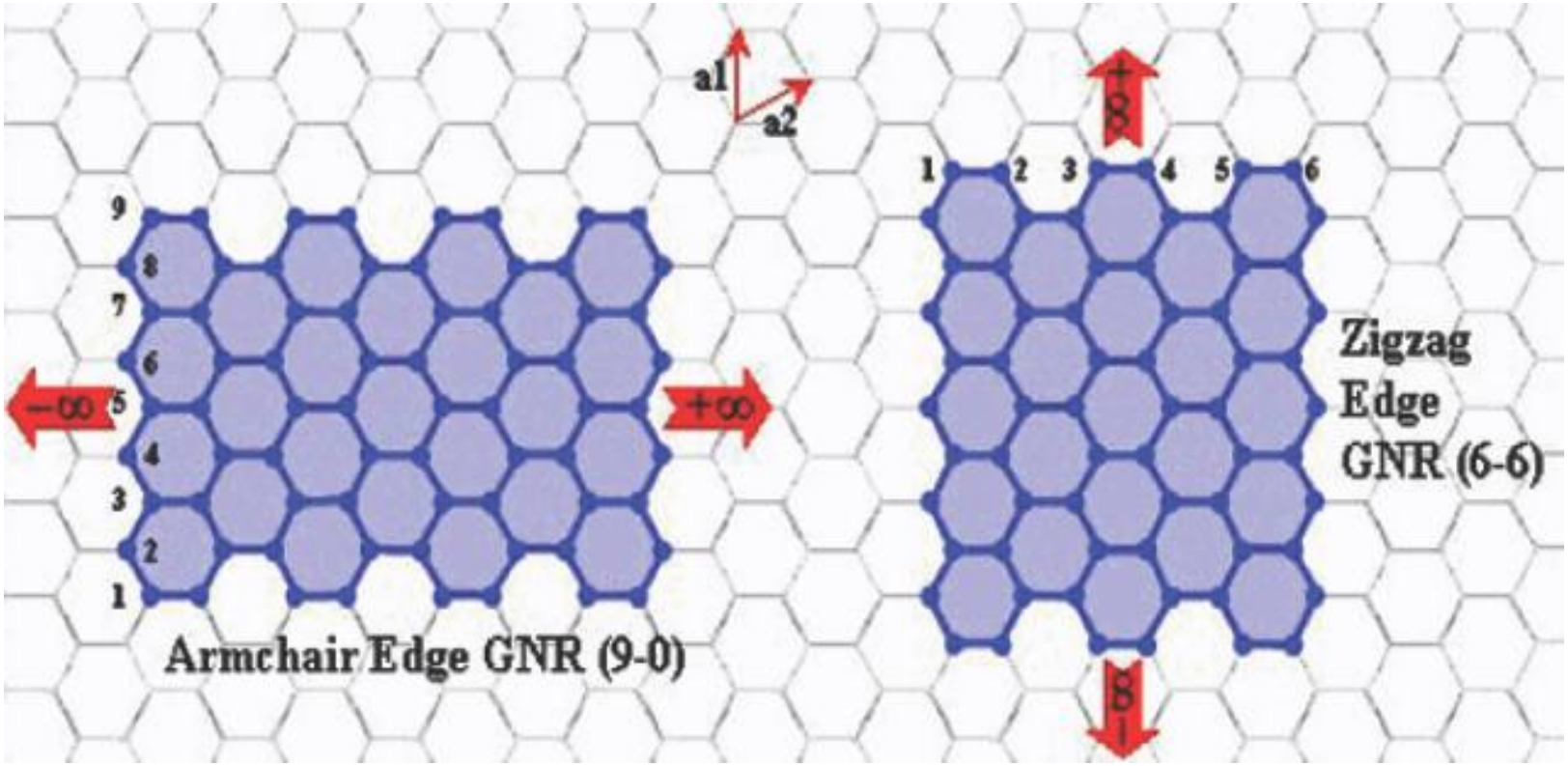
Plasma



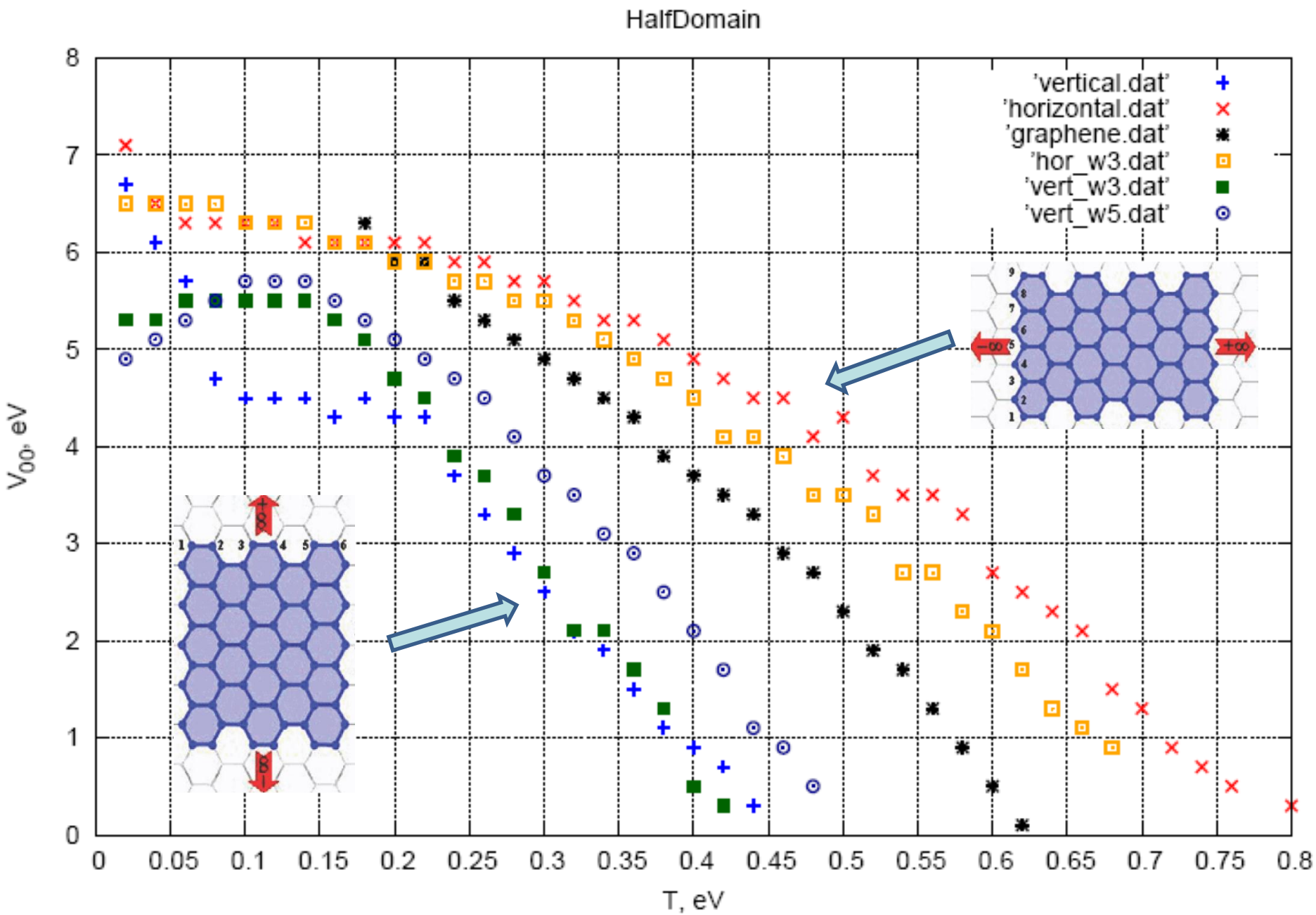
Chiral domains



Graphene nano-ribbons

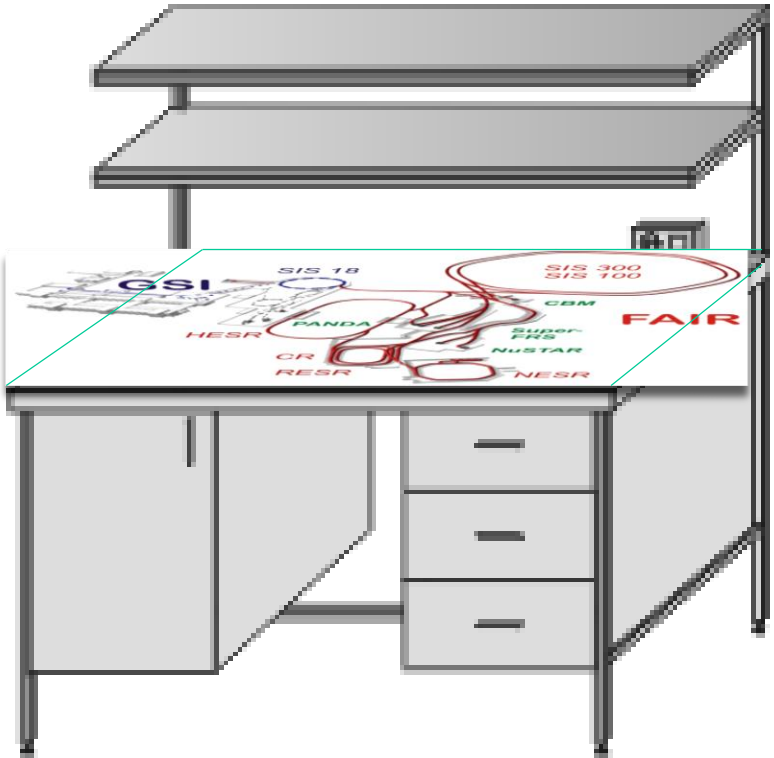


Graphene nano-ribbons: phase diagram



Темы исследований

Эффект критического заряда в графене



Historical Remark

Critical Charge phenomenon: qualitative approach

Non-relativistic particle:

$$p \approx \frac{\hbar}{R} \quad \Longrightarrow \quad E(R) \approx \frac{\hbar^2}{2mR^2} - \frac{Ze^2}{R}$$

$$\left(\frac{\partial E}{\partial R}\right)_{R=R_0} = 0 \quad \Longrightarrow \quad R_0 = \frac{\hbar^2}{mZe^2}$$

Historical Remark

Critical Charge phenomenon: qualitative approach

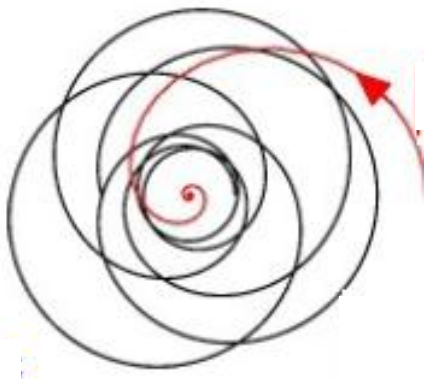
Relativistic particle:

$$p \approx \frac{\hbar}{R} \quad \Longrightarrow \quad E(R) \approx \sqrt{\left(\frac{\hbar c}{R}\right)^2 + (mc^2)^2} - \frac{Ze^2}{R}$$

$$\left(\frac{\partial E}{\partial R}\right)_{R=R_0} = 0 \quad \Longrightarrow \quad 1 + \left(\frac{mcR_0}{\hbar}\right)^2 = \left(\frac{\hbar c}{Ze^2}\right)^2$$

$$\Downarrow$$

$$Z < Z_c = \frac{\hbar c}{e^2} = \frac{1}{\alpha} \approx 137 \quad \Longrightarrow \quad R = 0 \quad \Longrightarrow$$



Historical Remark

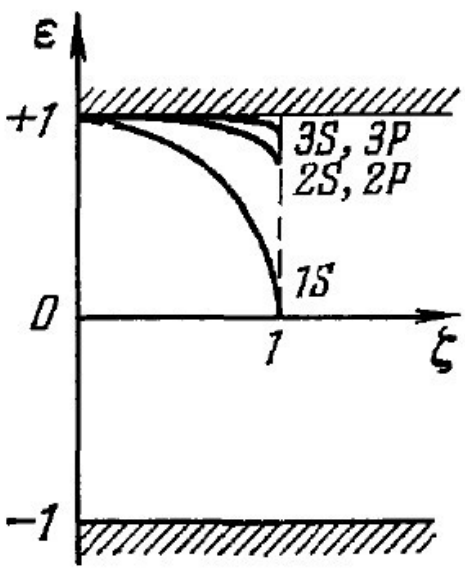
Little more Math: Dirac equation approach

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[c\,\vec{\alpha}\left(\vec{p} - \frac{e}{c}\vec{A}\right) - e\varphi + mc^2\,\hat{\beta}\right]\Psi$$

$$E_{n,j} = \frac{mc^2}{\sqrt{1 + \frac{(Z\alpha)^2}{\left(n - |j| + \sqrt{j^2 - (Z\alpha)^2}\right)^2}}}$$

$$\epsilon_1 = m\sqrt{1 - \zeta^2}$$

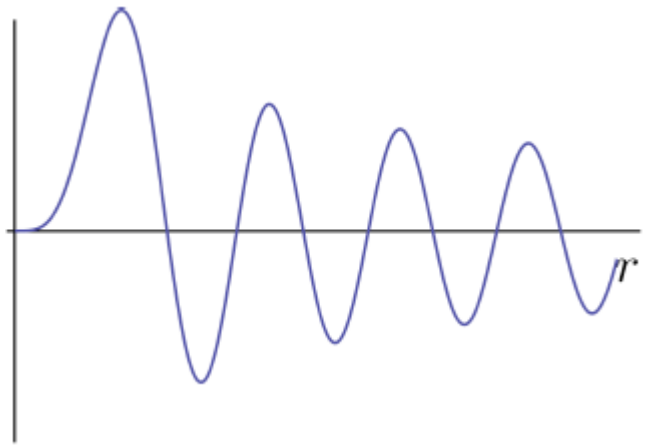
$$\zeta \equiv \frac{Ze^2}{\hbar c}$$



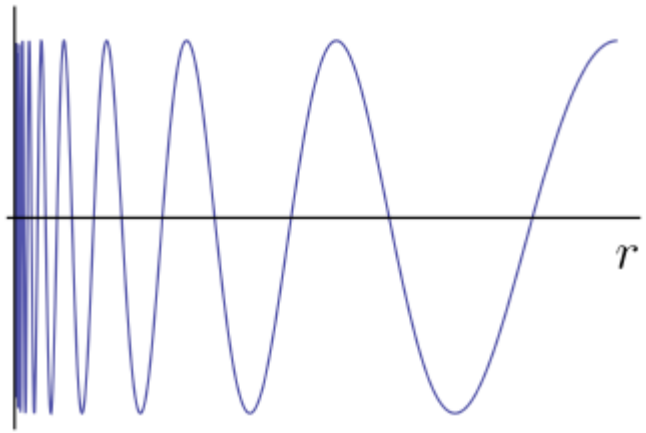
$$Z < Z_c = \frac{\hbar c}{e^2} = \frac{1}{\alpha} \approx 137$$

Historical Remark

Wave function and singularity at origin



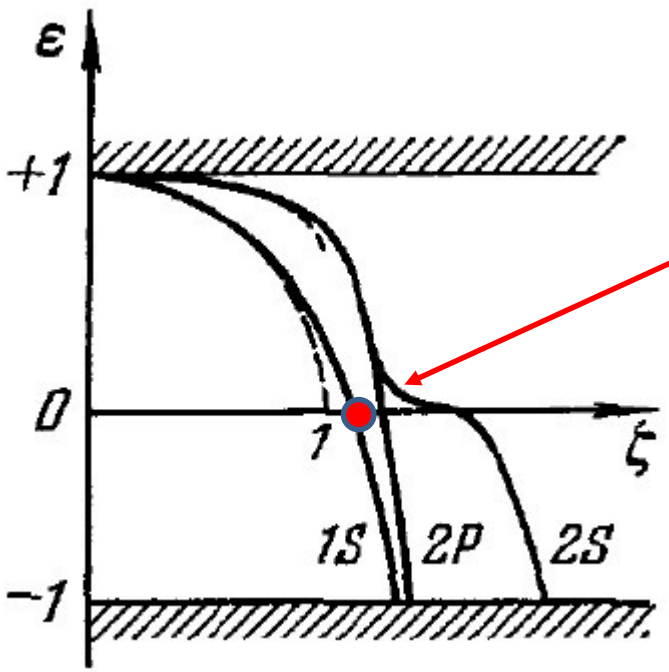
$Z < Z_{cr}$



$Z > Z_{cr}$

Historical Remark

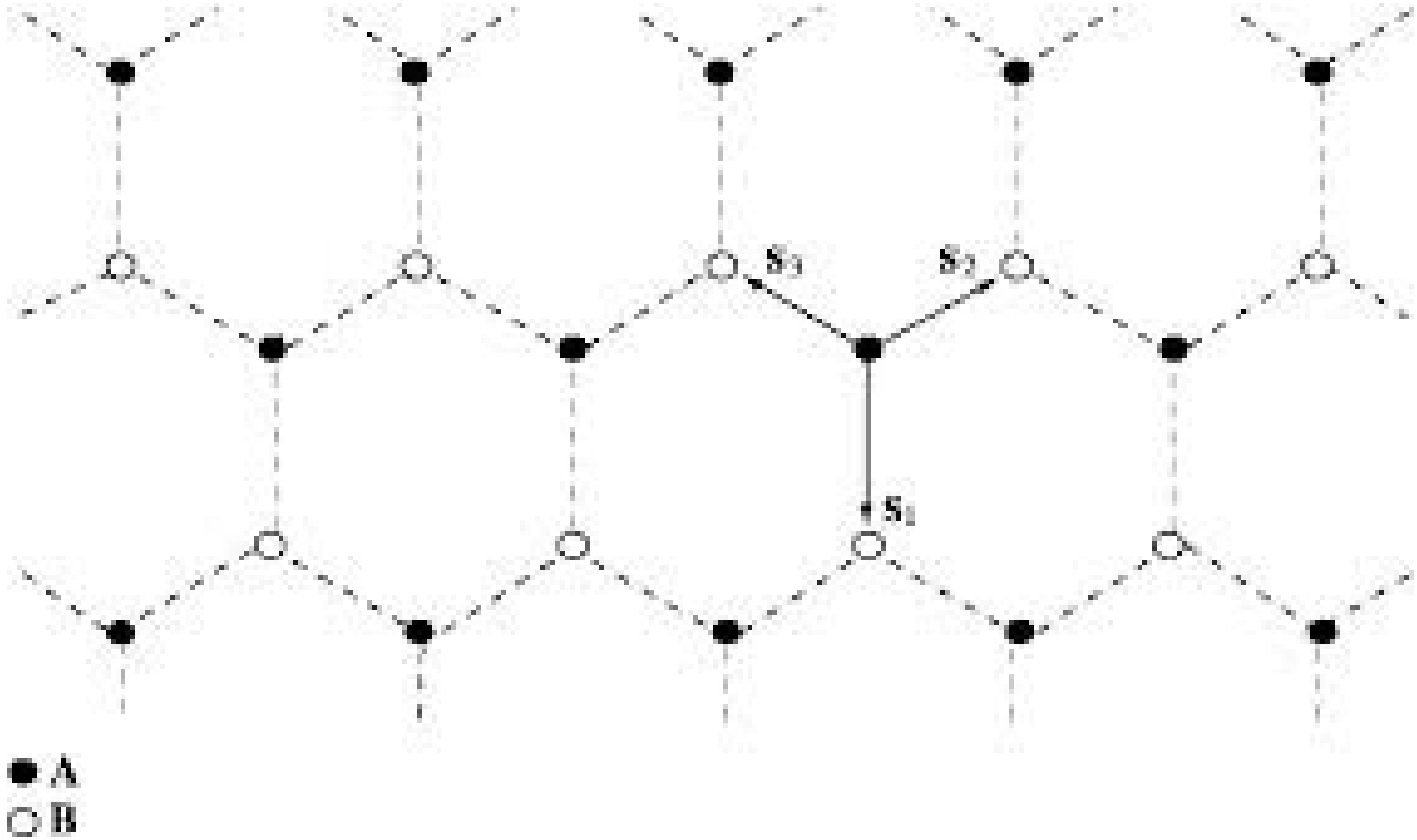
Little more Math: Dirac equation approach



$Z_{cr} = 170$

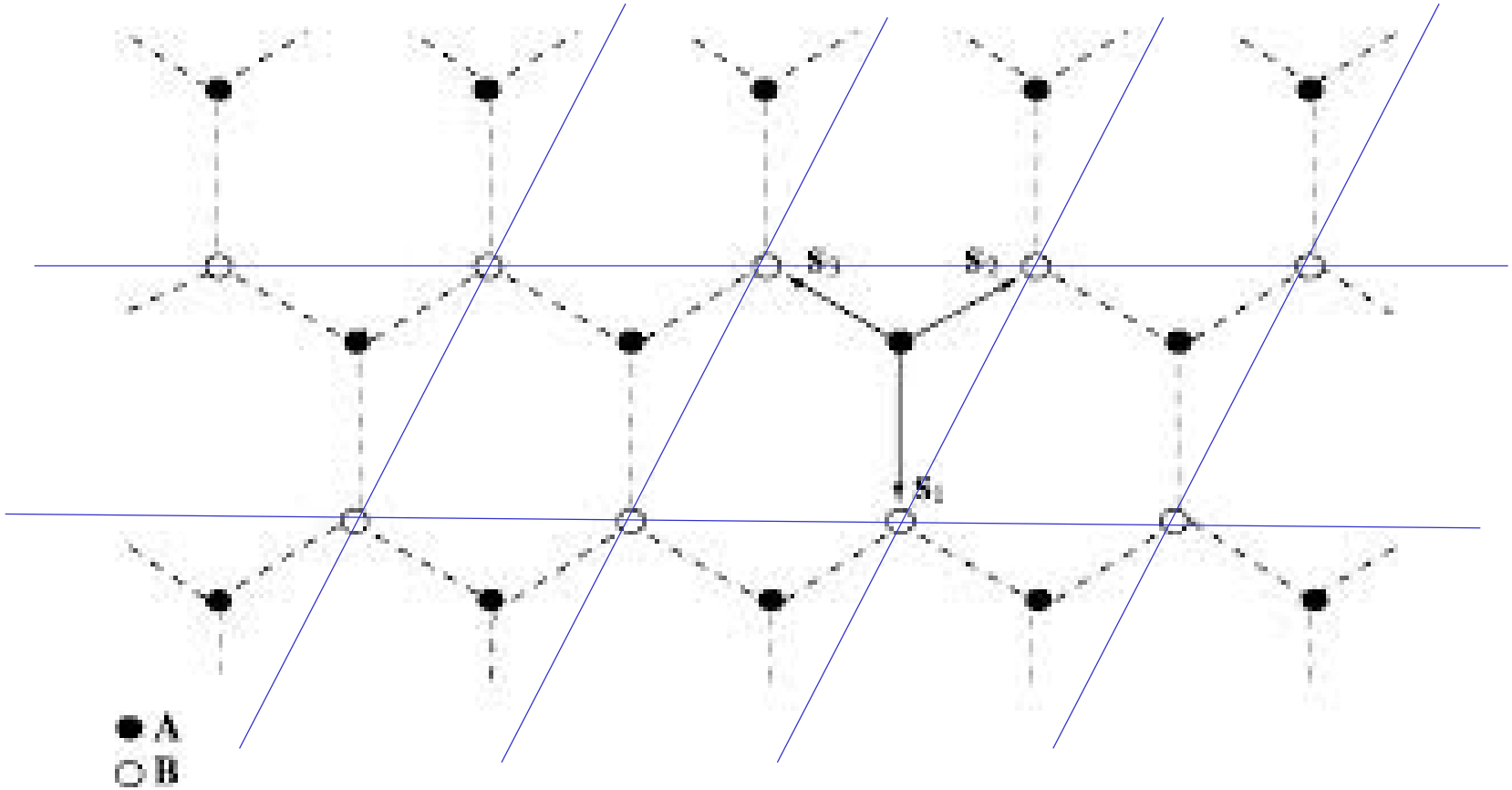
Gapped graphene

Violation of sub-lattice symmetry:



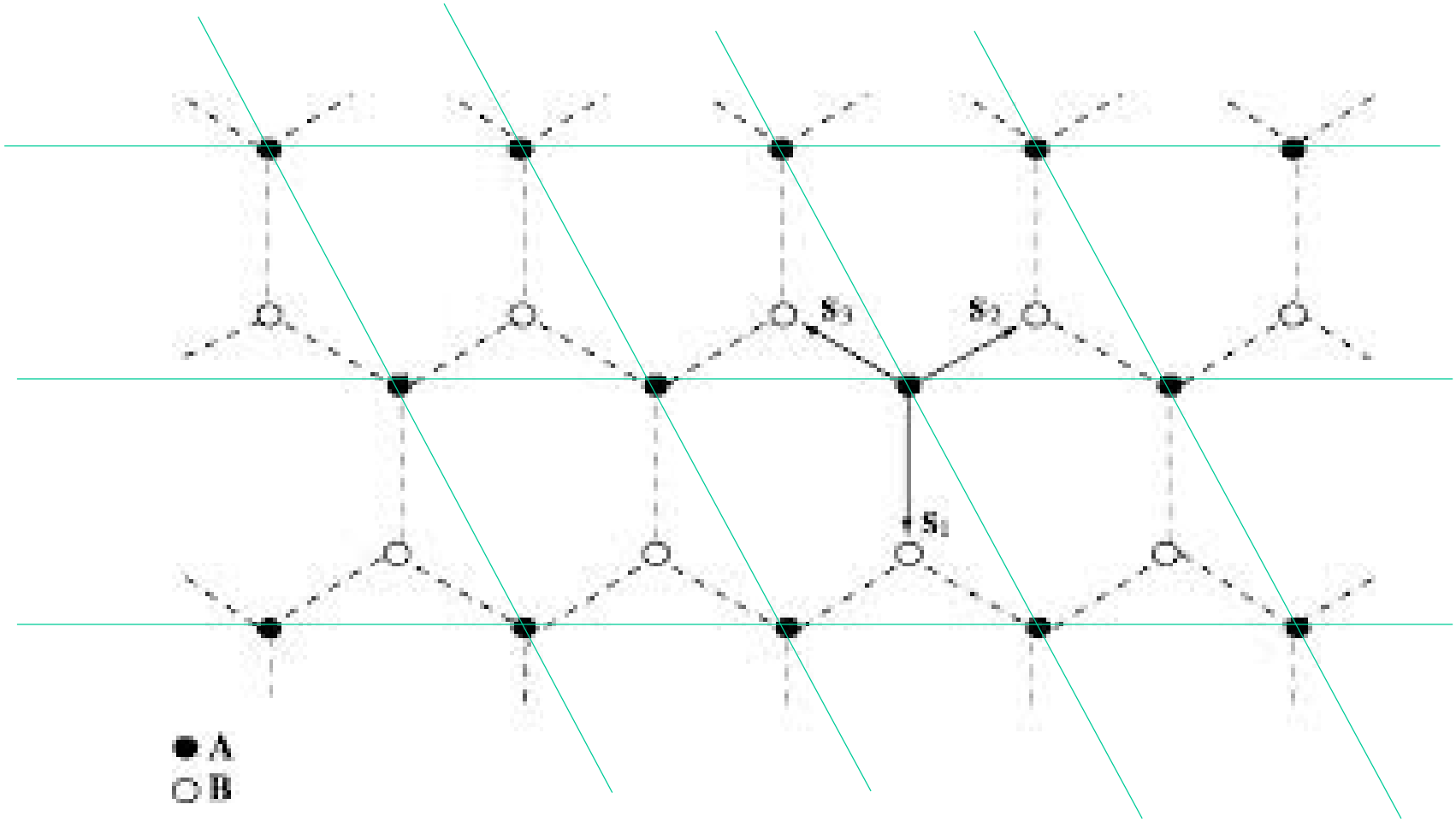
Gapped graphene

Violation of sub-lattice symmetry:



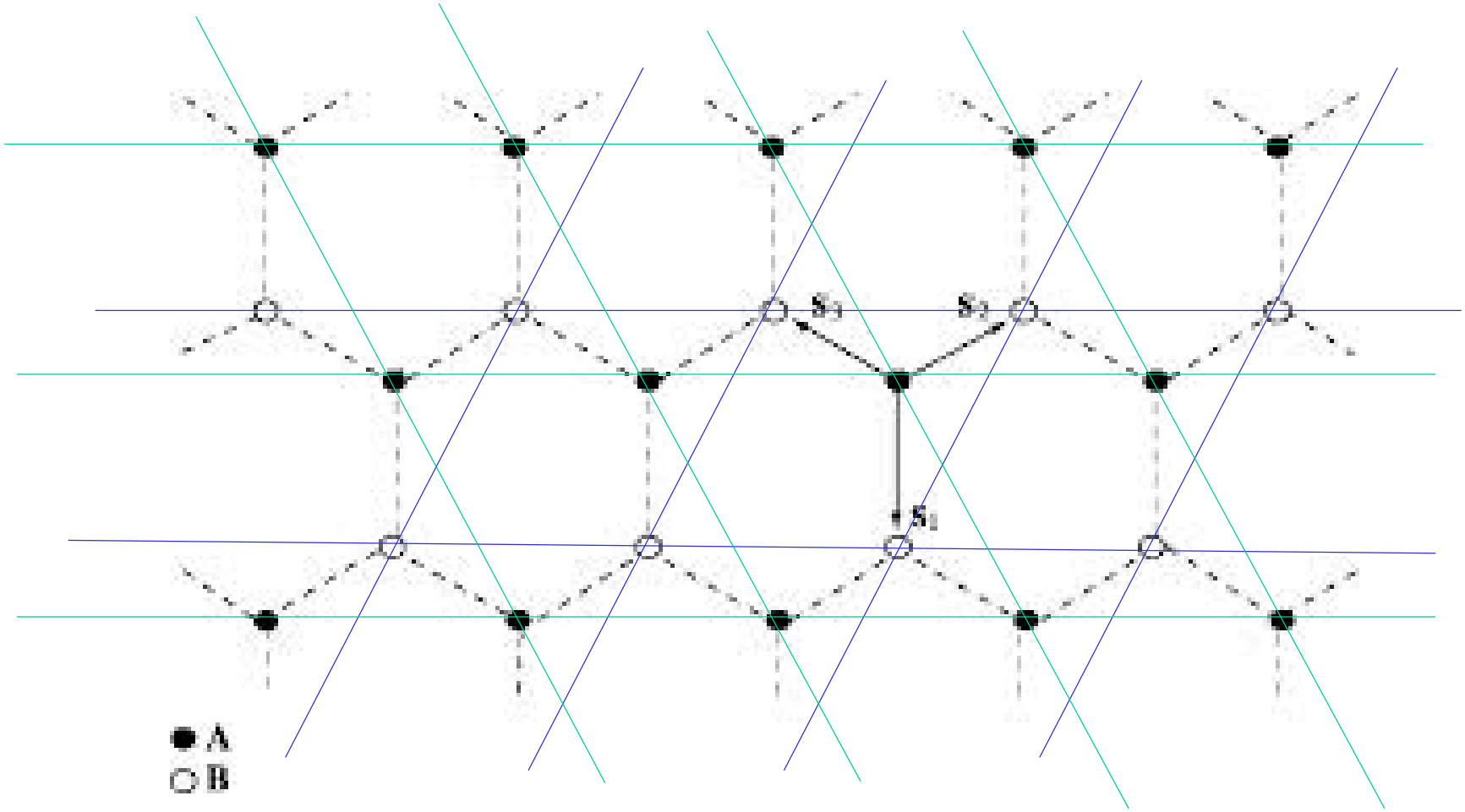
Gapped graphene

Violation of sub-lattice symmetry:



Gapped graphene

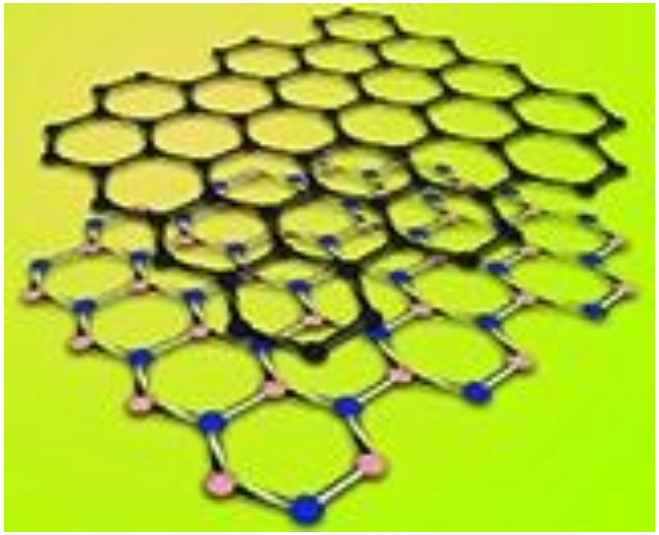
Violation of sub-lattice symmetry:

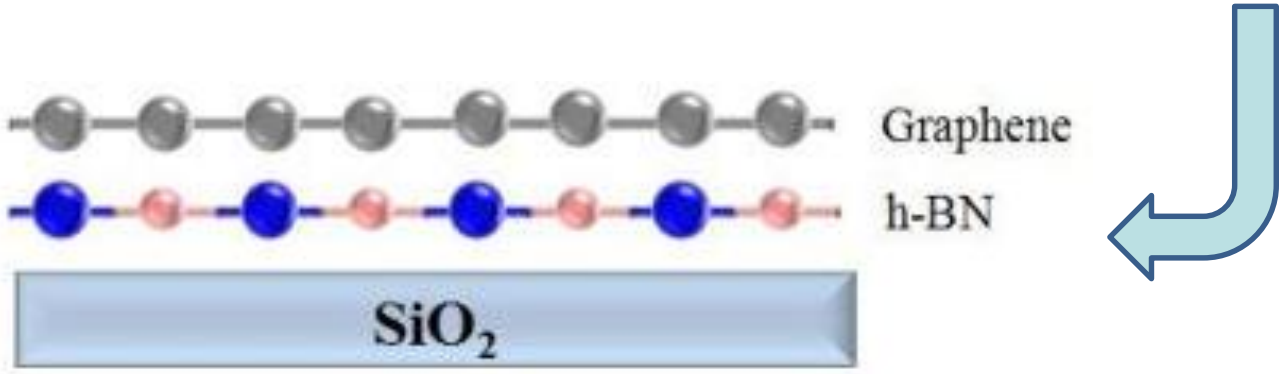


Gapped Graphene

Violation of sub-lattices symmetry

Graphene + Boron Nitride

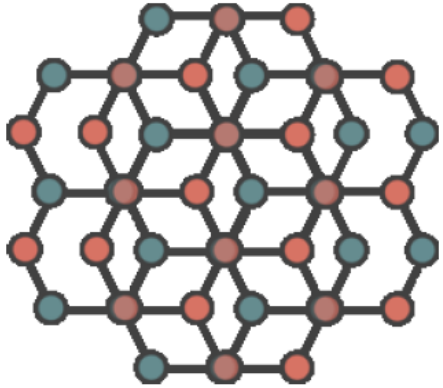


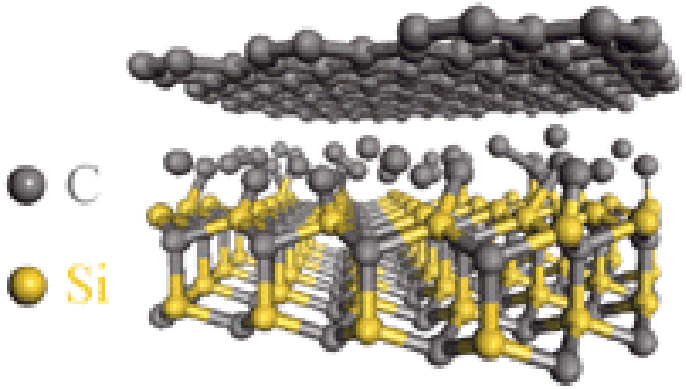


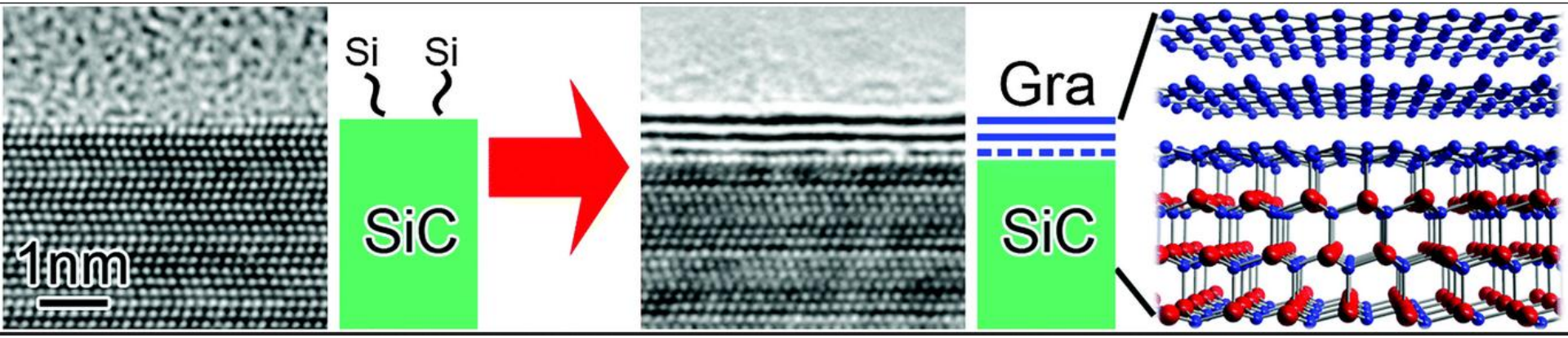
Gapped Graphene

Violation of sub-lattices symmetry

Graphene + Silicone Carbide



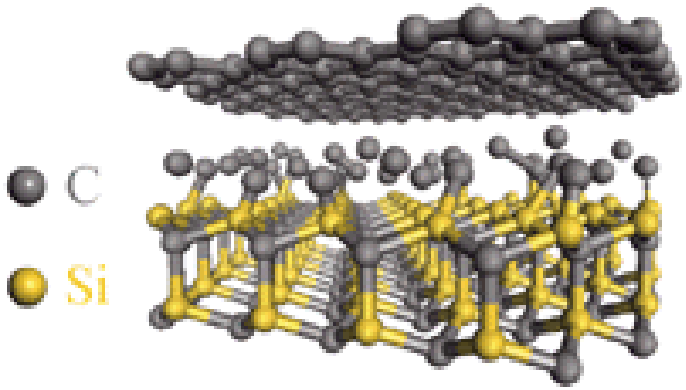




Gapped Graphene

Violation of sub-lattices symmetry

Graphene + Silicone Carbide



Critical charge in Graphene: Theory

Solution of Dirac equation:

$$(-i\hbar V_F(\sigma * \nabla) - \frac{Ze^2}{r+a} + mV_F^2\sigma_z)\psi(\mathbf{r}) = \epsilon\psi(\mathbf{r})$$

$$\psi_j(r,\phi) = \frac{1}{\sqrt{r}}\begin{pmatrix} e^{-i(j-1/2)\phi}A(r) \\ ie^{-i(j+1/2)\phi}B(r) \end{pmatrix}$$

$$\begin{bmatrix} \left(\epsilon + \frac{g}{r+a} - mV_F^2\right) & -\hbar V_F\left(\partial_r + \frac{j}{r}\right) \\ \hbar V_F\left(\partial_r - \frac{j}{r}\right) & \left(\epsilon + \frac{g}{r+a} + mV_F^2\right) \end{bmatrix} \begin{bmatrix} A(r) \\ B(r) \end{bmatrix} = 0.$$

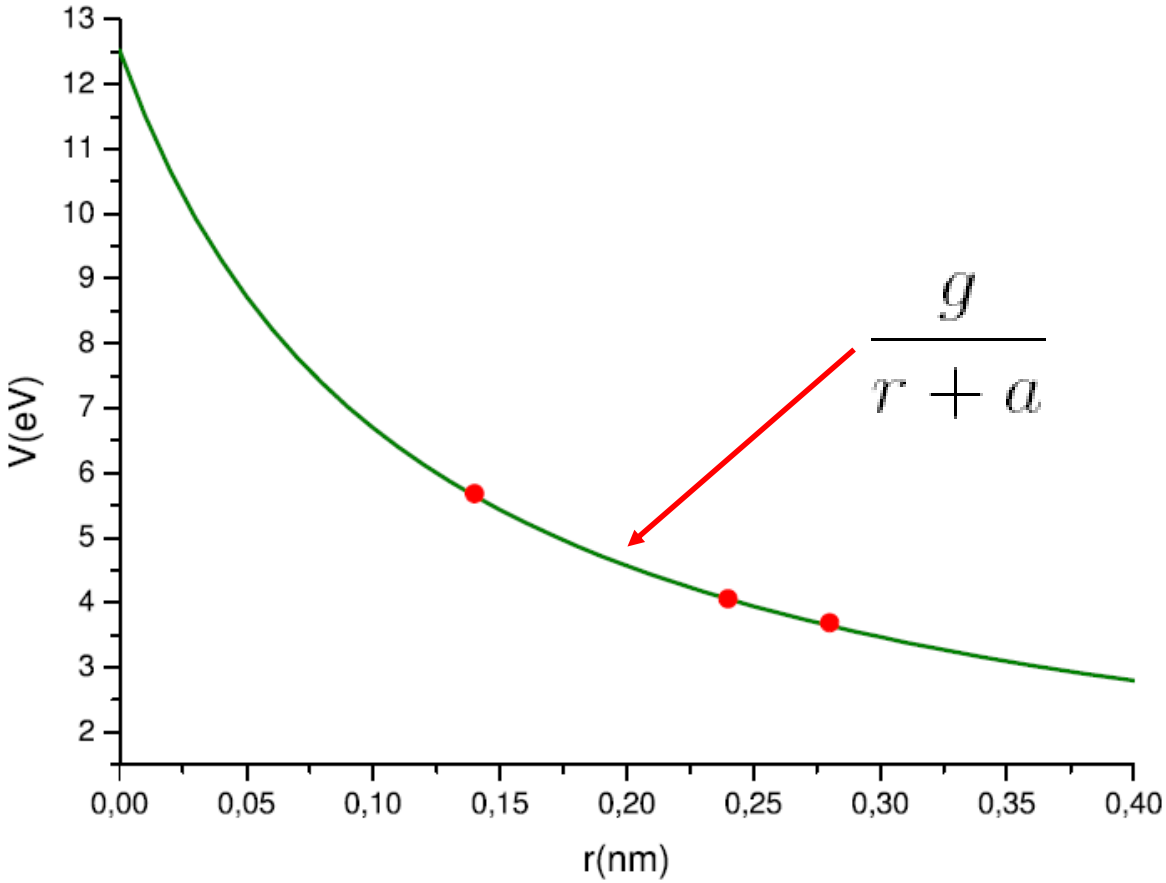
Role of the Terms in Hamiltonian of Graphene

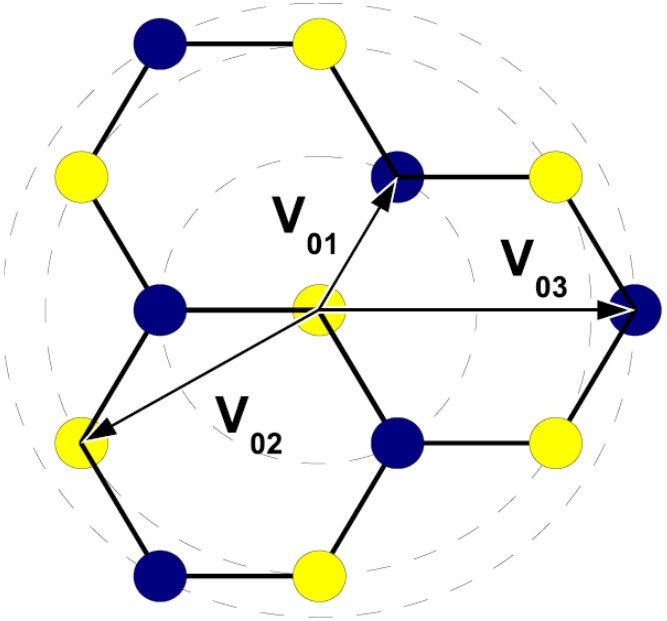
$$H_h = \sum_x q_x \; V_{x,x} \; q_x$$

$$H_c = \sum_{x \neq x'} q_x V_{x,x'} q'_x.$$

$$V(x,x) = 9.3 \quad \text{eV}$$

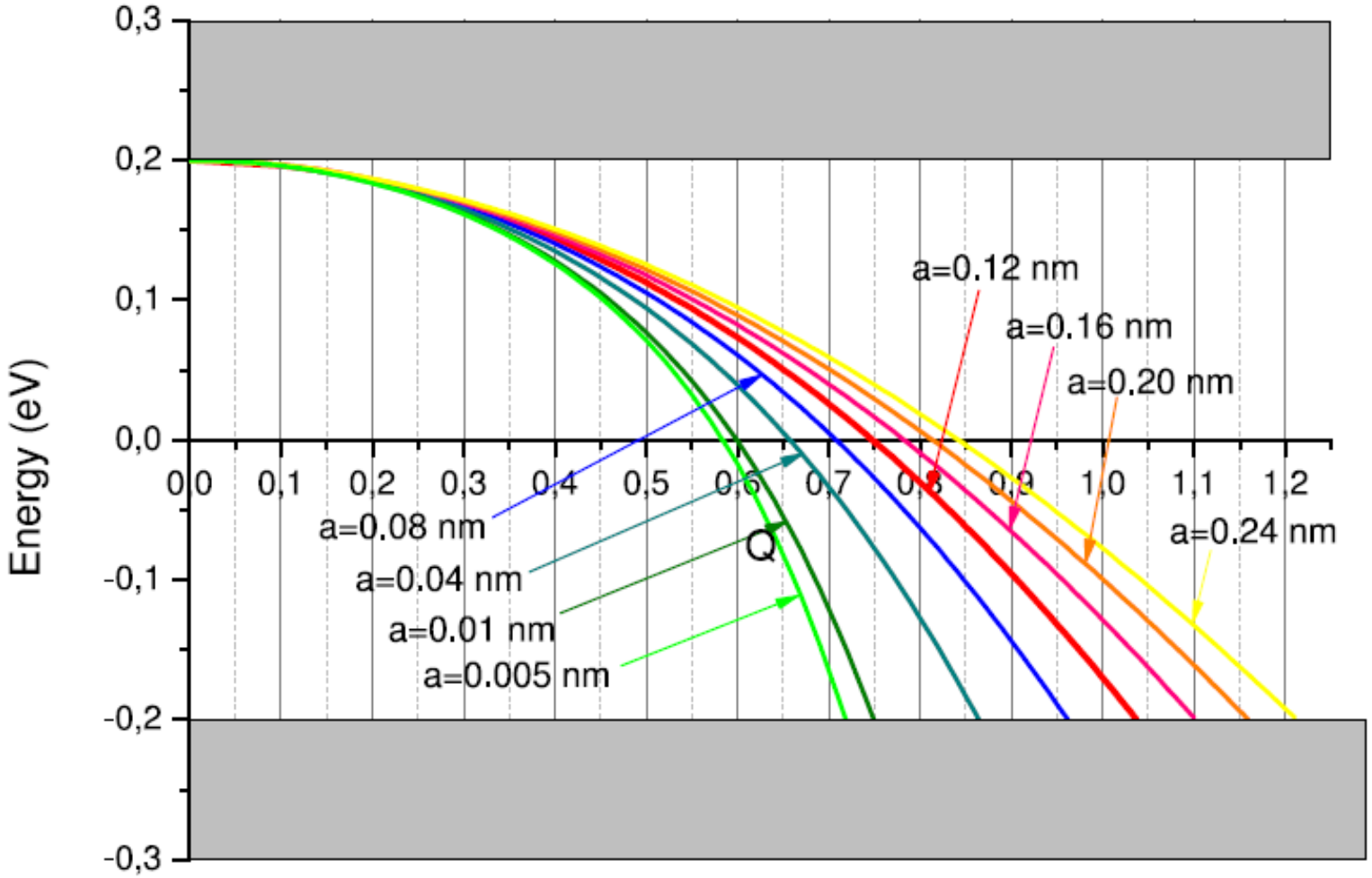
$$V(0,1) = 5.5 \quad \text{eV}$$





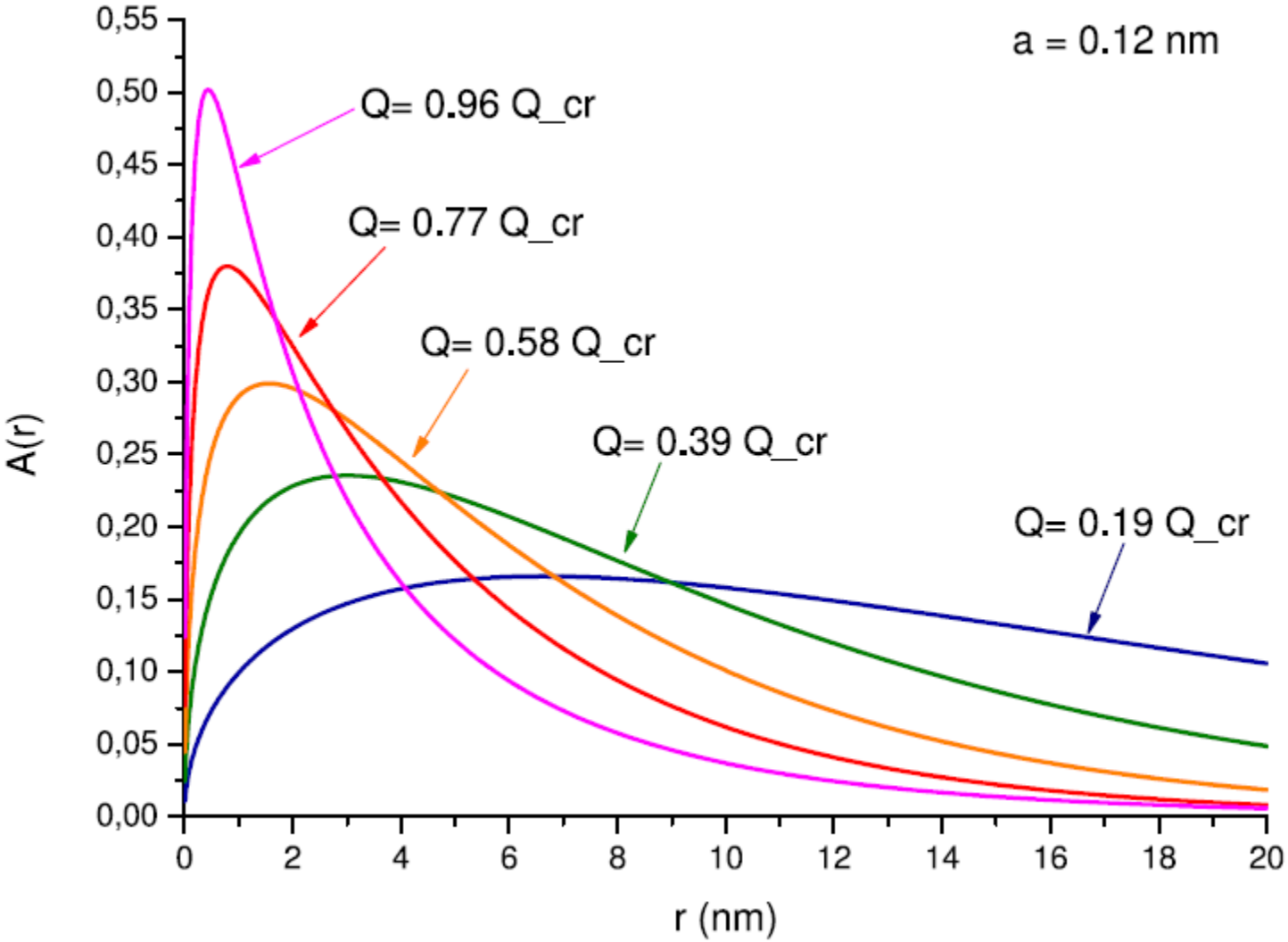
Critical charge in Graphene: Theory

Energy levels



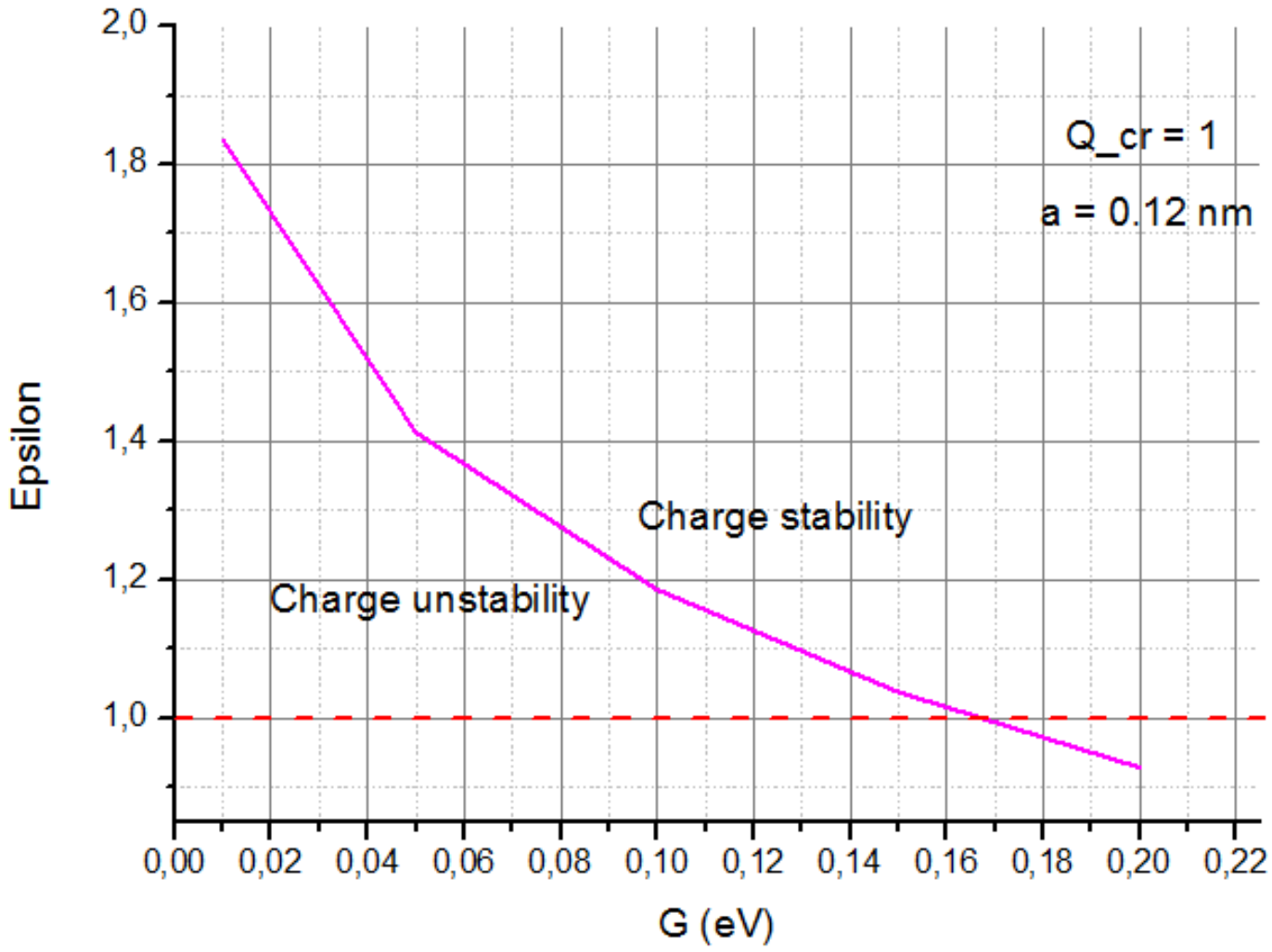
Критический заряд в графене: теория

Волновые функции



Критический заряд в графене: теория

Зависимость от величины массовой щели:



Критический заряд в графене: теория

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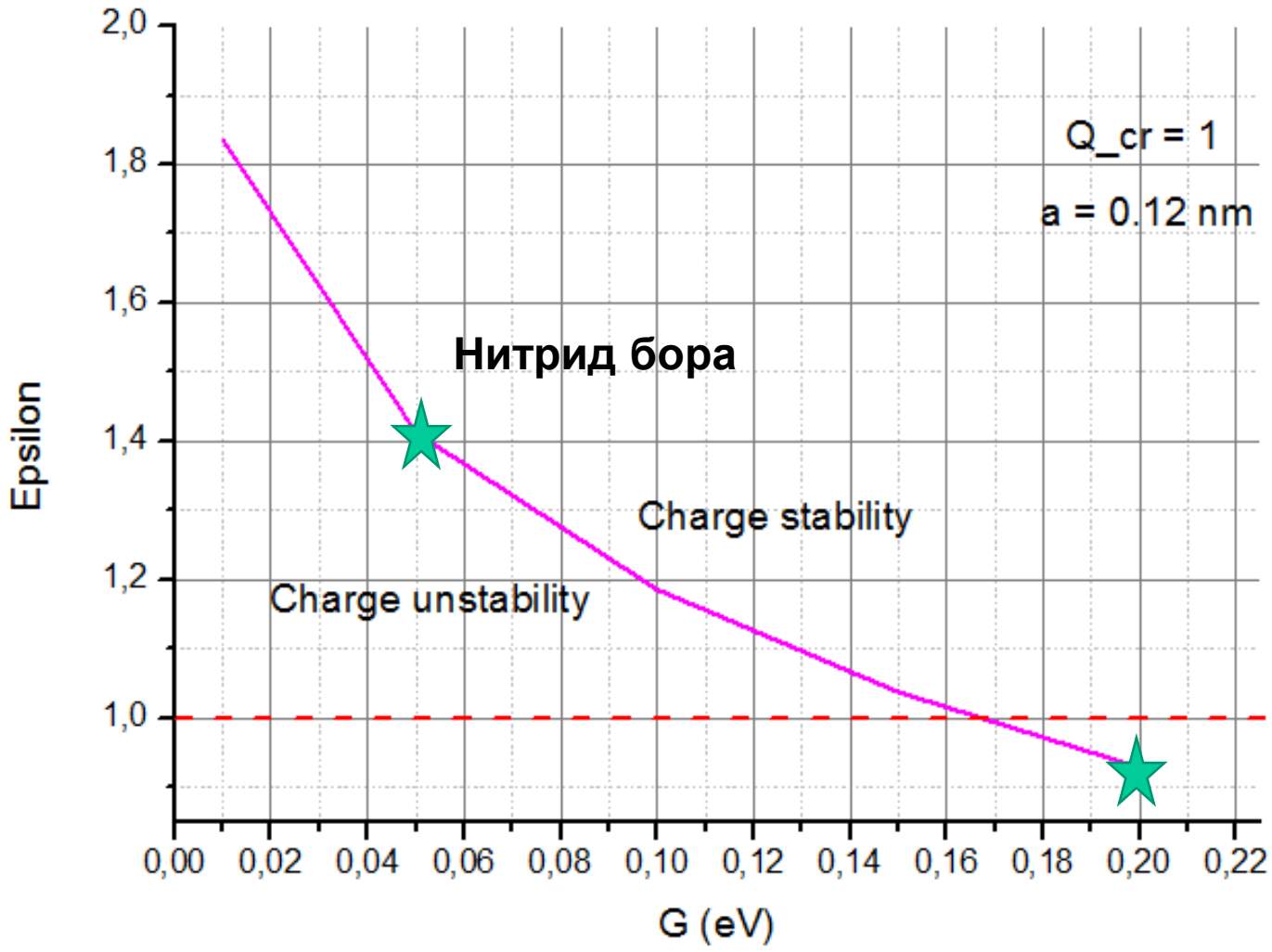

Критический заряд в графене: теория

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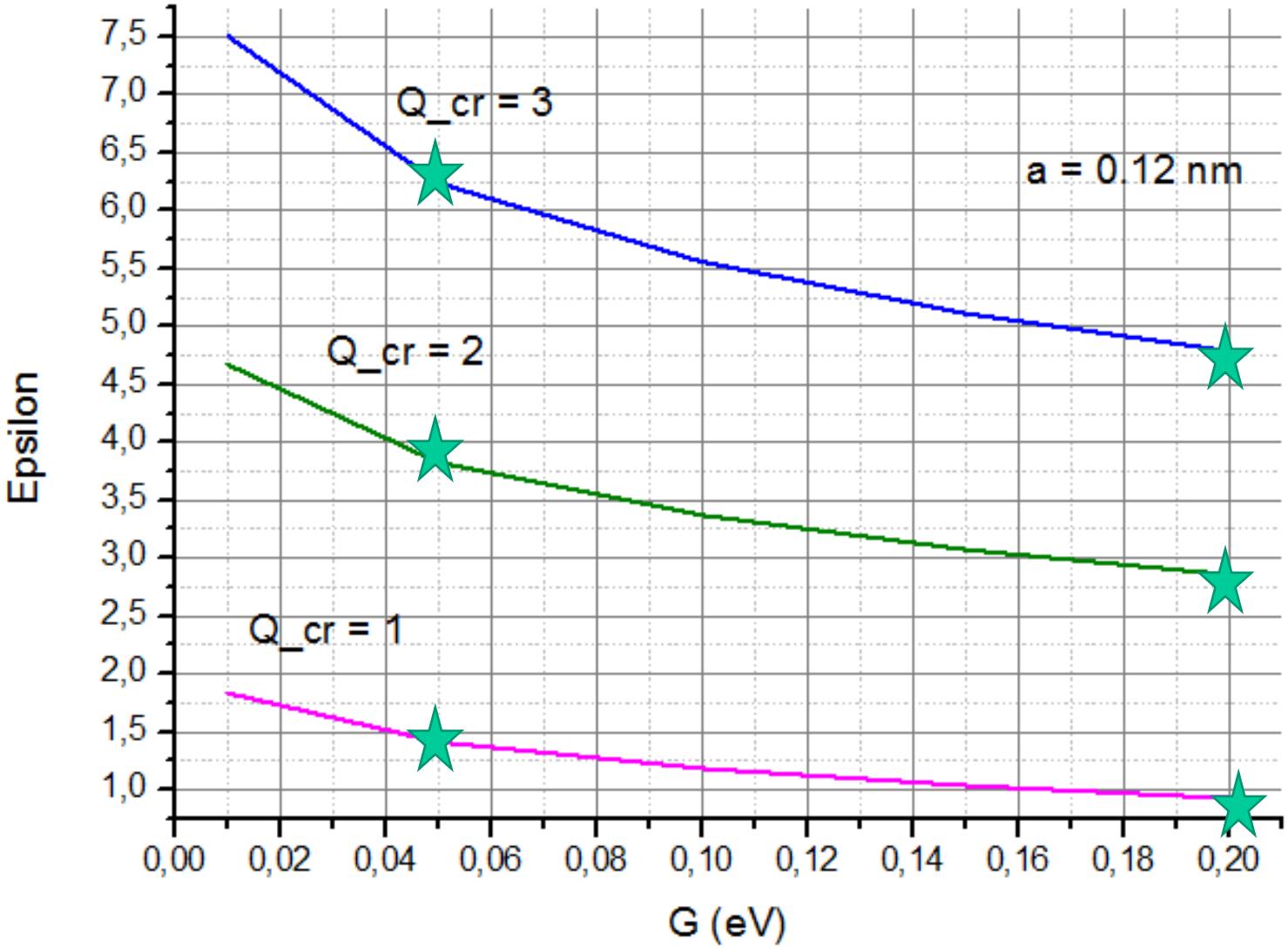
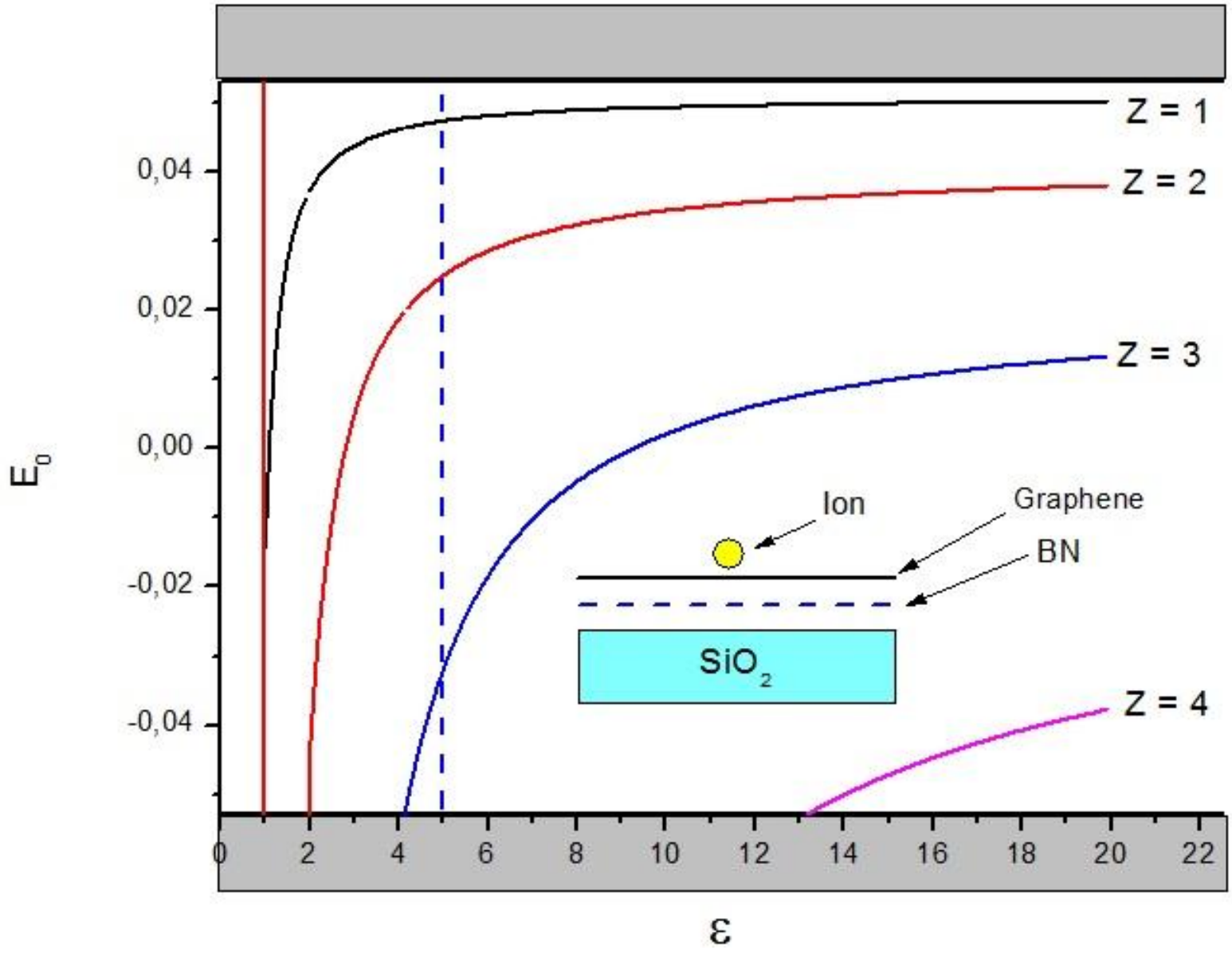
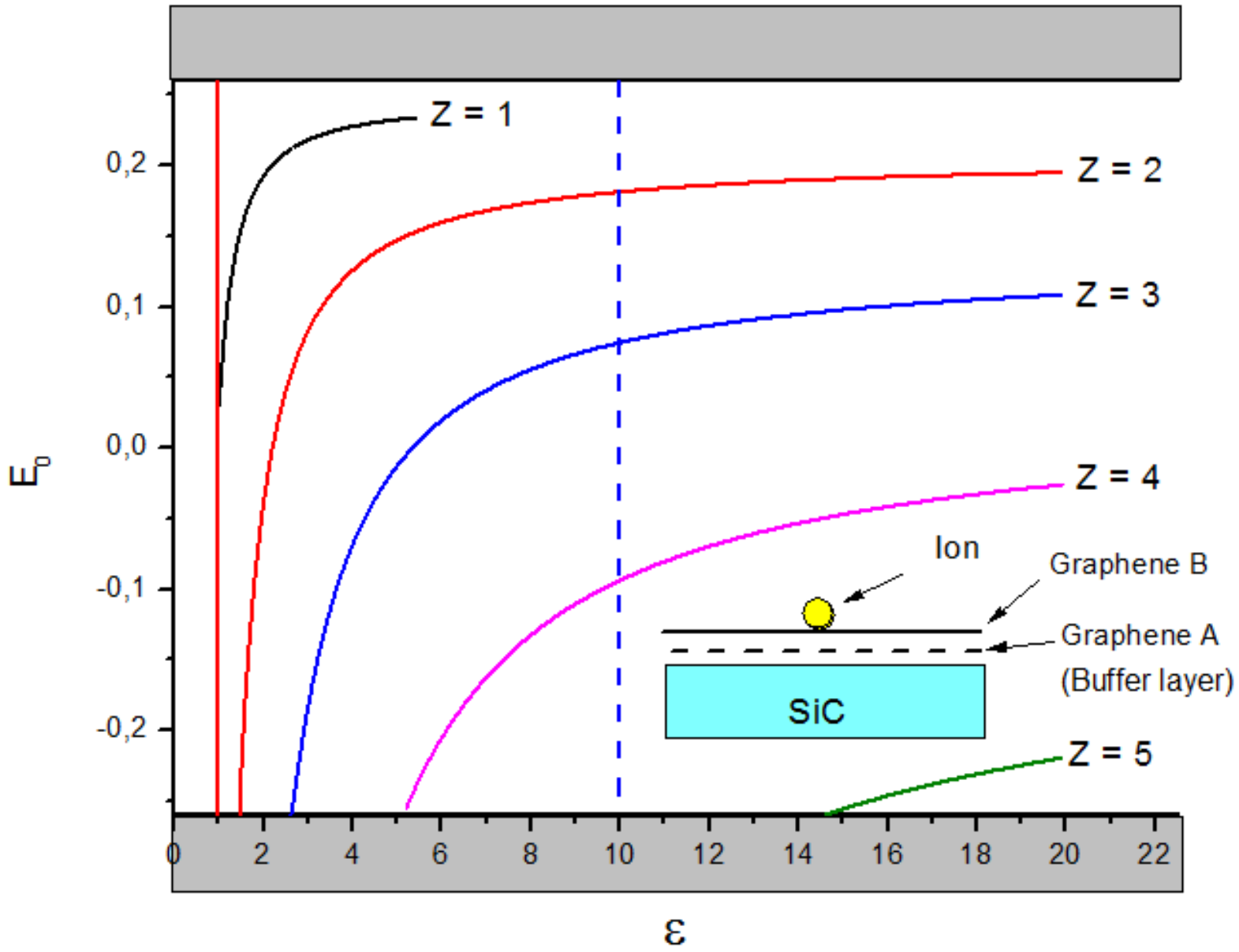


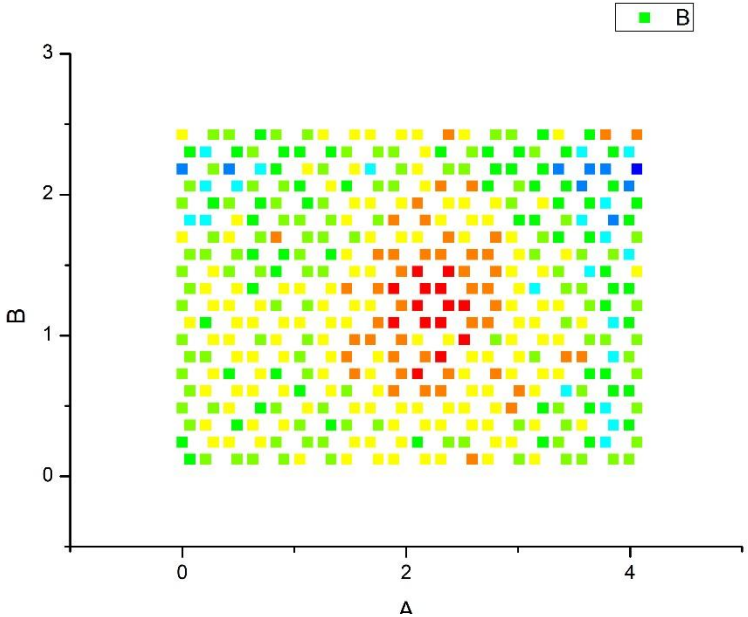
Critical charge in Graphene: Theory

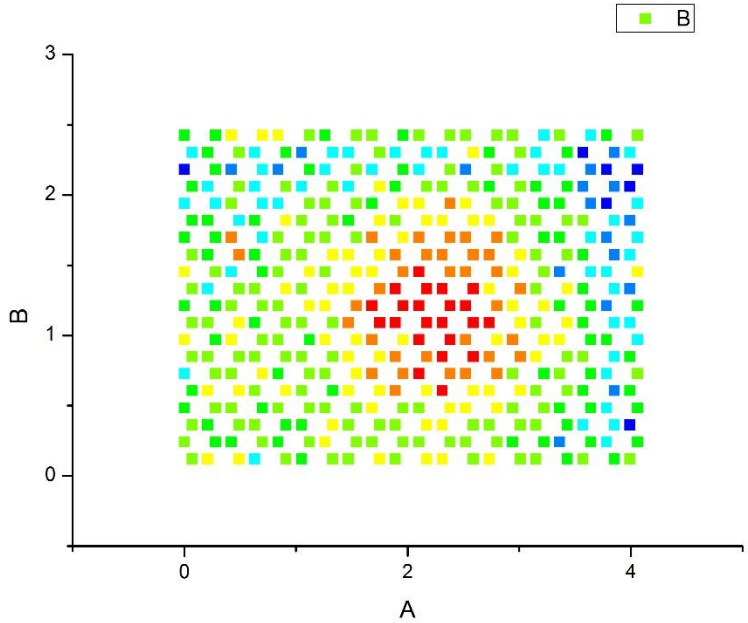


Critical charge in Graphene: Theory

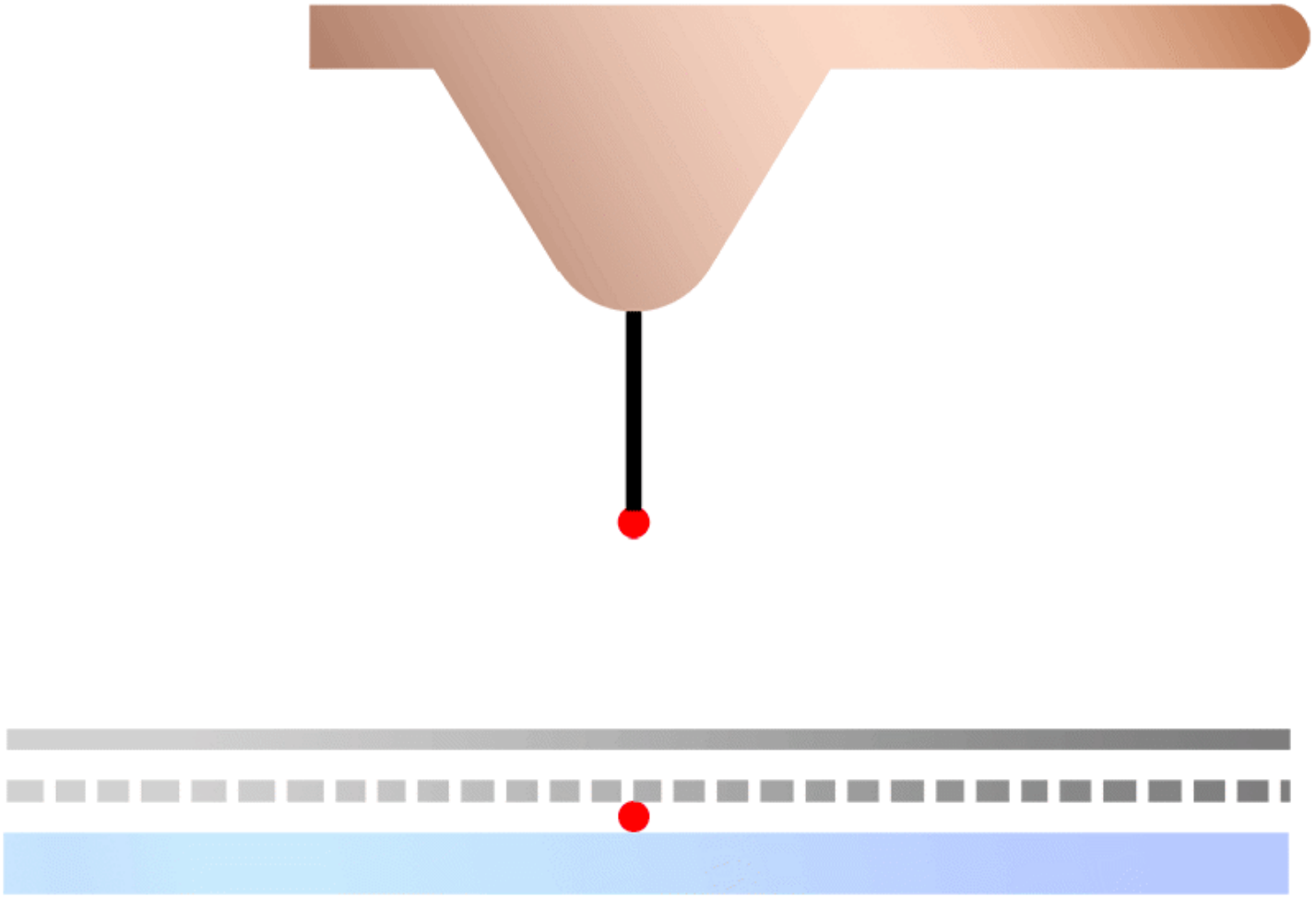


Critical charge in Graphene: MC





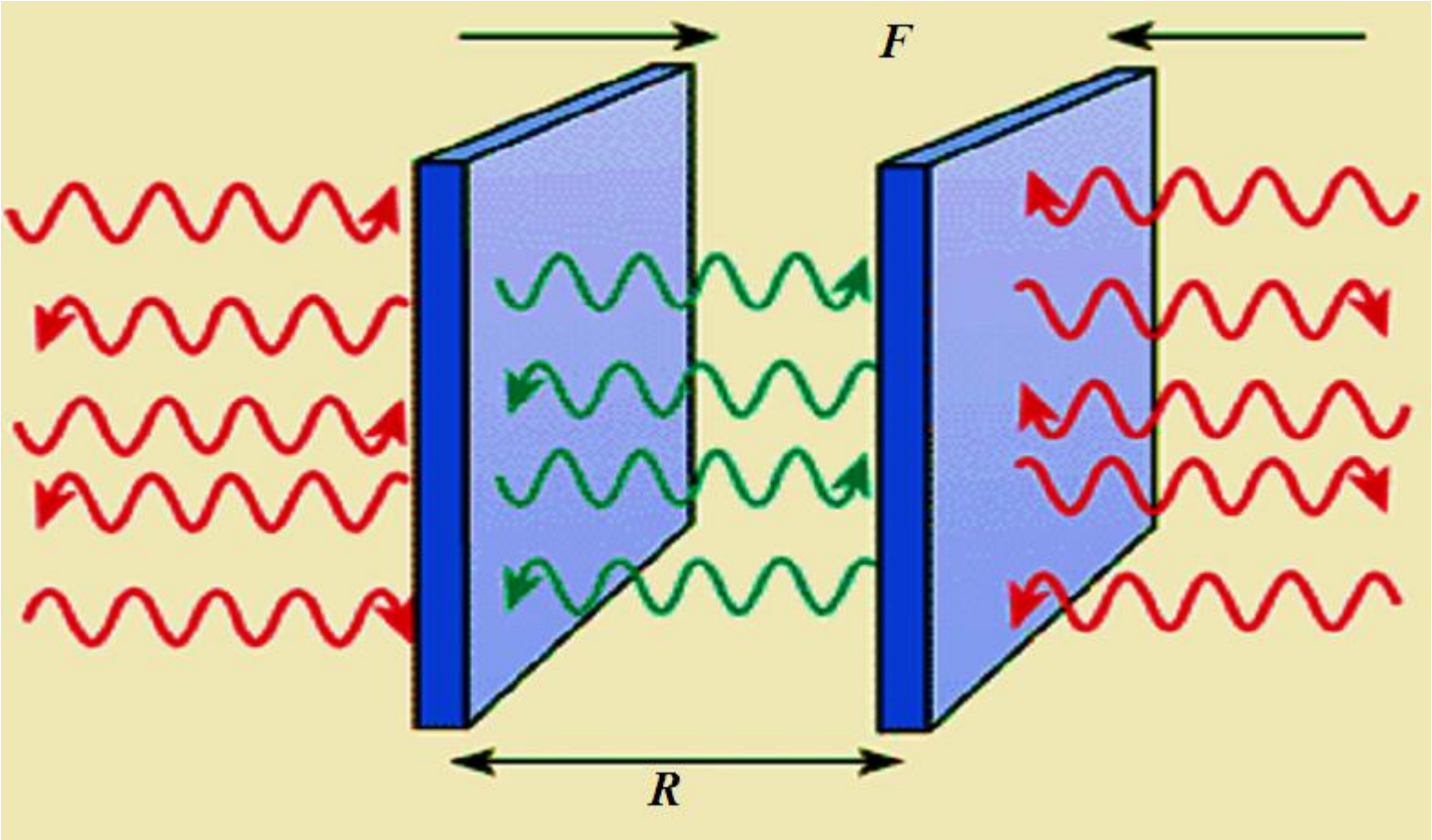
Critical charge in Graphene: Experiment



Темы исследований

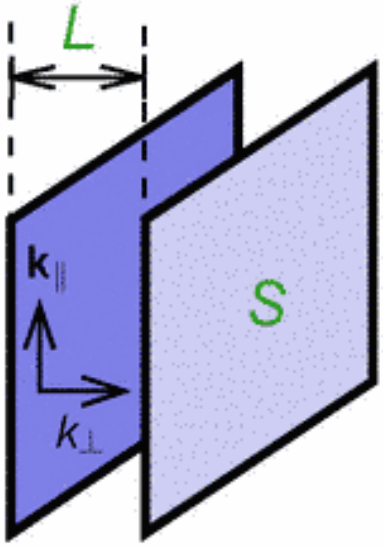
Эффект Казимира в наноструктурах

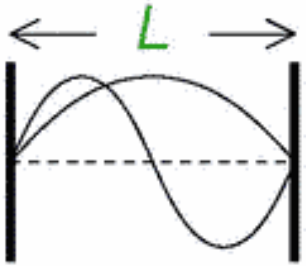
Эффект Казимира



$$E_{Cas} = -\frac{\pi^2 \hbar c}{720 R^3}$$

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

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

Зачем вычисляют силы Казимира?

- **Устойчивость микро- и нано-структур**

- **Микро- и нано-устройства, использующие эффект Казимира**

- **Применение в физике частиц и космологии**

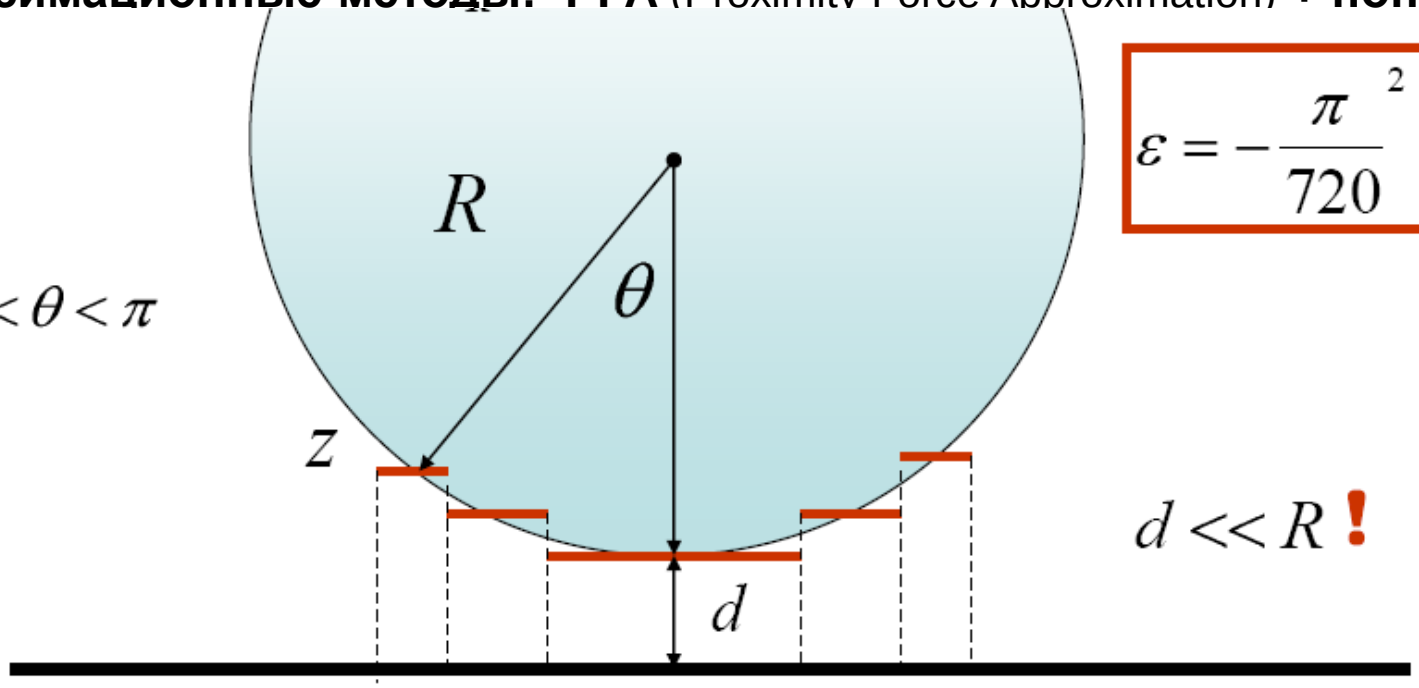
Как вычисляют силы Казимира?

- Метод прямого суммирования энергетических мод (применим только для задач с простой геометрией (плоскость-плоскость, плоскость-сфера и т.п.))

- **Апроксимационные методы: PFA** (Proximity Force Approximation) **+ поправки**

$$\varepsilon = -\frac{\pi^2}{720}\frac{\hbar c}{d^3}$$

$0 < \theta < \pi$



$d << R$!

Эффект Казимира для Черн-Саймонсовских поверхностей

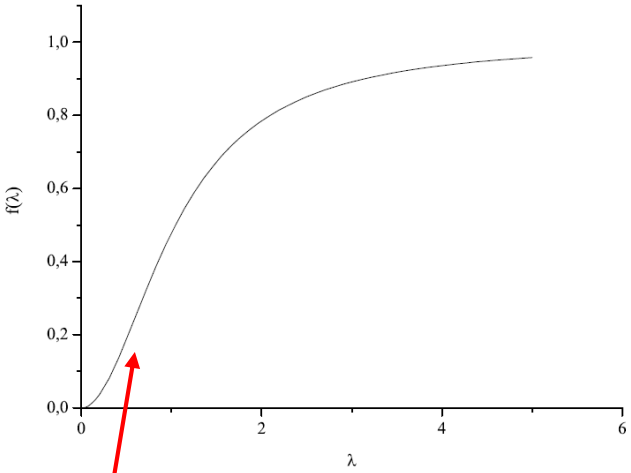
M. Bordag and D. V. Vassilevich, Phys. Lett. A 268 (2000) 75.
V. N. Markov and Yu. M. Pis'mak, J. Phys. A 39 (2006) 6525.

$$S = -\frac{1}{4}\int d^4x\ F_{\mu\nu}F^{\mu\nu} - \frac{\lambda}{2}\oint d^3s\,\varepsilon^{\sigma\mu\nu\rho}n_\sigma A_\mu(x)F_{\nu\rho}(x)$$

$$S_{CS} = \frac{\lambda}{2}\int(\delta(x_3)-\delta(x_3-R))\varepsilon^{3\mu\nu\rho}A_\mu(x)F_{\nu\rho}(x)d^4x$$

$$\Box A^\mu + \lambda(\delta(x_3)-\delta(x_3-R))\varepsilon^{3\sigma\nu\rho}A_\sigma\partial_\nu A_\rho = 0.$$

$$E_\parallel|_S = 0, \qquad H_n|_S = 0$$

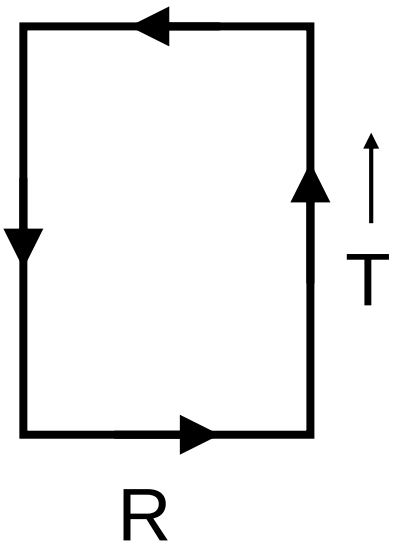


$$f(\lambda) = \frac{90}{\pi^4}\mathrm{Li}_4\left(\frac{\lambda^2}{\lambda^2+1}\right)$$

$$E_{Cas} = -\frac{\pi^2}{720R^3}f(\lambda) = -\frac{\lambda^2}{8\pi^2R^3} + O(\lambda^4)$$

$$\mathrm{Li}_4(x) = \sum_{k=1}^{\infty}\frac{x^k}{k^4} = -\frac{1}{2}\int_0^\infty k^2\ln(1-xe^{-k})dk.$$

Наблюдаемая для казимировской энергии: (Аналогия с петлей Вильсона)



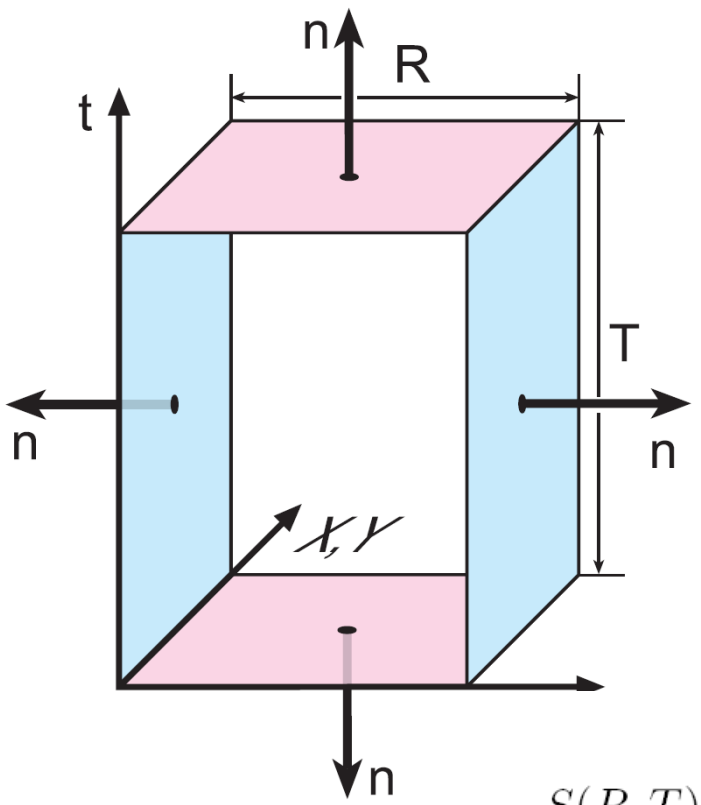
$$W_C = e^{ig\oint_C A_\mu dx^\mu} = e^{i\int J_\mu A^\mu dx^4}$$

$$J_\mu(x) = g\oint_C \delta(x-\xi)d\xi_\mu$$

$$\boxed{\langle W(R,T)\rangle \to Ce^{-V(R)T}}$$

$$V(R) = -\lim_{T\to\infty}\frac{1}{T}\ln\langle W_C(R,T)\rangle \approx C_1 + \frac{C_2}{R}$$

Наблюдаемая для казимировской энергии:



$$W_{Bag}(R,T) = e^{i\lambda S(R,T)}$$

$$= e^{i\lambda \oint_{\Sigma} \varepsilon_{\mu\nu\rho\sigma} A^{\nu} F^{\rho\sigma} dS^{\mu}}$$

$$\boxed{\langle W_{Bag}(R,T)\rangle \underset{T\to\infty}{\longrightarrow} C e^{-E_{cas}(R)T}}$$

$$S(R,T) = \int_0^T dt \iiint dxdydz(\delta(z-R)-\delta(z))\varepsilon_{3\nu\rho\sigma}A^{\nu}F^{\rho\sigma} +$$

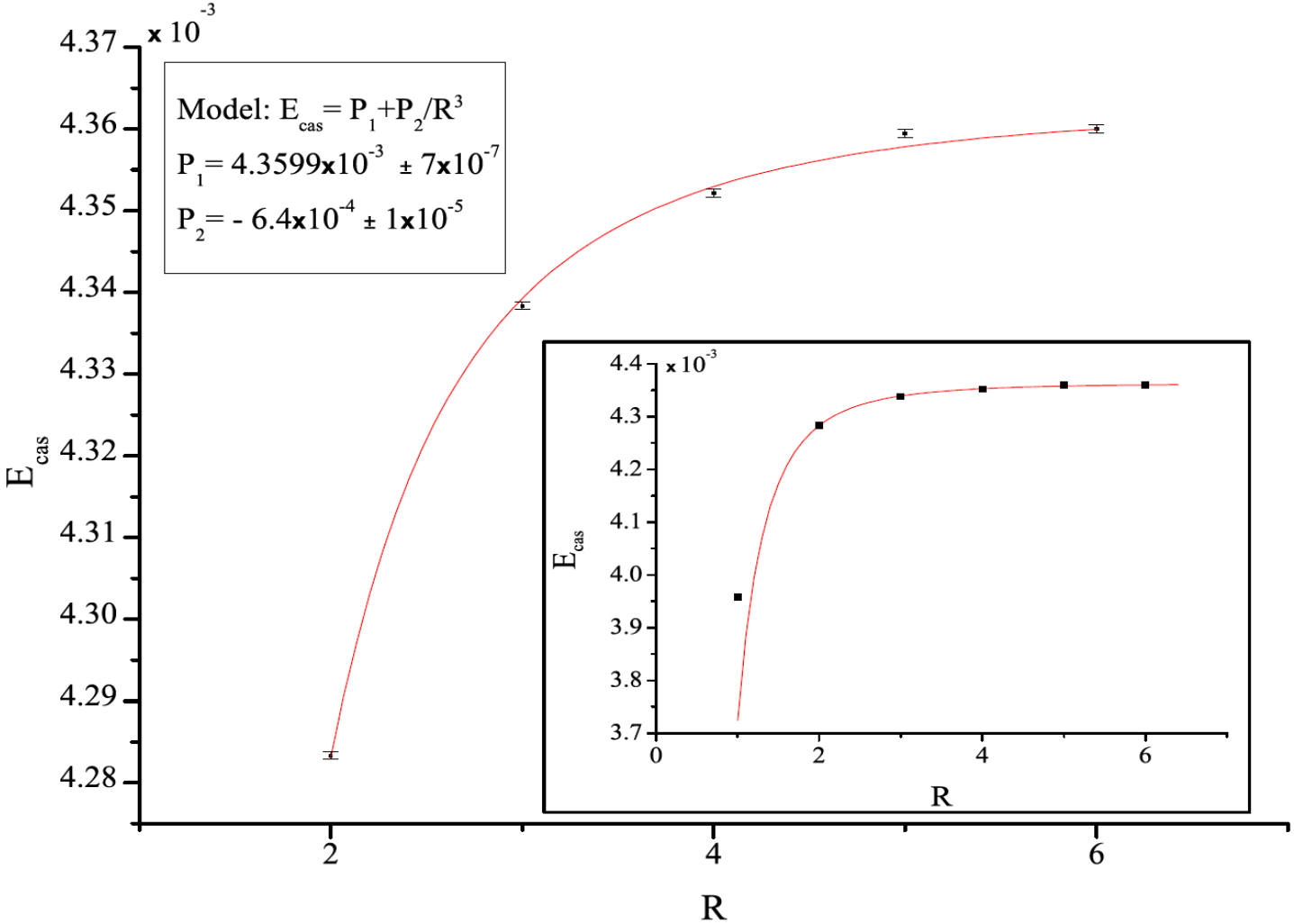
$$+ \int_0^R dz \iiint dxdydt(\delta(t-T)-\delta(t))\varepsilon_{0\nu\rho\sigma}A^{\nu}F^{\rho\sigma}.$$

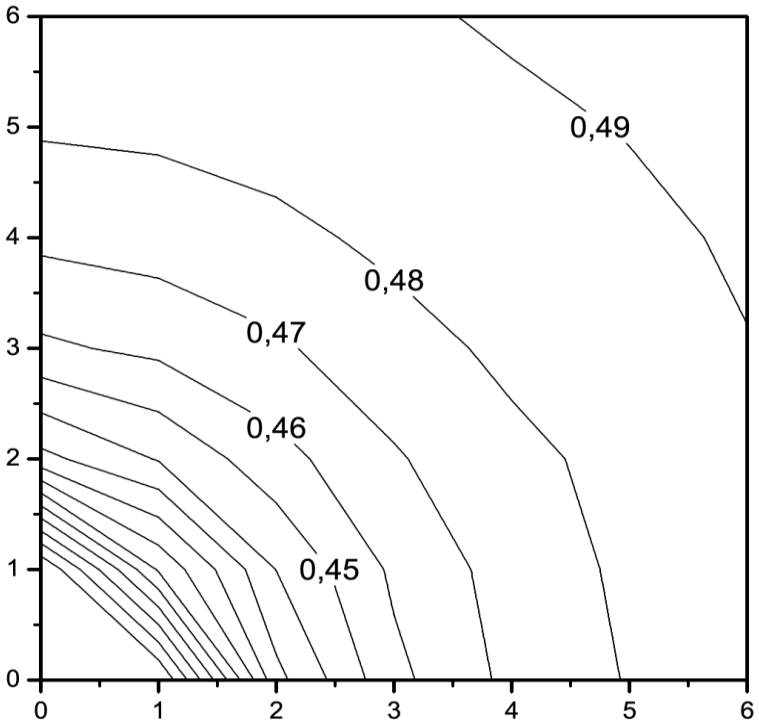
Величина, которую надо построить → $\boxed{A_\nu F_{\rho\sigma}}$

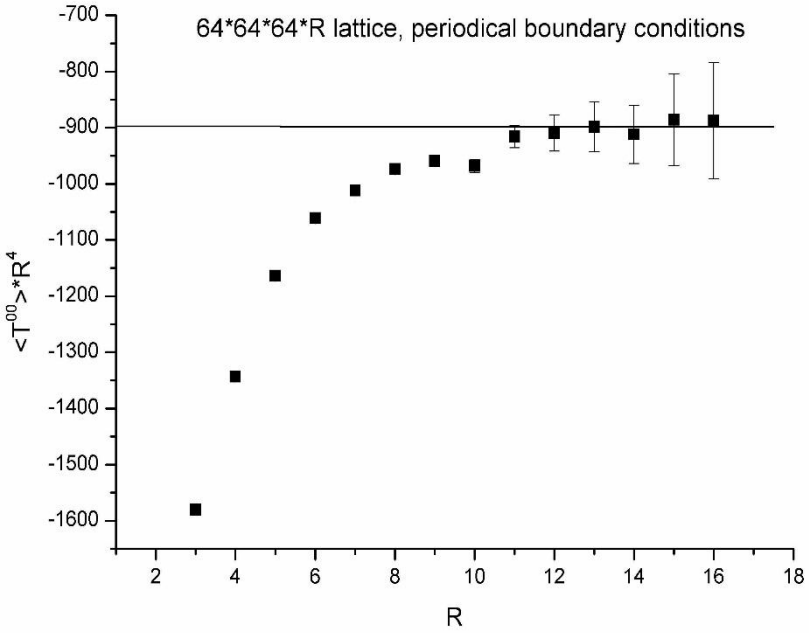
Решеточная реализация нашей наблюдаемой, вильсоновского “мешка”, должна отвечать следующим требованиям:

1) Калибровочная инвариантность. Полный интеграл по замкнутой поверхности для “вильсоновского мешка” должен быть калибровочным инвариантом.

2) “Локальность”. В предлагаемом решеточном представлении величины $A_\nu F_{\rho\sigma}$, A_ν и $F_{\rho\sigma}$ должны быть заданы в одной и той же точке x. Это требование нетривиально потому, что $\theta_{p,\rho\sigma}$ задает величину напряженности поля $F_{\rho\sigma}$ в центре плакета, в то время как θ_ν задает величину поля A_ν в центре линка, а это разные точки!

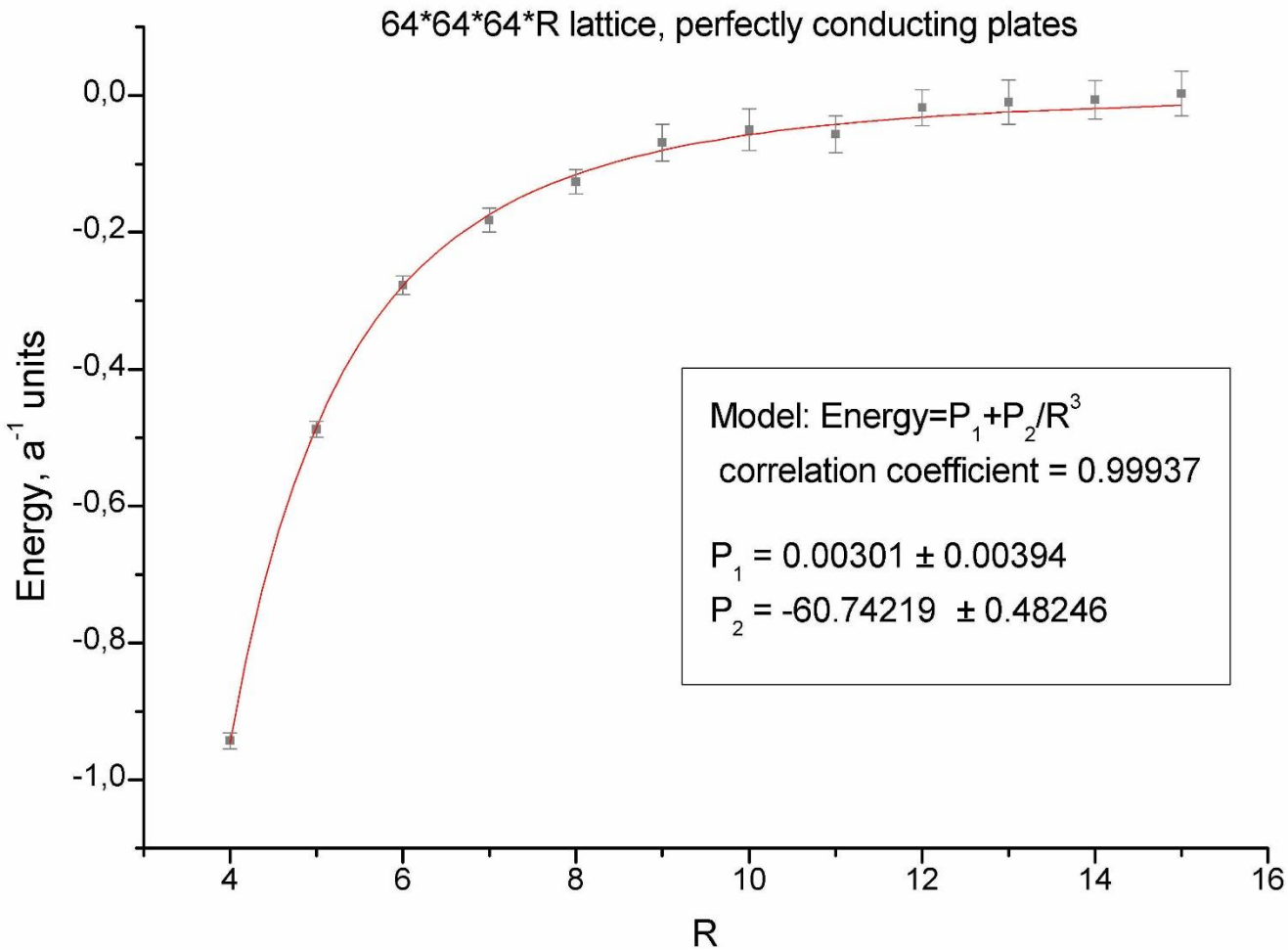

Model: $E_{cas} = P_1 + P_2/R^3$
$P_1 = 4.3599 \times 10^{-3} \pm 7 \times 10^{-7}$
$P_2 = -6.4 \times 10^{-4} \pm 1 \times 10^{-5}$
$\times 10^{-3}$
4.37
4.36
4.35
4.34
4.33
4.32
4.31
4.30
4.29
4.28
E_{cas}
2
4
6
R
$\times 10^{-3}$
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
E_{cas}
0
2
4
6
R

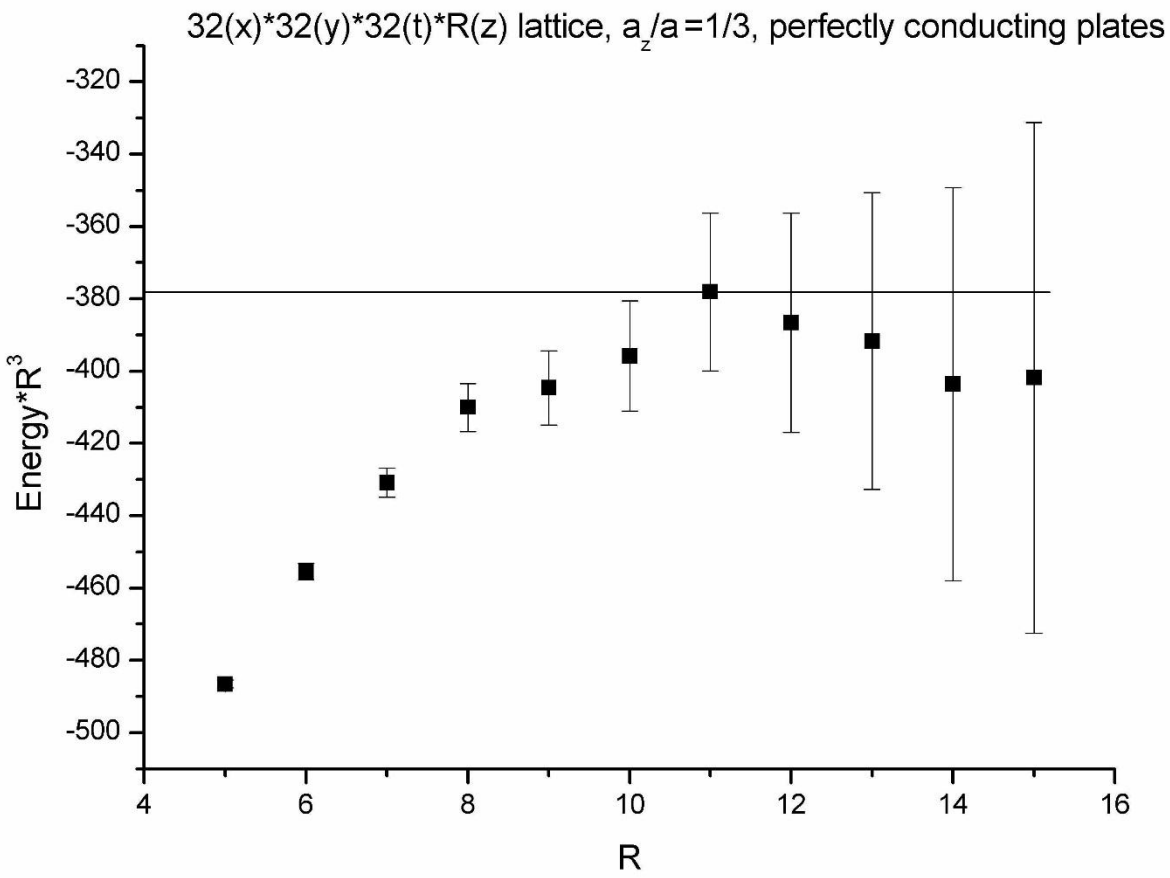

0,49
0,48
0,47
0,46
0,45
0
1
2
3
4
5
6


64*64*64*R lattice, periodical boundary conditions
<T^00>*R^4
R
-700
-800
-900
-1000
-1100
-1200
-1300
-1400
-1500
-1600
2
4
6
8
10
12
14
16
18

$$E_{cas.} = \frac{C}{(Ra)^3}(aN)^2 = \frac{CN^2}{R^3}\frac{1}{a}$$

$$E_{cas} = P_1 + \frac{P_2}{R^3}$$

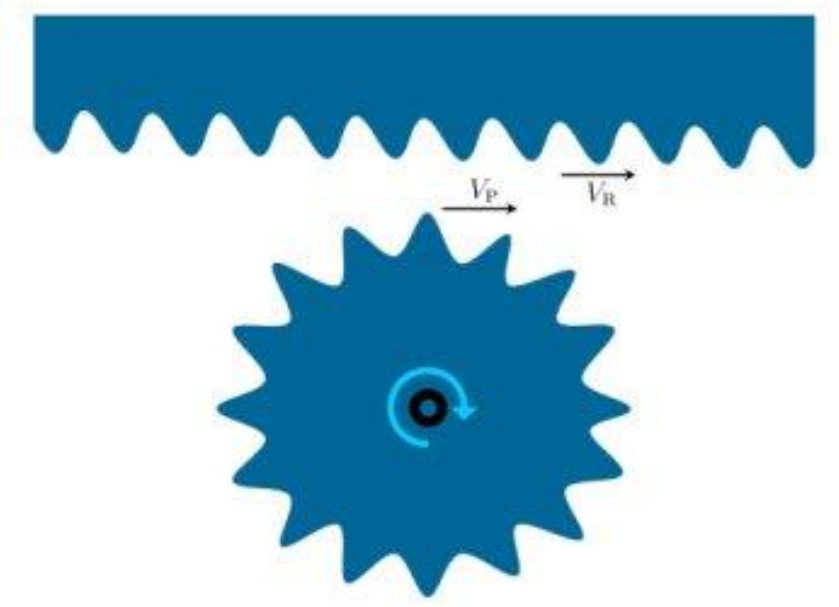

64*64*64*R lattice, perfectly conducting plates
Energy, a-1 units
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
4
6
8
10
12
14
16
R
Model: Energy=P1+P2/R3
correlation coefficient = 0.99937
P1 = 0.00301 ± 0.00394
P2 = -60.74219 ± 0.48246


32(x)*32(y)*32(t)*R(z) lattice, a_z/a =1/3, perfectly conducting plates
Energy*R^3
-320
-340
-360
-380
-400
-420
-440
-460
-480
-500
4
6
8
10
12
14
16
R

Энергия Казимира и квантовая теория поля на решетке

Актуальные задачи по расчету вакуумных сил (1).

Применение в задачах микромеханики – зубчатые передачи, шестеренки, функционирующие без зацепления.



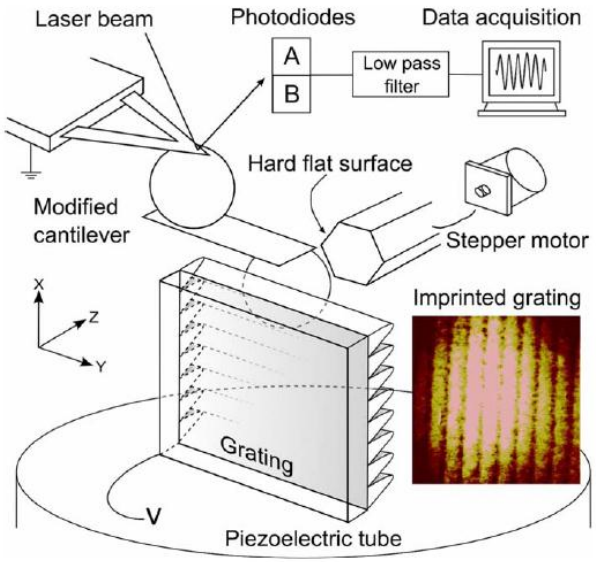


FIG. 1. (Color online) Schematic of the experimental setup (see text for further details). Insertion shows the imprinted corrugations on the second sphere. The lighter area shows higher points and hence demonstrates the sphericity of the imprinted surface.

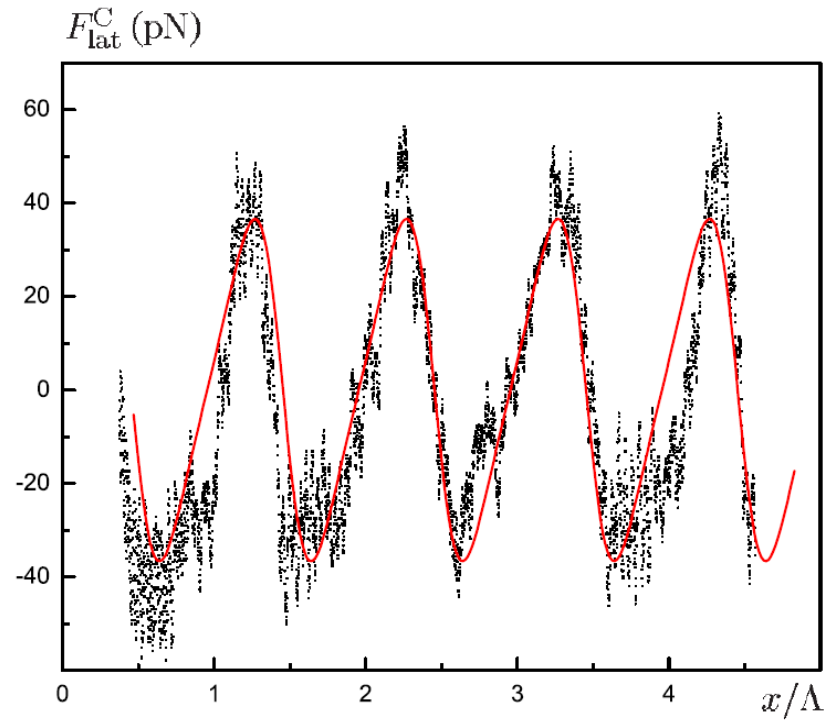
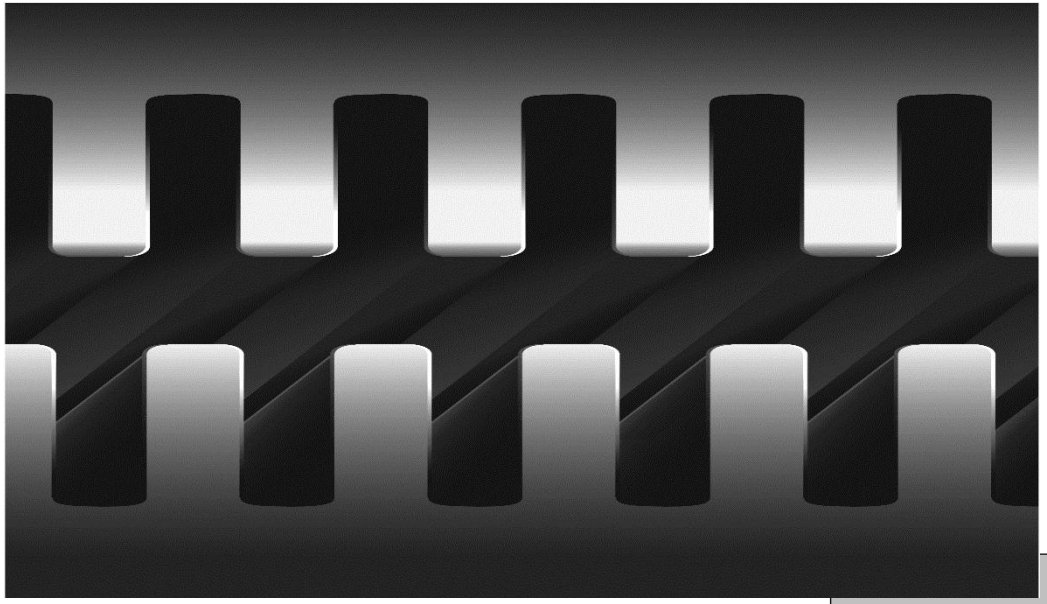
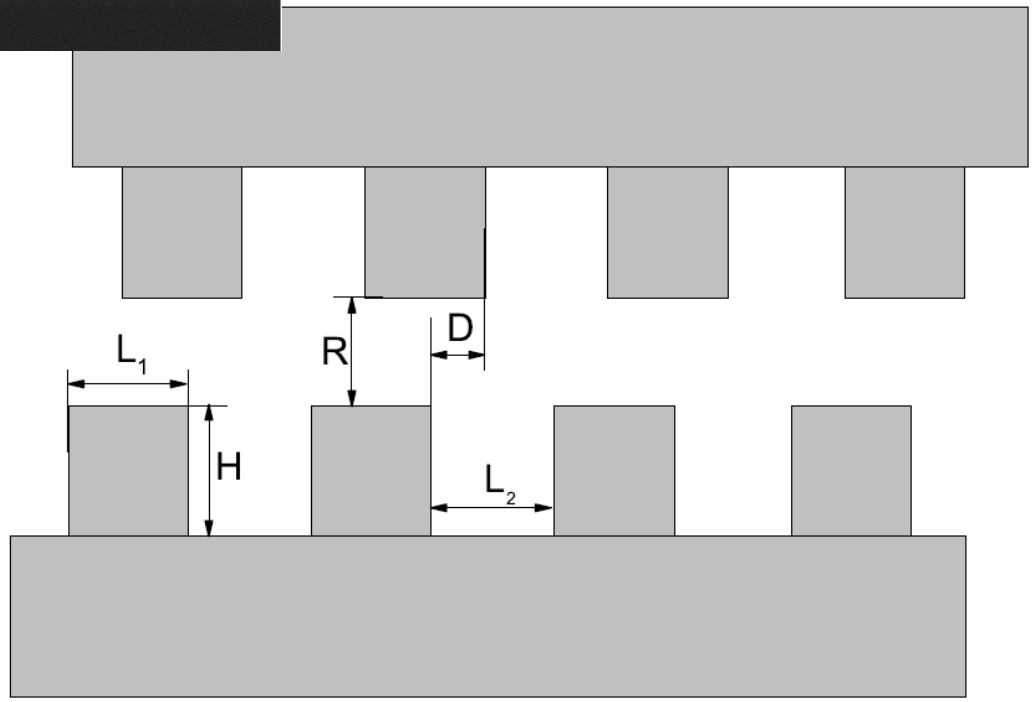
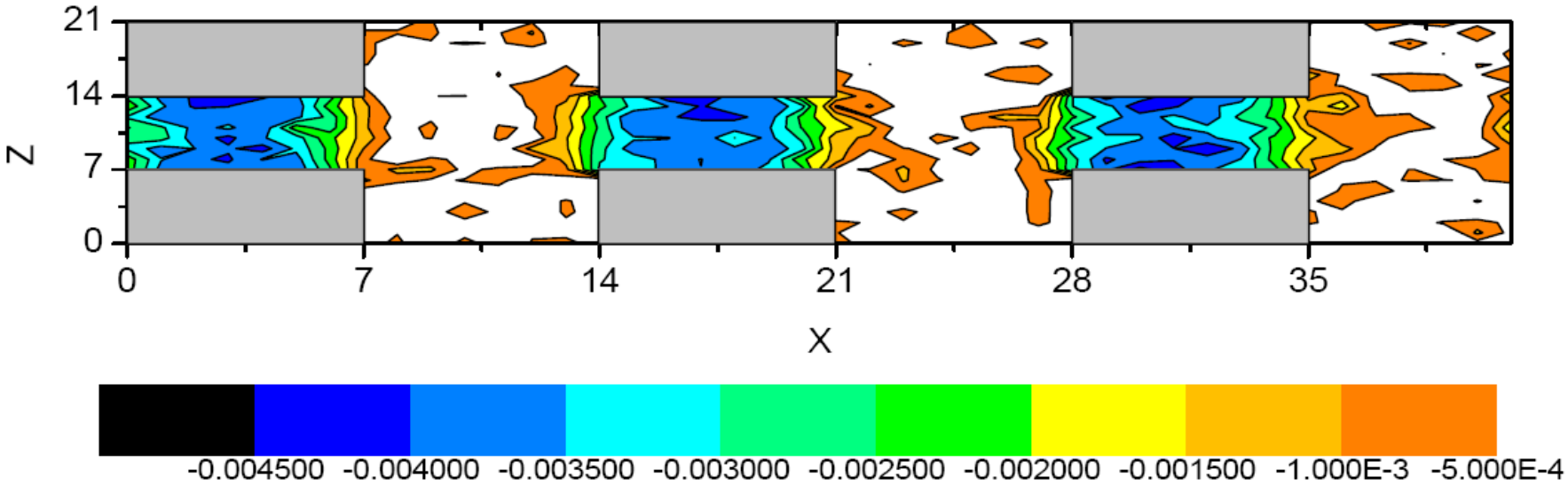
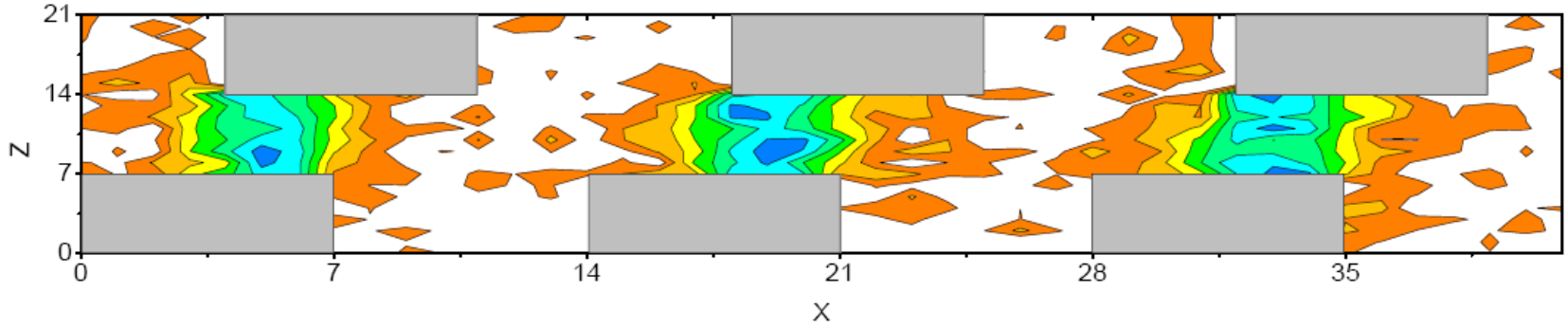


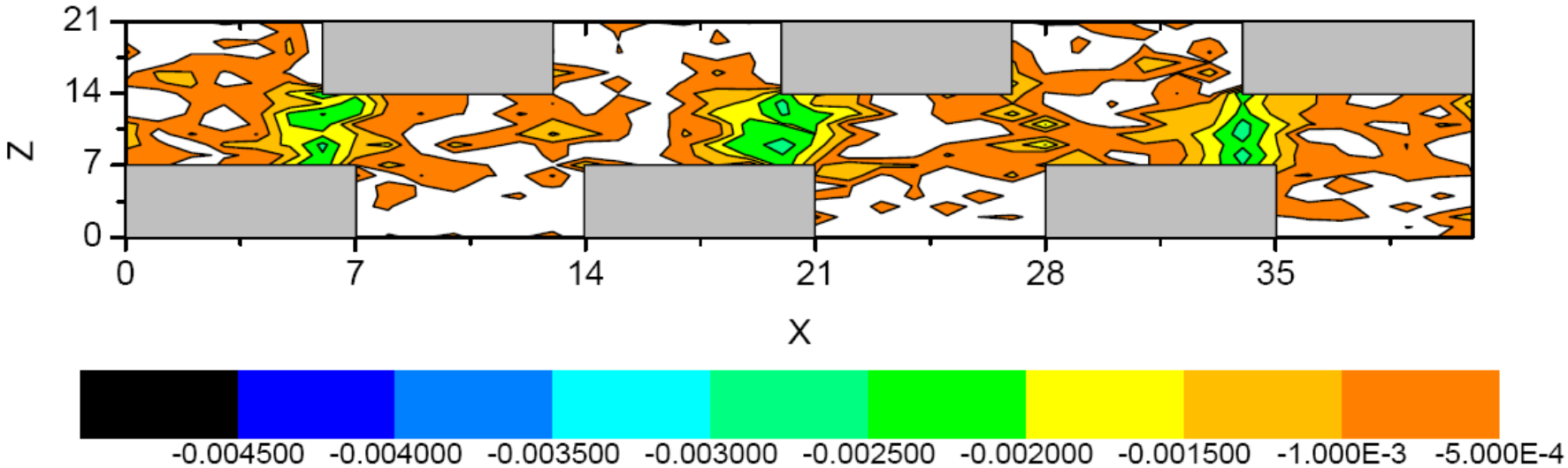
FIG. 2. (Color online) The phase dependence of the lateral Casimir force. The measurement data are shown as dots. The solid line is the exact theory.

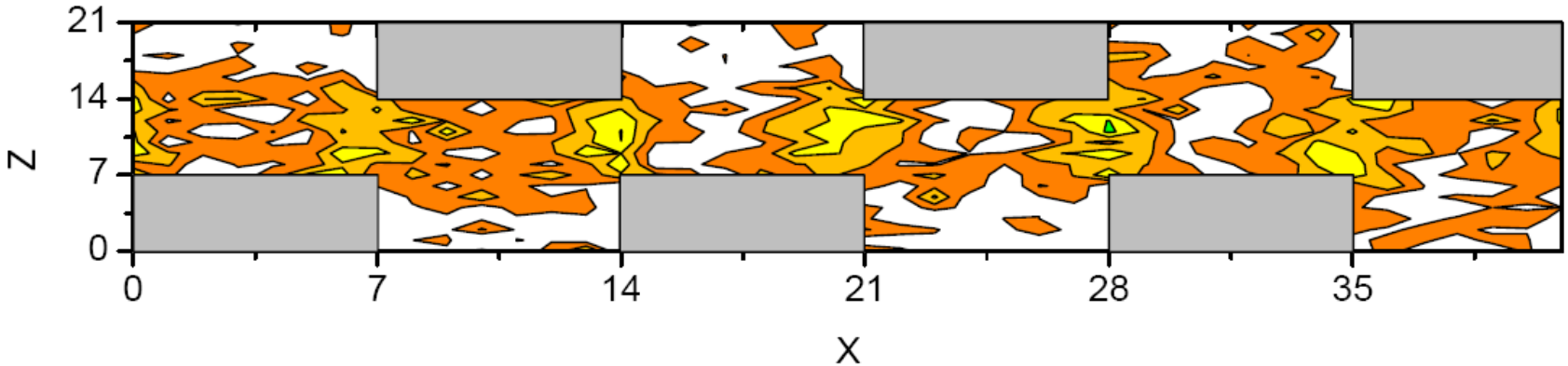



L1
R
D
H
L2


21
14
7
0
Z
0
7
14
21
28
35
X
-0.004500
-0.004000
-0.003500
-0.003000
-0.002500
-0.002000
-0.001500
-1.000E-3
-5.000E-4


21
14
7
0
Z
0
7
14
21
28
35
X

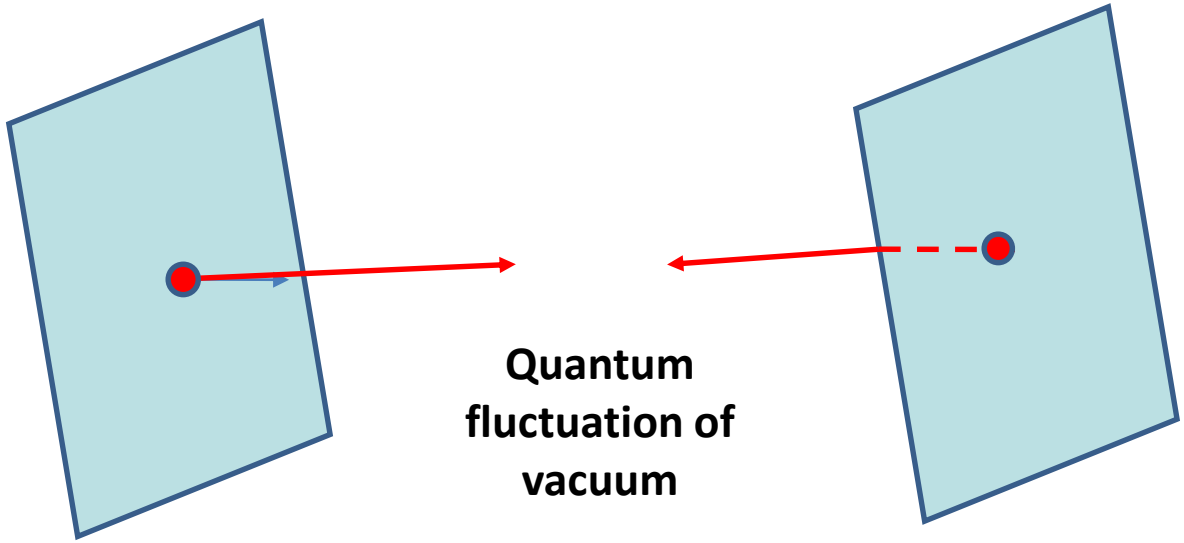

21
14
7
0
Z
0
7
14
21
28
35
X
-0.004500
-0.004000
-0.003500
-0.003000
-0.002500
-0.002000
-0.001500
-1.000E-3
-5.000E-4


21
14
7
0
Z
0
7
14
21
28
35
X

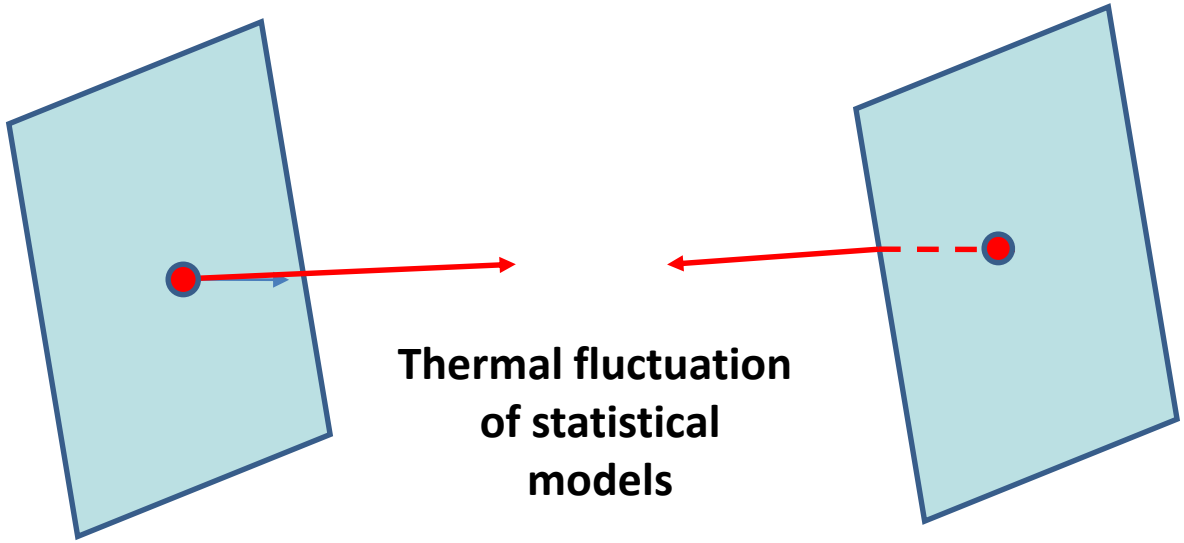
Темы исследований

Критический эффект Казимира в статистических моделях

Critical Casimir Effect: Casimir Effect in statistical model



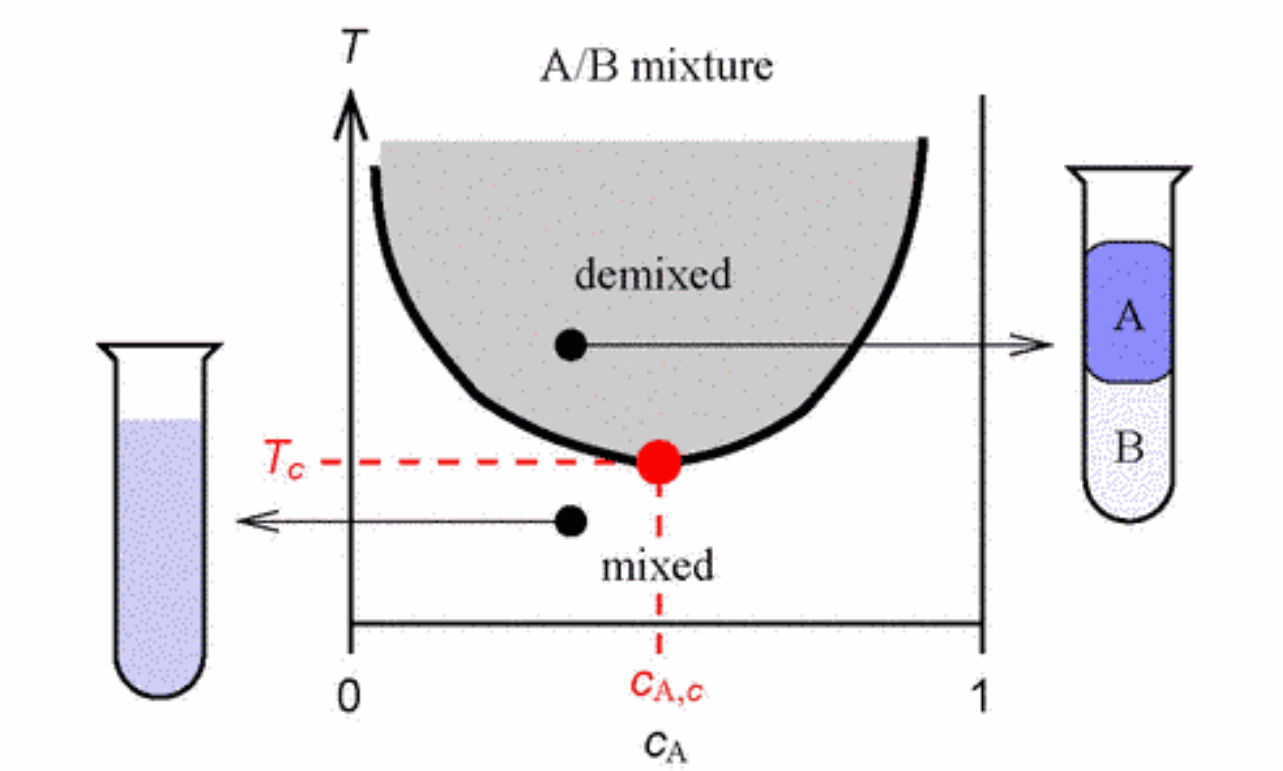
Critical Casimir Effect: Casimir Effect in statictical model



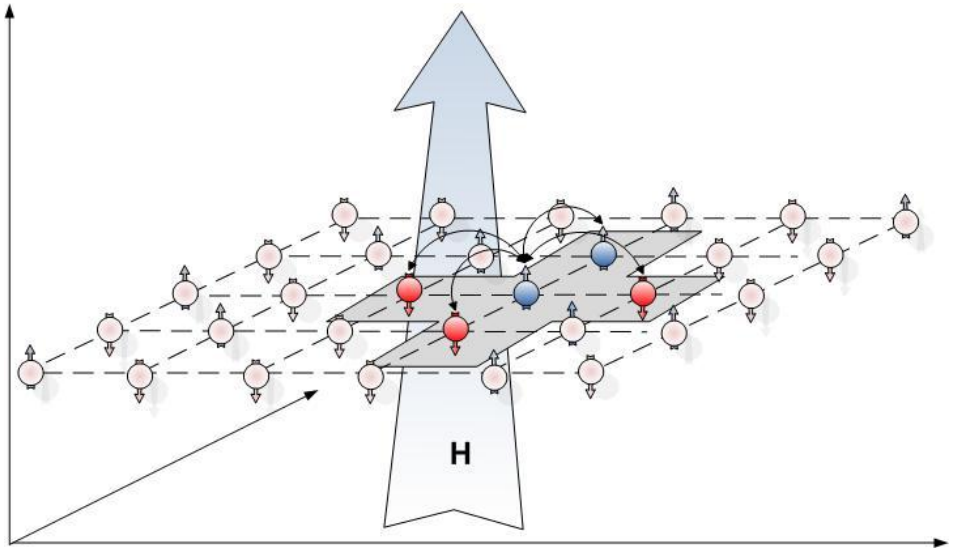
M. E. Fisher, P.-G. de Gennes, C. R. Acad. Sci. Paris Ser. B **287** , 207 (1978).

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

^{3}He – ^{4}He mixture



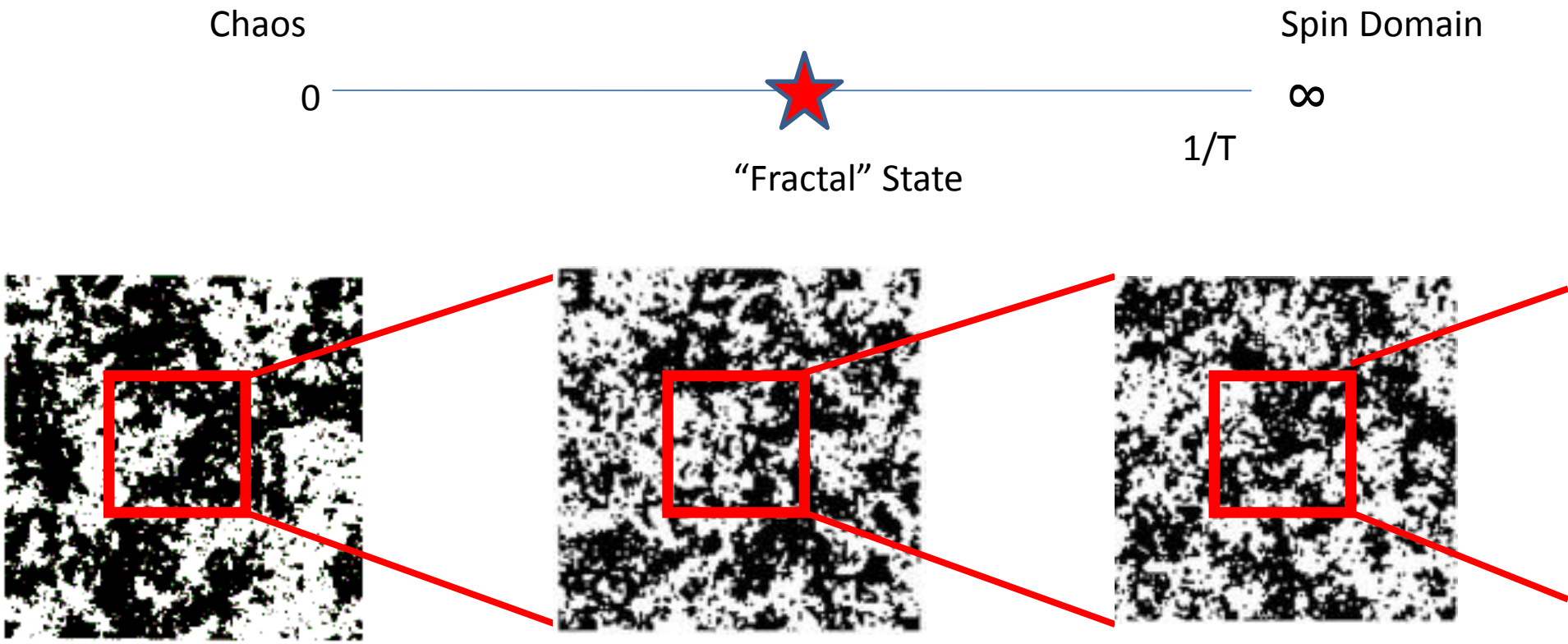
Conformal symmetry and phase transition: Ising model illustration



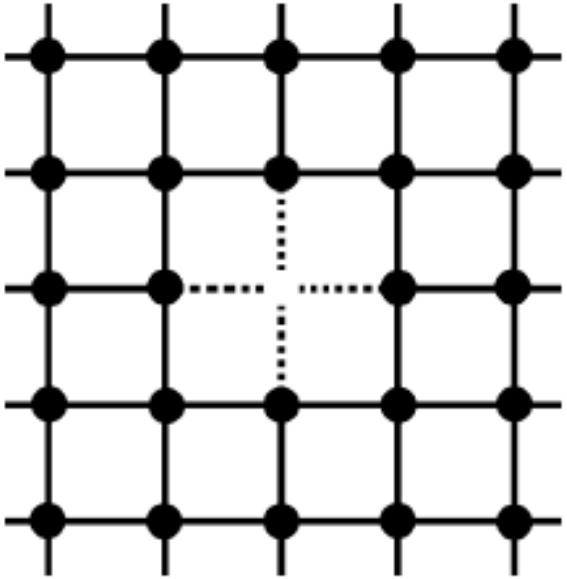
$$E(Conf) = -J \sum_{x,\mu} \sigma_x \sigma_{x+\mu} + H \sum_x \sigma_x,$$

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

Scale invariance at “Fractal” State



Ising model with defect



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

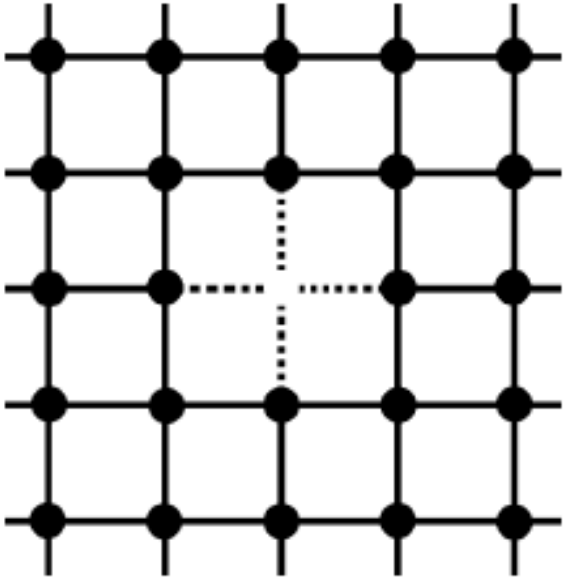
$$P(Conf) = \frac{1}{Z}e^{-\beta E(Conf)}, \qquad \varkappa = \beta J$$

Mass of defect:

$$m_d = E_d - E_0,$$

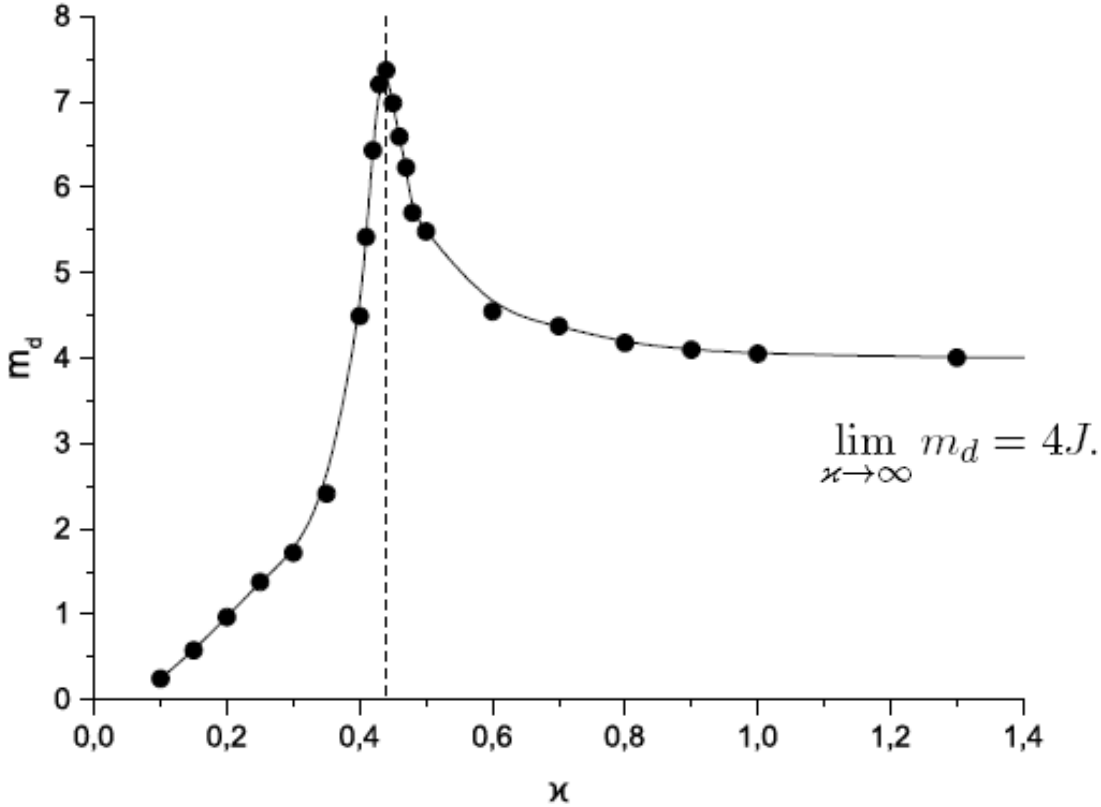
Subtraction procedure

MC of Ising model with defects

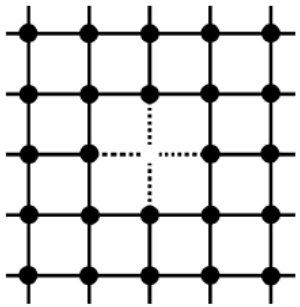


Mass of defect:

$$m_d = E_d - E_0,$$

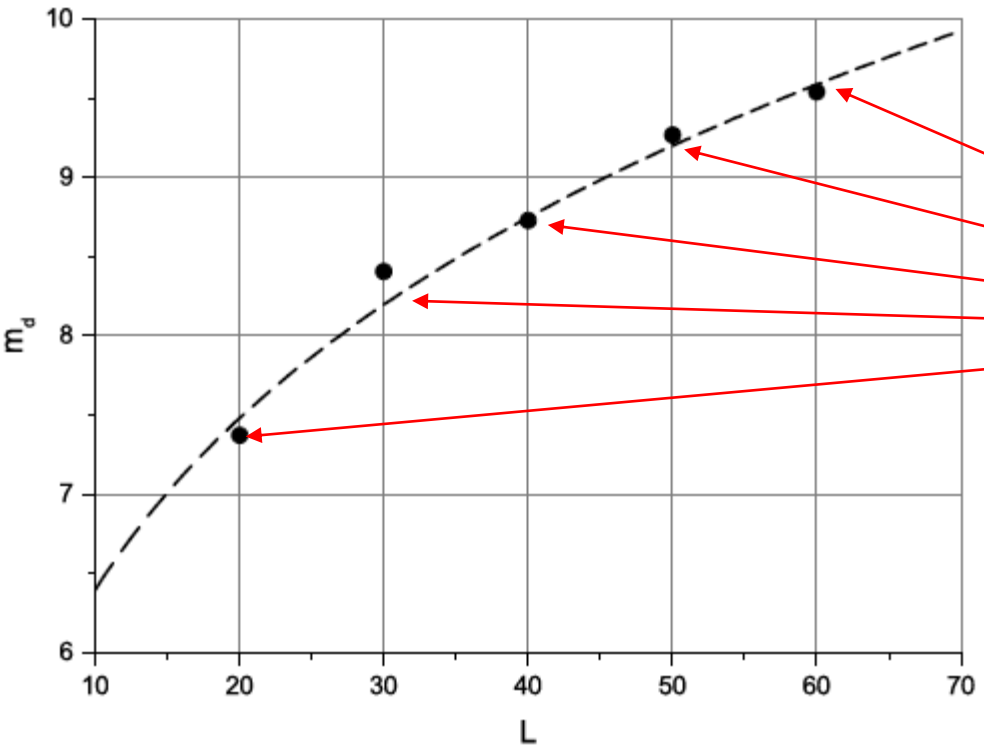


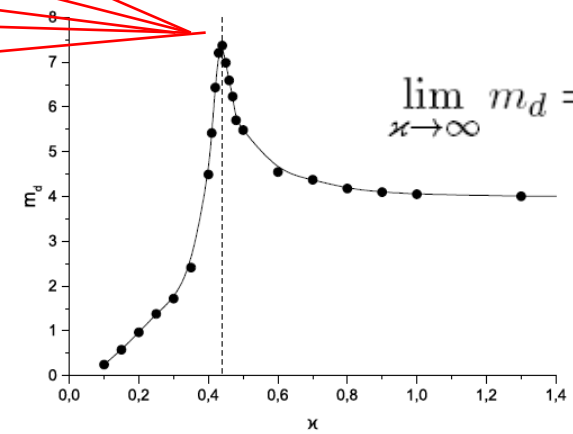
Mass of defect: volume dependence



Масса дефекта:

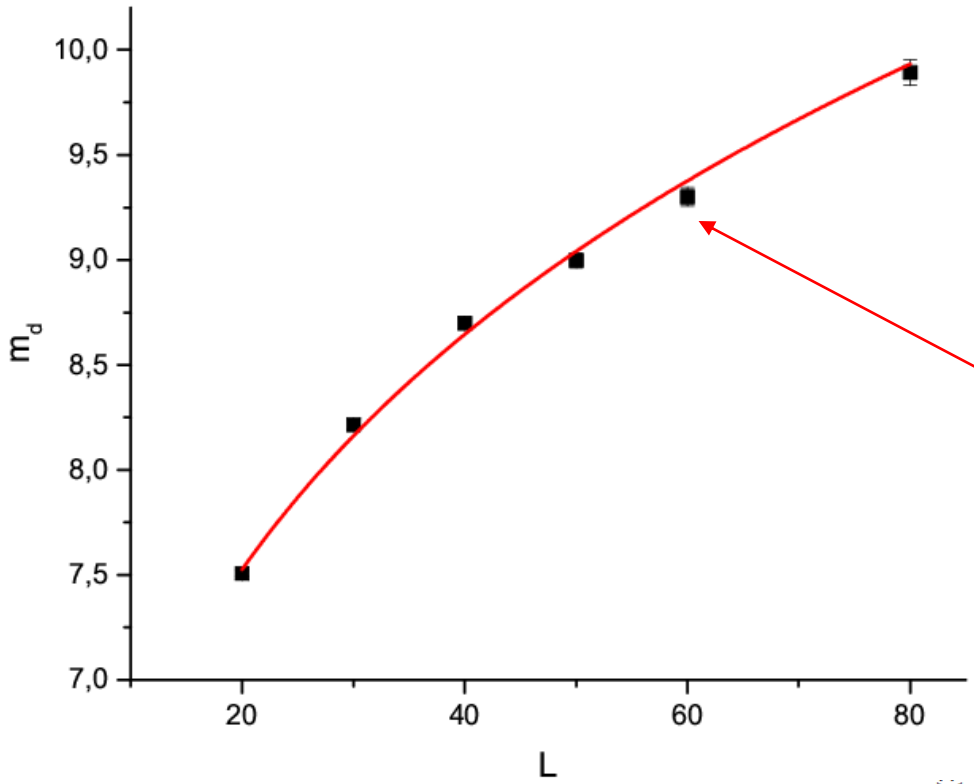
$$m_d = E_d - E_0,$$

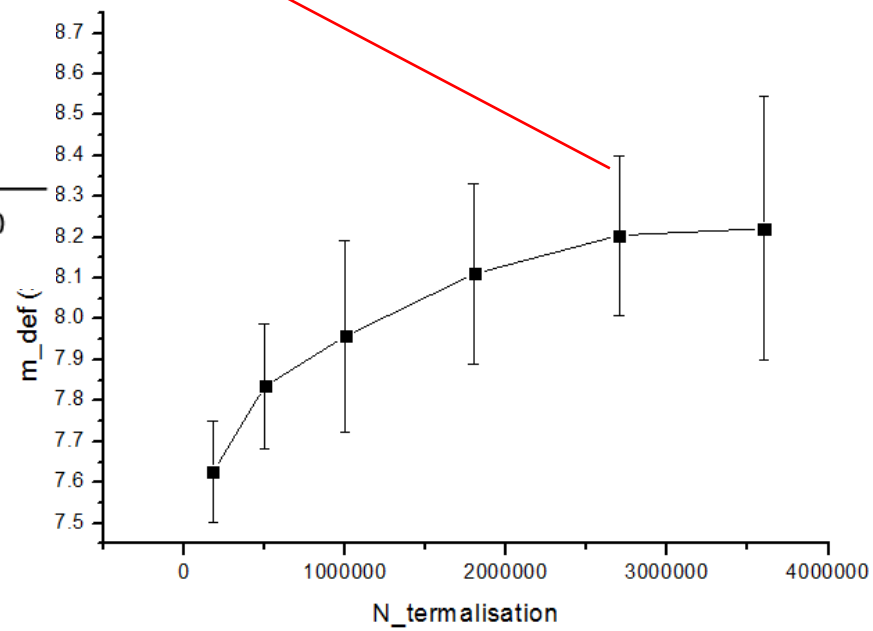




$$\lim_{\varkappa \to \infty} m_d = 4J.$$

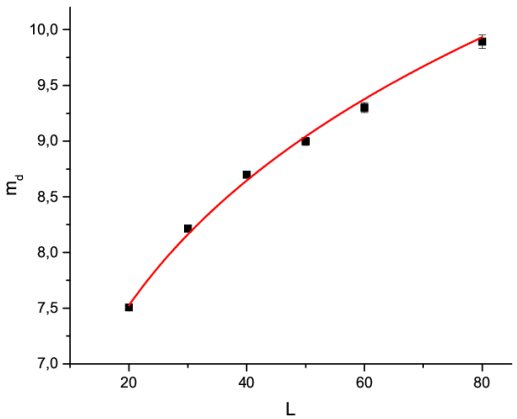
MC of defect mass: lattice volume dependence and thermalisation problems





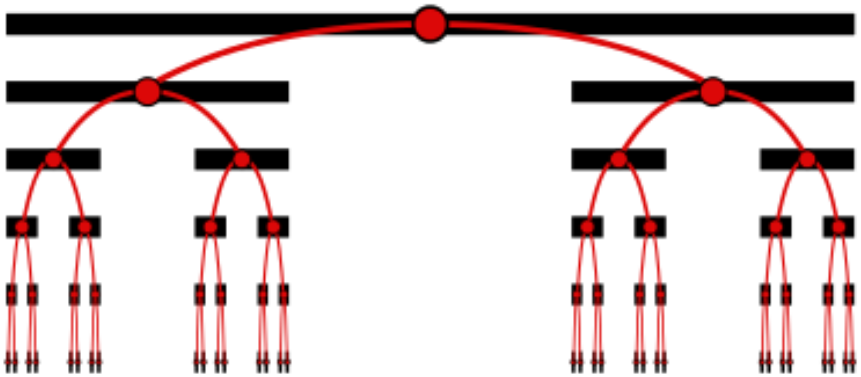
$$m_d^{\mathrm{cr}} = AL^n, \quad n \approx \frac{1}{5}$$

Defect in critical point: fractal dim object and Cantor set



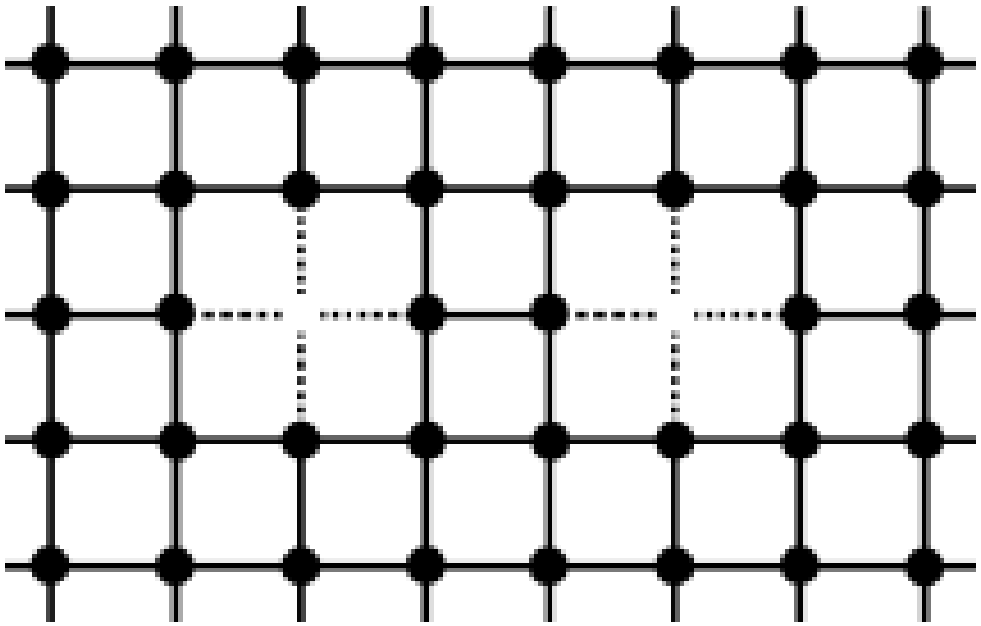
$$m_d^{\mathrm{cr}} = AL^n, \qquad n \approx \frac{1}{5}$$

Cantor set



Reflection in broken (fractal) mirror

Critical Casimir Forces between two defects



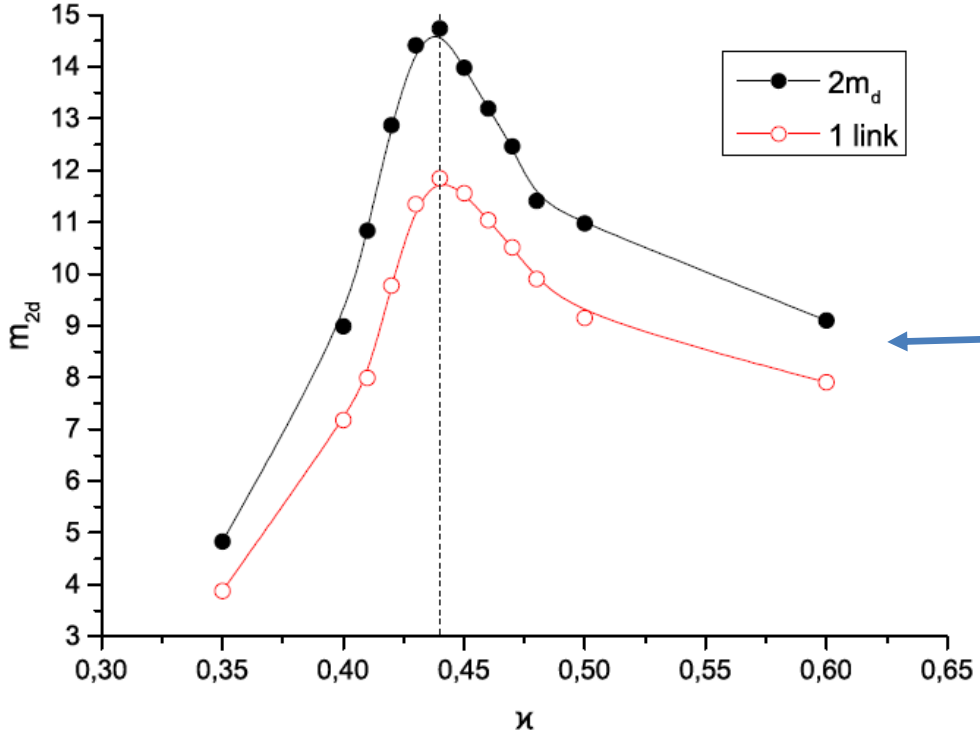
Two defects Bound Energy

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

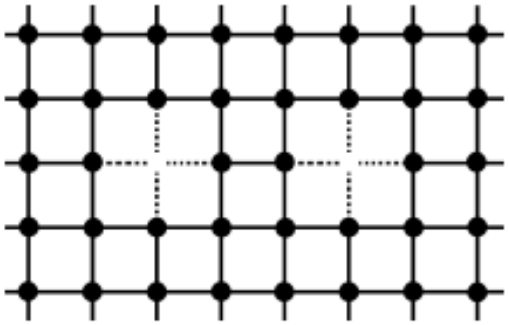
Subtraction procedure

Critical Casimir Forces between two defects

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



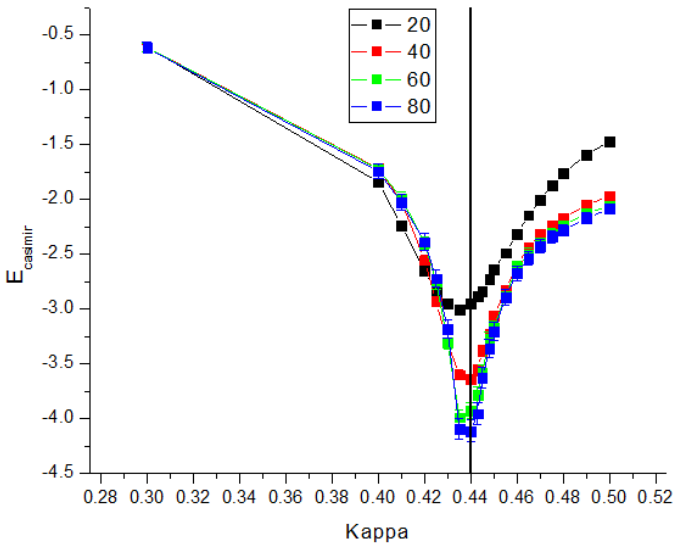
$m_{2d} < 2m_d$



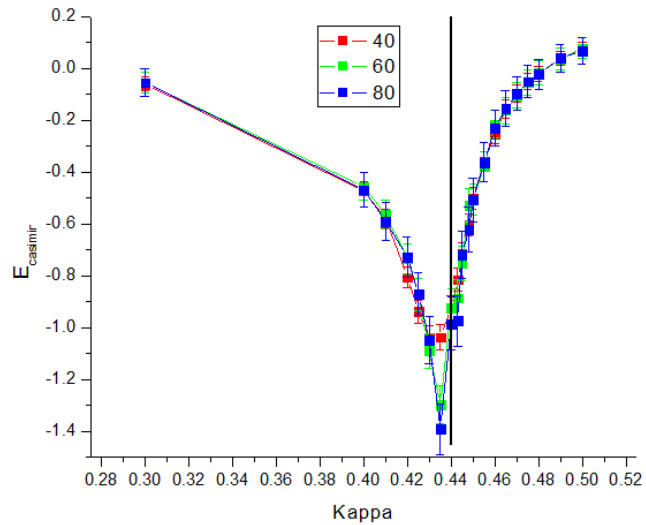
Critical Casimir Forces between two defects

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

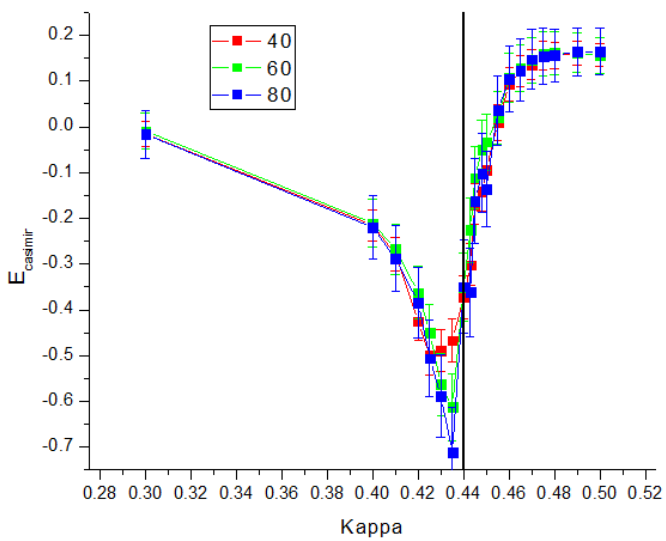
Dist. between def's = 1

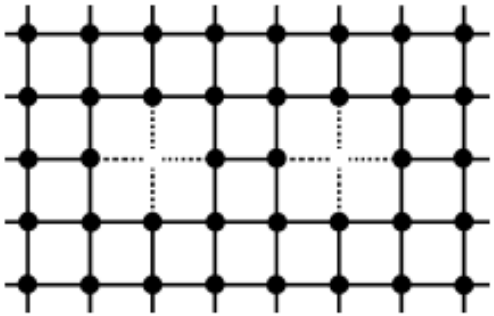


Dist. between def's = 2



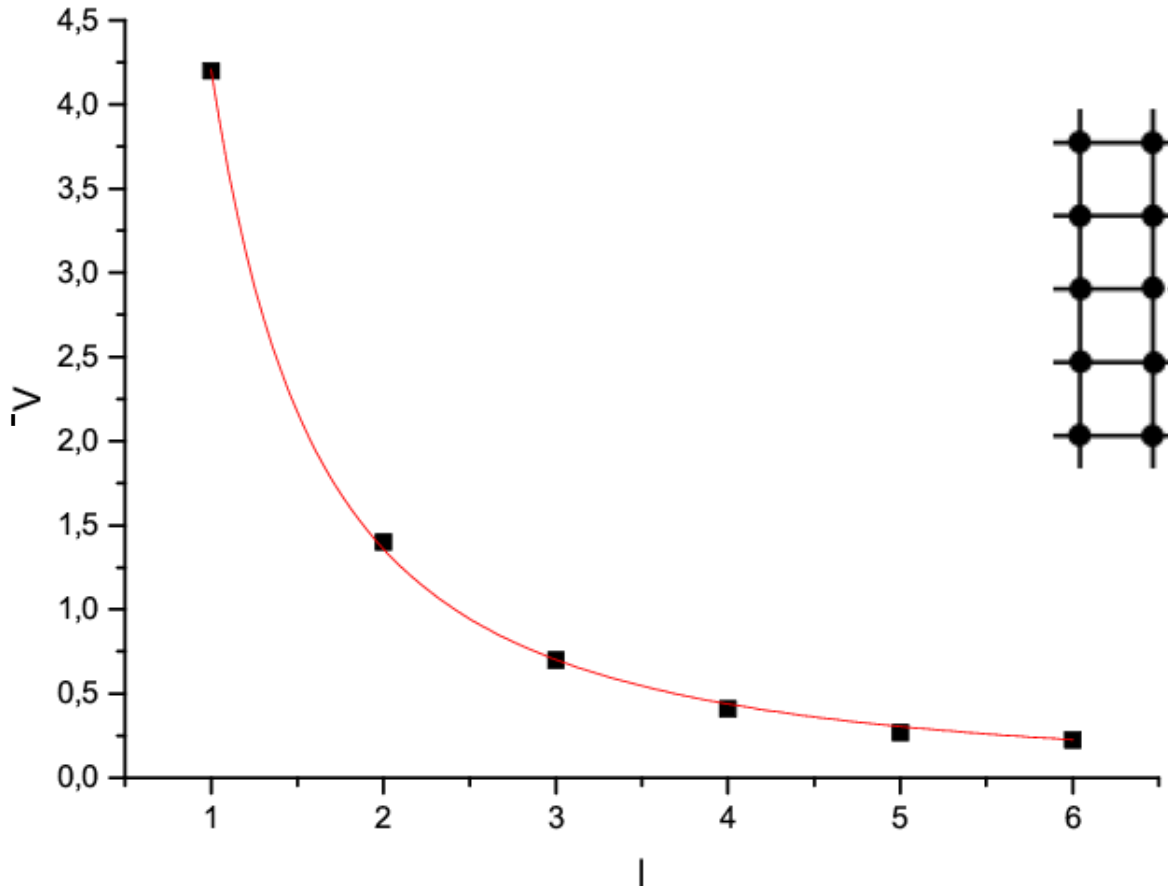
Dist. between def's = 3

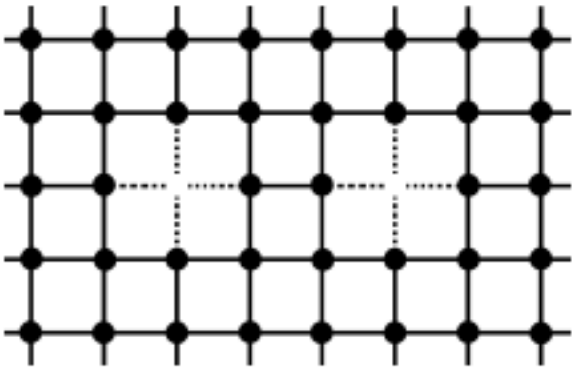




Critical Casimir Forces between two defects

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

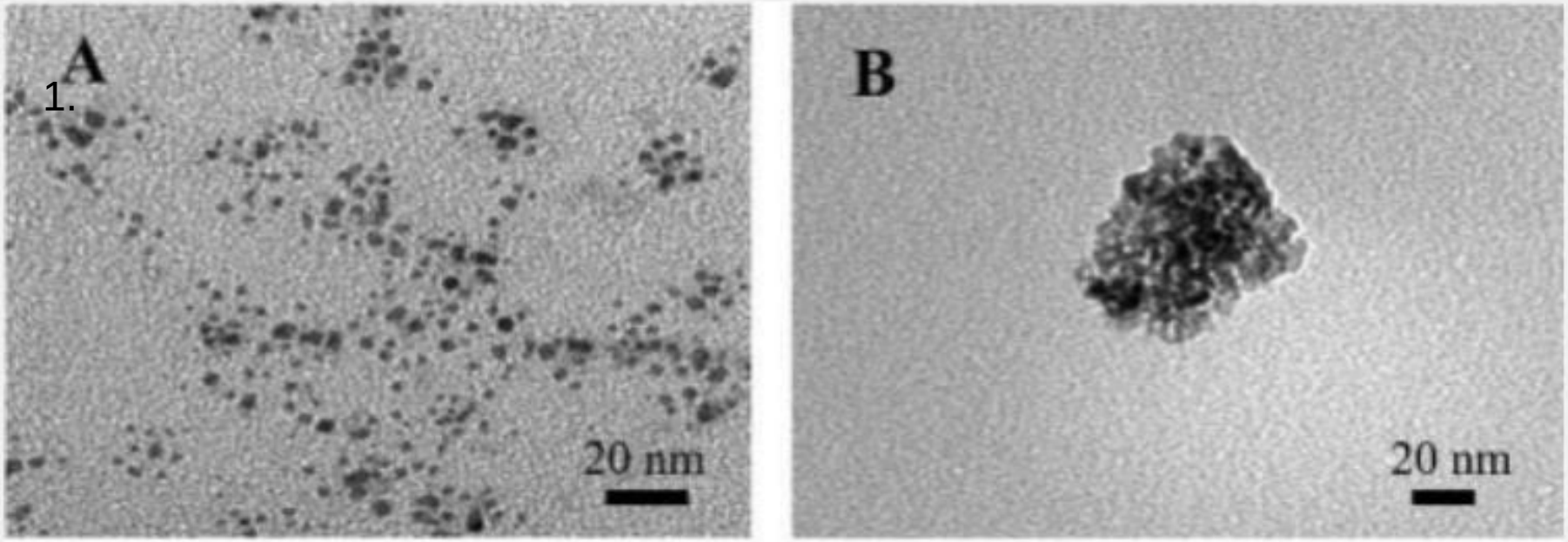




$$F(l) \sim \frac{1}{l^3}$$

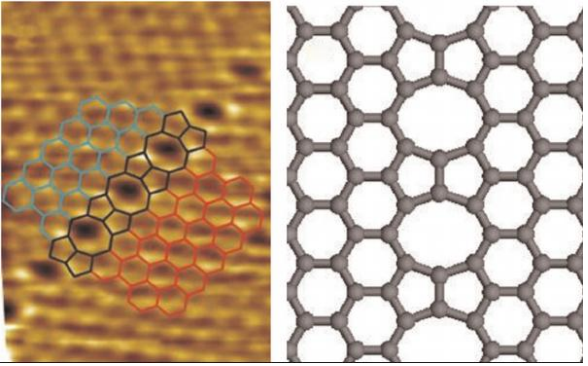
P. Nowakowski, A. Maciolek, S. Dietrich,
Critical Casimir forces between defects in the 2D Ising model,
J. Phys. A: Mathematical and Theoretical, **49**, 48 (2016)

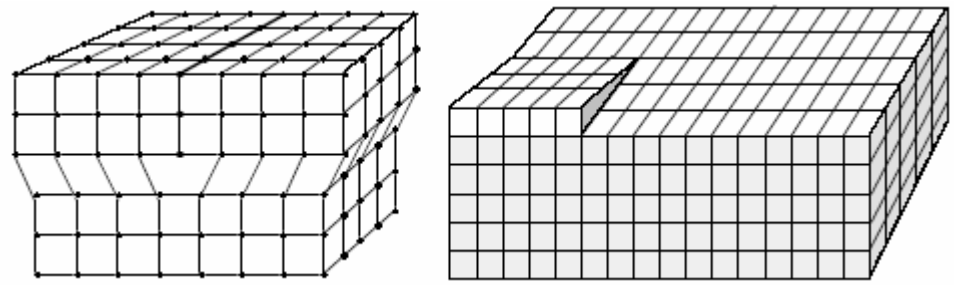
Defects aggregation



Dispersed nanoparticles

Aggregated nanoparticles





Critical Casimir Effect in defect lines

Critical Casimir Effect: BioPhysics Applications

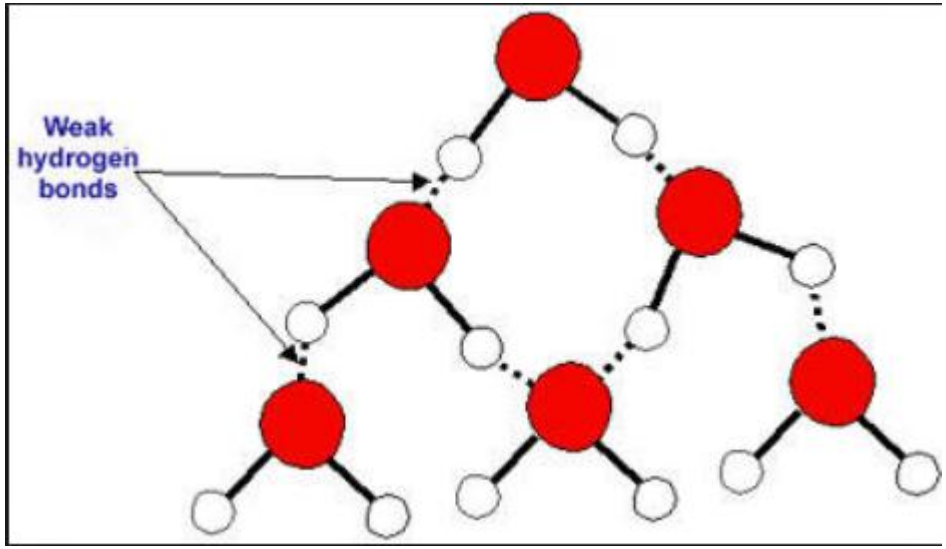
Biological processes in a medium of polarized molecules:

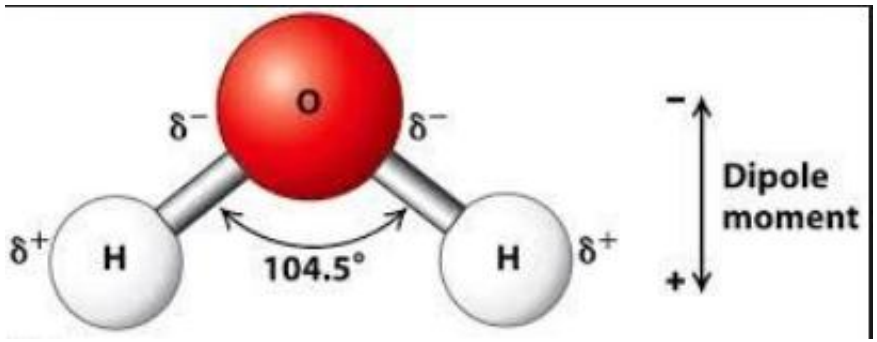
- Protein folding
- Cell membranes formation and lipid rafts
- Biological catalyst
- …

Critical Casimir Effect: BioMedical Application

1. Global protein structure formation

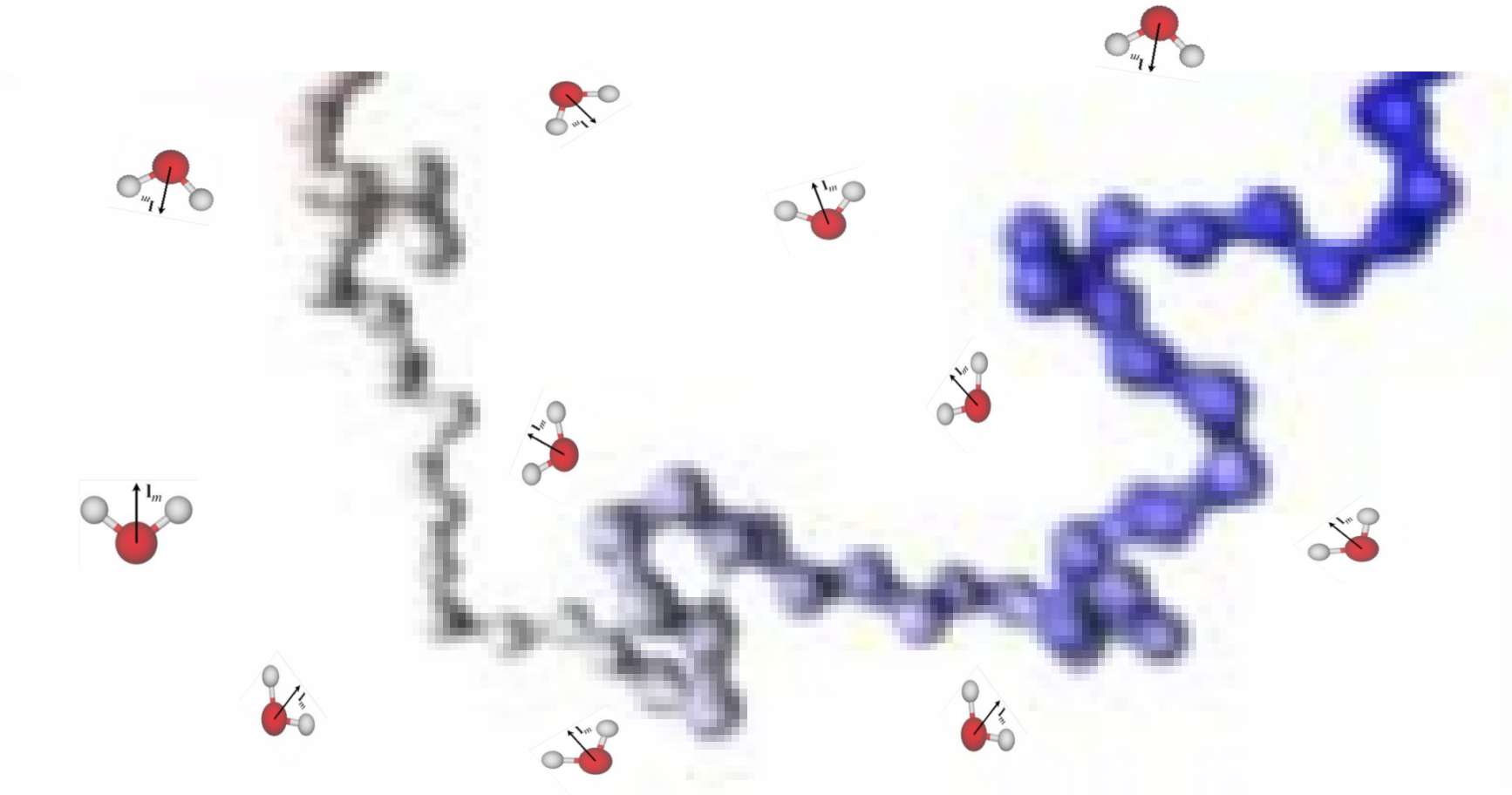
We have to take into account medium in which the protein folding is taken place.





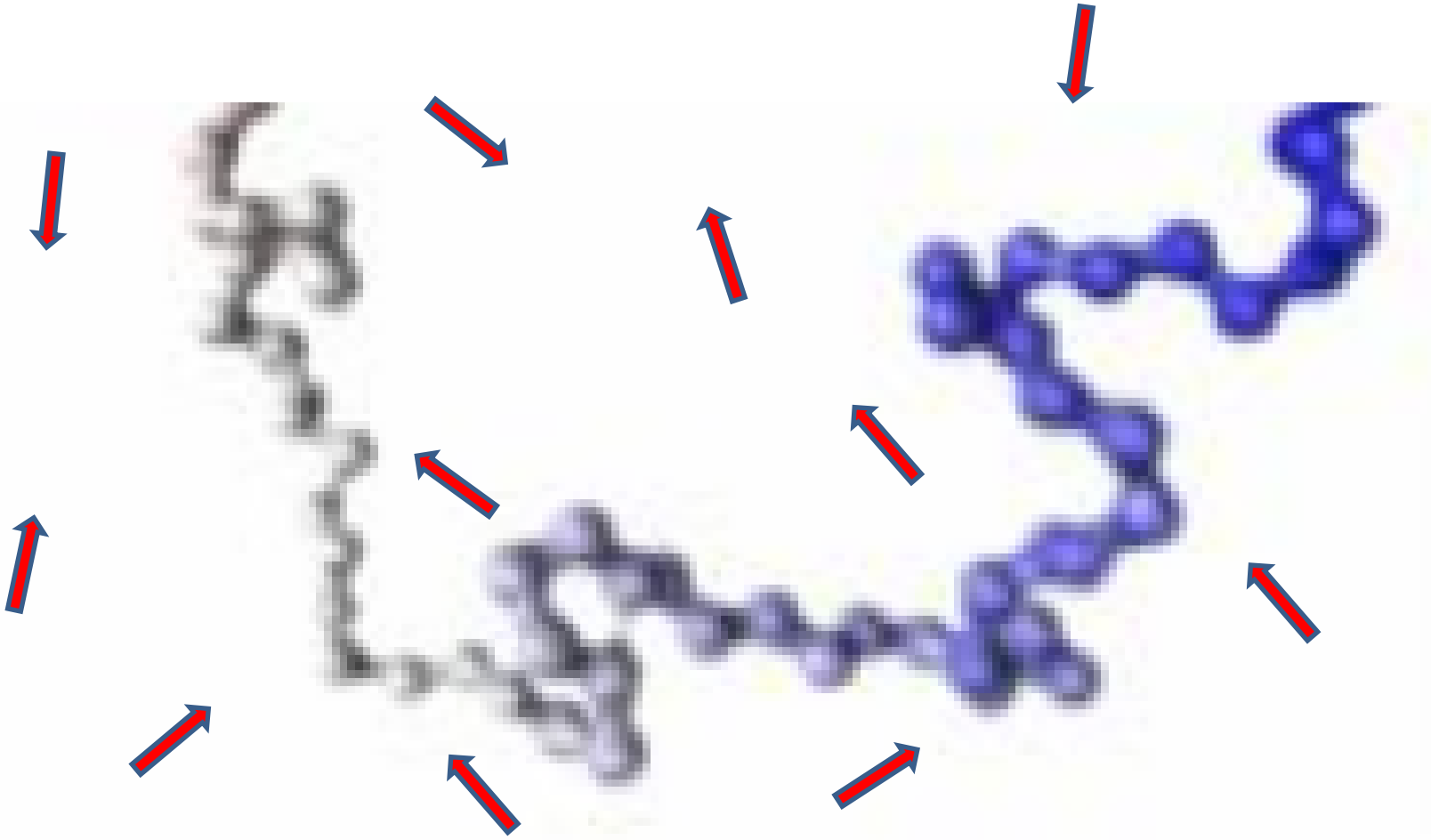
Critical Casimir Effect: BioMedical Application

1. Global protein structure formation



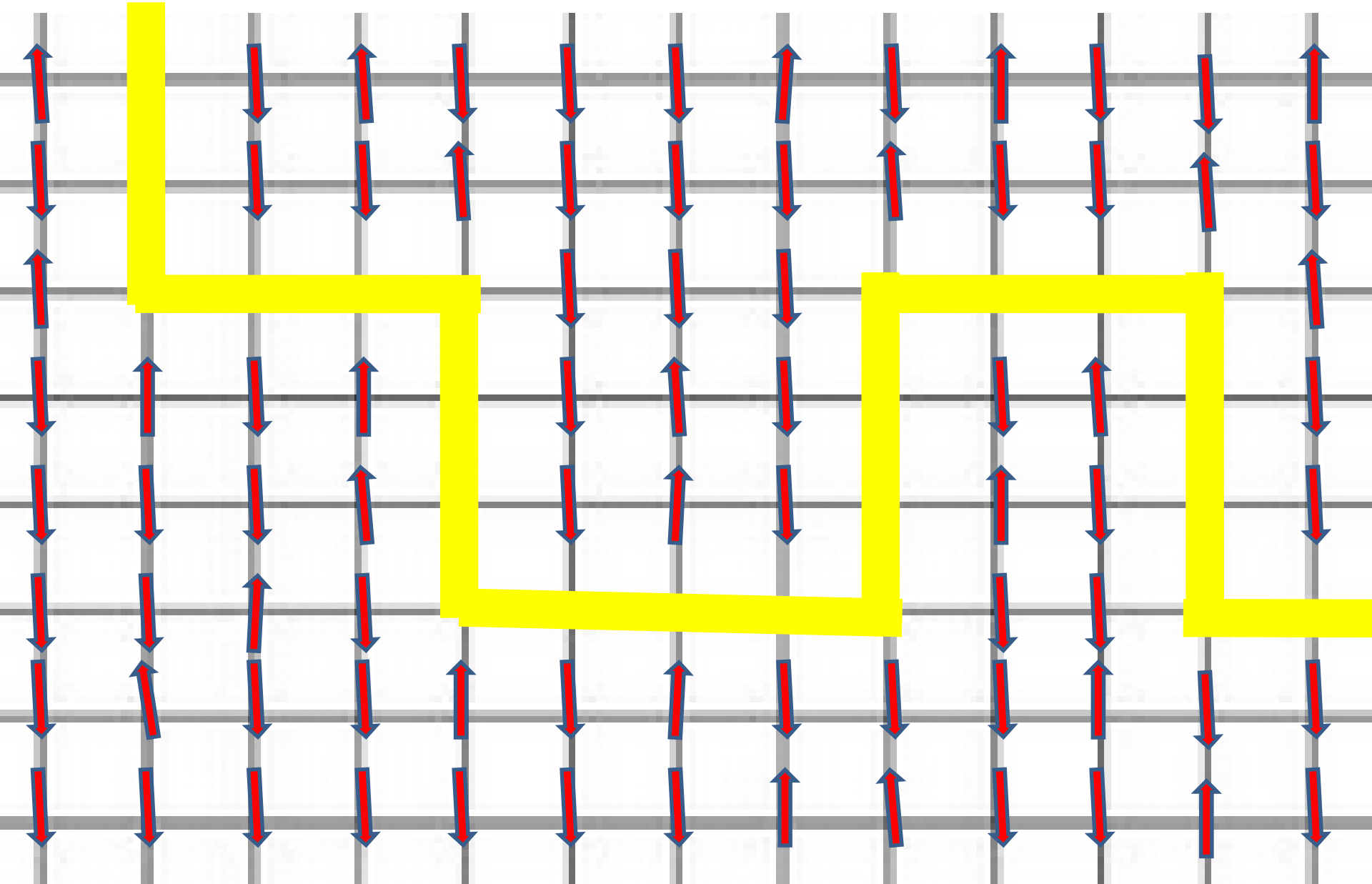
Critical Casimir Effect: BioMedical Application

1. Global protein structure formation

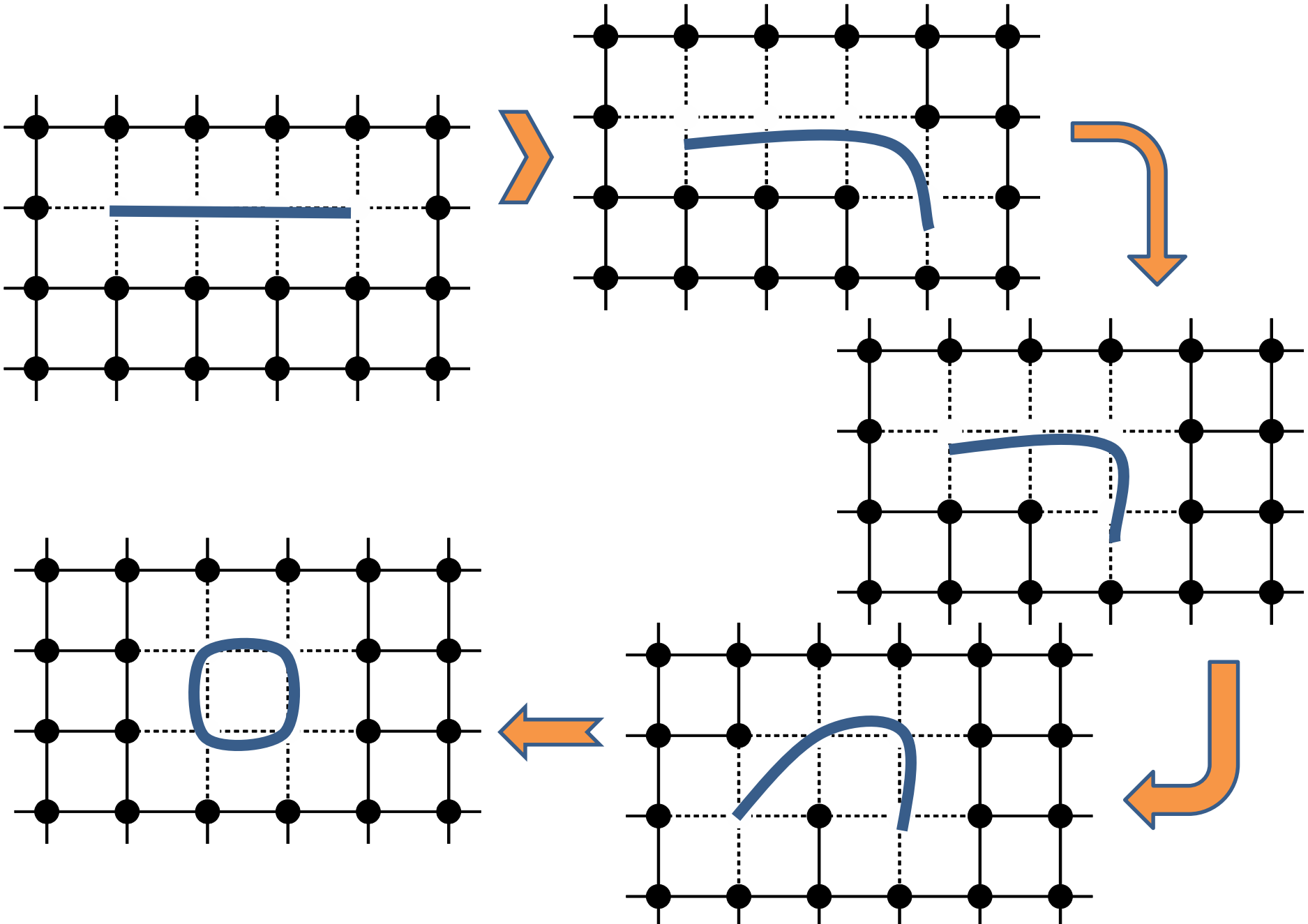


Critical Casimir Effect: BioMedical Application

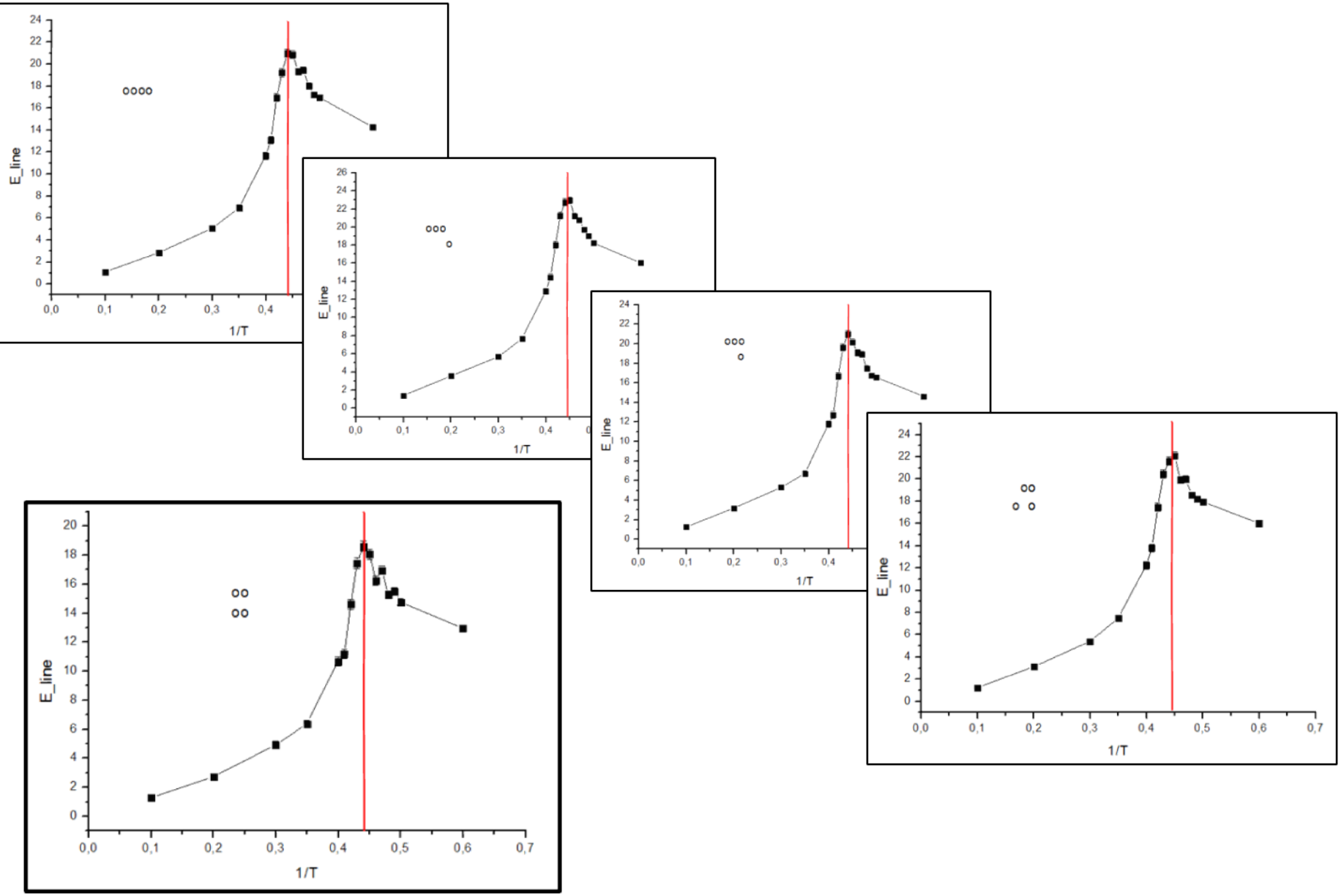
Discretization of the Model

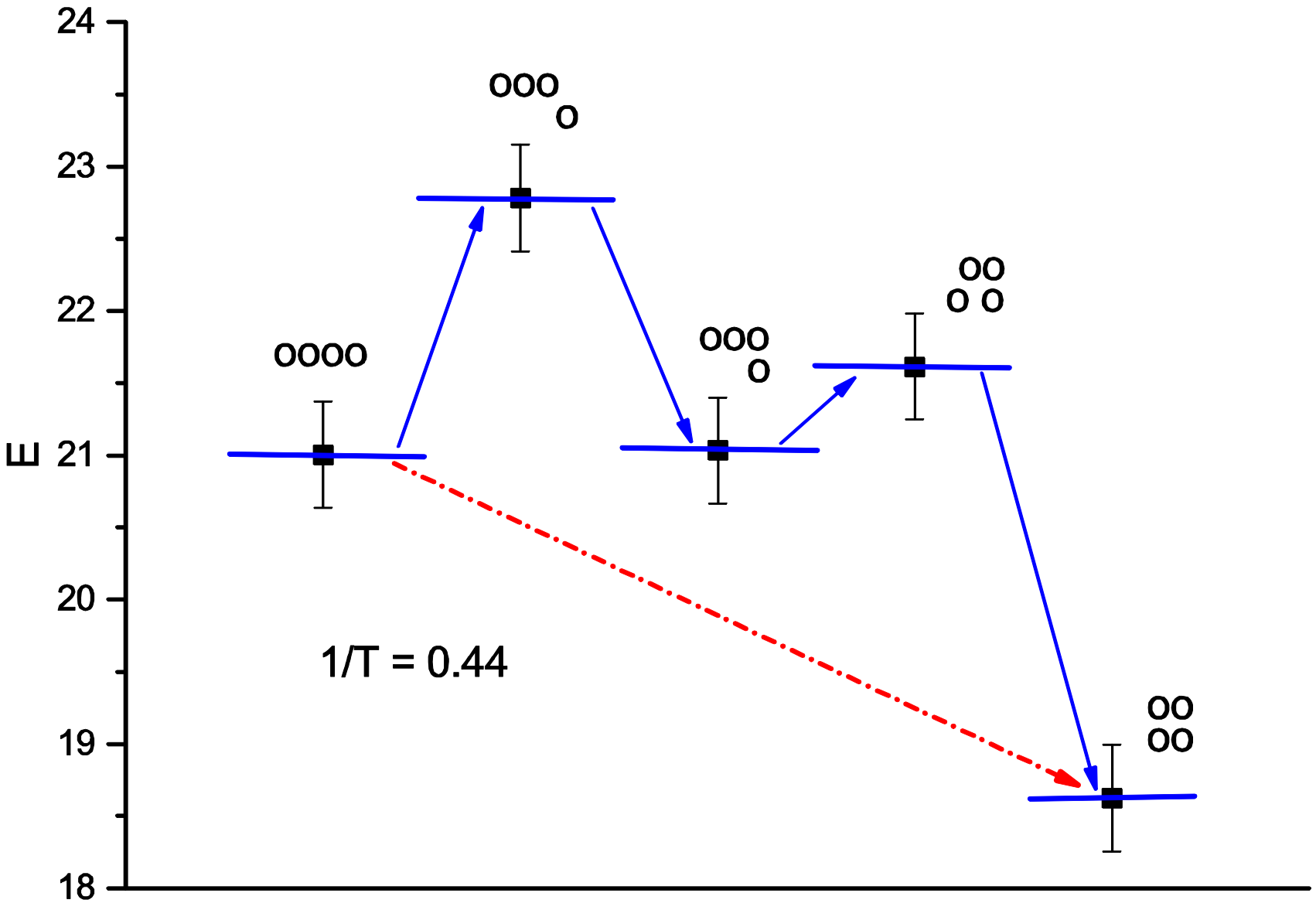


Simple example: collapse of 4 defects line

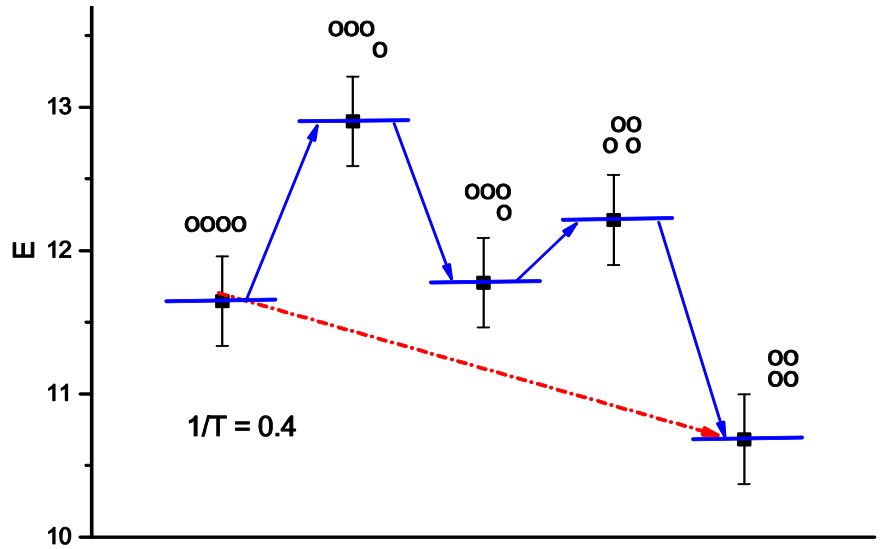


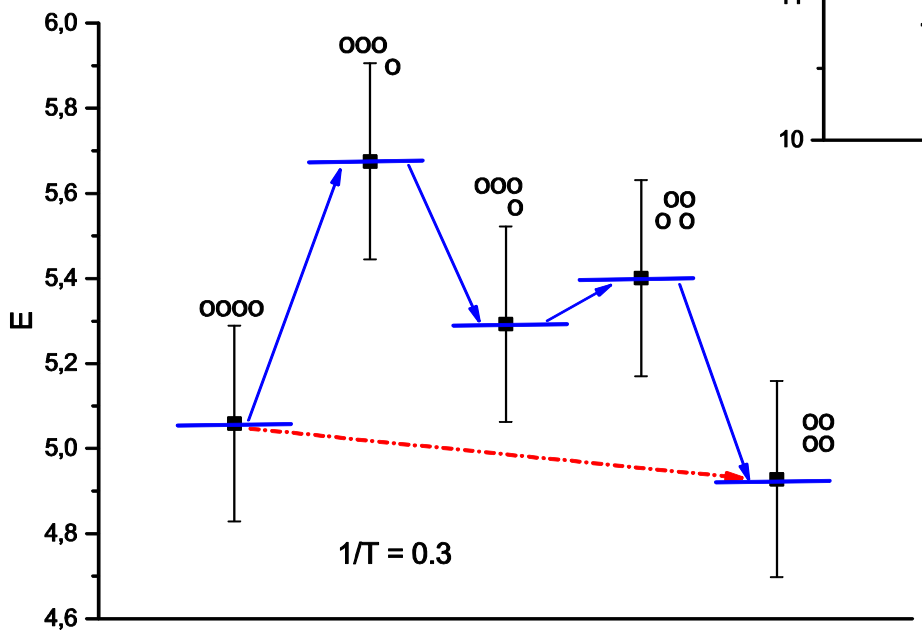
Defects aggregation - small line



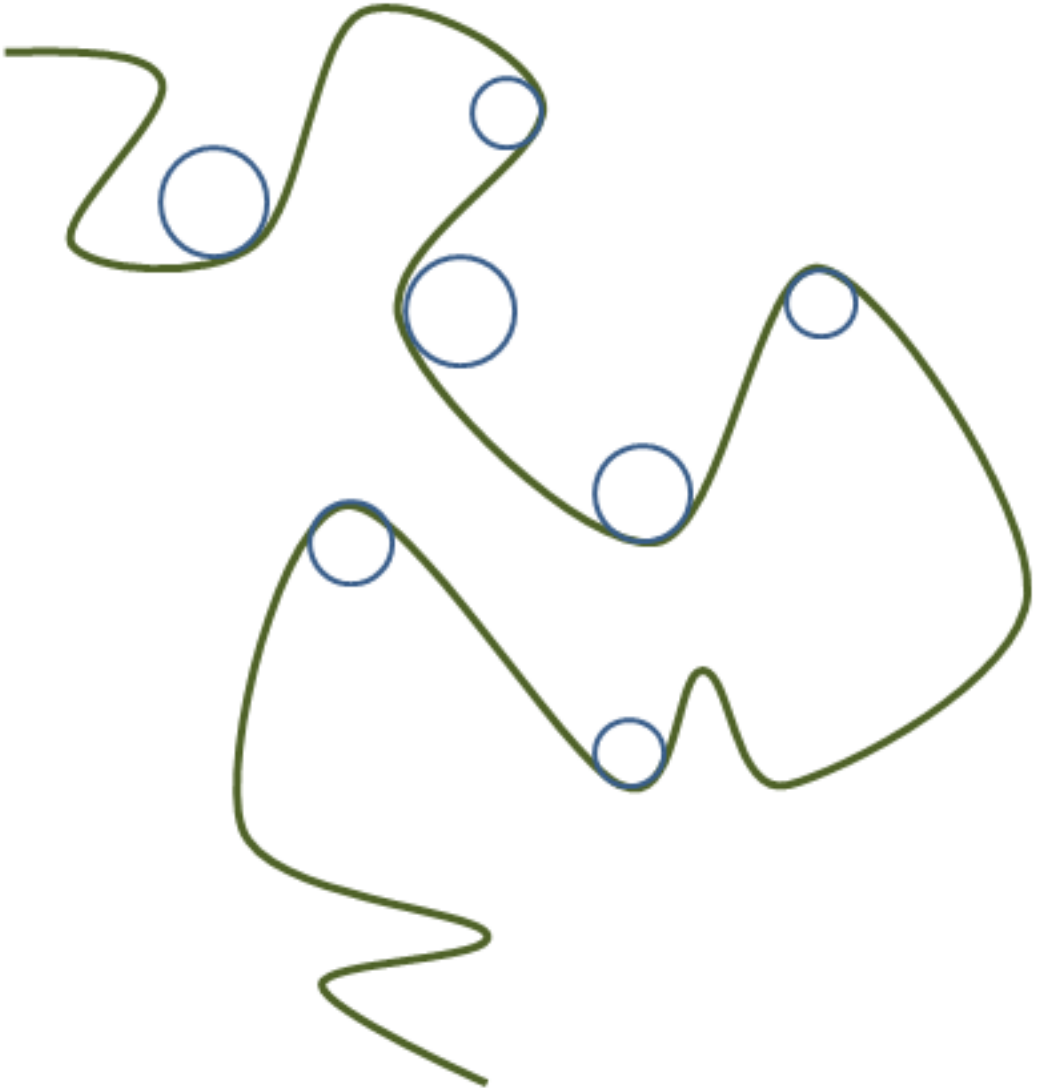

24
23
22
21
20
19
18
E
OOOO
OOO
O
OOO
O
OO
O O
OO
OO
1/T = 0.44

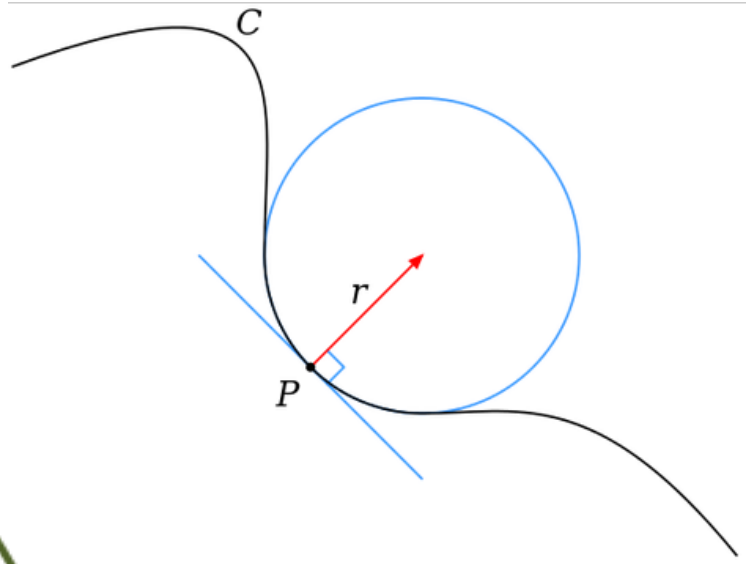
$1/T$	E
0.3	0.13
0.4	0.96
0.44	2.38

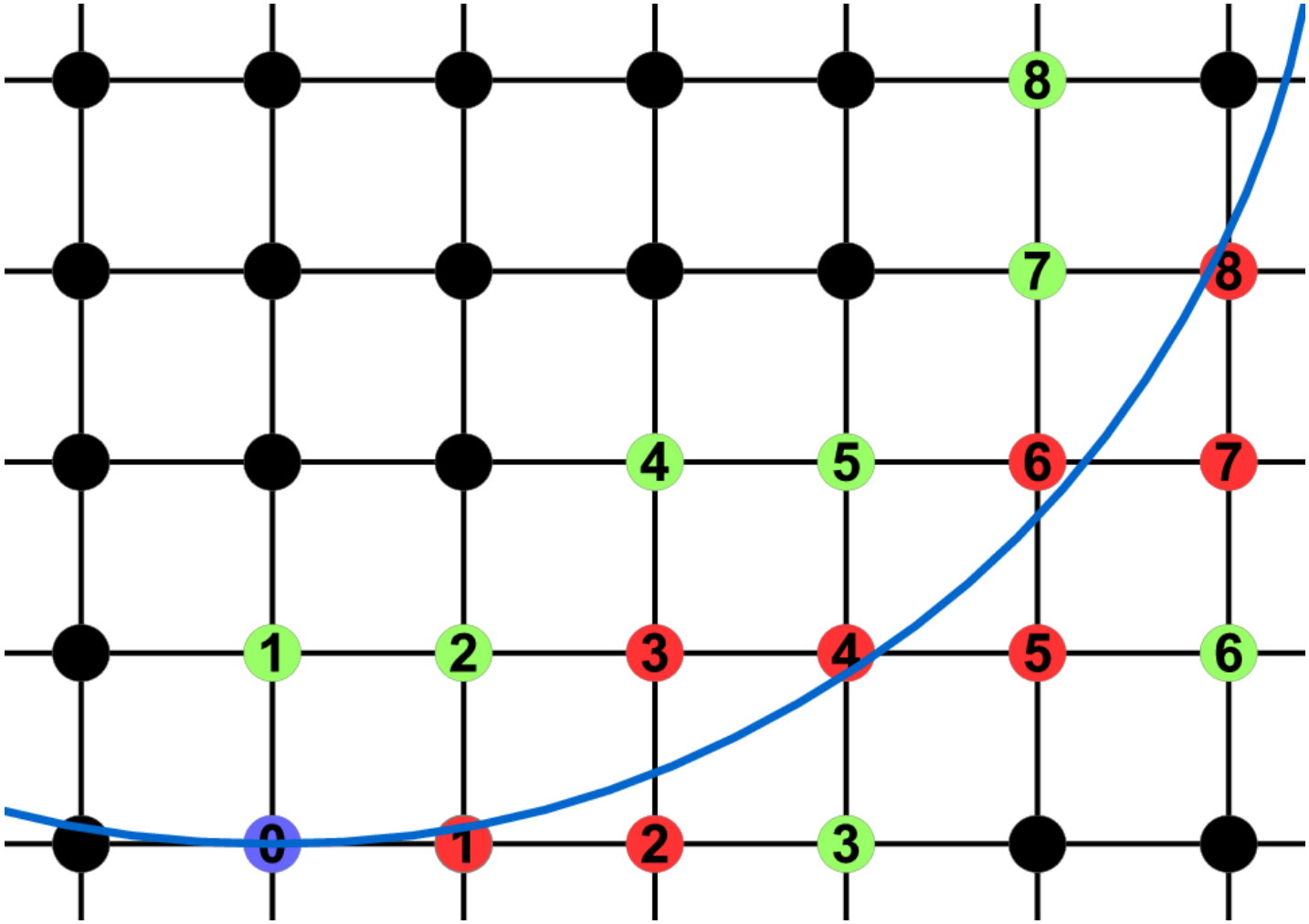


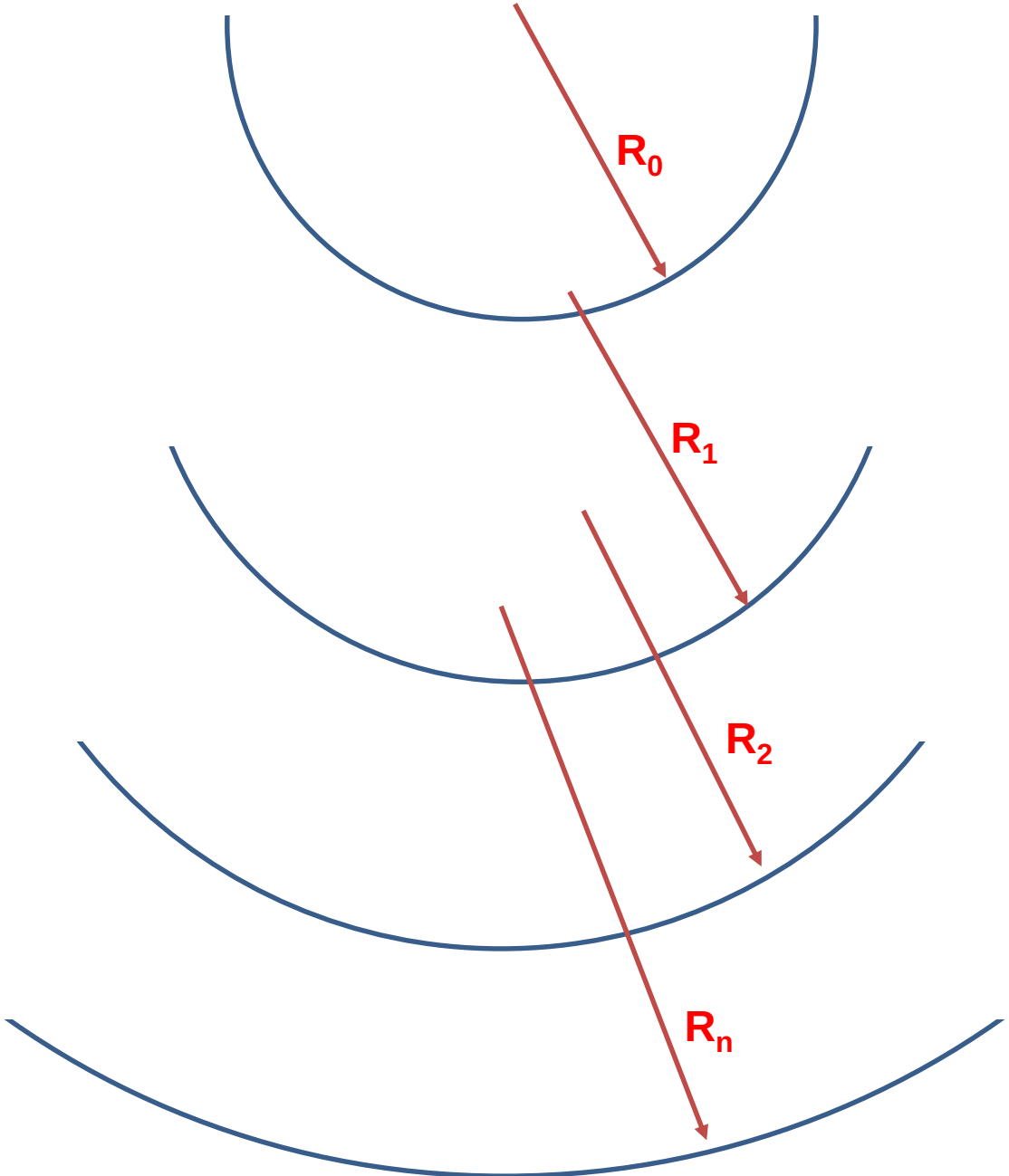


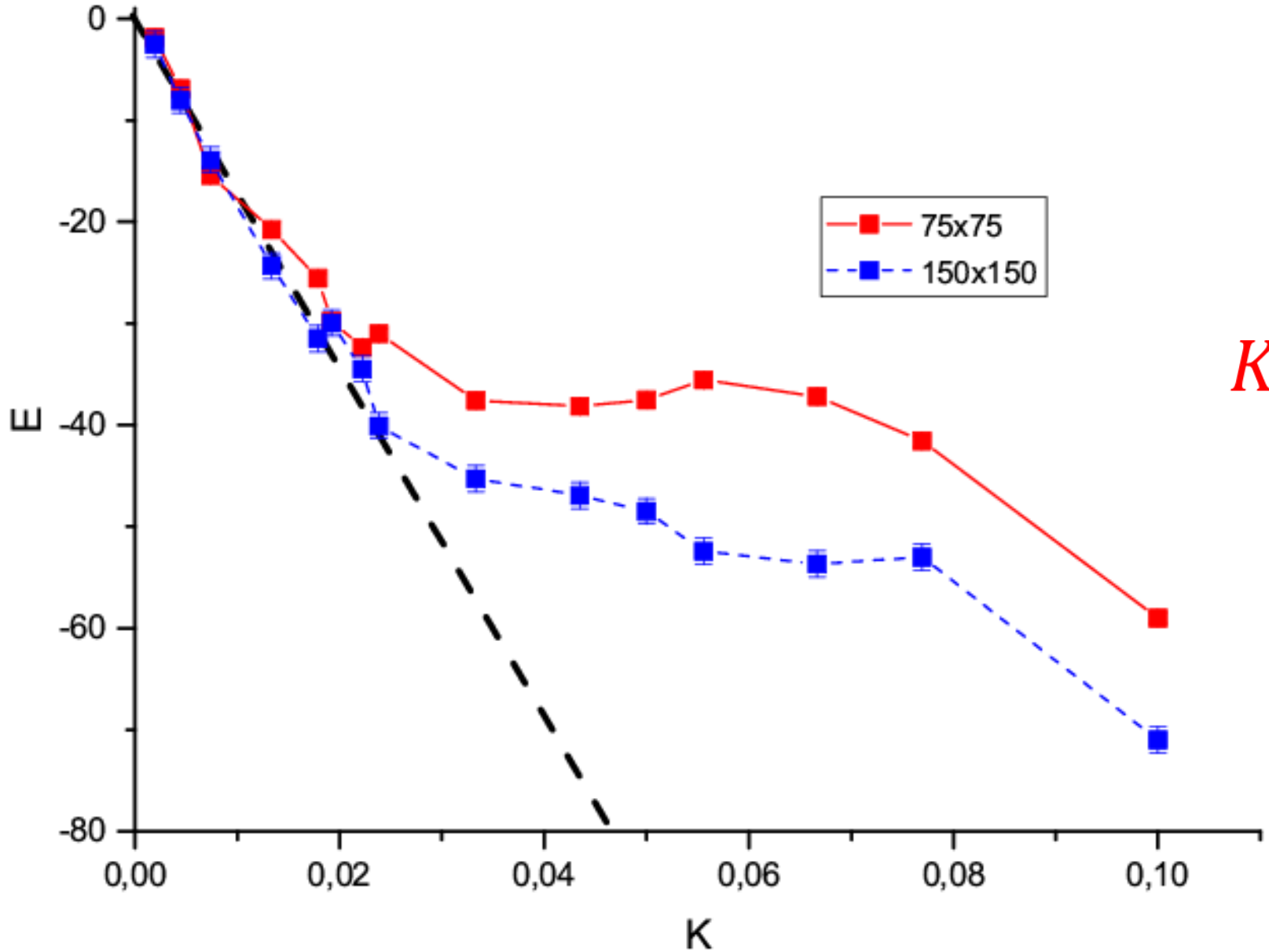
Elasticity of defect curves



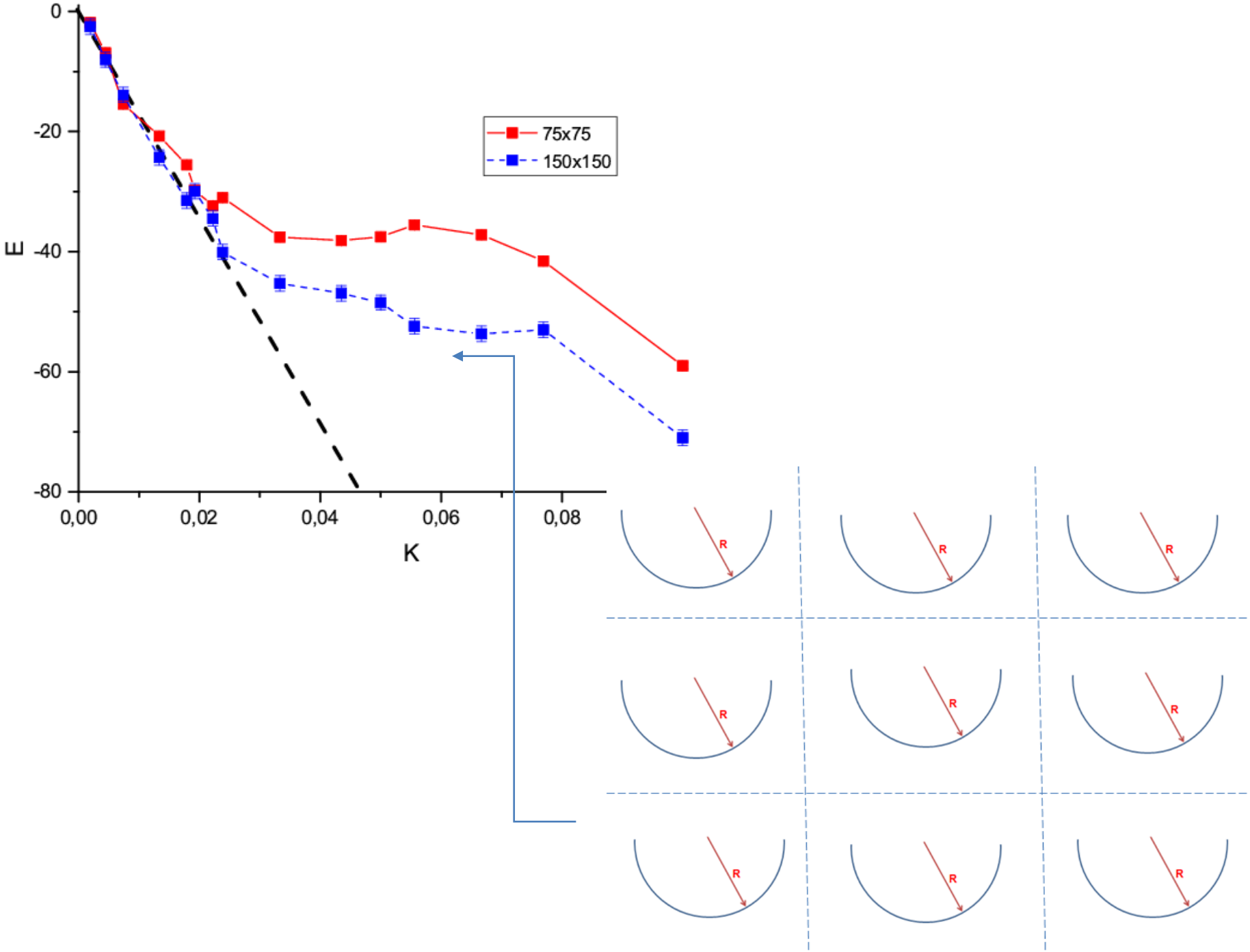


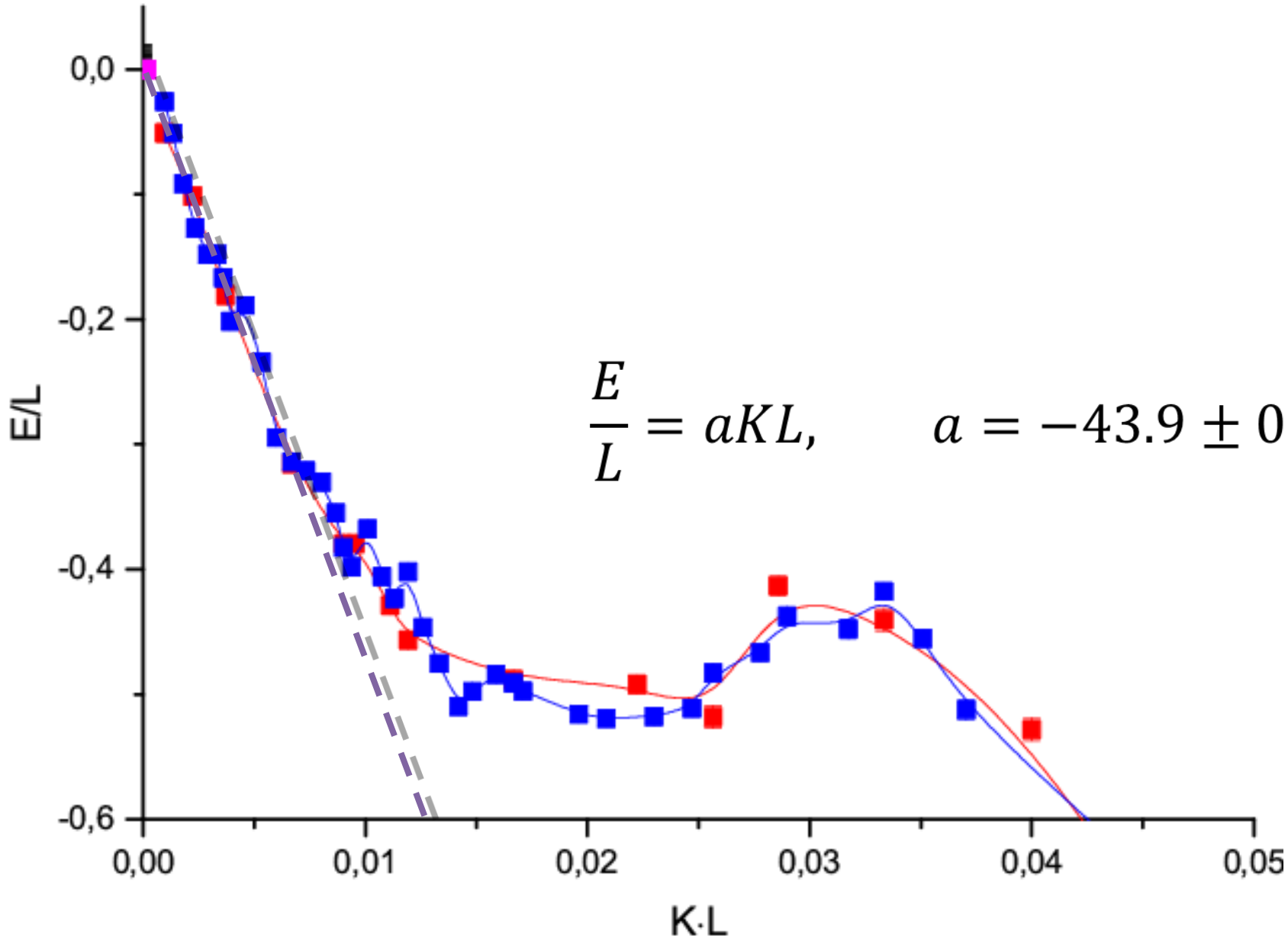

8
7
8
4
5
6
7
1
2
3
4
5
6
0
1
2
3


R_0
R_1
R_2
R_n



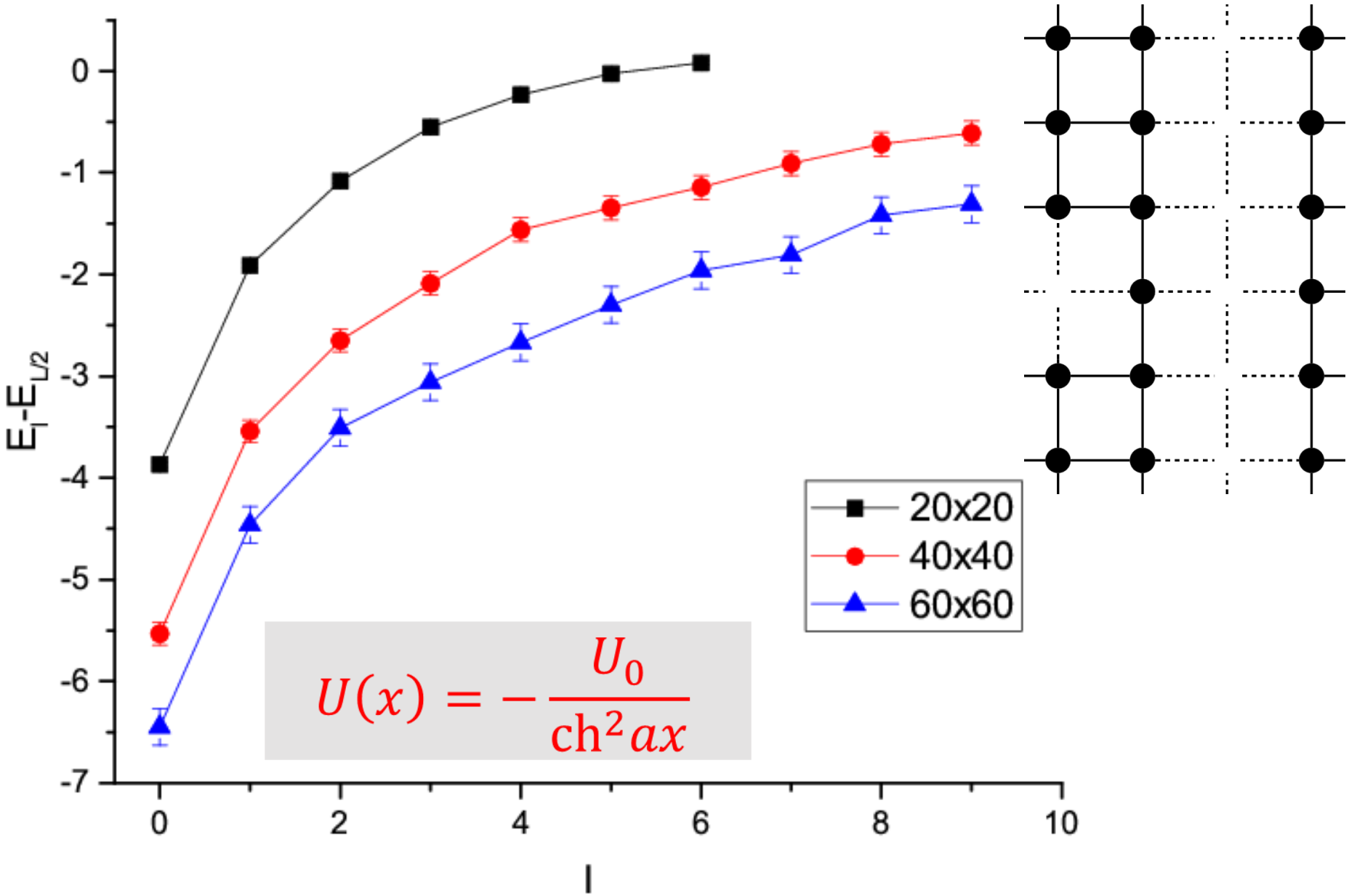
$$K = \frac{1}{R}$$


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



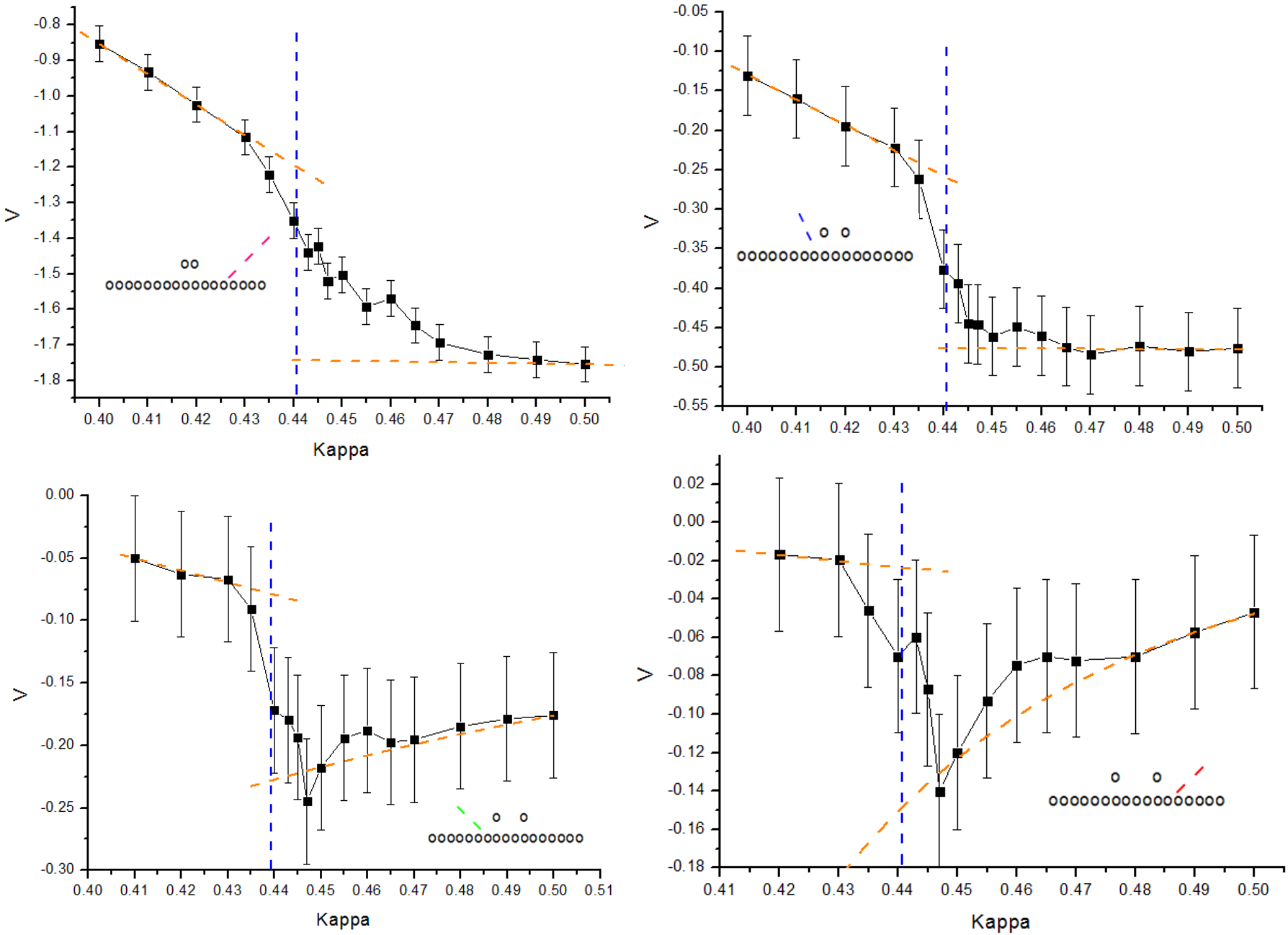
$$\frac{E}{L} = aKL, \qquad a = -43.9 \pm 0.9$$

Defect Confinement on Defect line

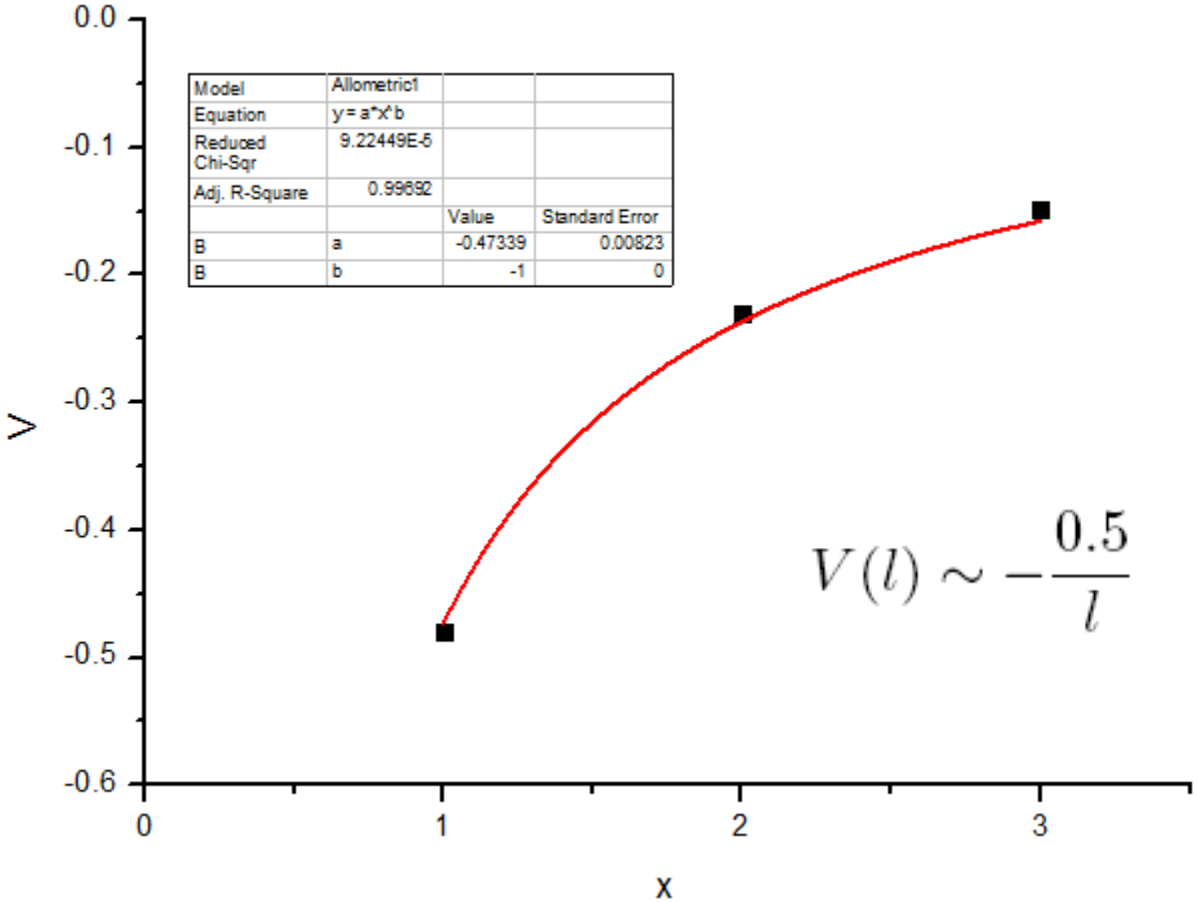

0
-1
-2
-3
-4
-5
-6
-7
E_l-$E_{L/2}$
0
2
4
6
8
10
l
20x20
40x40
60x60
$U(x) = -\frac{U_0}{\mathrm{ch}^2 ax}$

Two Defects on the defect line

Two defects on the defect line



Two defects on the defect line
Interaction potential

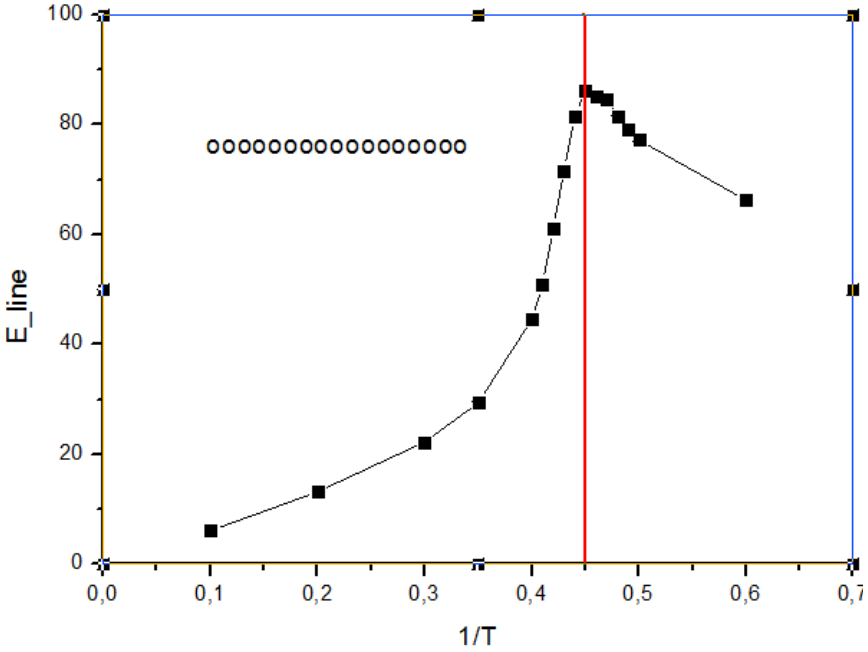


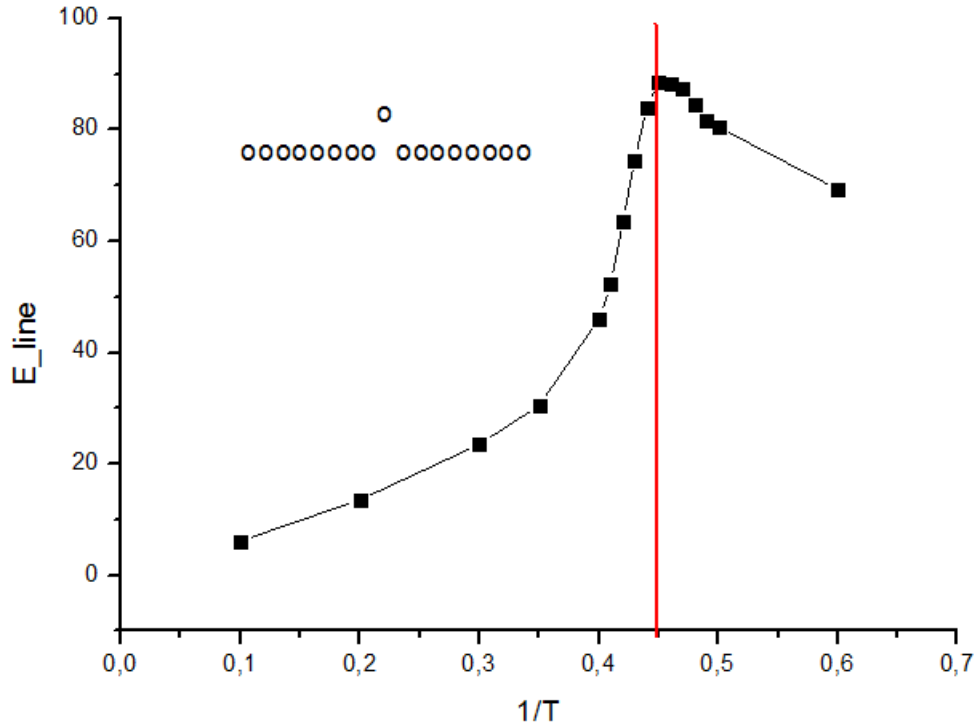
Model	Allometric1		
Equation	y = a*x^b		
Reduced Chi-Sqr	9.22449E-5		
Adj. R-Square	0.99692		
		Value	Standard Error
B	a	-0.47339	0.00823
B	b	-1	0

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

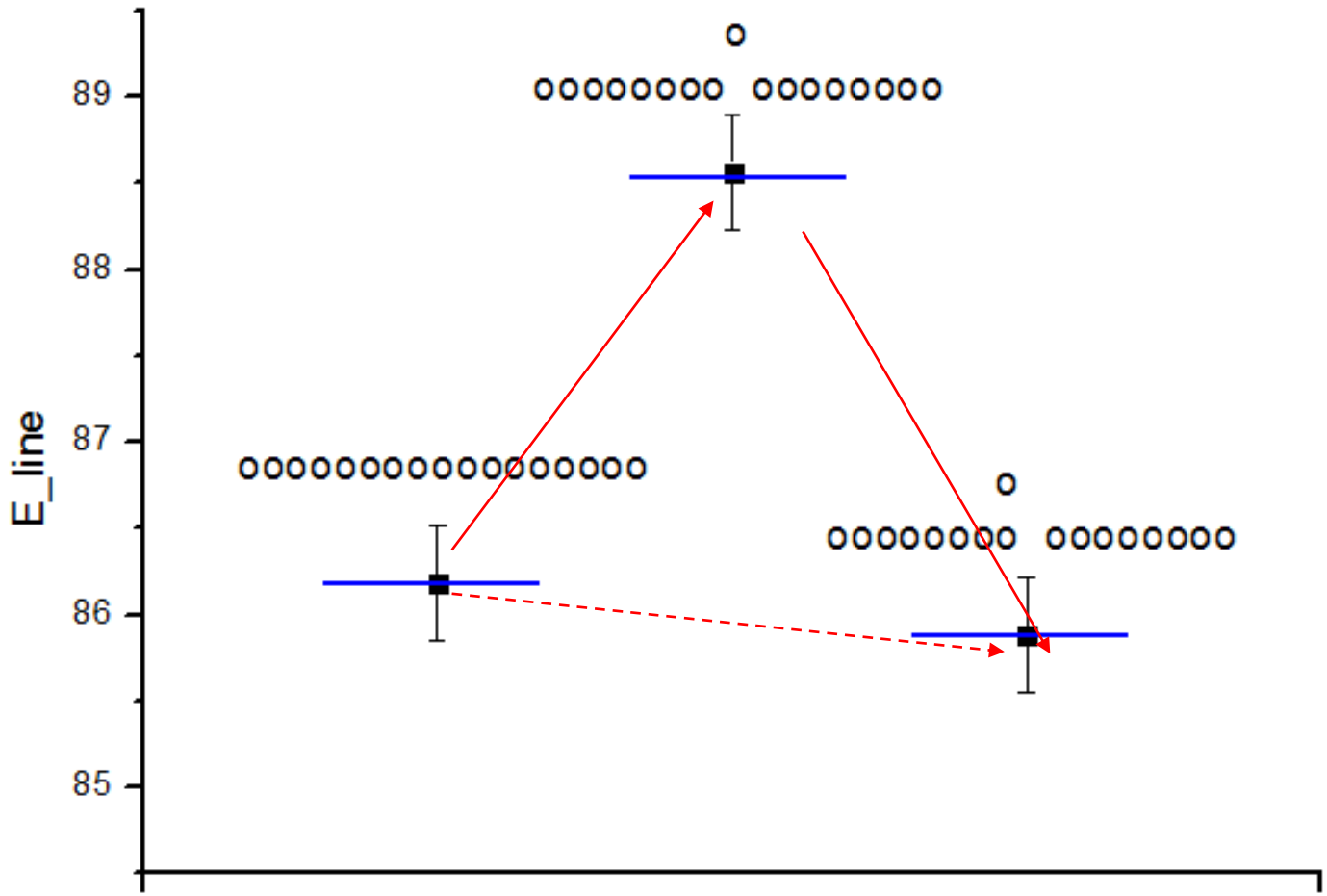
Defect – Anti-Defect pier creation

Defects aggregation - global line.
Def – AntiDef pier creation

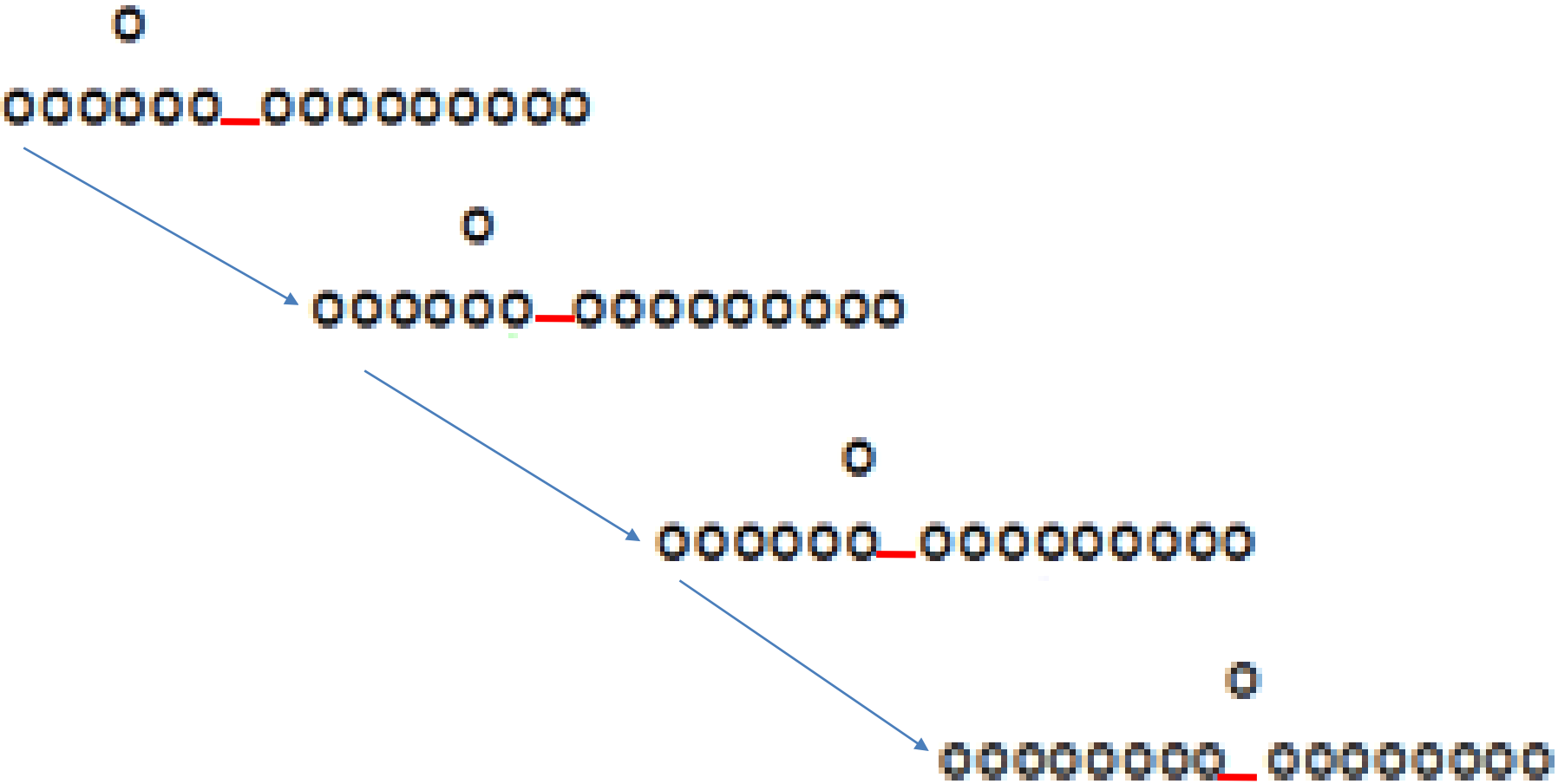




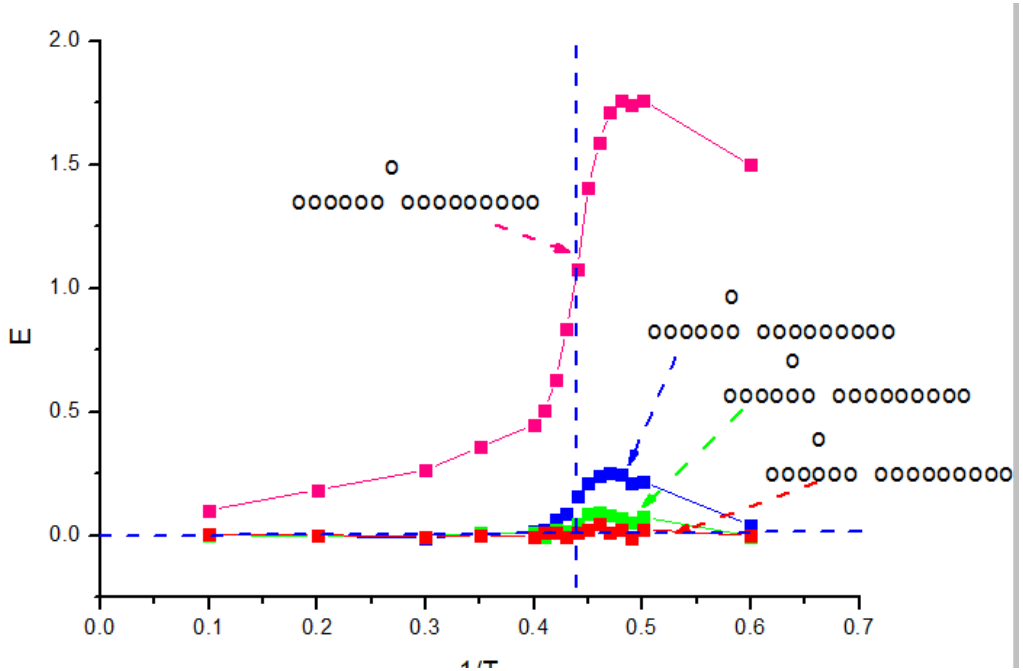
Defects aggregation - Def – AntiDef pier creation

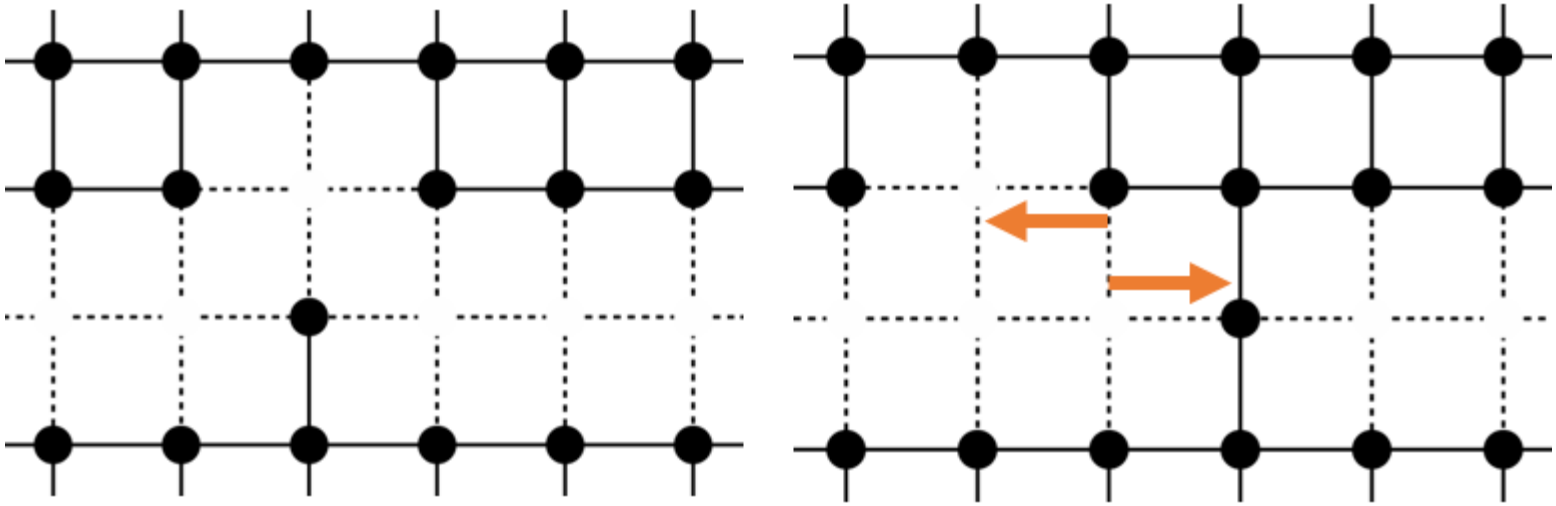


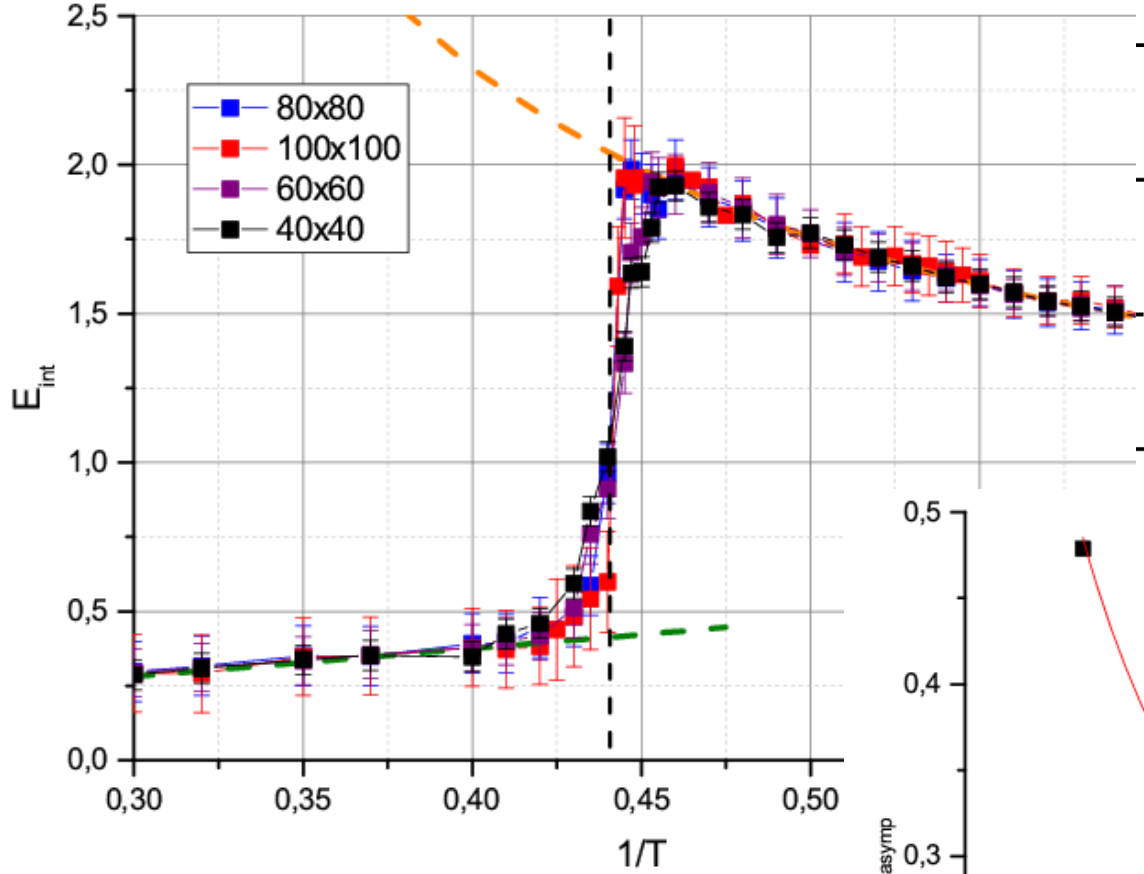
Defect – Anti-Defect intraction

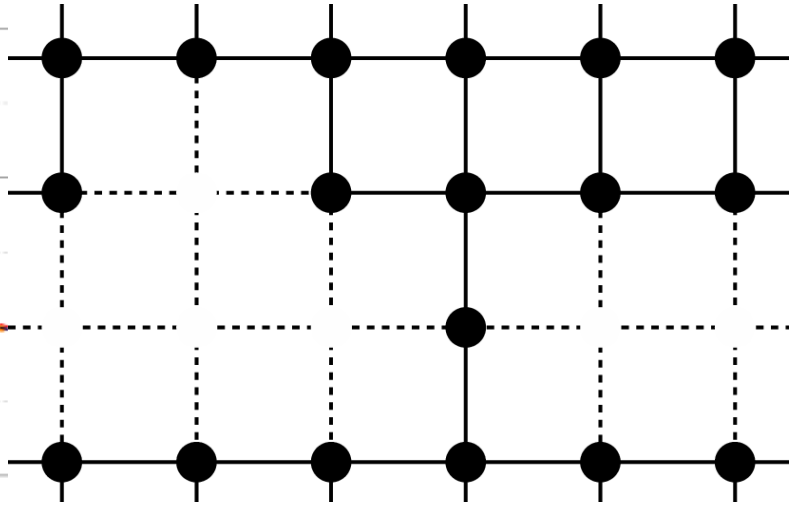


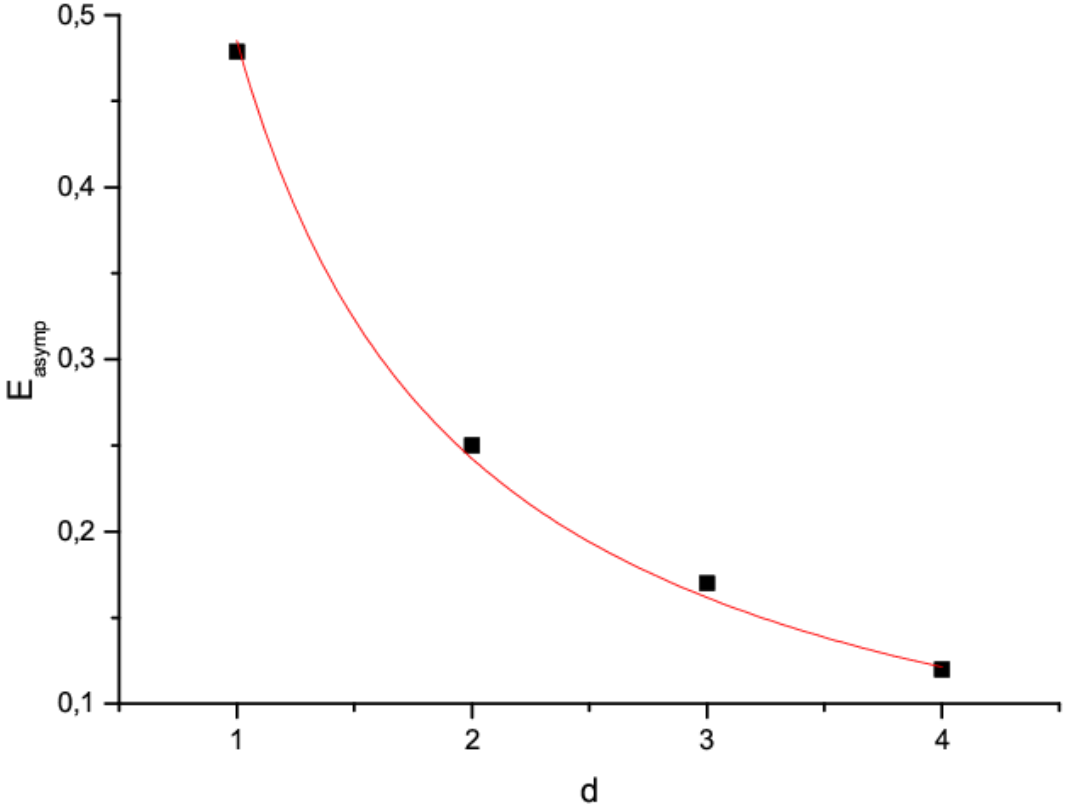
Def – AntiDef on the def line. Repulsion









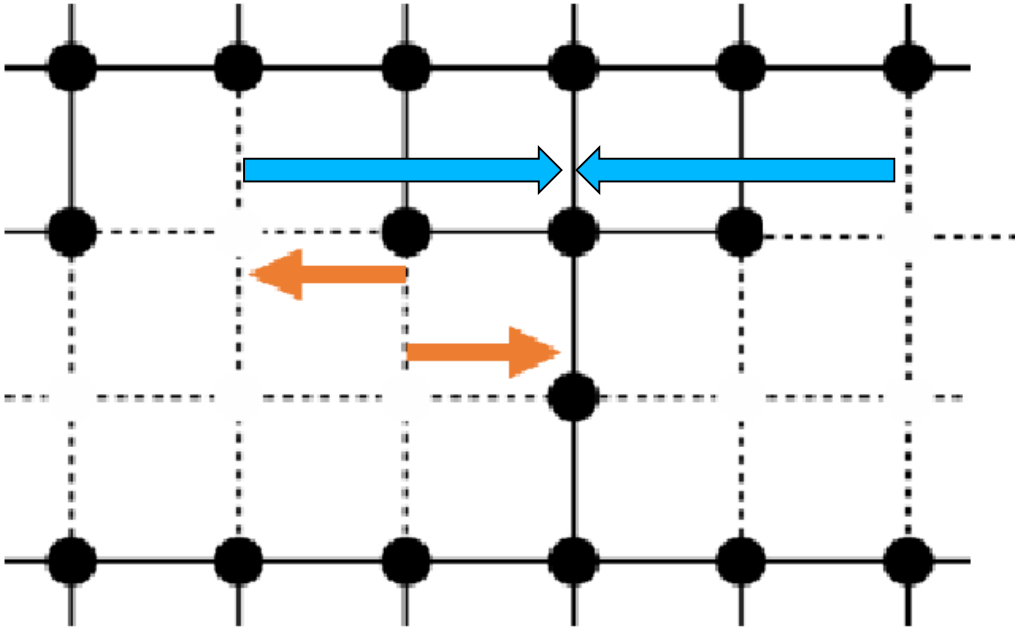


$$V(d) = ad^{-1},$$
$$a = 0.485 \pm 0.006$$

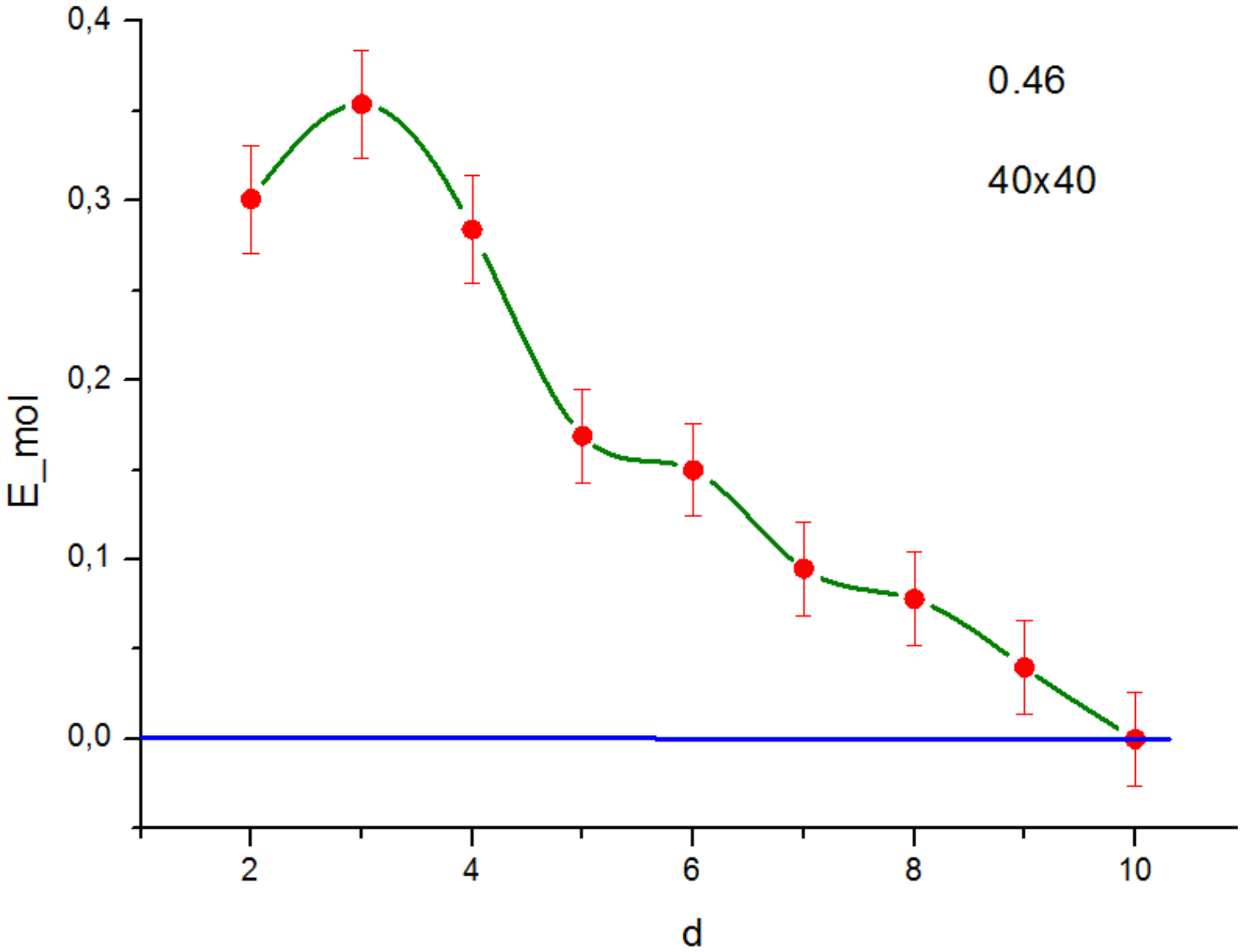
Казимировское отталкивание и самоорганизация дефектов на дефектной линии

Простейший пример самоорганизации – образование связанных состояний

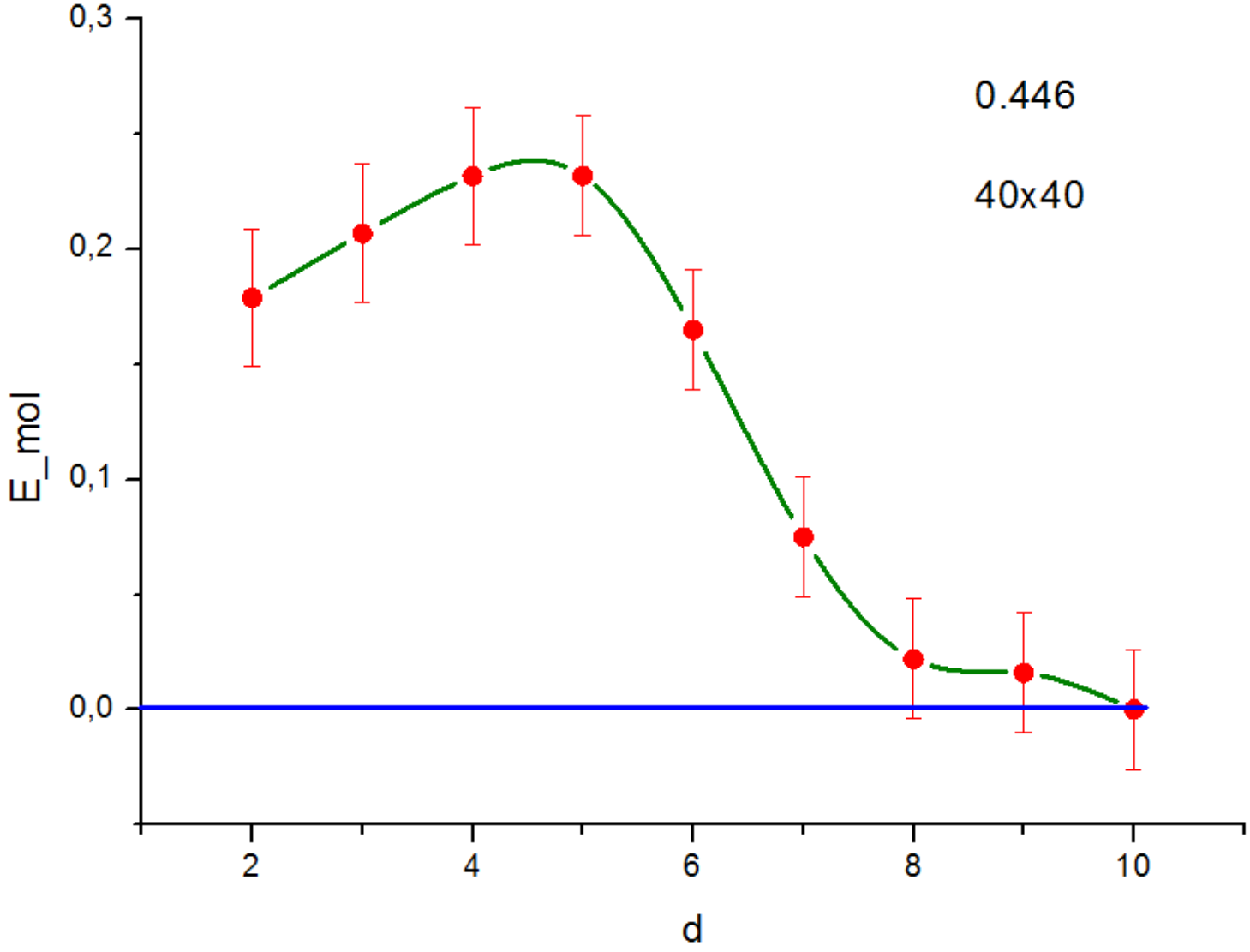
Дефект – антидефект – дефект (Д-А-Д) молекула



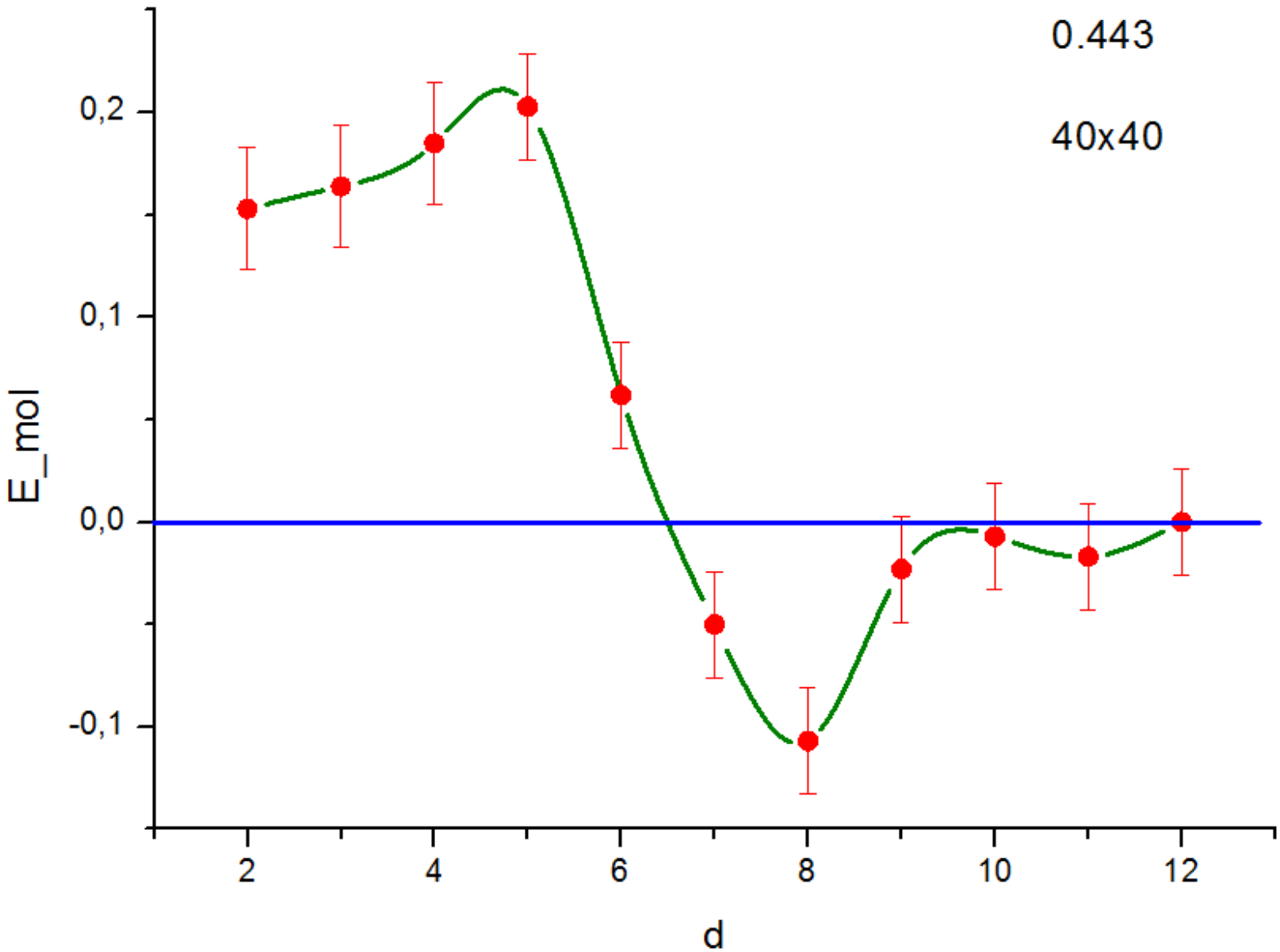
Казимировское отталкивание и самоорганизация дефектов на дефектной линии



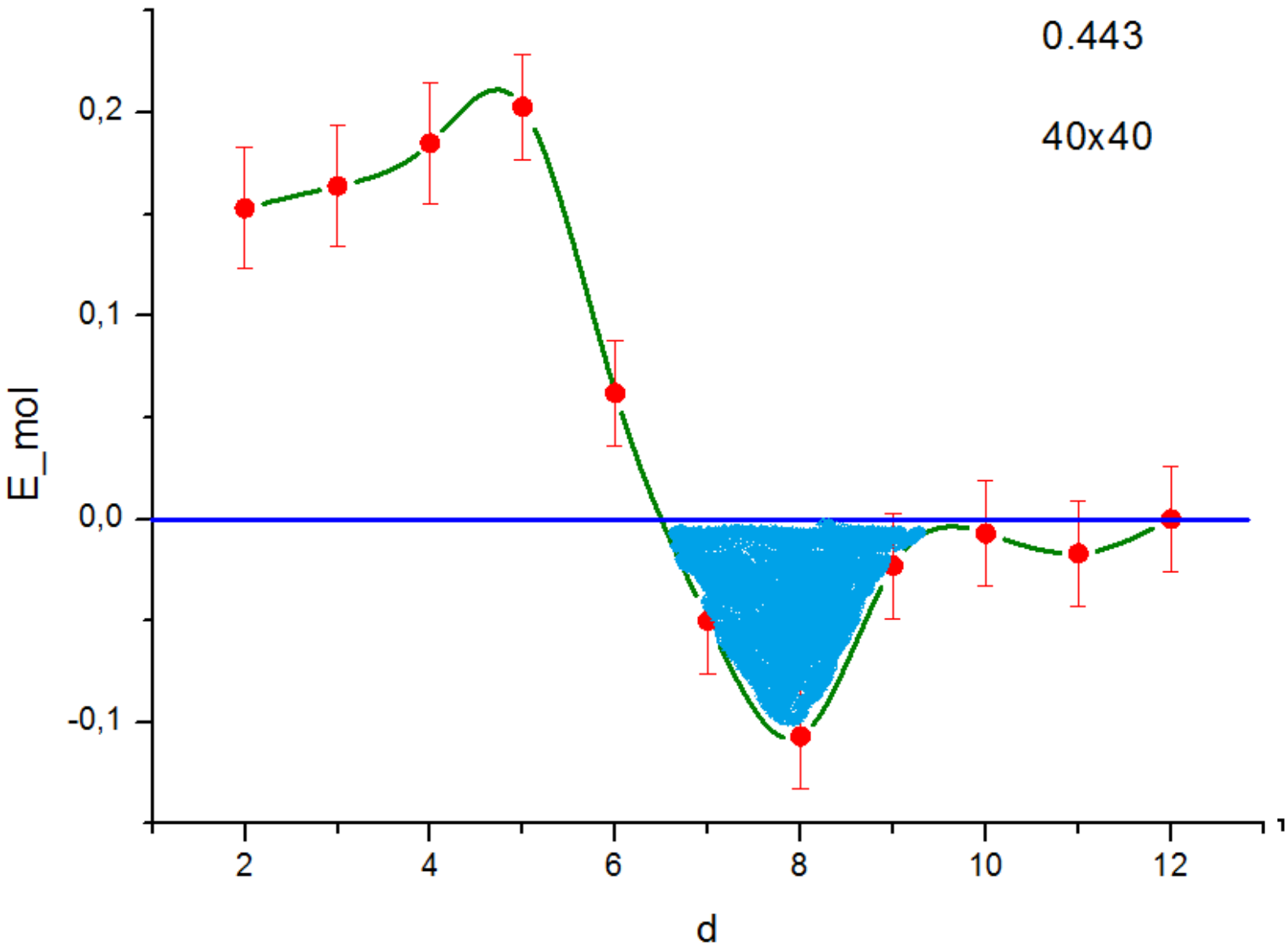
Казимировское отталкивание и самоорганизация дефектов на дефектной линии



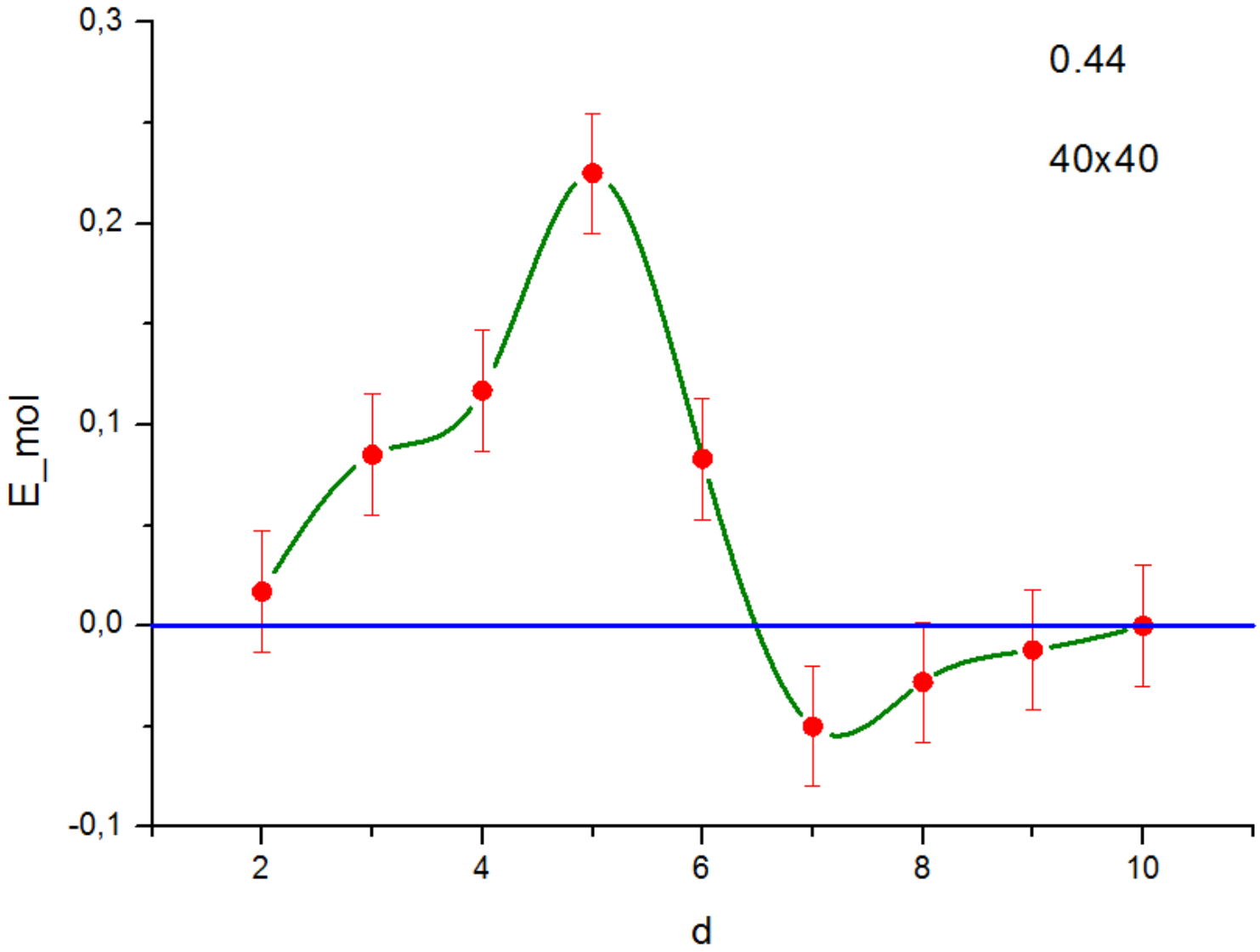
Казимировское отталкивание и самоорганизация дефектов на дефектной линии



Казимировское отталкивание и самоорганизация дефектов на дефектной линии



Казимировское отталкивание и самоорганизация дефектов на дефектной линии



Темы исследований

Искусственные нейронные сети на основе двойных квантовых точек

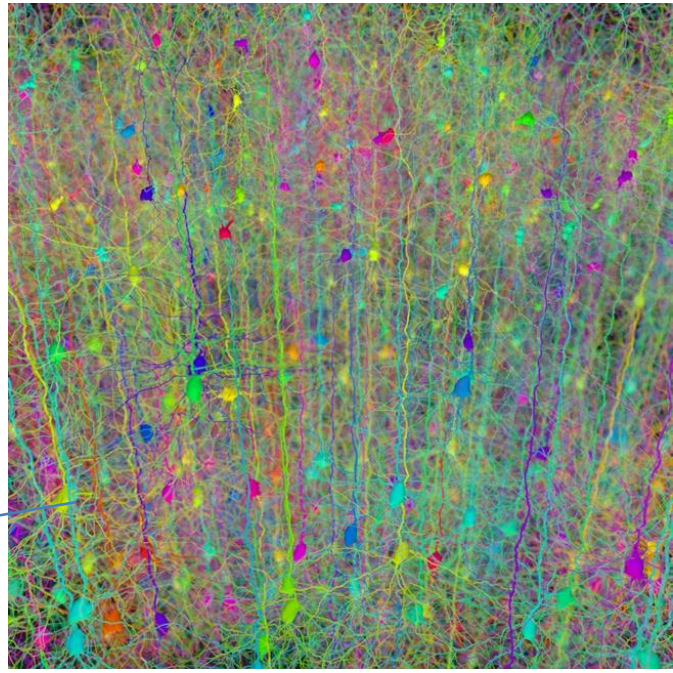
Programmers / Biologists

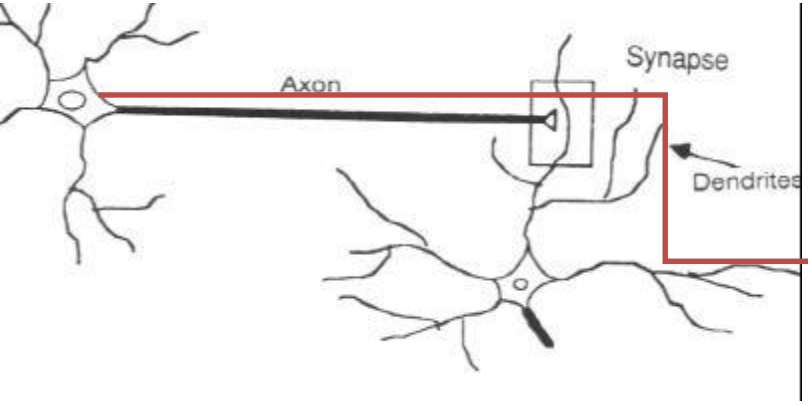
Two point of view on neural networks

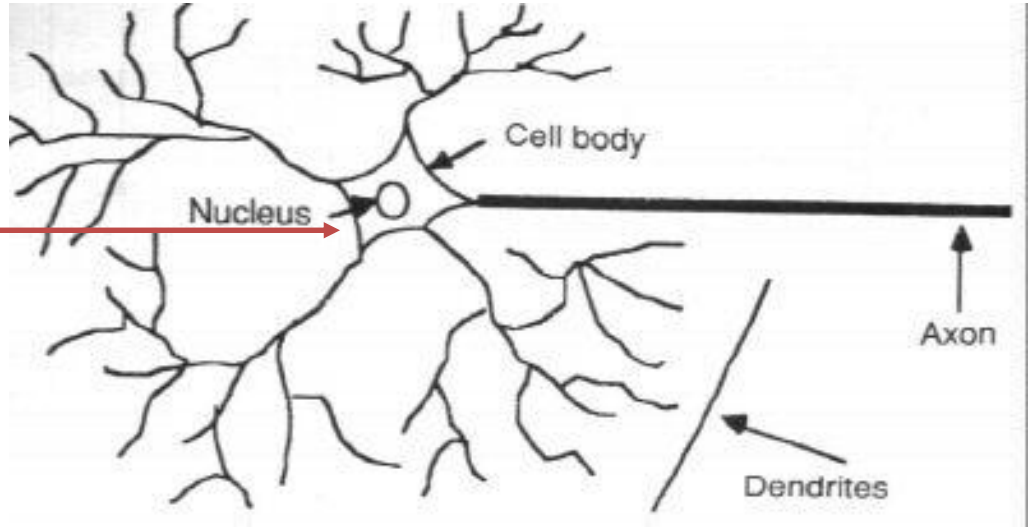
Programmers

Biologists

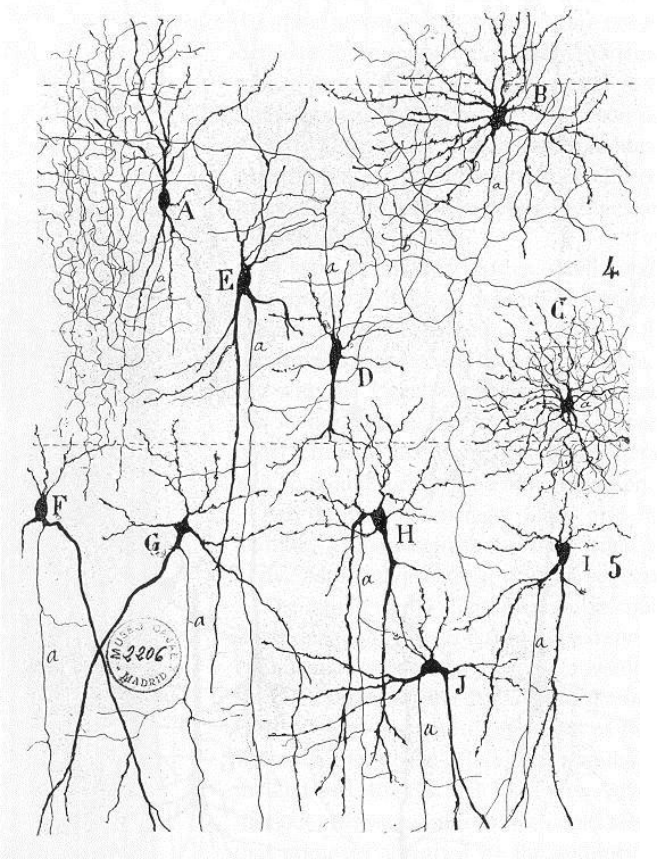
Neural network: Biology

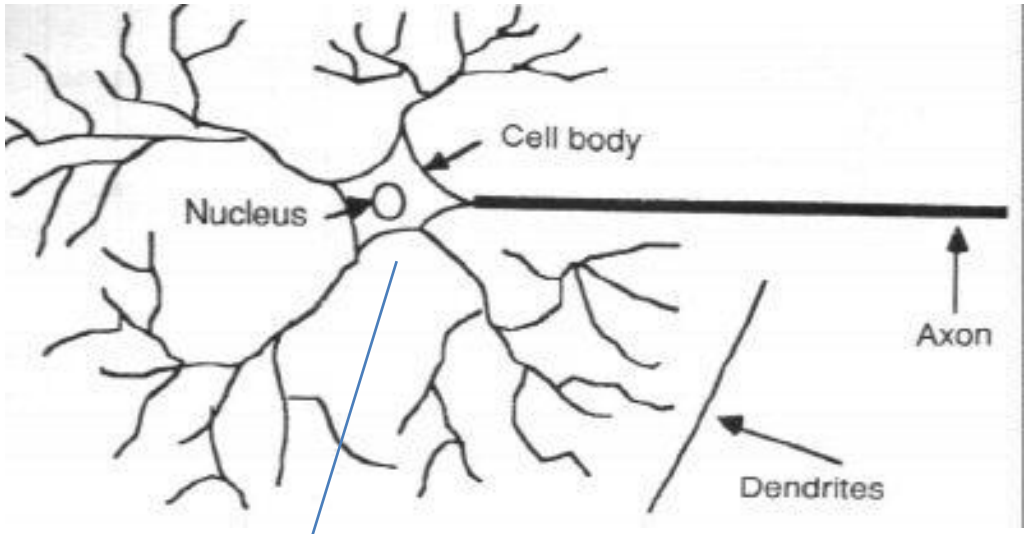


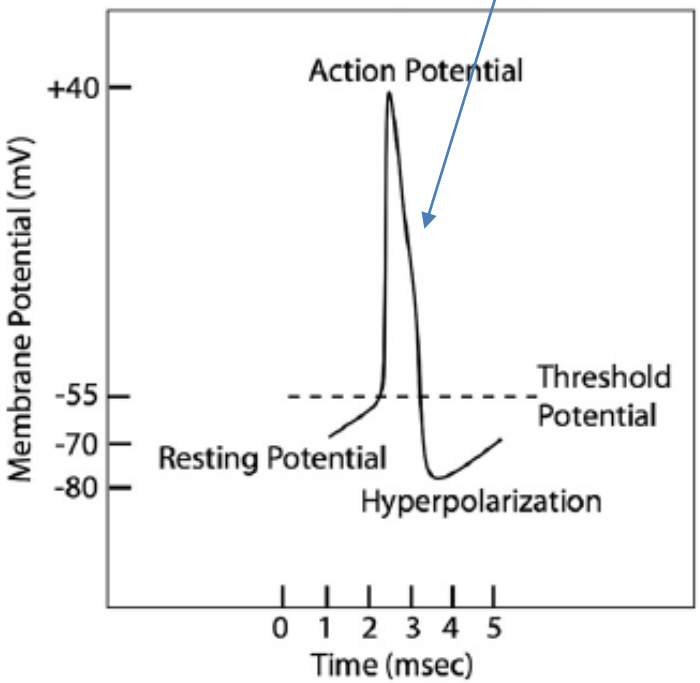




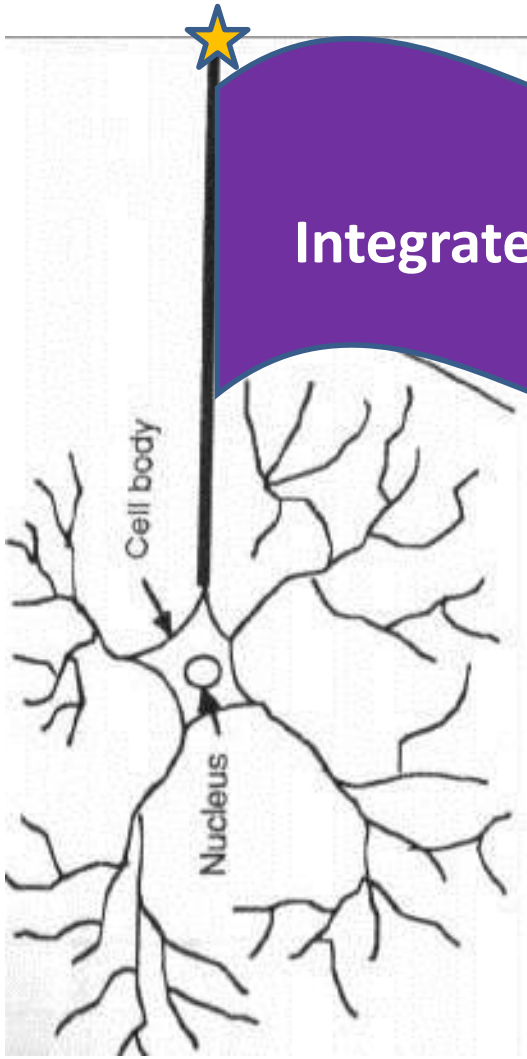
How Neuron Works: Biology



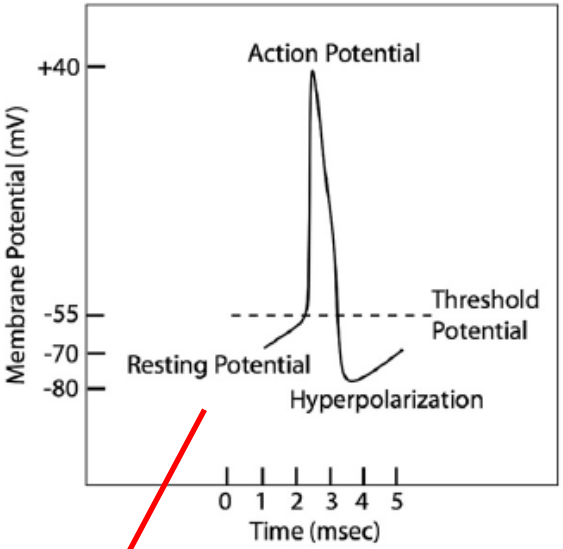




The models of Biological Neuron



Integrate-and-fire



$$I(t) = C_{\mathrm{m}} \frac{dV_{\mathrm{m}}}{dt}$$

Different for Different Models

Artificial Neural Network: main idea

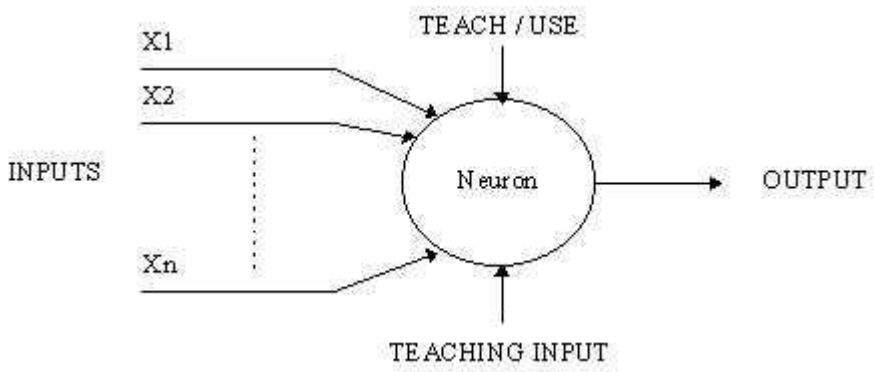
Main idea of Artificial Neural Network:

Artificial Neural Network (ANN) is an information system that is inspired by the biological nervous systems, such as the brain.

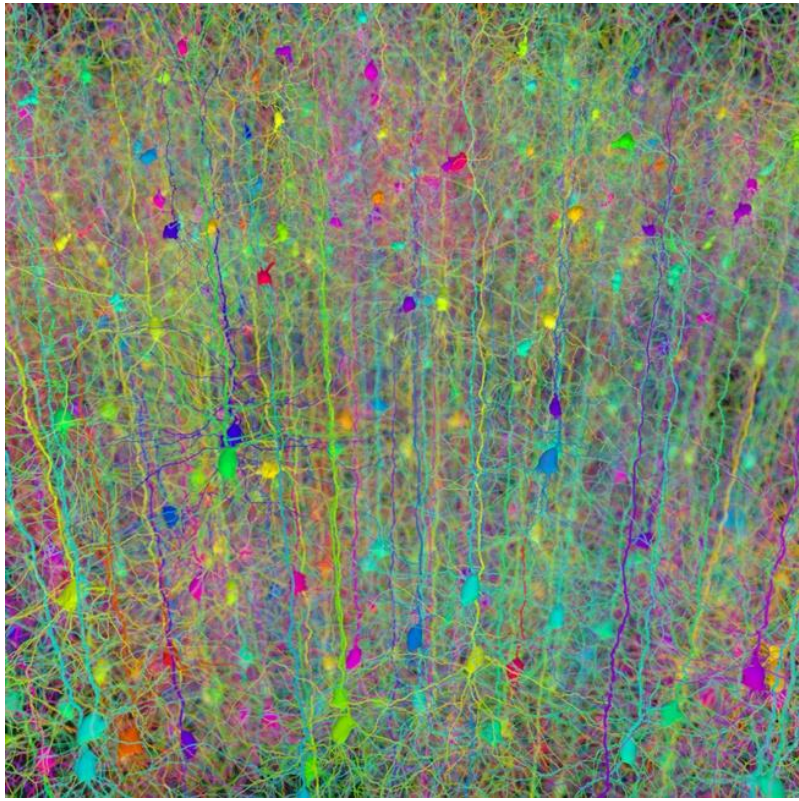
The key element of ANN is a large number of highly interconnected processing elements (neurones) working in unison to solve specific problems.

ANN, like brain, learn by examples or patterns.

Typical ANN problems: pattern recognition, data classification and so on.



New era in biological neural networks



Biological (real) neural networks are VERY complicated systems.

Models of neuron – stochastic diff. equations.

So…

Only qualitative analysis is possible now.

Statistical mechanics approach can be used

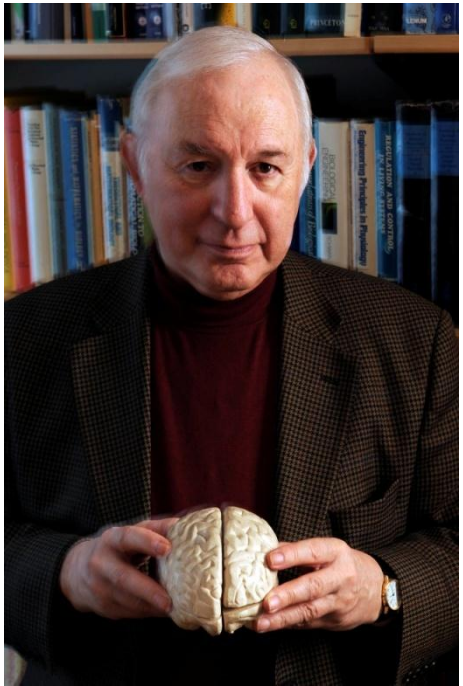
Idea of the universality classes: biological details may be not so essential in contrast with Symmetries and Topology of the Network.

Conformity in neural networks

Main question is:

What is the mechanism of the big correlation on the neural network?

Statistical mechanics gives the possible answer: Conformity near the phase transition. (Michael A. Buice and Jack D. Cowan, 2008-2009)



Conformity in neural networks

Jack D. Cowan: "Strange and interesting things happen in the neighborhood of a phase transition"

Statistical mechanics gives the possible answer: Conformity near the phase transition. (Michael A. Buice and Jack D. Cowan, 2008-2009)

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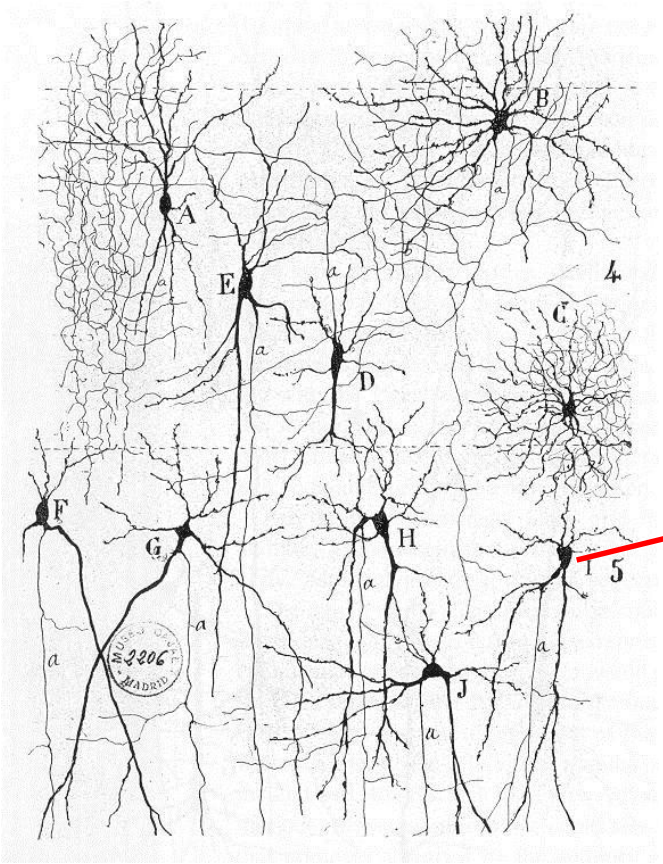
journal homepage: www.elsevier.com/locate/pbiomolbio

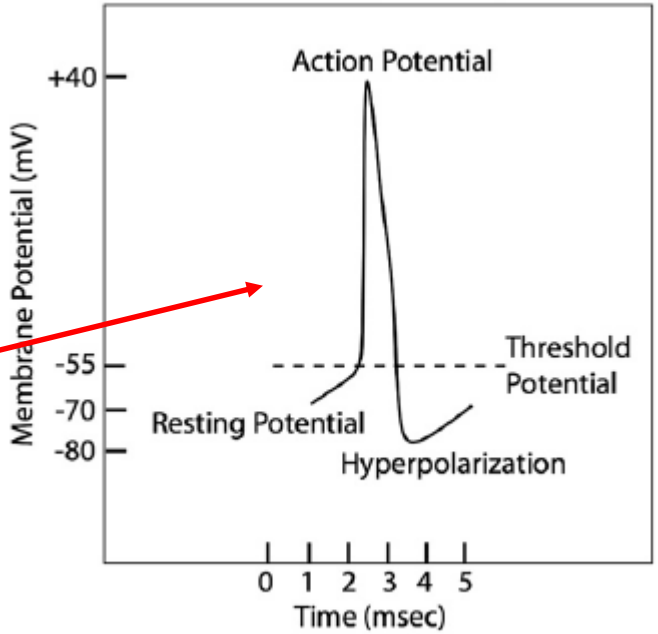
Review

Statistical mechanics of the neocortex

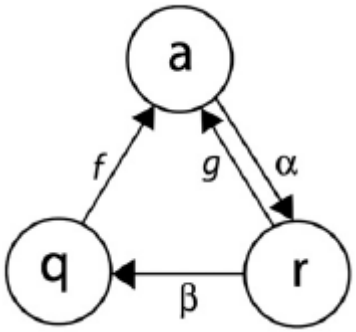
Michael A. Buice [a], Jack D. Cowan [b,*]

Neural network as statistical model





3–state model of neuron



Main idea

If the brain is statistical machine,
Why ANN is classical one?

Main idea

If the brain is statistical machine,
Why ANN is classical one?

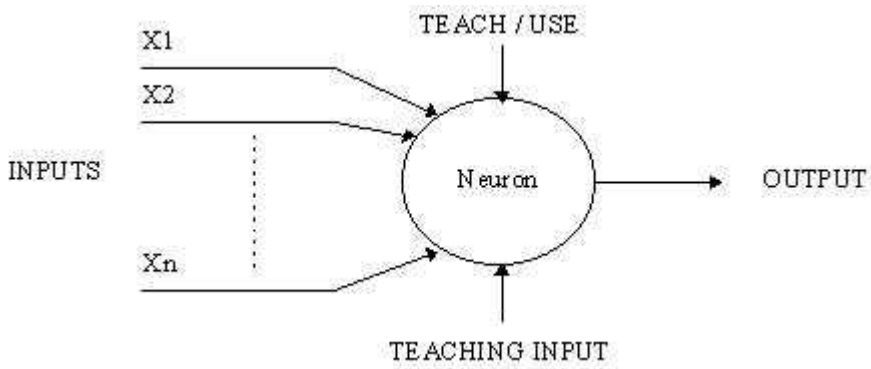
Artificial Neuron must be stochastic ….

Main idea

If the brain is statistical machine,
Why ANN is classical one?

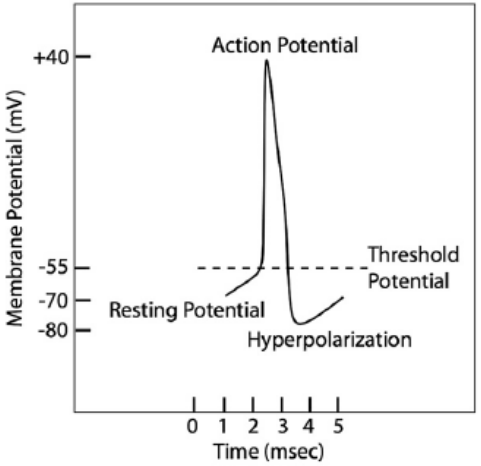
Artificial Neuron must be stochastic or Quantum.

Neuron: classical VS stochastic

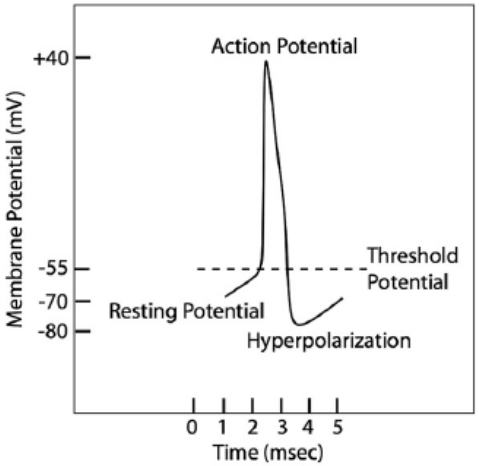


If $\Sigma (W\_1 X\_1 + W\_2 X\_2 + \ldots + W\_n X\_n) > I\_treshold$

then neuron generates spike

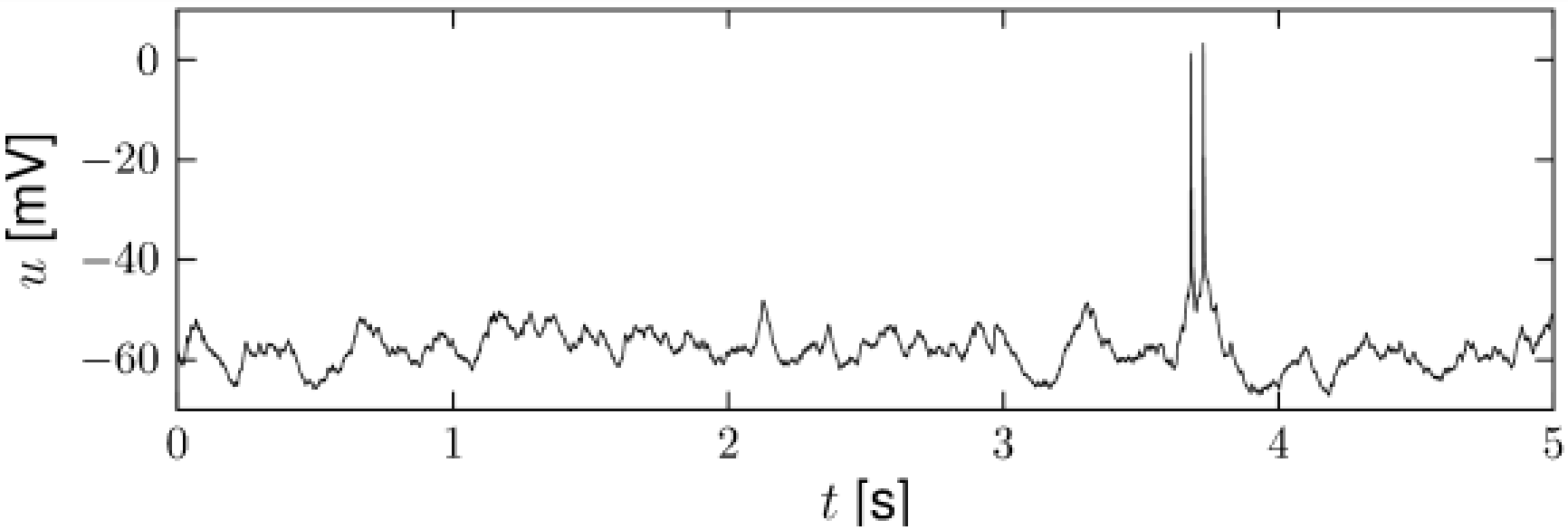


Neuron: classical VS stochastic

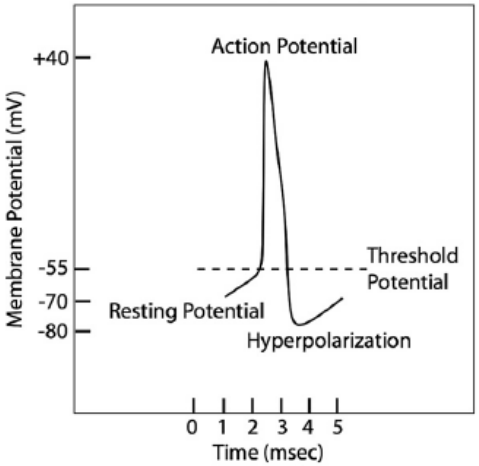


Simplification

Real neuron potential

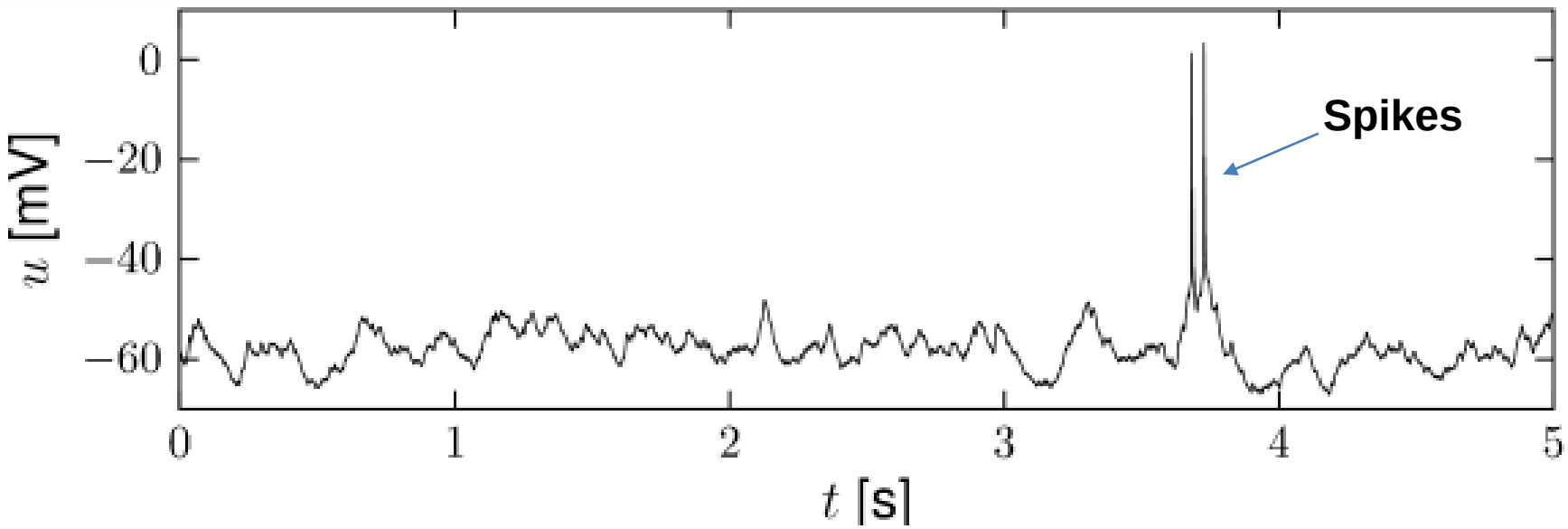


Neuron: classical VS stochastic

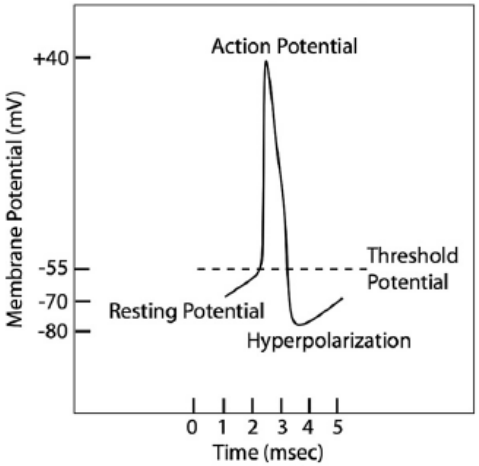


Simplification

Real neuron potential

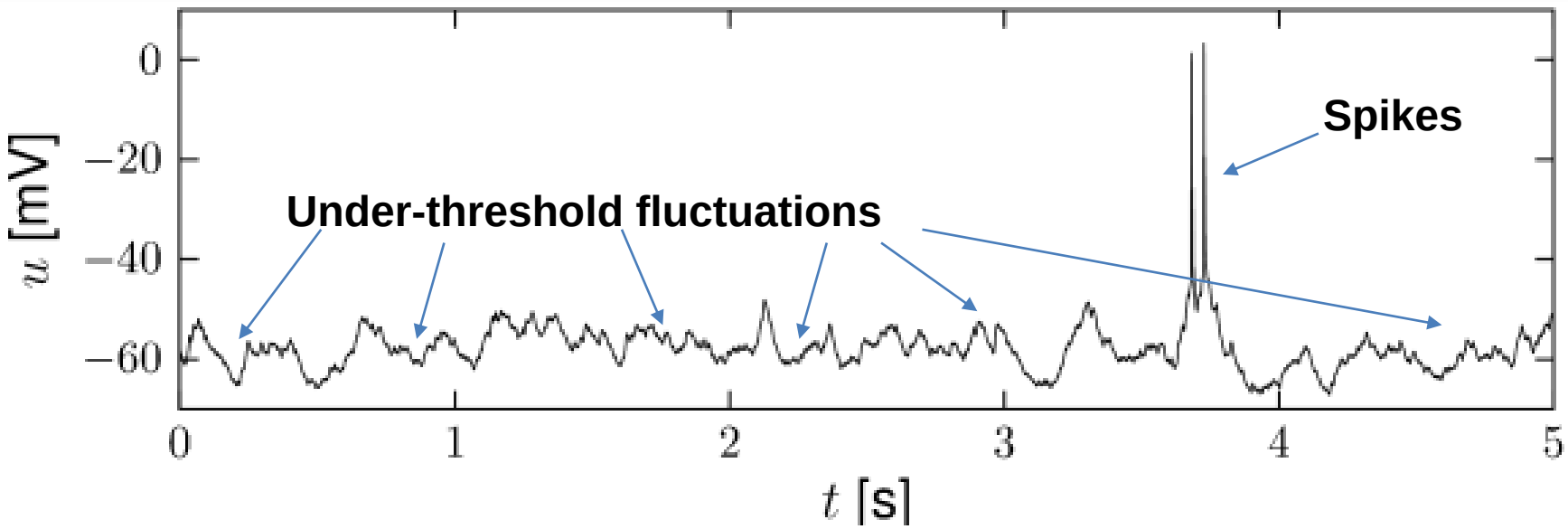


Neuron: classical VS stochastic

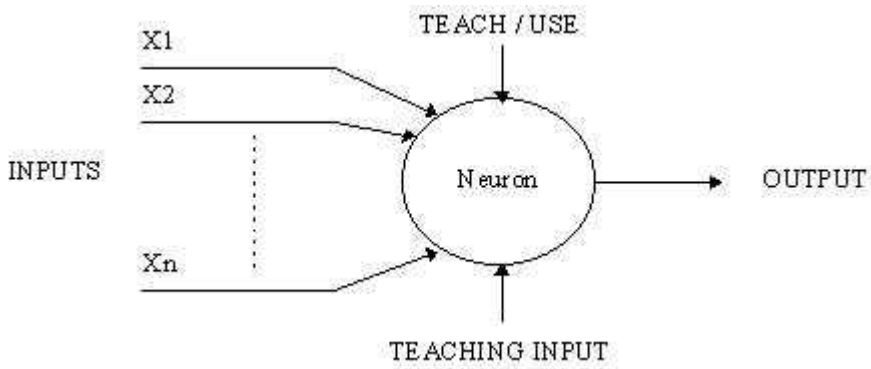


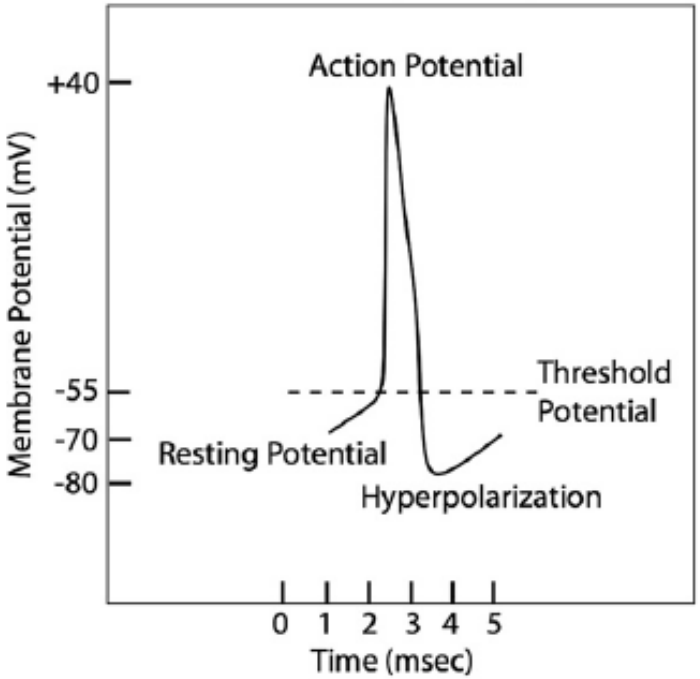
Simplification

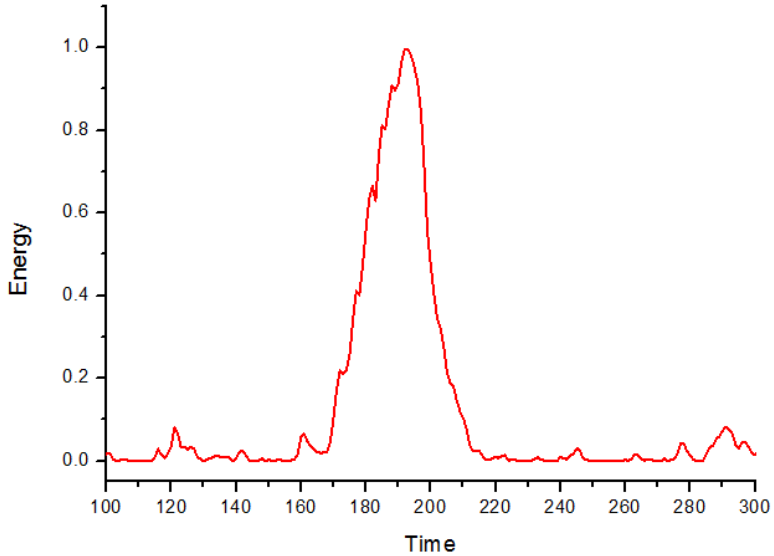
Real neuron potential



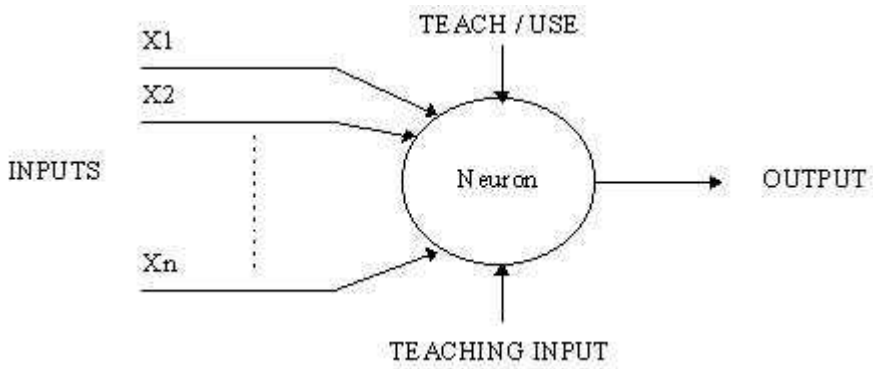
Quantum neuron = Q-neuron

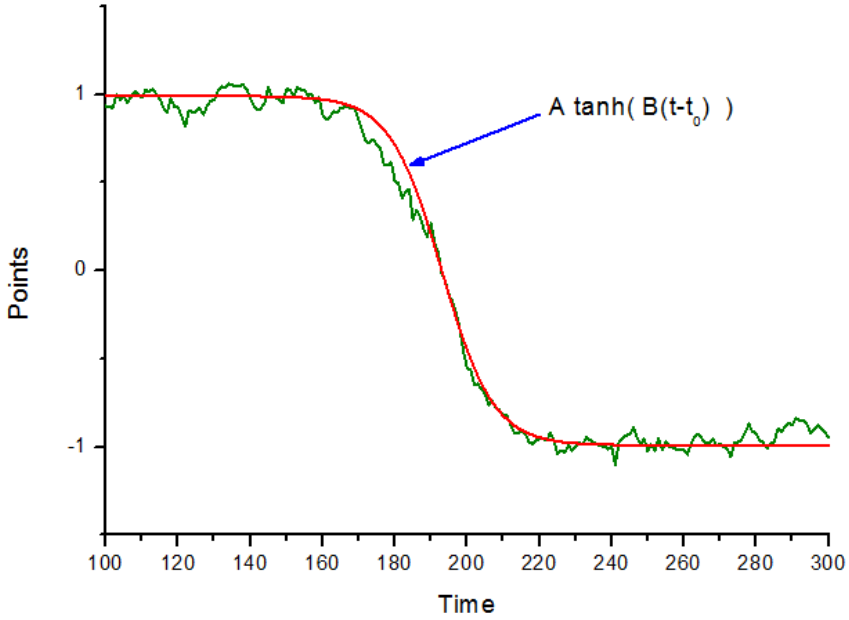


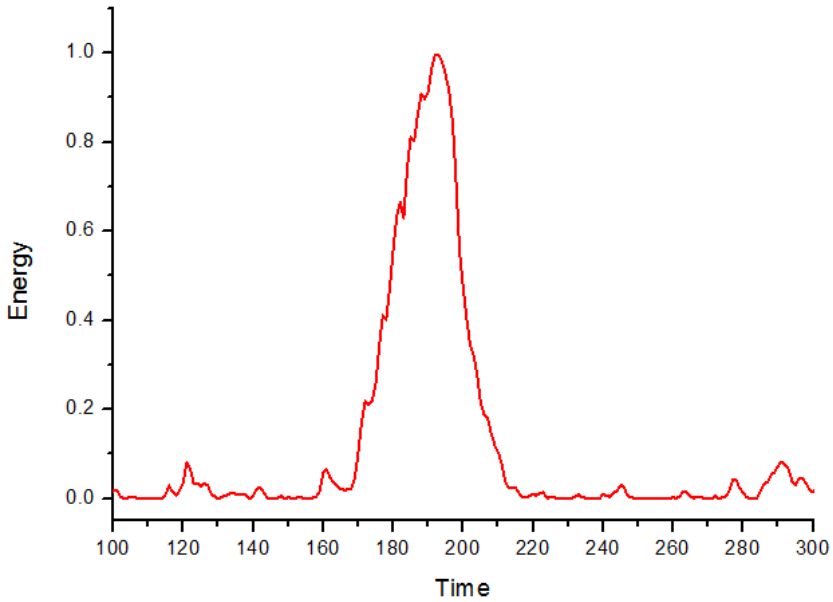




Quantum neuron = Q-neuron



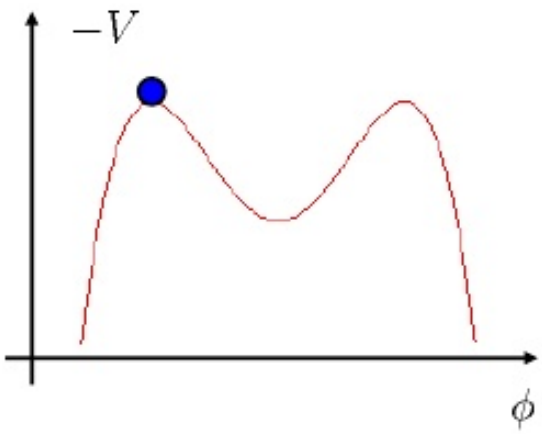


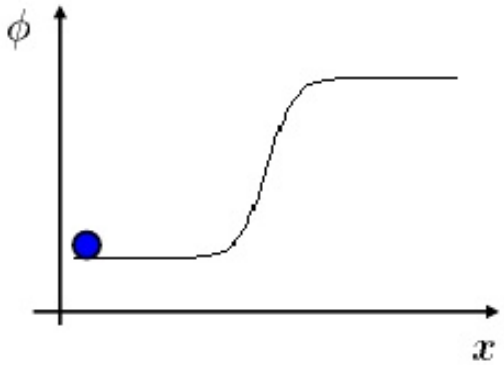


Quantum neuron

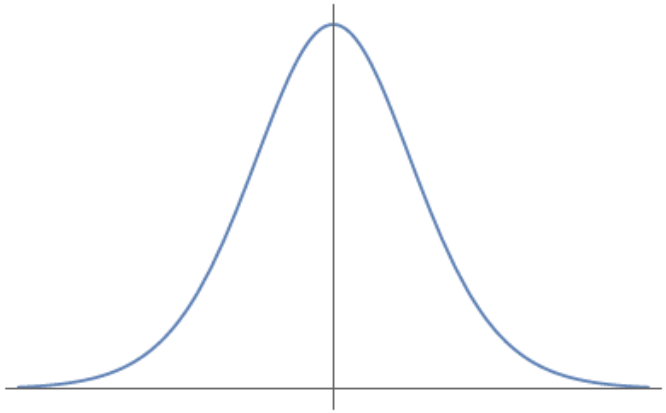
$$\hat{H}_i = \frac{1}{2}\hat{p}_i^2 + V_0\left(\hat{\varphi}_i\right).$$

$$V_0(\varphi_i) = \frac{\Lambda}{4}\left(\varphi^2 - \frac{\mu^2}{\Lambda}\right)^2.$$

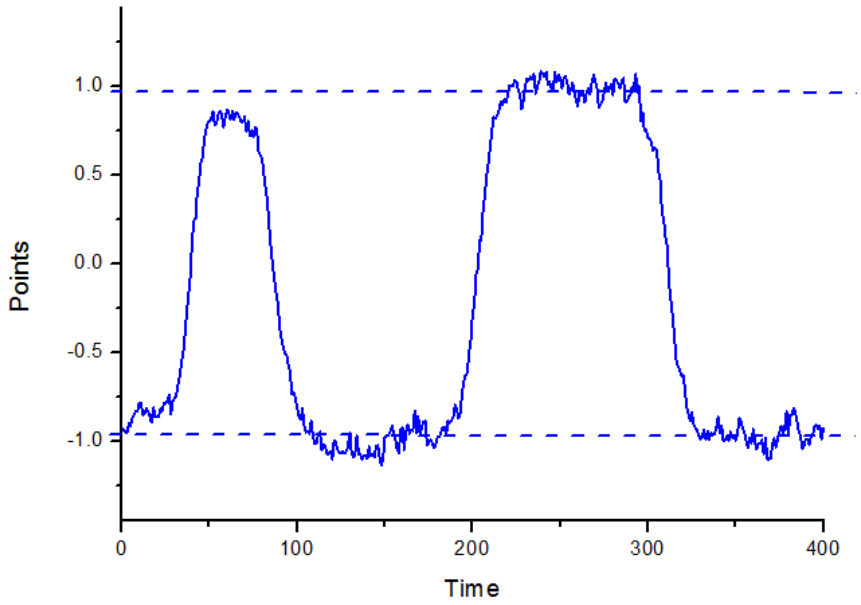


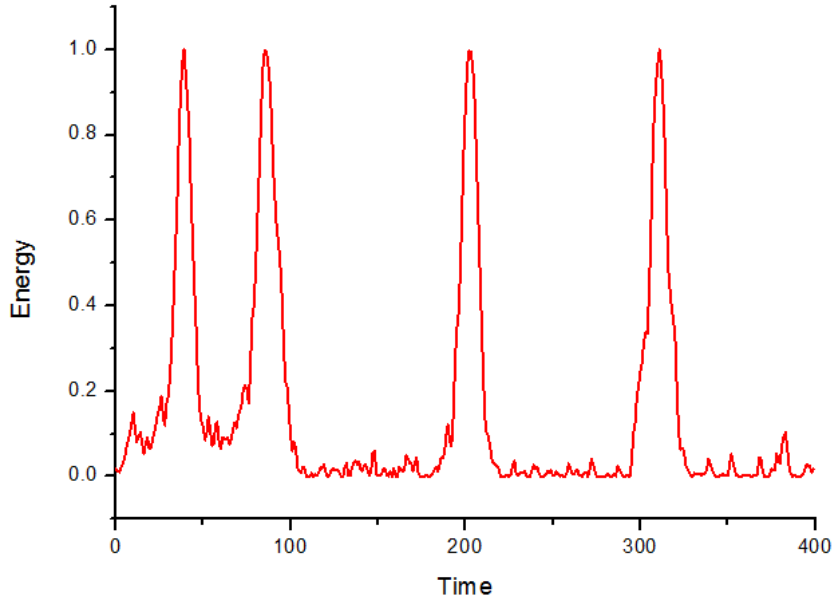


$$\phi(x,t) = \frac{m}{\sqrt{\lambda}}\tanh\left(\frac{m}{\sqrt{2}}(x - x_0)\right)$$

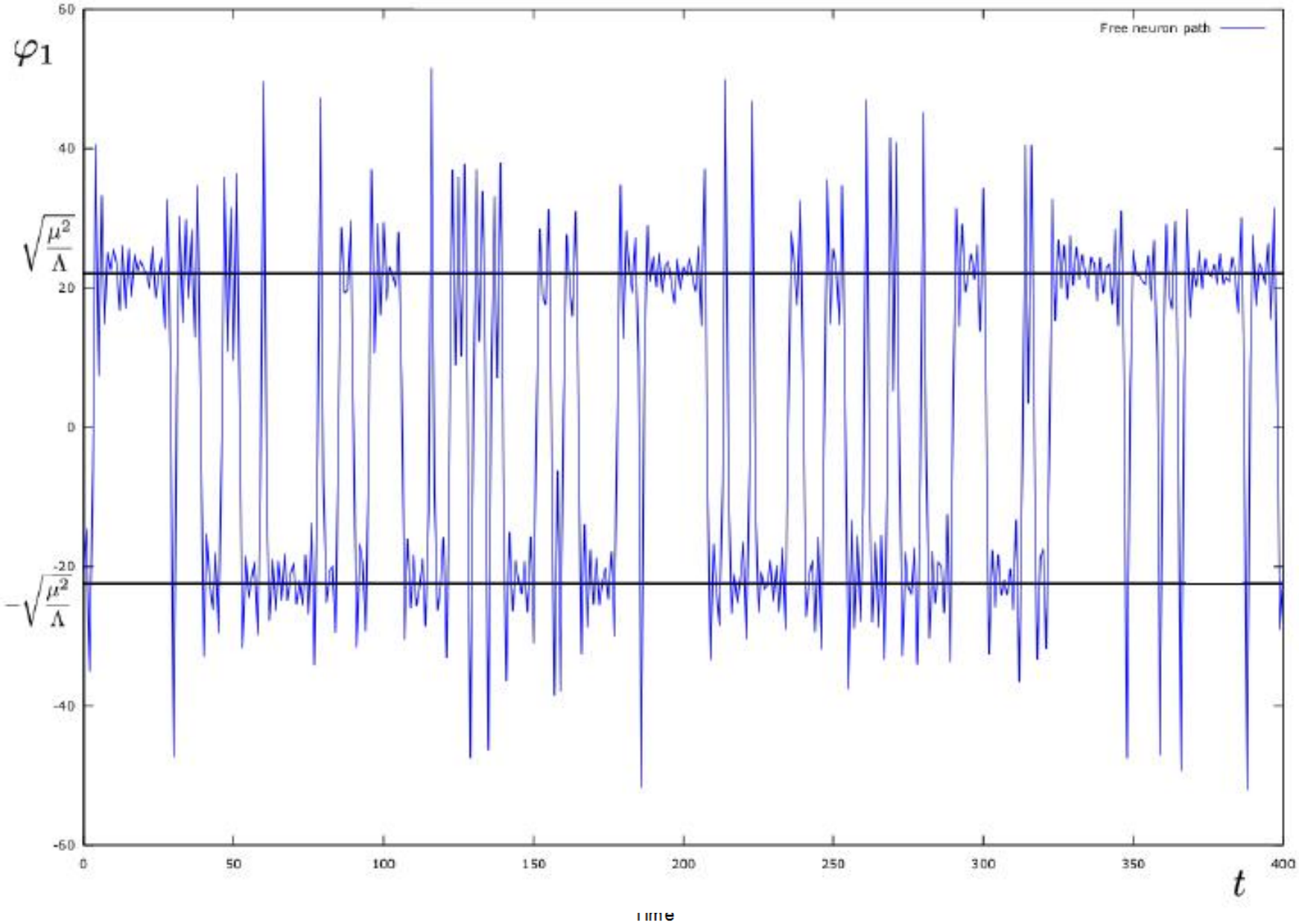


Quantum neuron = Q-neuron

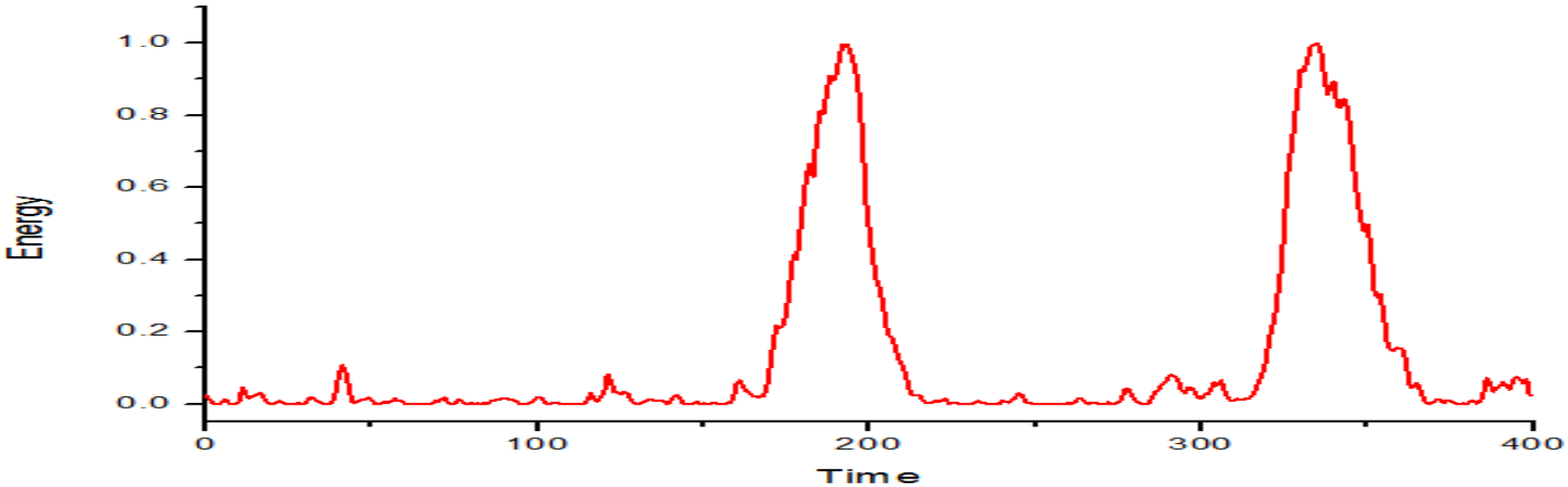


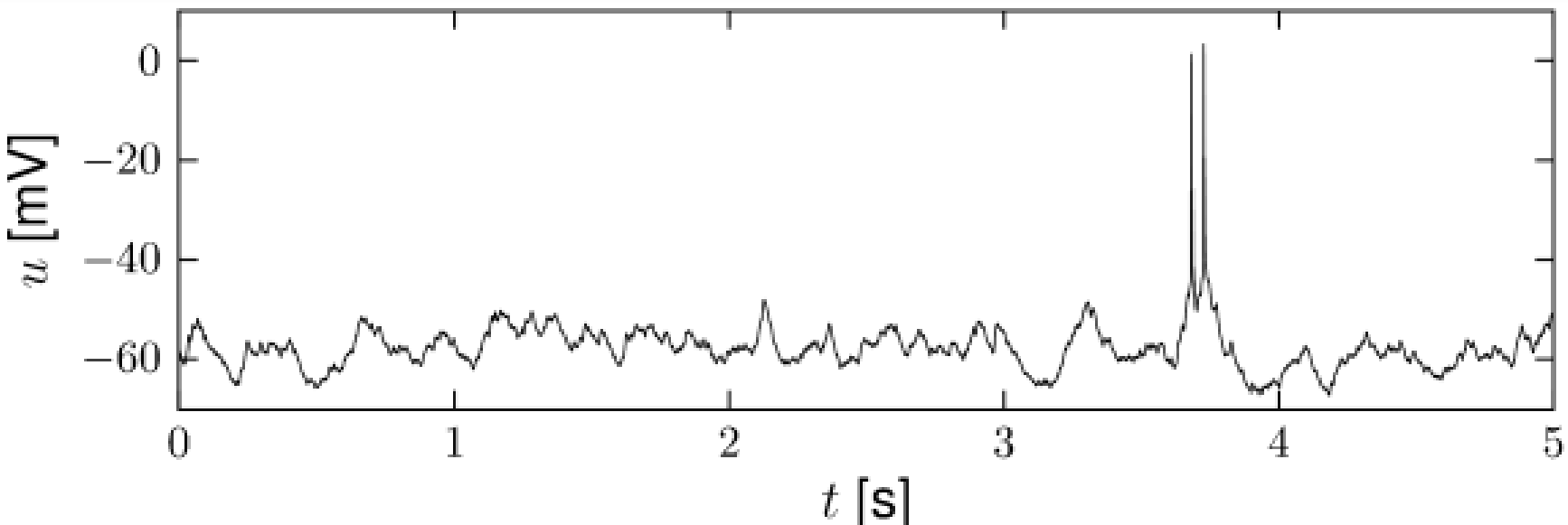


Quantum neuron = Q-neuron



Quantum neuron = Q-neuron

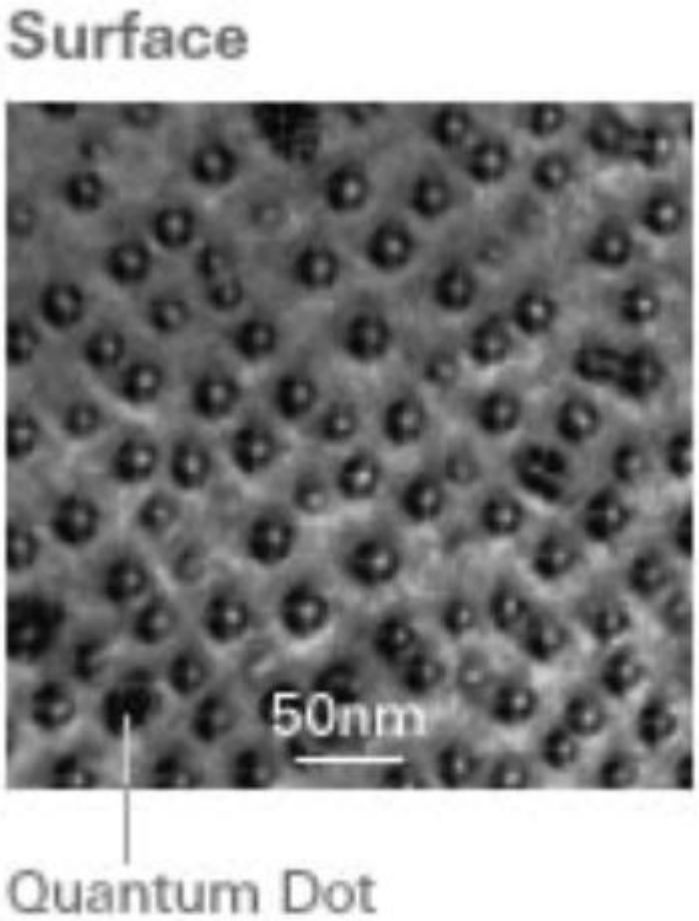




Nano-technological realizations

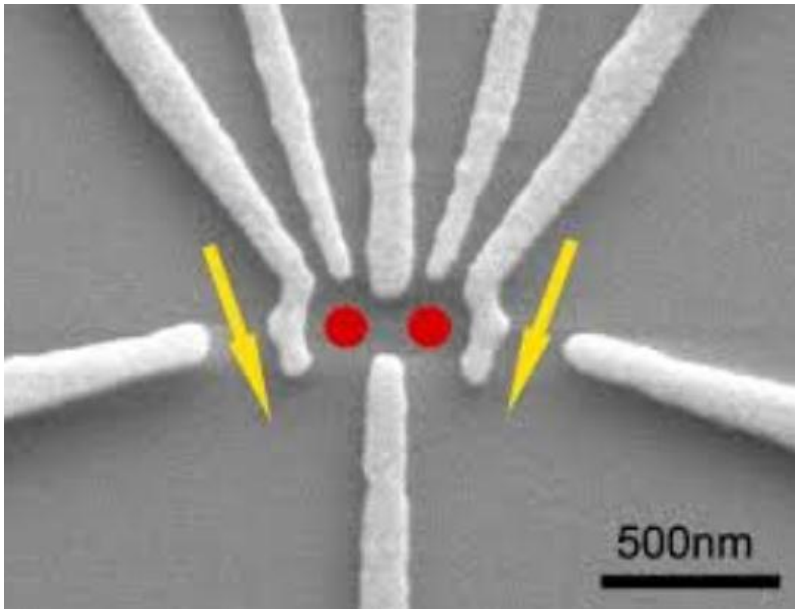
We need in Nano-technological platform for realization of QNN.

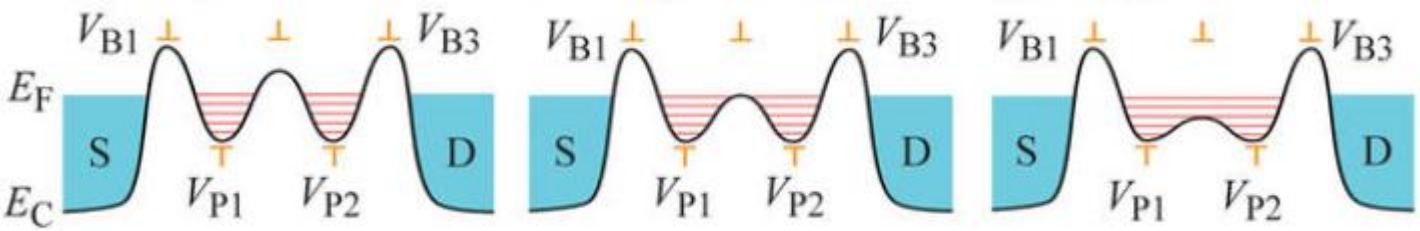
One possible way: **quantum double dots**.



Nano-technological realizations

Quantum double dots.

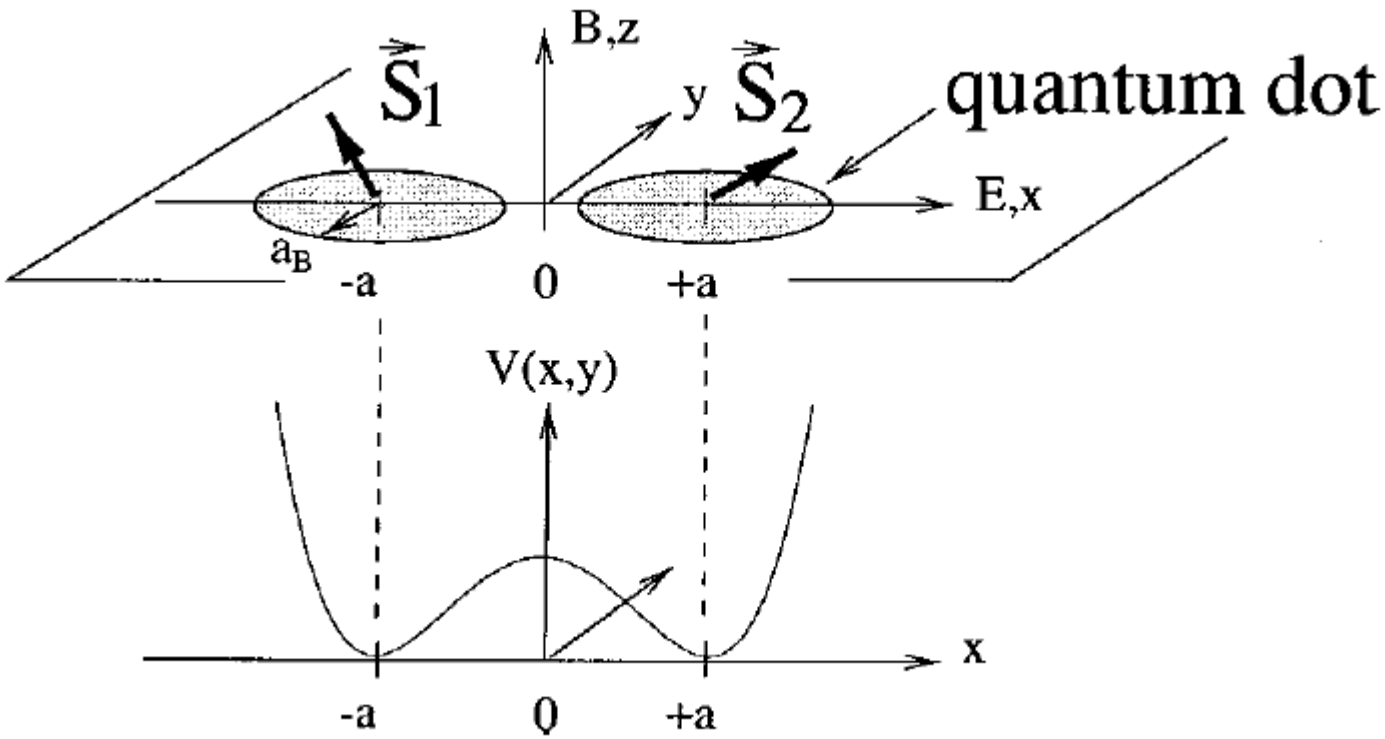




Scientific Reports **1**, Article number: 110 (2011)

Nano-technological realizations

Quantum double dots.



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Coupled quantum dots as quantum gates

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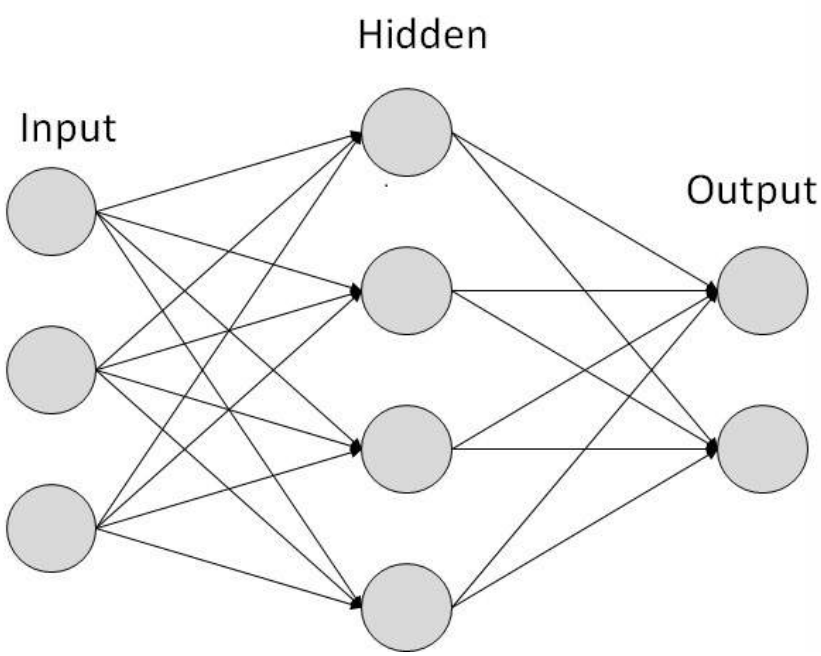
(Received 3 August 1998)

Quantum neural network as quantum many body system

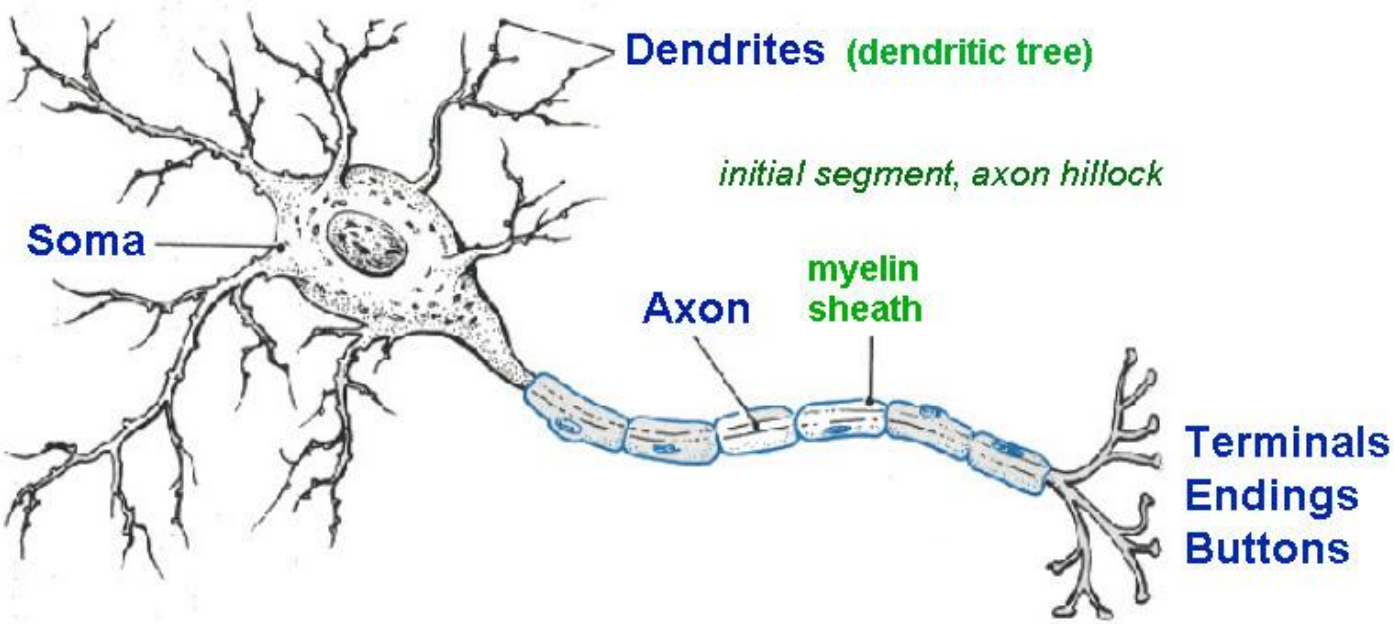
$$Z = \int \prod_i \mathcal{D}\varphi_i(\tau) \exp(-S(\varphi_i(\tau))), \varphi_i(0) = \varphi_i(T)$$

$$S = \int_0^T d\tau \left[\sum_i \left(\frac{1}{2}\dot{\varphi}_i^2 + V_0(\varphi_i) \right) + \sum_{i>j} V_{int}(\varphi_i, \varphi_j) \right]$$

$$\langle \mathcal{O}(\varphi_1, ..., \varphi_i) \rangle = \frac{1}{Z} \int \prod_i \mathcal{D}\varphi_i(\tau) \mathcal{O}(\varphi_1, ..., \varphi_i) \exp(-S(\varphi_i))$$



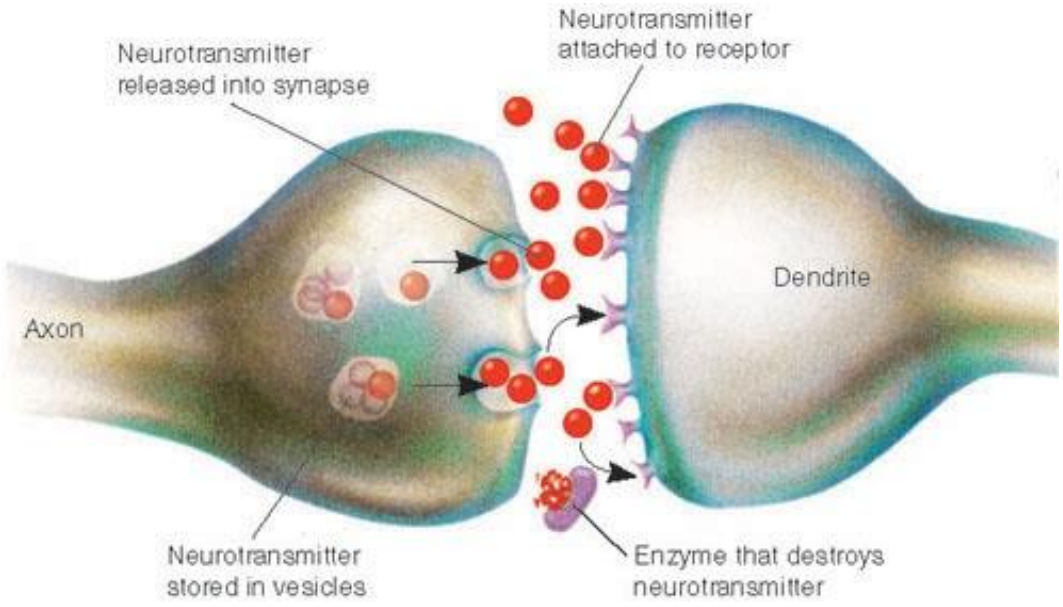
Axons in neural net



“Axon” is output information line from neuron.
So neural net is very non-local system.

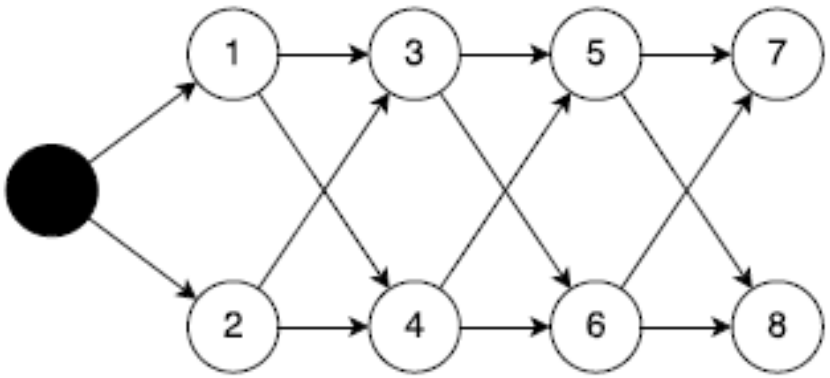
Role of Synepse

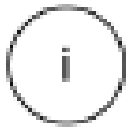
Role of Synepse is the contact coefficient, the measure of neuron connection.



Excitation connection

$$S = \int_0^T d\tau \left[\sum_i \left(\frac{1}{2}\dot{\varphi}_i^2 + V_0(\varphi_i) \right) + \sum_{i>j} V_{int}(\varphi_i, \varphi_j) \right]$$



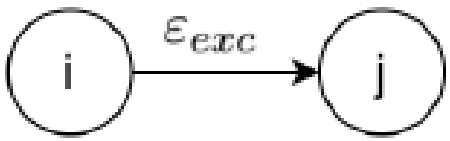
1. 

$$- \mathcal{L}_0 = \frac{1}{2}\dot{\varphi}_i^2 + \frac{\Lambda}{4}\left(\varphi_i^2 - \frac{\mu^2}{\Lambda}\right)^2$$

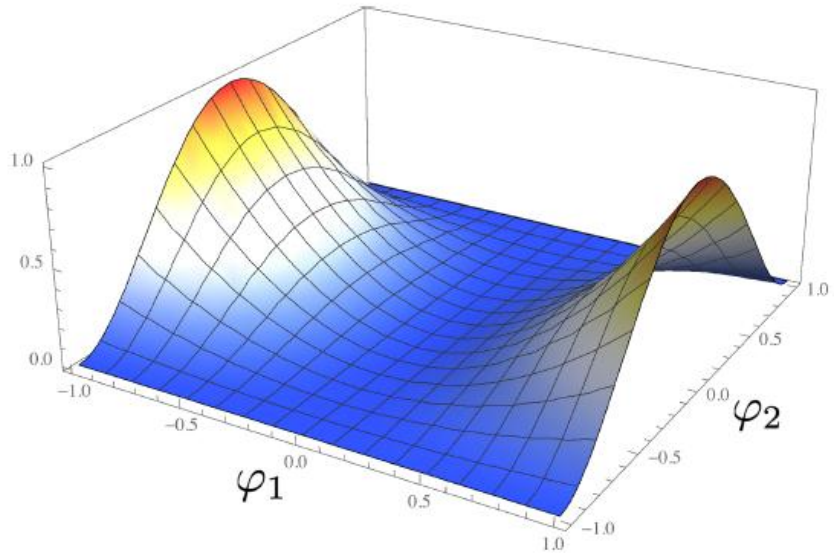
2. 

$$- \mathcal{L}_{int} = \varepsilon_{exc}\varphi_j^2\left(\varphi_i^2 - \frac{\mu^2}{\Lambda}\right)^2$$

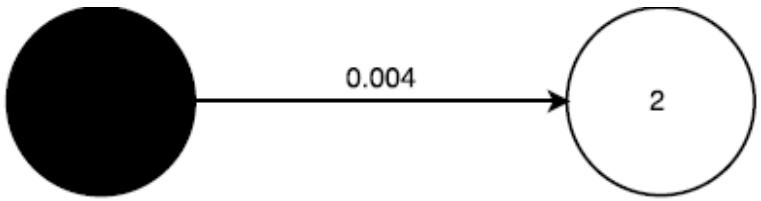
Excitation connection



$$-\mathcal{L}_{int} = \varepsilon_{exc}\varphi_j^2\left(\varphi_i^2 - \frac{\mu^2}{\Lambda}\right)^2$$

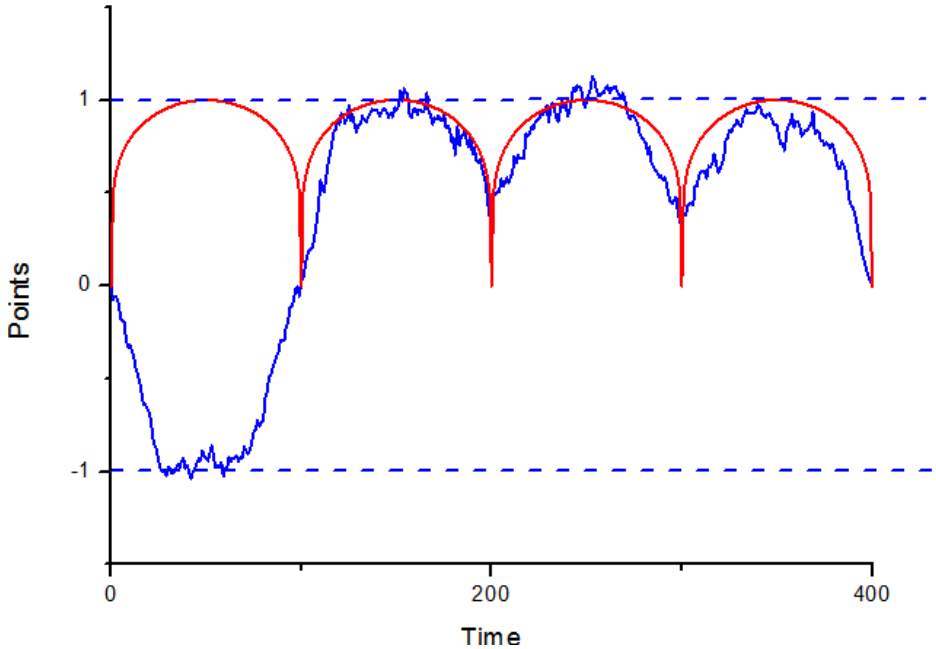


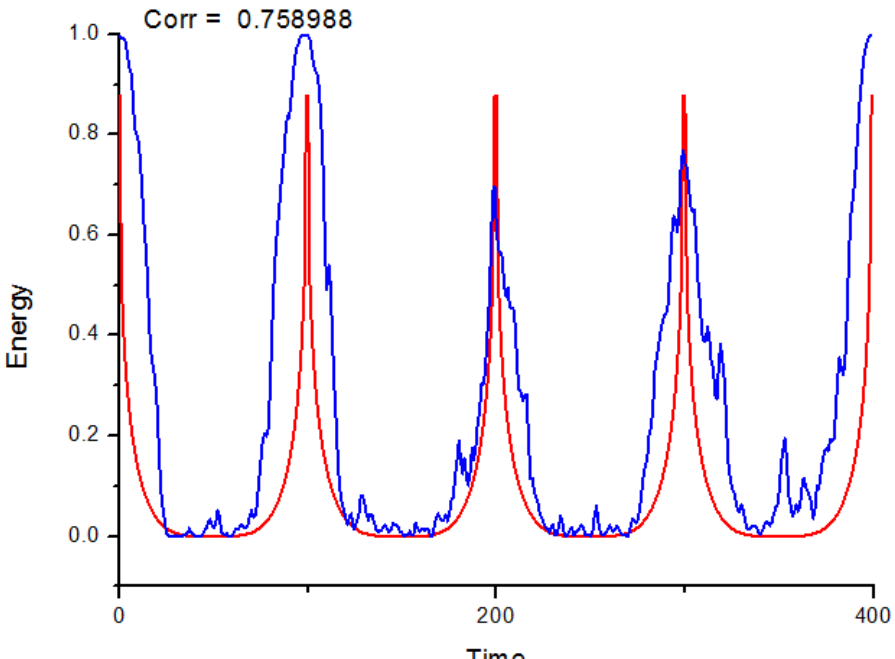
Excitation connection: simple test



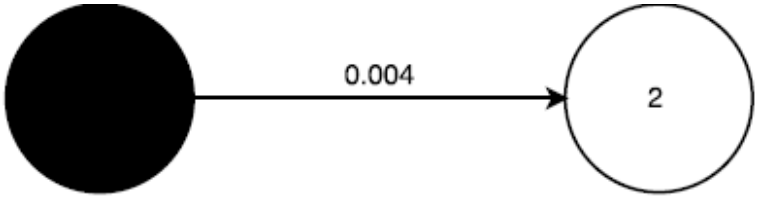
$$Z = \int \prod_i \mathcal{D}\varphi_i(\tau) \exp(-S(\varphi_i(\tau))), \varphi_i(0) = \varphi_i(T)$$

$$S = \int_0^T d\tau \left[\sum_i \left(\frac{1}{2}\dot{\varphi}_i^2 + V_0(\varphi_i) \right) + \sum_{i>j} V_{int}(\varphi_i, \varphi_j) \right]$$



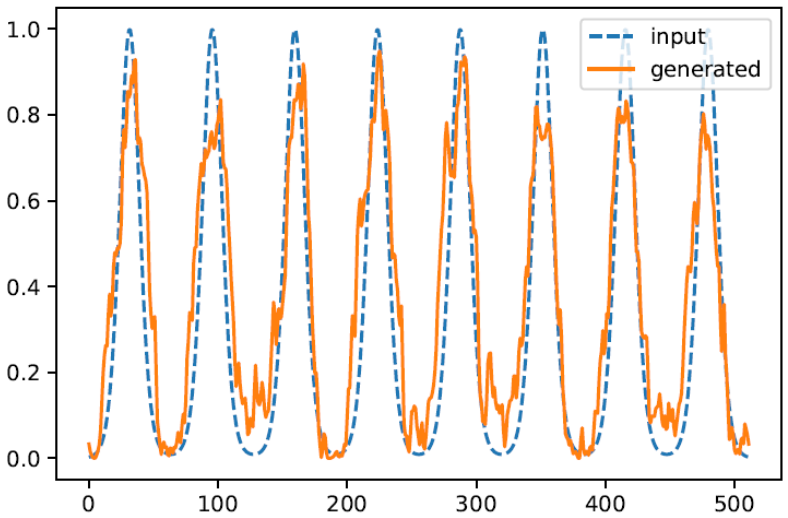


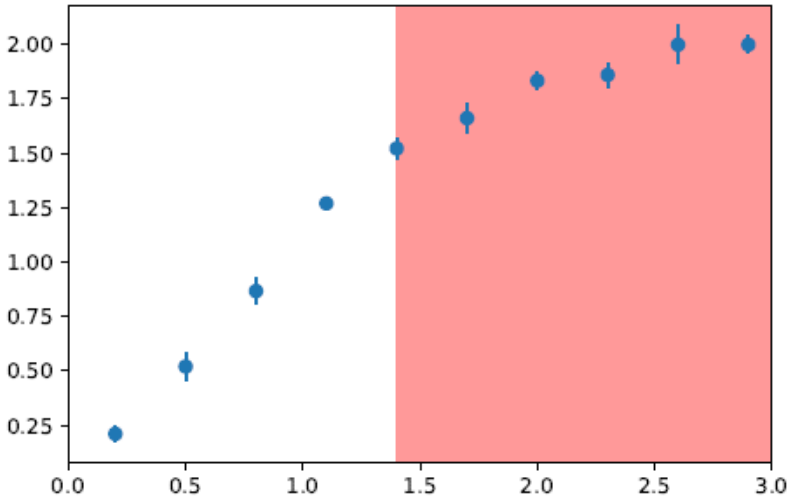
Excitation connection: simple test



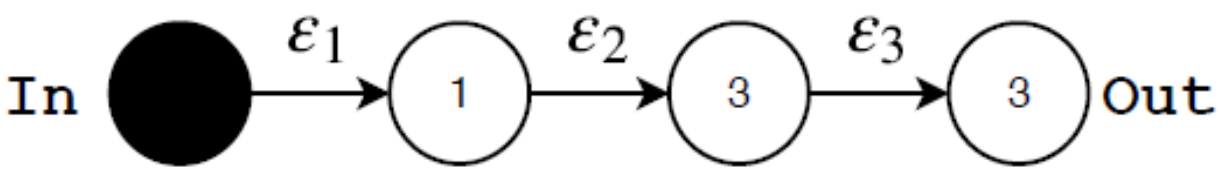
Activity of Q-neuron

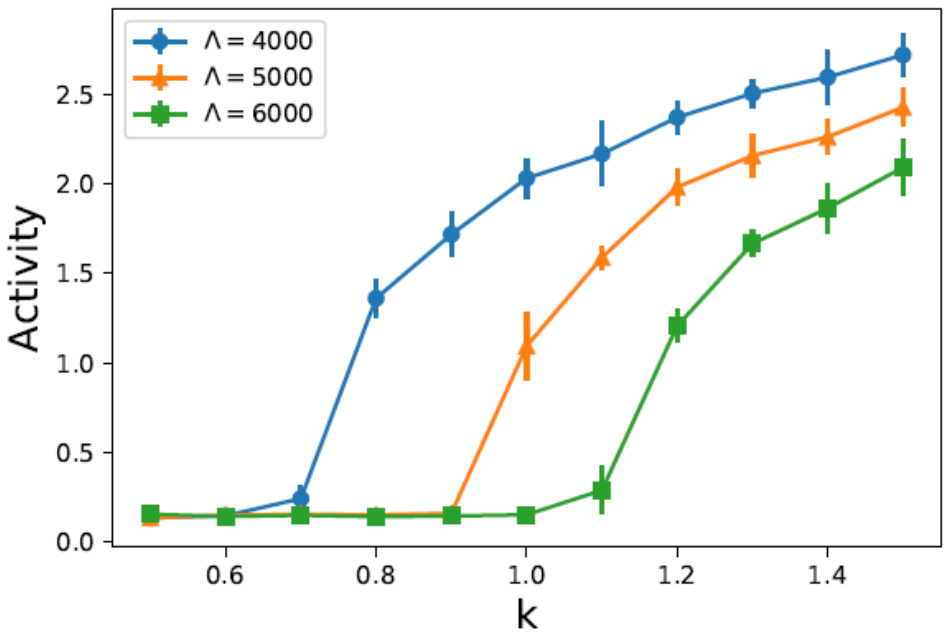
$$\left(\varphi_2^2 - 1\right)^2$$



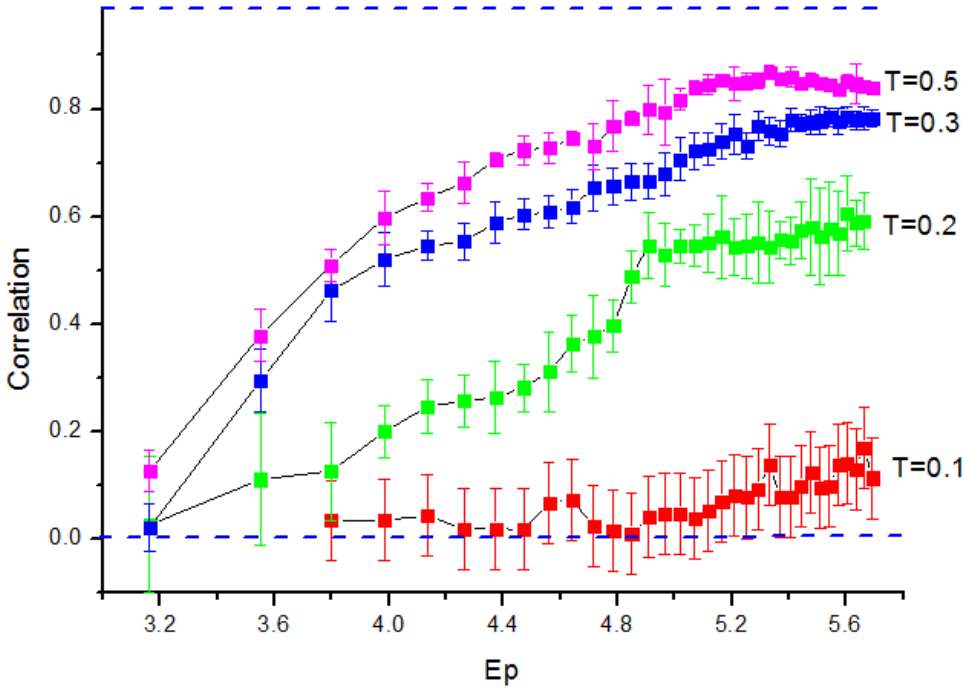


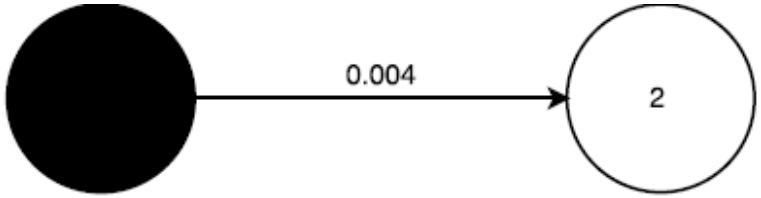
Excitation connection: 3 Q-neurons transport

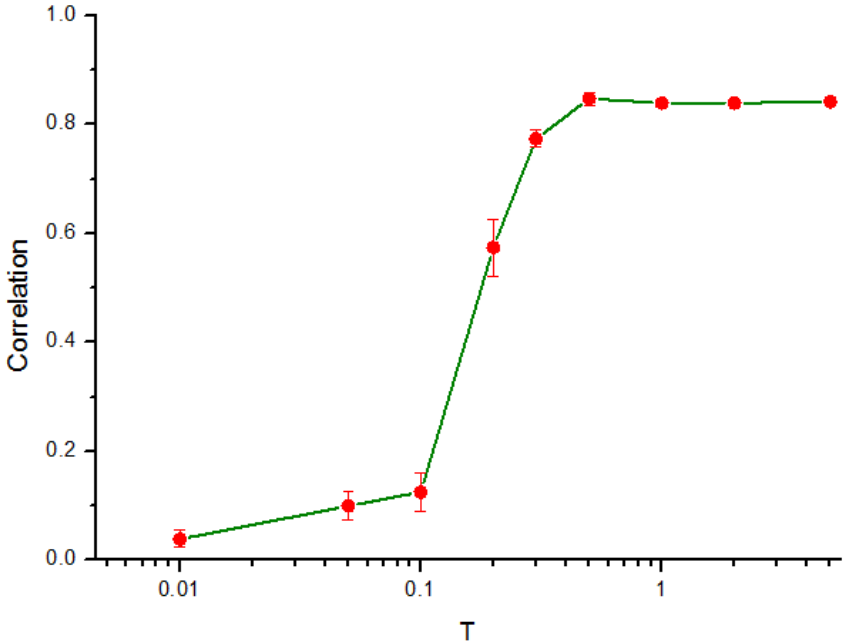




Quantum neuron

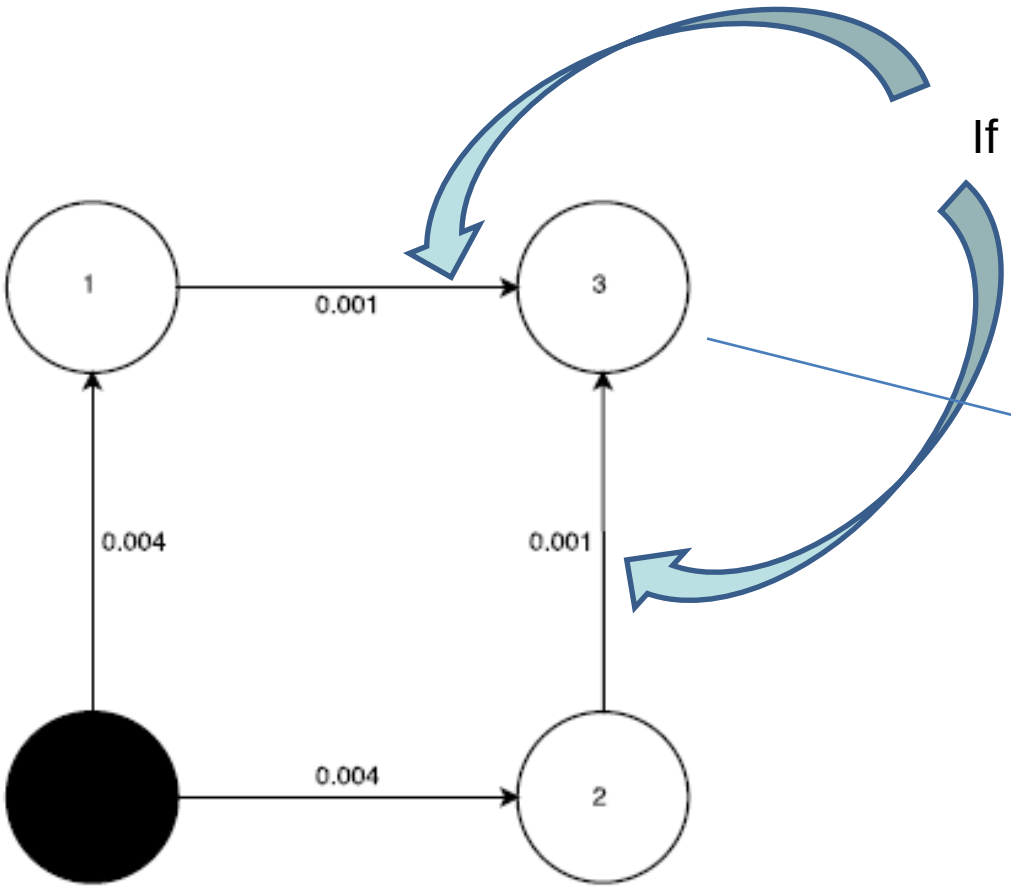




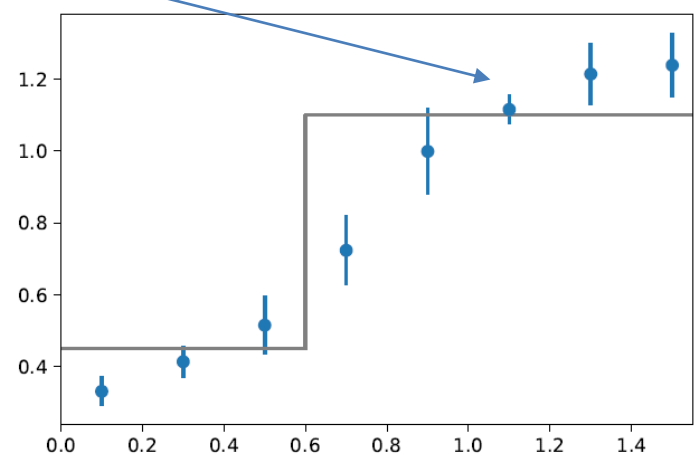


Quantum neural network logical elements

Logical AND

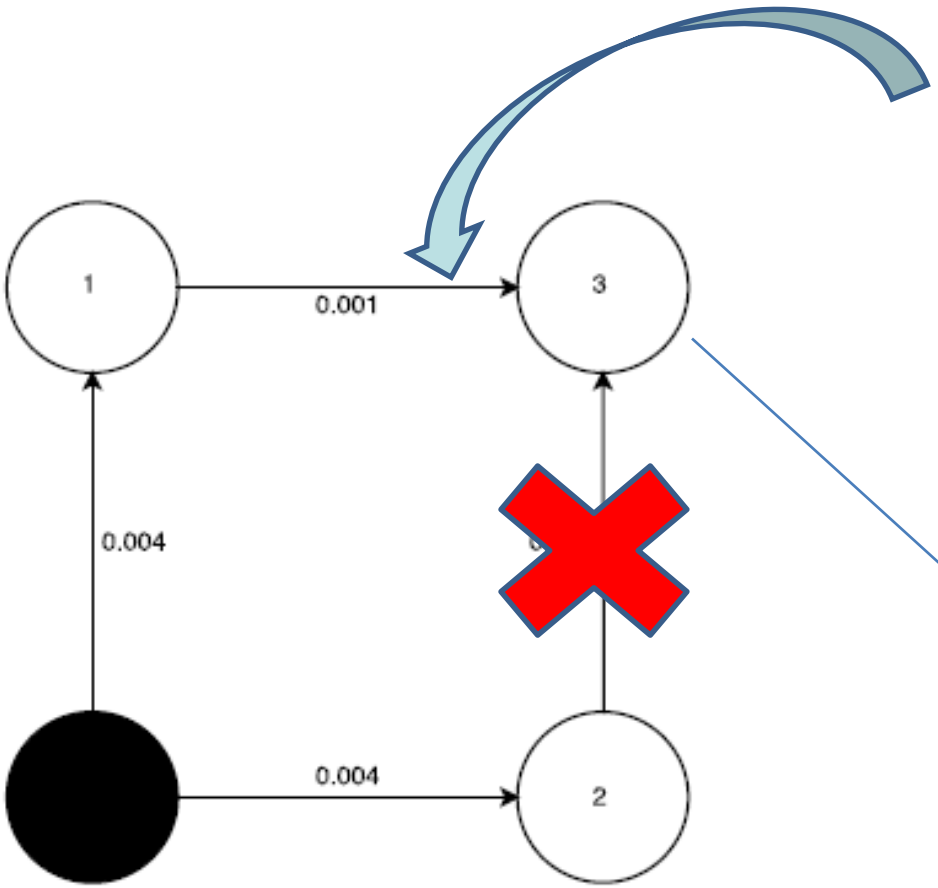


If both Paths are active,
Correlation more 70 %

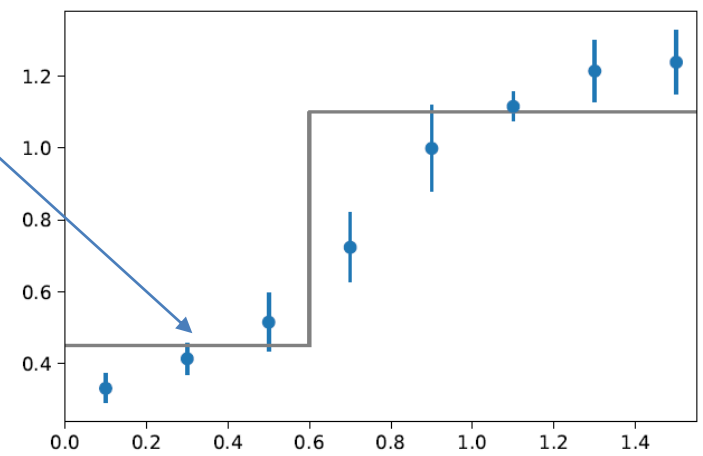


Quantum neural network logical elements

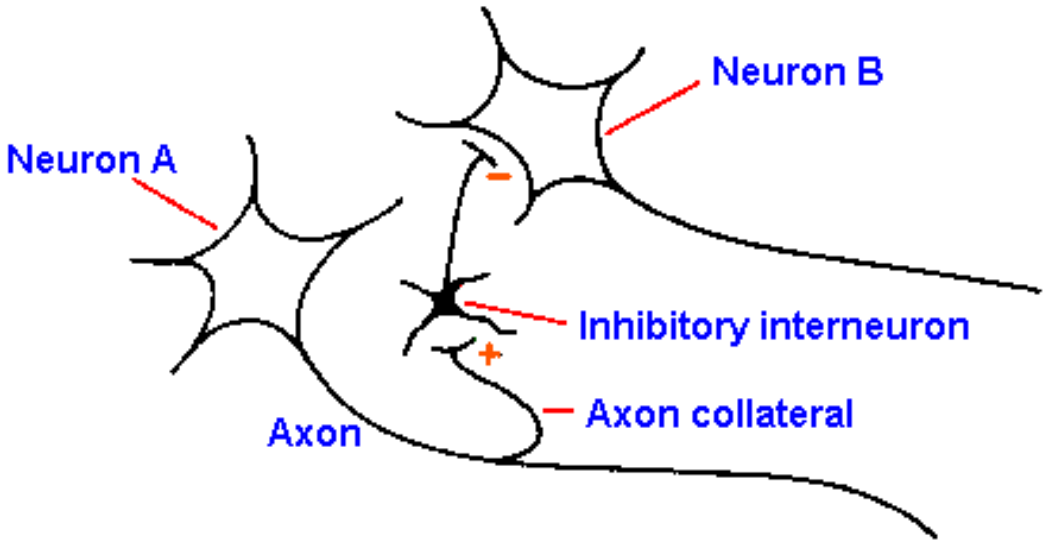
Logical AND



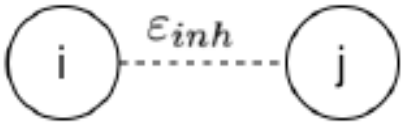
If only one Path is active,
Correlation less 20 %



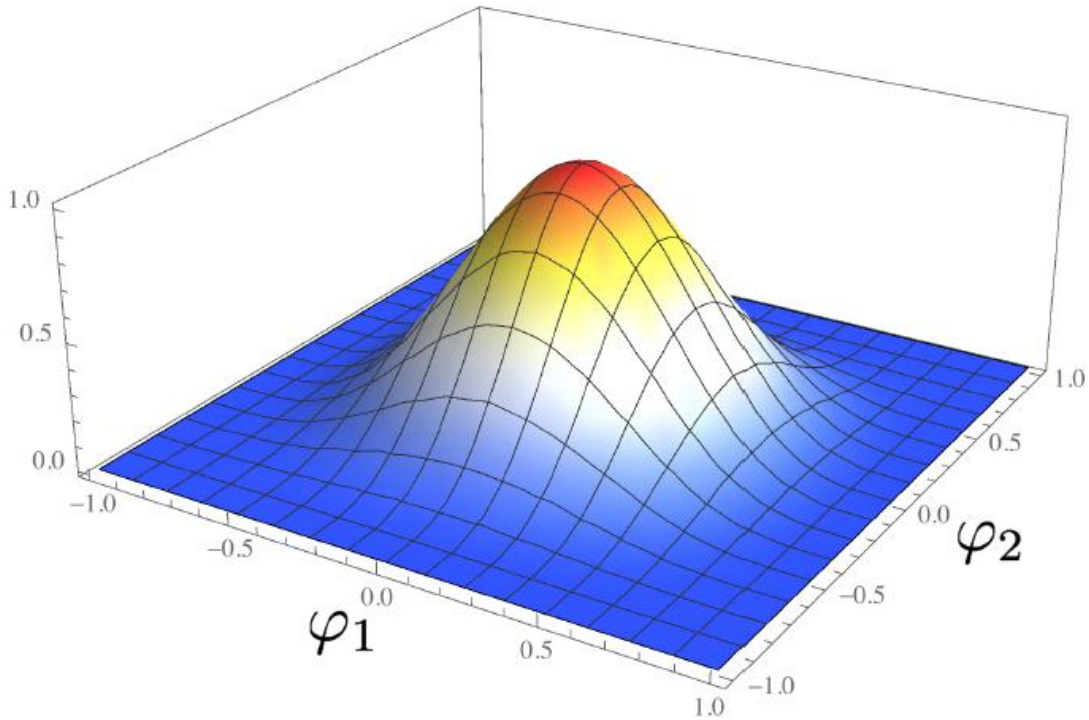
Inhibiting potential



Inhibiting potential

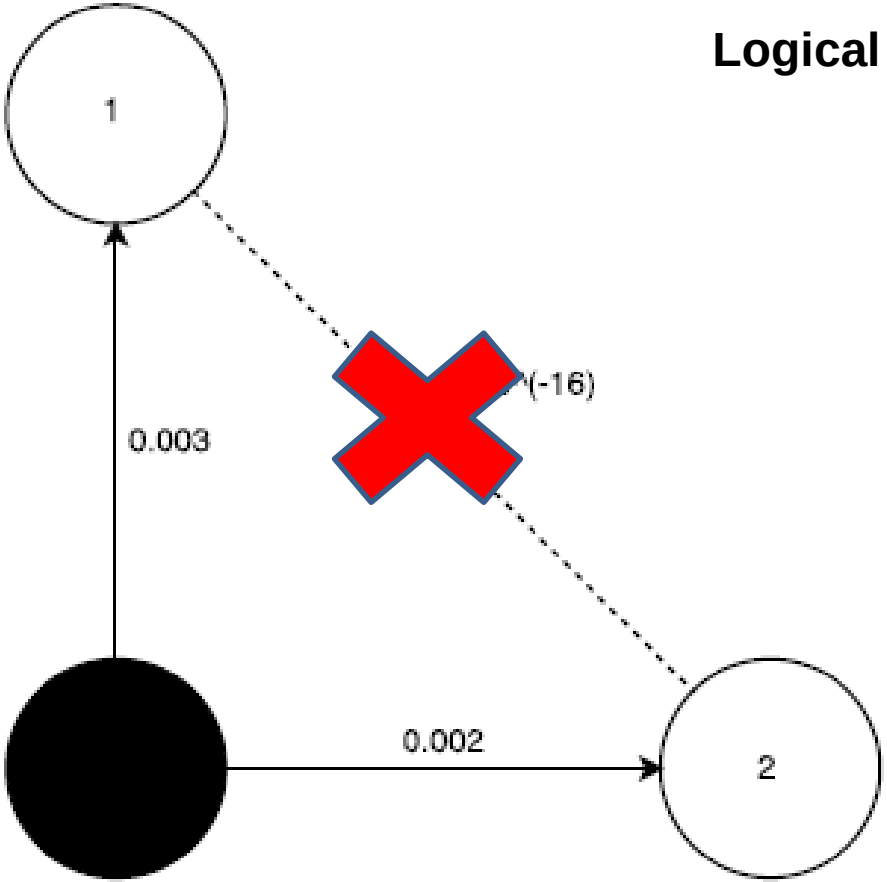


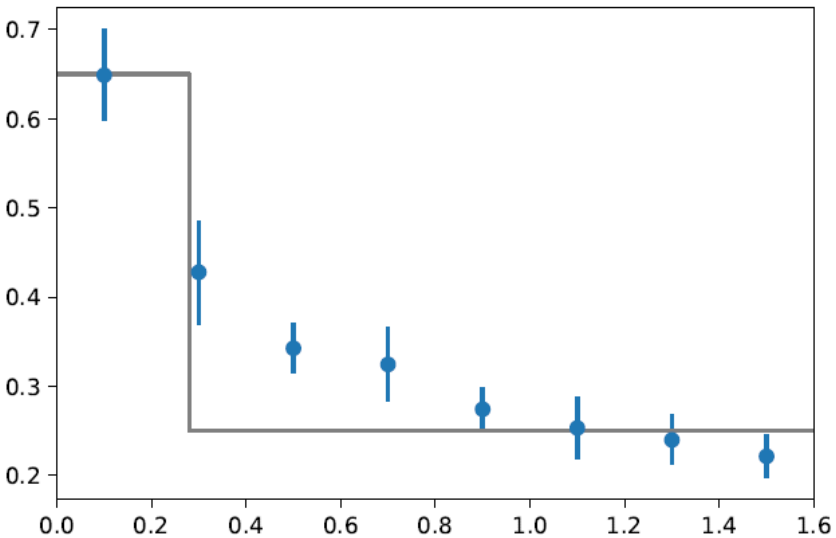
$$-\mathcal{L}_{int} = \varepsilon_{inh}\left(\varphi_i^2 - \frac{\mu^2}{\Lambda}\right)^4\left(\varphi_j^2 - \frac{\mu^2}{\Lambda}\right)^4$$



Quantum neural network logical elements

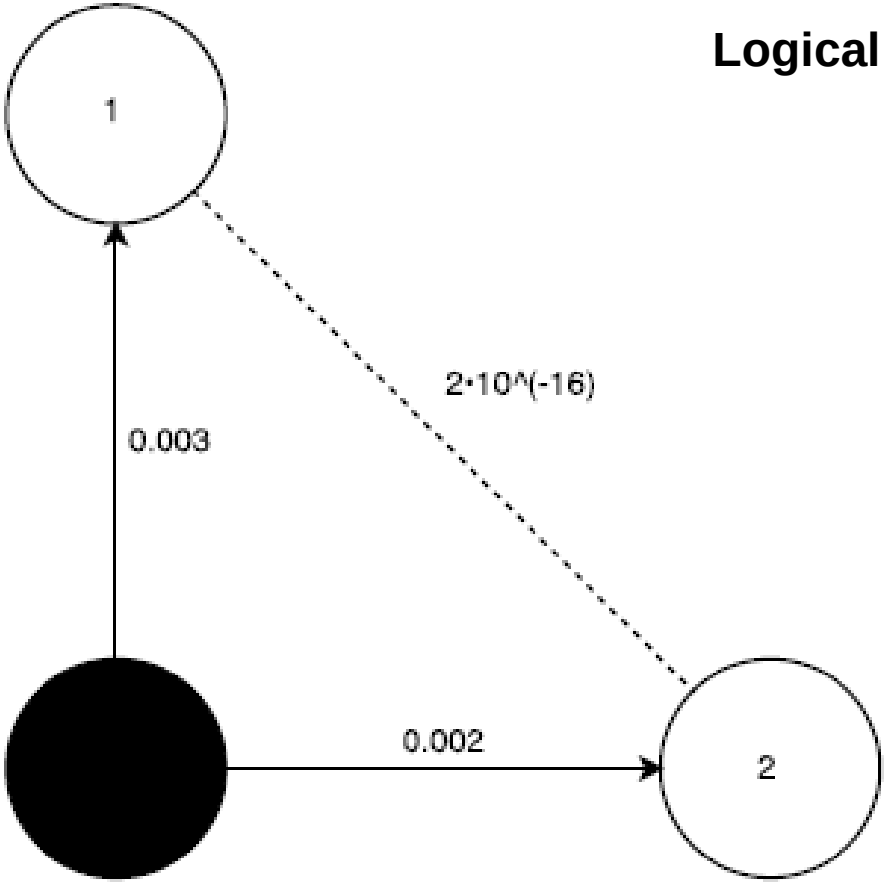
Logical NOT

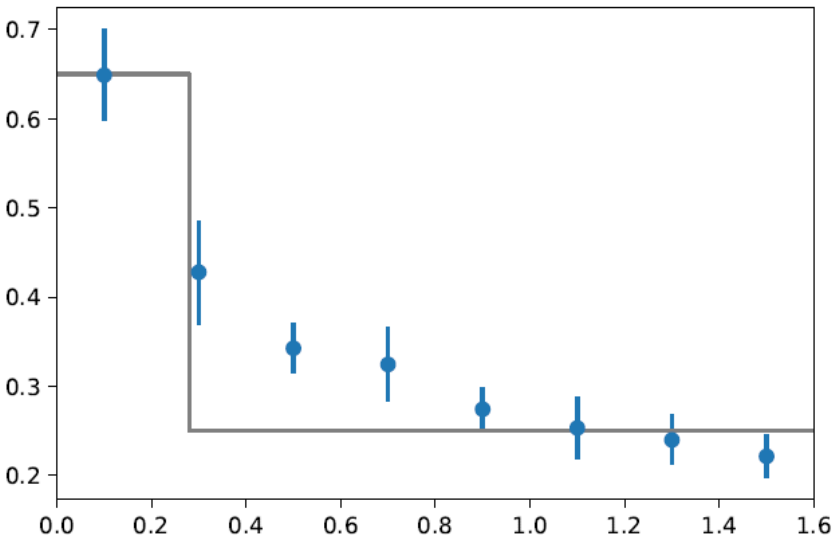




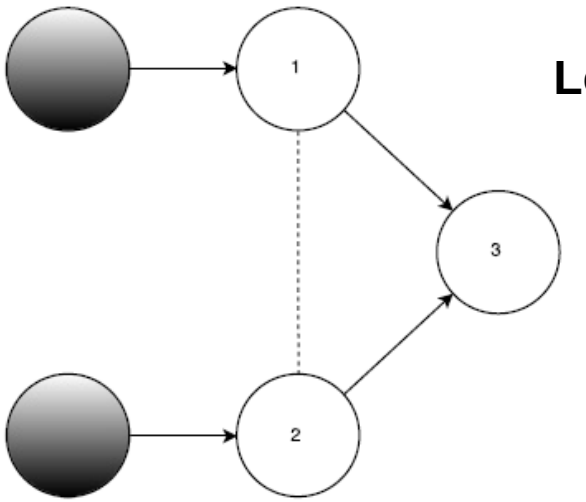
Quantum neural network logical elements

Logical NOT

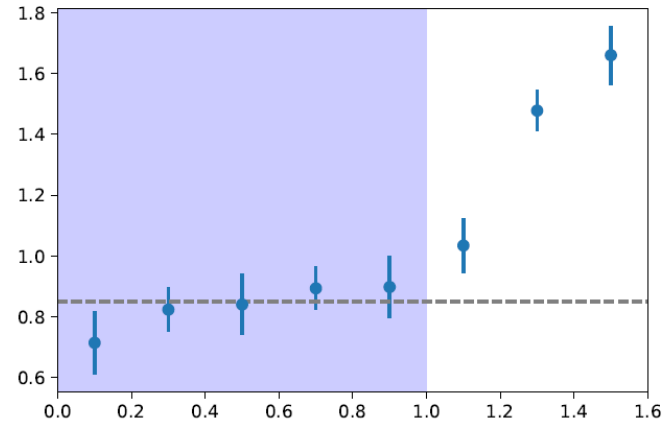




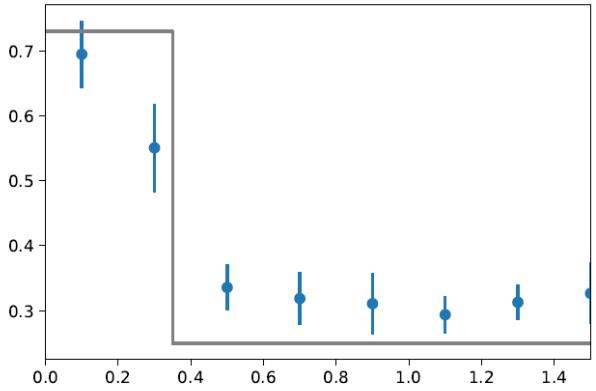
Quantum neural network logical elements

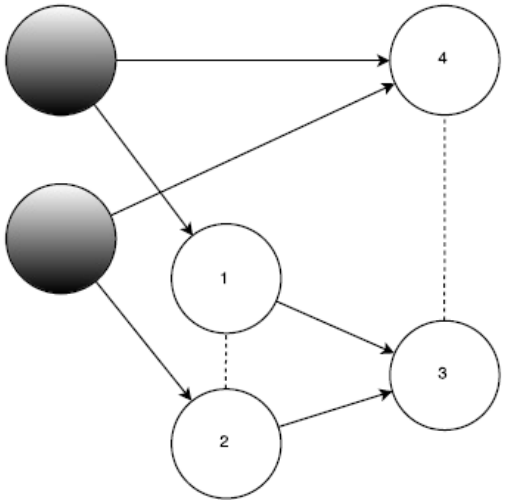


Logical OR

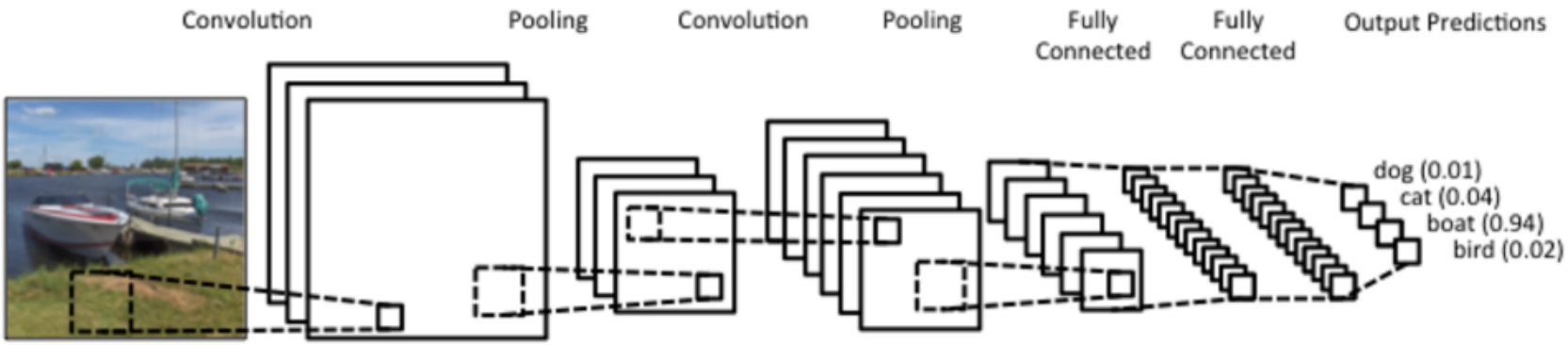


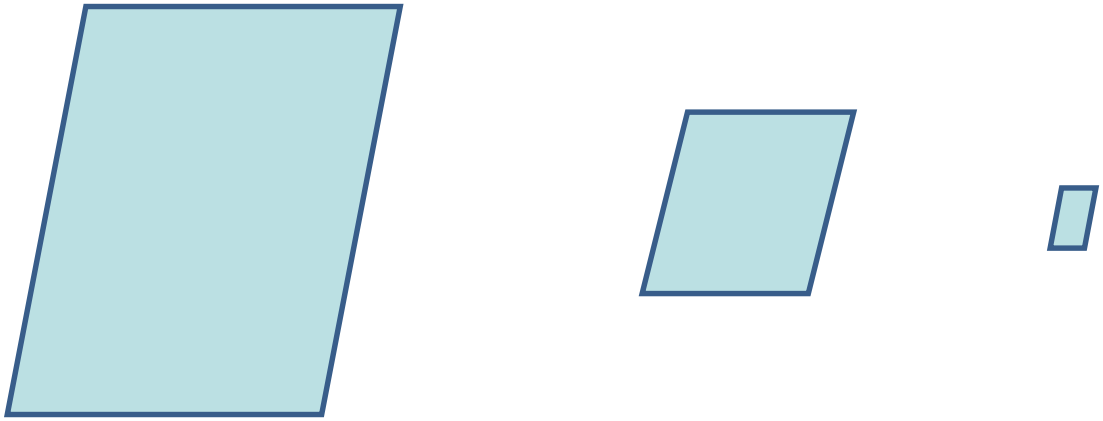
Logical exclusive OR (XOR)



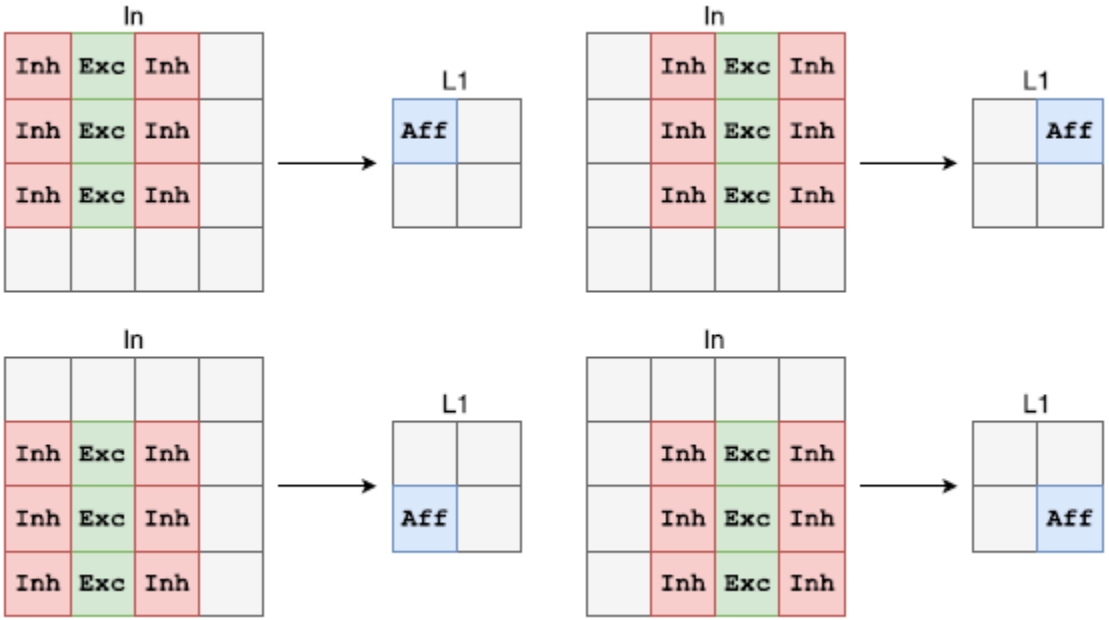


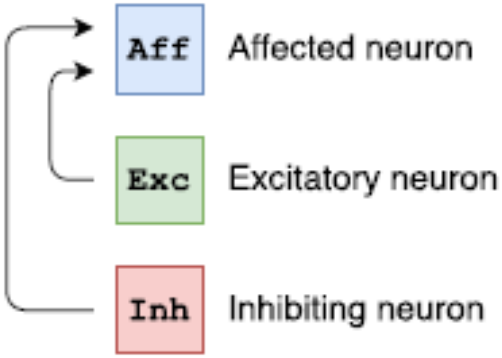
Convolution neural network



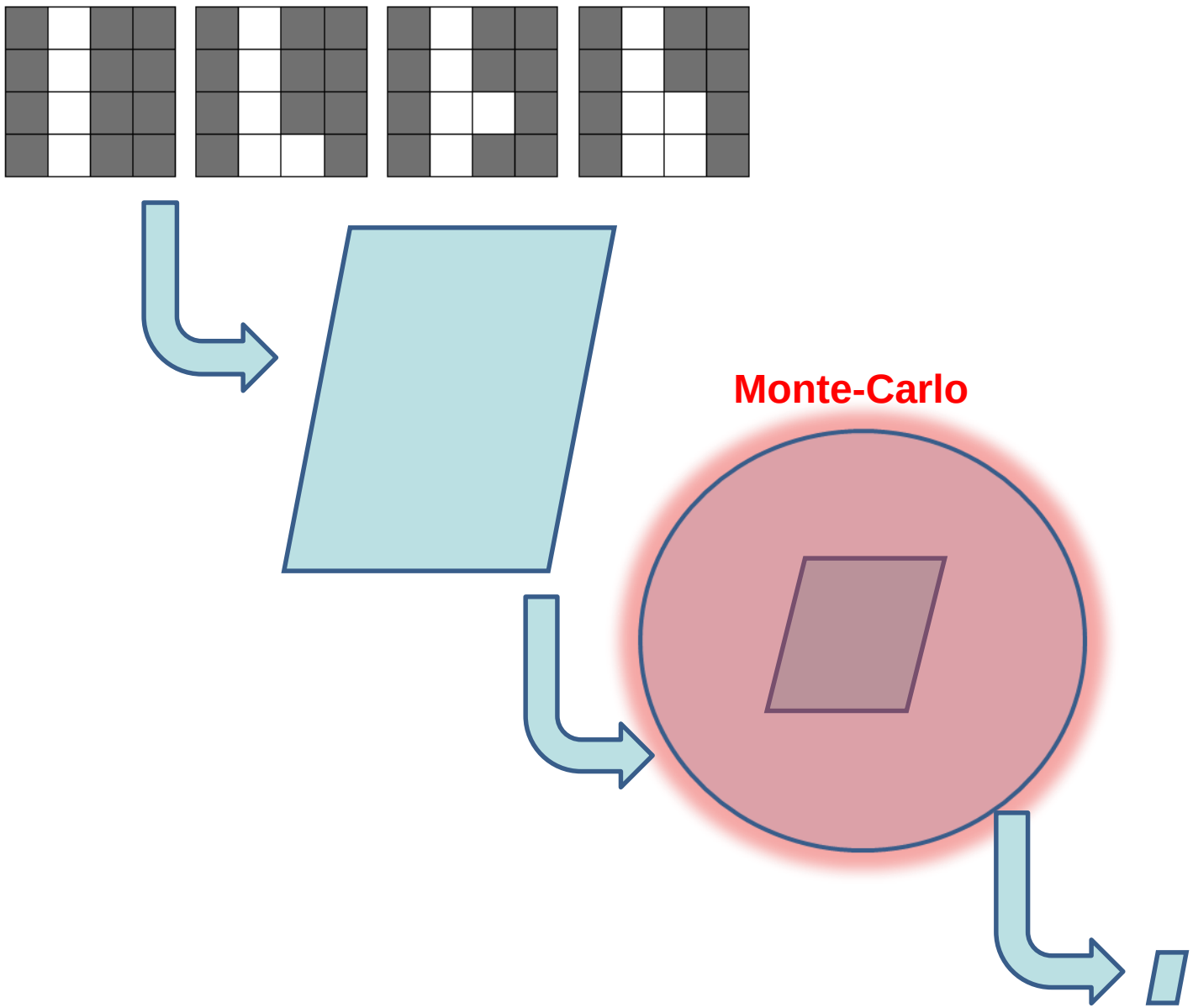


Convolution neural network

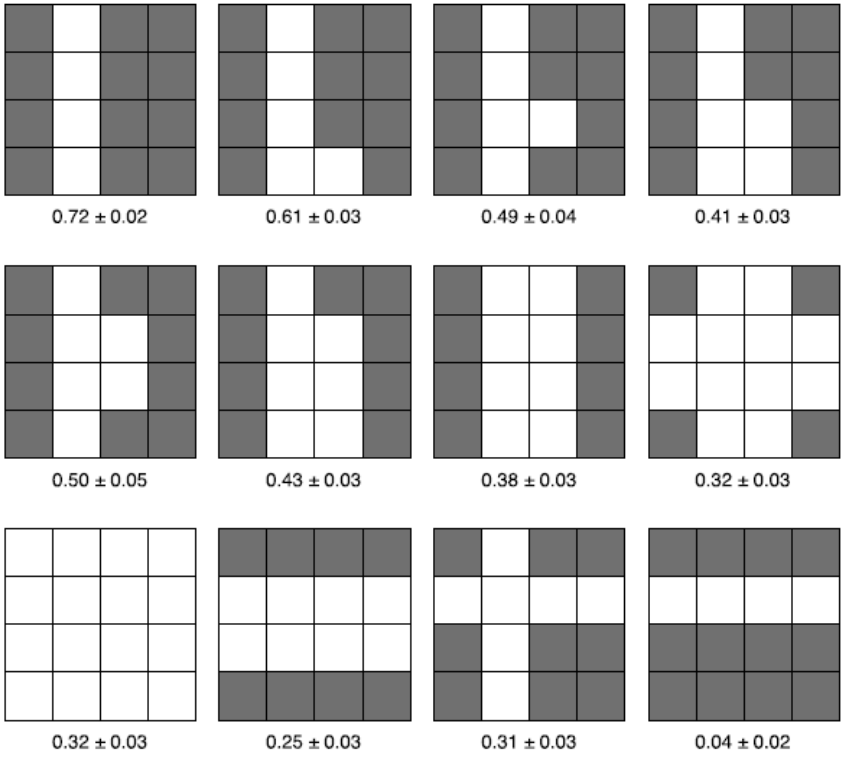


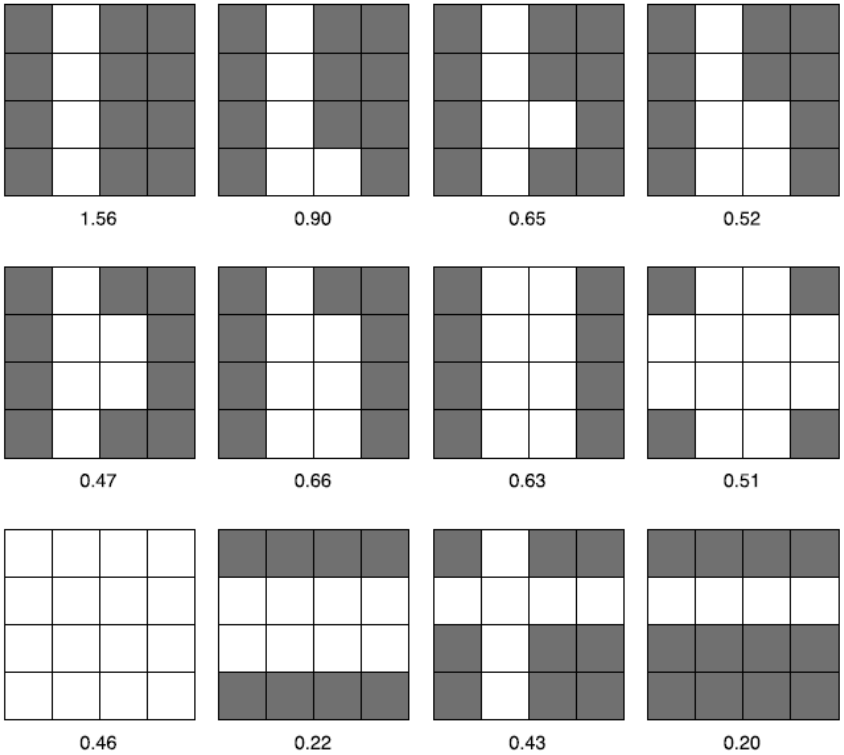


Convolution neural network



Convolution neural network

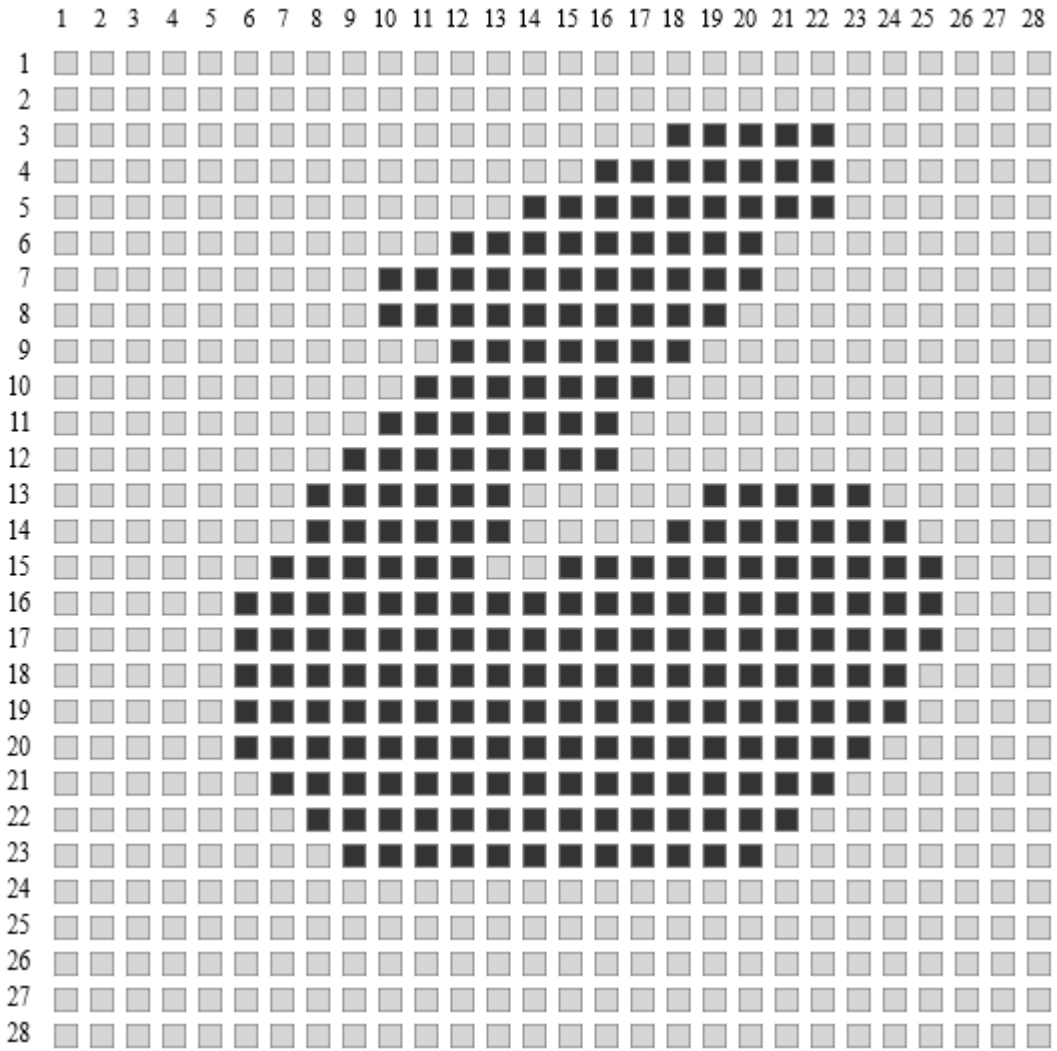




Digit recognition

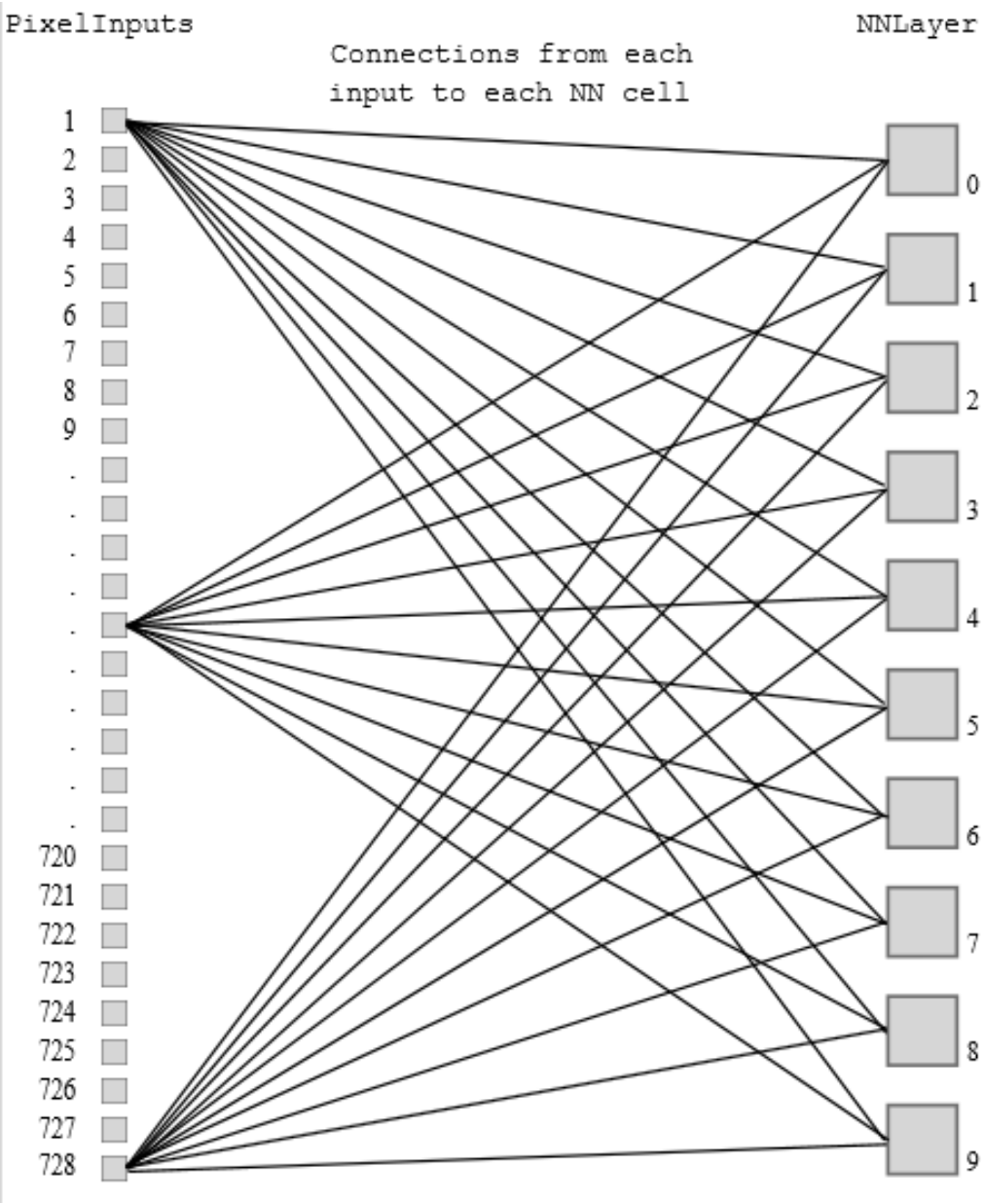
MNIST database

Digit recognition



MNIST database: **MNIST image has a size of 28*28 = 784 pixels**

Digit recognition



Digit recognition

$$\mathcal{L}_0 = \sum_{i=0}^{784} \left[\frac{1}{2}\dot{\psi}_i^2 + \frac{\Lambda}{4}\left(\psi_i^2 - \frac{\mu^2}{\Lambda}\right)^2 \right] + \sum_{j=0}^{10} \left[\frac{1}{2}\dot{\varphi}_j^2 + \frac{\Lambda}{4}\left(\varphi_j^2 - \frac{\mu^2}{\Lambda}\right)^2 \right]$$

$$\mathcal{L} = \mathcal{L}_0 + \sum_{i=0}^{784}\sum_{j=0}^{10} k\left(\varepsilon_{ij} - b\right) A_i \varphi_j^2 \left(\psi_i^2 - \frac{\mu^2}{\Lambda}\right)^2 + \\ + 10^{-17} \sum_{k>j}^{10}\sum_{j=0}^{10} \left(\varphi_j^2 - \frac{\mu^2}{\Lambda}\right)^4 \left(\varphi_k^2 - \frac{\mu^2}{\Lambda}\right)^4,$$

$$Z = \int \prod_i \mathcal{D}\varphi_i\left(\tau\right) \exp(-S(\varphi_i(\tau))), \varphi_i(0) = \varphi_i(T)$$

Digit recognition

$X \in \mathbb{R}^{N \times M}$ brightness of j-th pixel in i-th image.

$$S = XW$$

score of i-th image treated as j-th number.

$$p_{ij} = \frac{exp(S_{ij})}{\sum_{j=0}^{9} (exp(S_{ij}))}.$$

$$\mathcal{L} = -\frac{1}{N} \sum_{i=0}^{N-1} ln(p_{ij}) \delta^{i}_{correct} + \lambda \sum_{i=0}^{M-1} \sum_{j=0}^{9} max(-W_{ij}, 0), \lambda \to \infty$$

Digit recognition

$$\hat{\psi}_i = \hat{\psi}(b_i) = \sqrt{\sqrt{b_i}\psi^2 - \sqrt{b_i} + 1}$$

$$\hat{\varepsilon}_{ij}\varphi_j^2\left(\hat{\psi}_i^2 - 1\right)^2 = \hat{\varepsilon}_{ij}b_i\varphi_j^2\left(\psi_i^2 - 1\right)^2 = \varepsilon_{ij}\varphi_j^2\left(\psi_i^2 - 1\right)^2$$

We can now use W as connection matrix for ε connecting input and output

Digit recognition

```
P(0) = 0.338608
P(6) = 0.13097
P(7) = 0.104982
P(2) = 0.0962352
P(5) = 0.0873339
P(4) = 0.0781002
P(9) = 0.0714371
P(3) = 0.0662971
P(8) = 0.0260371
P(1) = 0
```

```
P(1) = 0.655741
P(8) = 0.0840482
P(3) = 0.0834241
P(2) = 0.0605042
P(7) = 0.0424982
P(0) = 0.037828
P(4) = 0.0180404
P(9) = 0.0130295
P(6) = 0.00488656
P(5) = 0
```

```
P(2) = 0.451795
P(6) = 0.207845
P(3) = 0.12158
P(5) = 0.0695778
P(0) = 0.0440336
P(8) = 0.0399262
P(9) = 0.0267228
P(7) = 0.0263385
P(4) = 0.012181
P(1) = 0
```

```
P(4) = 0.362327
P(8) = 0.16814
P(2) = 0.14839
P(1) = 0.104967
P(9) = 0.0852715
P(3) = 0.0759215
P(5) = 0.0338338
P(6) = 0.0196095
P(0) = 0.00153889
P(7) = 0
```

```
P(7) = 0.605863
P(9) = 0.153816
P(8) = 0.0527513
P(3) = 0.0501808
P(1) = 0.0482902
P(0) = 0.0334645
P(5) = 0.0295938
P(2) = 0.0167923
P(4) = 0.00924887
P(6) = 0
```

Основные результаты

был построен формализм для исследования квантовых эффектов в релятивистских и нерелятивистских системах многих частиц, построены эффективные численные алгоритмы Монте-Карло моделирования таких систем, которые были протестированы на примере модельной задачи о релятивистском гармоническом осцилляторе;

с помощью разработанных численных методов Монте-Карло интегрирования была исследована актуальная задача о фазовом повелении атомарного металлического водорода, построено уравнение состояния этой системы;

построен решеточный формализм исследования вакуумных эффектов в квантовой электродинамике, разработаны алгоритма учета влияния различных граничных условий, диэлектрических особенностей среды, температурных эффектов на величину казимировский вакуумных сил, исследована важная для наномеханики задача о тангенциальных (касательных) силах Казимира и реечной передачи механического воздействия без зацепления за счет вакуумных сил;

Основные результаты

методы Монте-Карло моделирования эффекта Казимира в теории поля были перенесены в исследовании критических сил Казимира в классических спиновых системах, были исследованы критические силы взаимодействия двух дефектов, притяжение (конфаймент) уединенного дефекта к дефектной линии, взаимодействие двух дефектов, притянутых к одной линии, а также дефекта и анти-дефекта (разрыва в дефектной линии), рассмотрен процесс коллапса систем дефектов в кластер, исследовано влияние искривленности дефектной линии на ее казимировскую энергию;

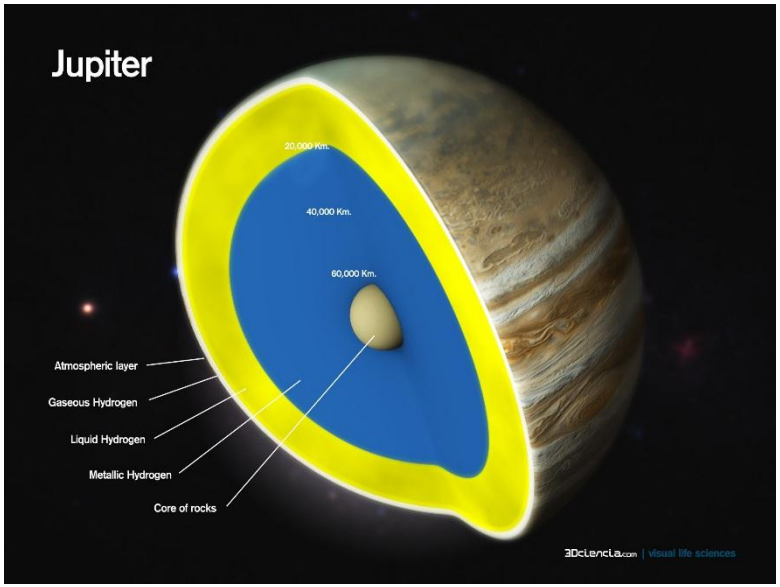
разработаны теоретико-полевые и решеточные монте-карловские методы исследования фазовых и критических явлений в графене, исследована фазовая картина перехода в состояния со спонтанным зарядовым разделением (экситонный конденсат) в графене как функция параметром системы, рассмотрен случай как
листа графена, так и графеновых нанолент, теоретико-полевыми решеточными методами исследована фазовая картина перехода в разделенное по спину состояние (антиферромагнитных конденсат), исследовано влияние внешних факторов среды (диэлектрических свойств подложки, внешнего магнитного поля, концентрации дефектов) на эту фазовую картину;

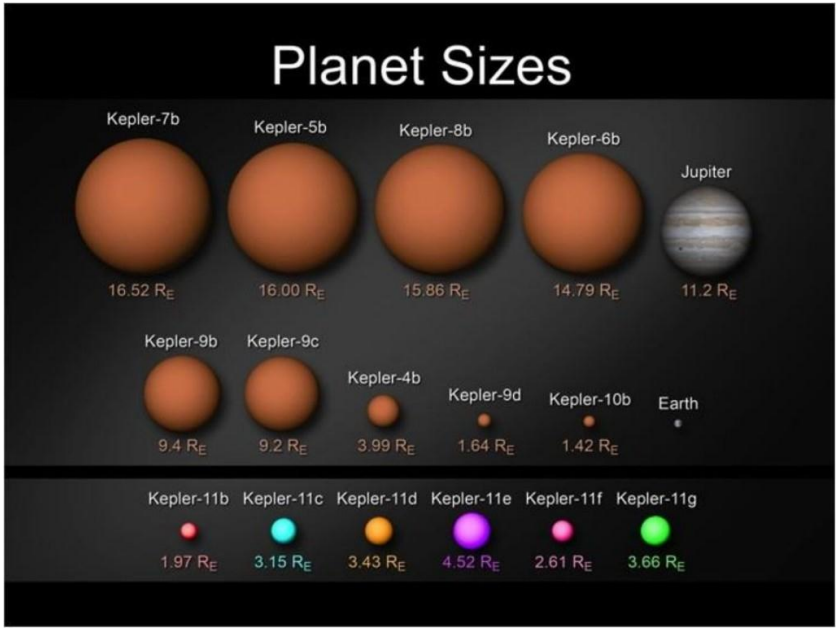
предложена схема создания базовых элементов спинтроники на основе критических явлений в графене;

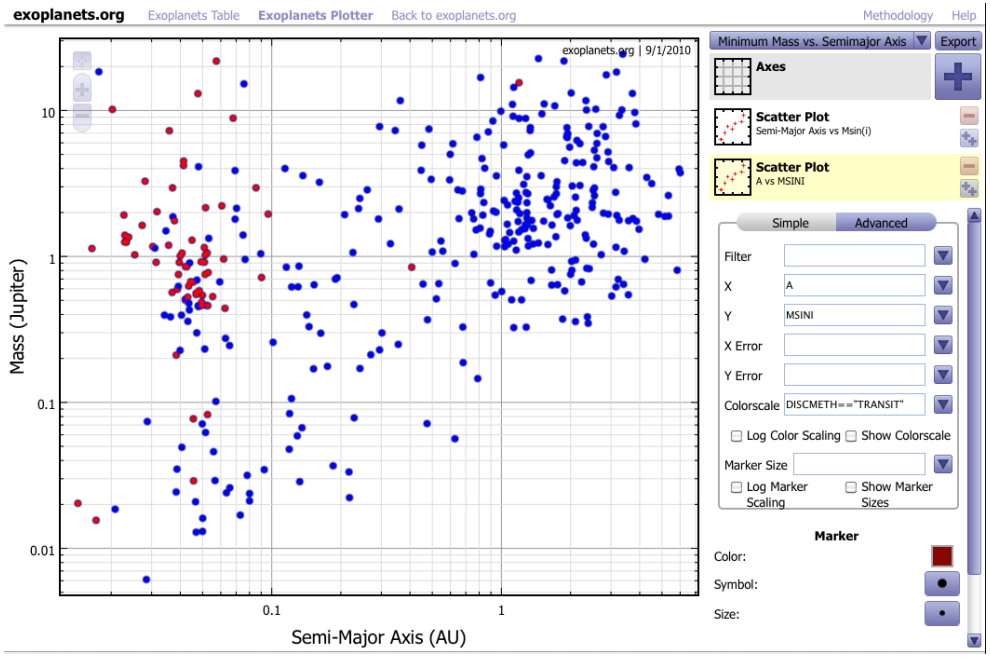
Темы исследований

Металлический водород

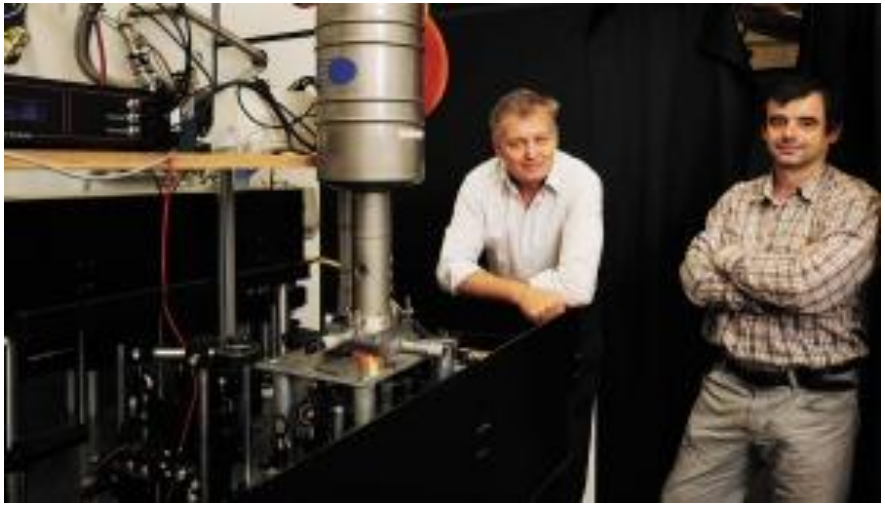
Металлический водород



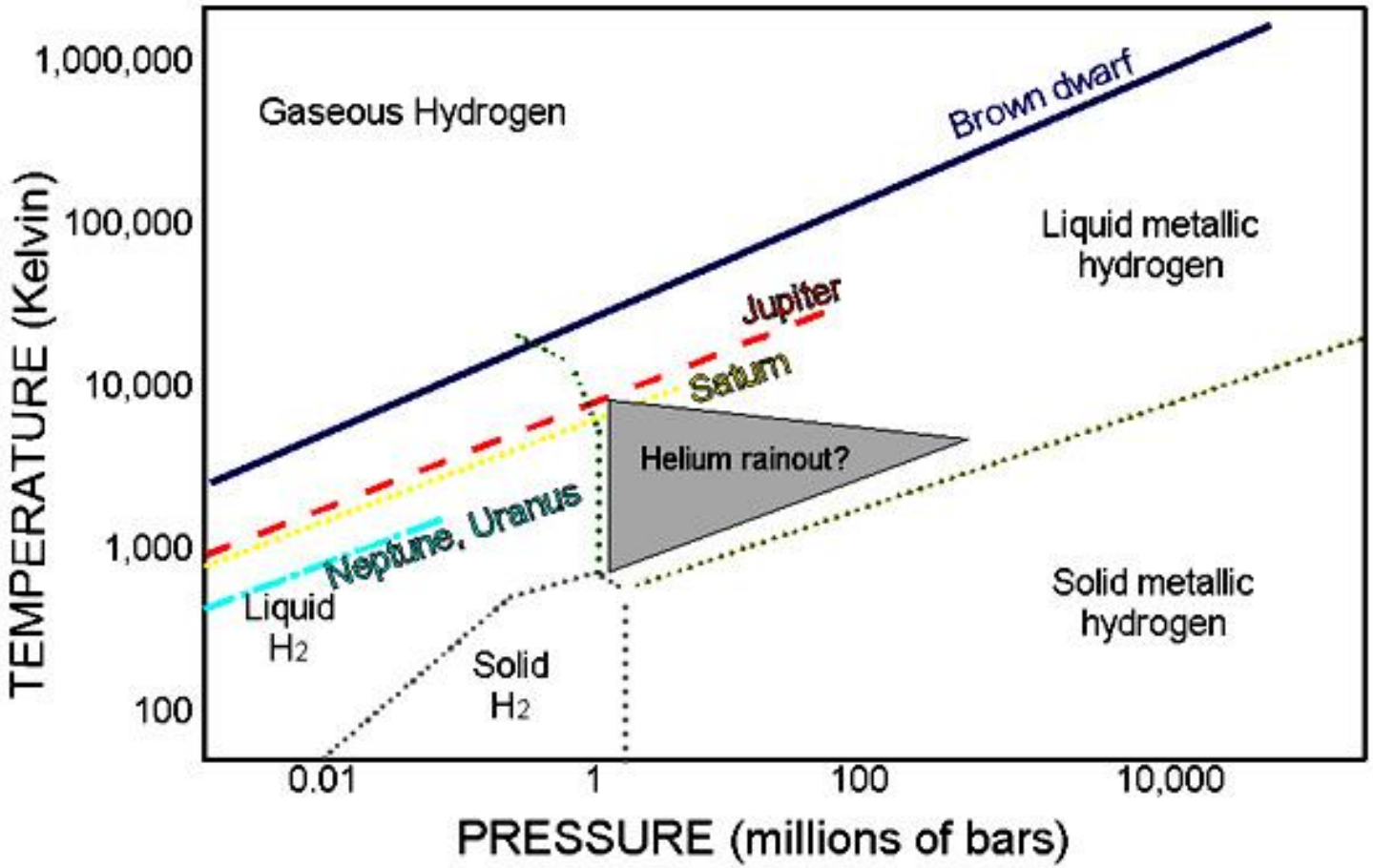




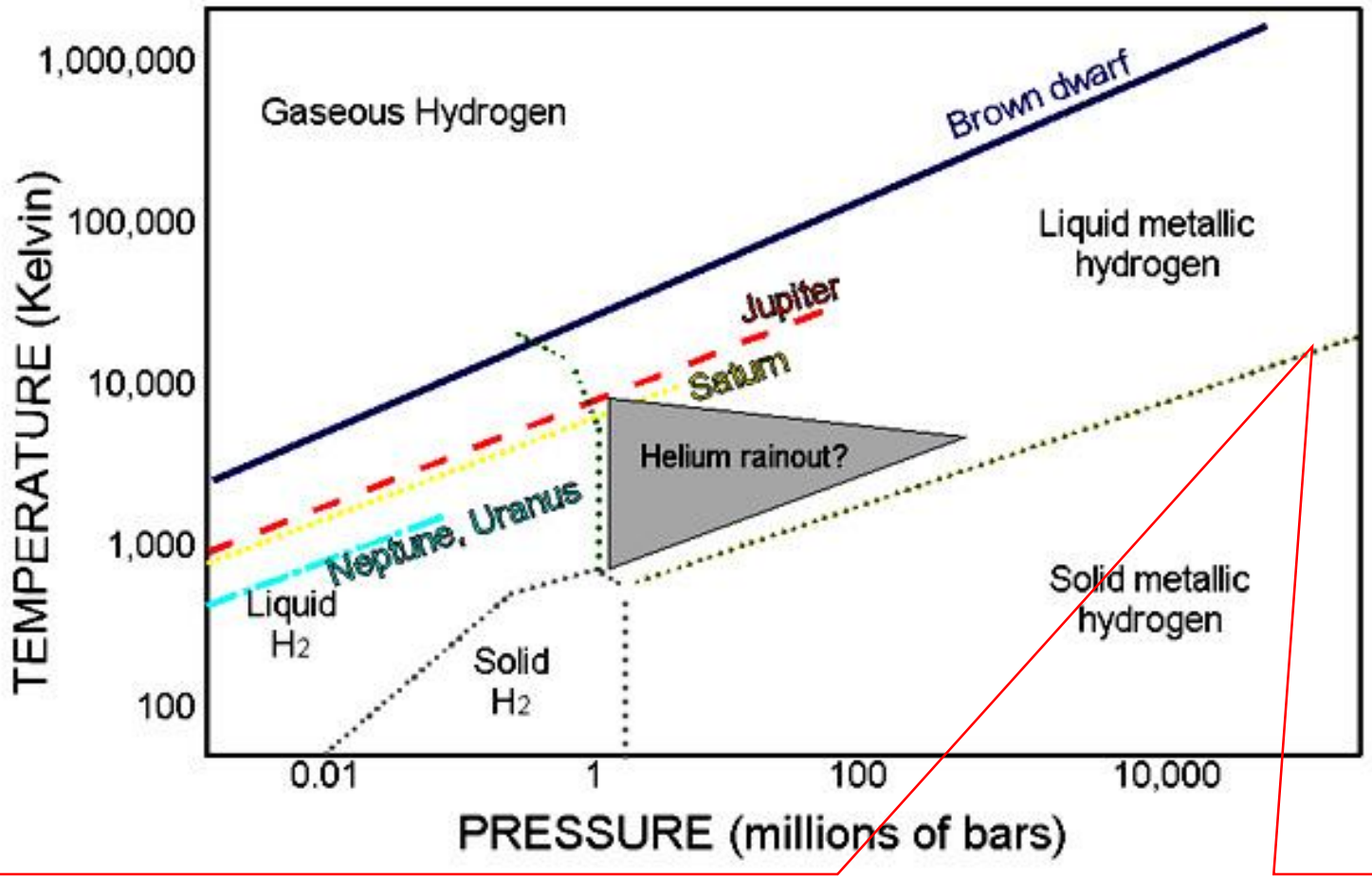
Металлический водород на Земле



Водород при высоких давлениях

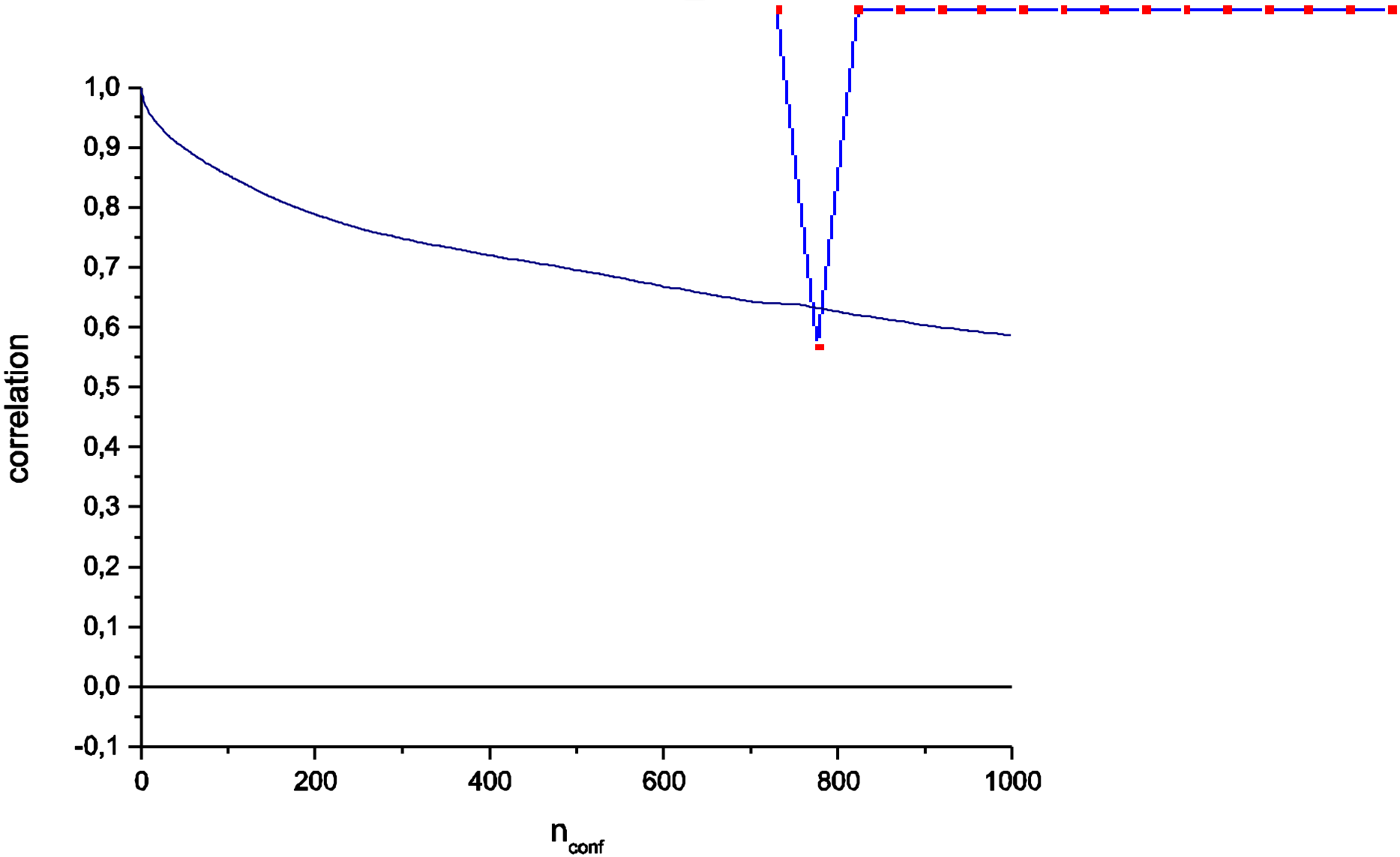


Водород при высоких давлениях

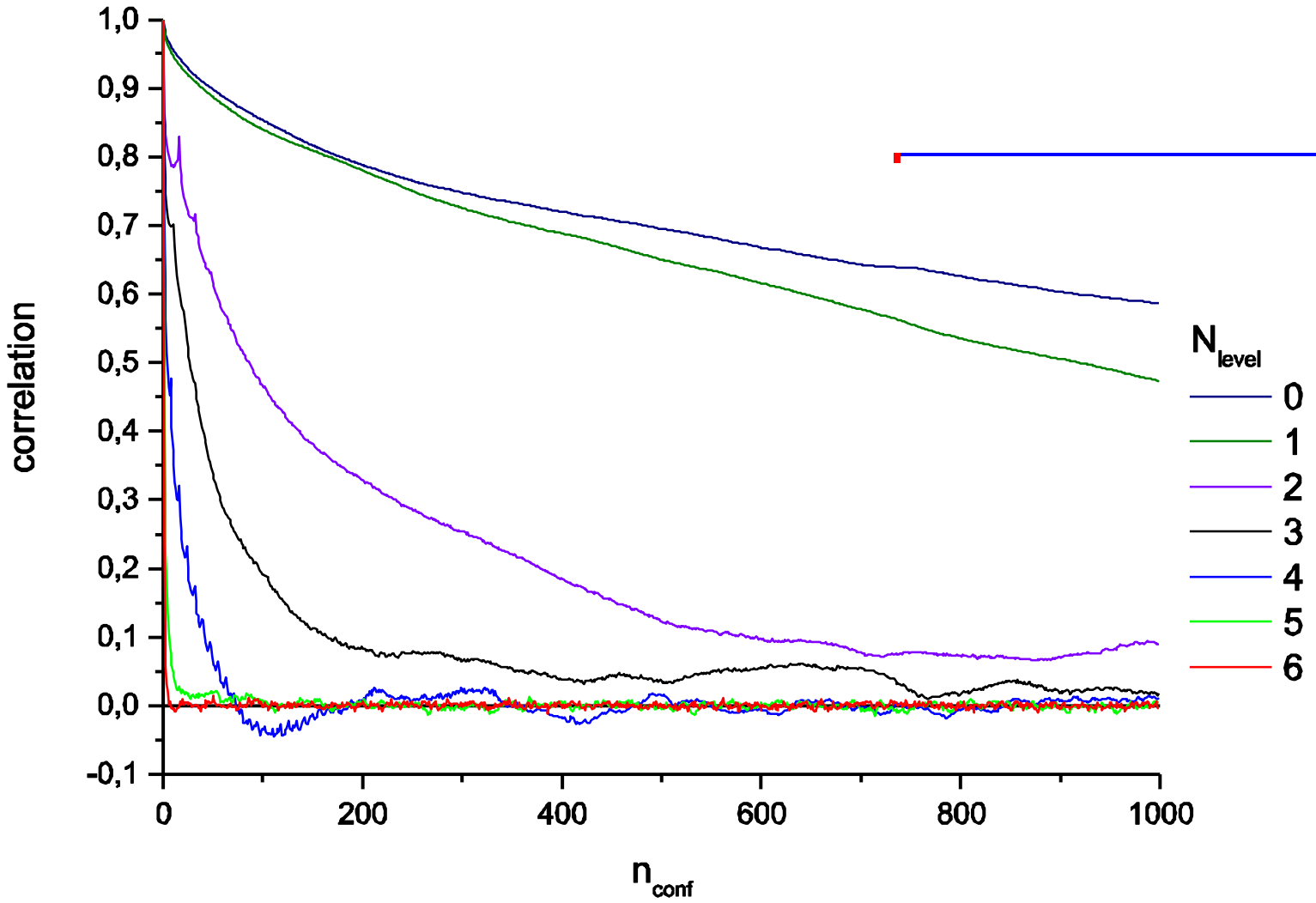


Вигнеровский кристалл протонов $$V(r) = \frac{e^2}{r}\exp\{-r/R\}$$

Алгоритм


1,0
0,9
0,8
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0,0
-0,1
correlation
0
200
400
600
800
1000
n conf

Многоуровневый алгоритм



Вычисление наблюдаемых

- Кинетическая энергия
- Давление

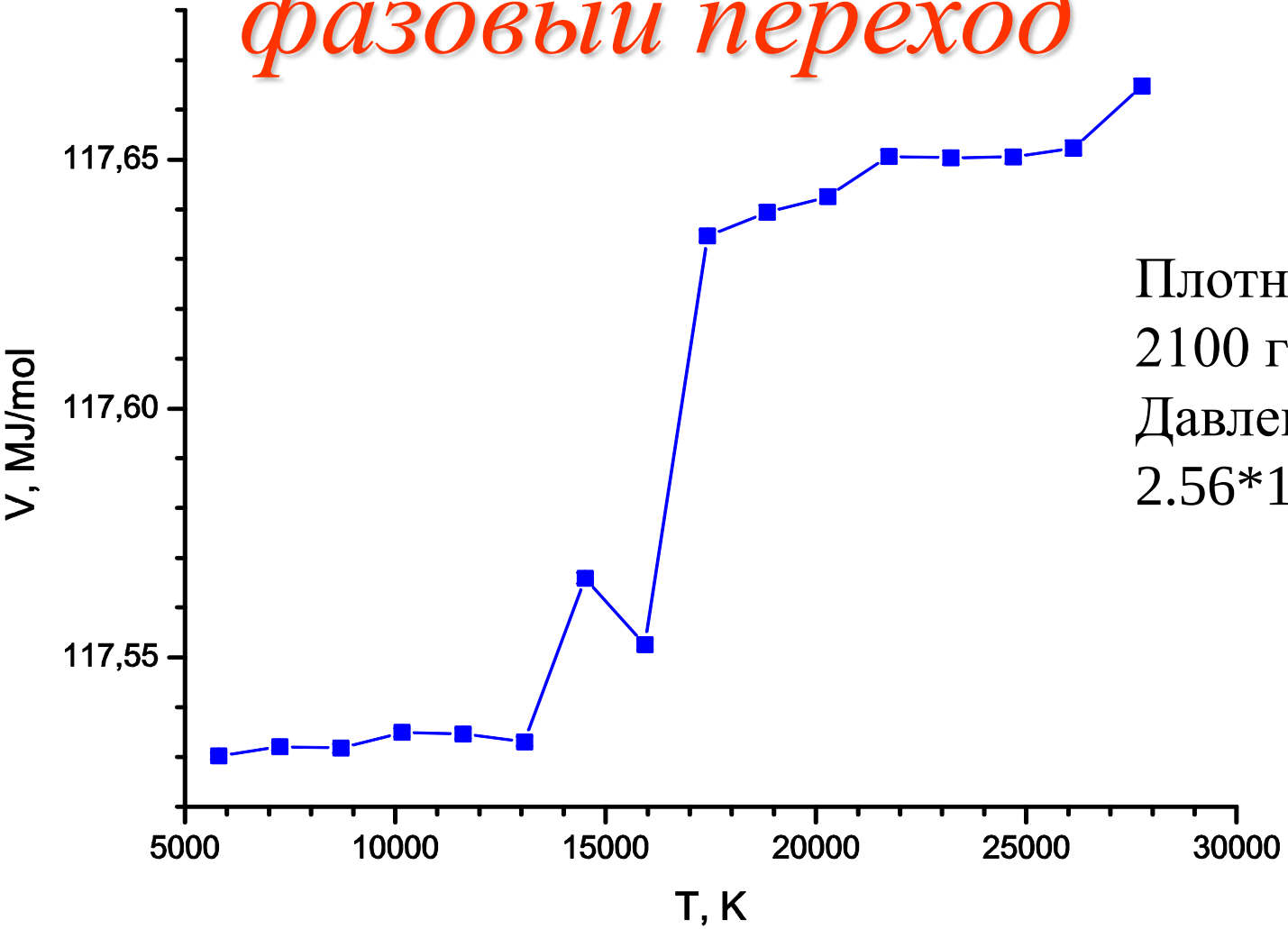
$$\langle K \rangle = \left\langle \frac{m(v_i - v_{cm})^2}{2} + \frac{m}{2} \right\rangle$$

$$\langle P \rangle = \frac{1}{3L^3} \left\langle \left(mv^2 + \sum_{ij} \frac{r_{ij} \cdot F_{ij}}{} \right) \right\rangle$$

- Потенциальная энергия рассчитывалась как сумма энергий взаимодействия протонов

Атомарный металлический водород:

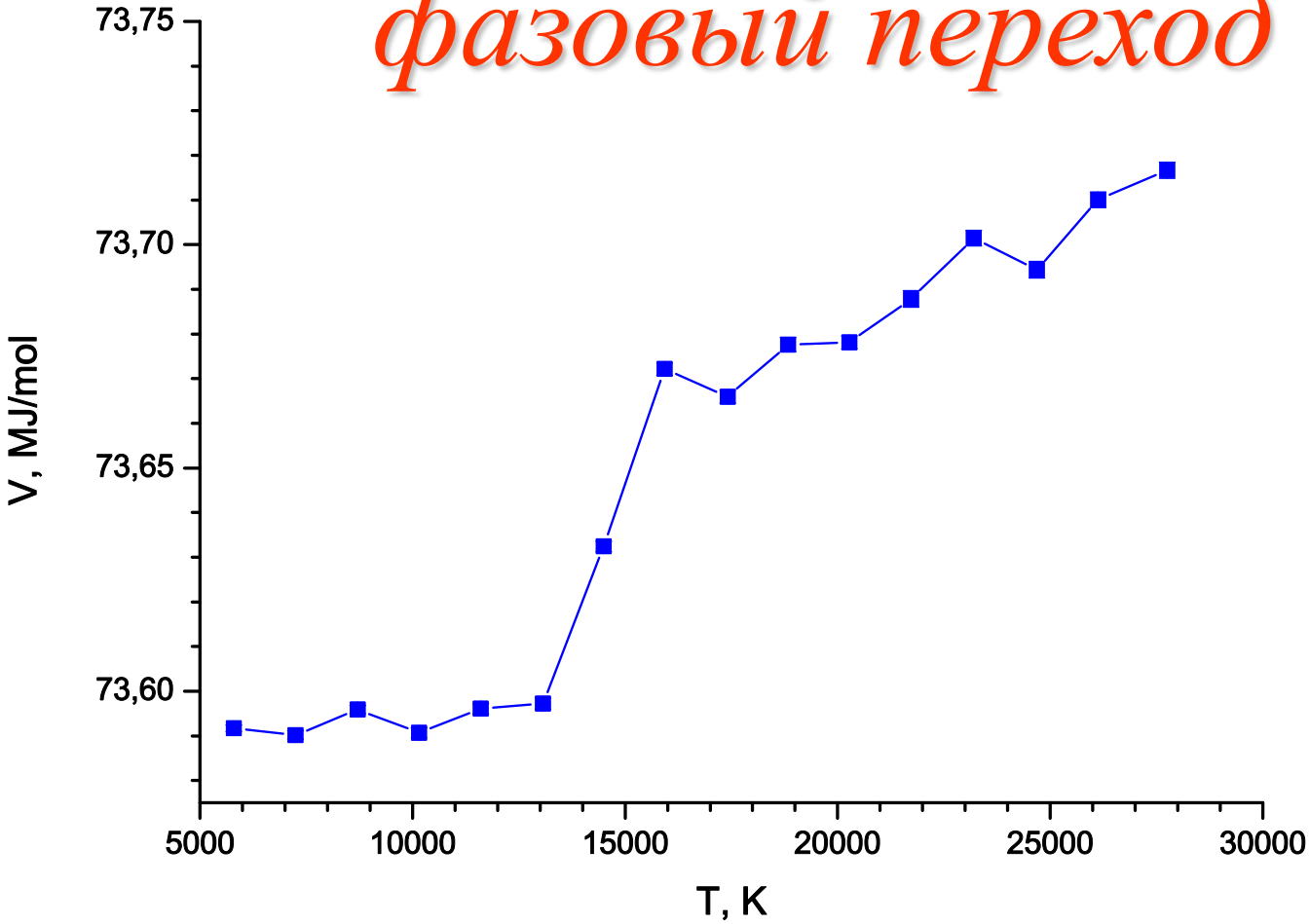
фазовый переход



Плотность:
2100 г/см^3
Давление:
2.56*10^{17} Па

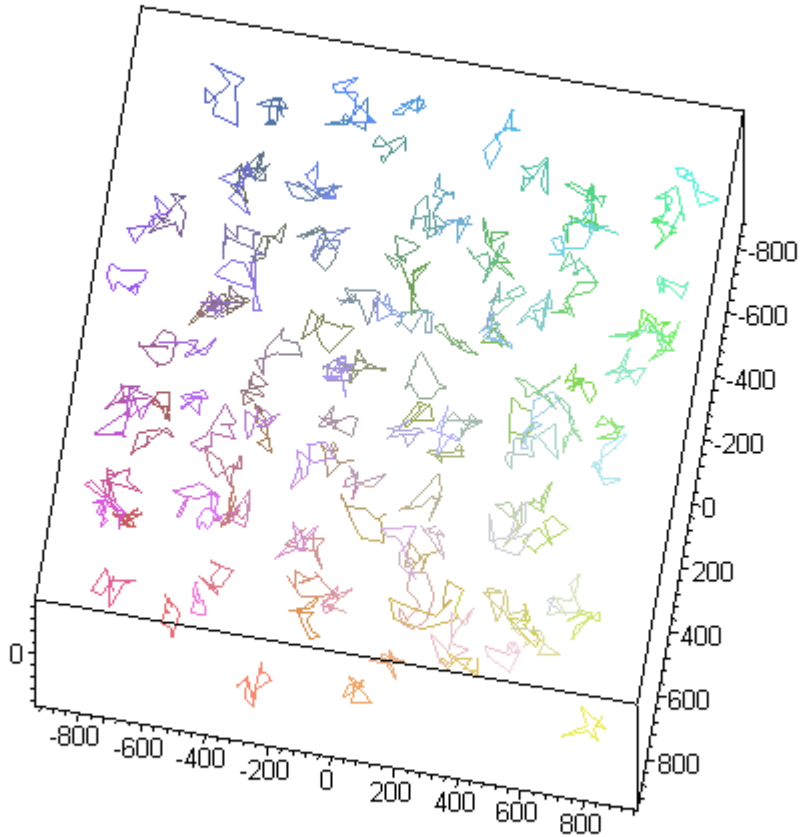
Атомарный металлический водород:

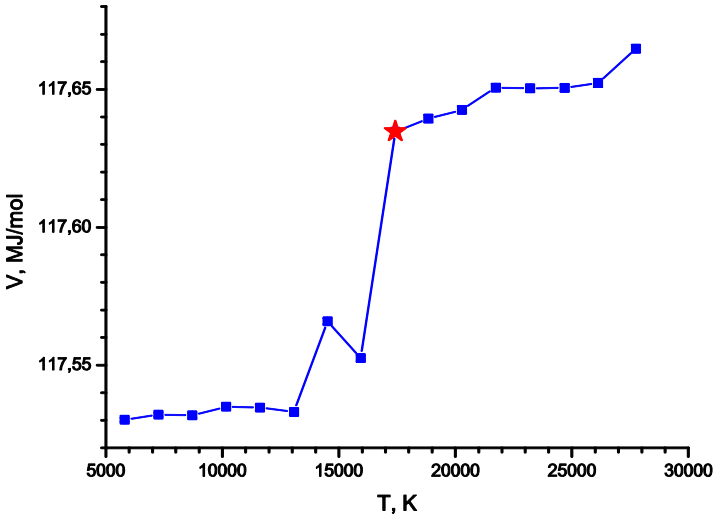
фазовый переход



Плотность:
1075 г/см^3
Давление:
0.84*10^{17} Па

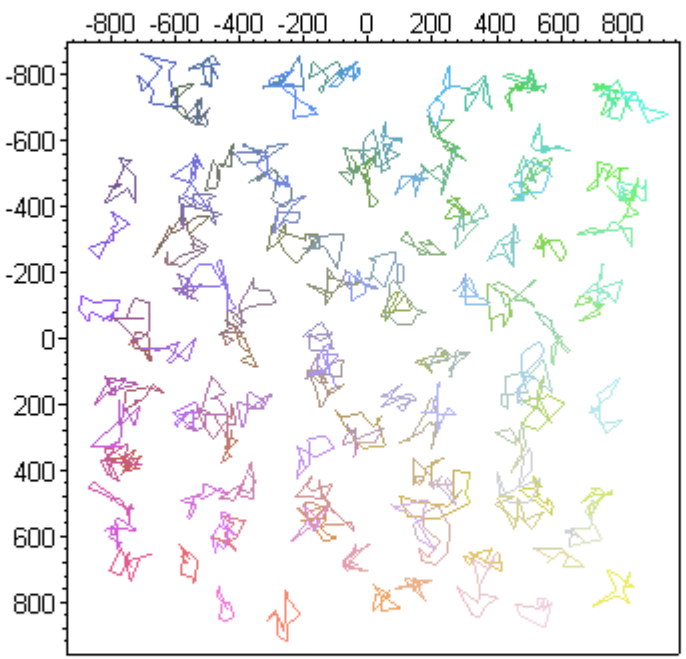
Атомарный металлический водород

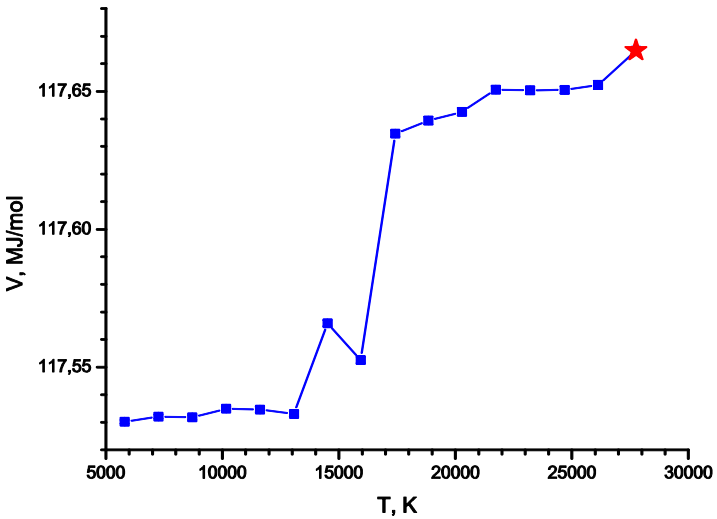




$$T = 17 \cdot 10^3 K$$

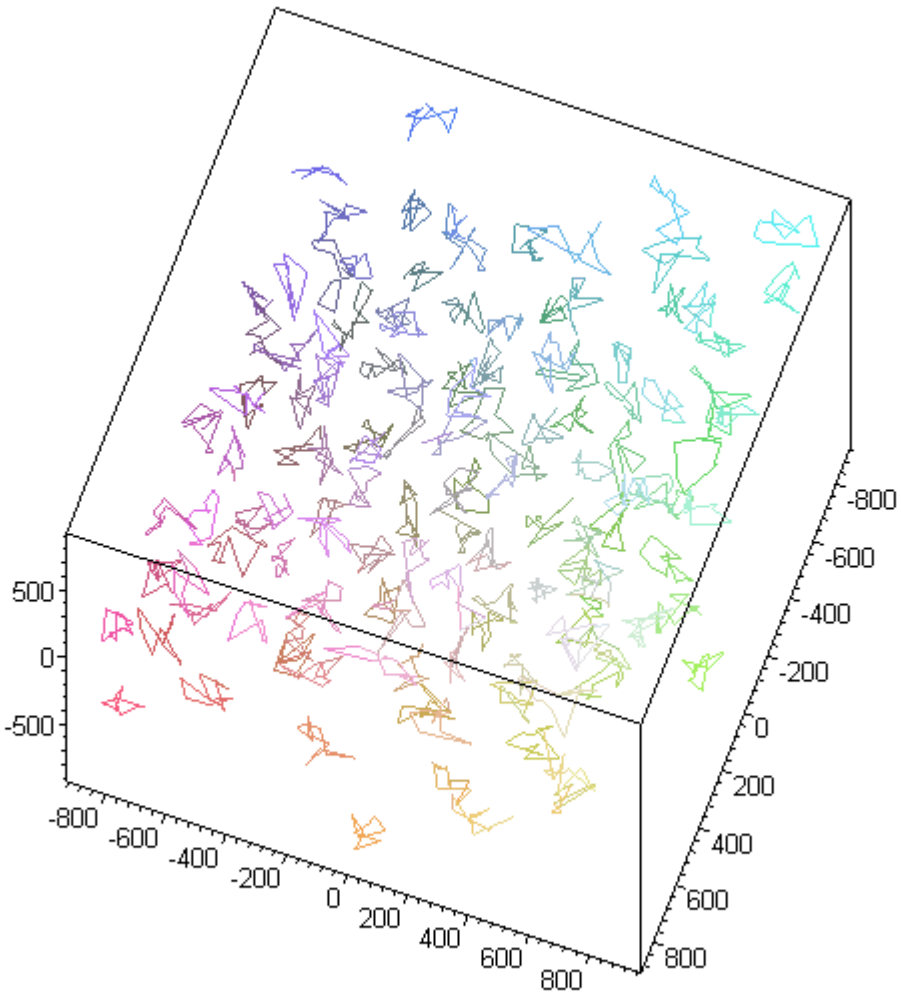
Атомарный металлический водород

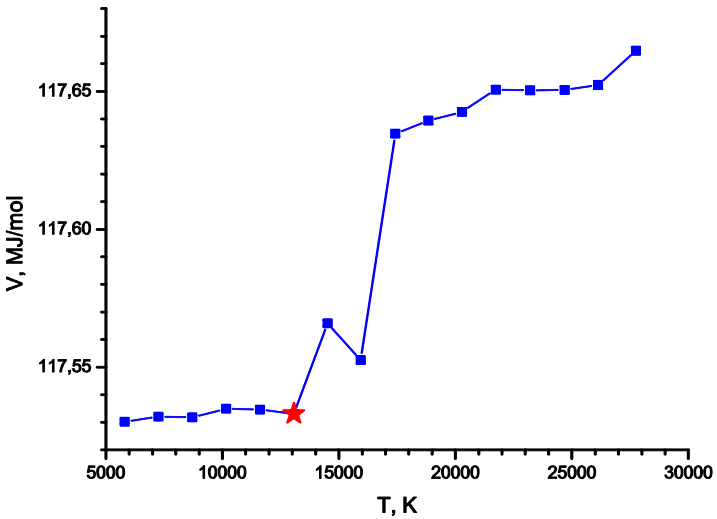




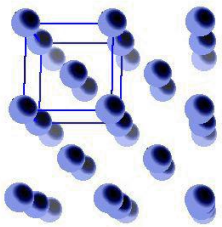
$$T = 28 \cdot 10^3 K$$

Атомарный металлический водород

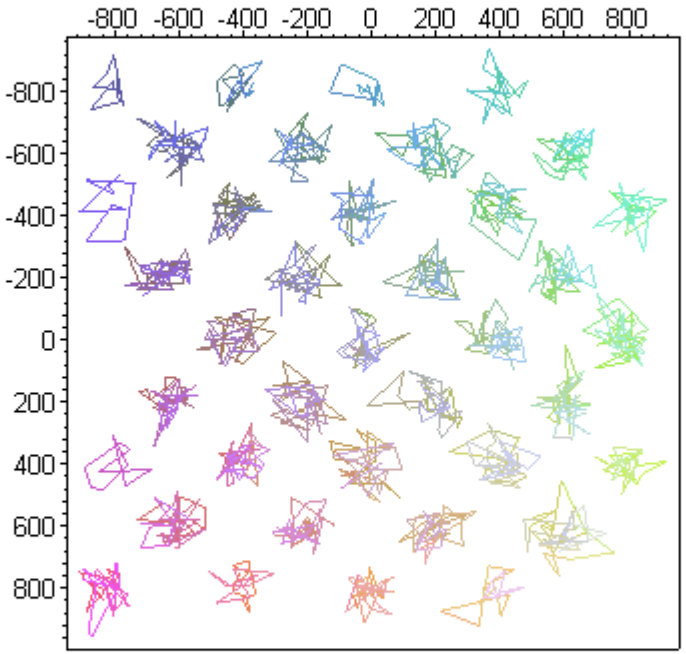


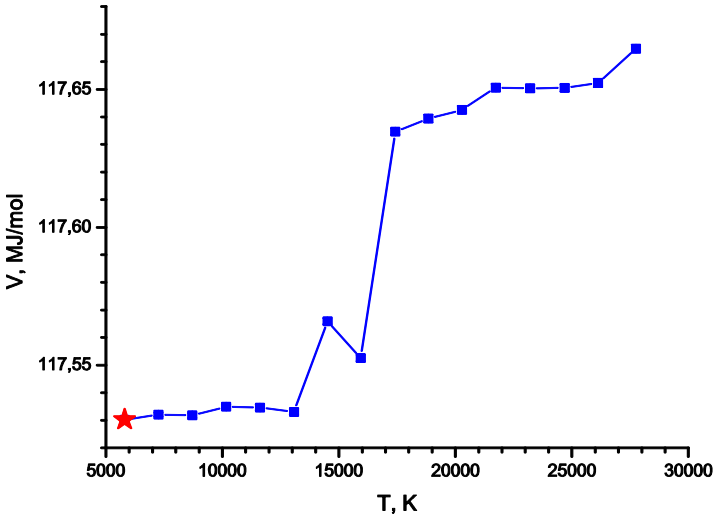


$$T = 13 \cdot 10^3 K$$

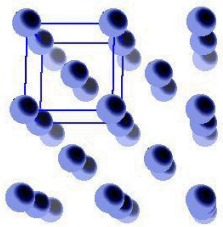


Атомарный металлический водород

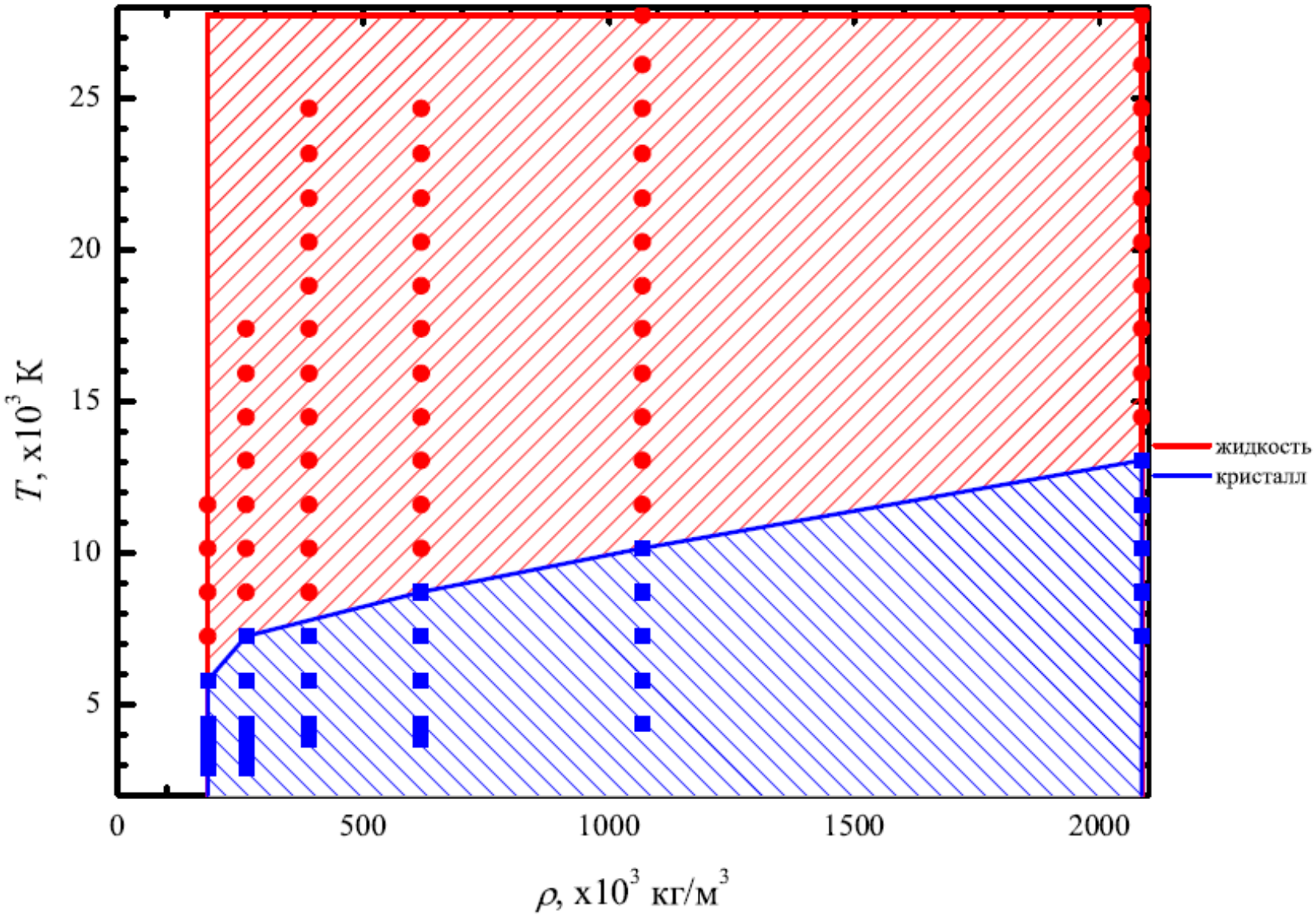




$$T = 6 \cdot 10^3 K$$

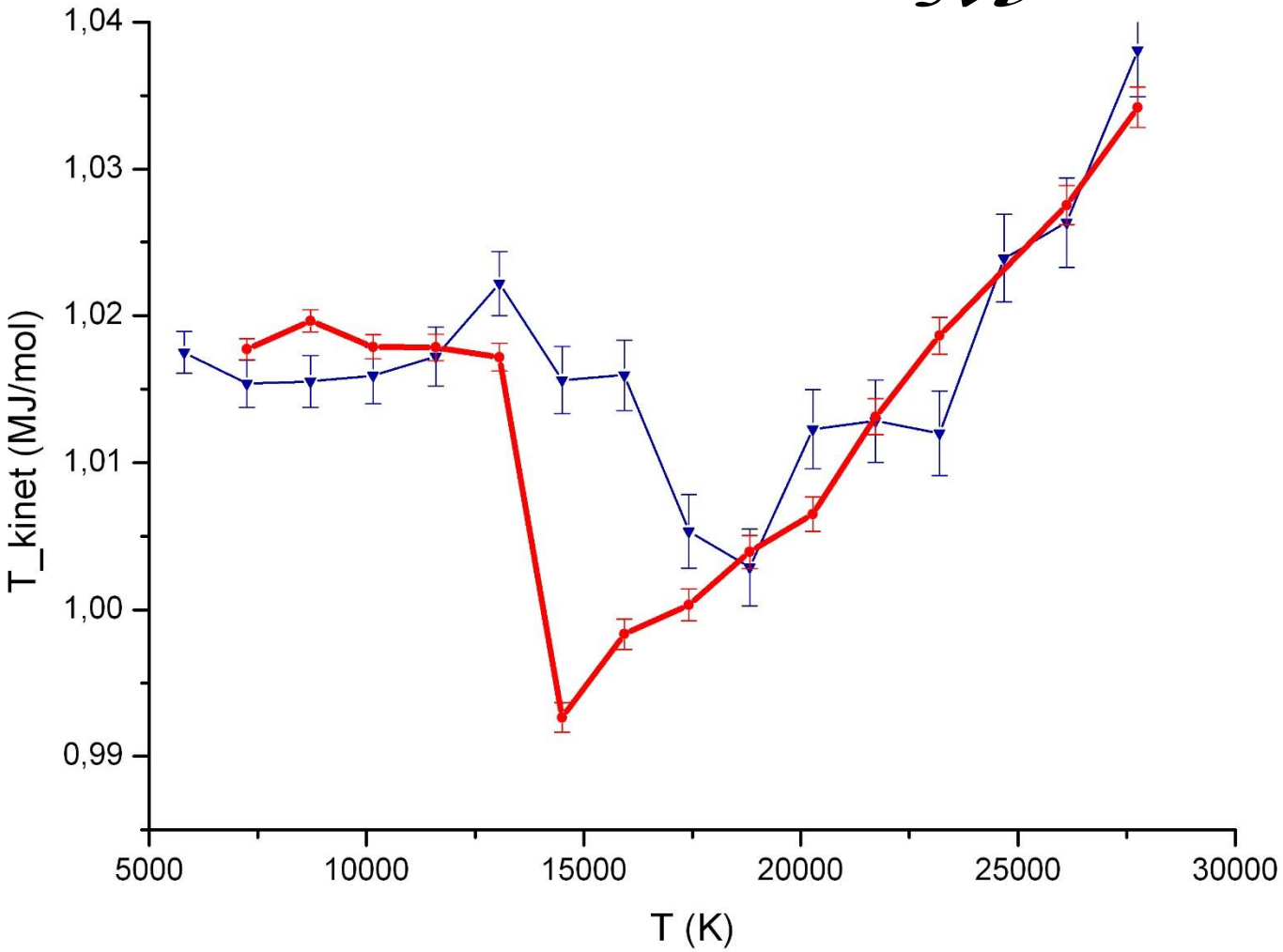


Фазовая диаграмма

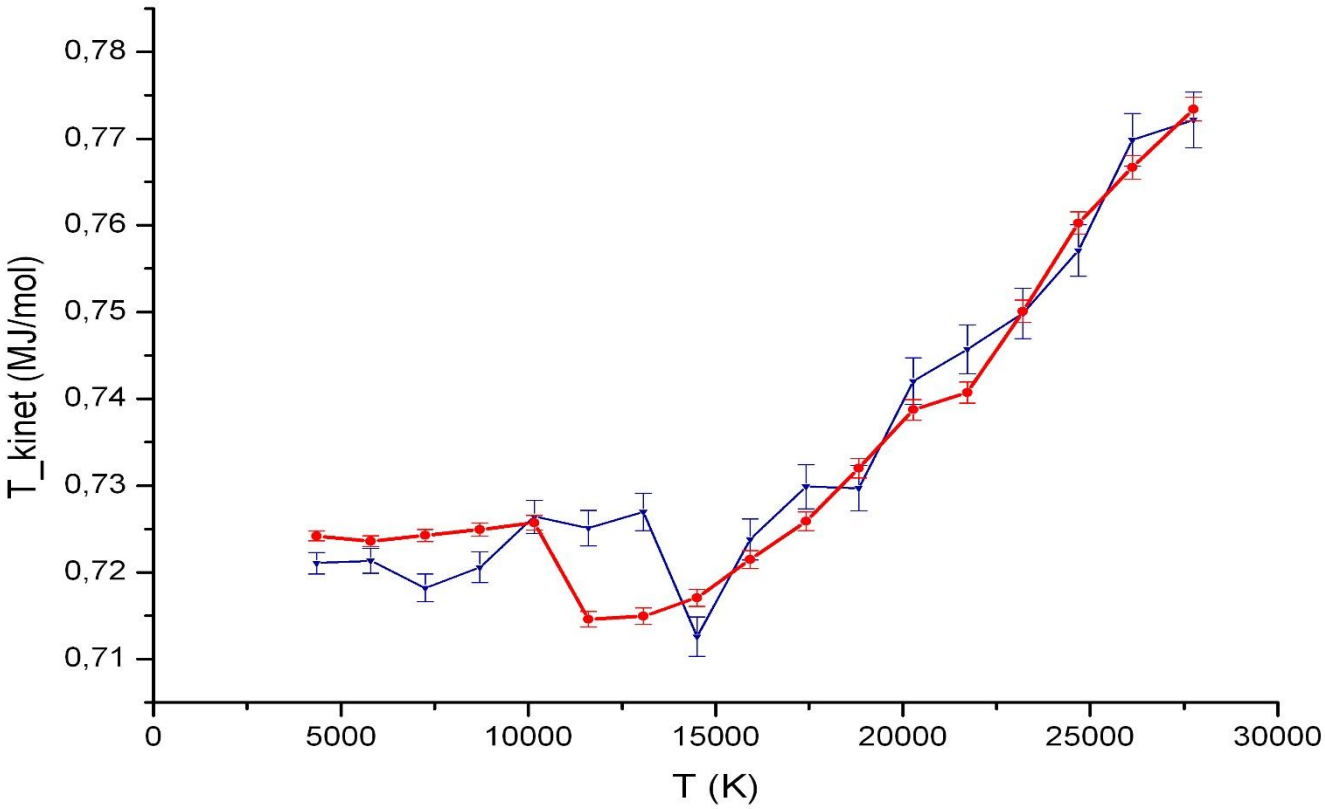


Кинетическая энергия при rs=200

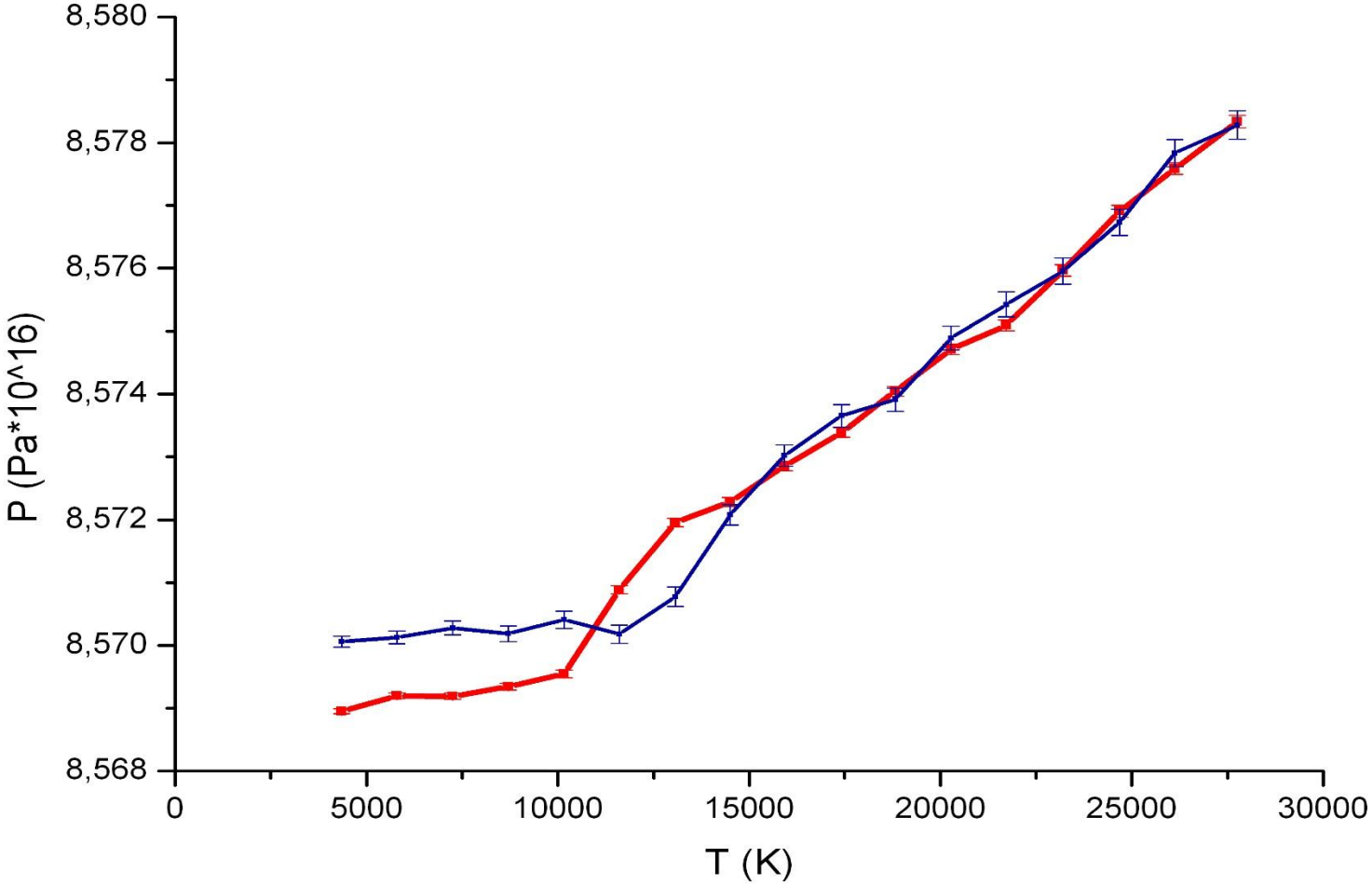
$$(\rho = 2,14 \cdot 10^{6} \frac{кг}{м^3})$$



Кинетическая энергия при rs=250
(ρ=1,046*10^6 кг/м^3)



Давление при rs=250 (ρ=1,046*10^6 кг/м^3)

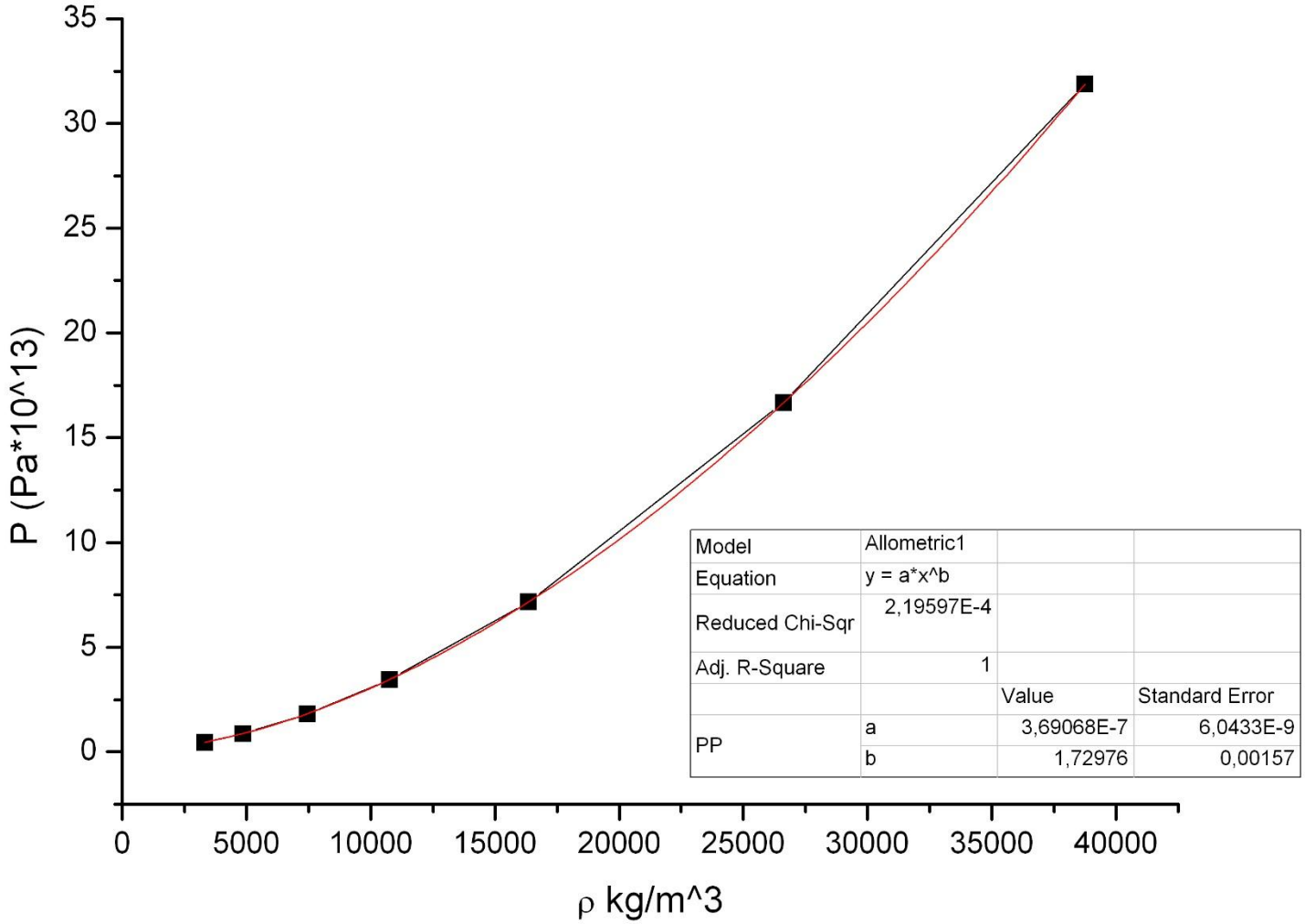


Изотермы

- Для трёх выбранных температур зависимость давления от плотности для жидкой фазы хорошо ложится на степенной закон

$$P = k \cdot \rho^{\gamma}$$

График зависимости P(ρ) для T=5800K



Model	Allometric1		
Equation	y = a*x^b		
Reduced Chi-Sqr	2,19597E-4		
Adj. R-Square	1		
		Value	Standard Error
PP	a	3,69068E-7	6,0433E-9
	b	1,72976	0,00157

Темы исследований

Фазовые явления
в
графене