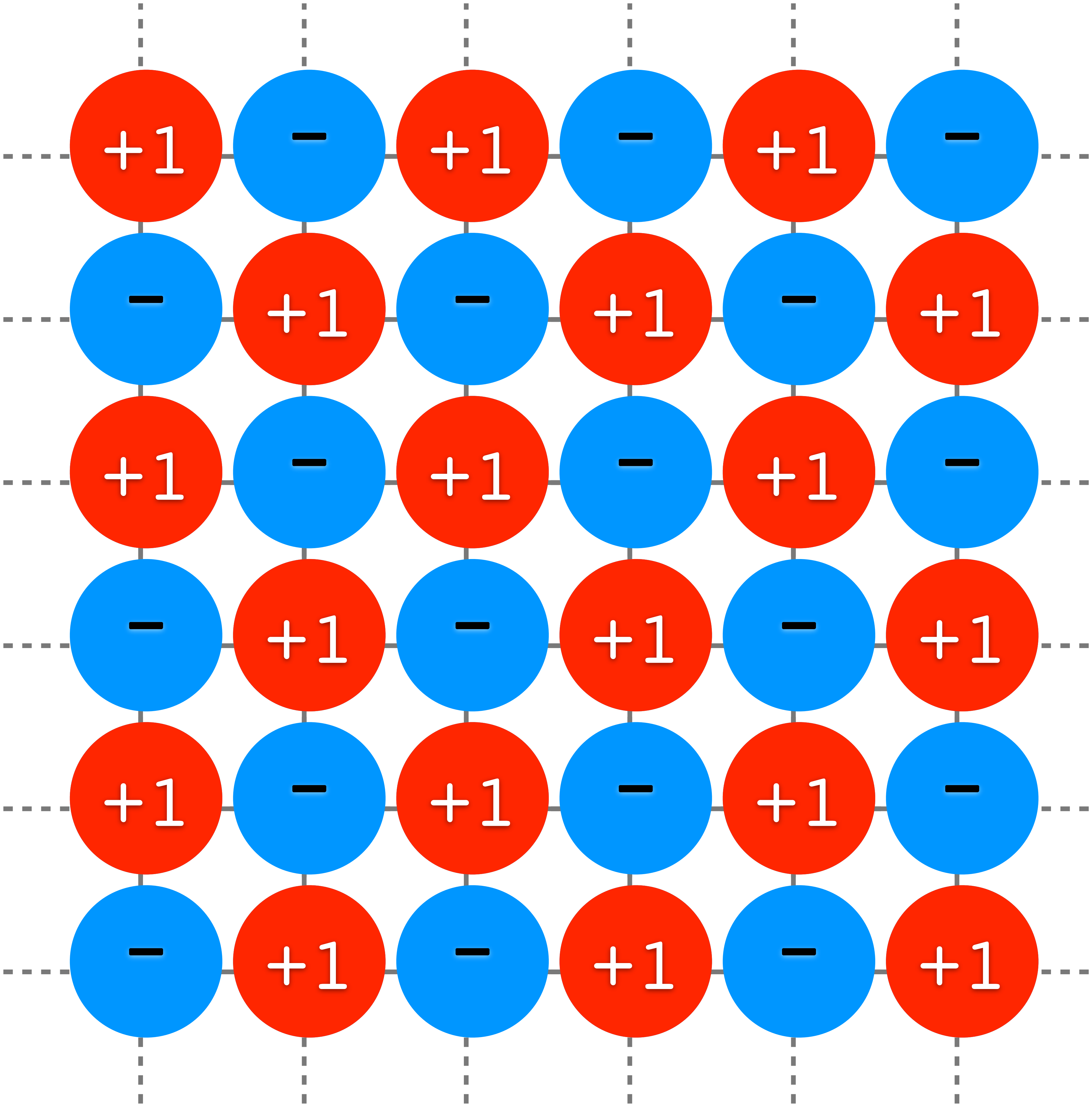
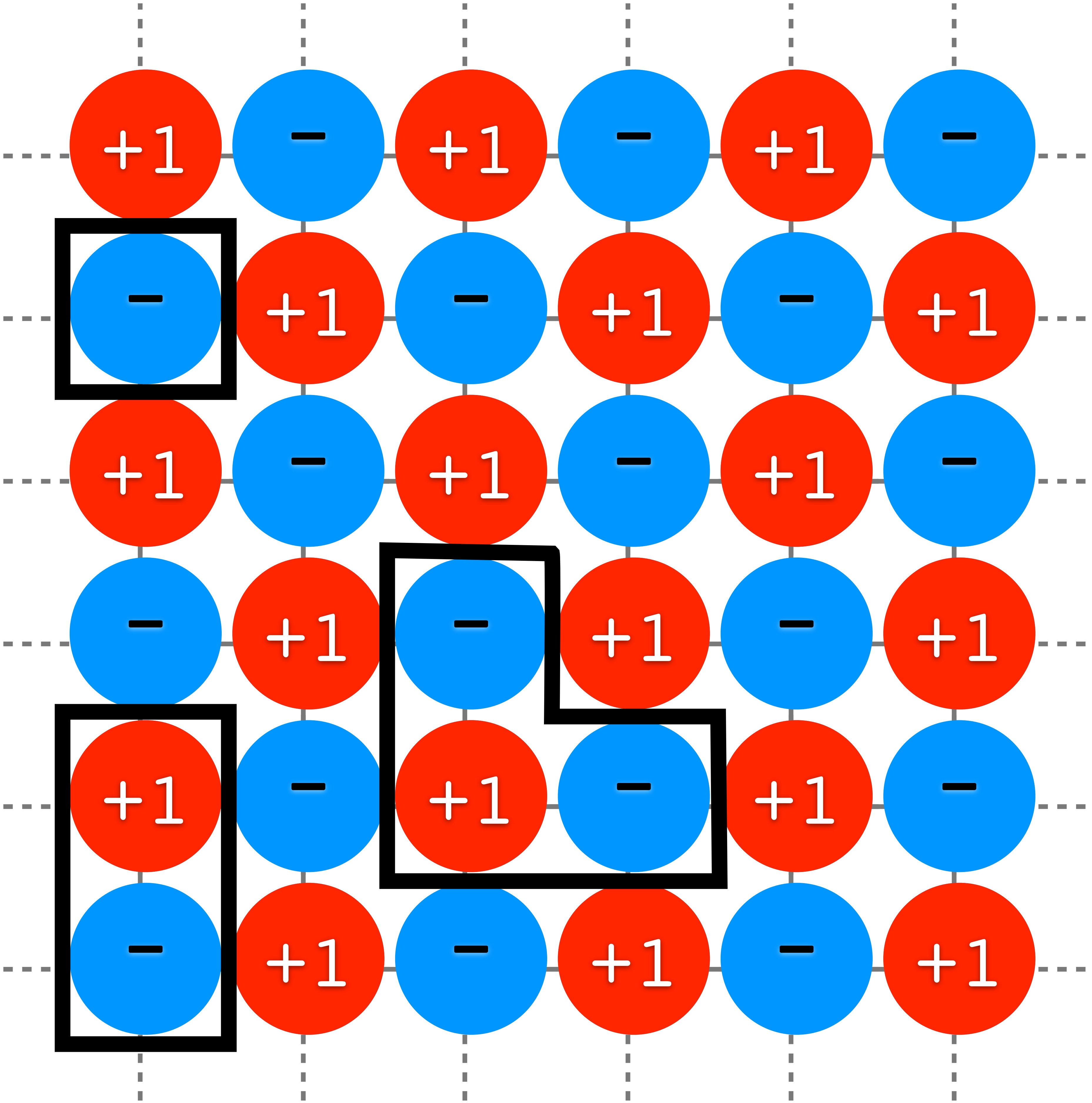
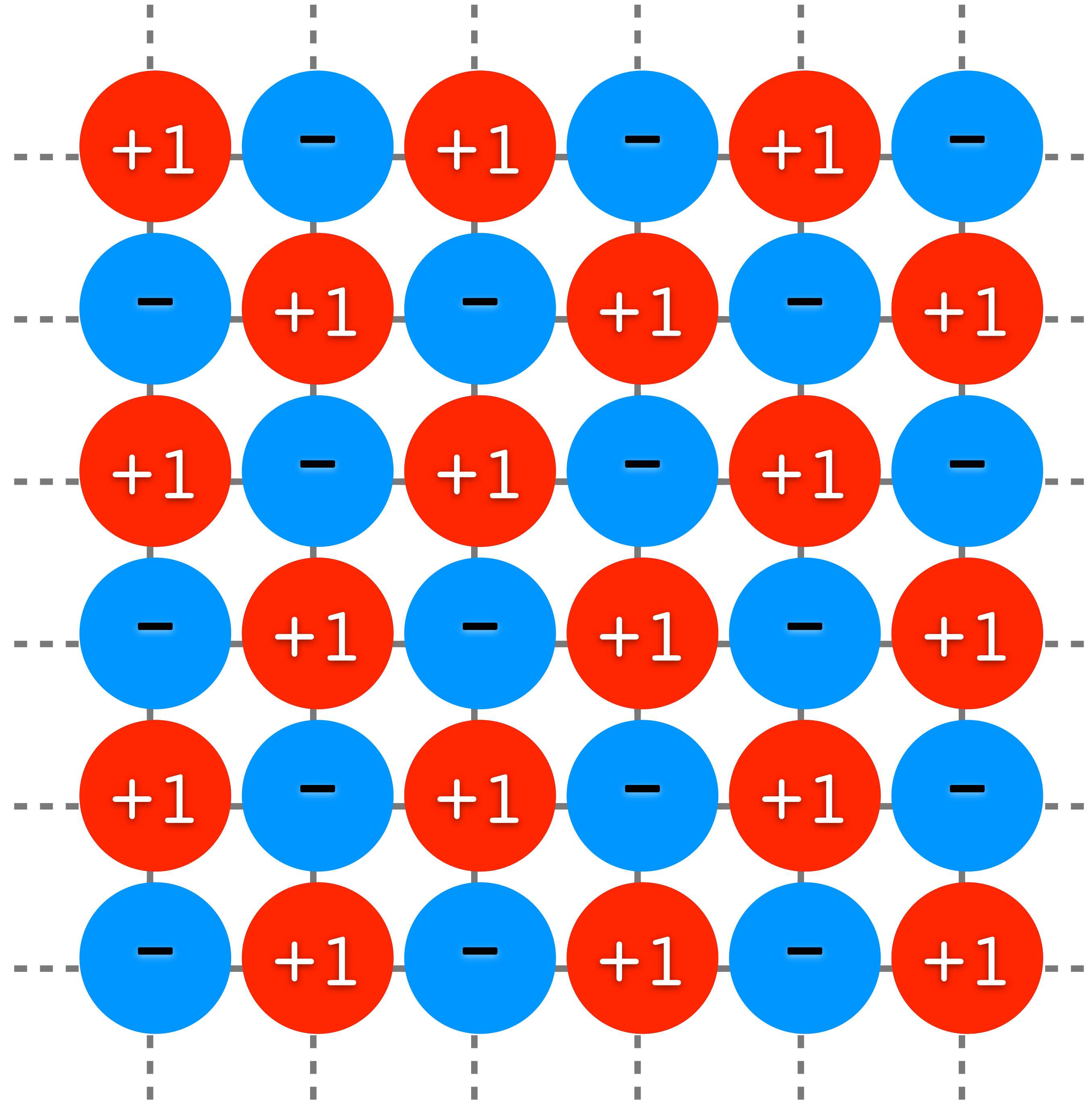

+1
−


+1
−

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 + J_1 \bigcirc + J_2 \bigcirc\bigcirc + J_3 \bigcirc\bigcirc\bigcirc + \cdots$$

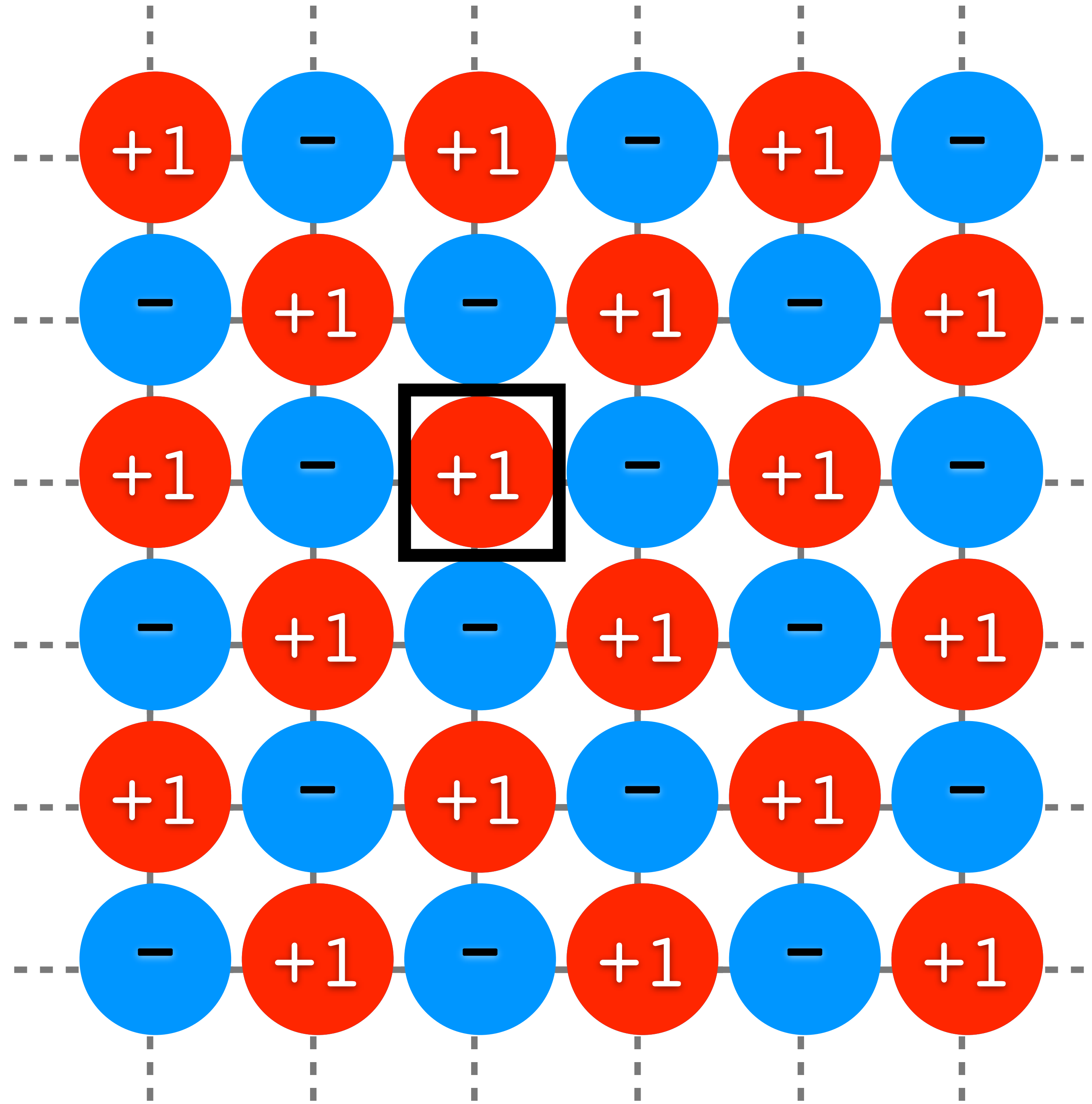
Empty cluster is trivial

$$1 = \frac{1}{N} \sum_{i}^{\text{lattice}} S_i^0$$



$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 \, \bigcirc + J_1 \, \bigcirc + J_2 \, \bigcirc\bigcirc + J_3 \, \bigcirc\bigcirc\bigcirc + \cdots$$

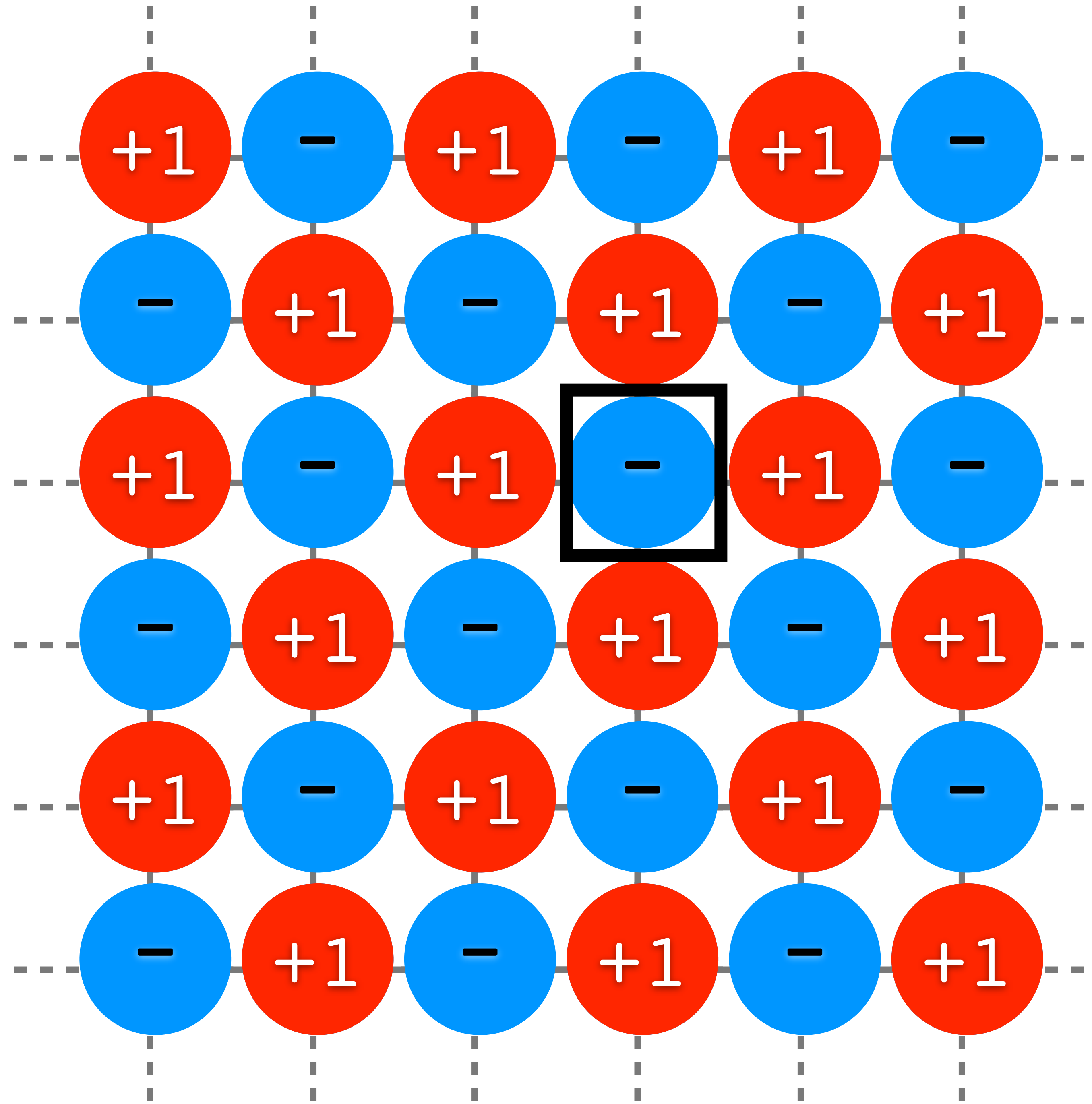
$$? = \frac{1}{N} \sum_{i}^{\text{lattice}} S_i$$



$$0 = (-1) + (+1) + (-1) + (+1) + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 \, \bigcirc + J_1 \, \bigcirc + J_2 \, \bigcirc\bigcirc + J_3 \, \bigcirc\bigcirc\bigcirc + \cdots$$

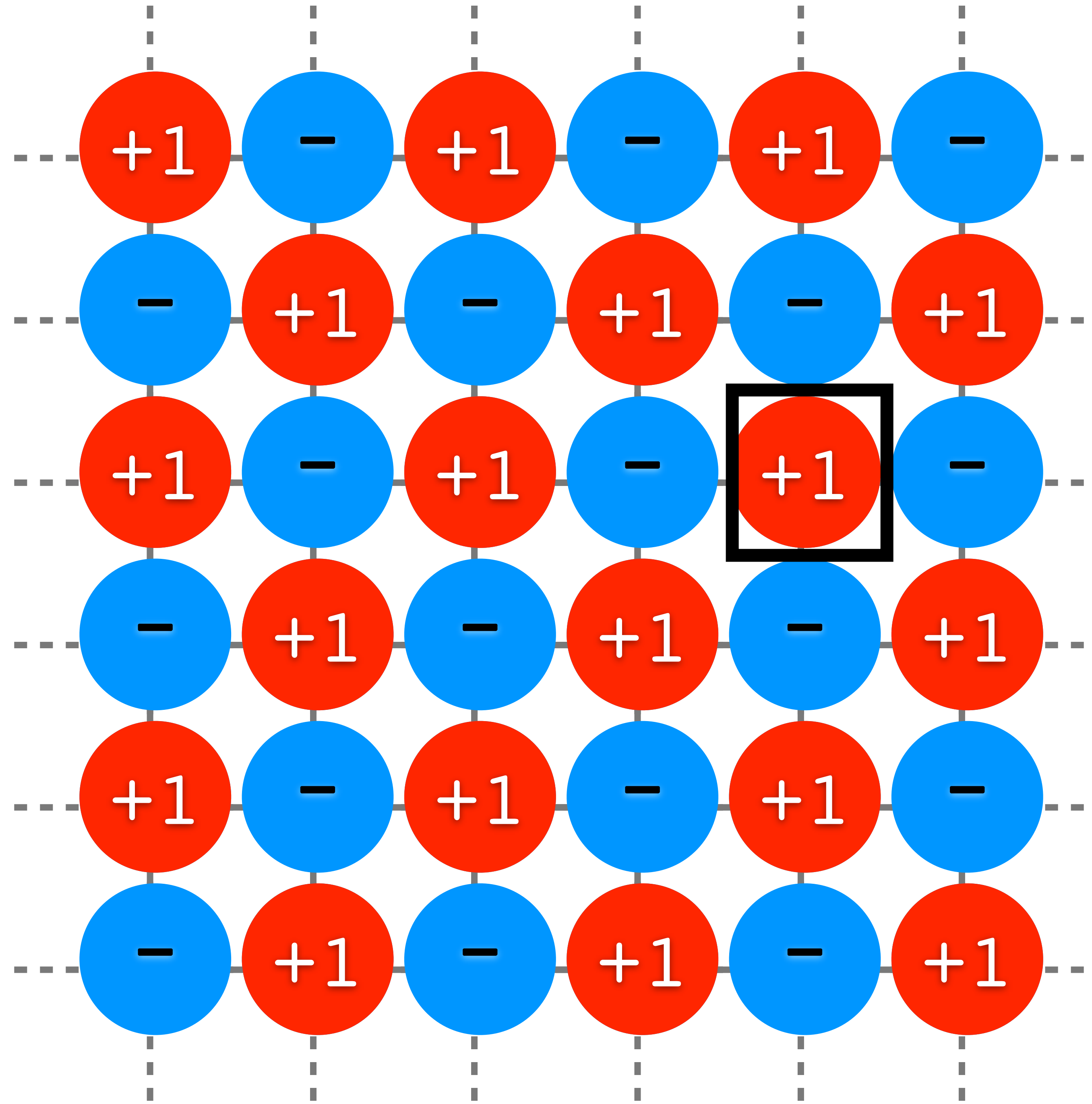
$$? = \frac{1}{N} \sum_{i}^{\text{lattice}} S_i$$



$$0 = (-1) + (+1) + (-1) + (+1) + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 \; + \; J_1 \; + \; J_2 \; + \; J_3 + \cdots$$

$$? = \frac{1}{N} \sum_{i}^{\text{lattice}} S_i$$



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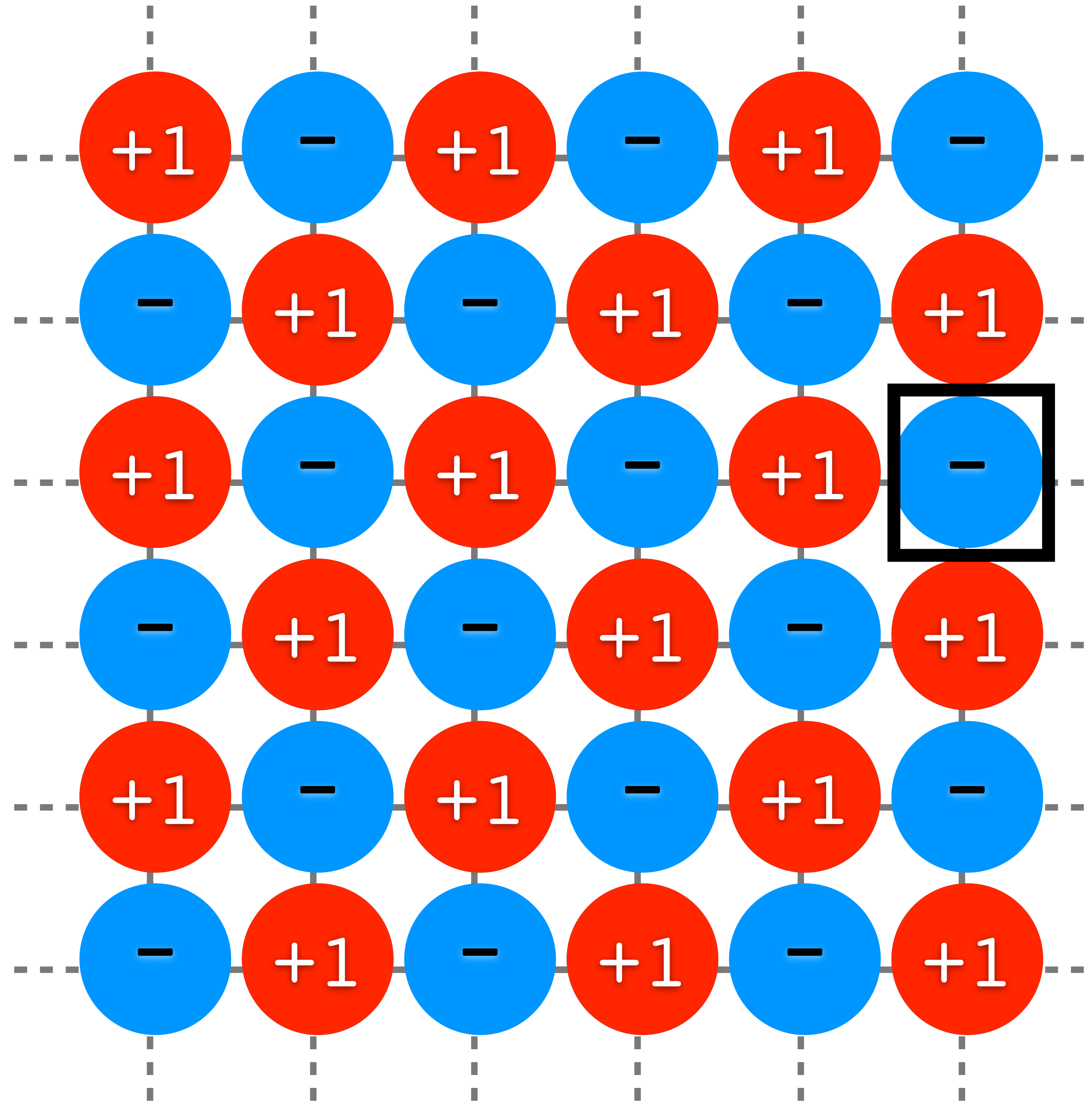
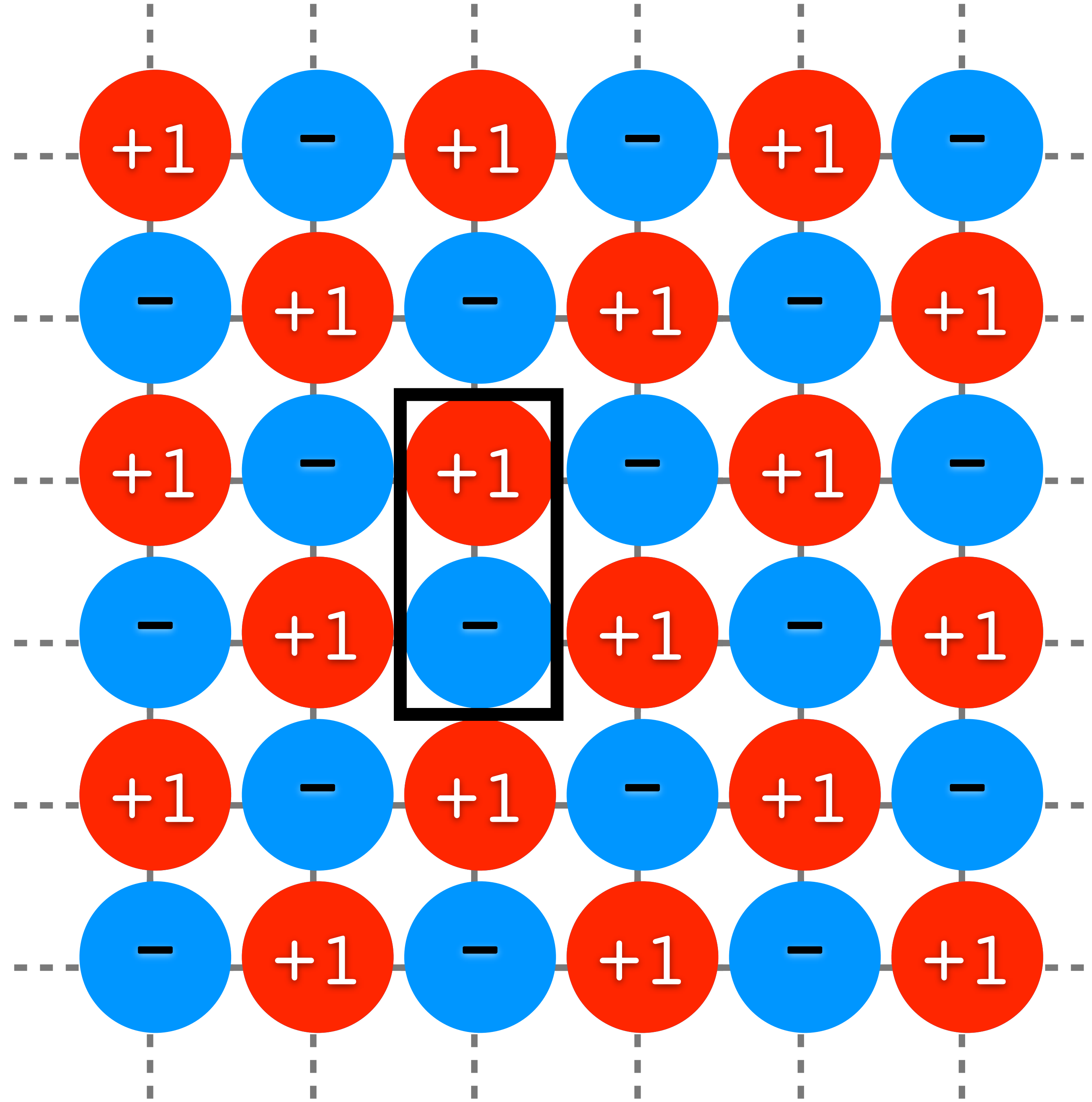


$$0 = (-1) + (+1) + (-1) + (+1) + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 \bigcirc + J_1 \bigcirc + J_2 \bigcirc\bigcirc + J_3 \bigcirc\bigcirc\bigcirc + \cdots$$

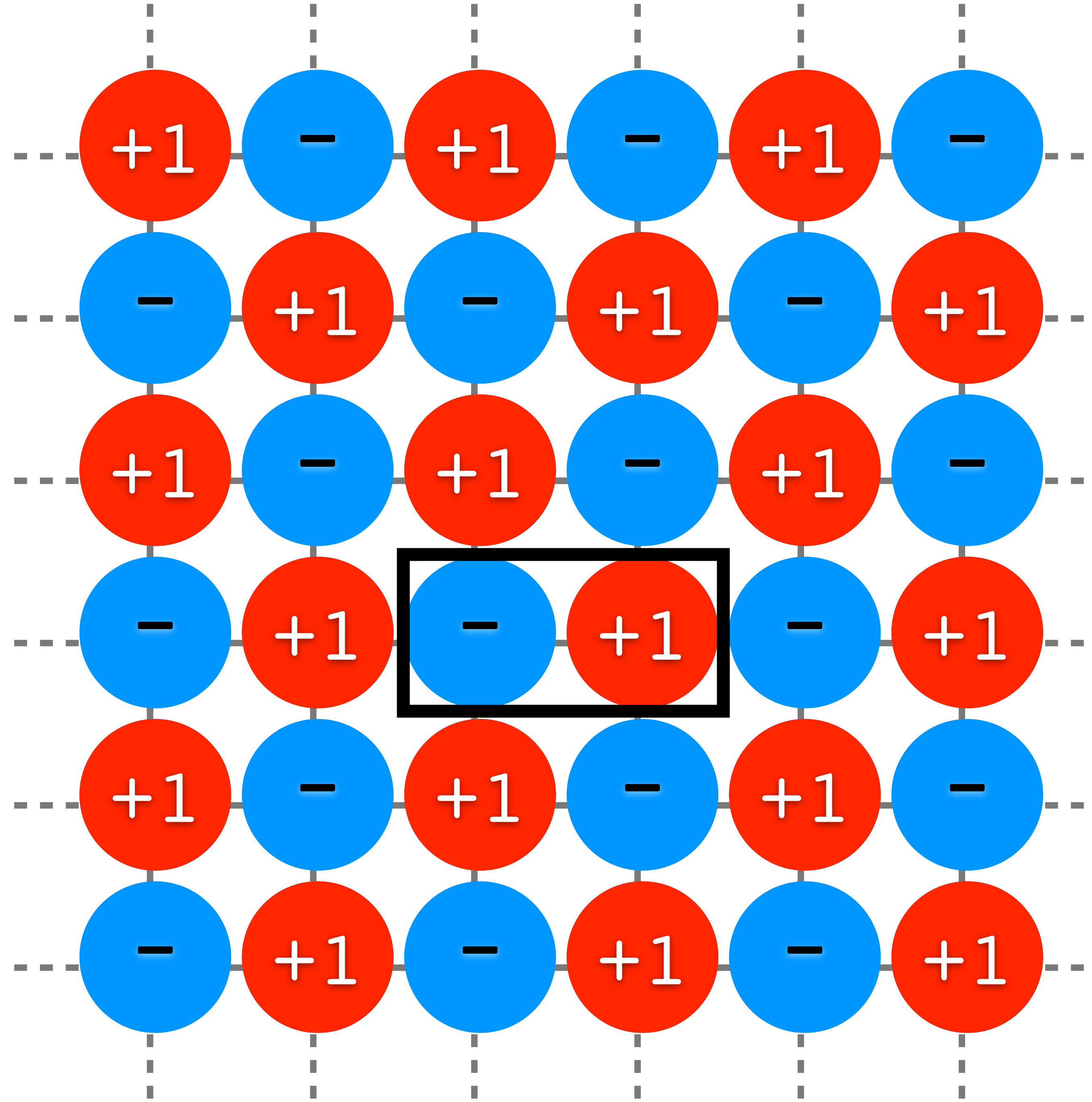
$$? = \frac{1}{N} \sum_{<i,j>_{\mathrm{N.N.}}}^{\text{lattice}} S_i S_j$$



$$-1 = \left(\frac{1}{2}\right)\left(\frac{1}{4}\right)[(-1)(+1) + (-1)(+1) + (-1)(+1) + (-1)(+1)$$

$$[(-1)(+1) + (-1)(+1) + (-1)(+1) + (-1)(+1)]$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 \bigcirc + J_1 \bigcirc + J_2 \bigcirc\bigcirc + J_3 \bigcirc\bigcirc\bigcirc + \cdots$$



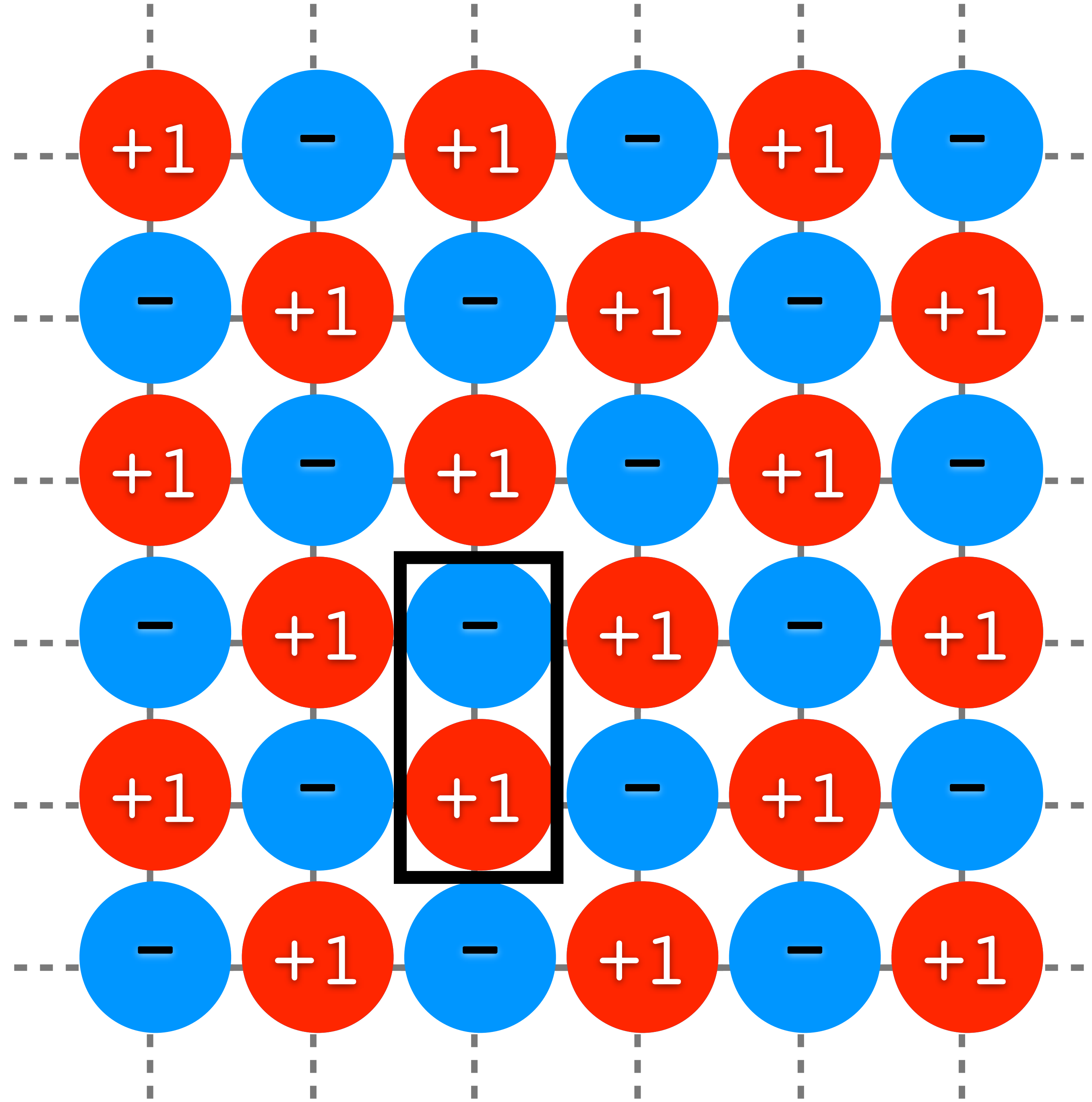
$$? = \frac{1}{N} \sum_{<i,j>_{\mathrm{N.N.}}}^{\mathrm{lattice}} S_i S_j$$

$$-1 = \left(\frac{1}{2}\right)\left(\frac{1}{4}\right)[(-1)(+1) + (-1)(+1) + (-1)(+1) + (-1)(+1)$$

$$[(-1)(+1) + (-1)(+1) + (-1)(+1) + (-1)(+1)]$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 \, \bigcirc + J_1 \, \bigcirc + J_2 \, \bigcirc\bigcirc + J_3 \, \bigcirc\bigcirc\bigcirc + \cdots$$

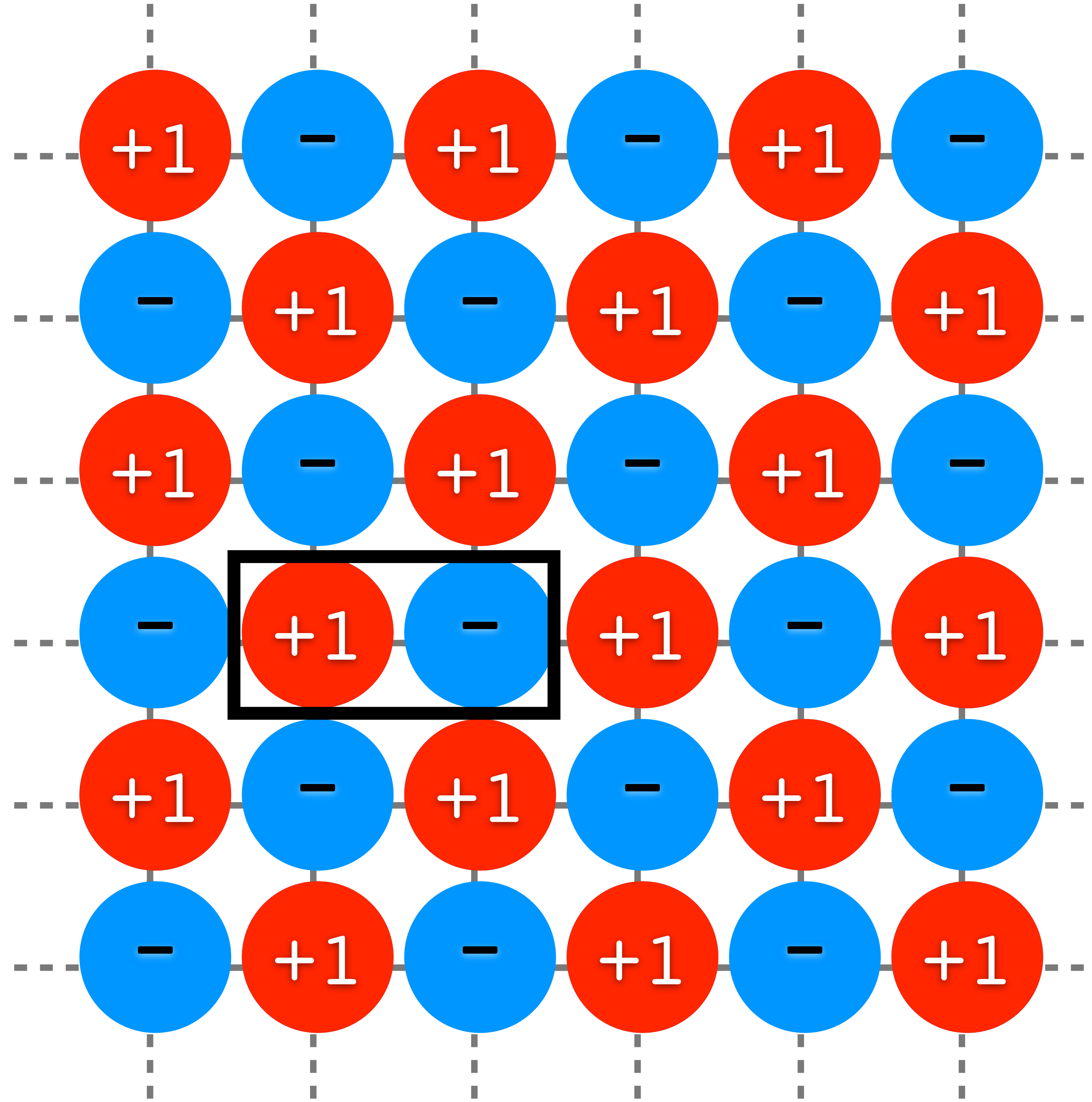
$$? = \frac{1}{N} \sum_{<i,j>_{\mathrm{N.N.}}}^{\mathrm{lattice}} S_i S_j$$



$$-1 = \left(\frac{1}{2}\right)\left(\frac{1}{4}\right)\left[(-1)(+1) + (-1)(+1) + (-1)(+1) + (-1)(+1)\right.$$

$$\left.\left[(-1)(+1) + (-1)(+1) + (-1)(+1) + (-1)(+1)\right]\right.$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 \bigcirc + J_1 \bigcirc + J_2 \bigcirc\bigcirc + J_3 \bigcirc\bigcirc\bigcirc + \cdots$$

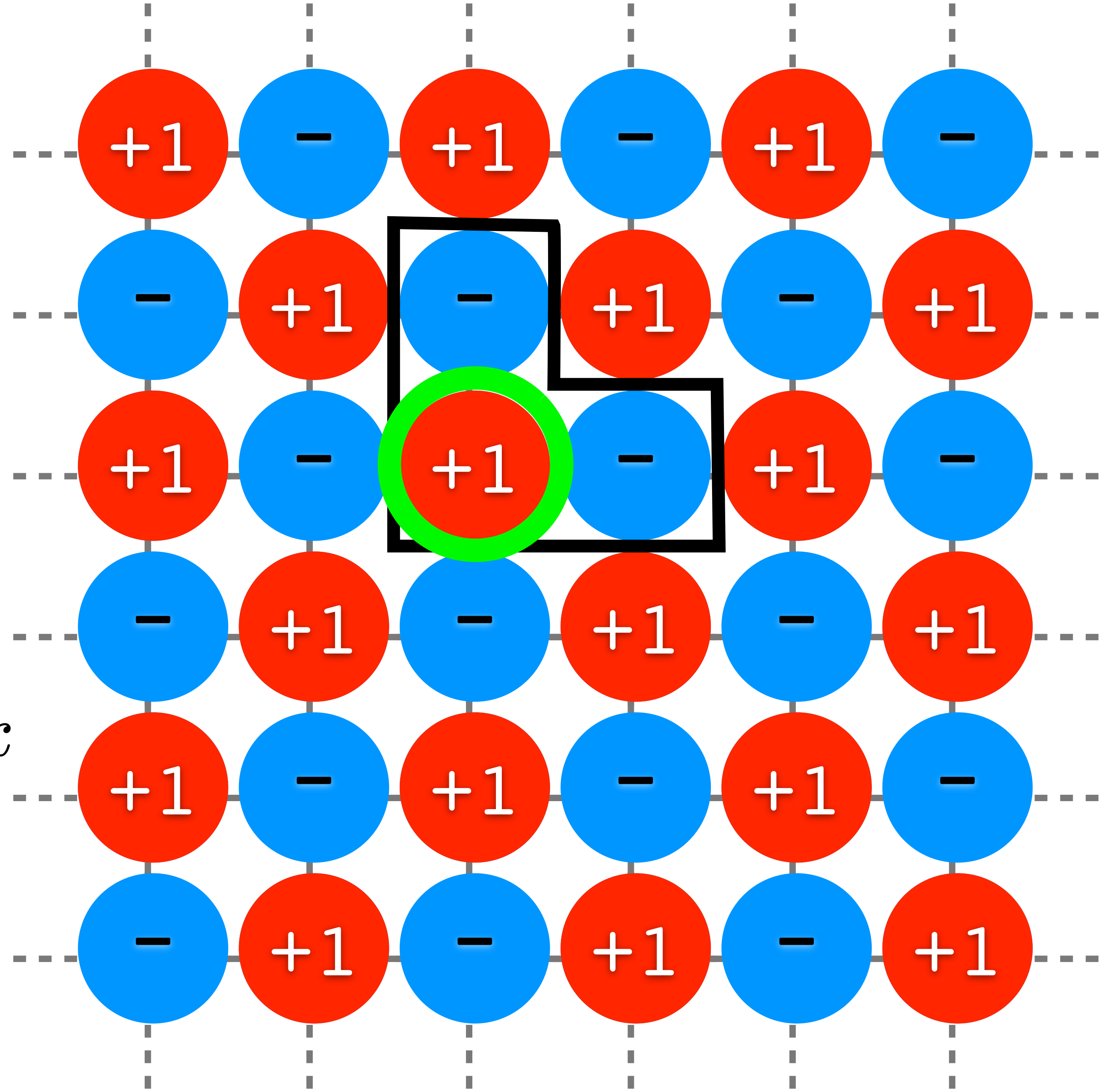


$$? = \frac{1}{N} \sum_{<i,j>_{\mathrm{N.N.}}}^{\mathrm{lattice}} S_i S_j$$

$$-1 = \left(\frac{1}{2}\right)\left(\frac{1}{4}\right)\left[(-1)(+1) + (-1)(+1) + (-1)(+1) + (-1)(+1)\right.$$

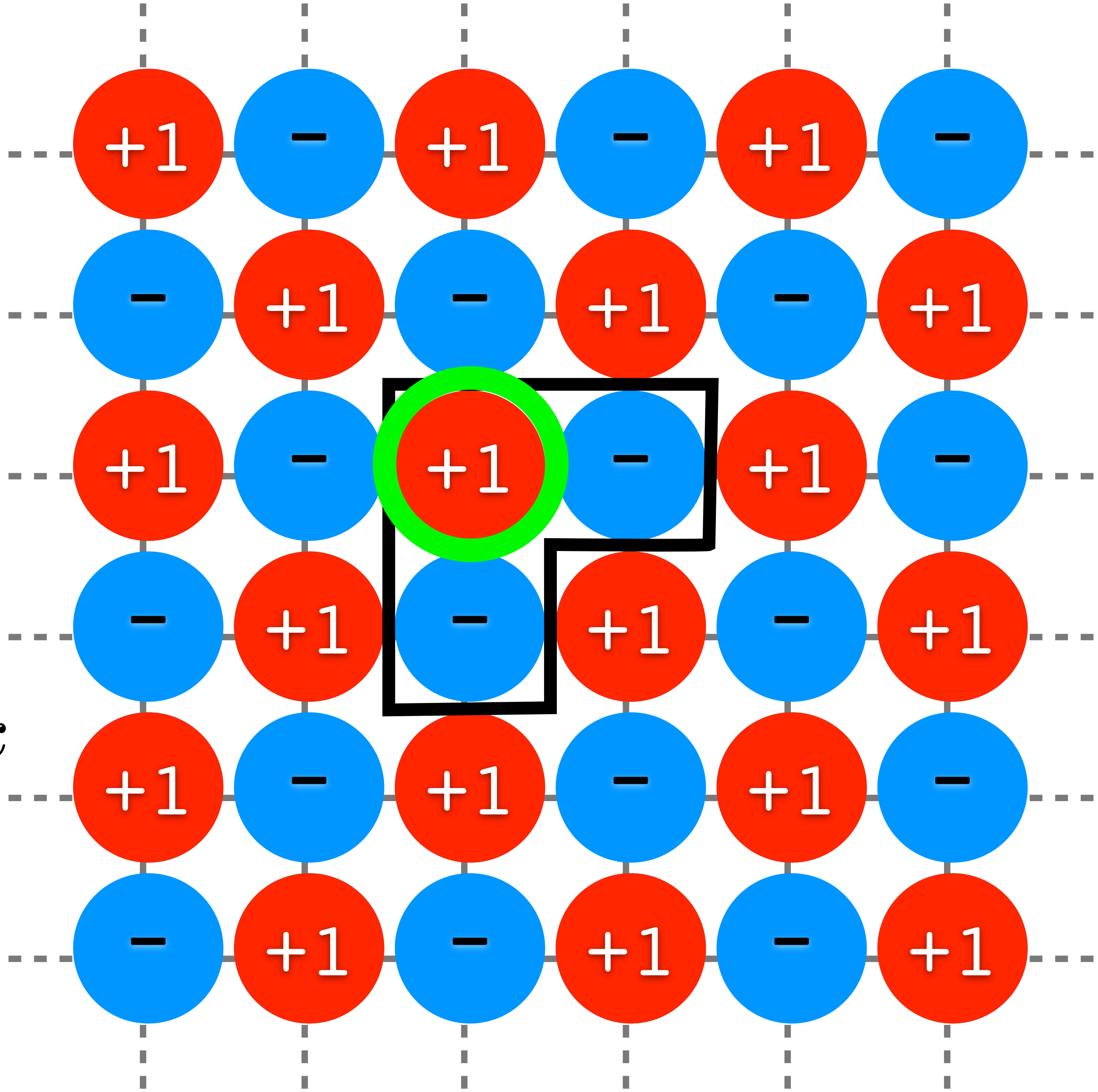
$$\left.\left[(-1)(+1) + (-1)(+1) + (-1)(+1) + (-1)(+1)\right]\right.$$

$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\text{lattice}} S_i S_j S_k$$



?

$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\mathrm{lattice}} S_i S_j S_k$$



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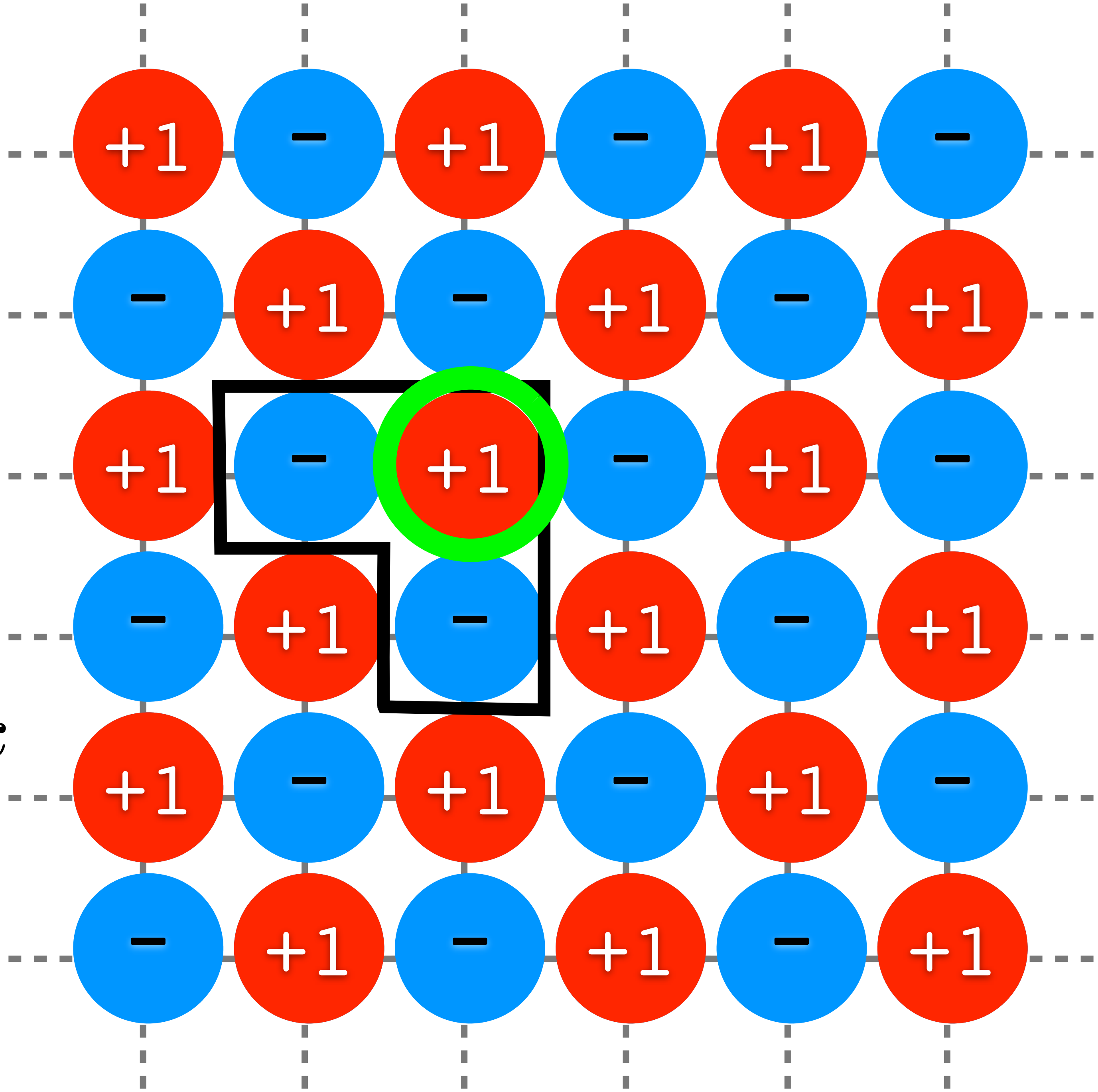
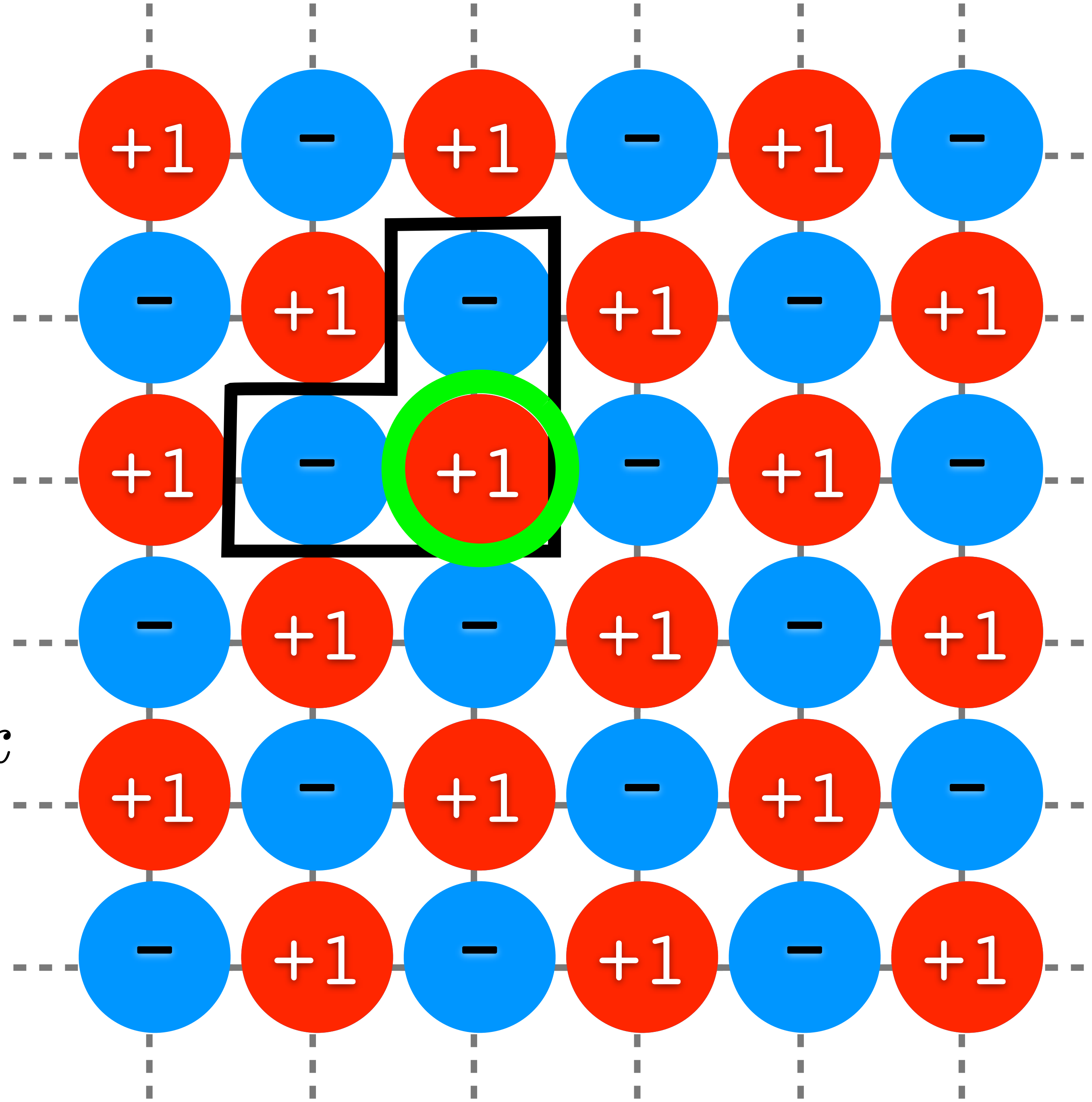
$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\text{lattice}} S_i S_j S_k$$



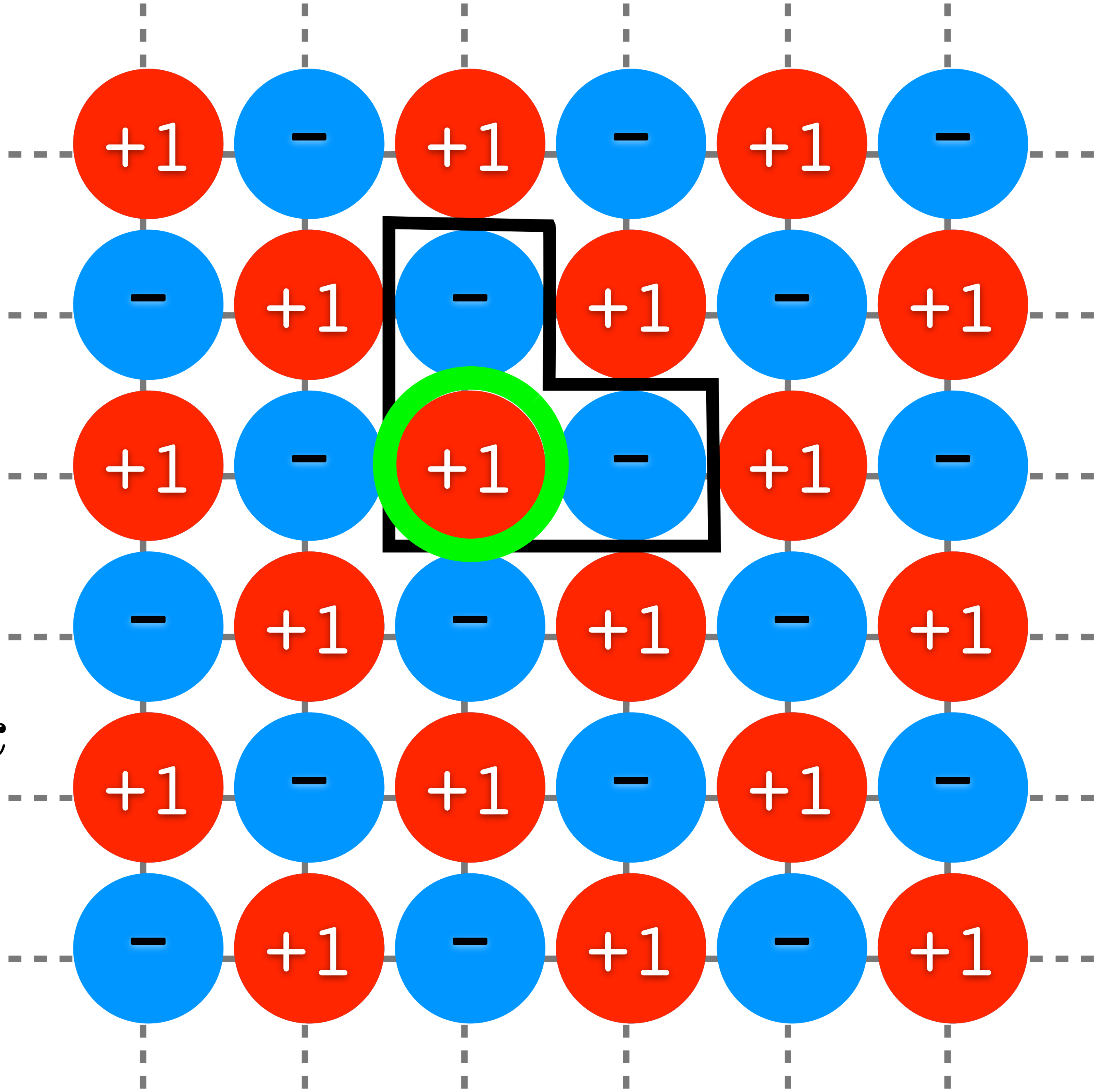
?

$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\mathrm{lattice}} S_i S_j S_k$$



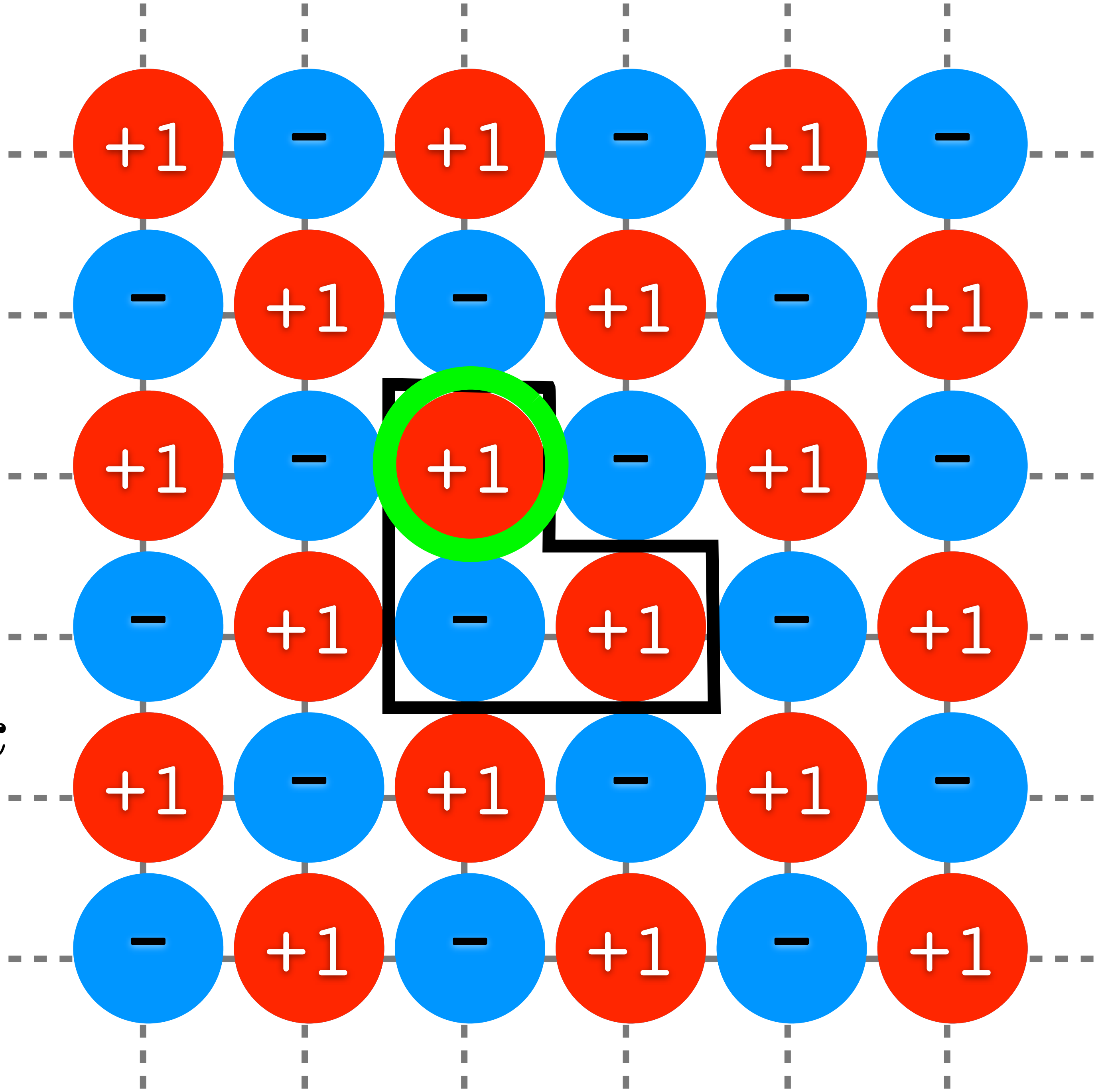
?

$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\mathrm{lattice}} S_i S_j S_k$$



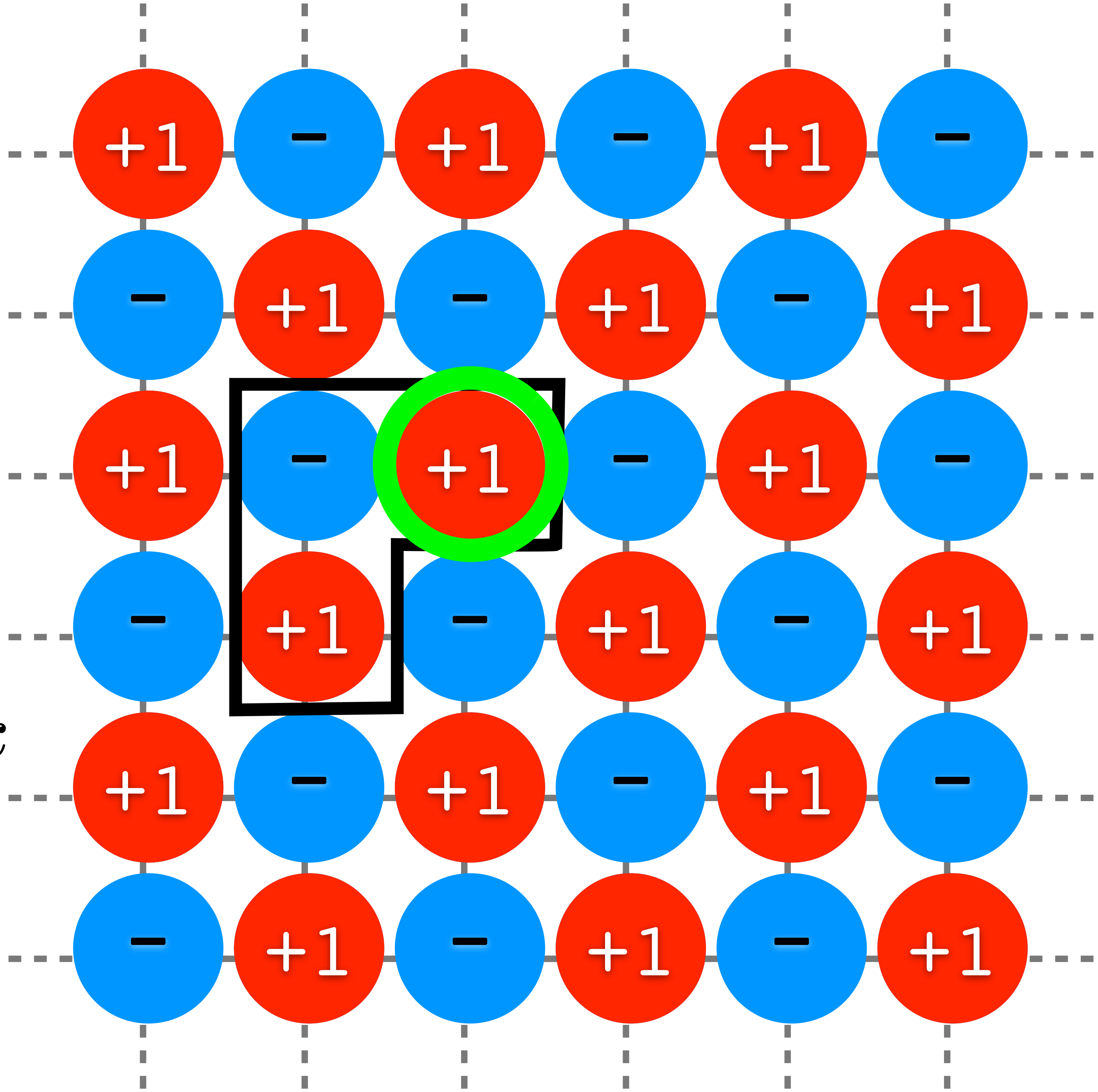
?

$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\text{lattice}} S_i S_j S_k$$



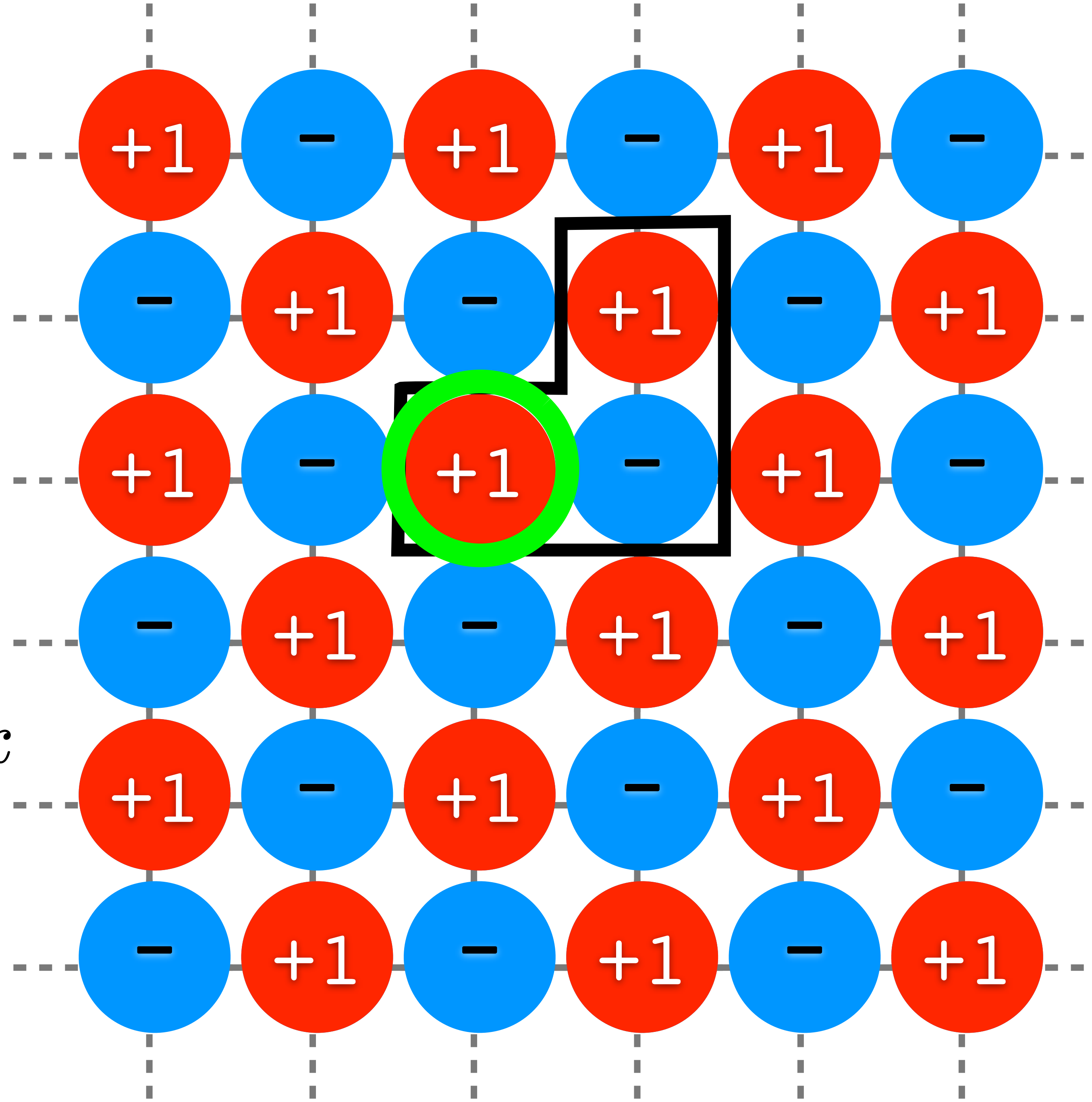
?

$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\mathrm{lattice}} S_i S_j S_k$$



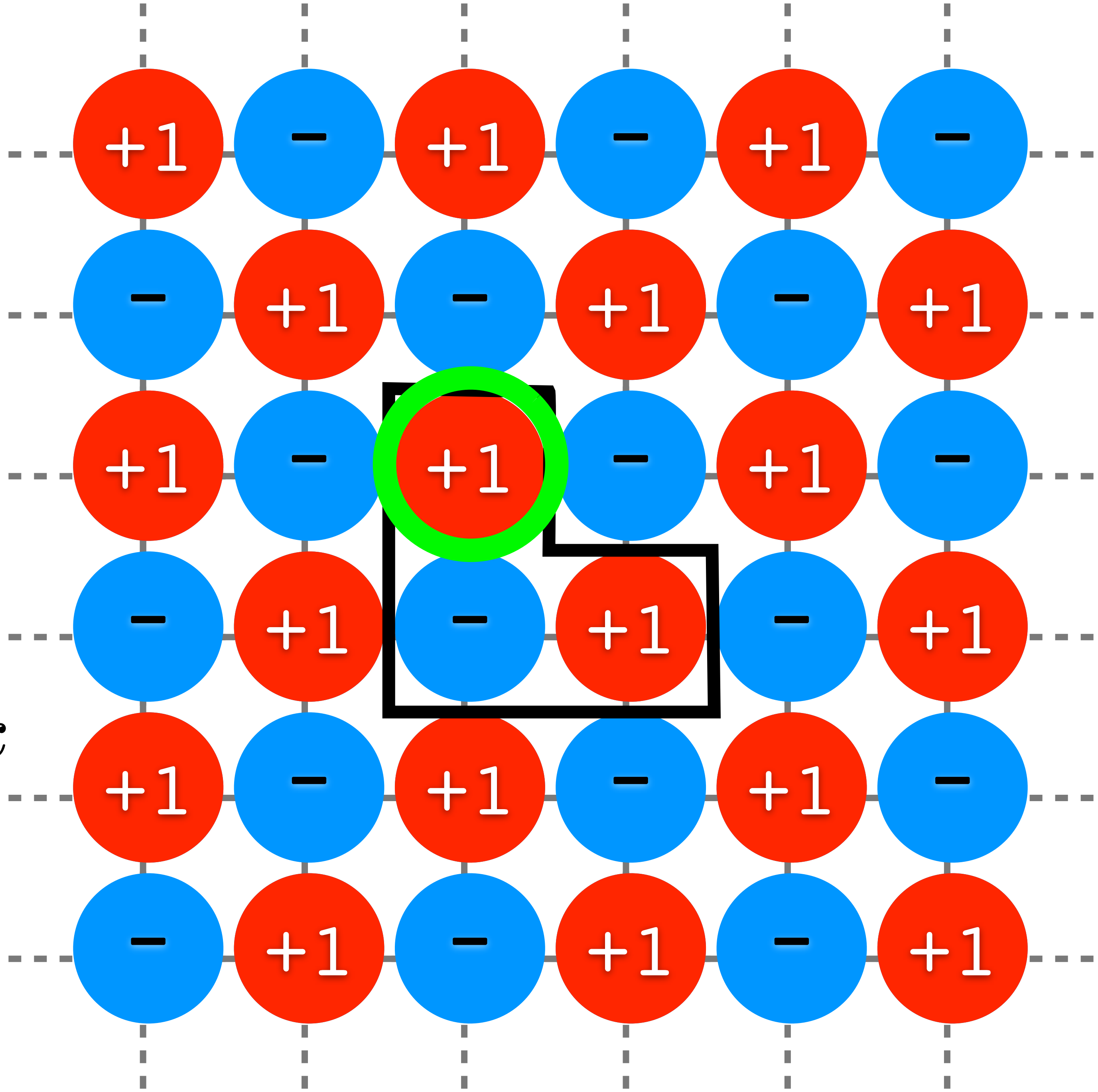
?

$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\mathrm{lattice}} S_i S_j S_k$$



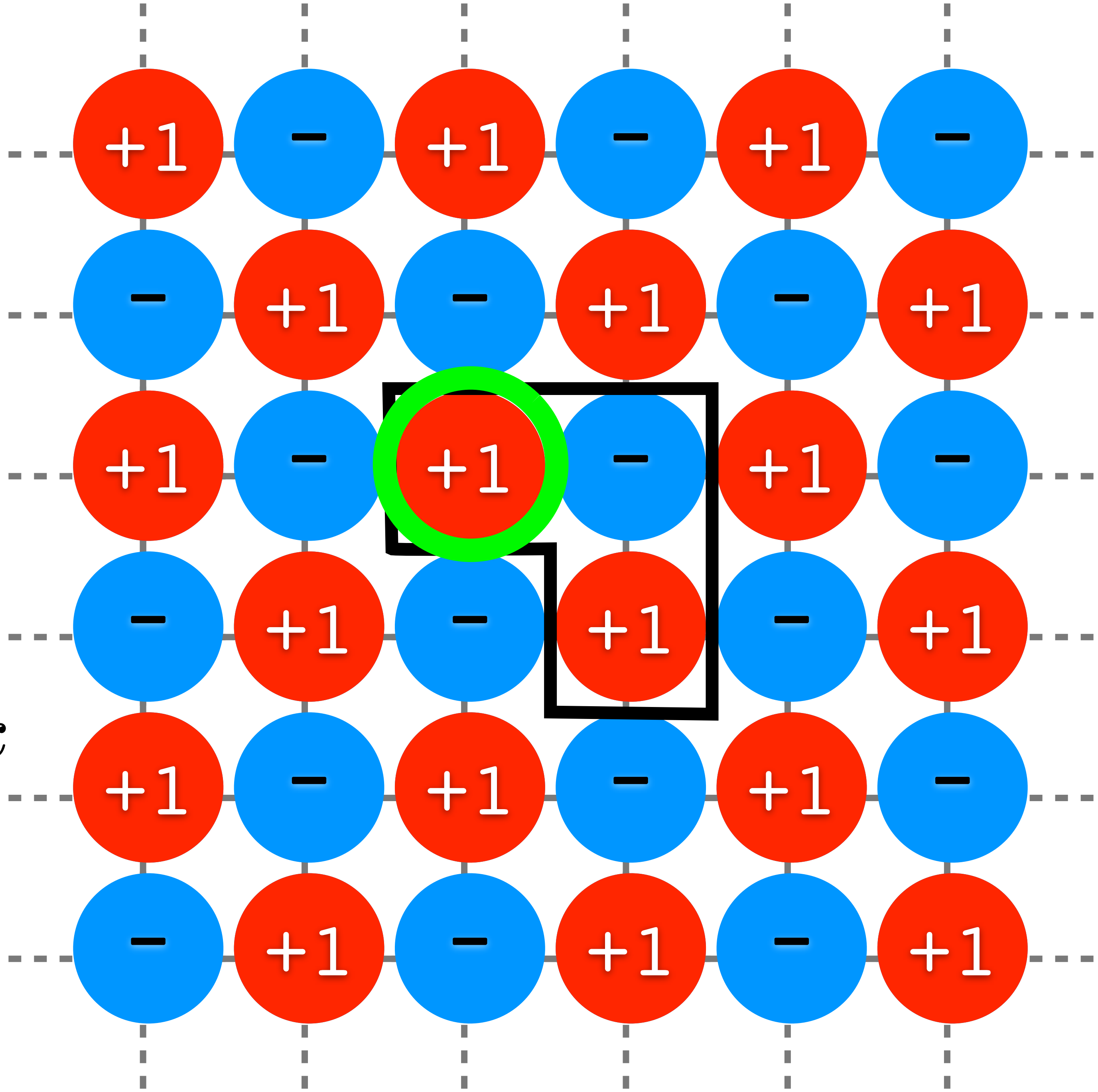
?

$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\text{lattice}} S_i S_j S_k$$

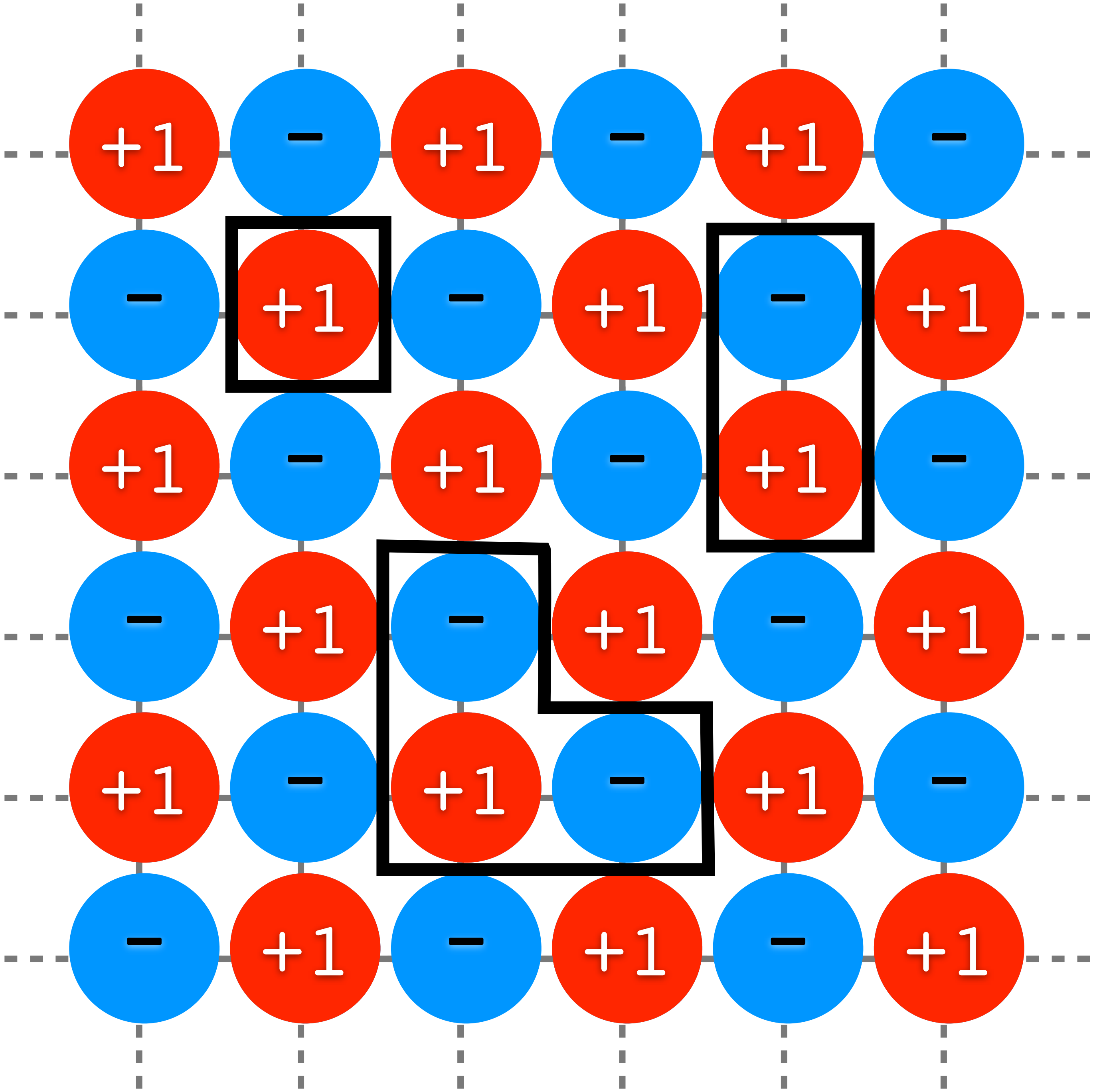


?

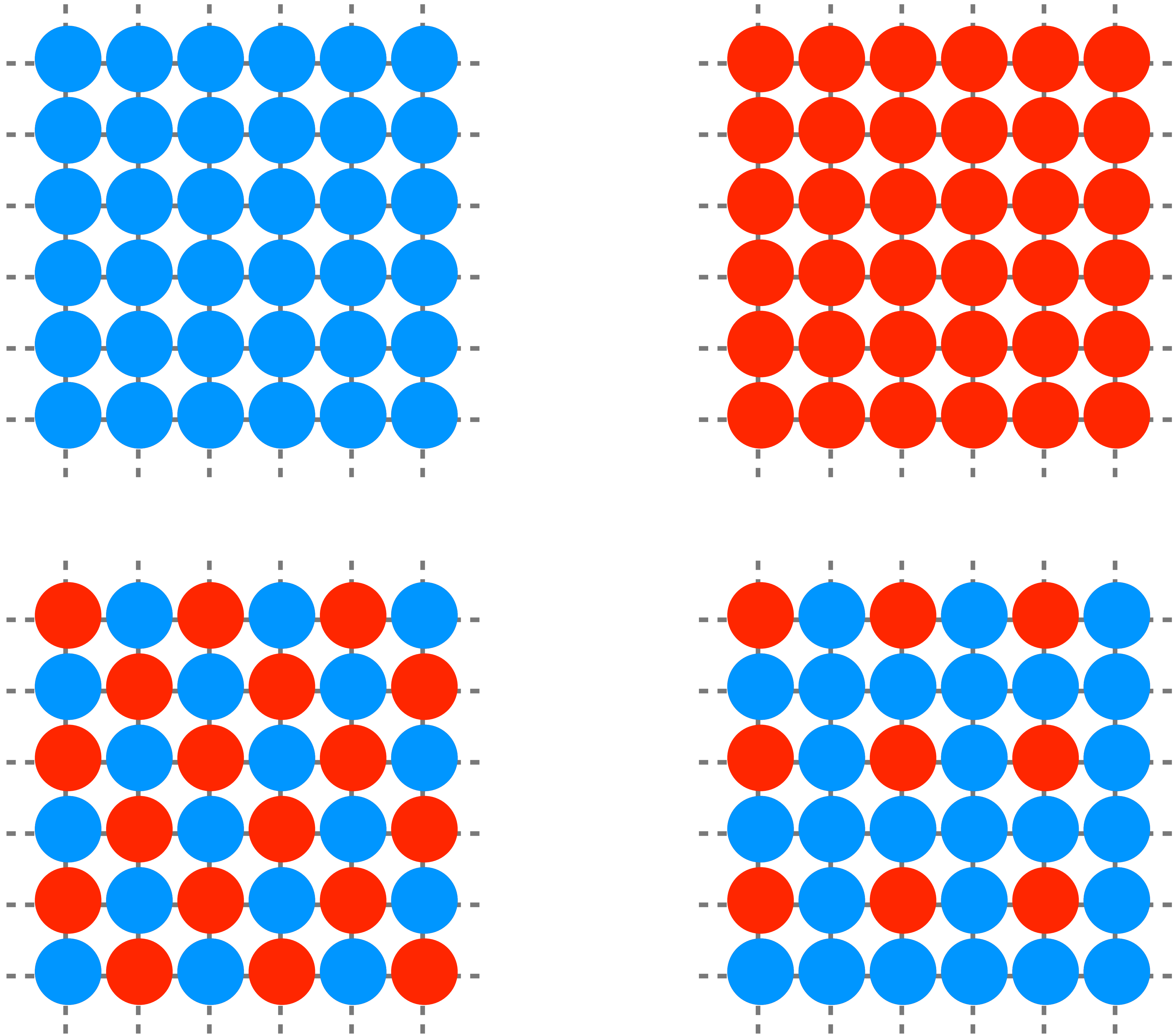
$$? = \frac{1}{N} \sum_{<i,j,k>_{\mathrm{N.N.}}}^{\text{lattice}} S_i S_j S_k$$

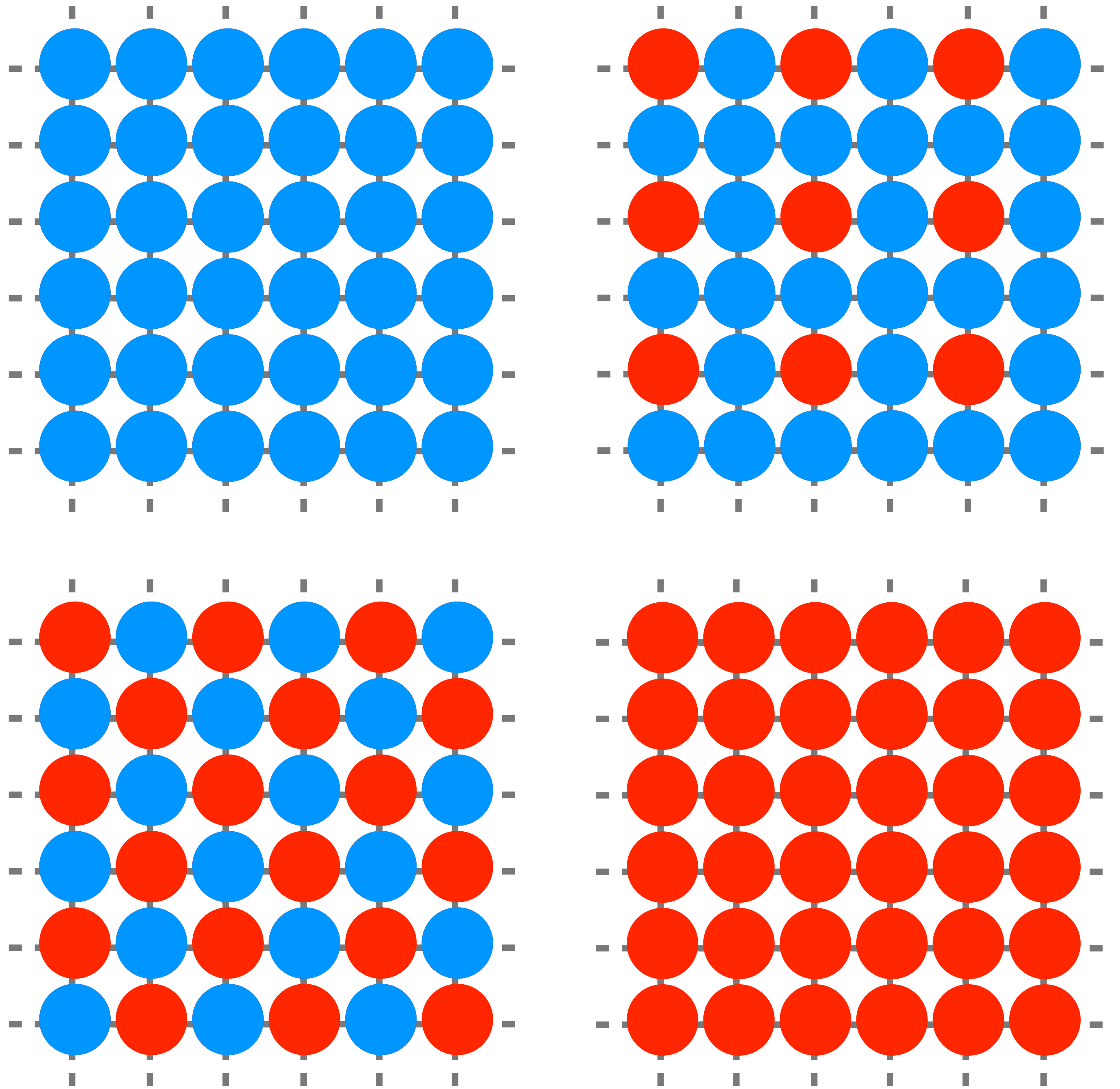


?



$$(\bar{\Pi}_0, \bar{\Pi}_1, \bar{\Pi}_2, \bar{\Pi}_3) = (1, 0, -1, 0)$$





$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & -1 & 0 \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$\begin{pmatrix} E_1 \\ E_2 \\ E_3 \\ E_4 \end{pmatrix} = \begin{pmatrix} \Pi_{1,1} & \Pi_{1,2} & \Pi_{1,3} & \Pi_{1,4} \\ \Pi_{2,1} & \Pi_{2,2} & \Pi_{2,3} & \Pi_{2,4} \\ \Pi_{3,1} & \Pi_{3,2} & \Pi_{3,3} & \Pi_{3,4} \\ \Pi_{4,1} & \Pi_{4,2} & \Pi_{4,3} & \Pi_{4,4} \end{pmatrix} \begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \end{pmatrix}$$

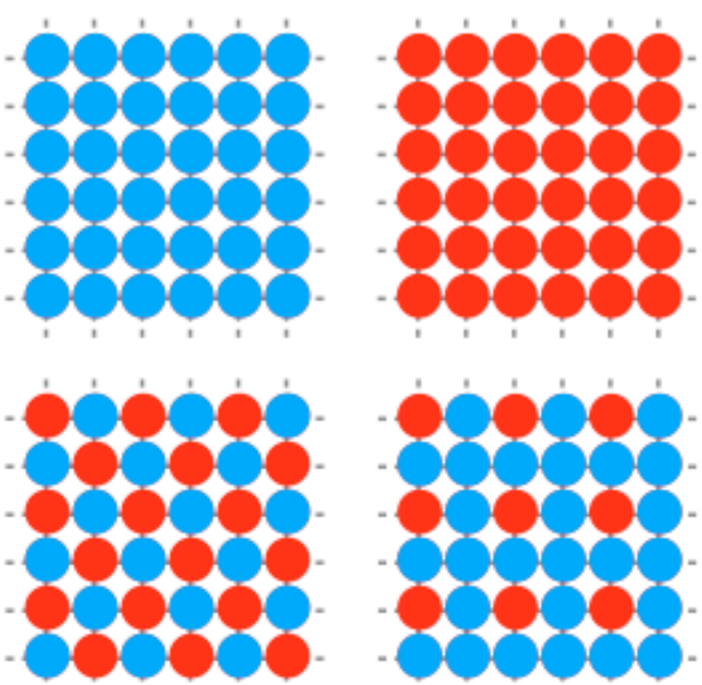
$$\Downarrow$$

$$\begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \end{pmatrix} = \begin{pmatrix} \Pi_{1,1} & \Pi_{1,2} & \Pi_{1,3} & \Pi_{1,4} \\ \Pi_{2,1} & \Pi_{2,2} & \Pi_{2,3} & \Pi_{2,4} \\ \Pi_{3,1} & \Pi_{3,2} & \Pi_{3,3} & \Pi_{3,4} \\ \Pi_{4,1} & \Pi_{4,2} & \Pi_{4,3} & \Pi_{4,4} \end{pmatrix}^{-1} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \\ E_4 \end{pmatrix}$$

$$\begin{pmatrix} E_1 \\ E_2 \\ E_3 \\ E_4 \end{pmatrix} = \begin{pmatrix} \Pi_{1,1} & \Pi_{1,2} & \Pi_{1,3} & \Pi_{1,4} \\ \Pi_{2,1} & \Pi_{2,2} & \Pi_{2,3} & \Pi_{2,4} \\ \Pi_{3,1} & \Pi_{3,2} & \Pi_{3,3} & \Pi_{3,4} \\ \Pi_{4,1} & \Pi_{4,2} & \Pi_{4,3} & \Pi_{4,4} \end{pmatrix} \begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \end{pmatrix}$$

$$\Downarrow$$

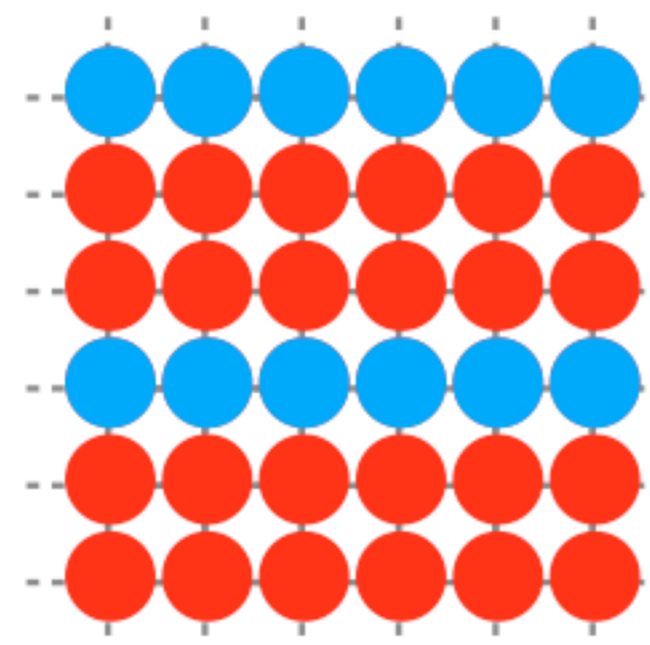
$$\begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \end{pmatrix} = \begin{pmatrix} \Pi_{1,1} & \Pi_{1,2} & \Pi_{1,3} & \Pi_{1,4} \\ \Pi_{2,1} & \Pi_{2,2} & \Pi_{2,3} & \Pi_{2,4} \\ \Pi_{3,1} & \Pi_{3,2} & \Pi_{3,3} & \Pi_{3,4} \\ \Pi_{4,1} & \Pi_{4,2} & \Pi_{4,3} & \Pi_{4,4} \end{pmatrix}^{-1} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \\ E_4 \end{pmatrix}$$



$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & -1 & 0 \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$\longrightarrow$

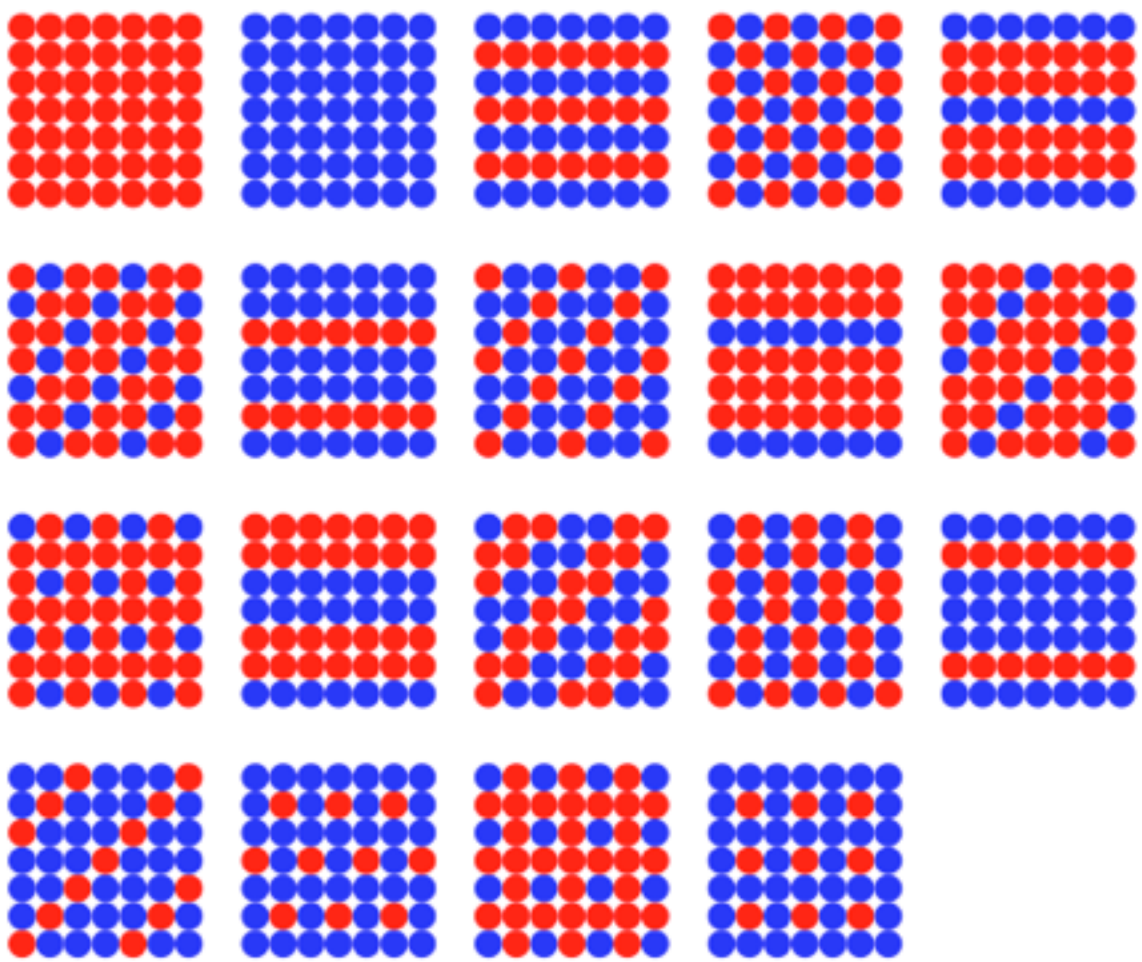
invert and predict by hand



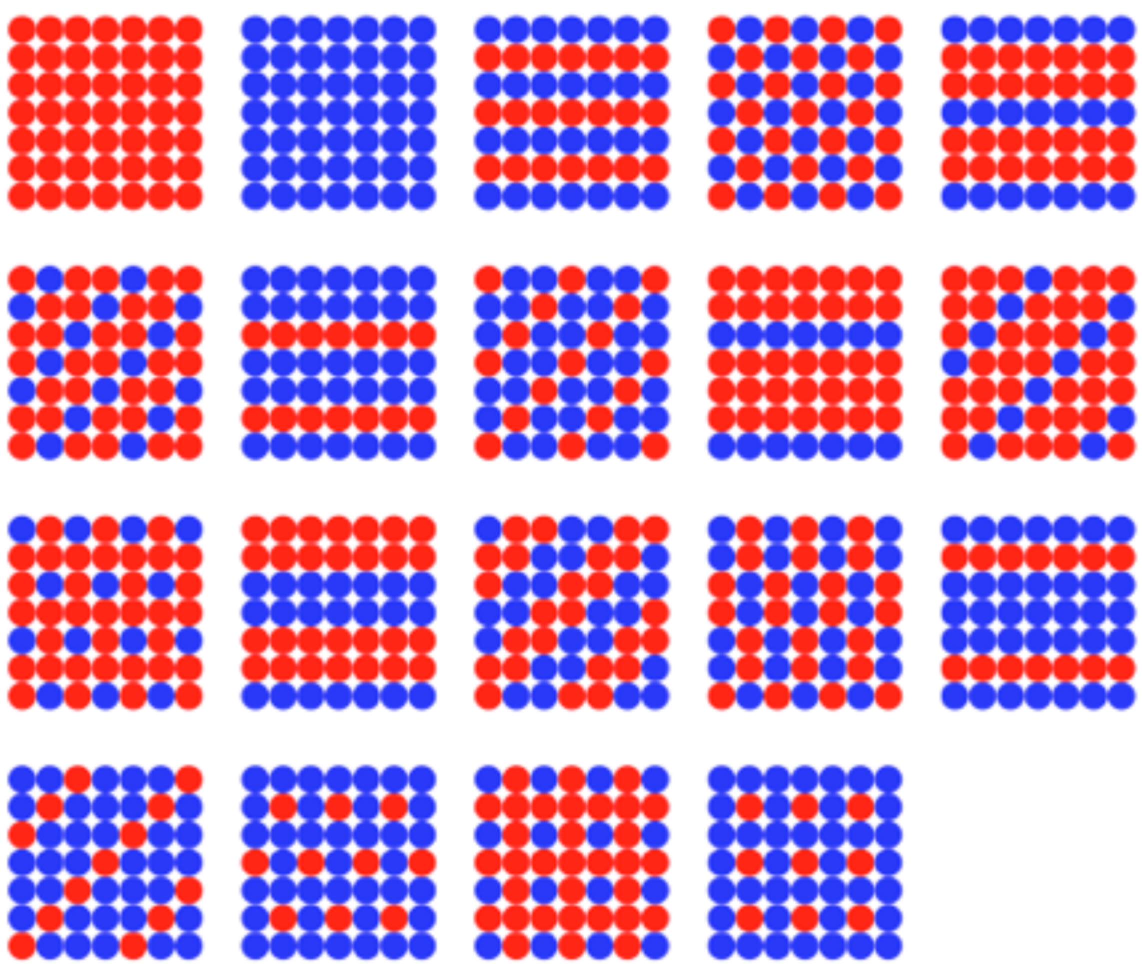
... now do the same problem again but using UNCLE

... now do the same problem again but using UNCLE
- and predict all structures up to four atoms

... now do the same problem again but using UNCLE
- and predict all structures up to four atoms



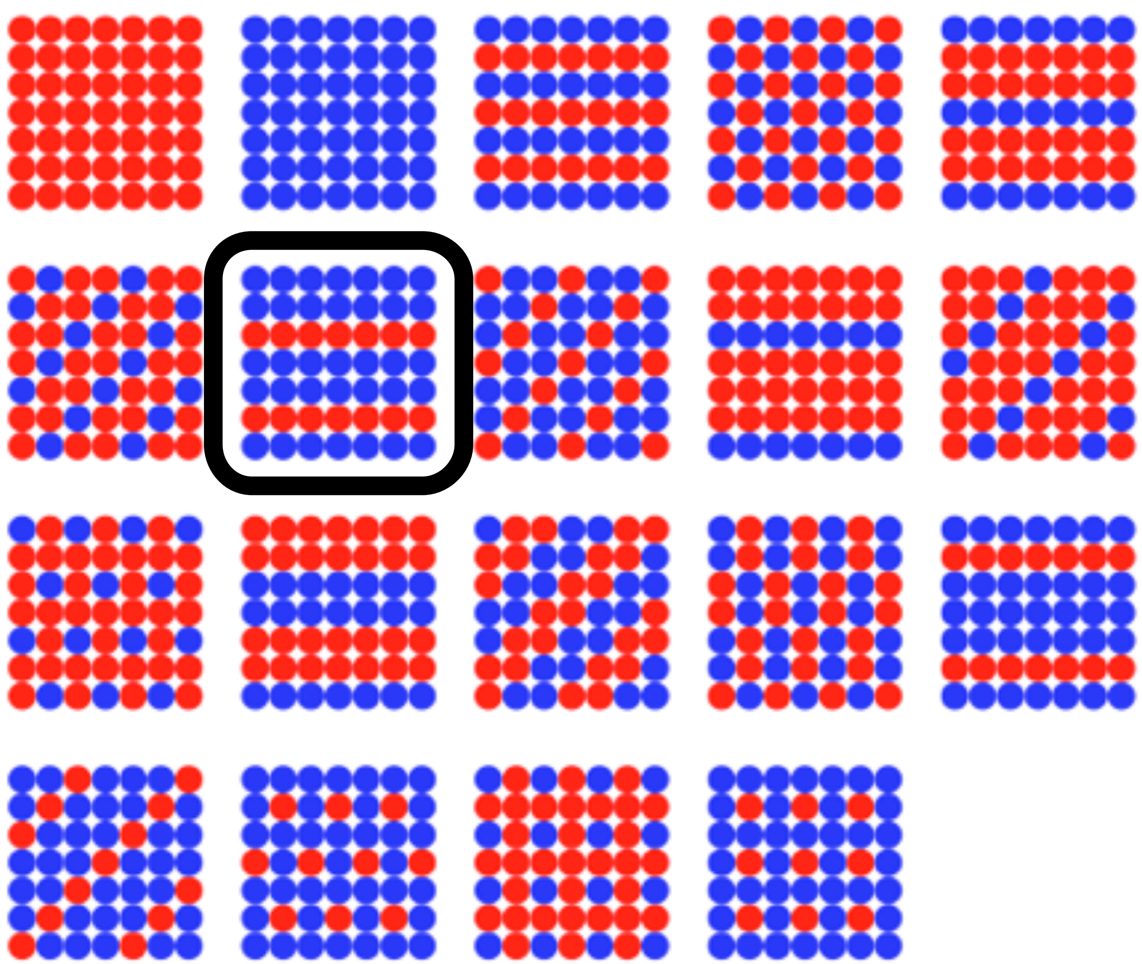
... now do the same problem again but using UNCLE
- and predict all structures up to four atoms



Matrix of $\overline{\Pi}$'s

1.000000	1.000000	1.000000	1.000000
1.000000	0.500000	0.500000	0.000000
1.000000	0.500000	0.000000	0.500000
1.000000	0.500000	0.000000	0.000000
1.000000	0.500000	0.000000	0.000000
1.000000	0.333333	0.333333	-0.333333
1.000000	0.333333	-0.333333	0.333333
1.000000	0.000000	0.500000	0.000000
1.000000	0.000000	0.000000	-1.000000
1.000000	0.000000	0.000000	0.000000
1.000000	0.000000	-0.500000	0.000000
1.000000	0.000000	-1.000000	1.000000
1.000000	-0.333333	0.333333	-0.333333
1.000000	-0.333333	-0.333333	0.333333
1.000000	-0.500000	0.500000	0.000000
1.000000	-0.500000	0.000000	0.000000
1.000000	-0.500000	0.000000	0.000000
1.000000	-0.500000	0.000000	0.500000
1.000000	-1.000000	1.000000	1.000000

... now do the same problem again but using UNCLE
- and predict all structures up to four atoms



Matrix of $\overline{\Pi}$'s

1.000000	1.000000	1.000000	1.000000
1.000000	0.500000	0.500000	0.000000
1.000000	0.500000	0.000000	0.500000
1.000000	0.500000	0.000000	0.000000
1.000000	0.500000	0.000000	0.000000
1.000000	0.333333	0.333333	-0.333333
1.000000	0.333333	-0.333333	0.333333
1.000000	0.000000	0.500000	0.000000
1.000000	0.000000	0.000000	-1.000000
1.000000	0.000000	0.000000	0.000000
1.000000	0.000000	-0.500000	0.000000
1.000000	0.000000	-1.000000	1.000000
1.000000	-0.333333	0.333333	-0.333333
1.000000	-0.333333	-0.333333	0.333333
1.000000	-0.500000	0.500000	0.000000
1.000000	-0.500000	0.000000	0.000000
1.000000	-0.500000	0.000000	0.000000
1.000000	-0.500000	0.000000	0.500000
1.000000	-1.000000	1.000000	1.000000

... now do the same problem again but using UNCLE
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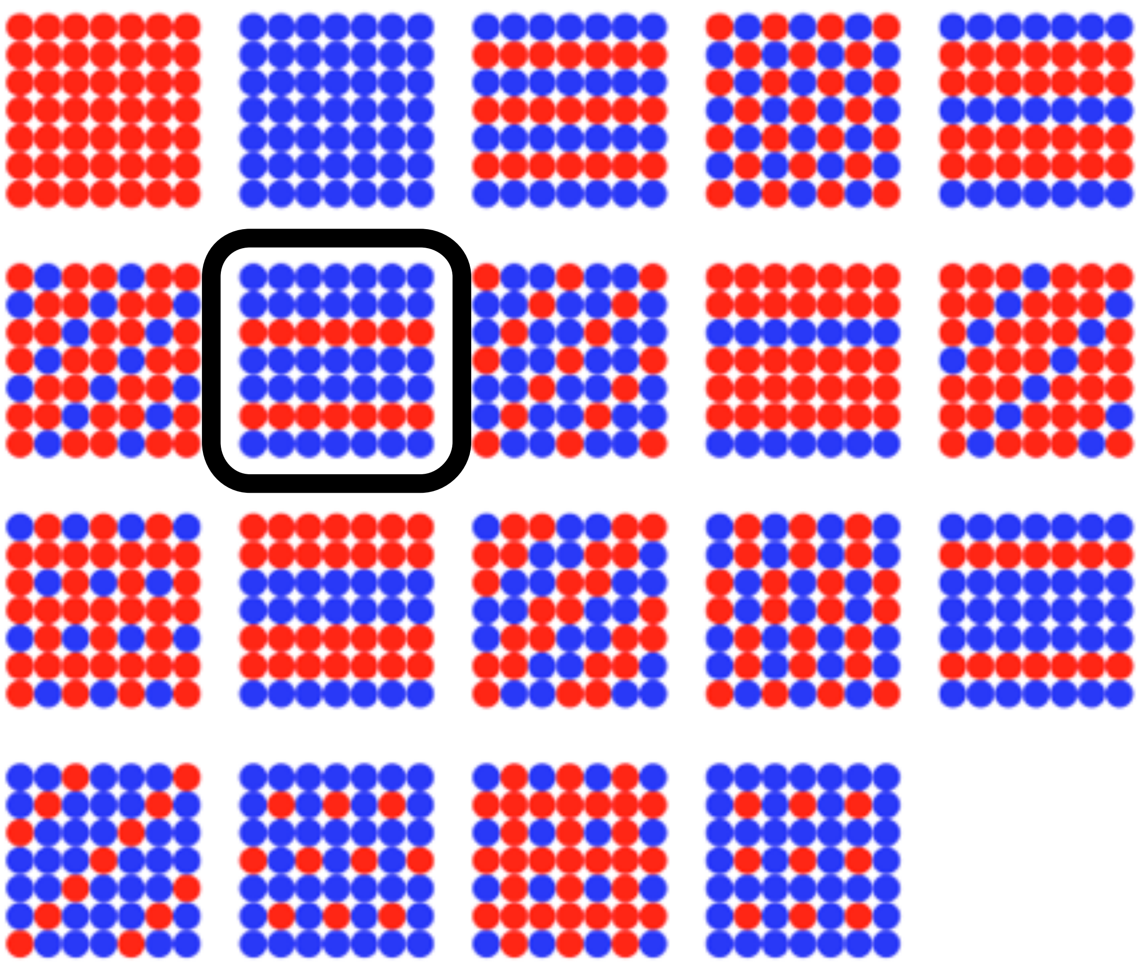
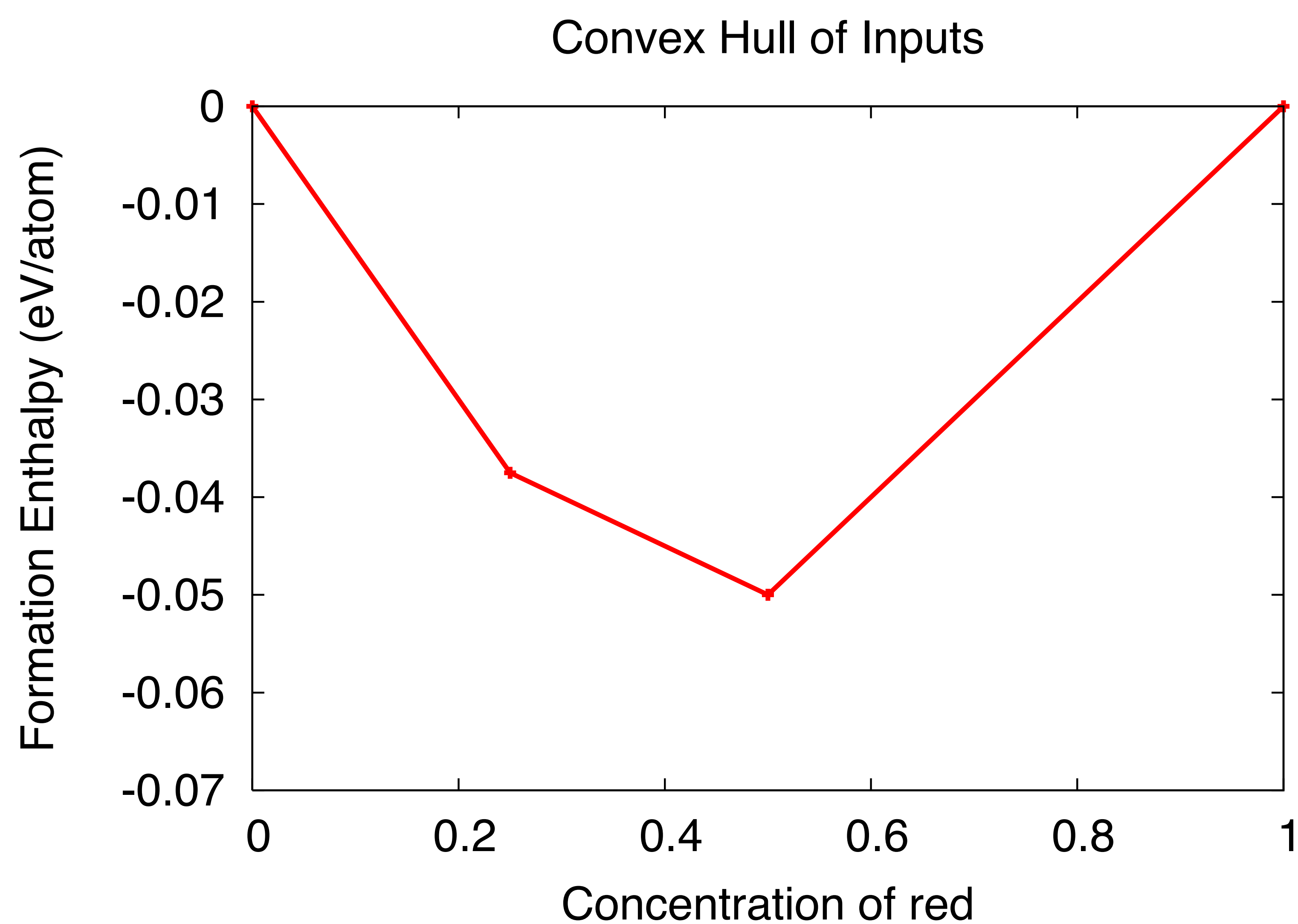


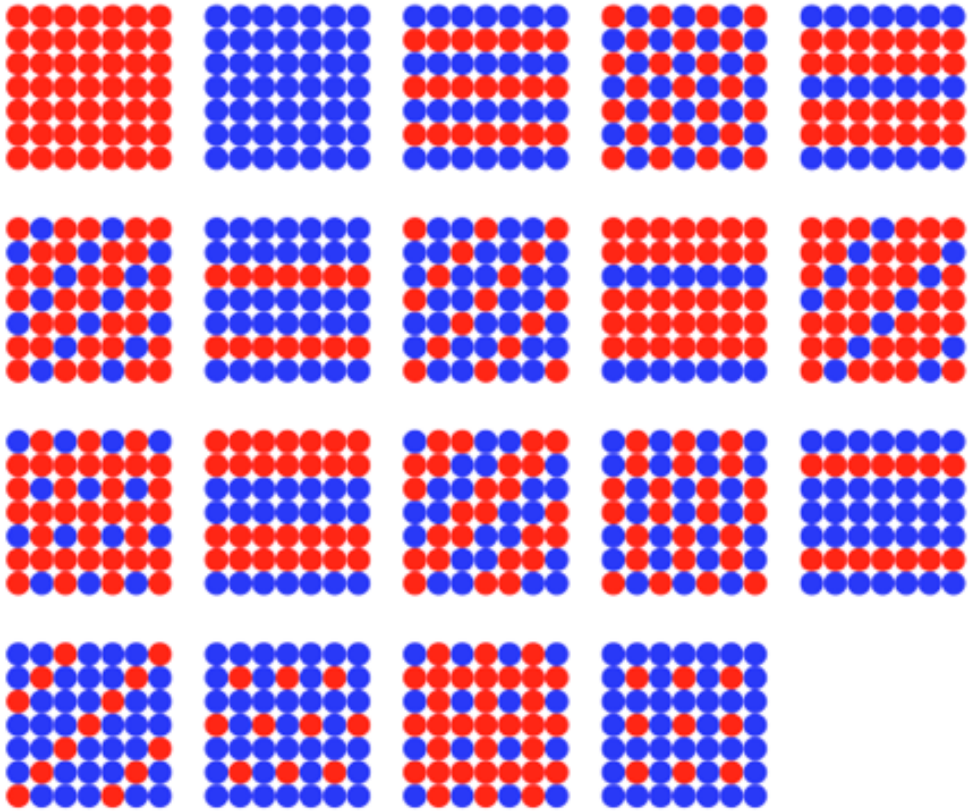
$$E = \vec{\overline{\overline{\Pi}}} \cdot \vec{J}$$

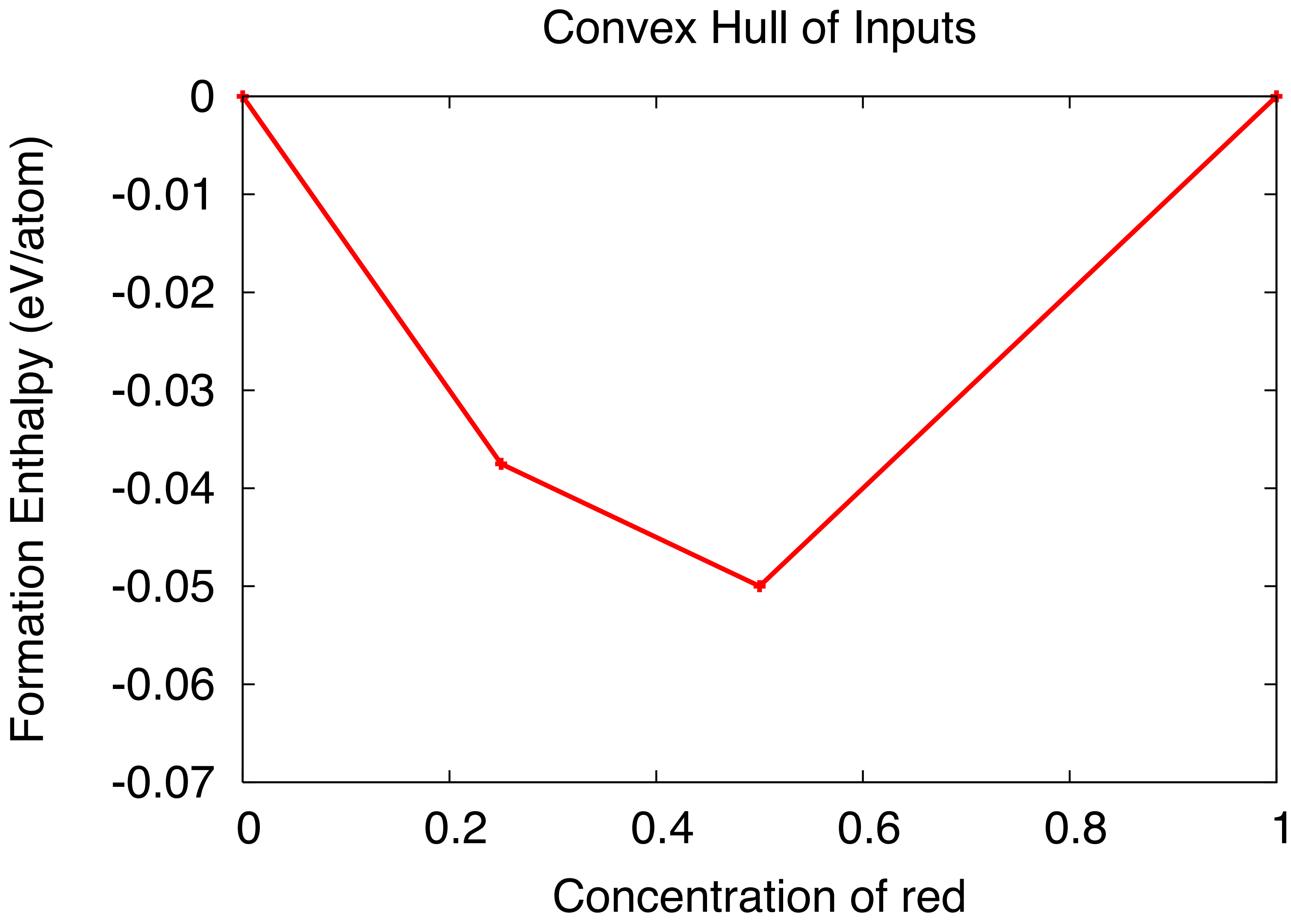
Matrix of $\overline{\Pi}$'s

1.000000	1.000000	1.000000	1.000000
1.000000	0.500000	0.500000	0.000000
1.000000	0.500000	0.000000	0.500000
1.000000	0.500000	0.000000	0.000000
1.000000	0.500000	0.000000	0.000000
1.000000	0.333333	0.333333	-0.333333
1.000000	0.333333	-0.333333	0.333333
1.000000	0.000000	0.500000	0.000000
1.000000	0.000000	0.000000	-1.000000
1.000000	0.000000	0.000000	0.000000
1.000000	0.000000	-0.500000	0.000000
1.000000	0.000000	-1.000000	1.000000
1.000000	-0.333333	0.333333	-0.333333
1.000000	-0.333333	-0.333333	0.333333
1.000000	-0.500000	0.500000	0.000000
1.000000	-0.500000	0.000000	0.000000
1.000000	-0.500000	0.000000	0.000000
1.000000	-0.500000	0.000000	0.500000
1.000000	-1.000000	1.000000	1.000000

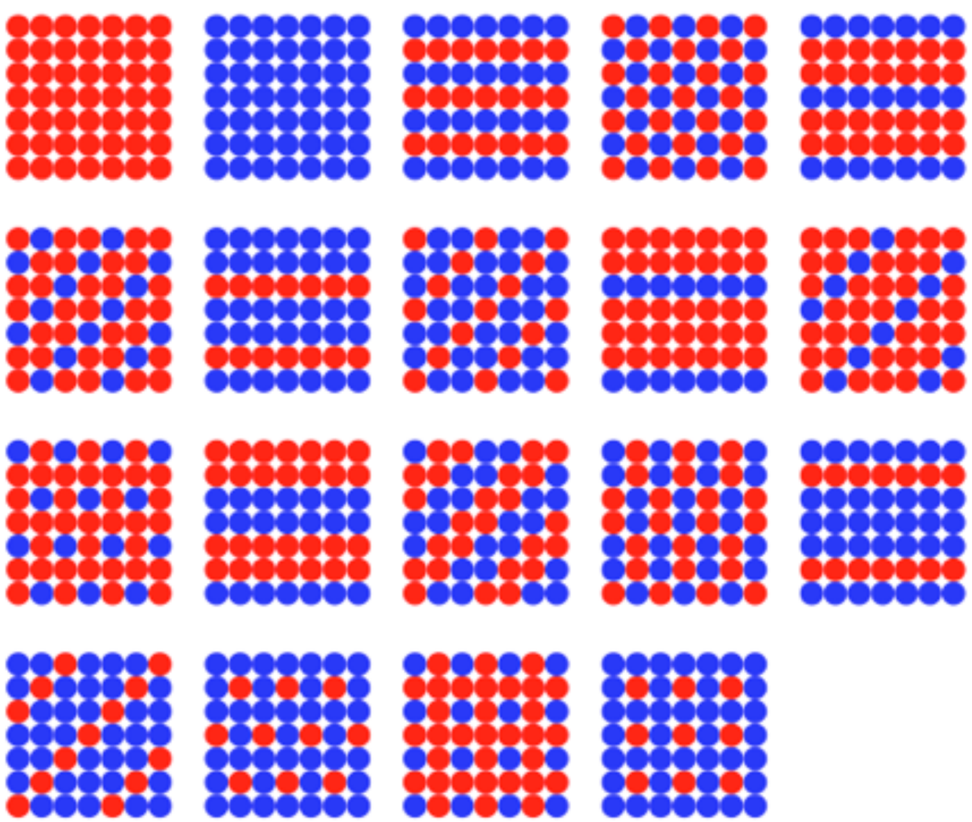


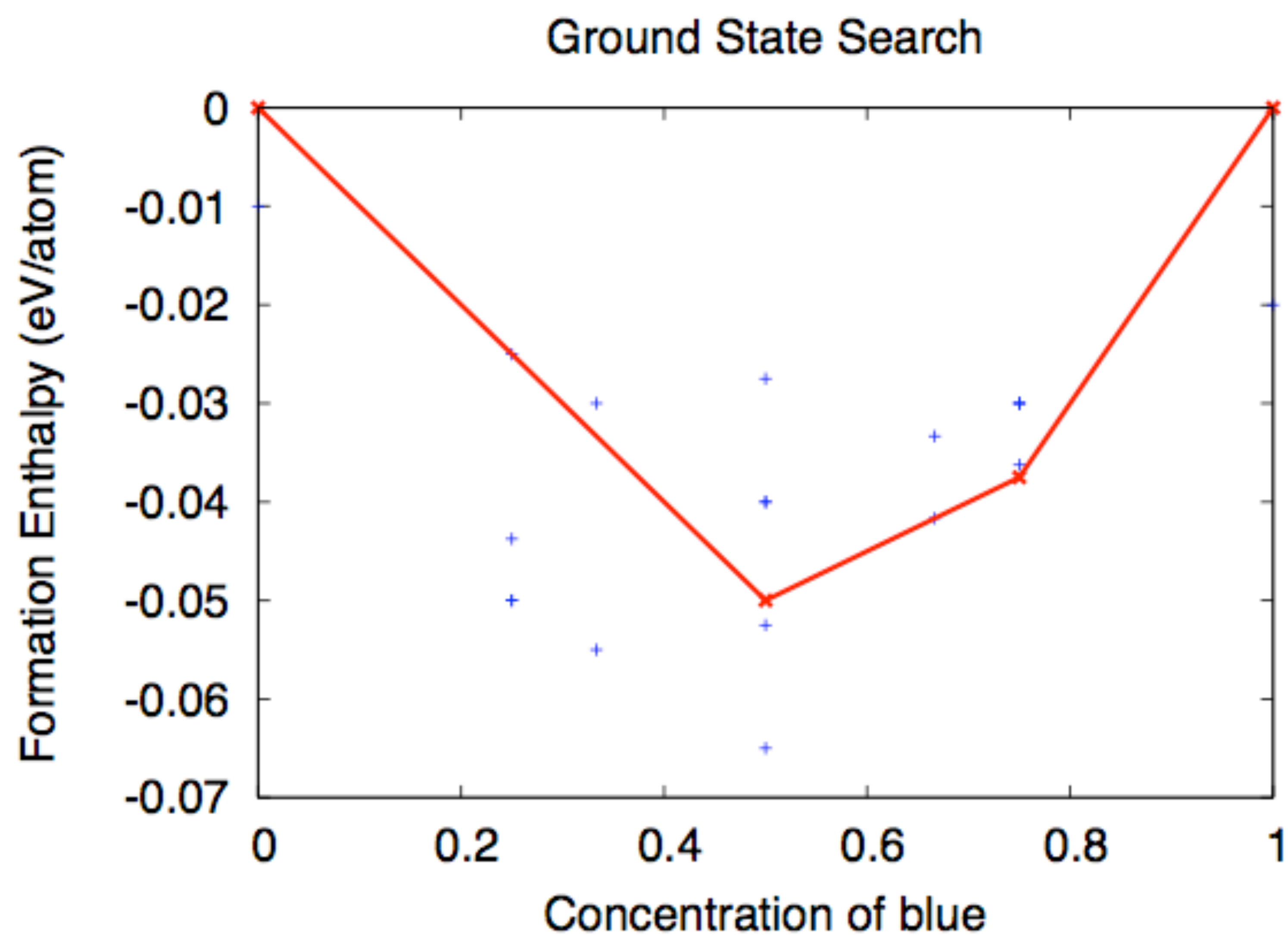
Constructing the **convex hull** from the predictions



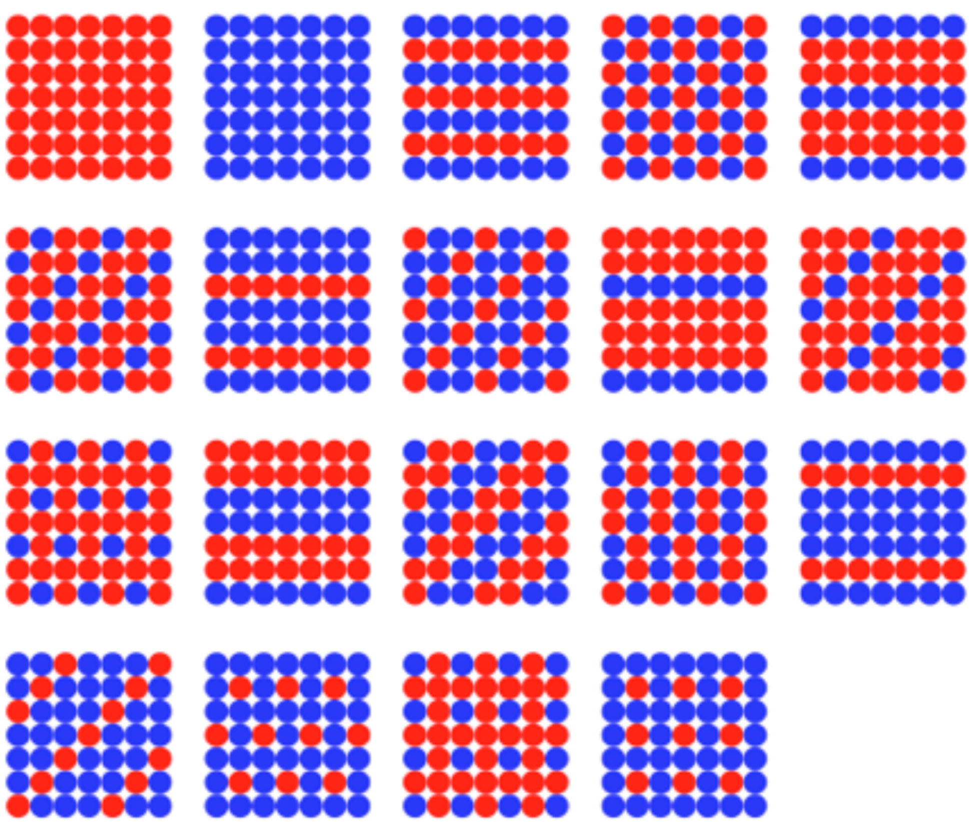


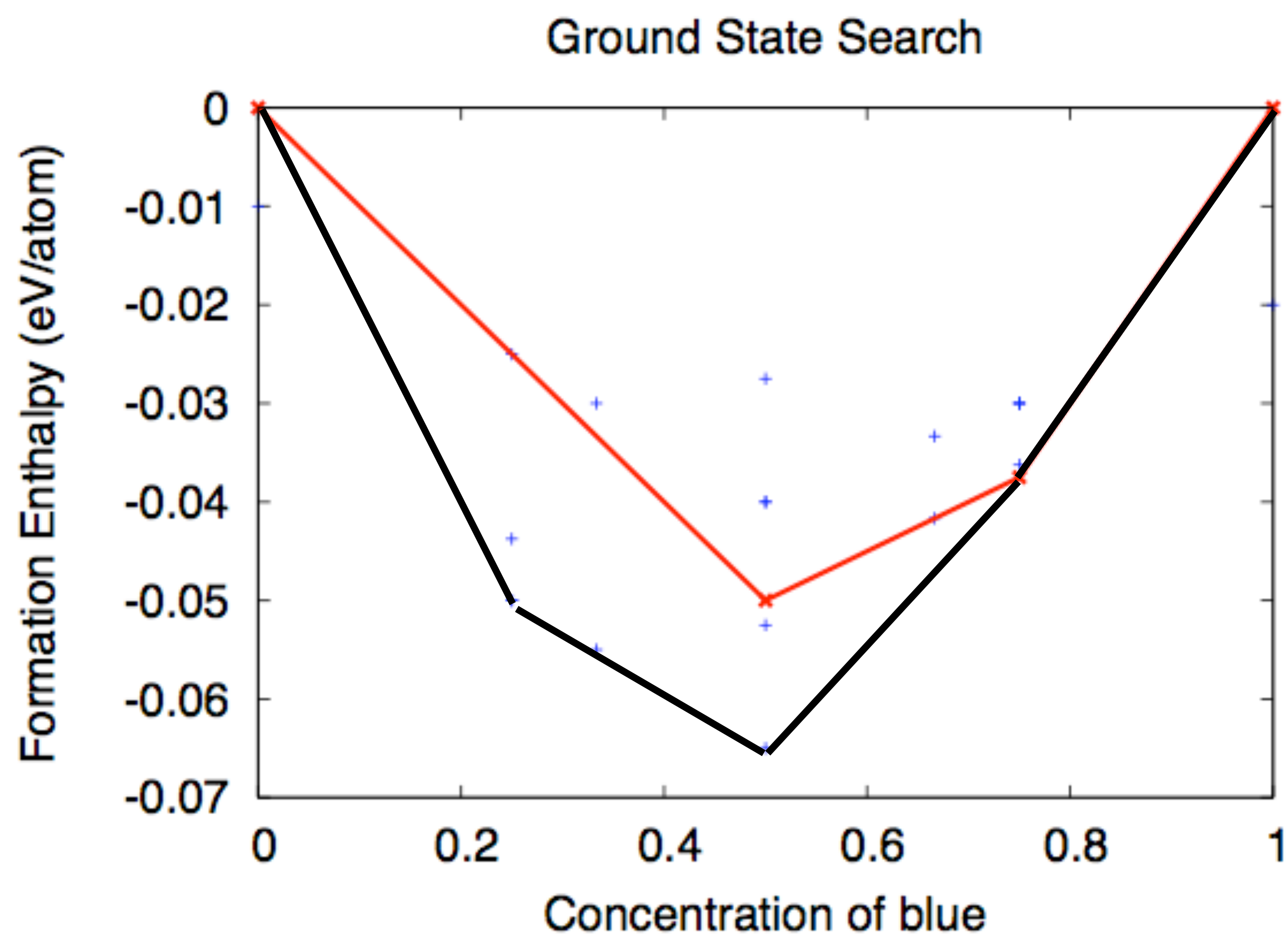
Constructing the **convex hull** from the predictions



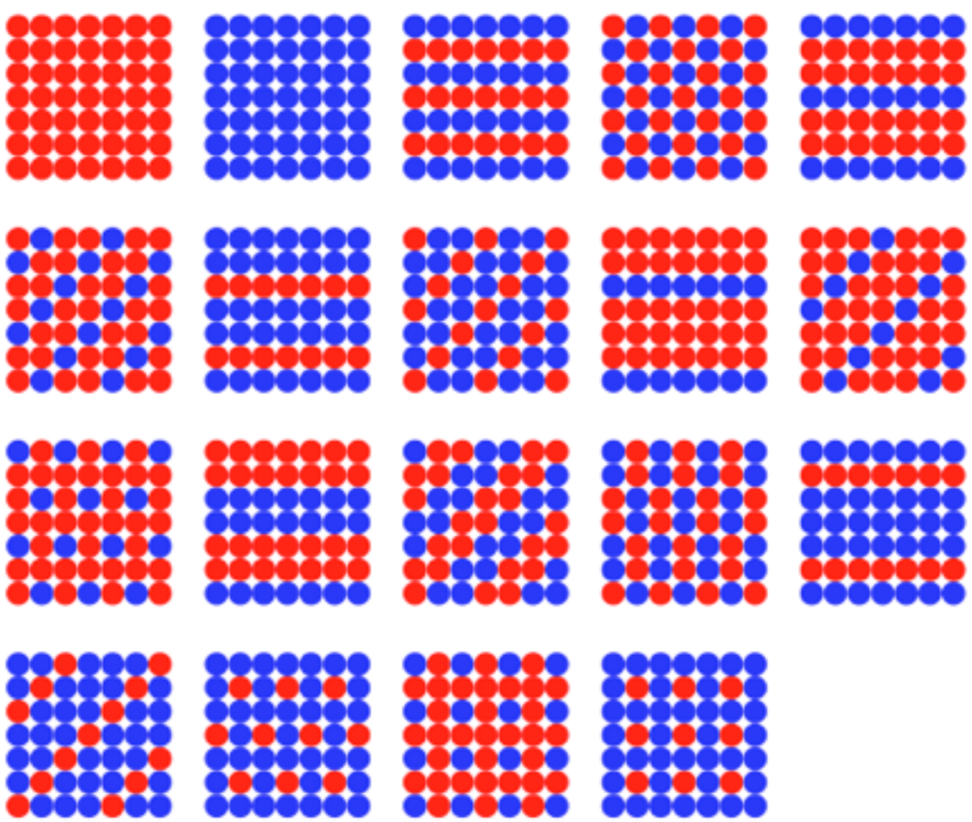


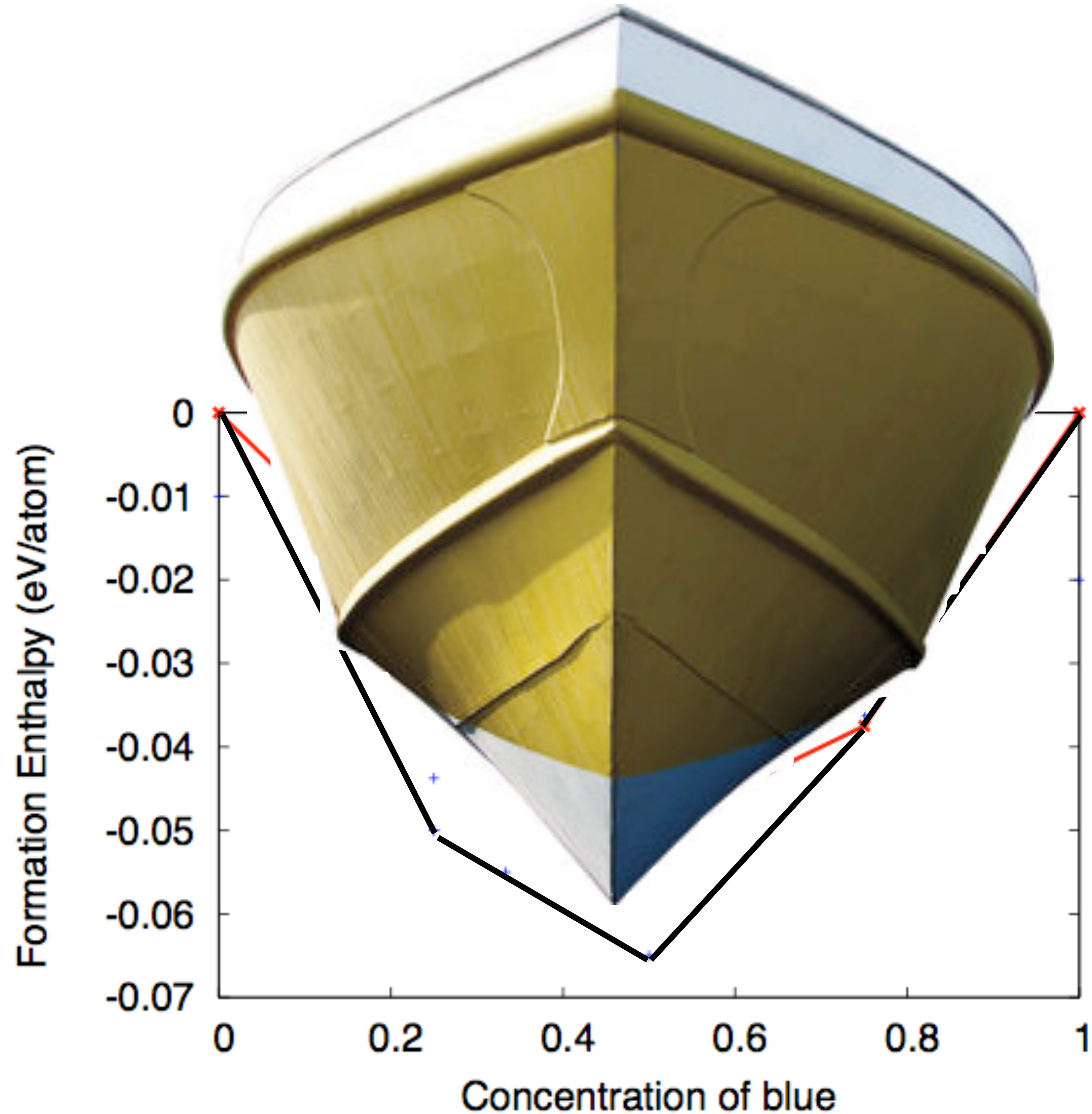
Constructing the **convex hull** from the predictions



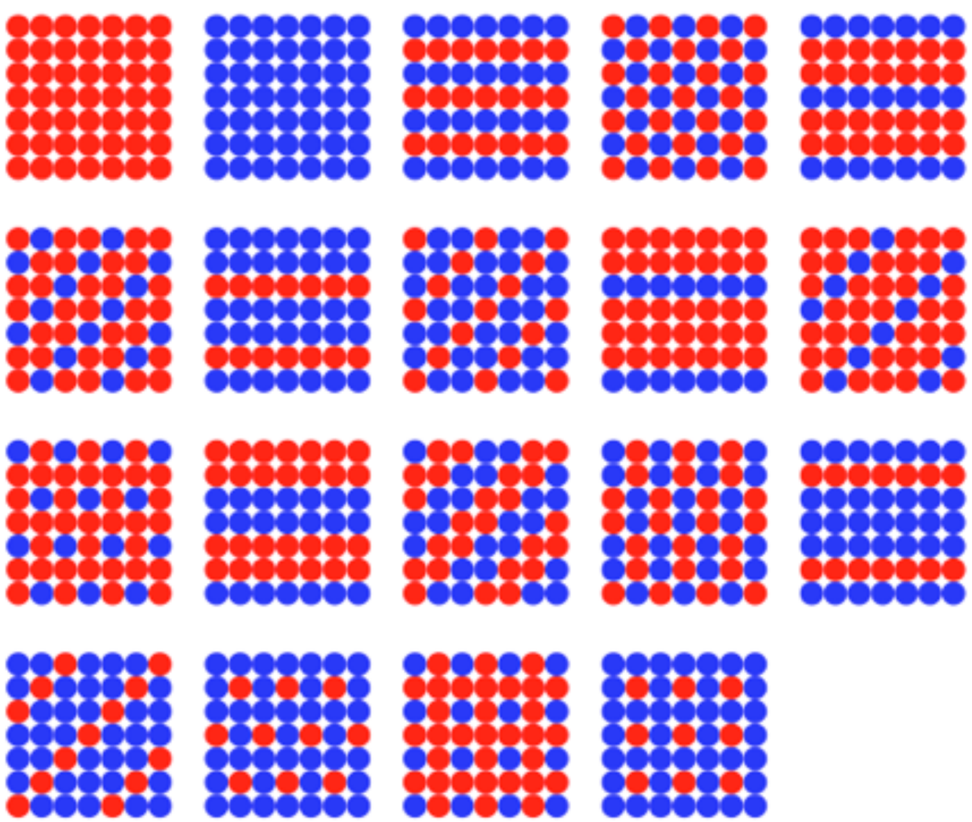


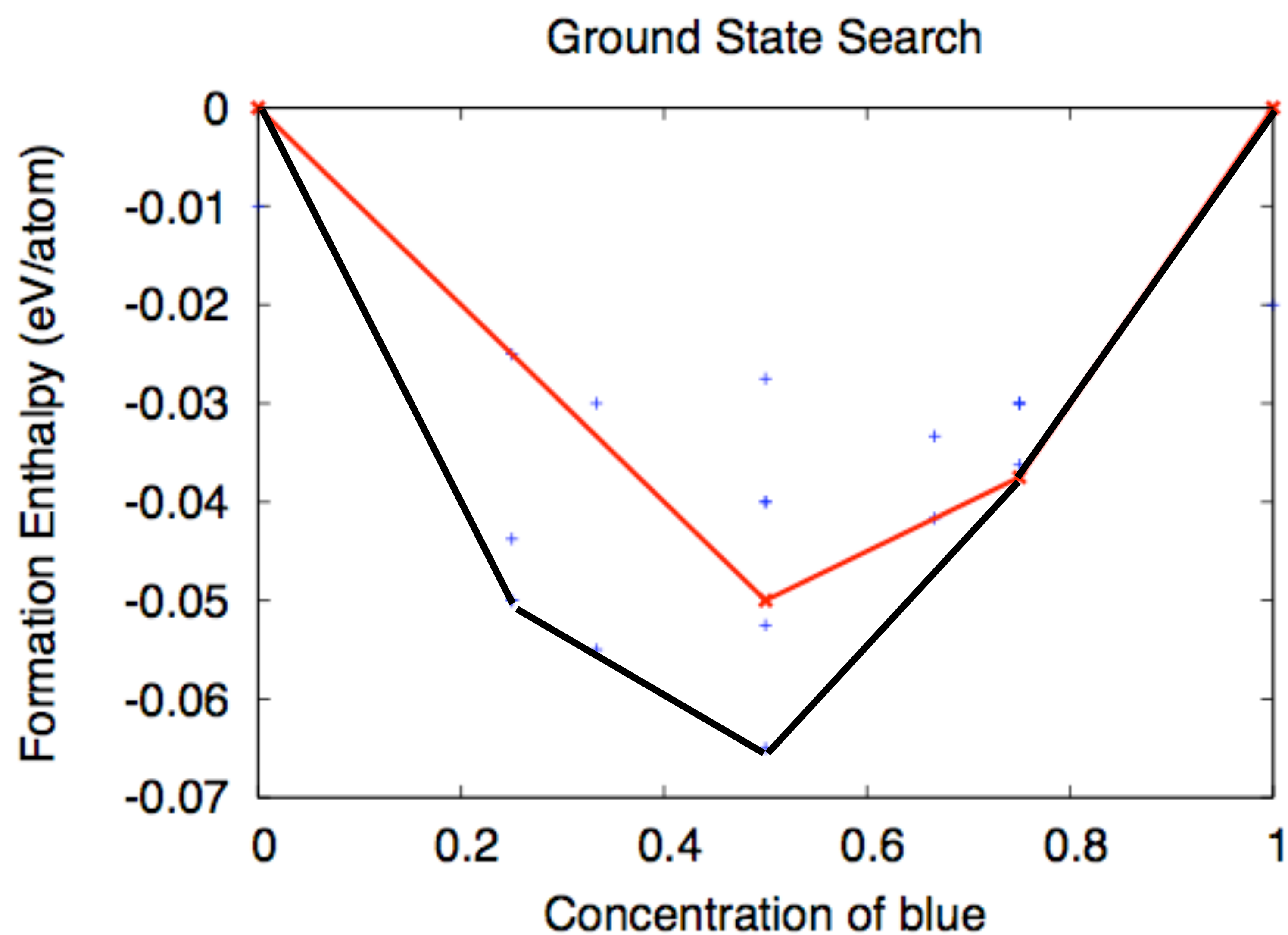
Constructing the **convex hull** from the predictions





Constructing the **convex hull** from the predictions





Constructing the **convex hull** from the predictions

Monte Carlo modeling in a nutshell

Monte Carlo modeling in a nutshell

Use random numbers to...

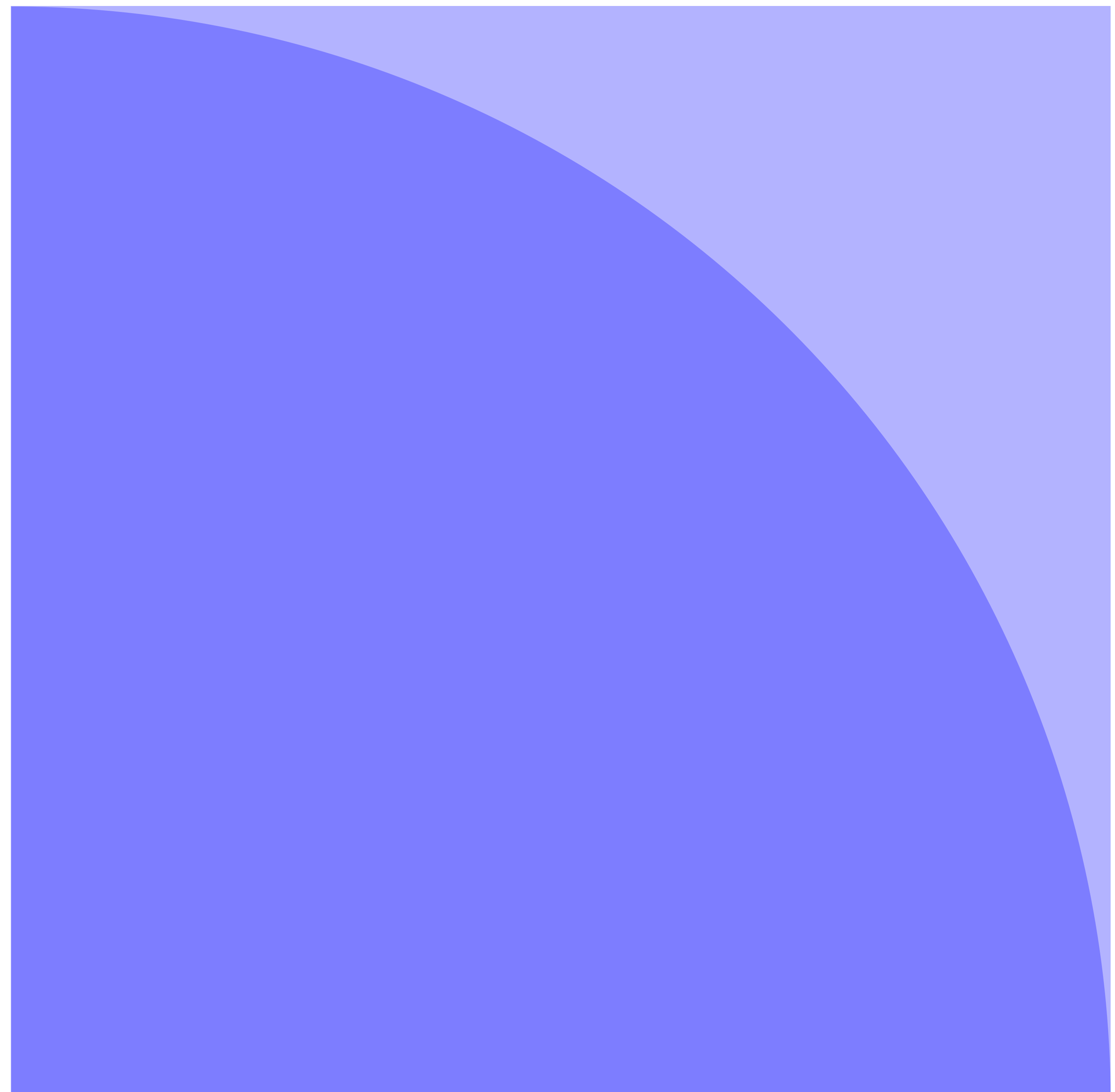
Find the thermodynamic equilibrium of a system as a function of temperature.

Monte Carlo modeling in a nutshell

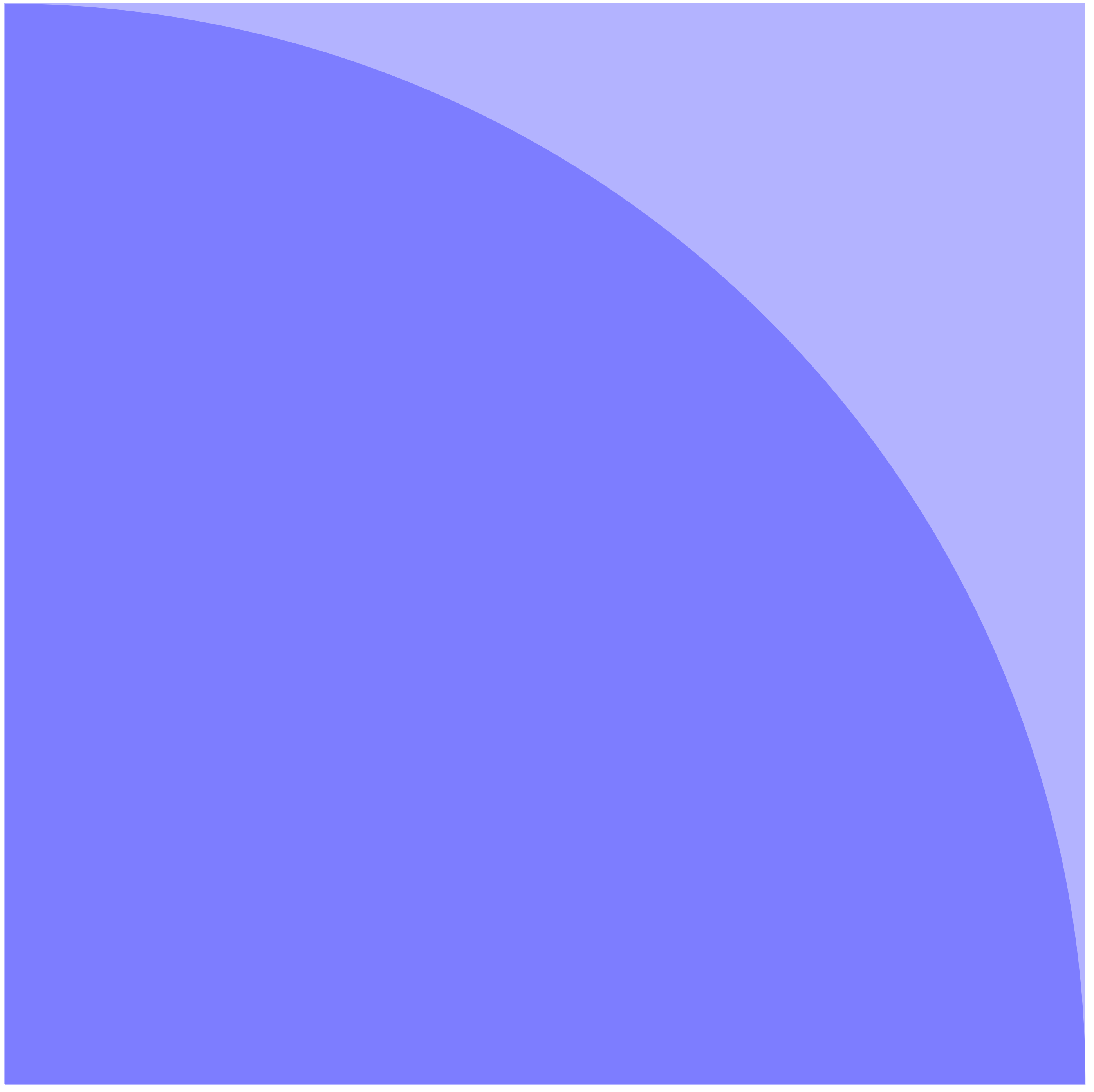
Use random numbers to...

Find the thermodynamic equilibrium of a system as a function of temperature.

- Is a material magnetic at a given T?
- Is a material ordered (stronger) at a given T?



$$\frac{A_{\text{circle}}}{A_{\text{square}}} = \frac{\pi}{4}$$



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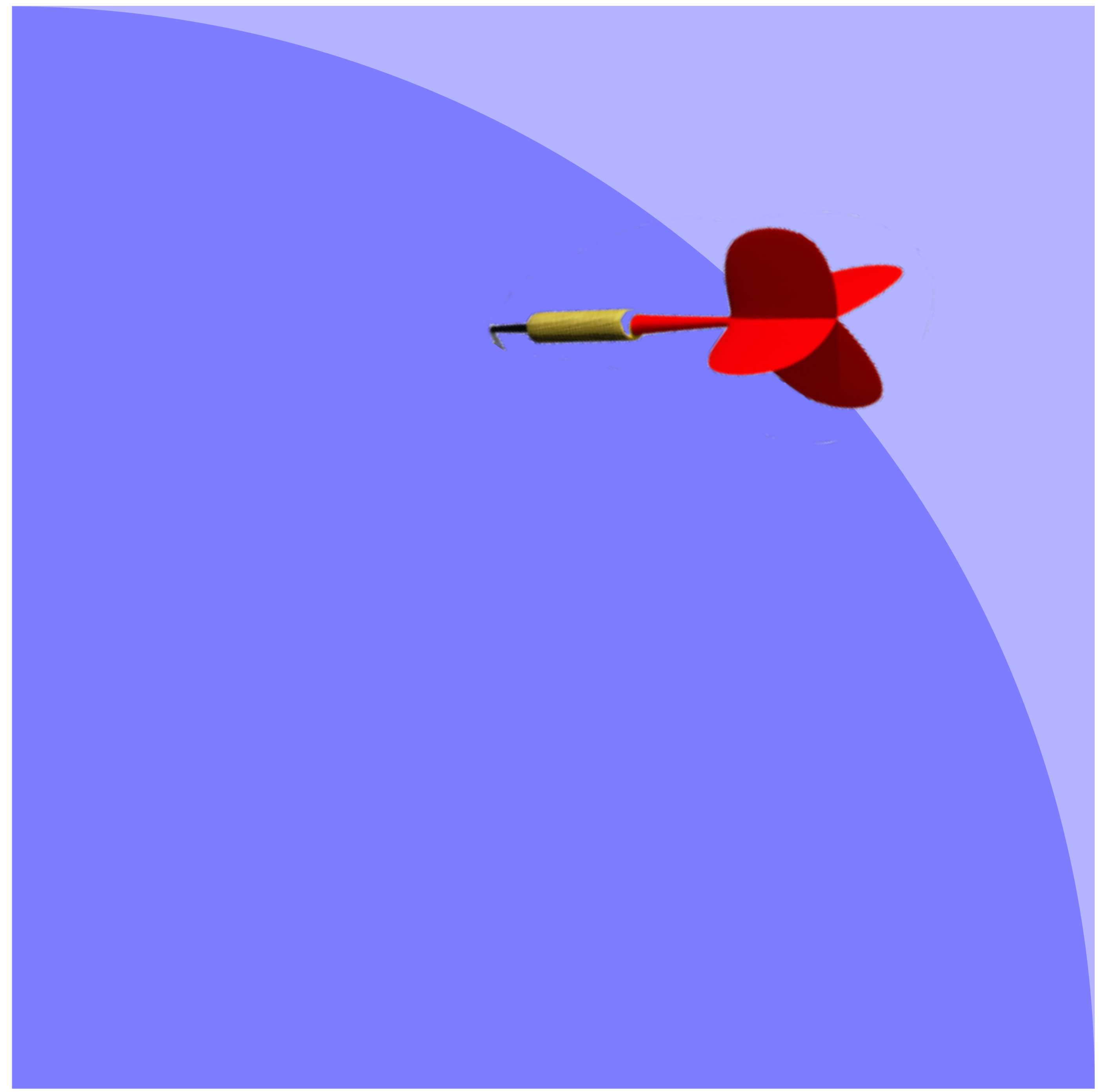

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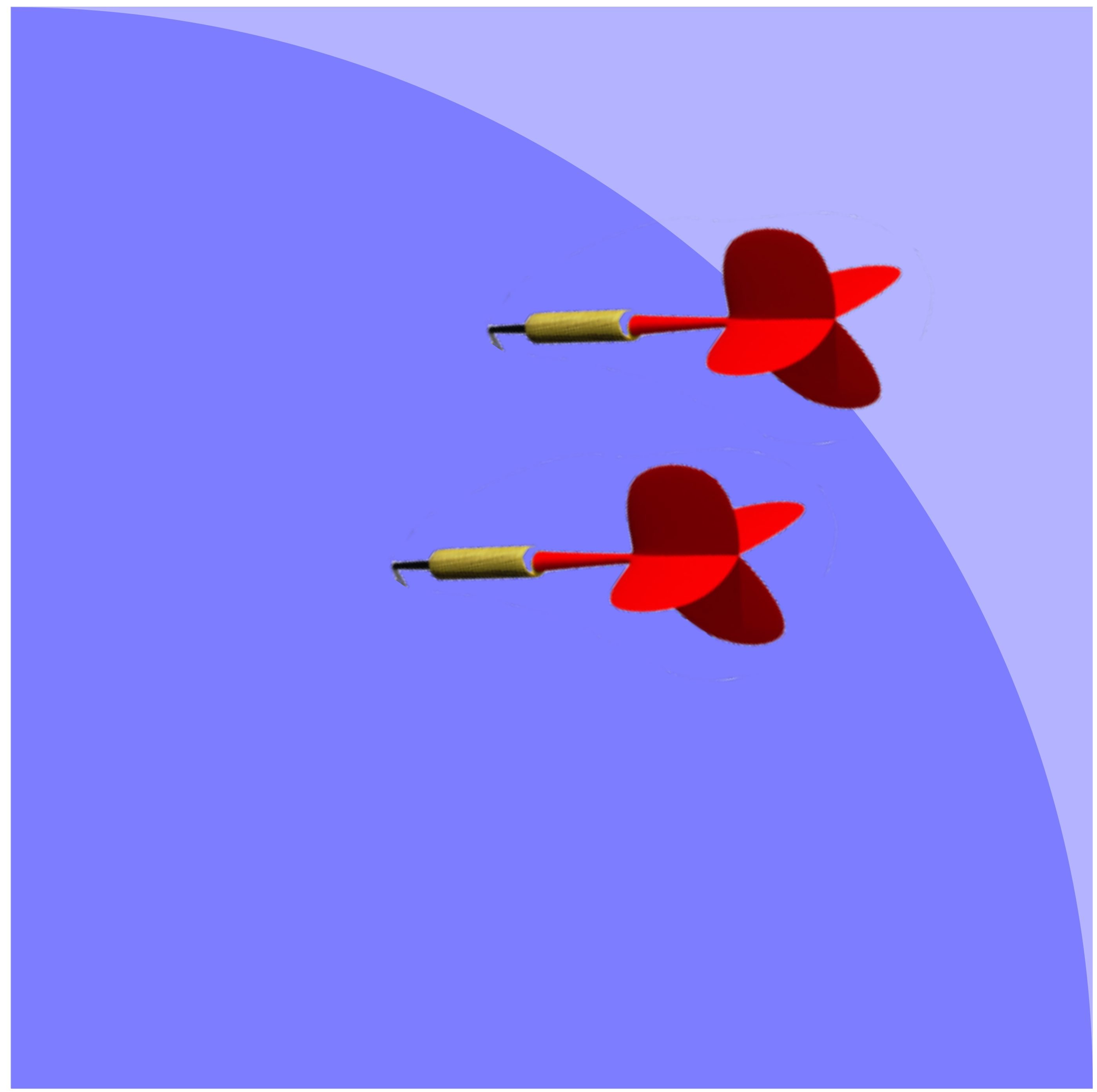
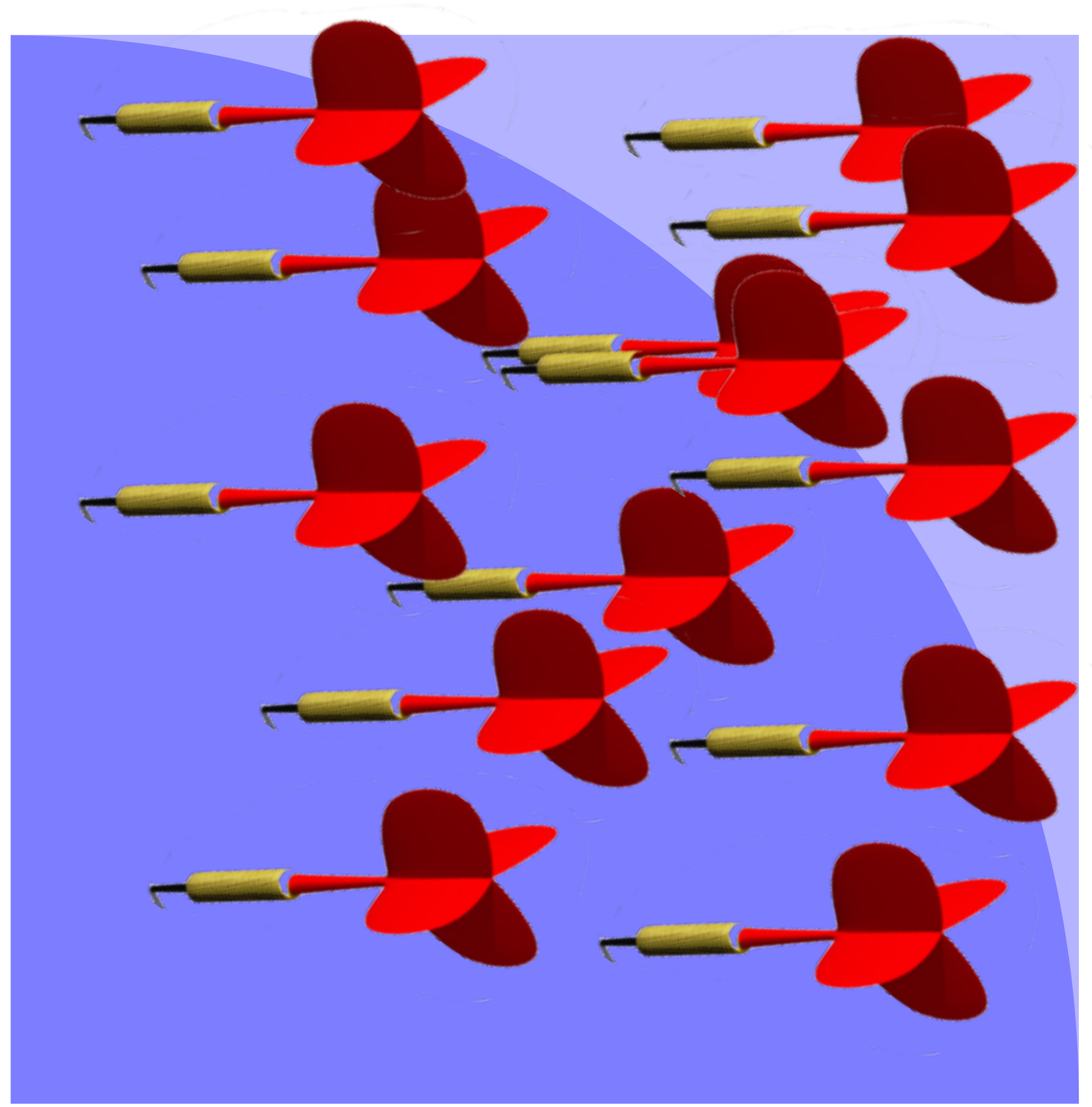
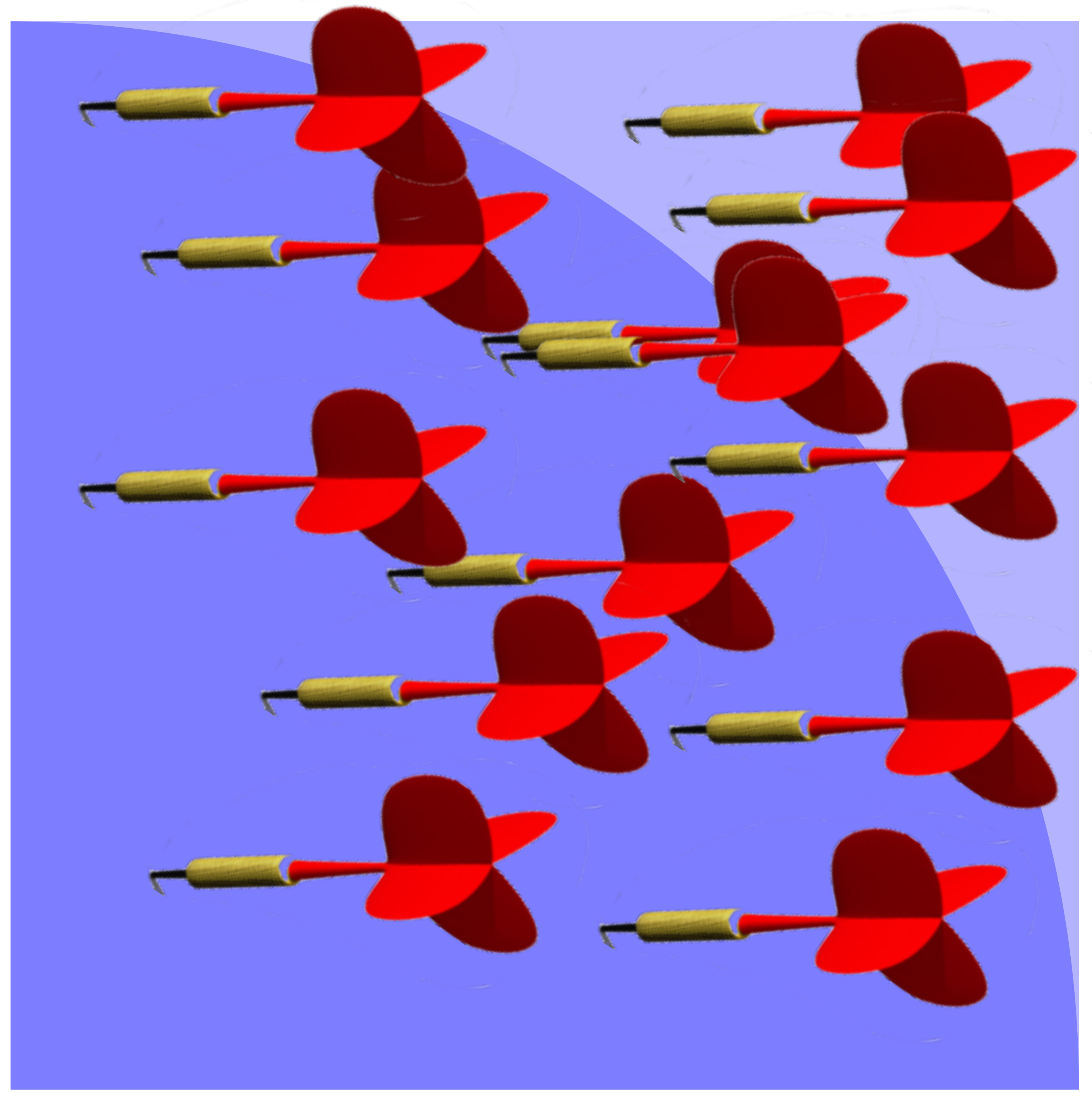


$$\frac{A_{\text{circle}}}{A_{\text{square}}} = \frac{\pi}{4}$$



$$\frac{A_{\text{circle}}}{A_{\text{square}}} = \frac{\pi}{4}$$

$$\frac{N_{\text{circle}}}{N_{\text{square}}} \approx \frac{\pi}{4}$$



Monte Carlo modeling in a nutshell

Find the thermodynamic equilibrium of a system as a function of temperature.

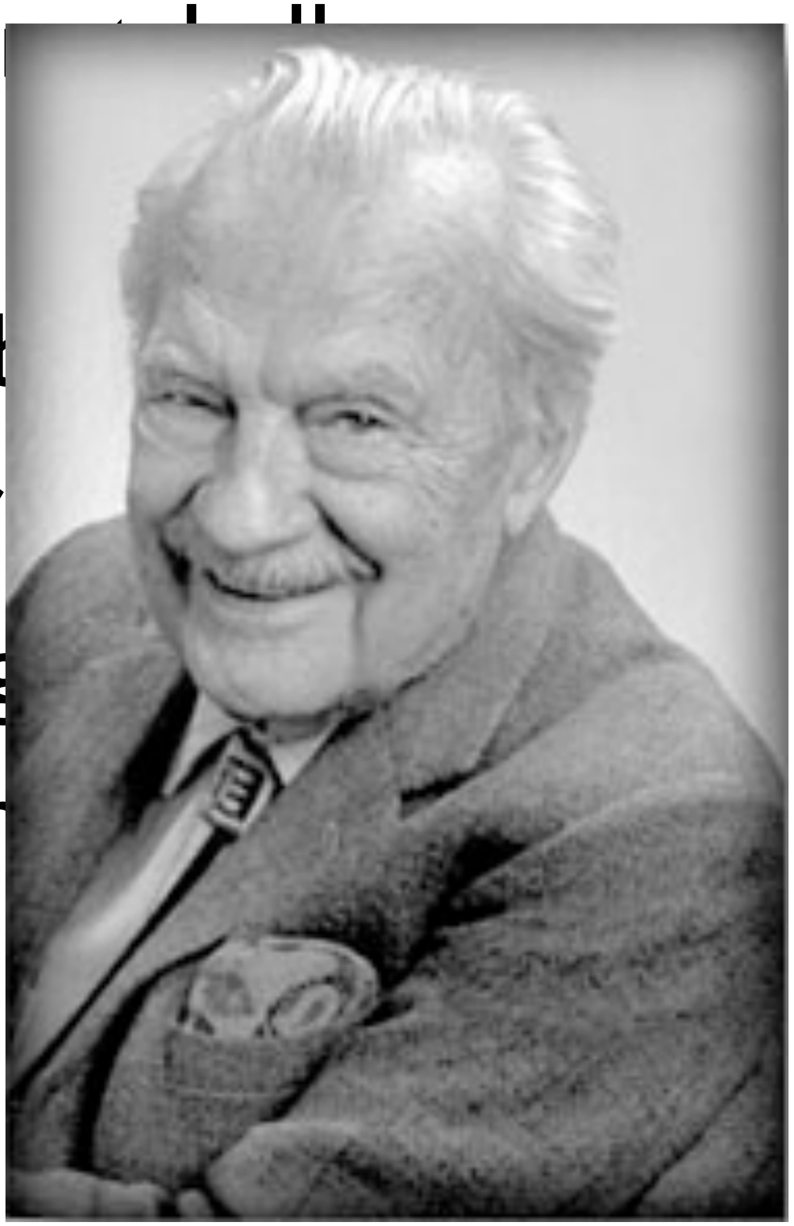
- Is a material magnetic at a given *T*?
- Is a material ordered (stronger) at a given *T*?

Metropolis algorithm:

Monte Carlo modeling in a

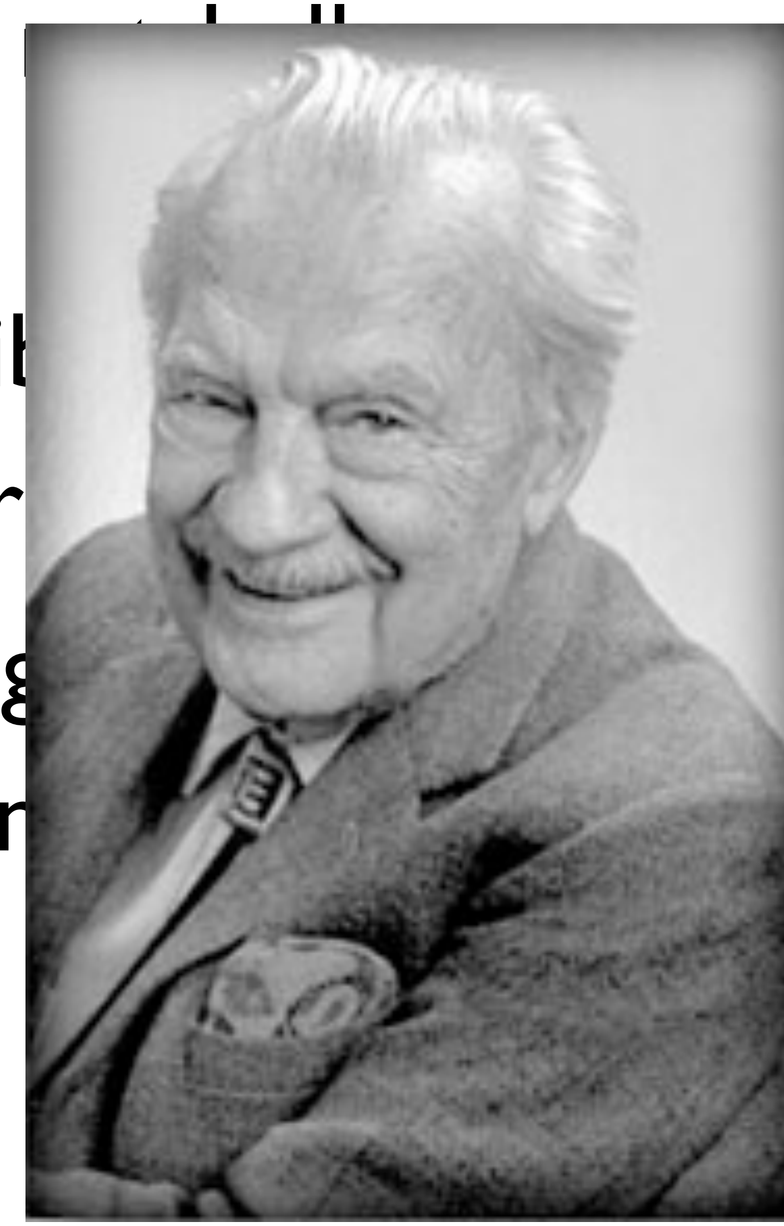
Find the thermodynamic equilib
system as a function of temper

- Is a material magnetic at a g
- Is a material ordered (stron



Metropolis algorithm:

Monte Carlo modeling in a



Find the thermodynamic equilib

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Metropolis algorithm:

- Choose a new configuration, compute ΔE
- If $\Delta E \leq 0$, keep it
- If $\Delta E > 0$, keep it only if $\exp \Delta E/kT > r$

Monte Carlo modeling in a

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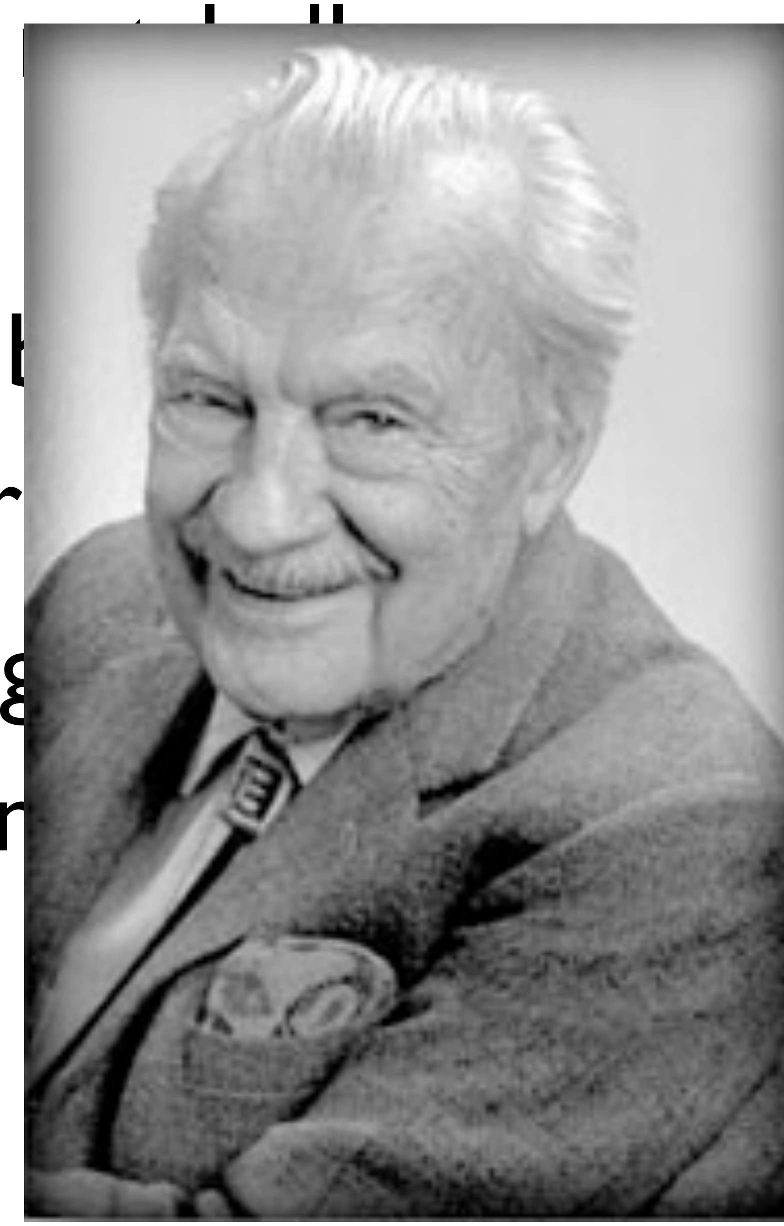

Metropolis algorithm:

At random

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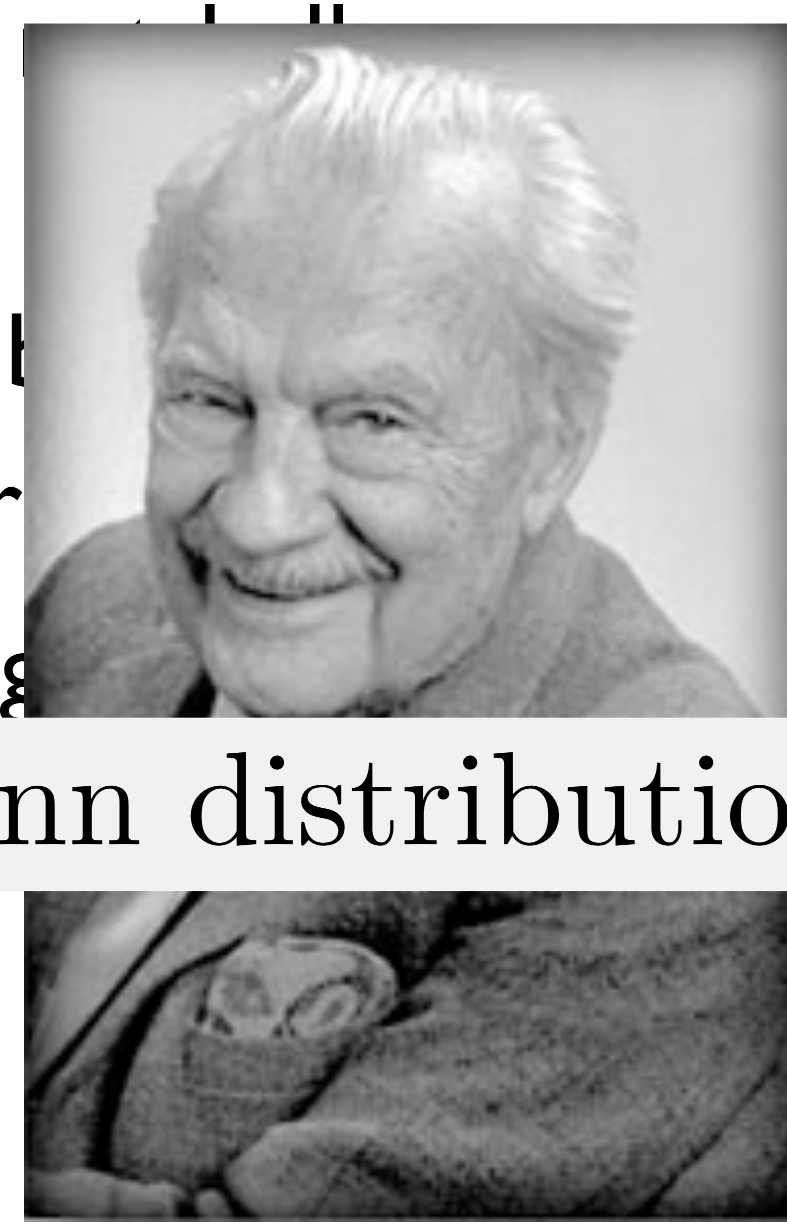
Monte Carlo modeling in a



Find the thermodynamic equilib

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Collection of states: Boltzmann distribution

Metropolis algorithm:

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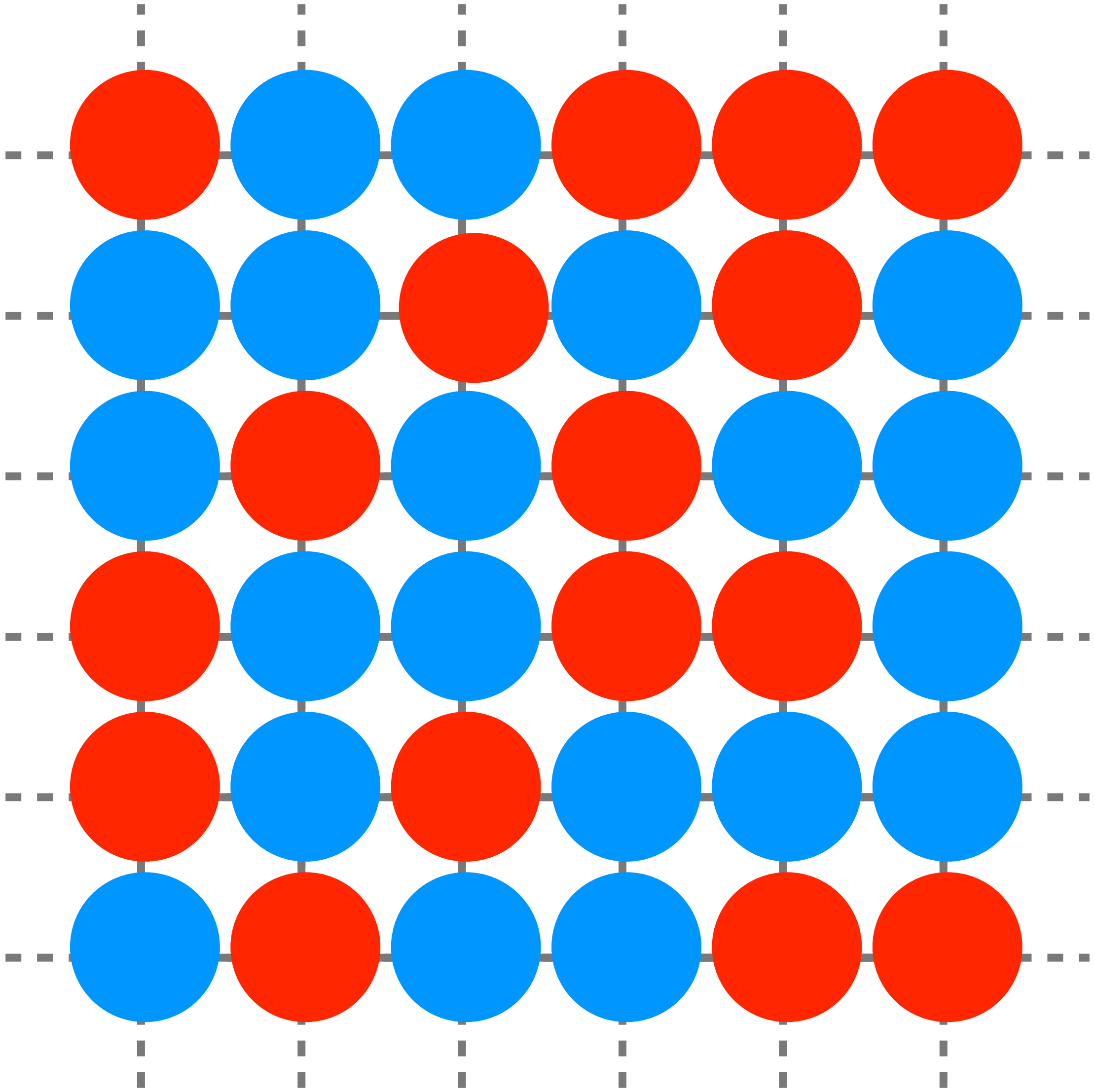

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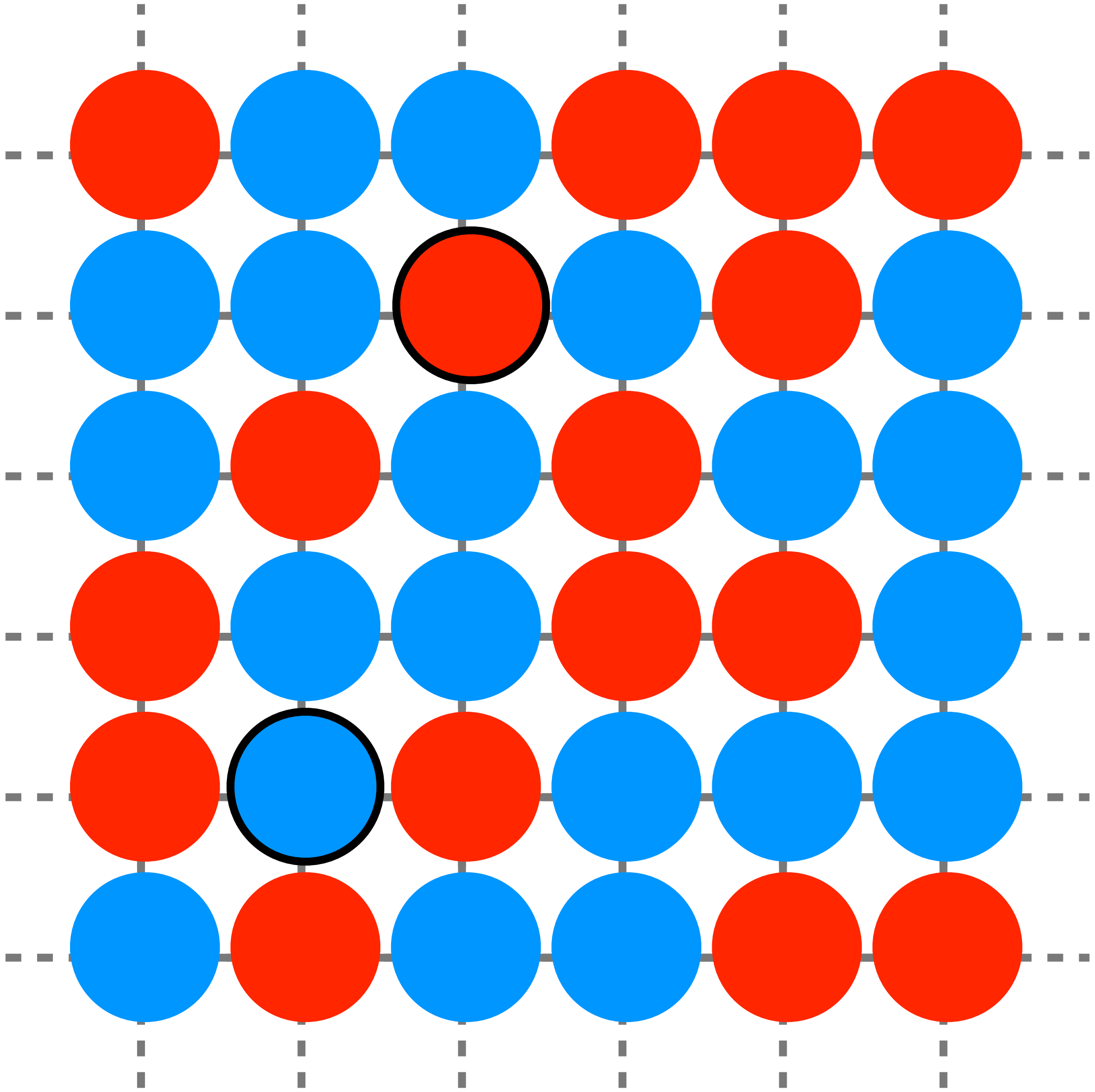

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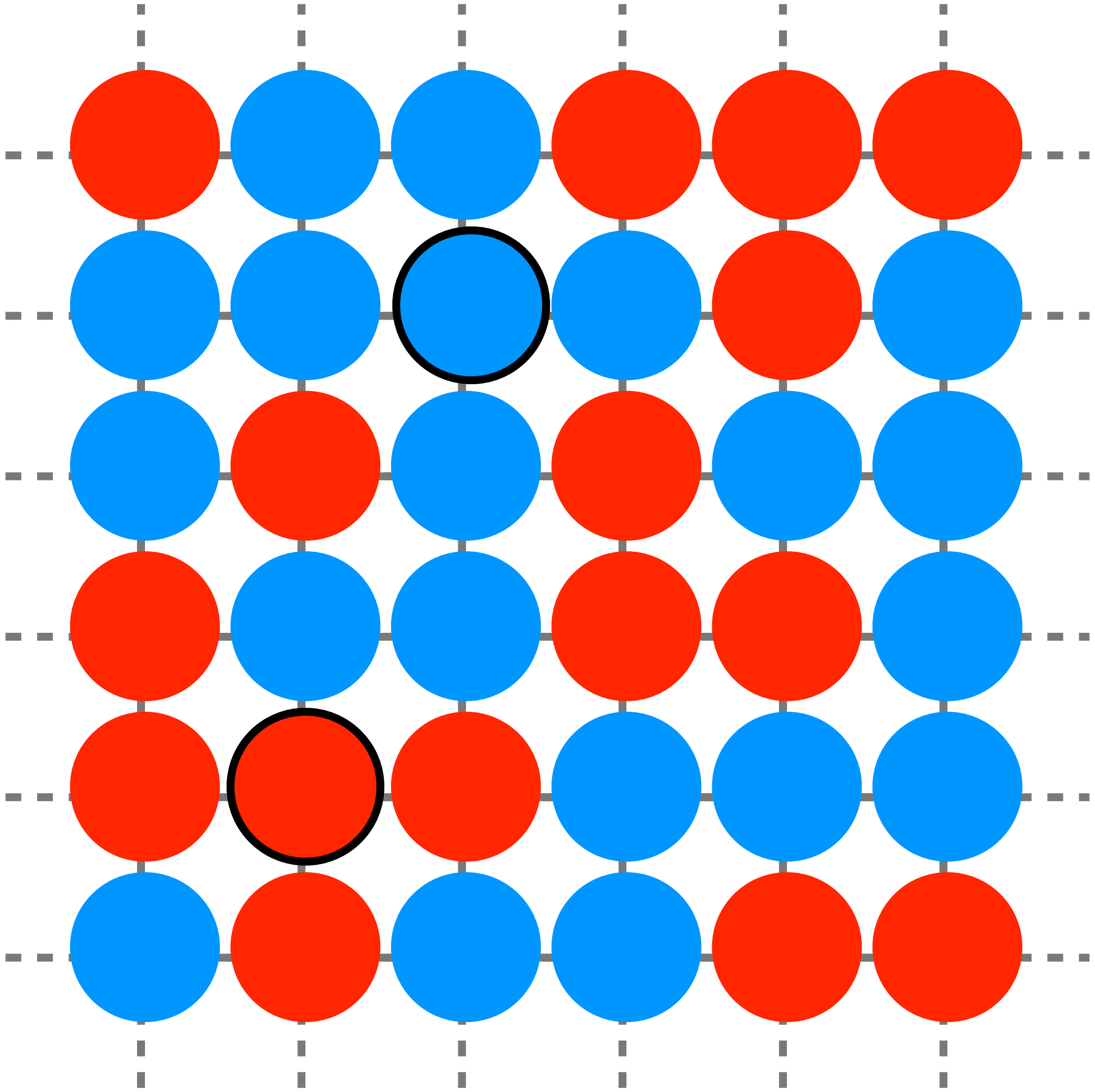

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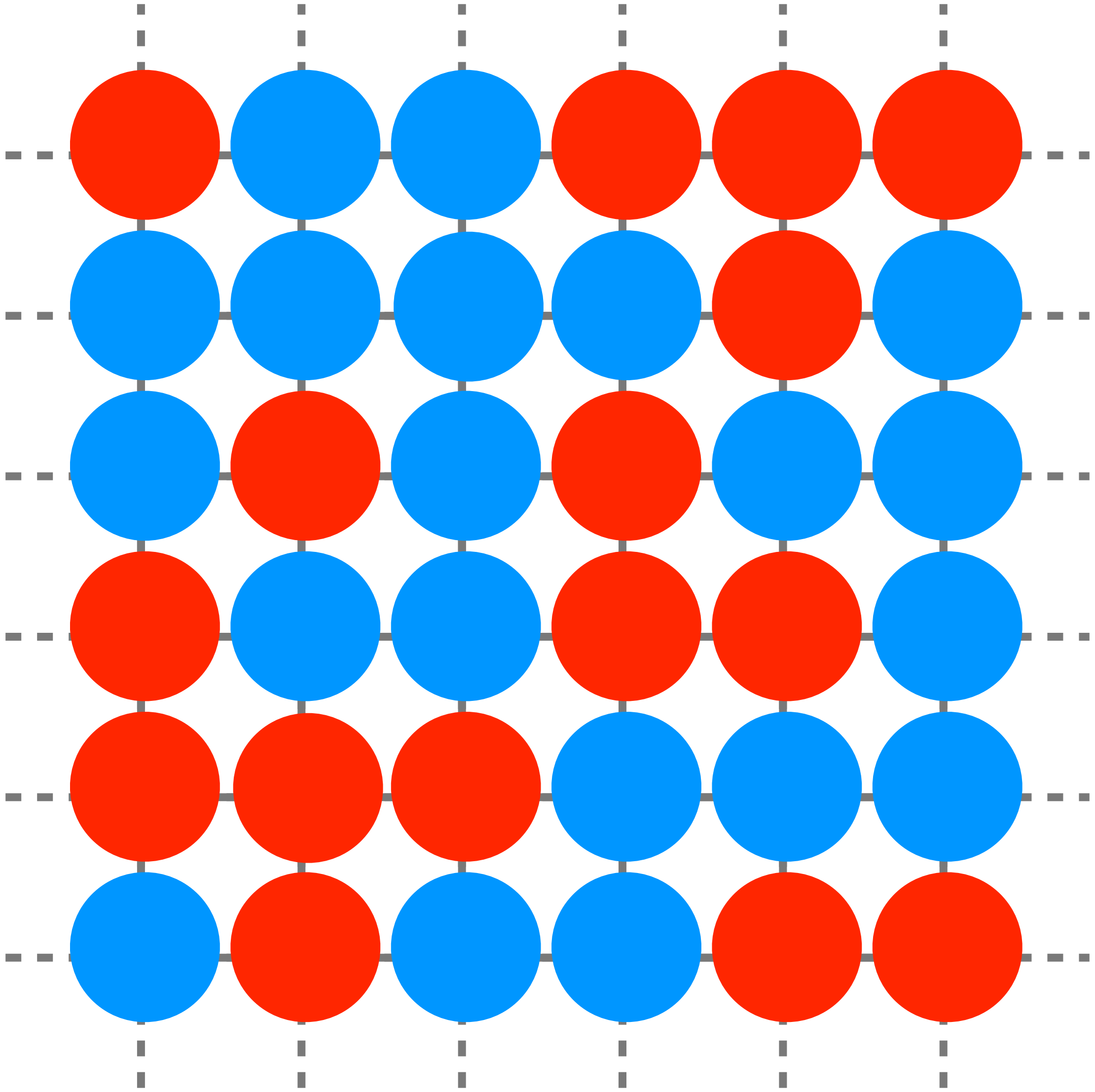

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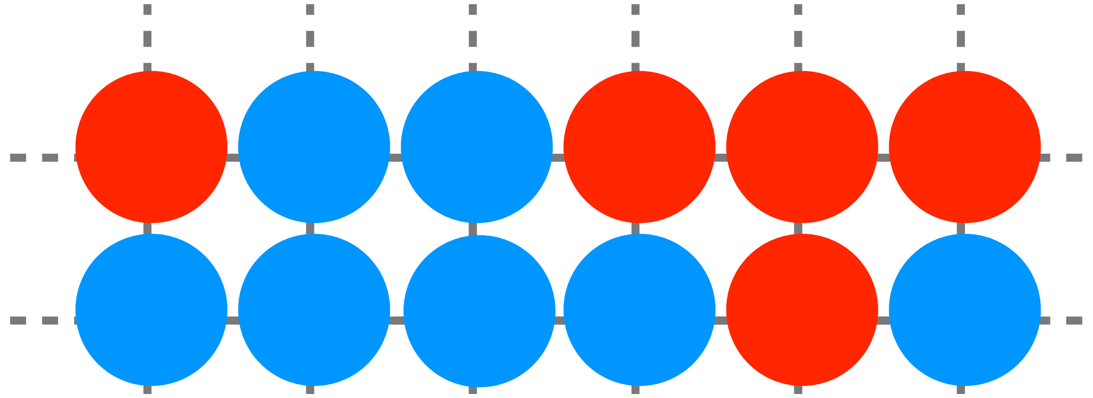
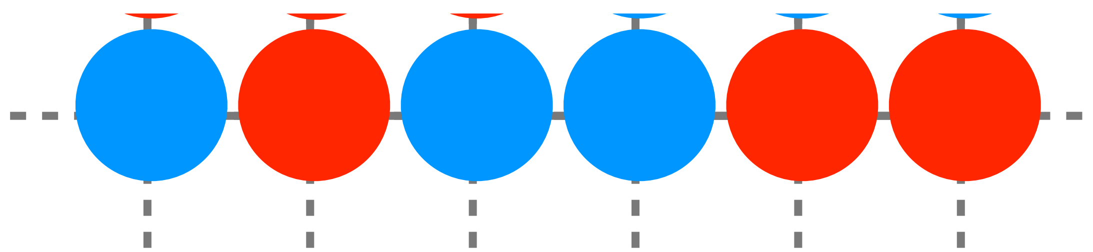


$$F = U - TS$$



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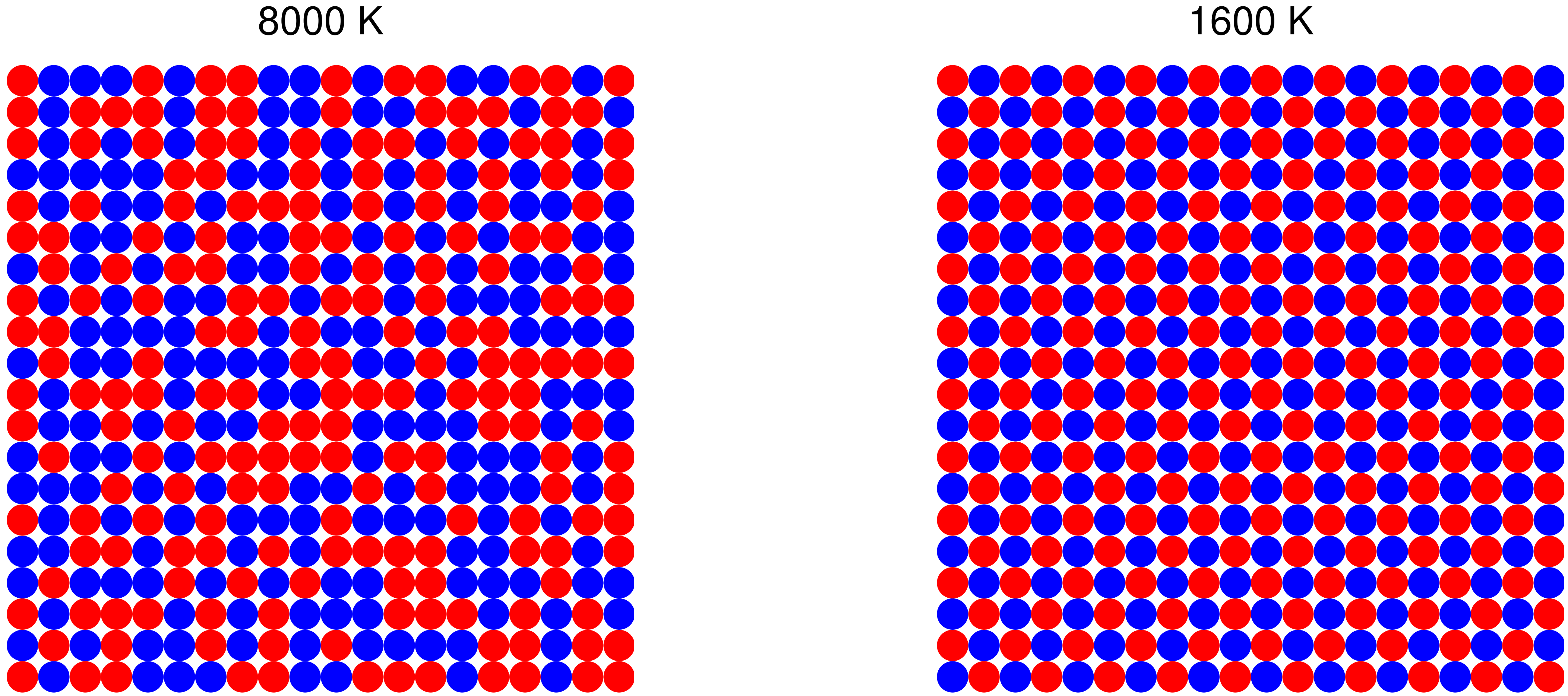
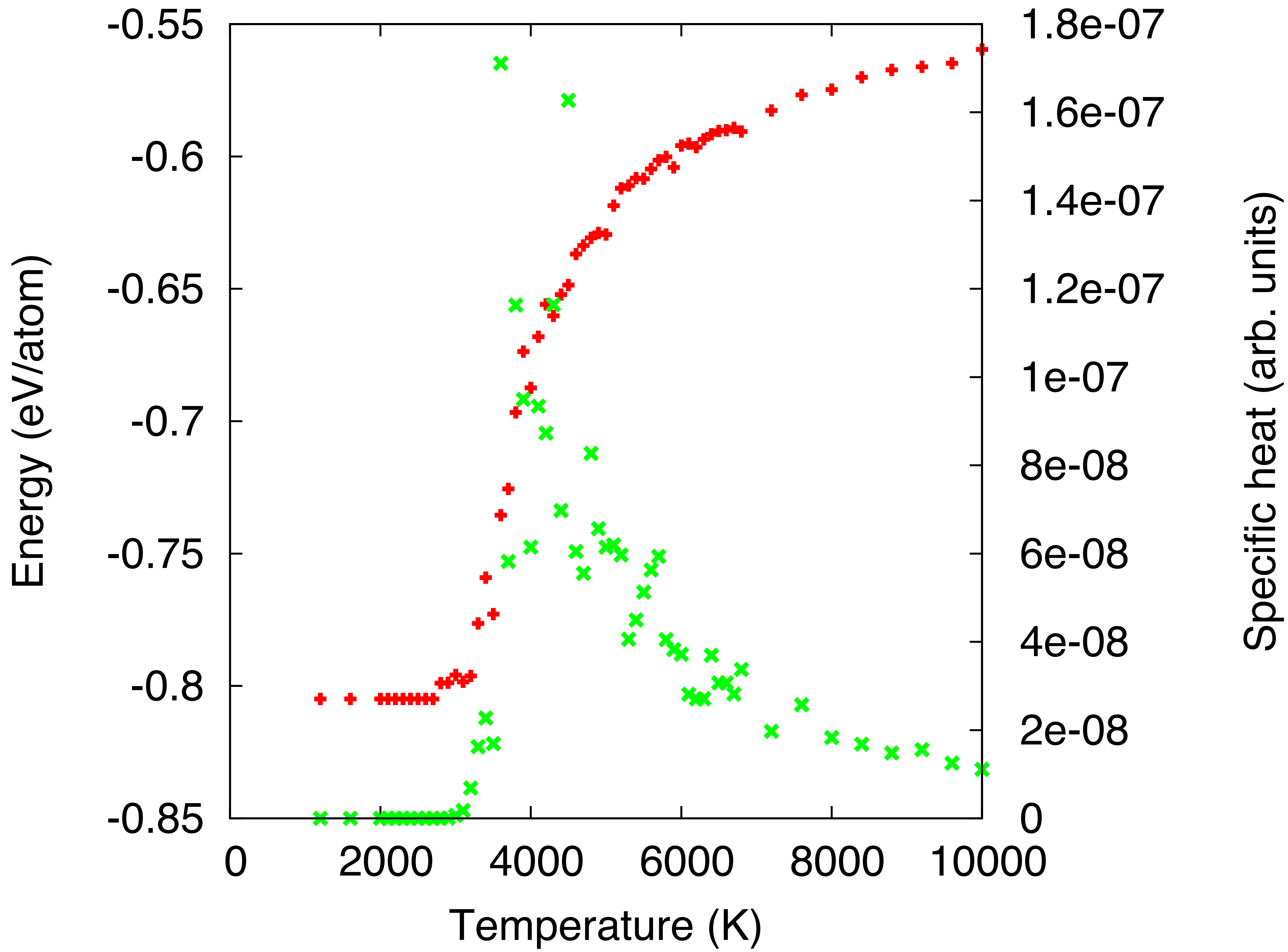
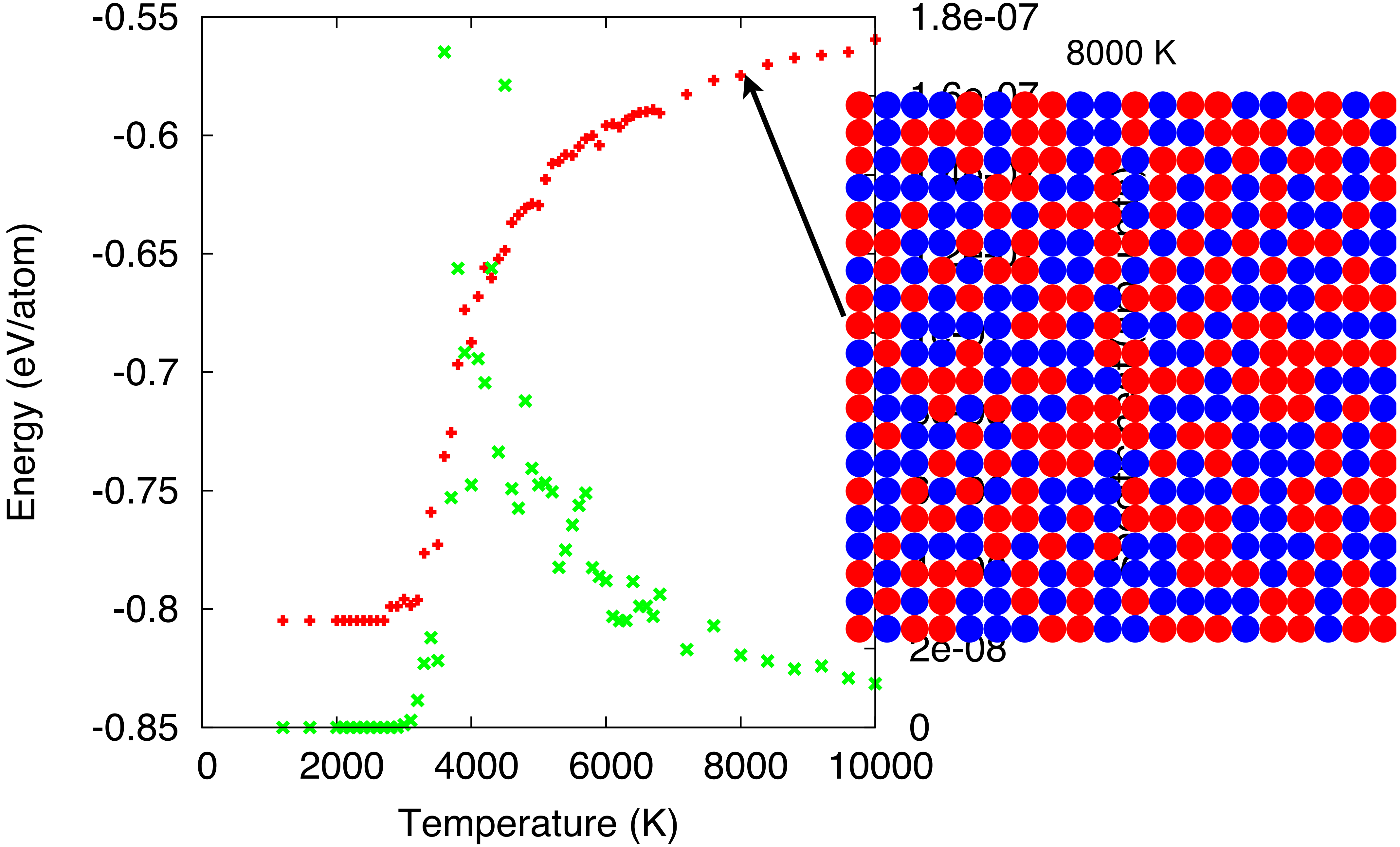

8000 K
1600 K



-0.55
-0.6
-0.65
-0.7
-0.75
-0.8
-0.85
Energy (eV/atom)
1.8e-07
1.6e-07
1.4e-07
1.2e-07
1e-07
8e-08
6e-08
4e-08
2e-08
0
Specific heat (arb. units)
0
2000
4000
6000
8000
10000
Temperature (K)



-0.55
-0.6
-0.65
-0.7
-0.75
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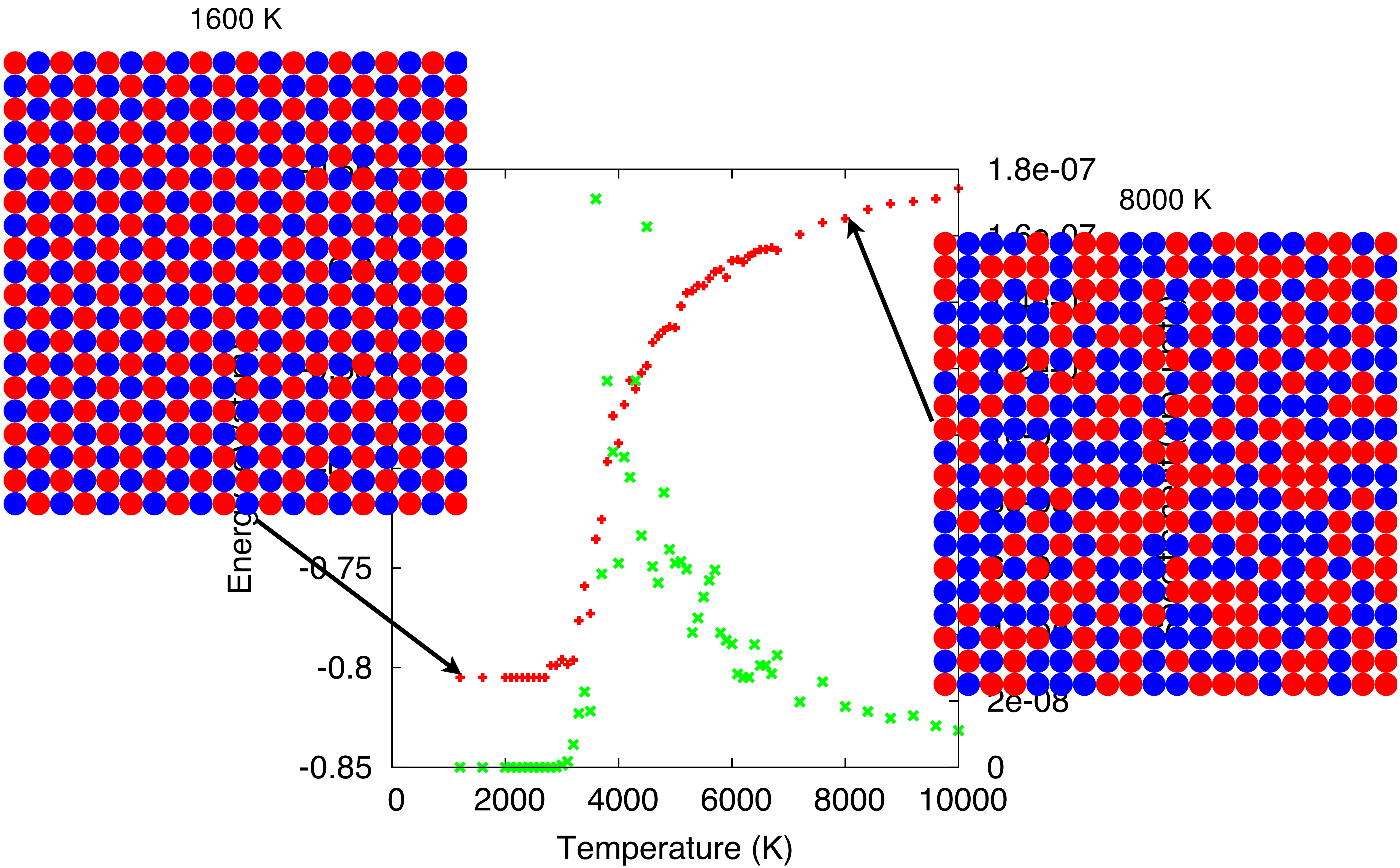
Energy (eV/atom)
0
2000
4000
6000
8000
10000
Temperature (K)
1.8e-07
0
8000 K



1600 K
8000 K
1.8e-07
2e-08
0
-0.75
-0.8
-0.85
0
2000
4000
6000
8000
10000
Temperature (K)