The bulk spectral gap is semi-decidable: a convergent family of certified upper bounds

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PhIQuS, Inria Saclay

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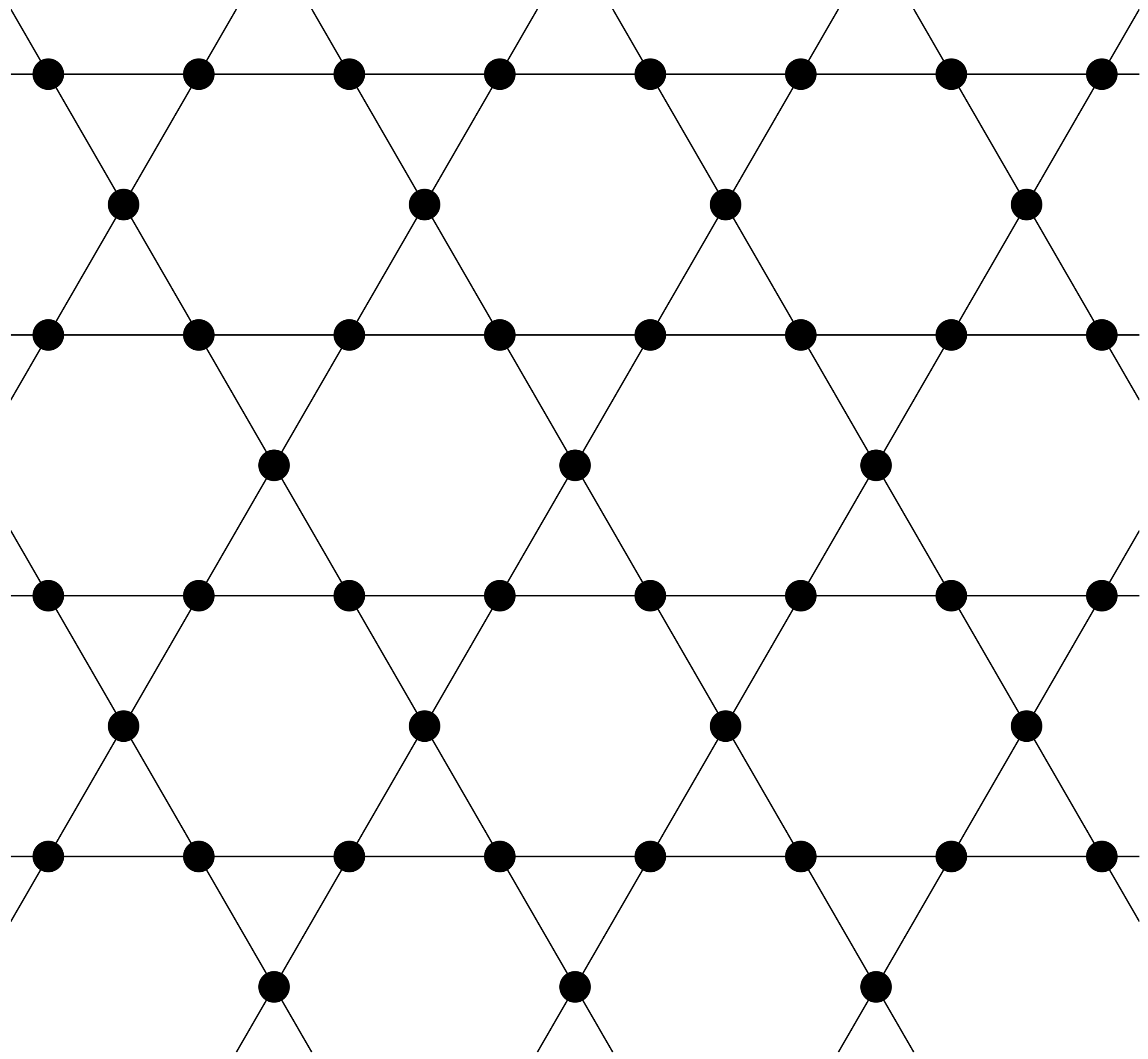
With Matthias Schötz, Jie Wang, Victor Magron, Igor Klep, Omar Fawzi and Marc-Olivier Renou

Certifying ground-state properties of quantum many-body systems

1. **Motivation**
2. Finite systems
3. Thermodynamic limit with boundaries
4. Thermodynamic limit: the bulk

Quantum many-body systems



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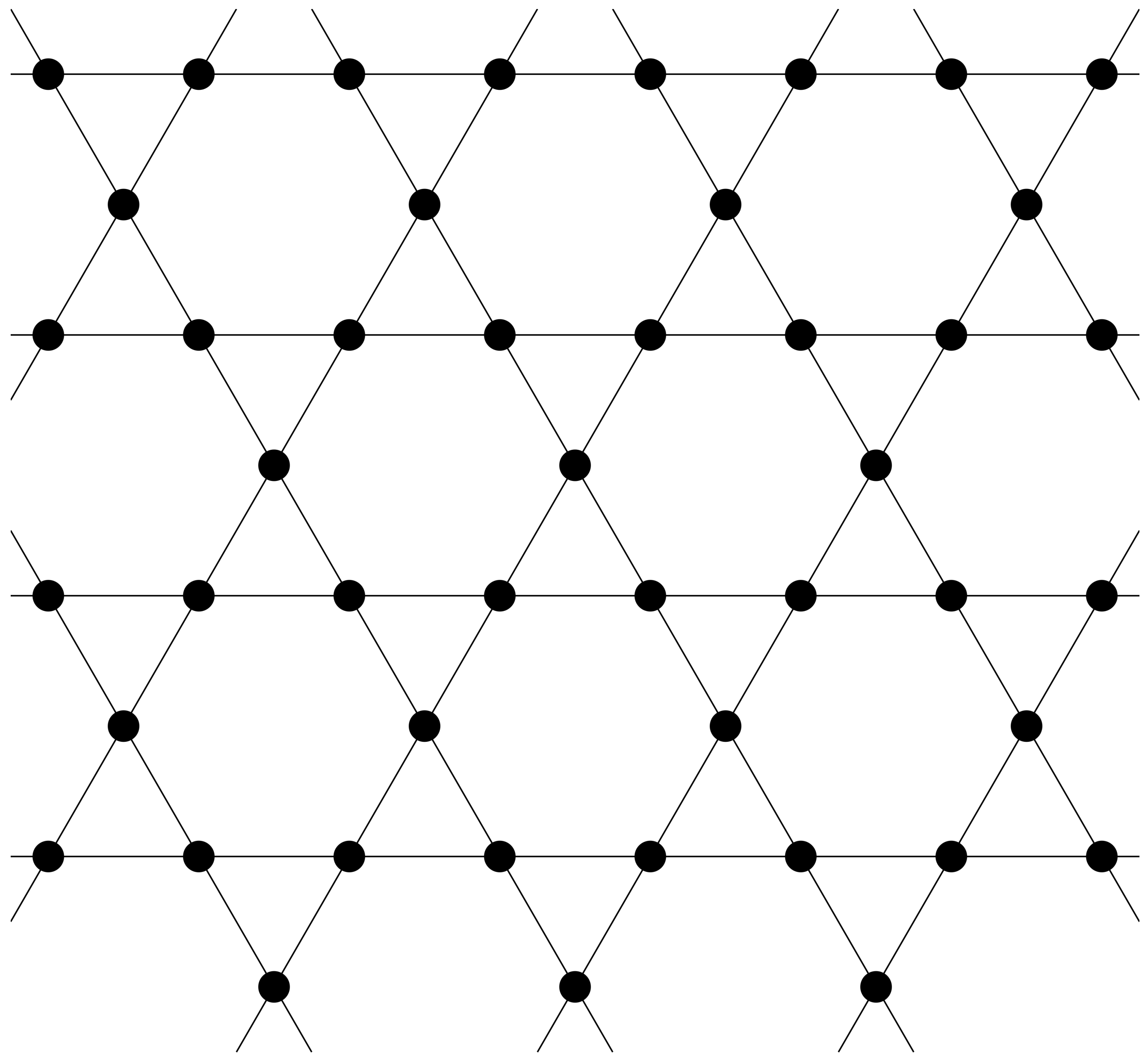

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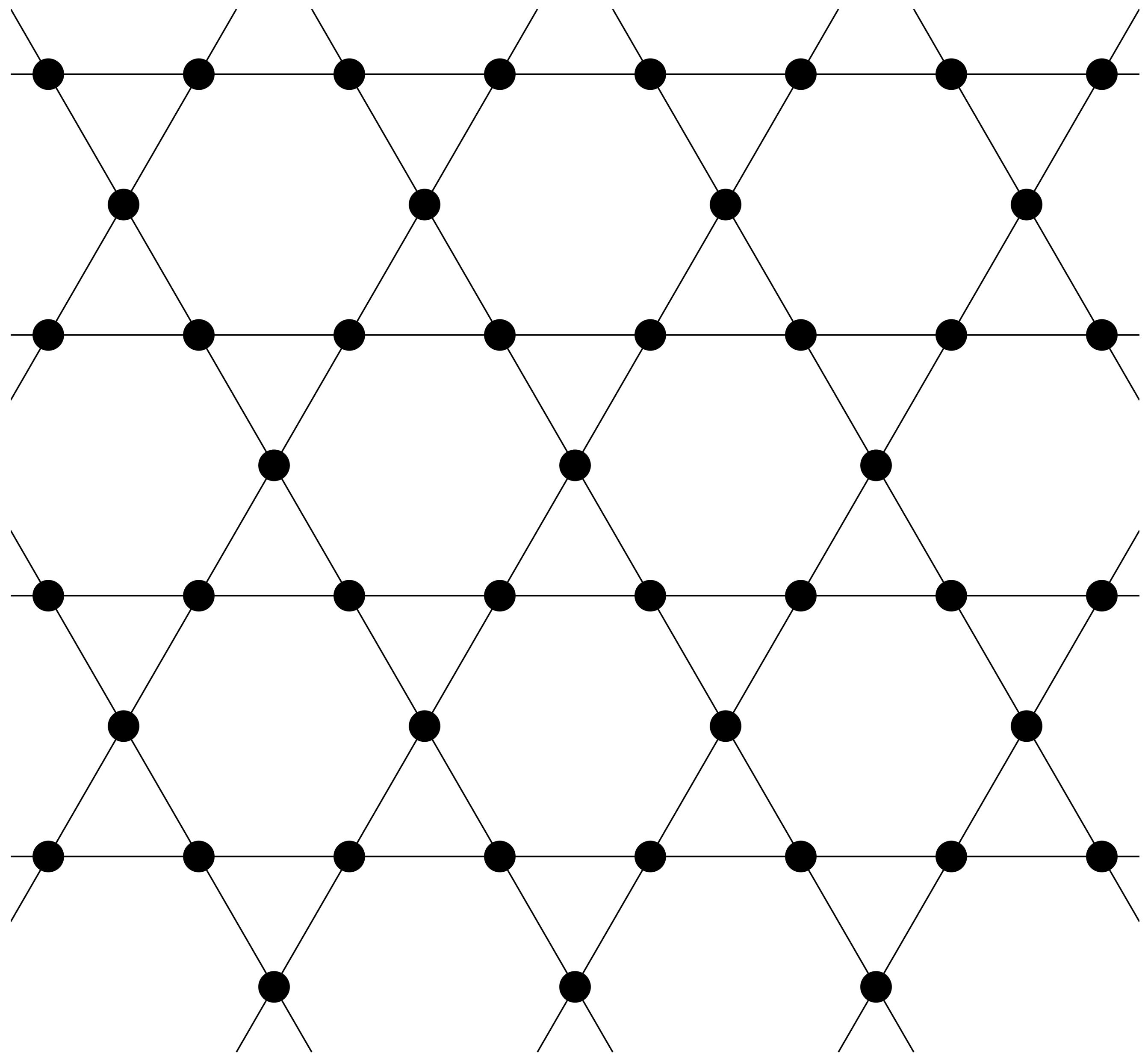

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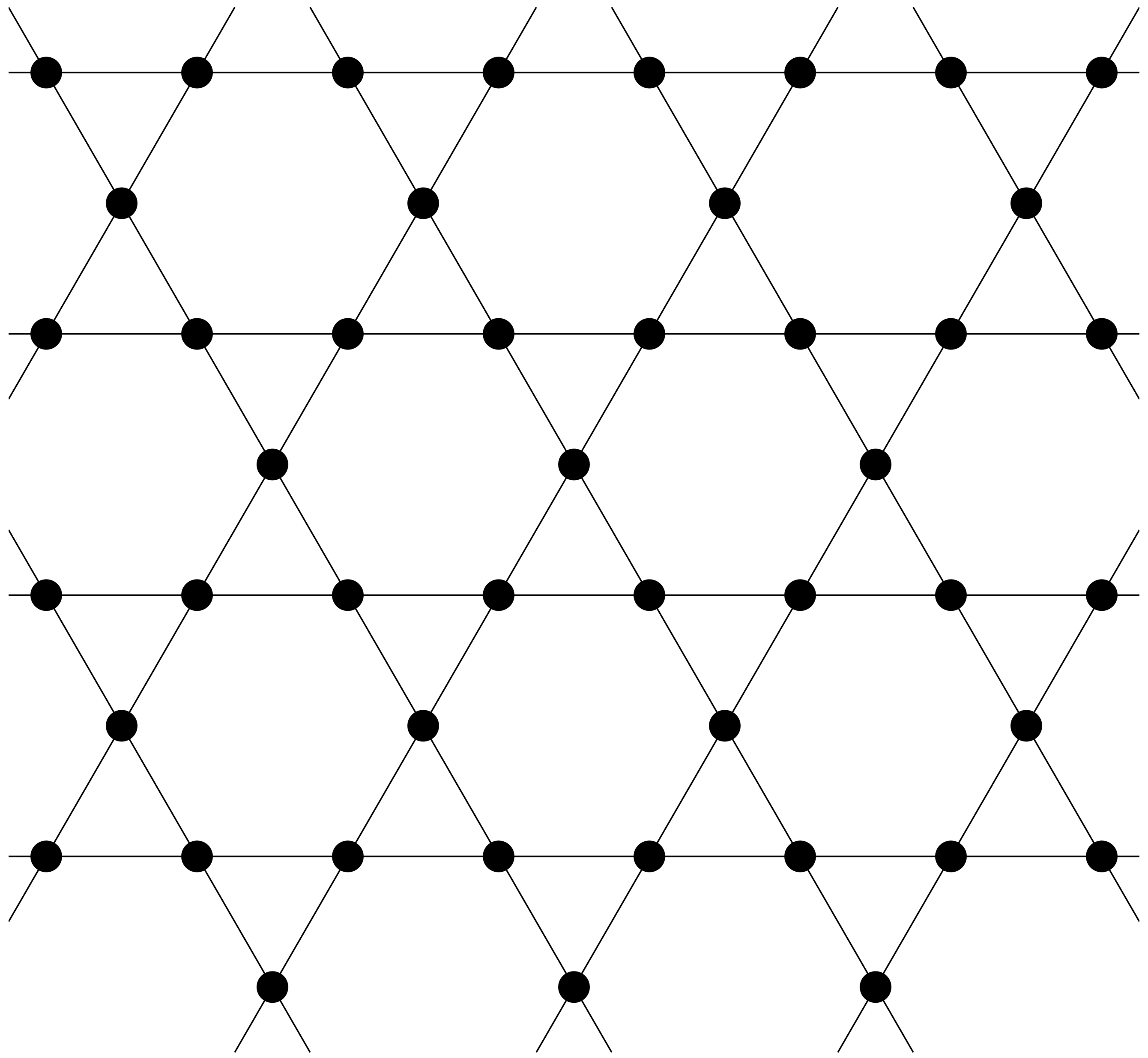

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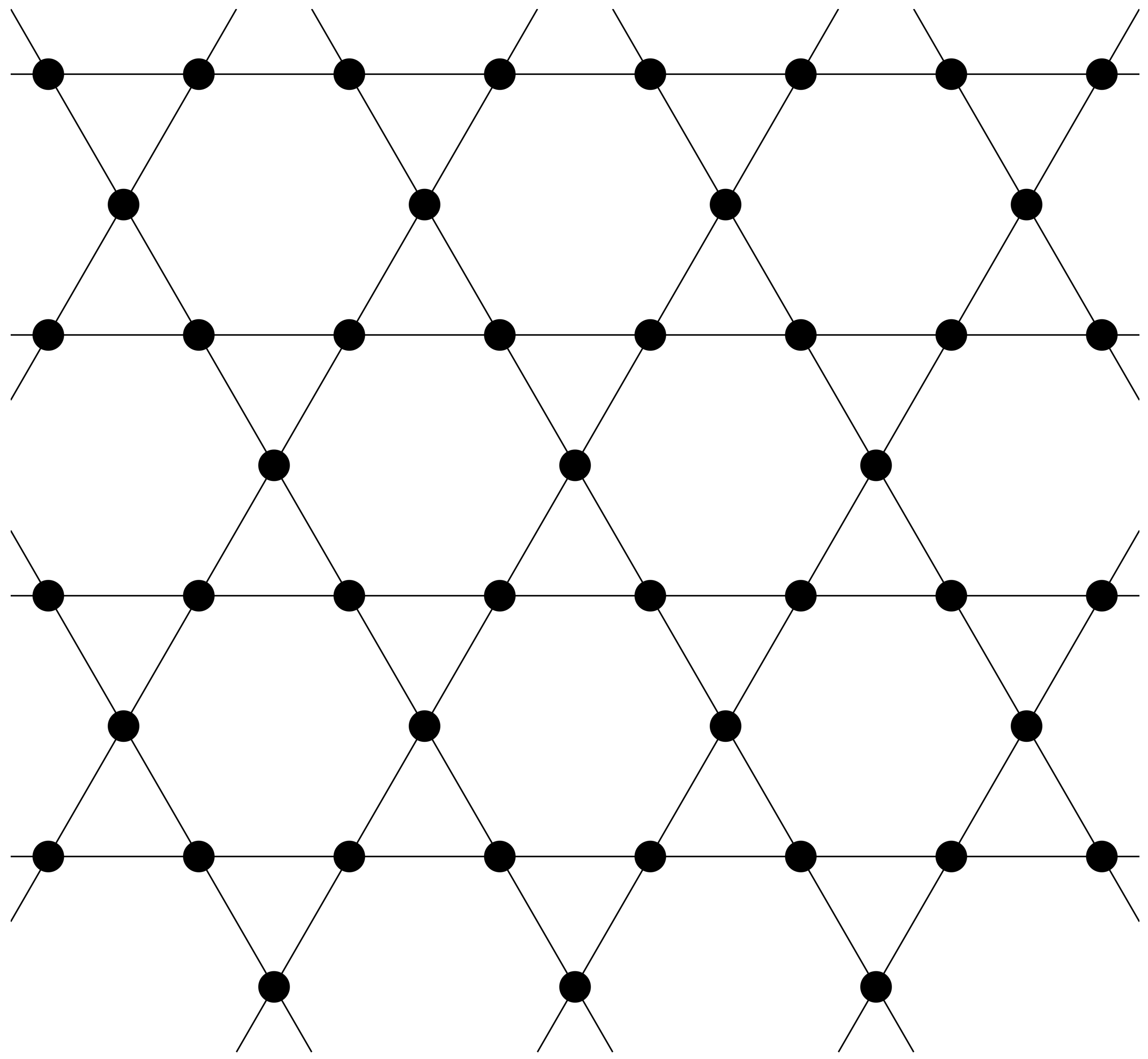

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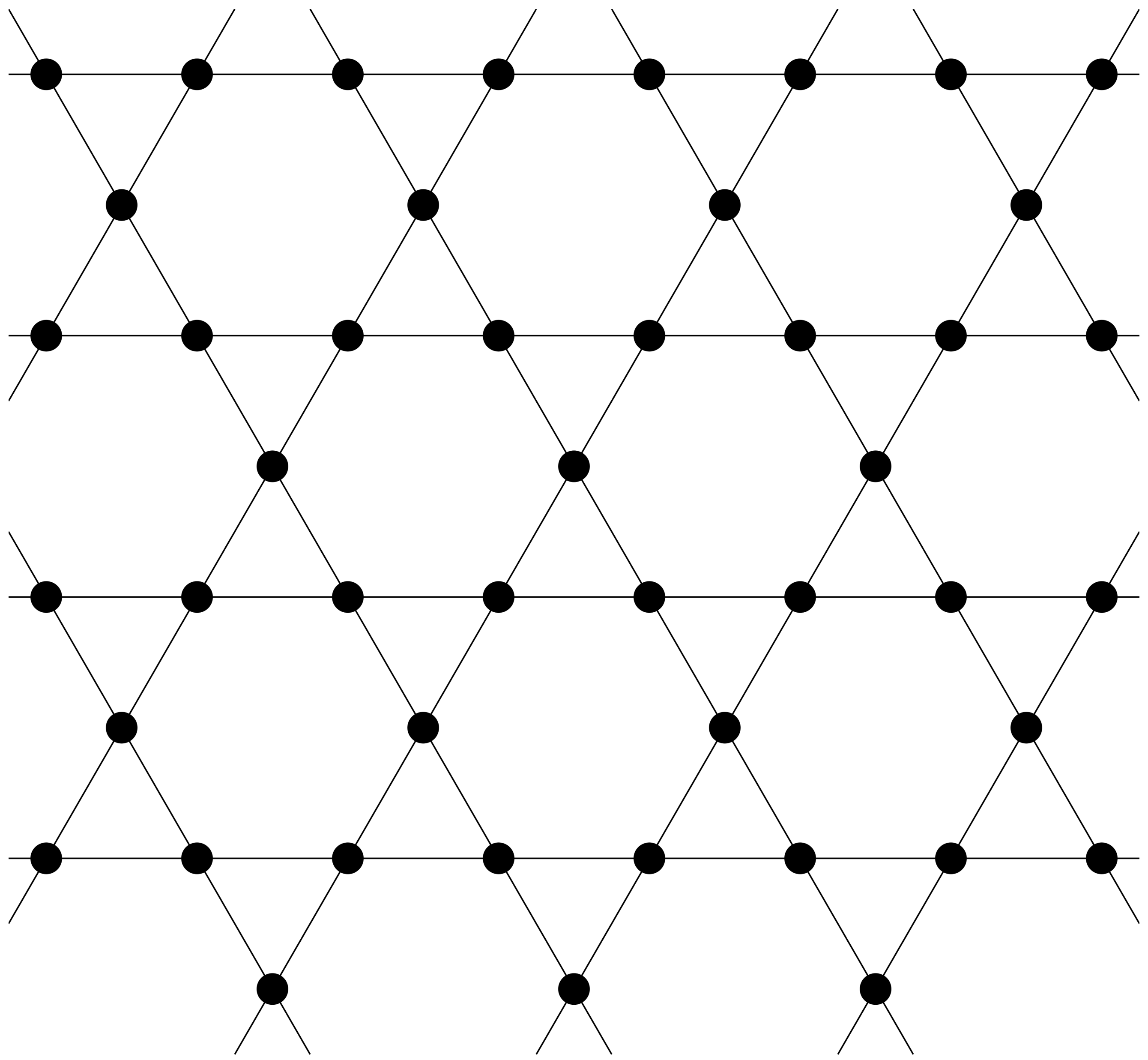

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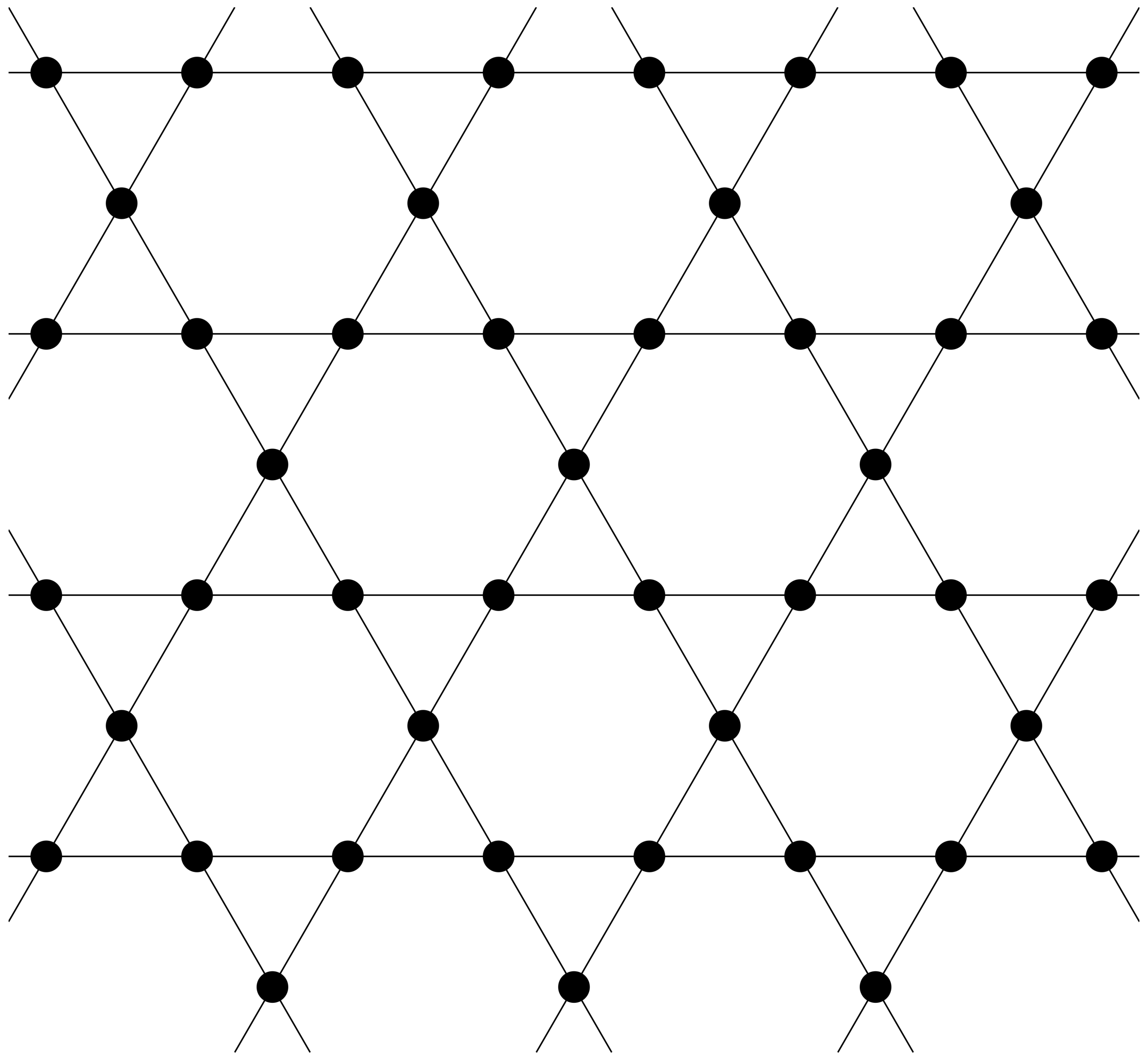

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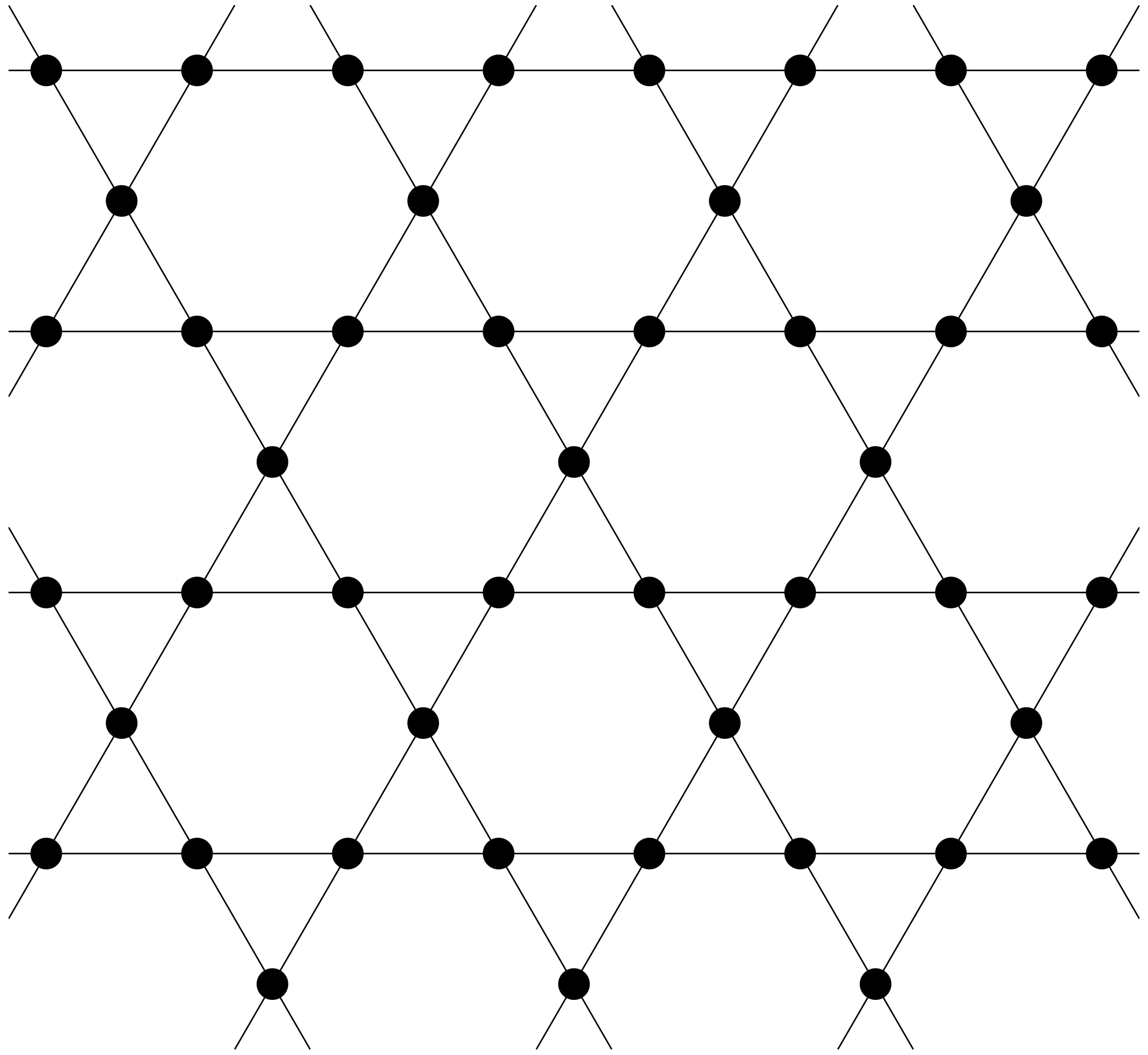
- It's a matrix of dim 2^N! Impossible to compute

Paradigmatic problem: spectral gap



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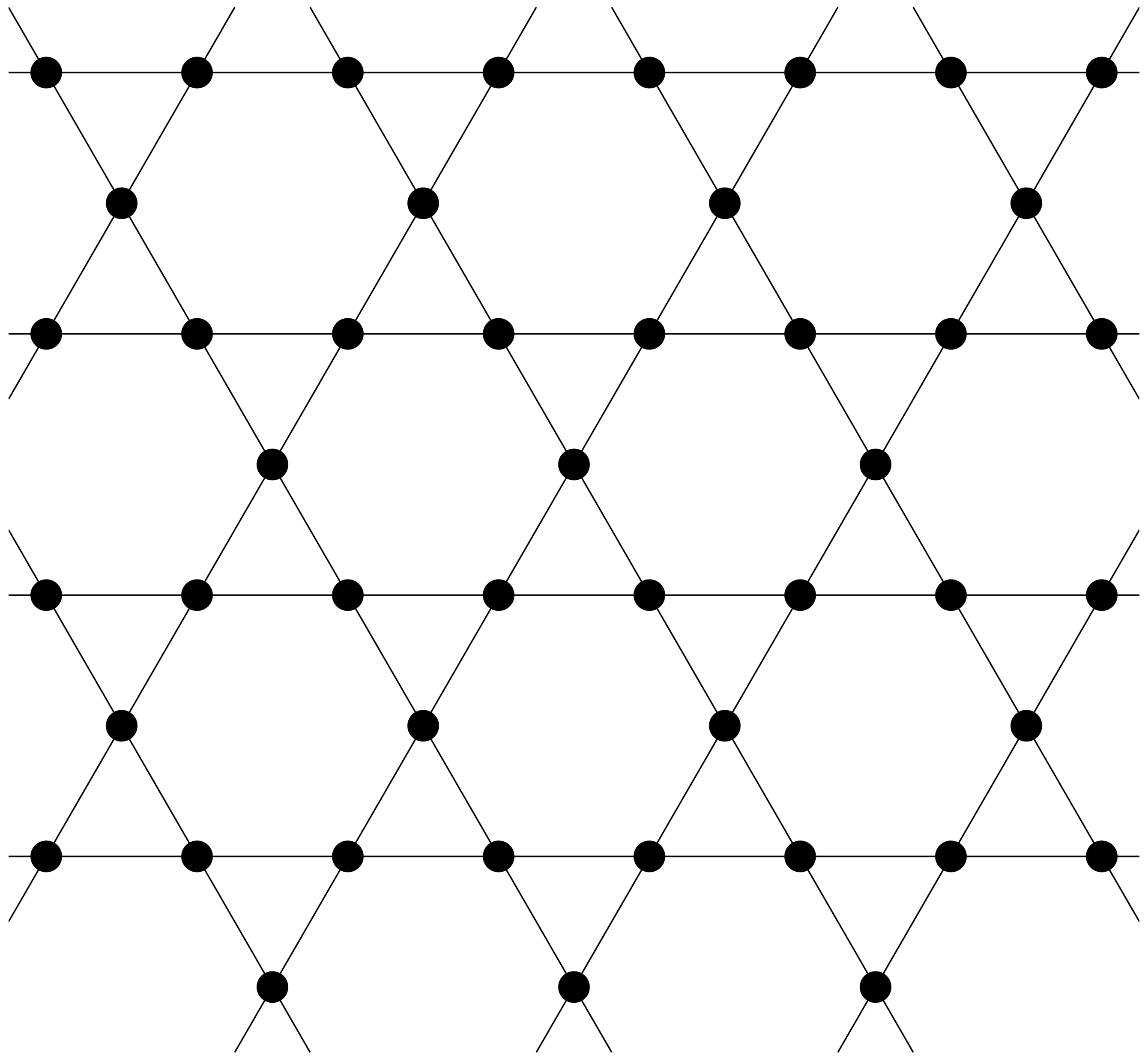

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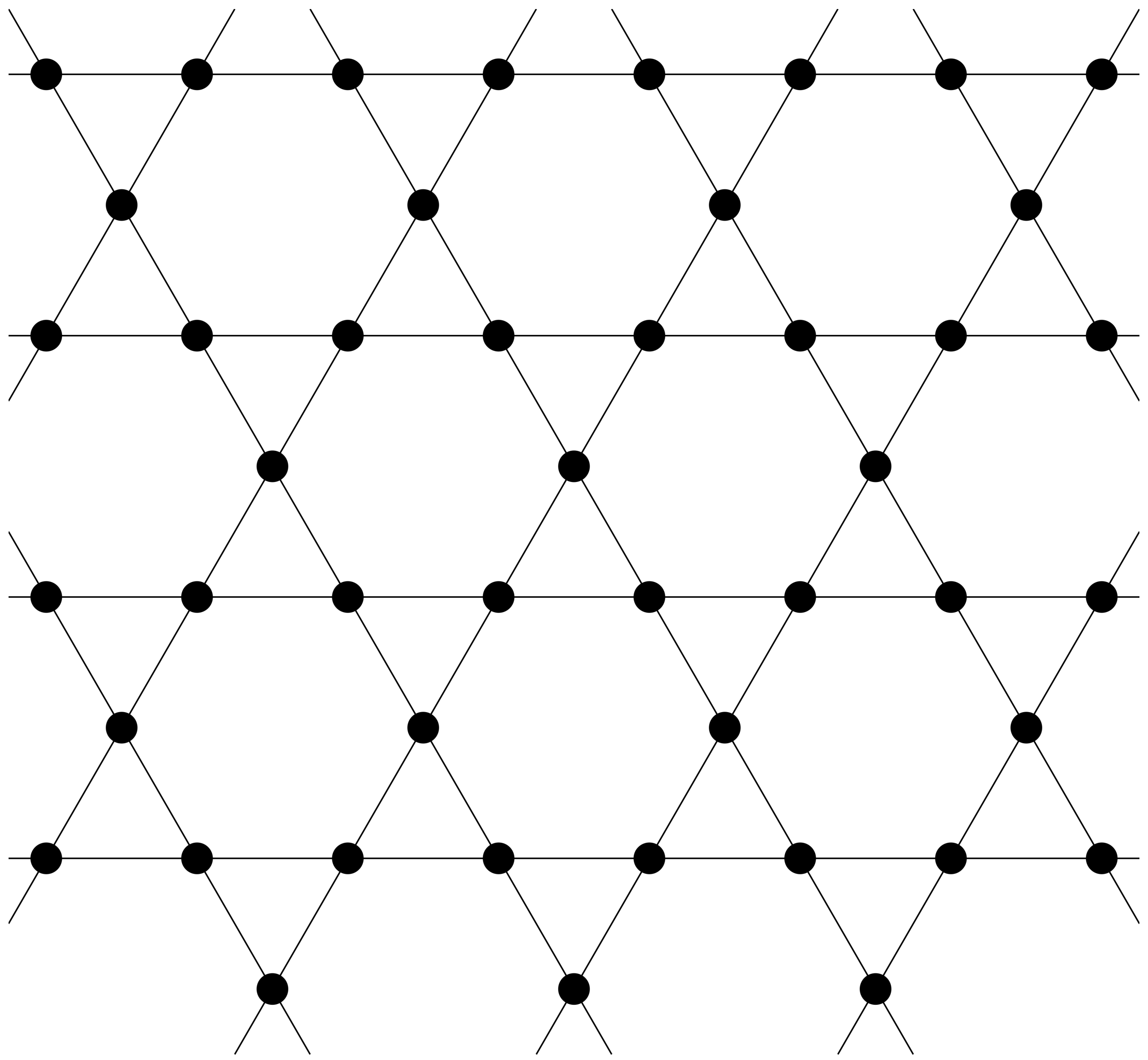

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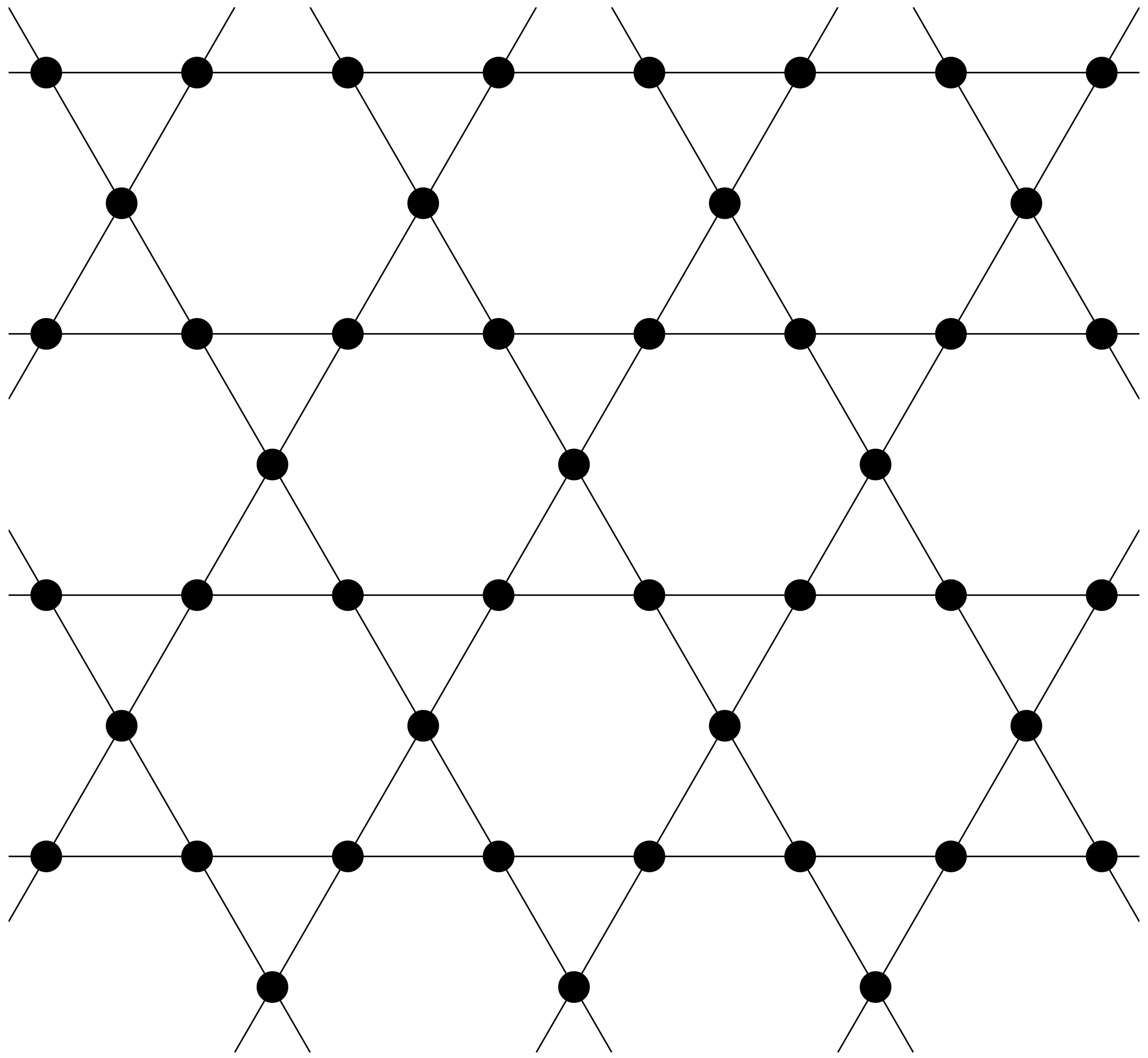

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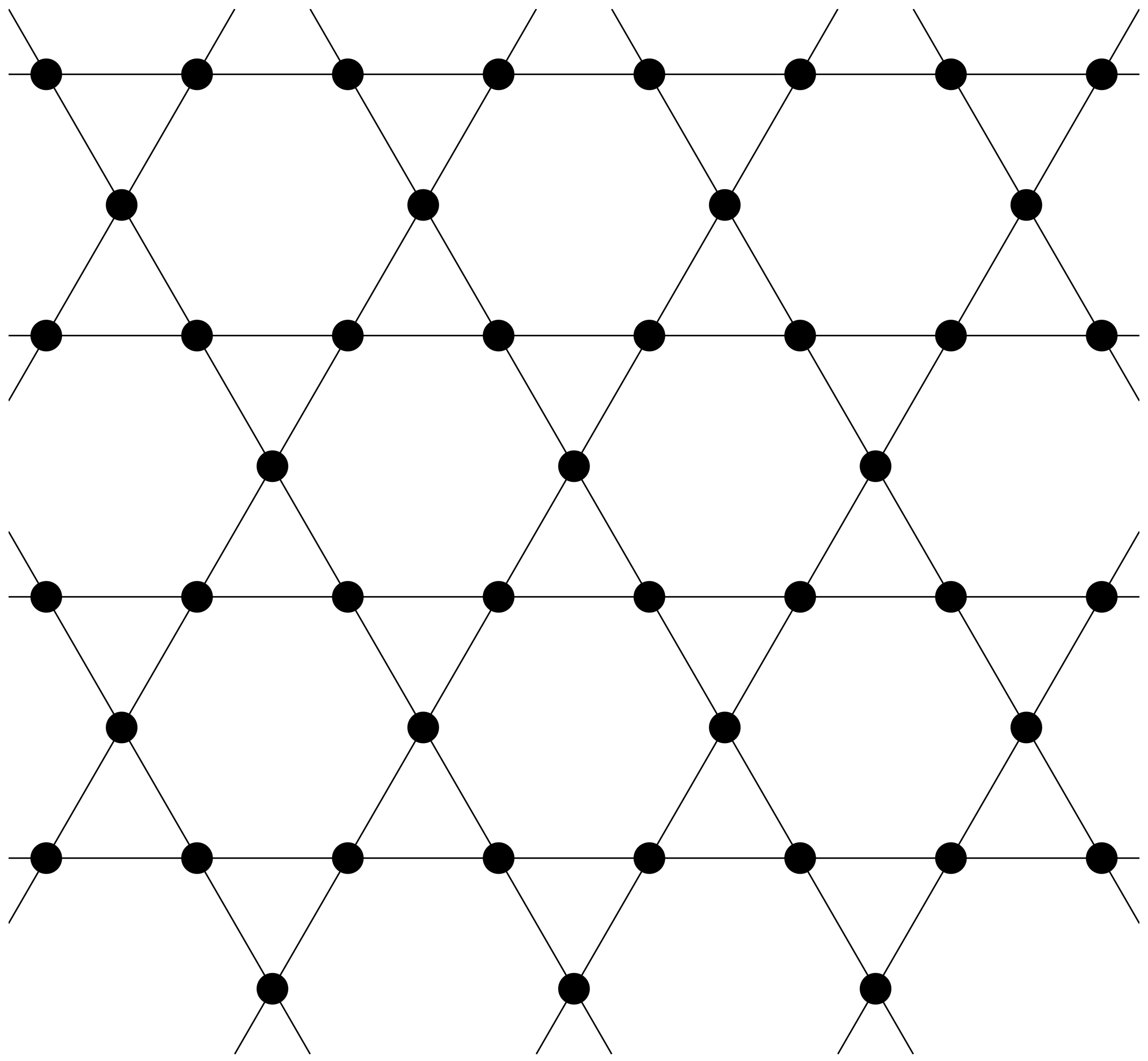

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- Energy needed for the lowest excitation
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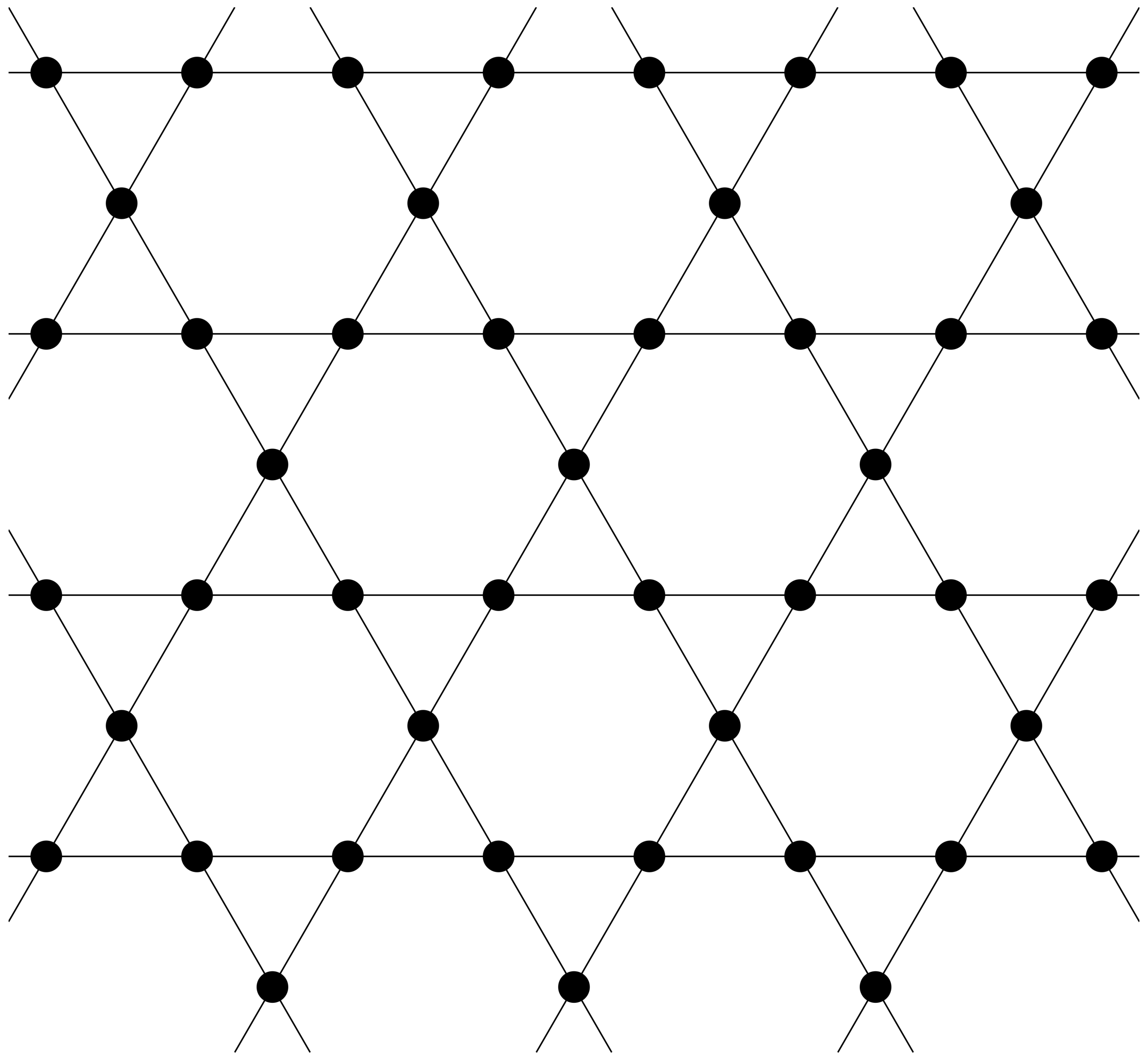
- Gapless: long-range correlation, unstable

Main result: first general algorithm



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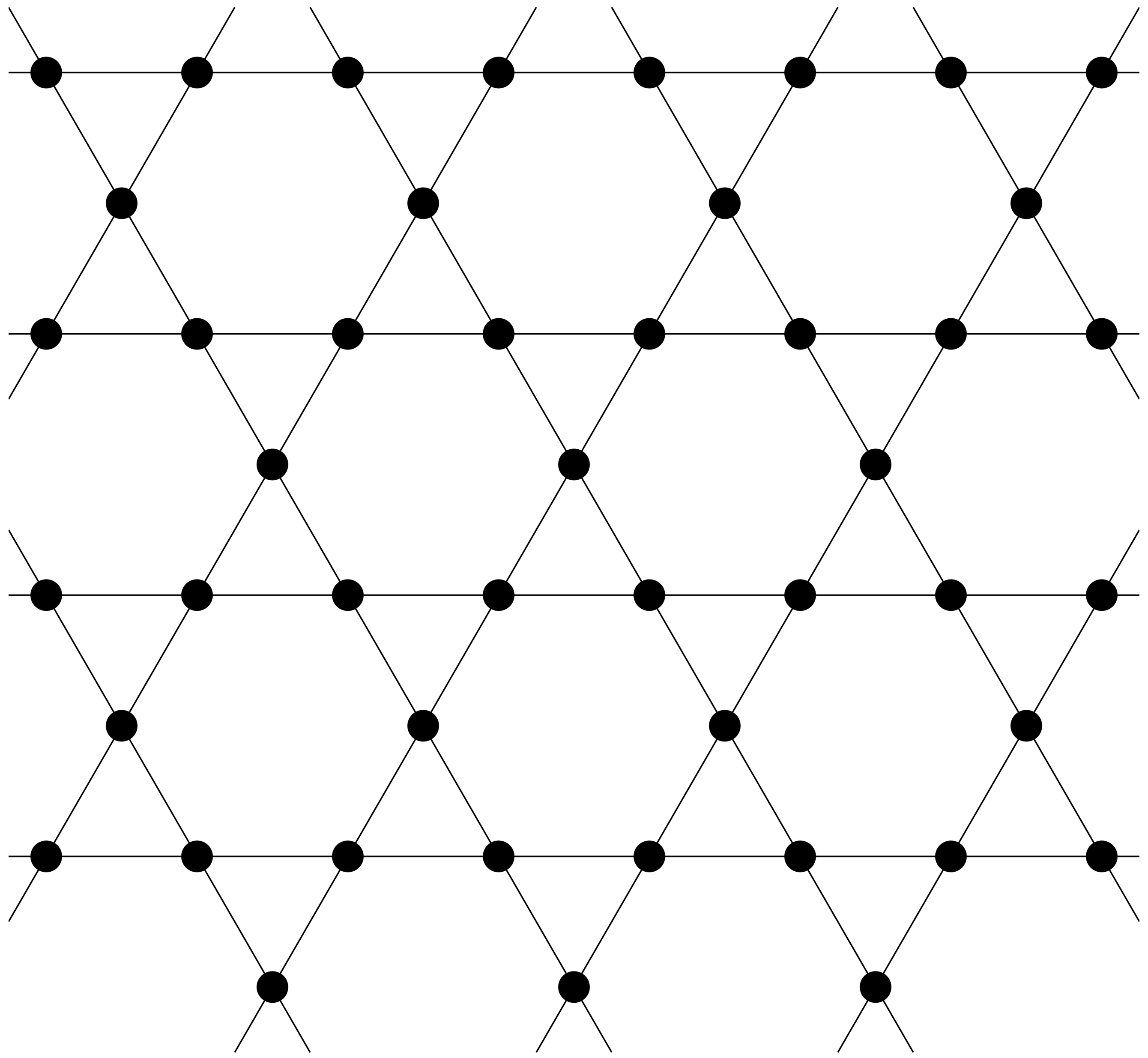

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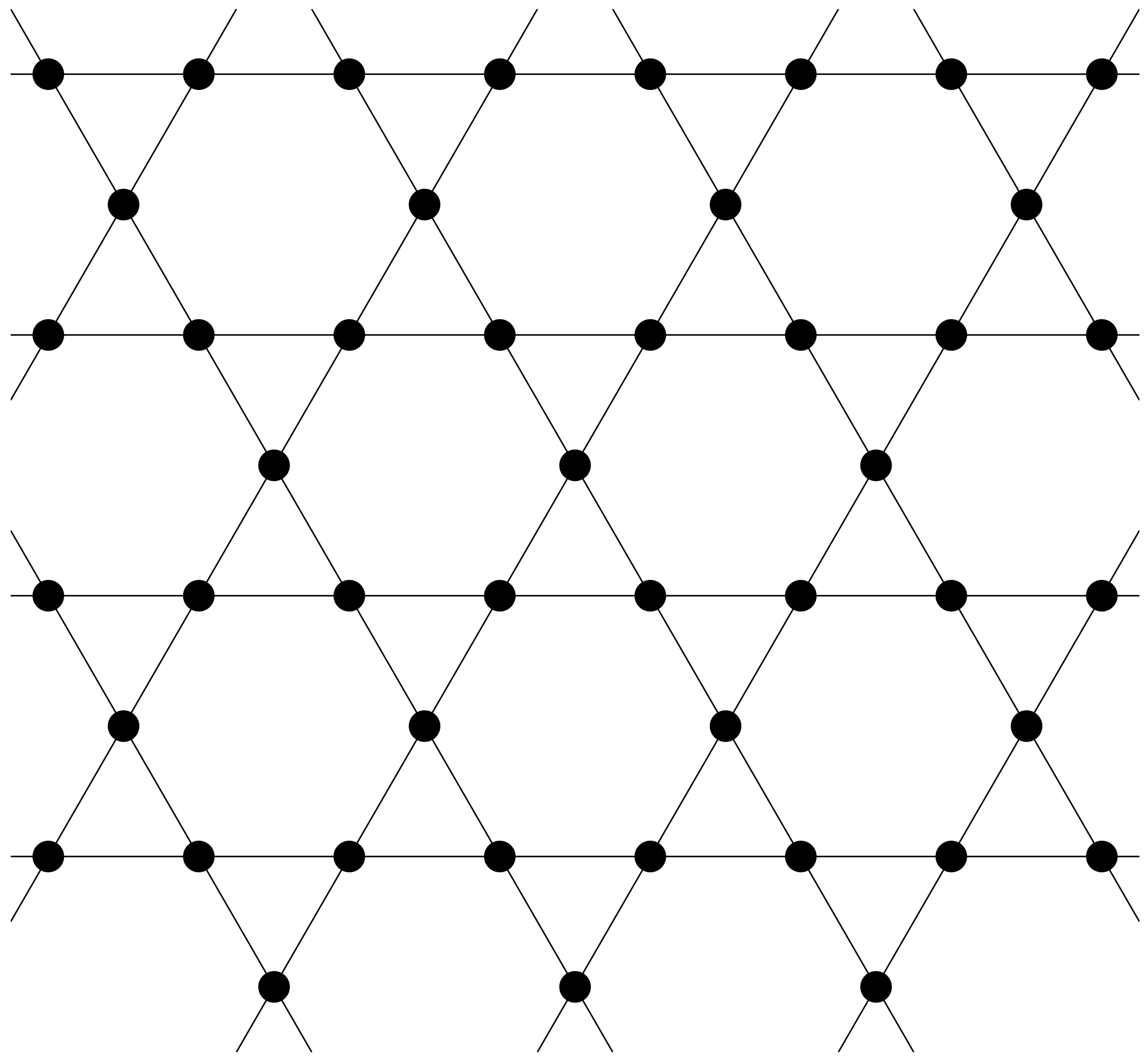

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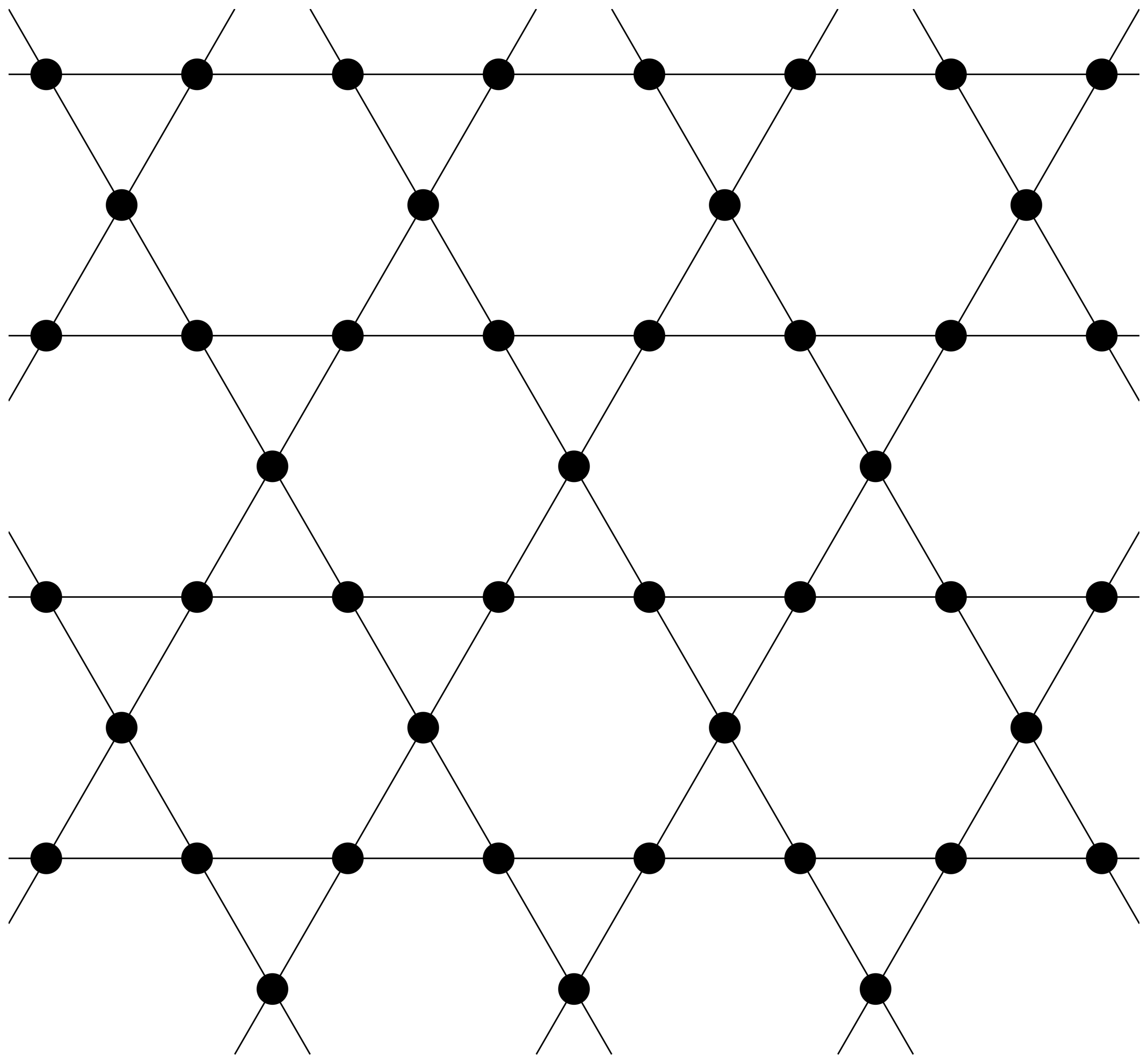

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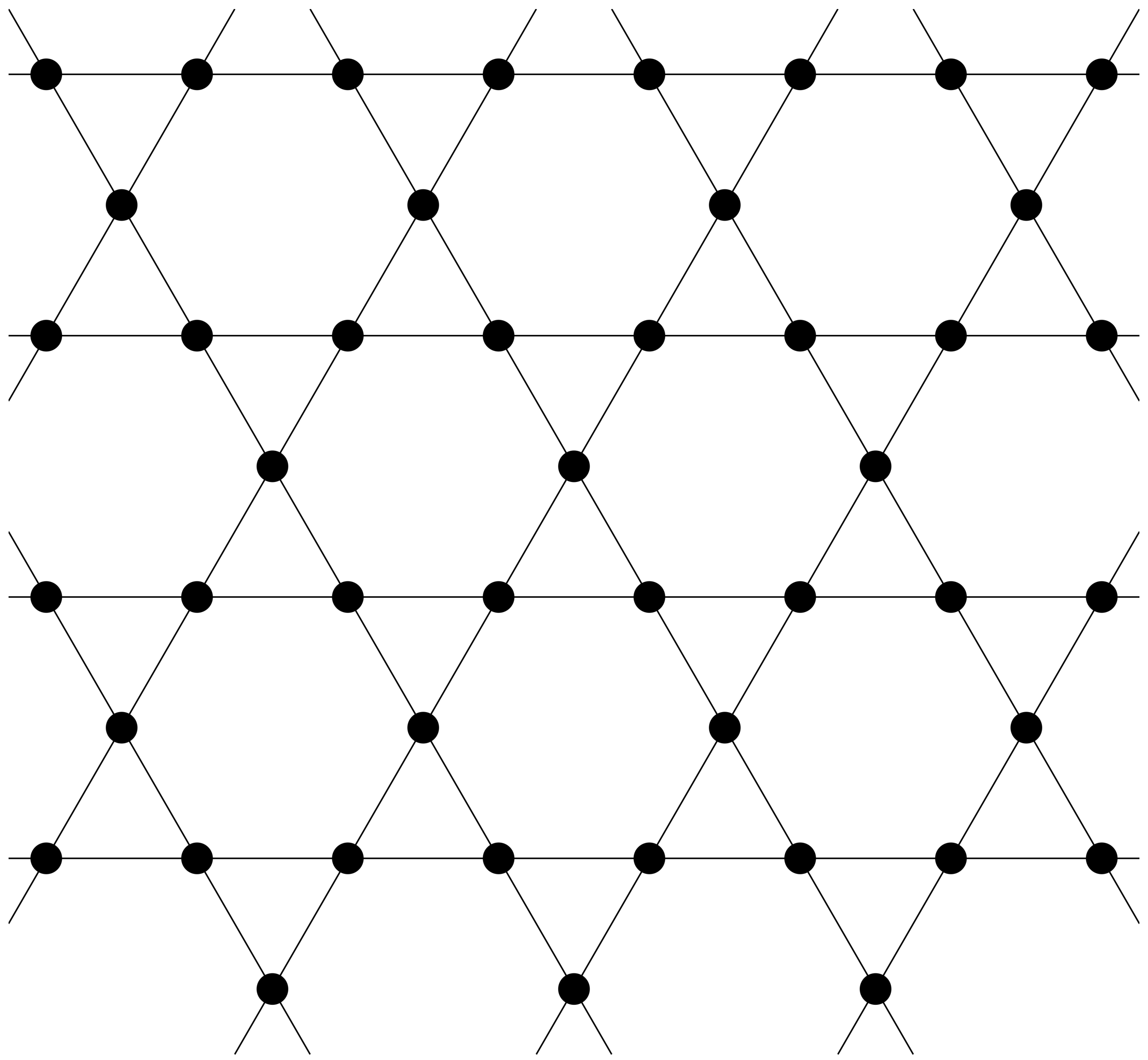

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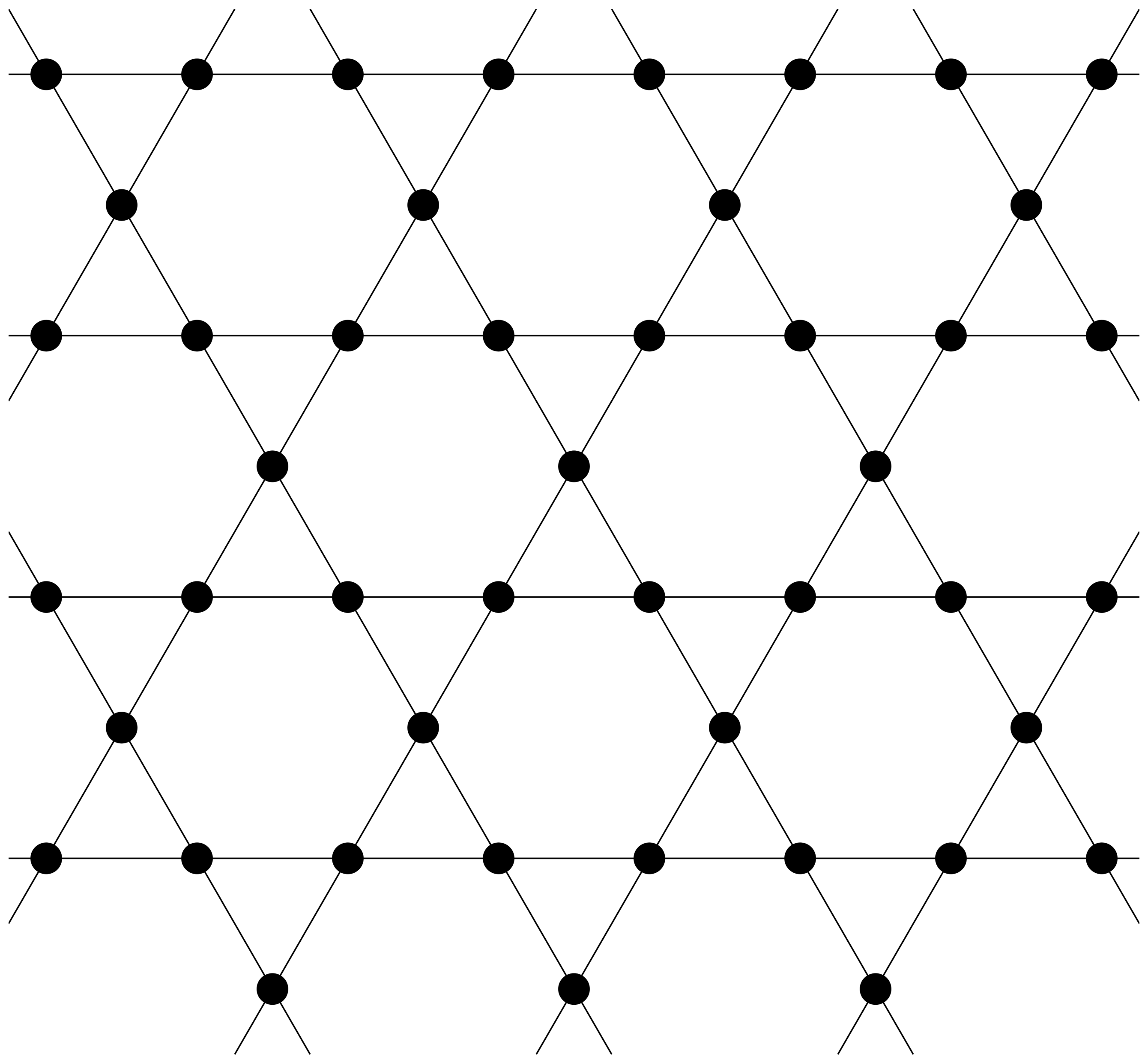

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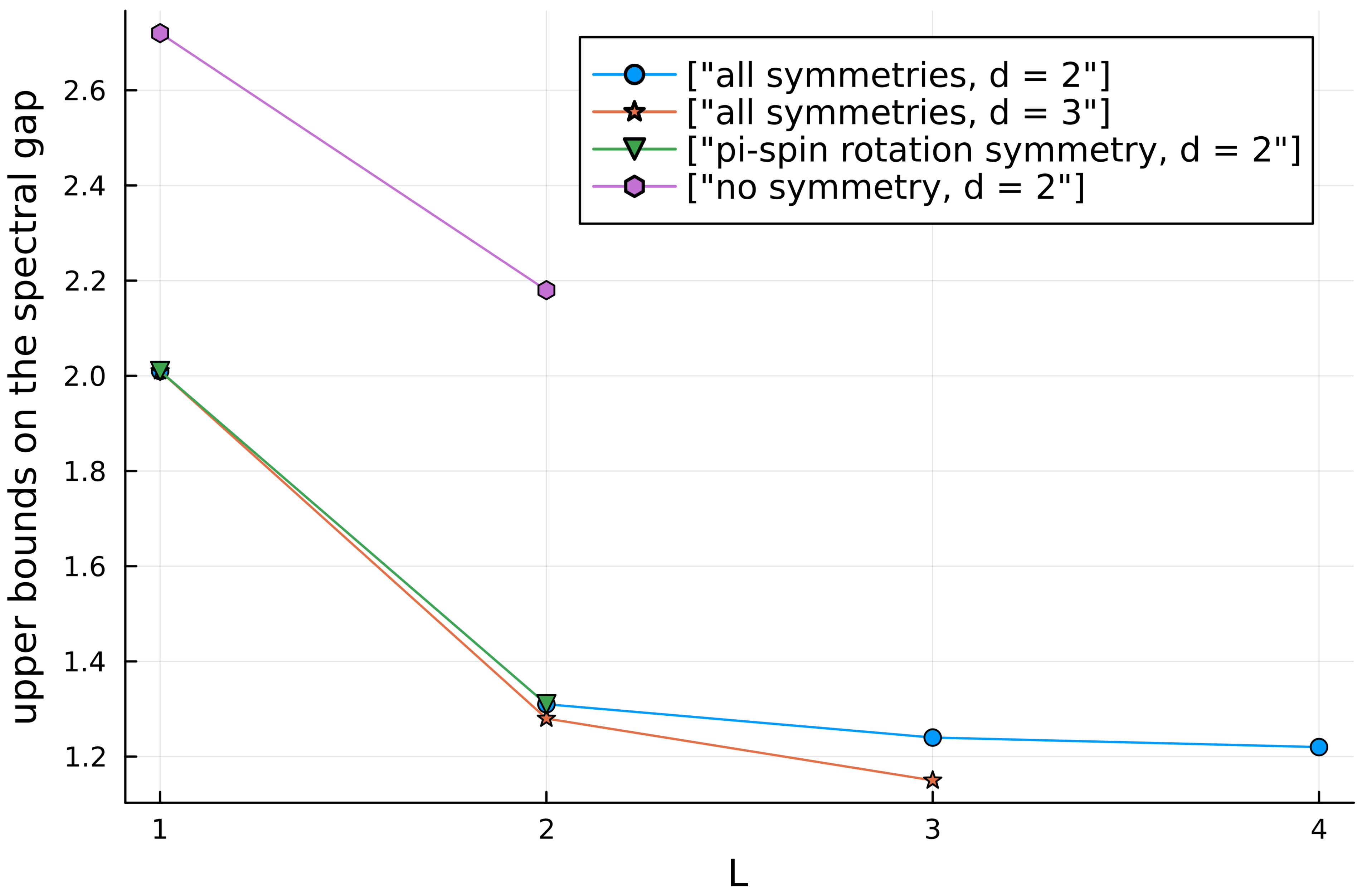

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Kagome Heisenberg model

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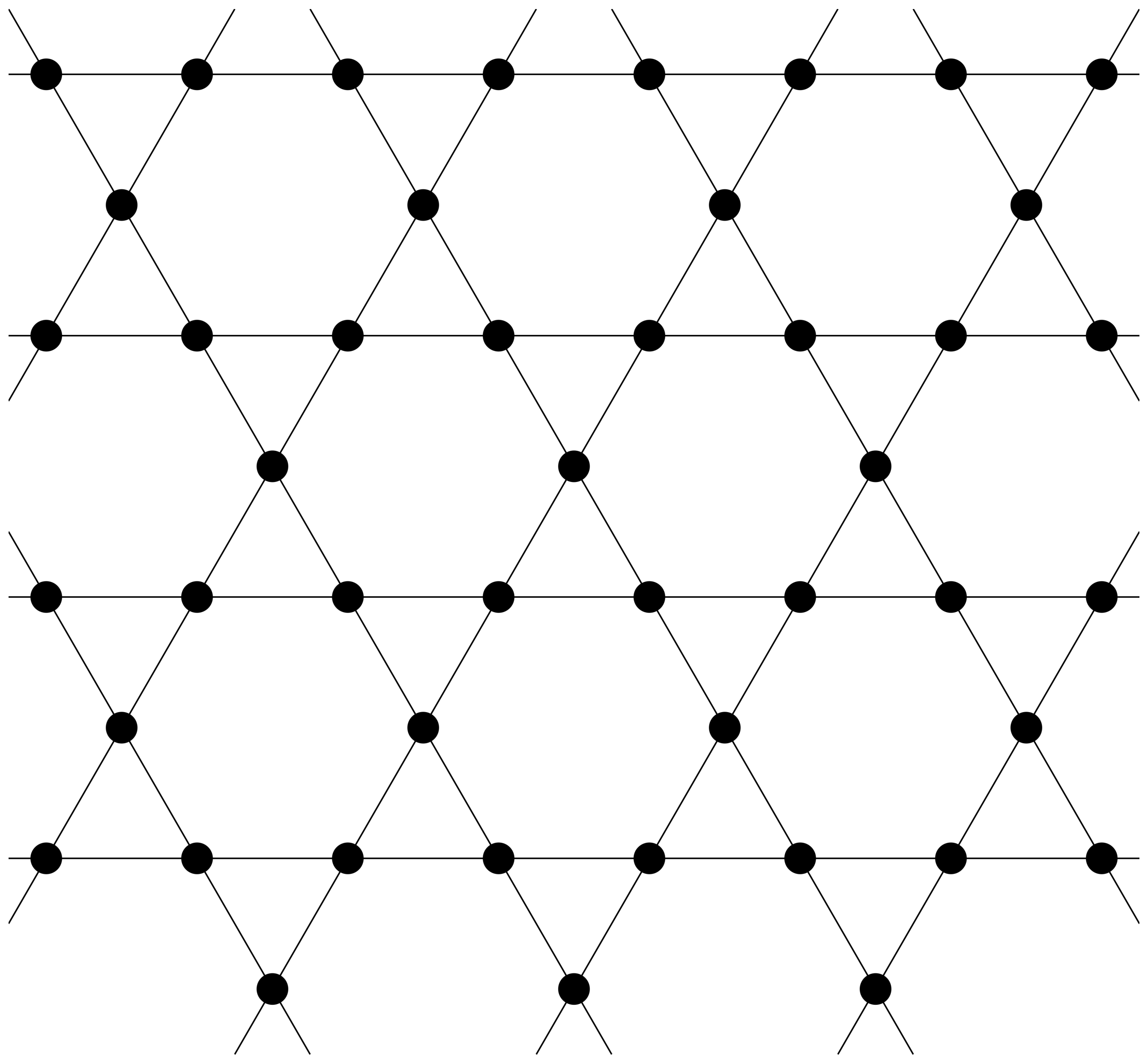

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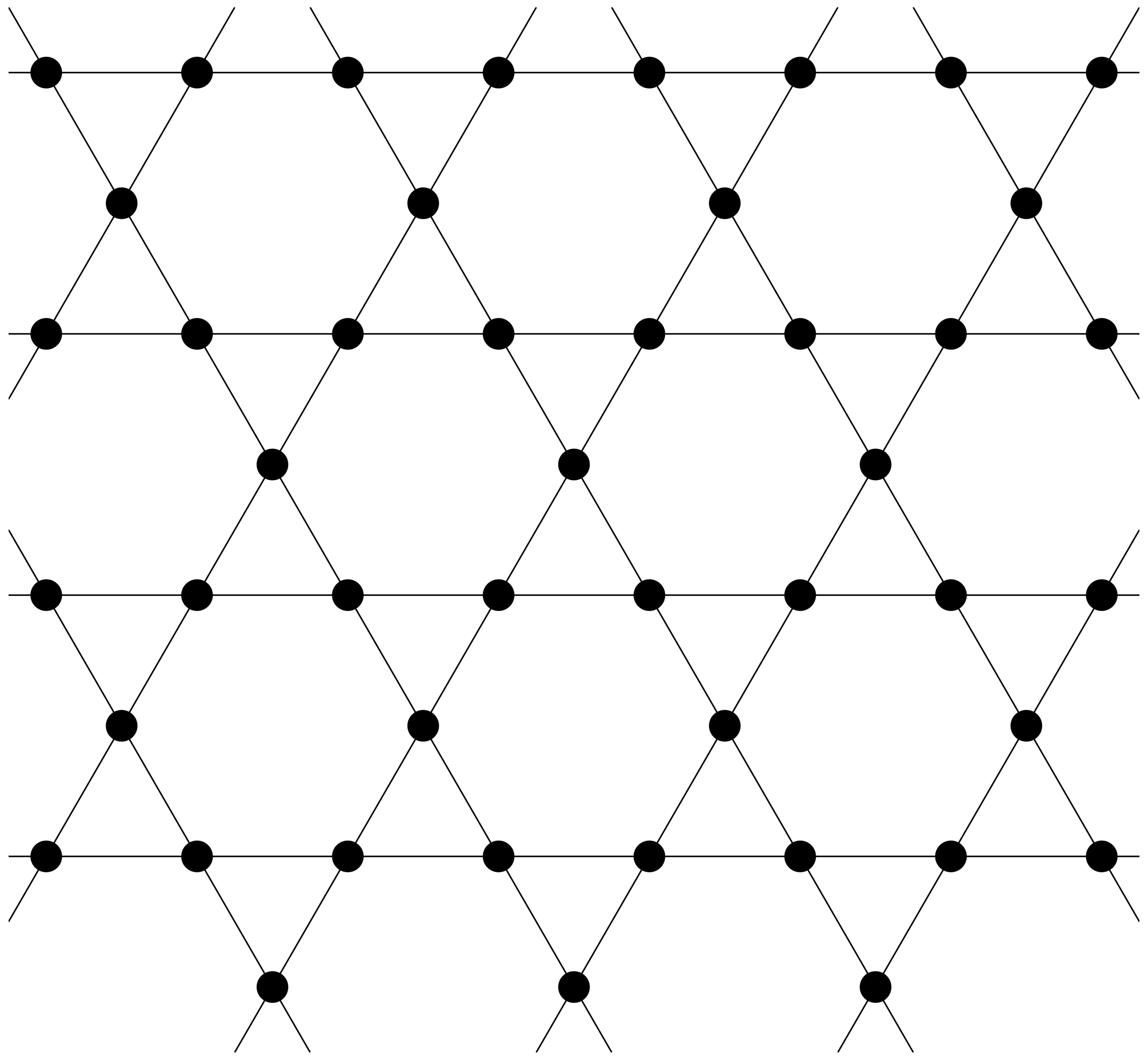

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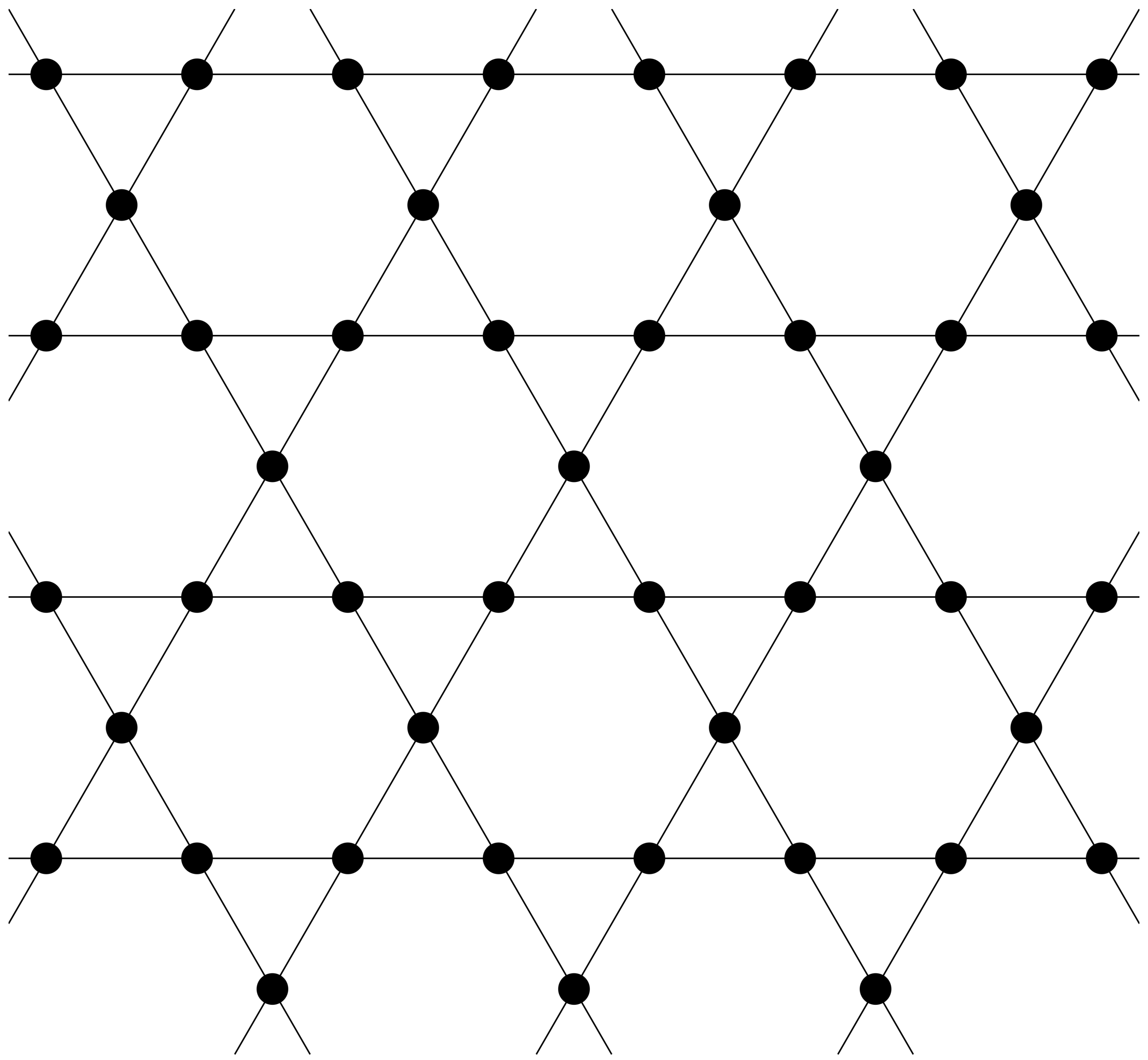

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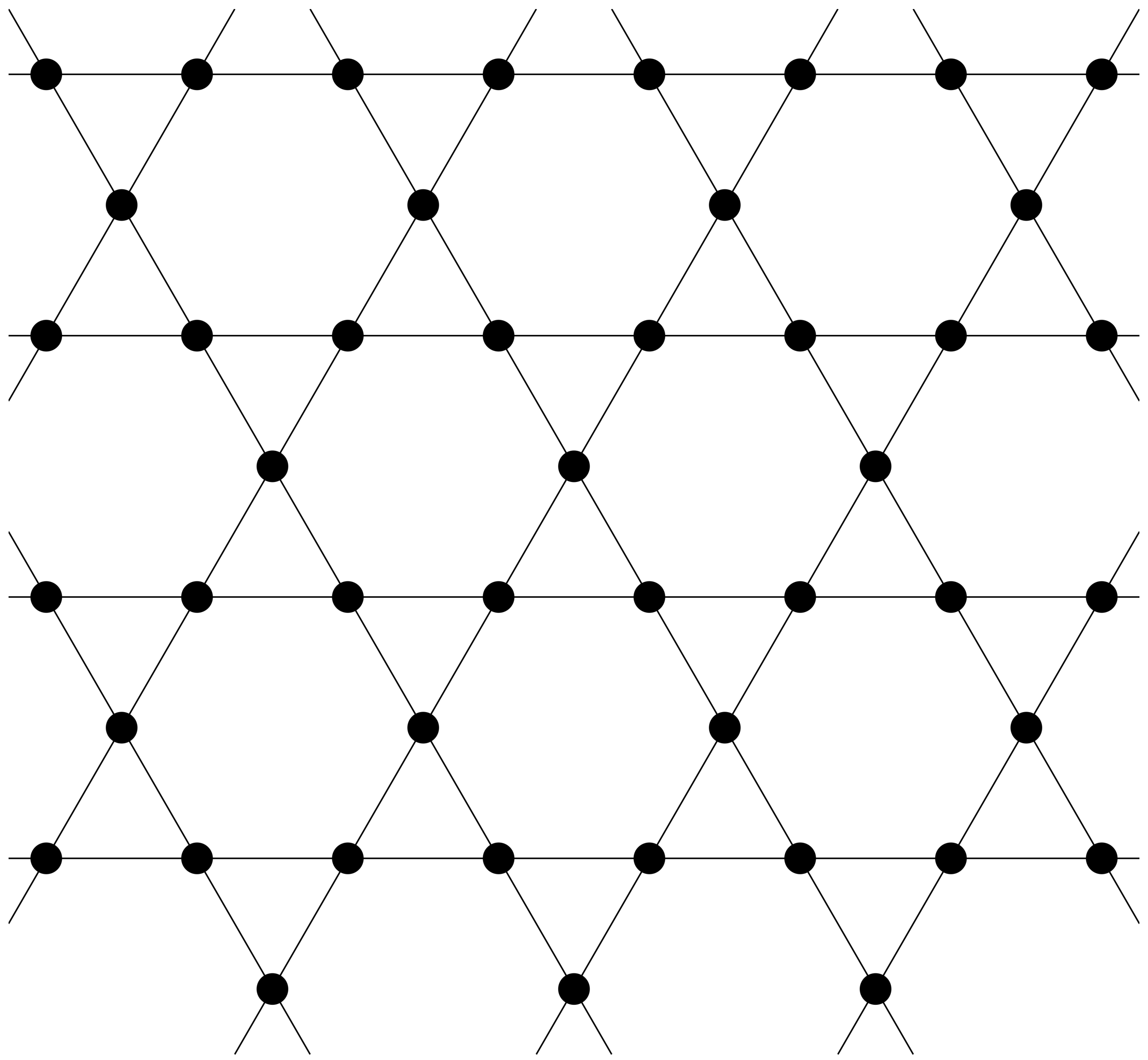

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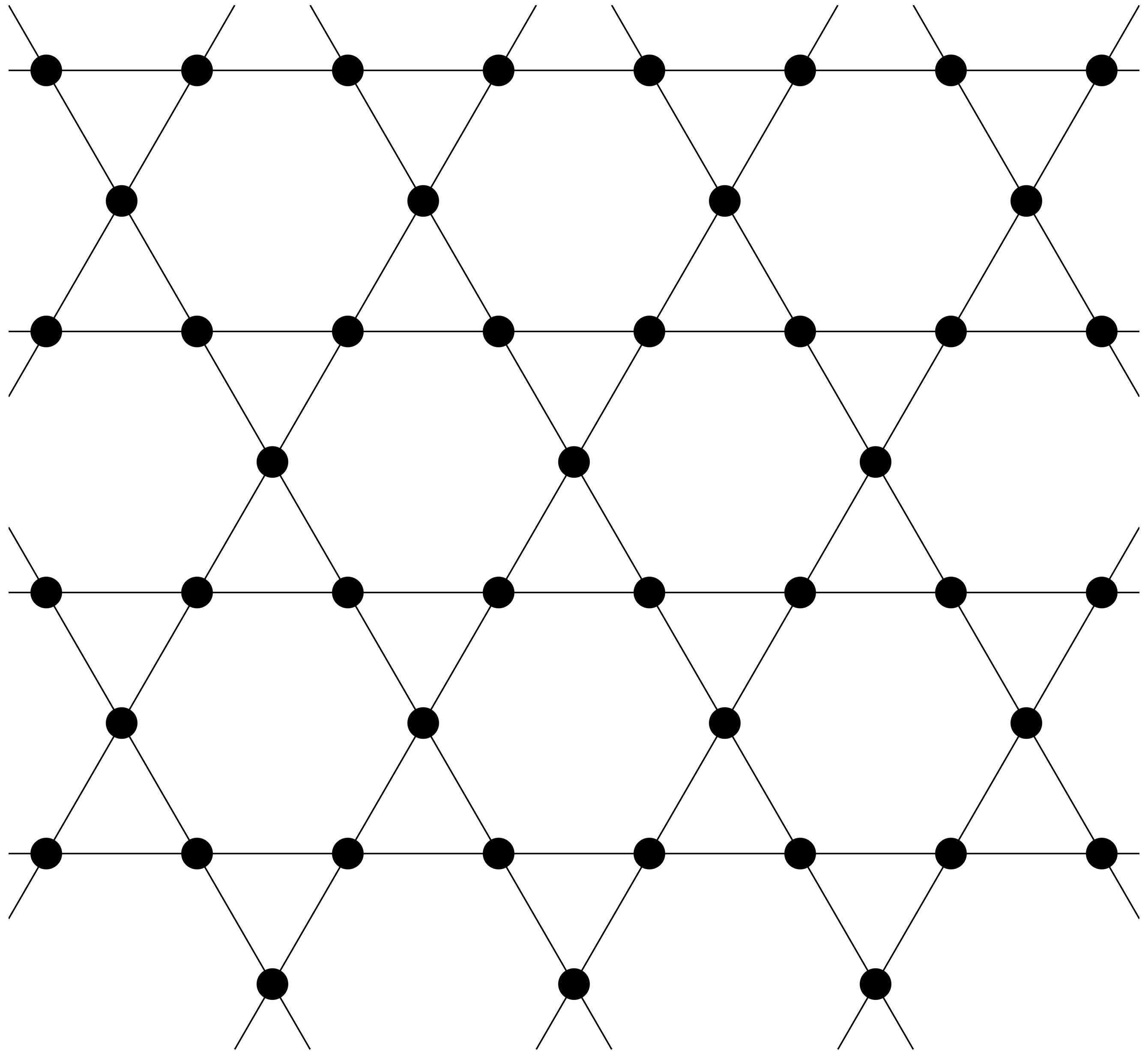

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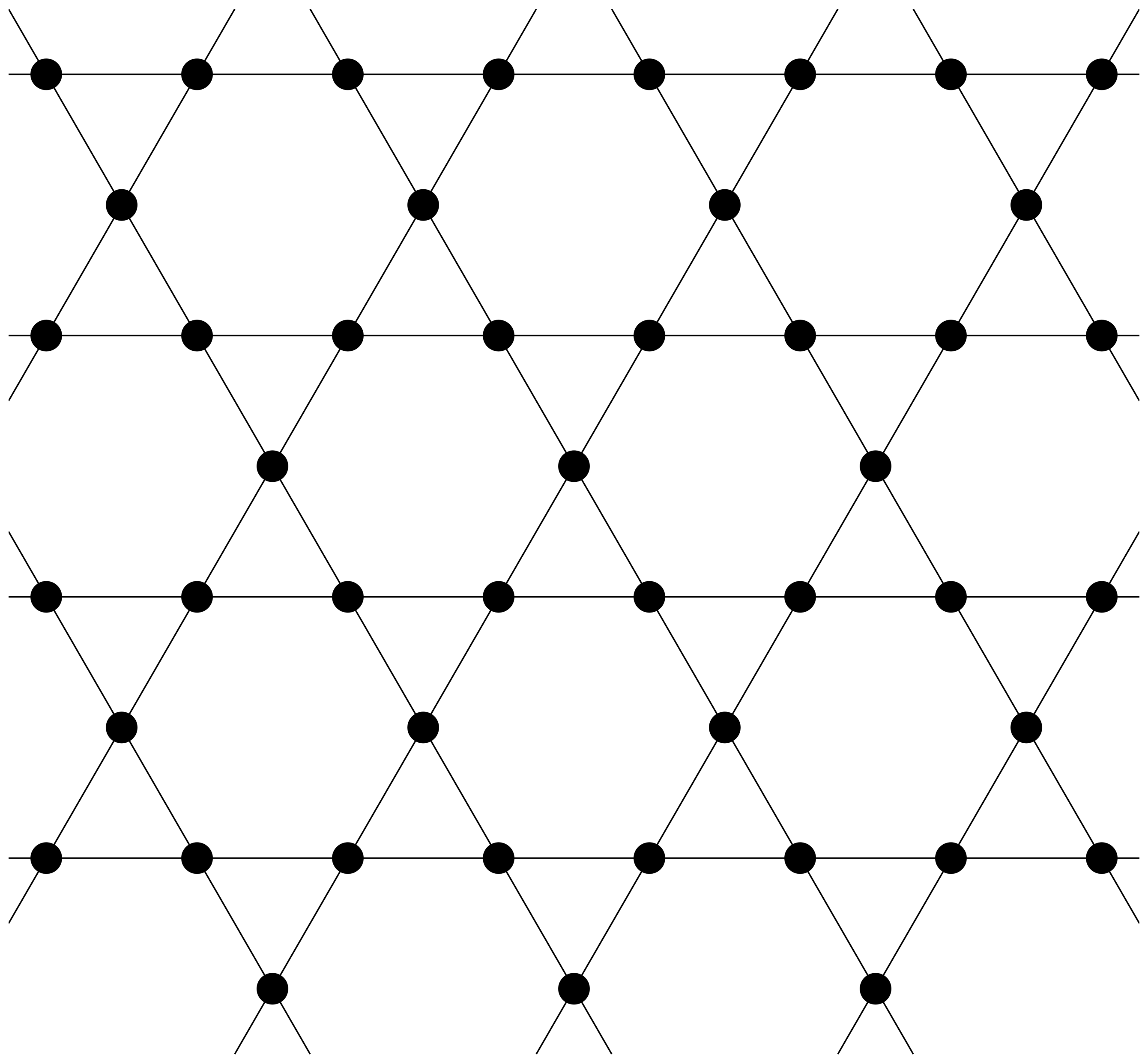
- Can we instead have a numerical result that remain true in 100 years with even quantum computers?

Motivation: decidability



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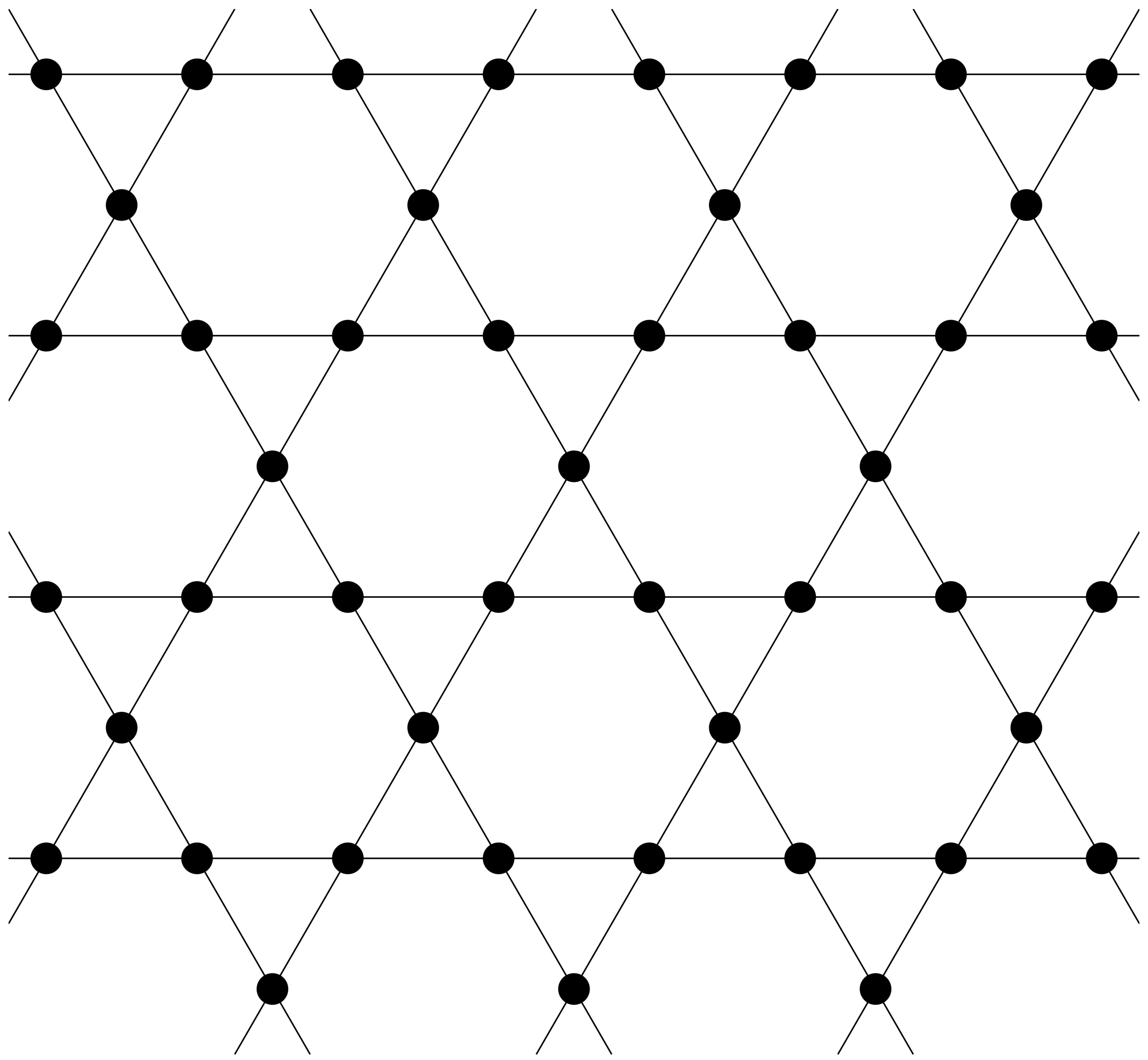

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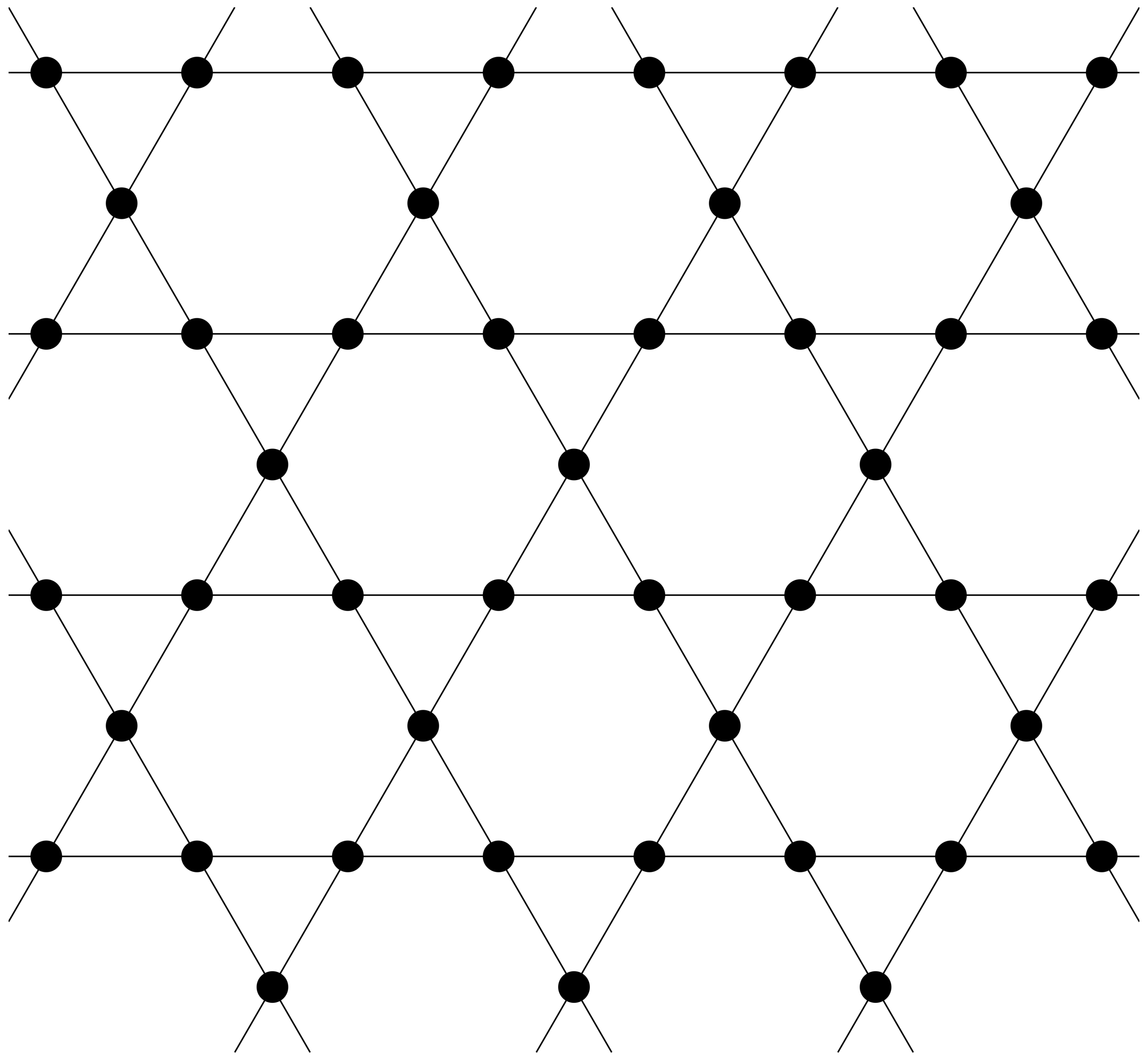

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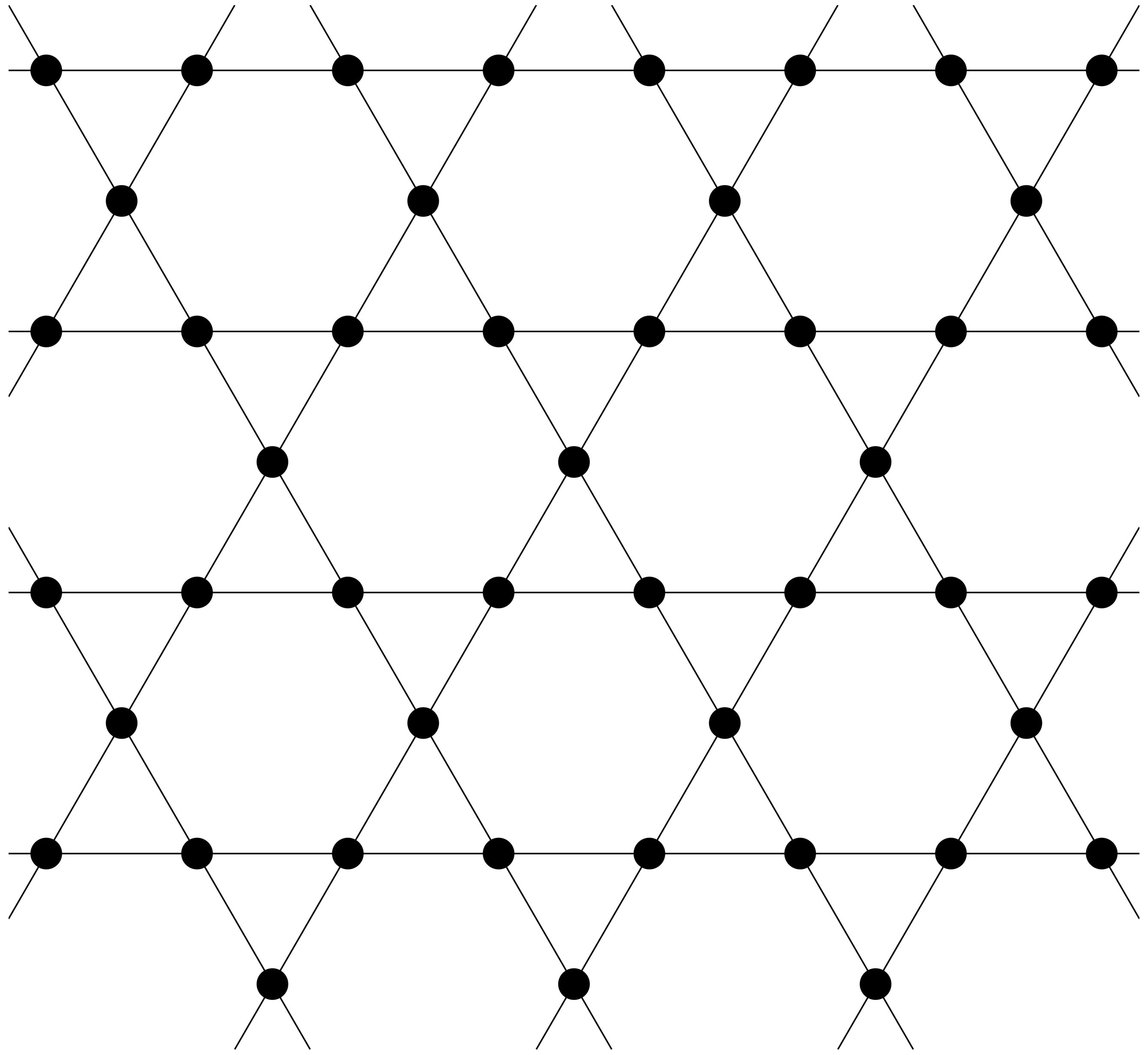

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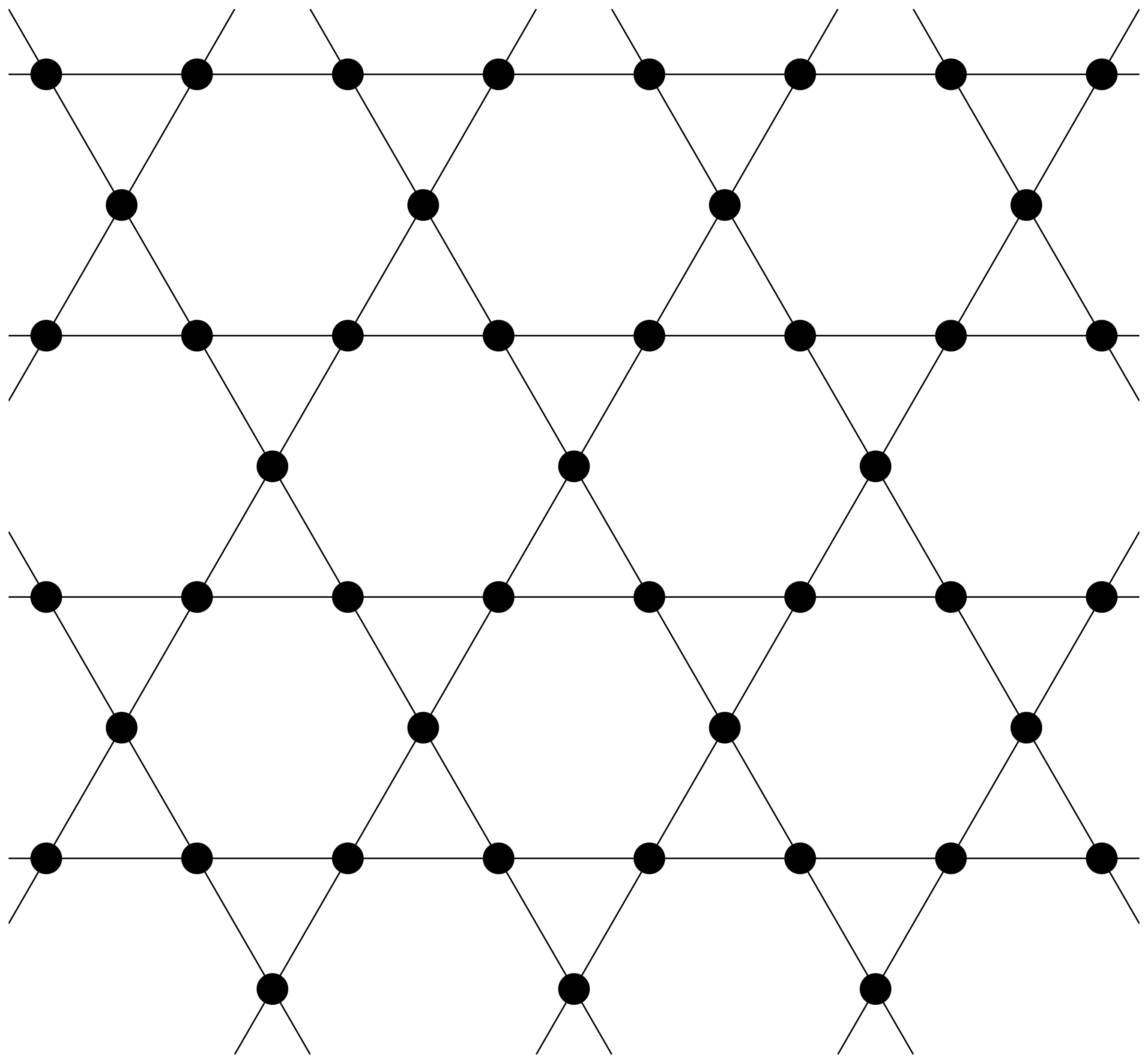

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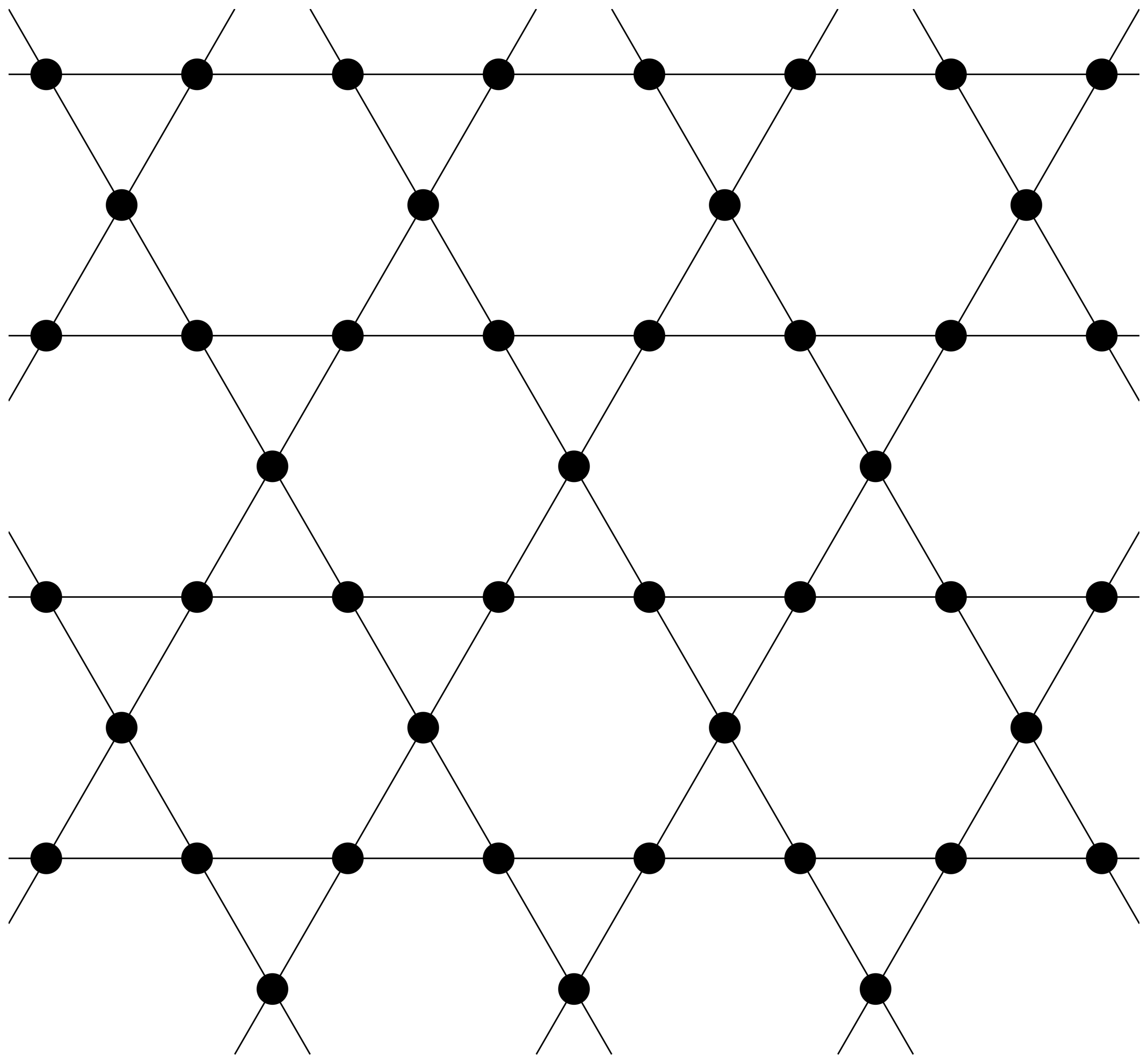

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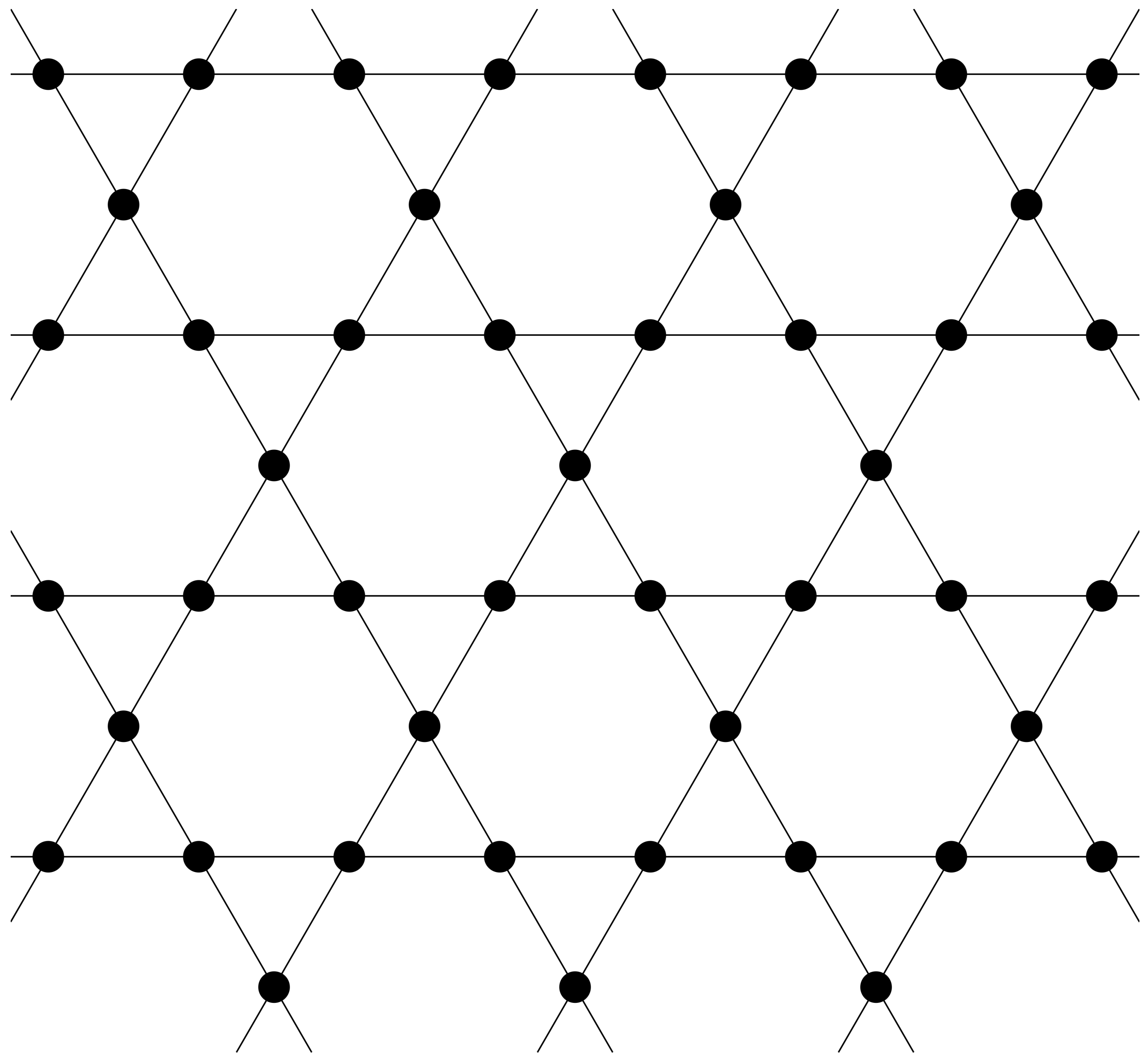

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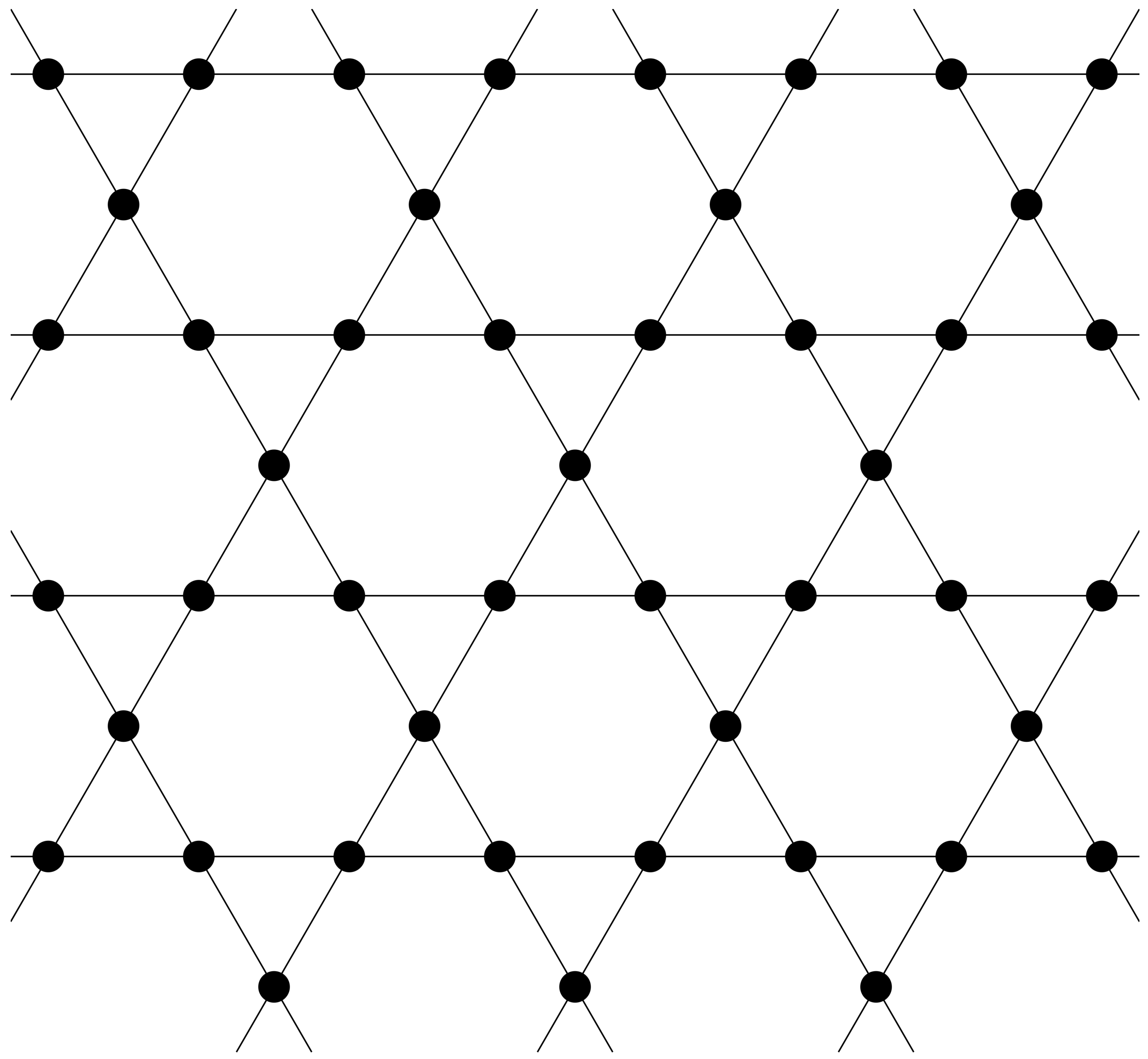

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- Different notions of thermodynamic limit
- “Open boundary condition” vs “bulk away from boundary”

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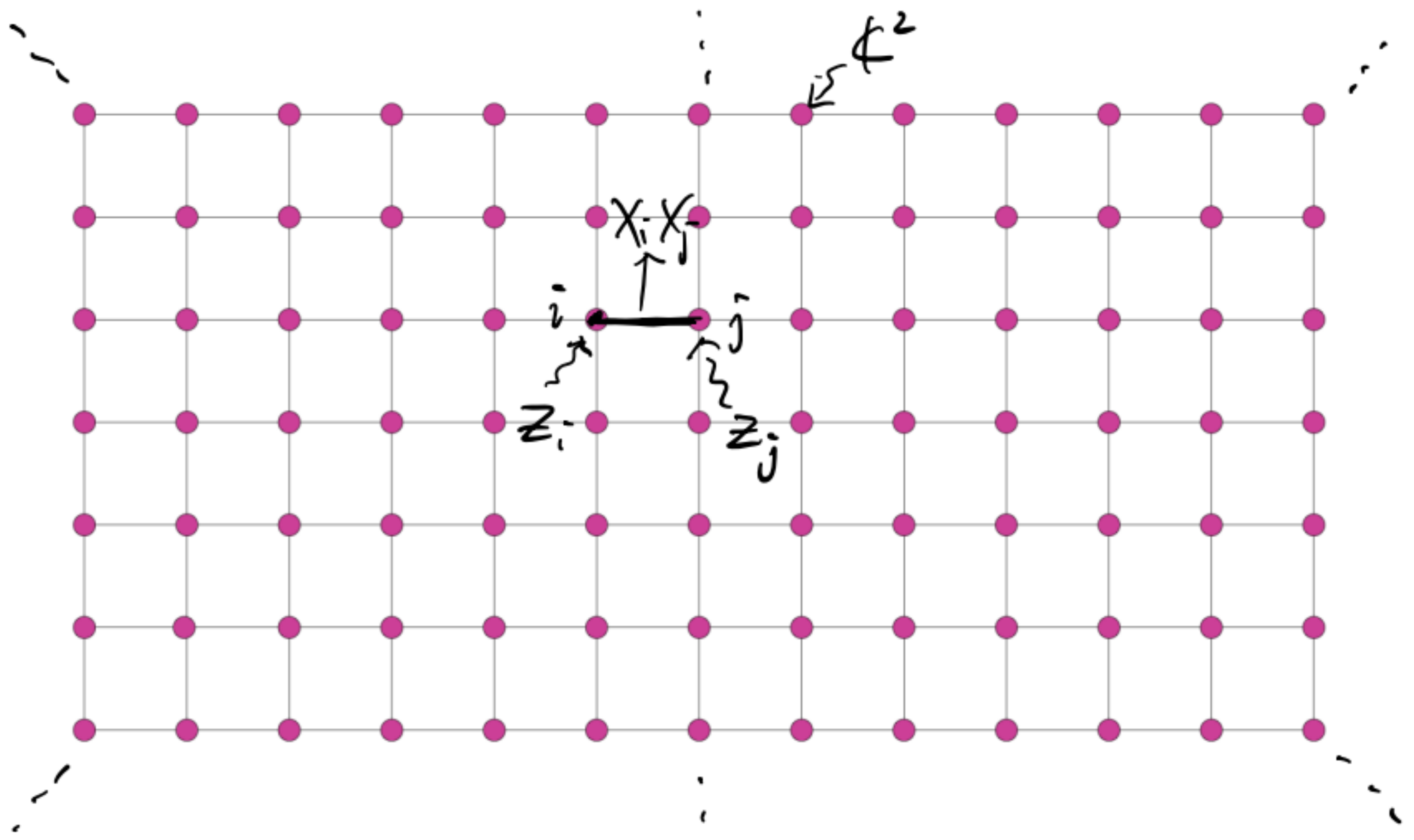
Finite size system



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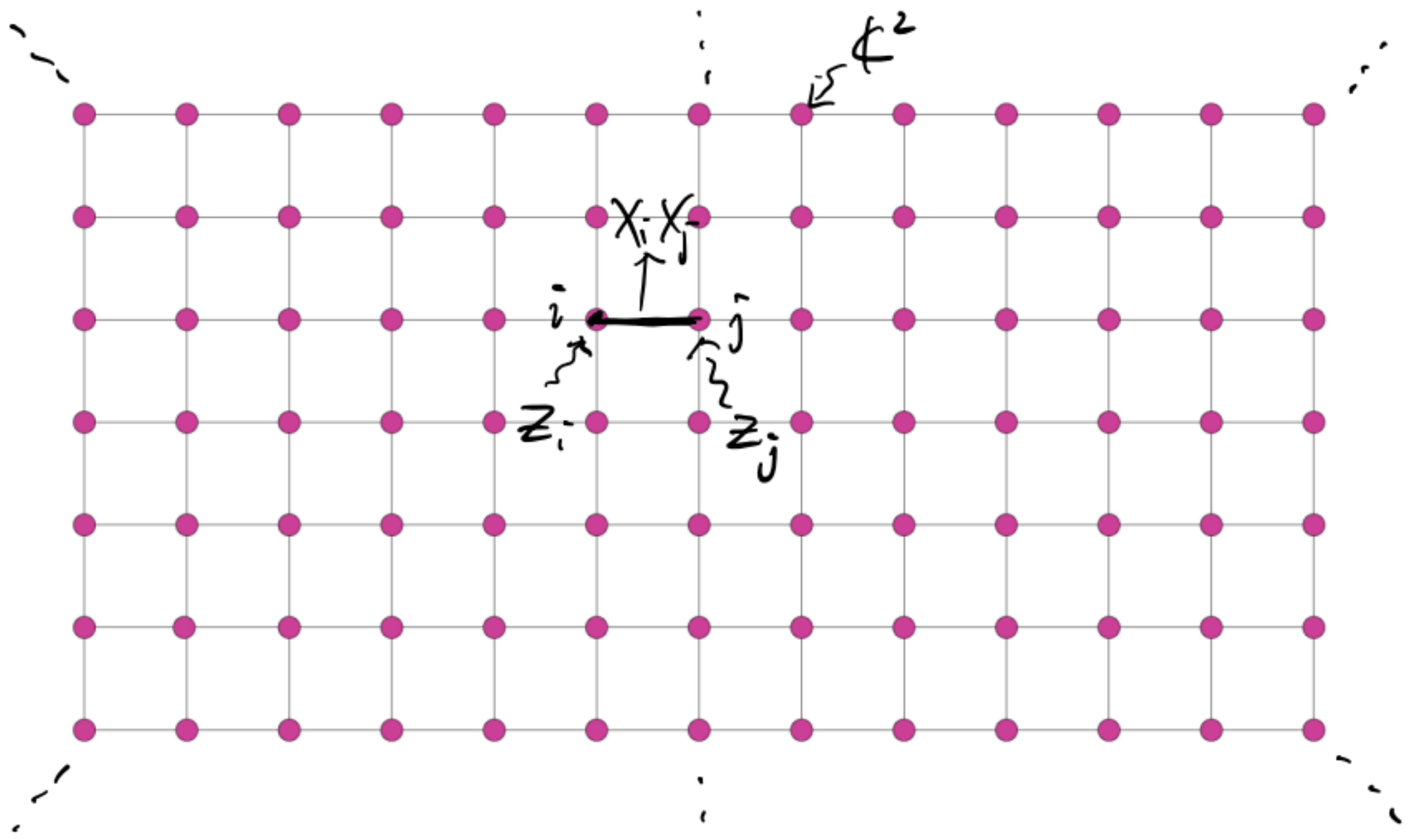

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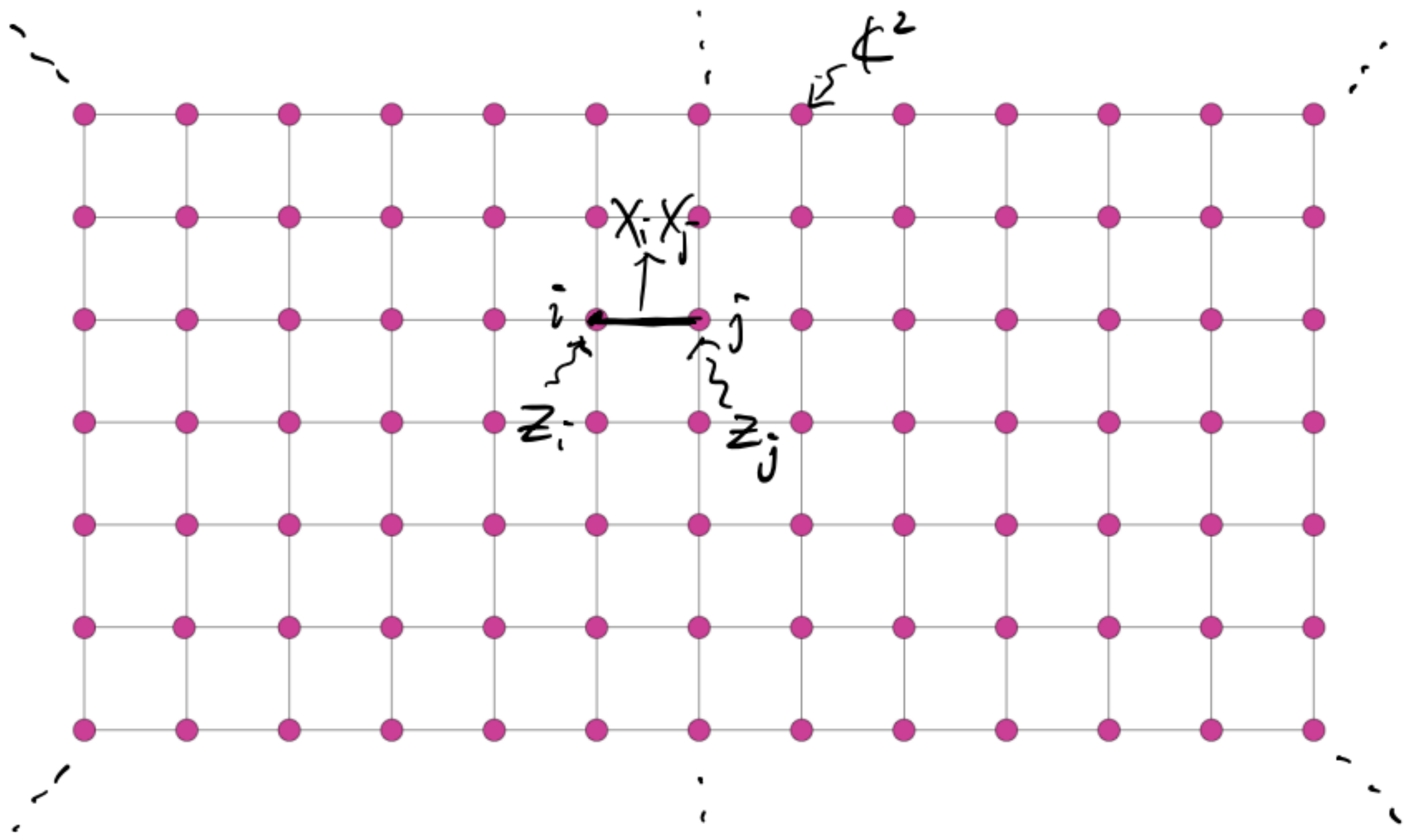

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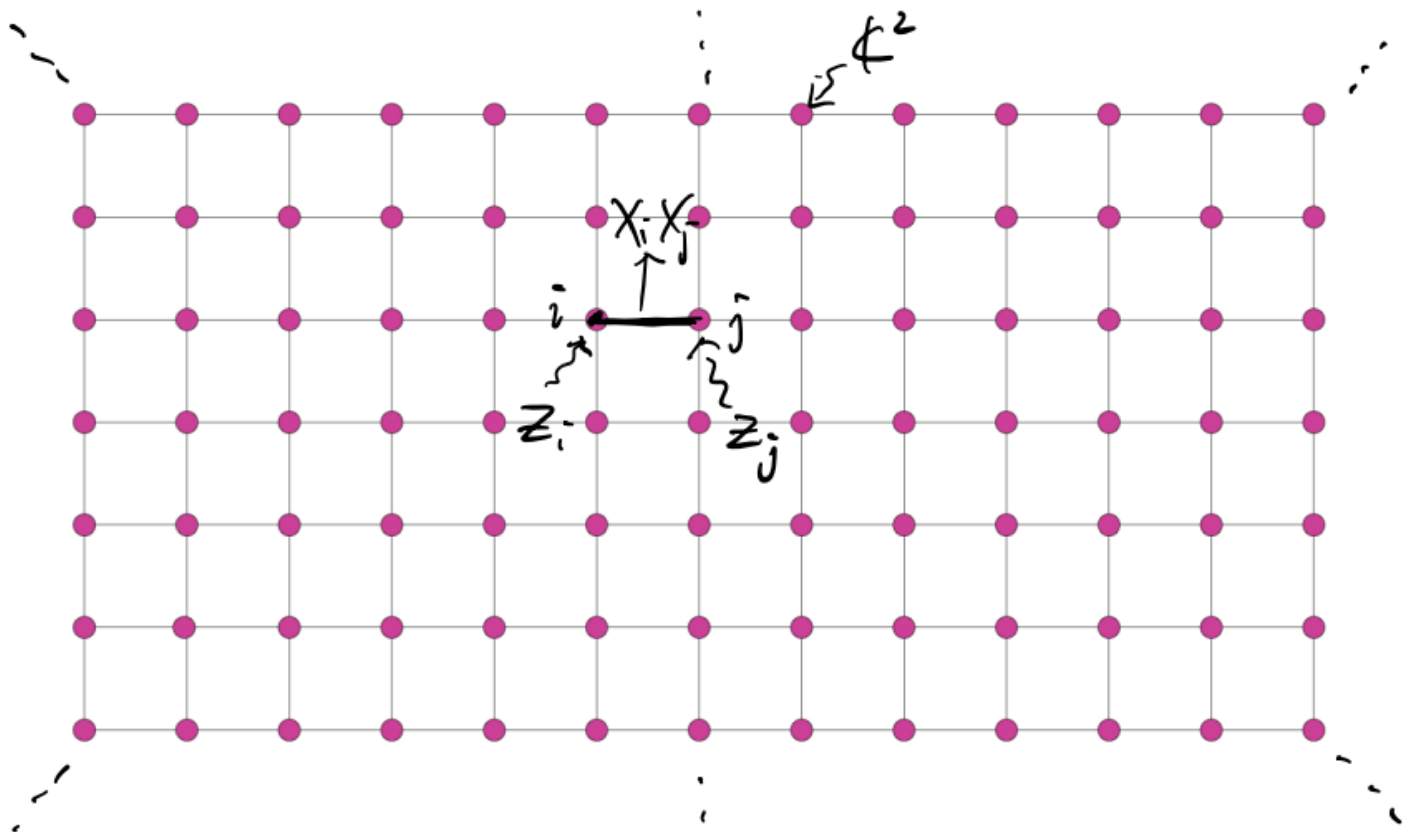

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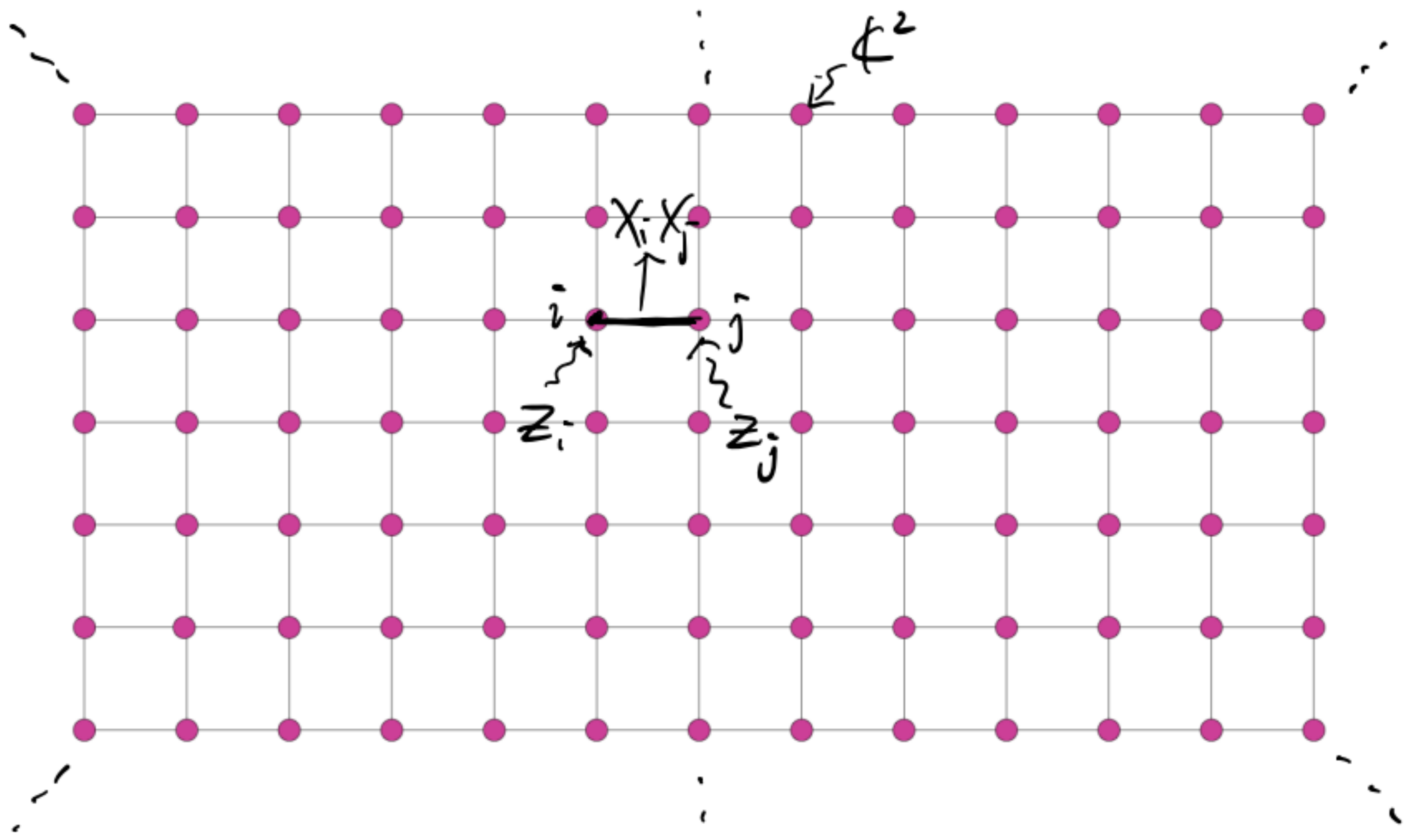

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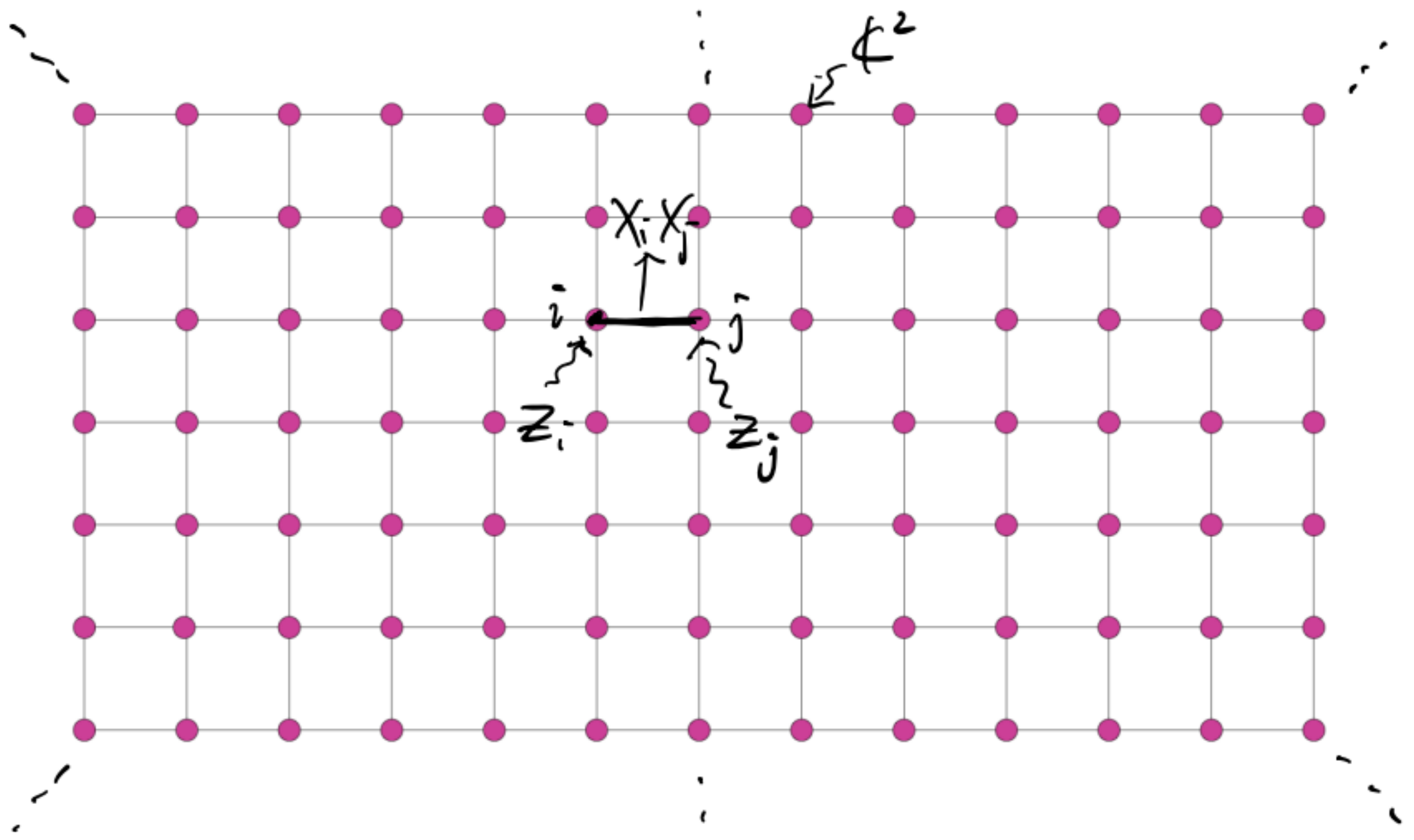

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- E.g.: $h_{ij} = X_iX_j + Z_i + Z_j$

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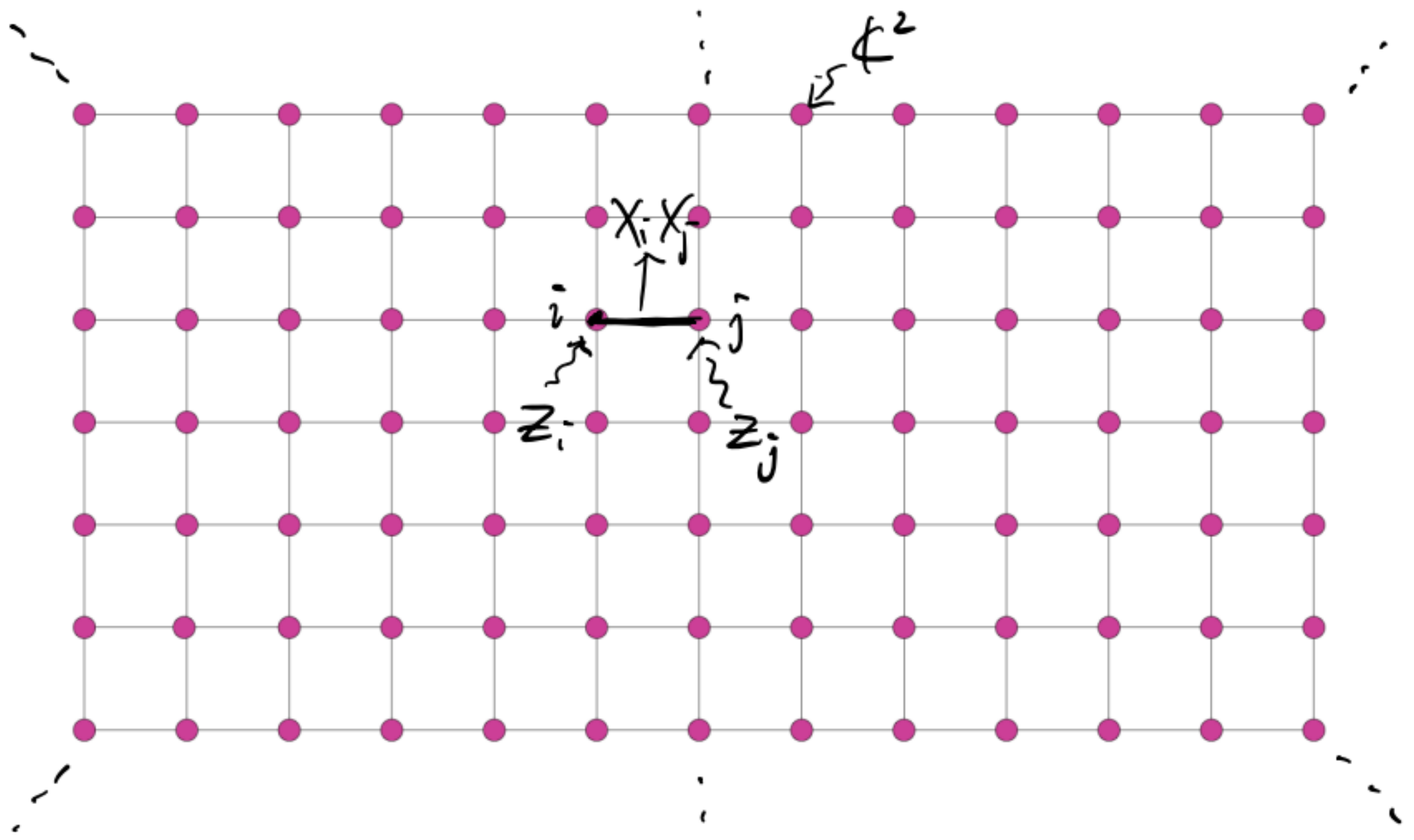

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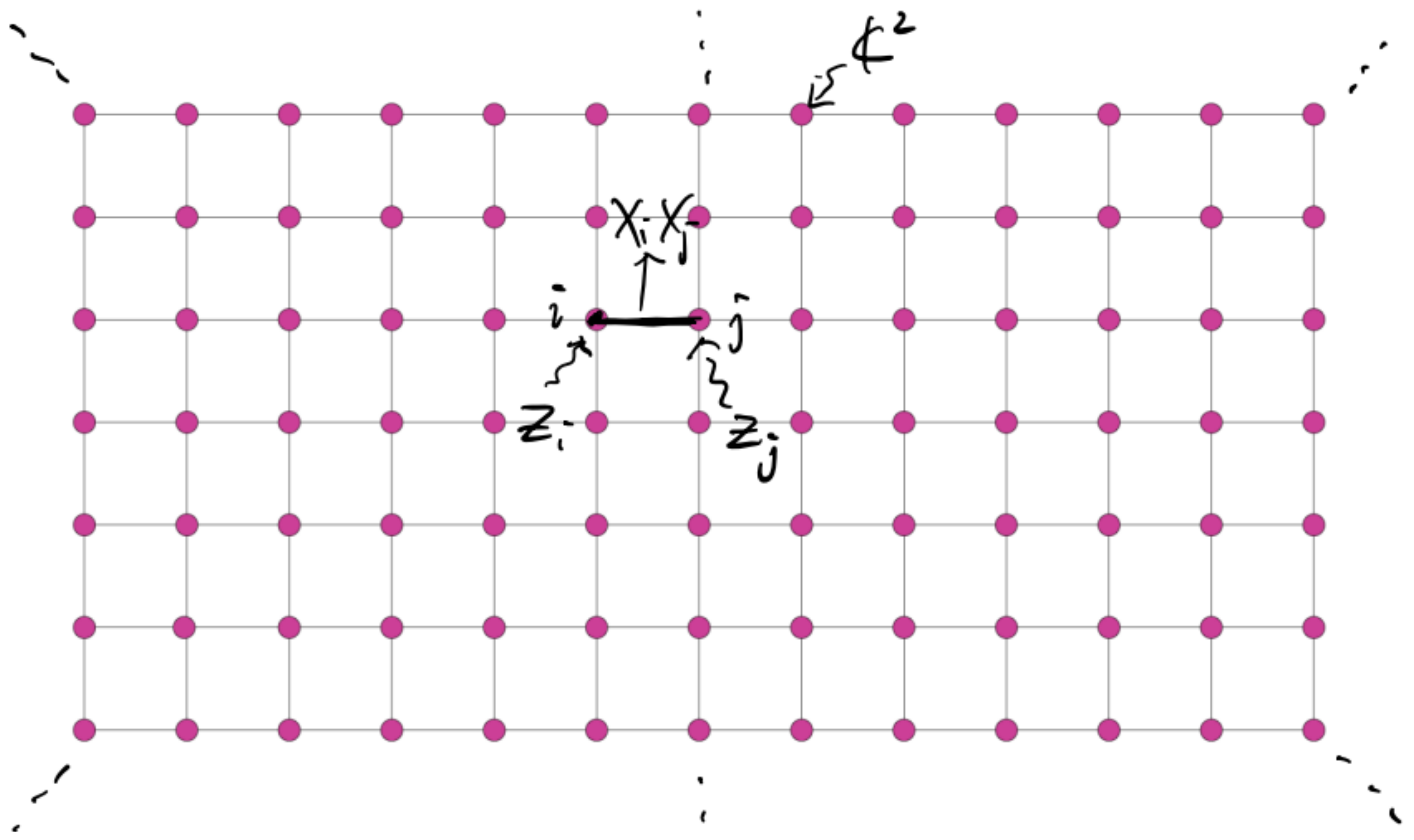

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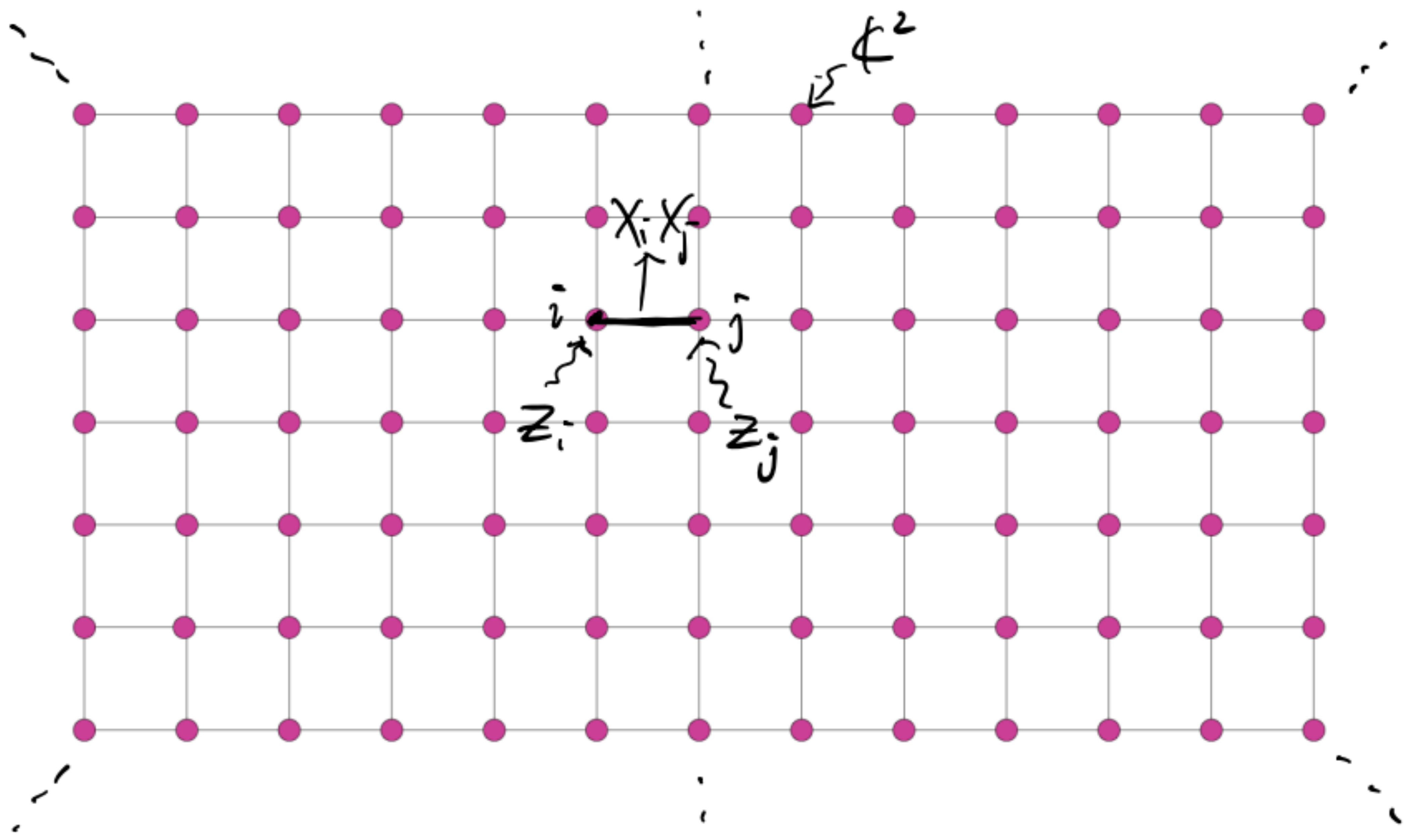

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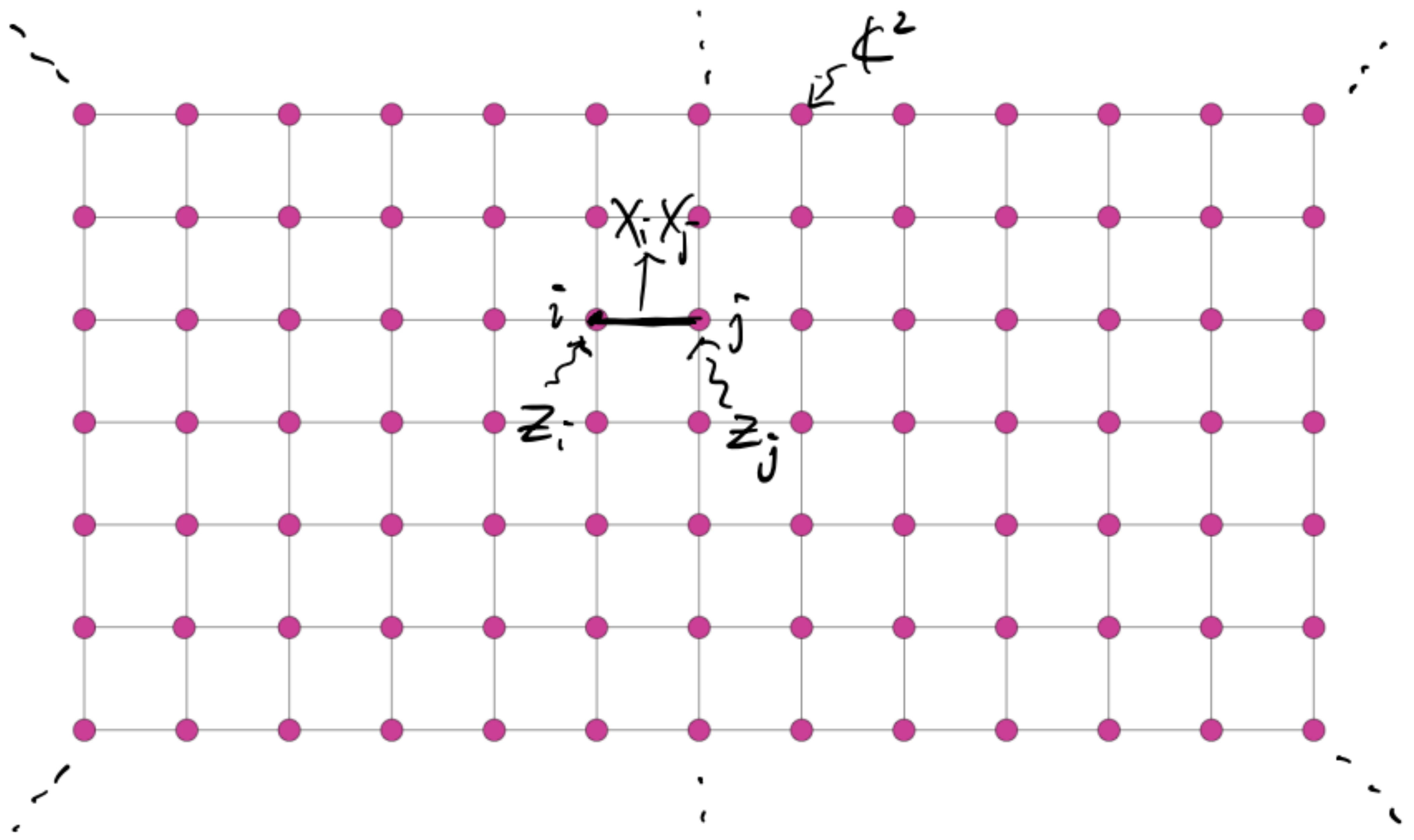

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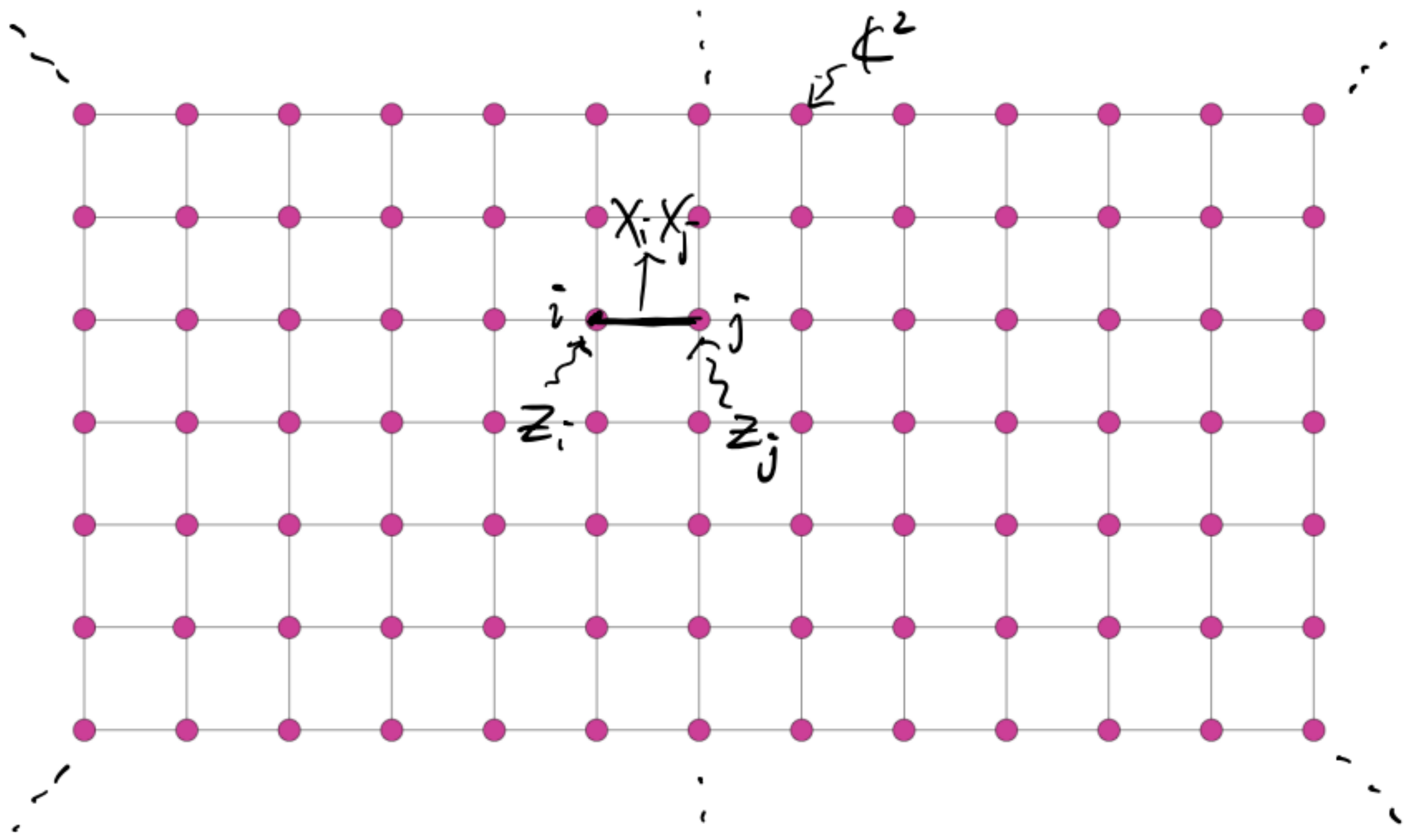

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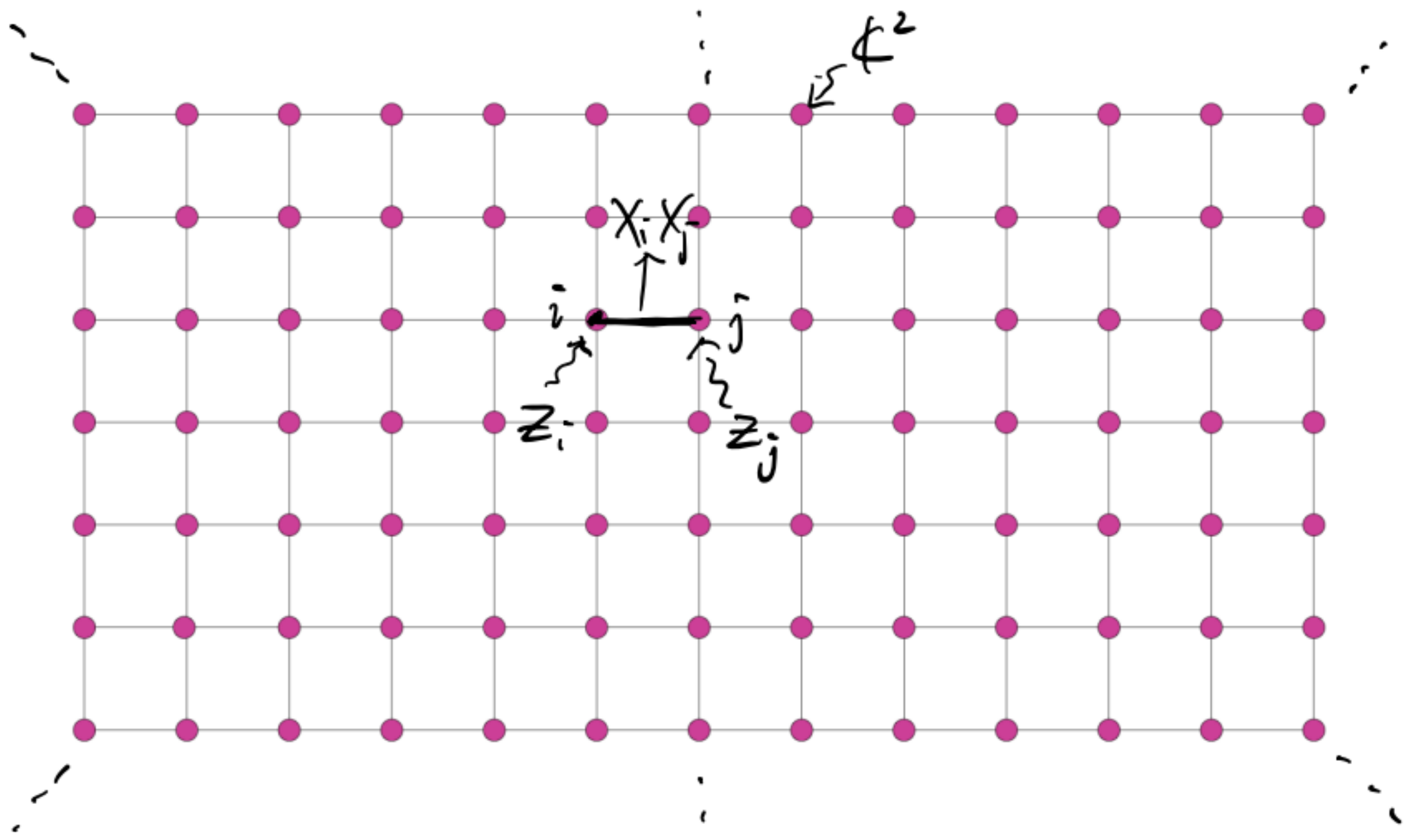
- Ground state ρ_{GS} has the smallest energy = projector on the lowest eigenvalue of H

Finite size system



- $\mathscr{H}_i = \mathbb{C}^2, H := \sum_{<i,j>} h_{ij}, N \sim 10^{23}$
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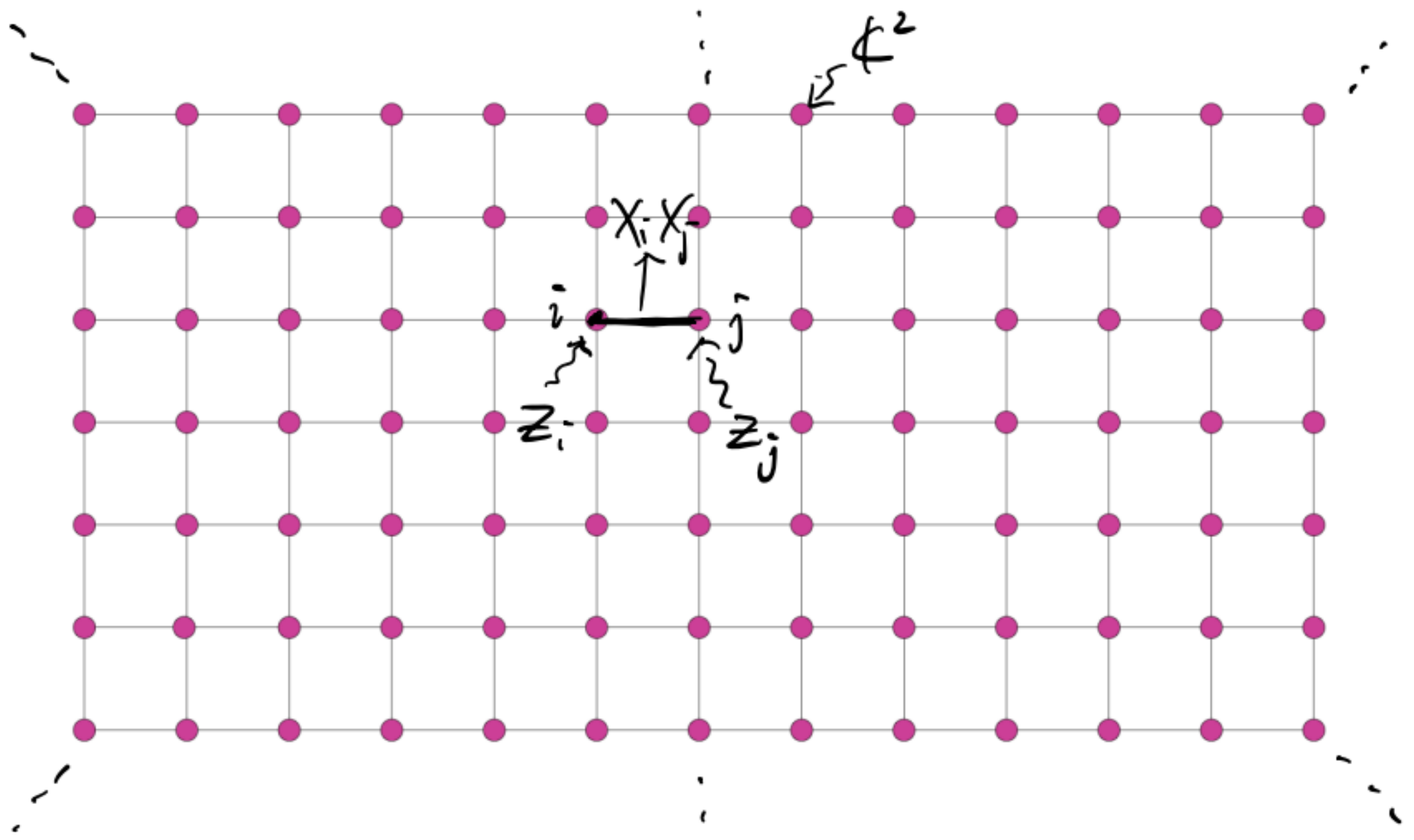

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- Gigantic matrices, impossible to compute

Certifying ground-state properties of quantum many-body systems

1. Motivation
2. Finite systems
3. **Thermodynamic limit with boundaries**
4. Thermodynamic limit: the bulk

Justification of thermodynamic limit

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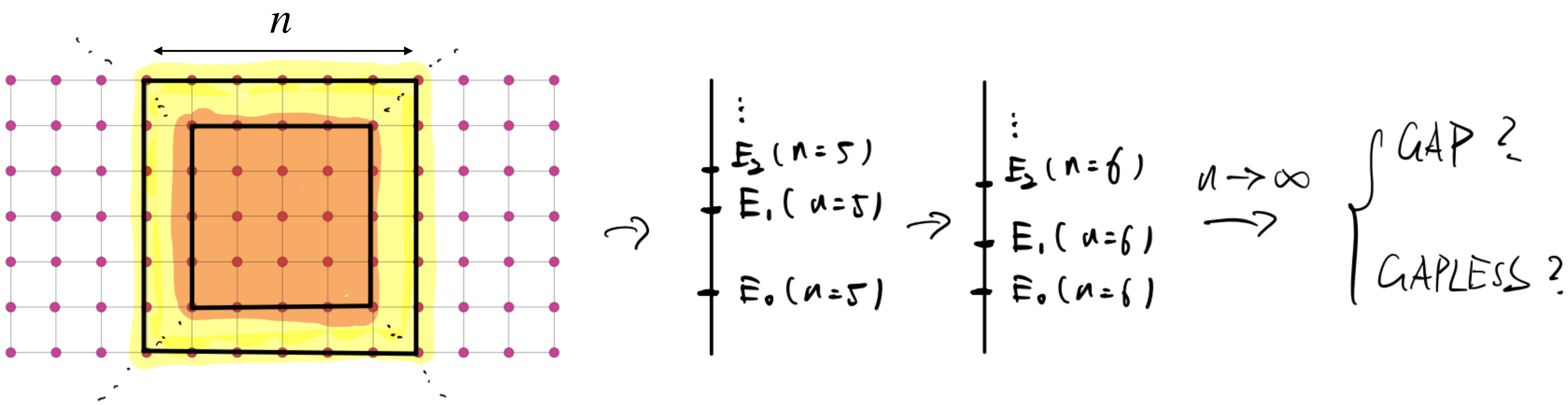
- How to take this limit?

Thermodynamic limit with boundaries



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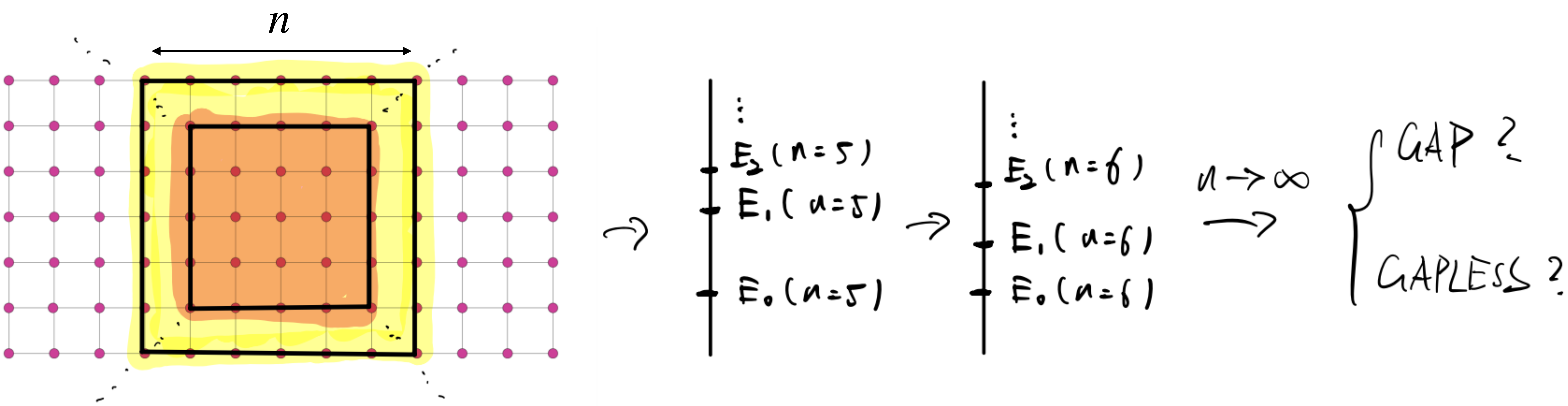

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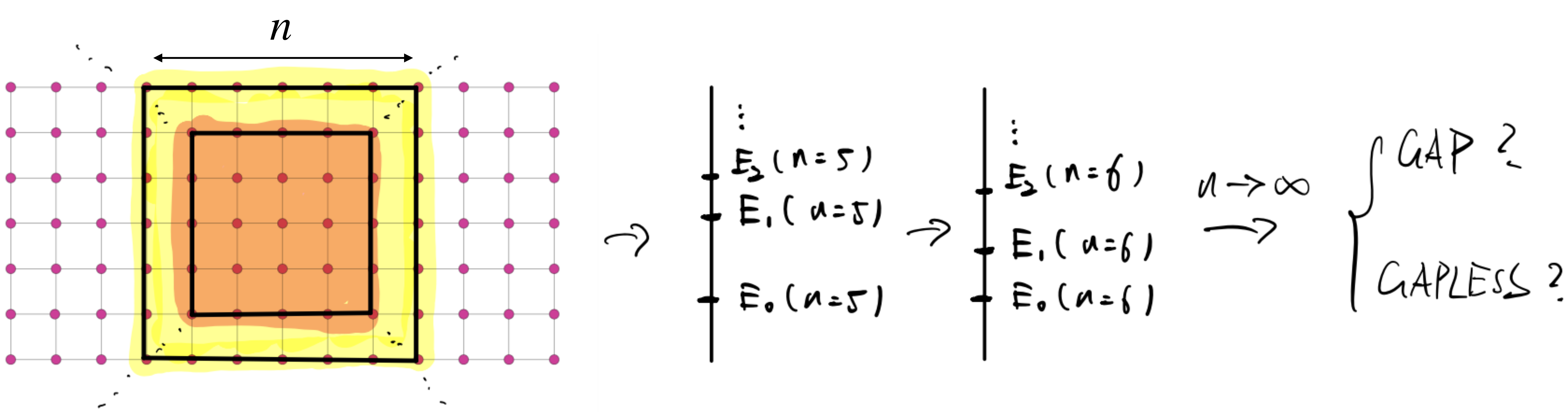

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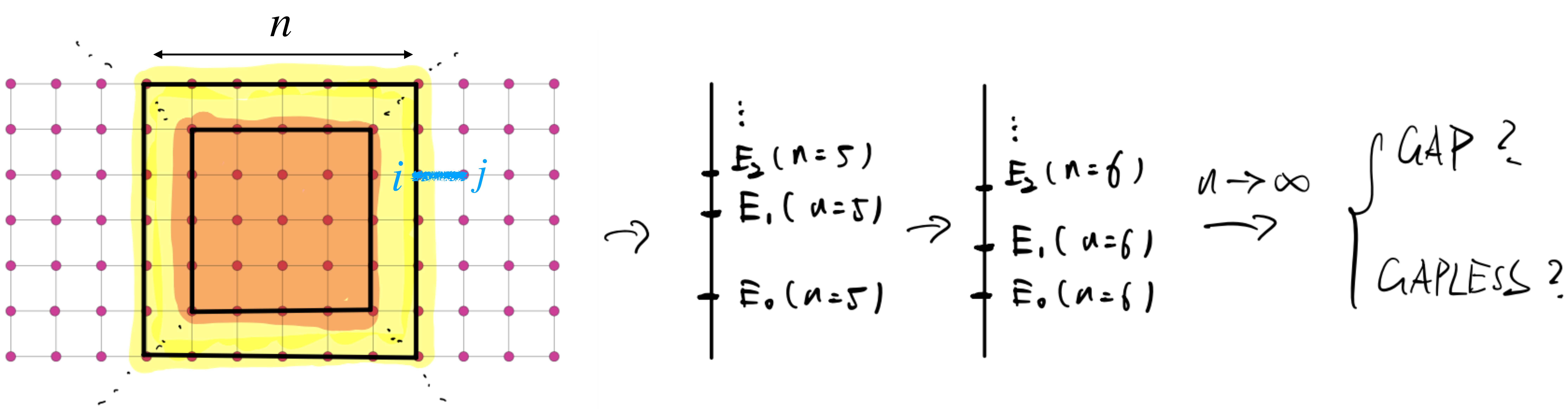
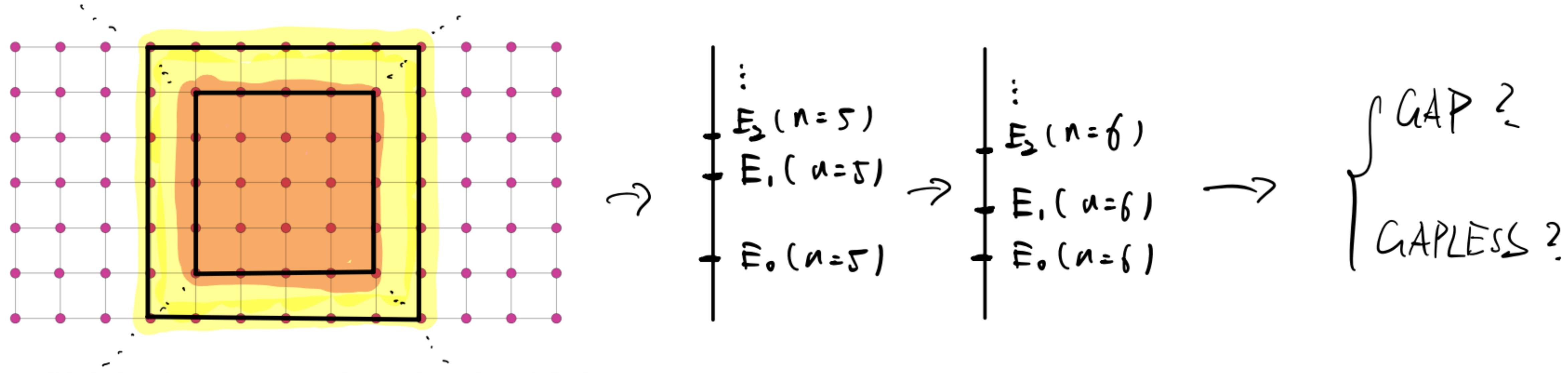
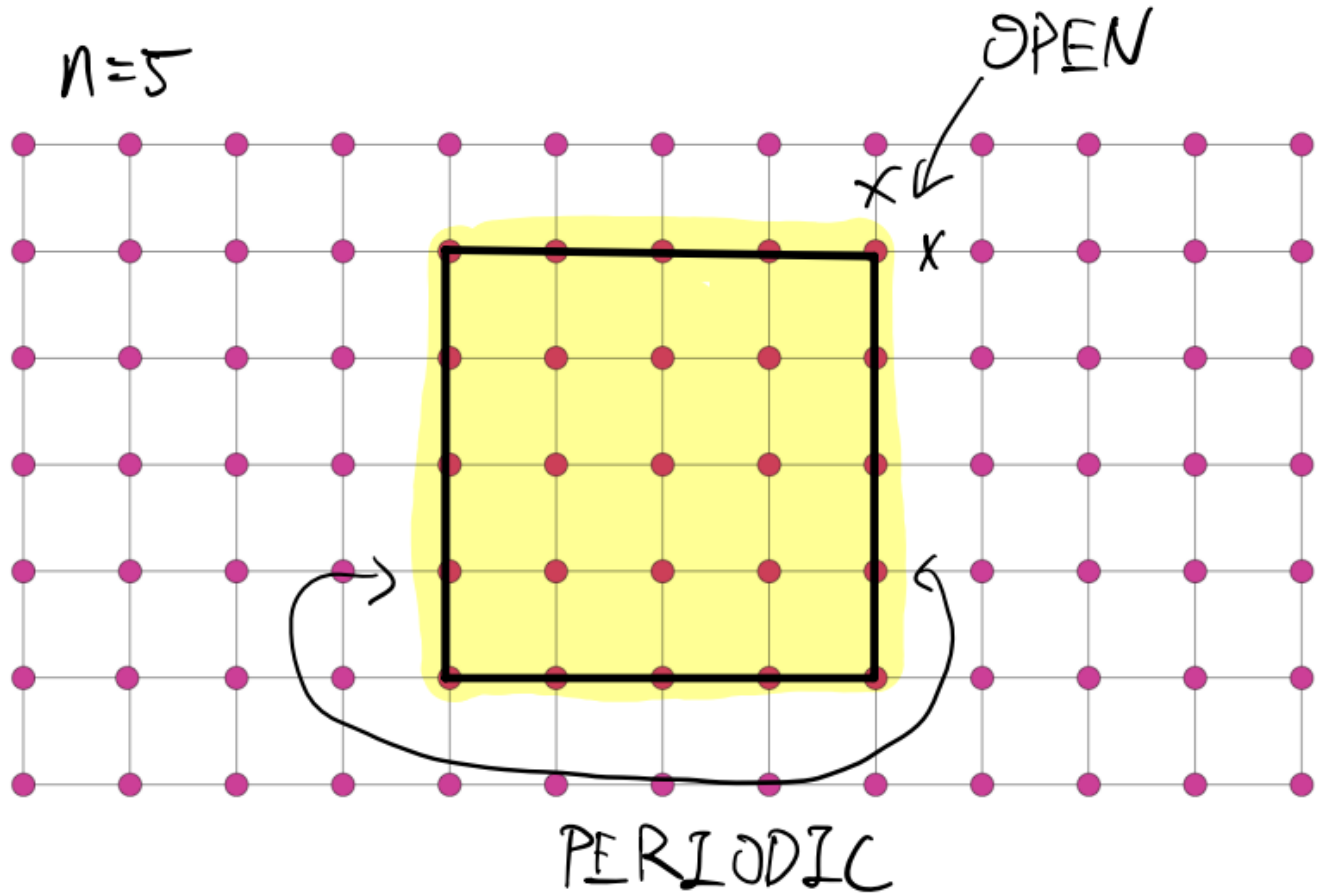


- Look at the $n \times n$ sub-lattice, finite size calculation get ρ^n_{GS} and $\Delta_n(H)$
- let $n \to \infty$
- Subtlety on boundary: what about h_{ij} when i inside $n \times n$, but j outside?

Thermodynamic limit with boundaries





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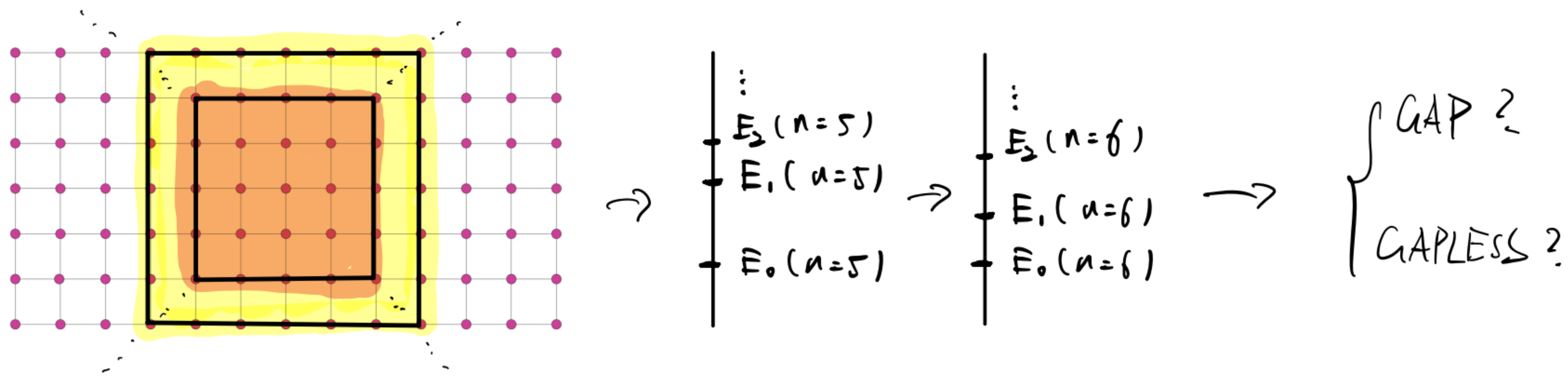
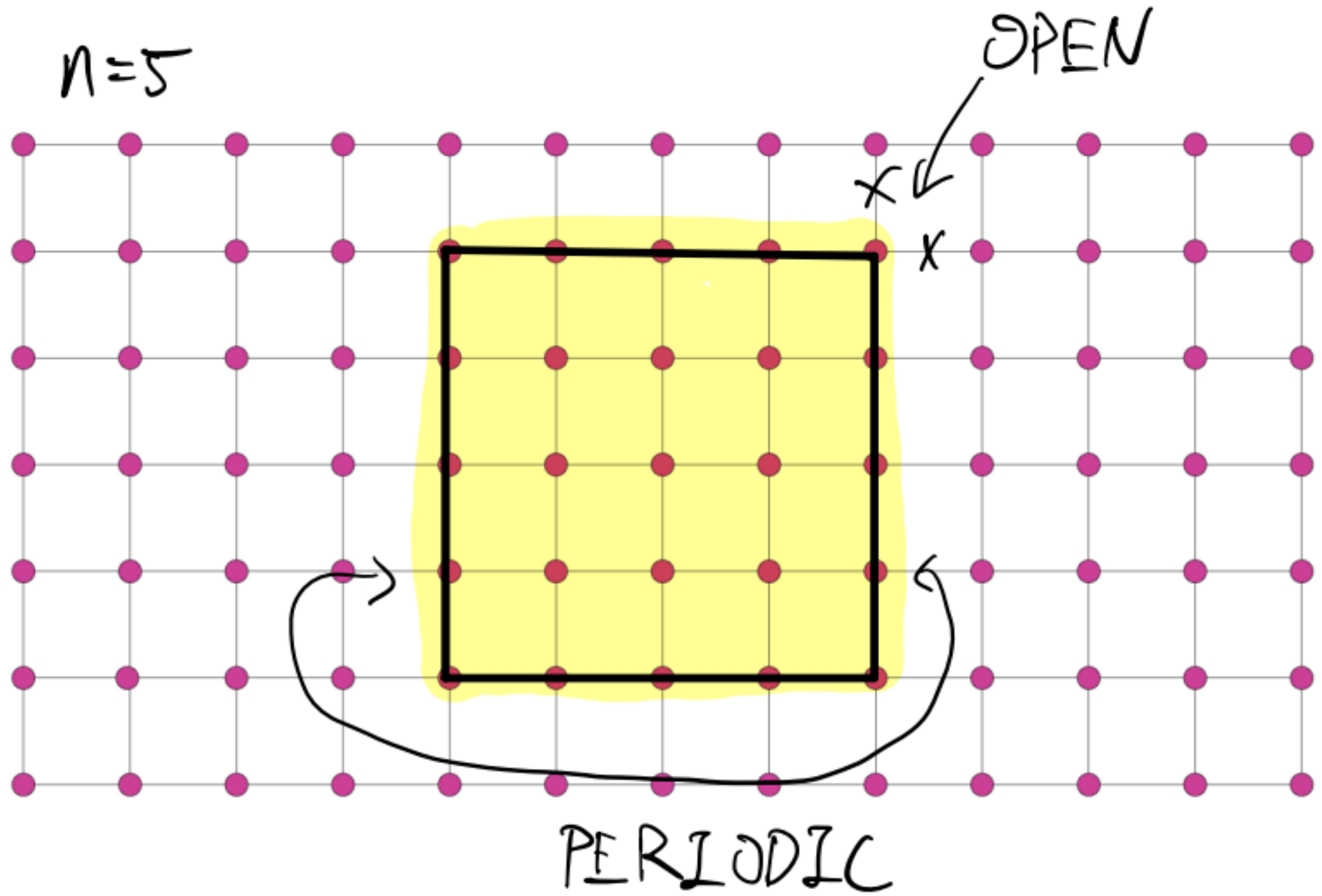
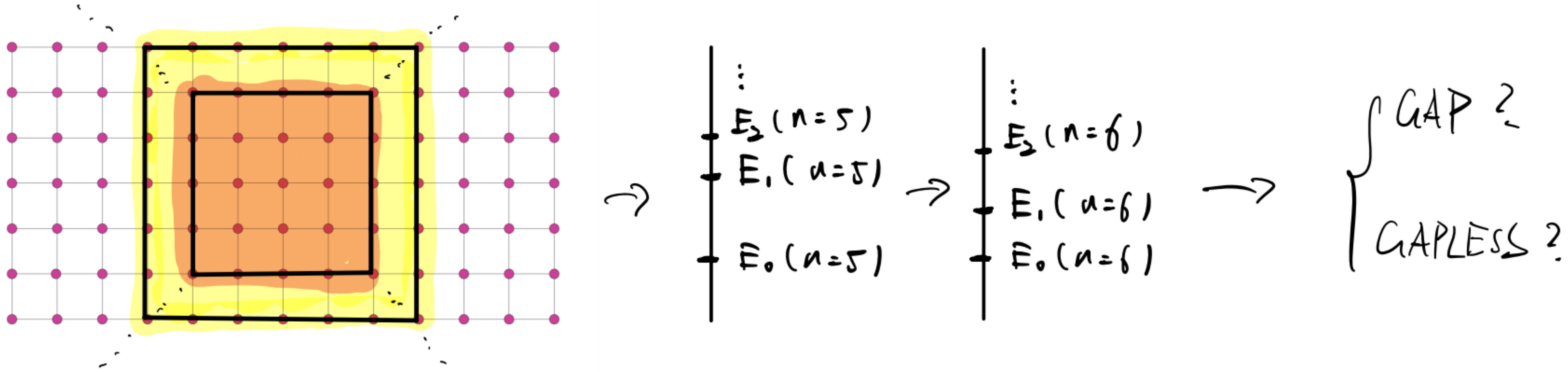
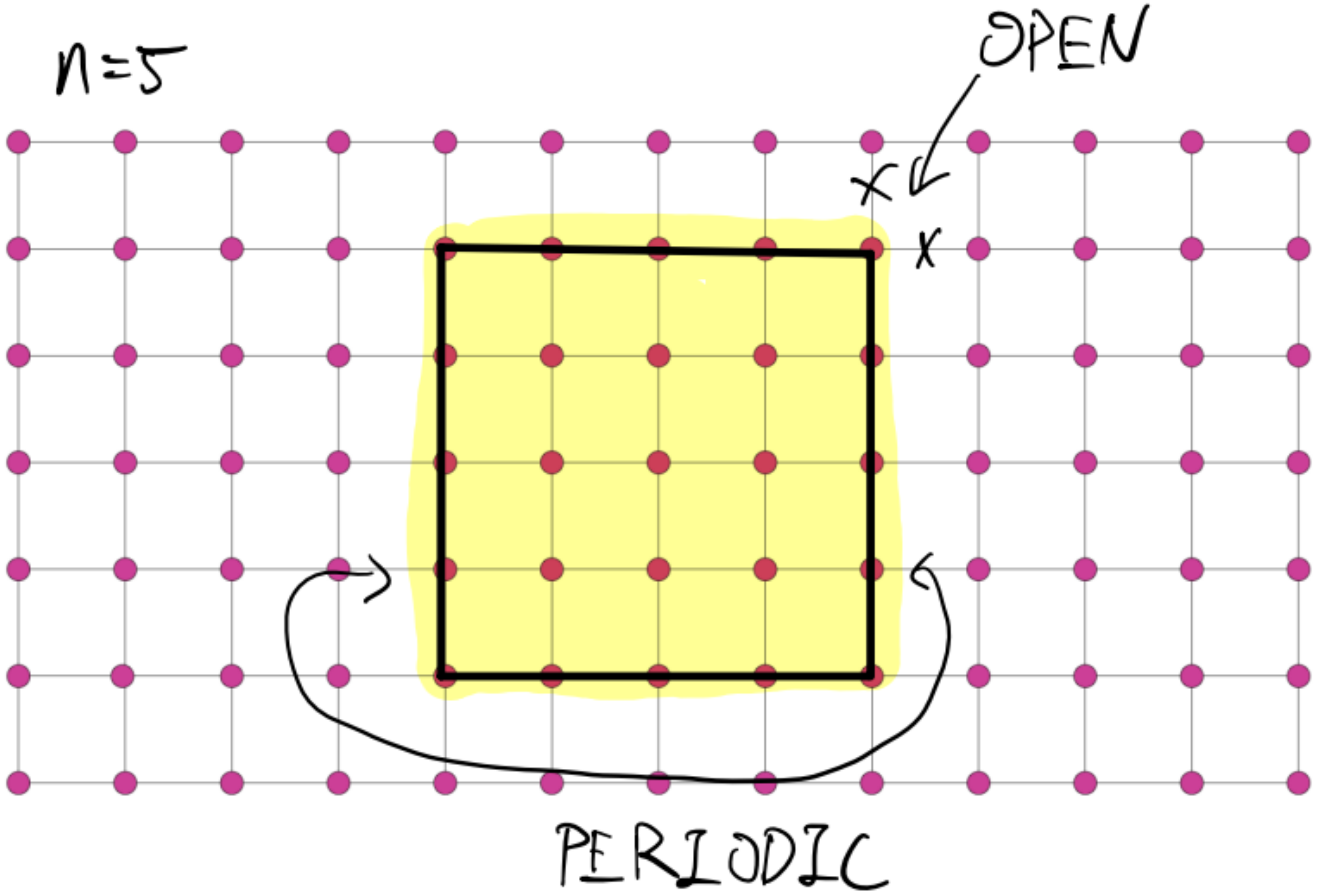




- Need to fix a boundary condition

Thermodynamic limit with boundaries





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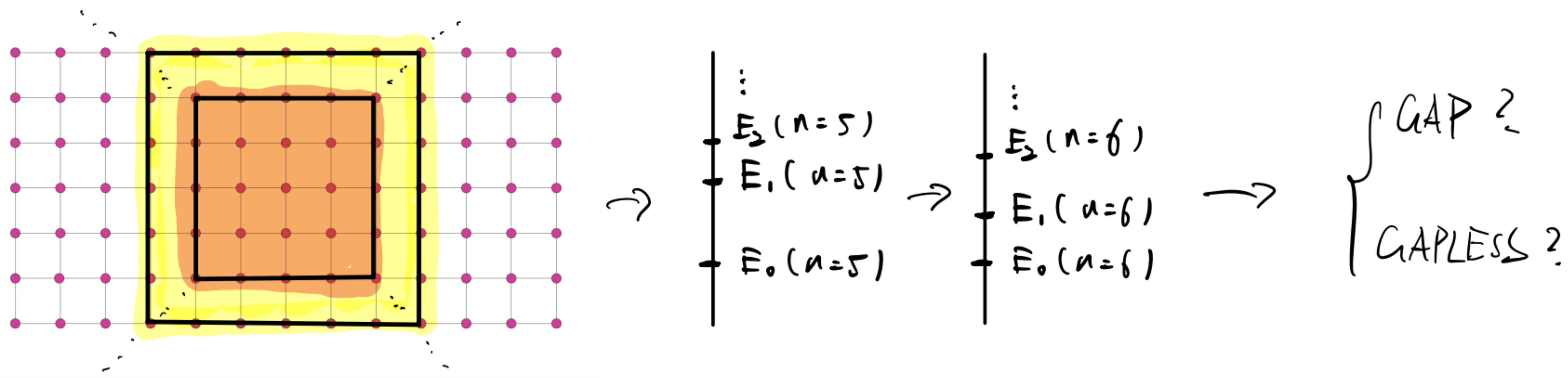
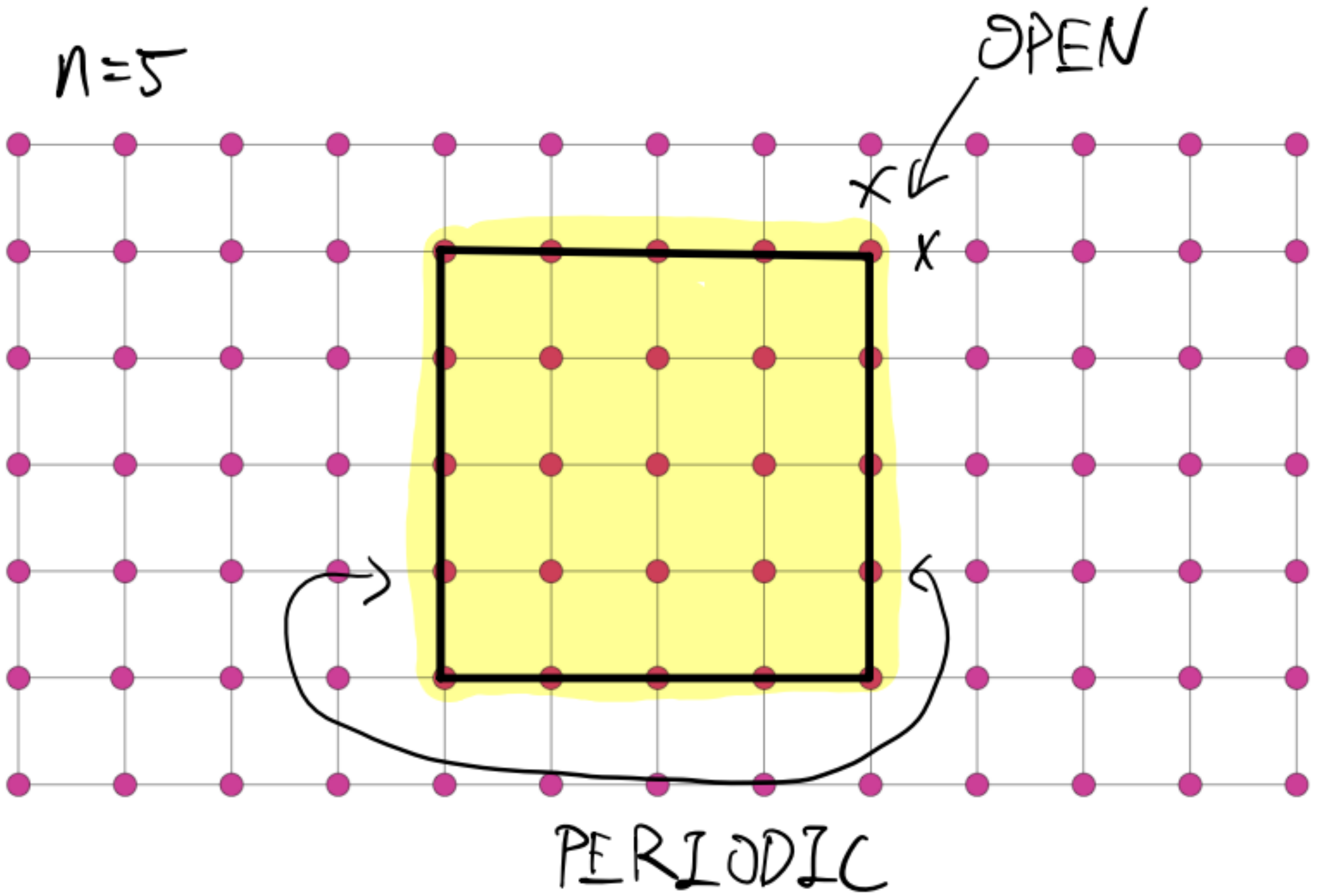
Thermodynamic limit with boundaries





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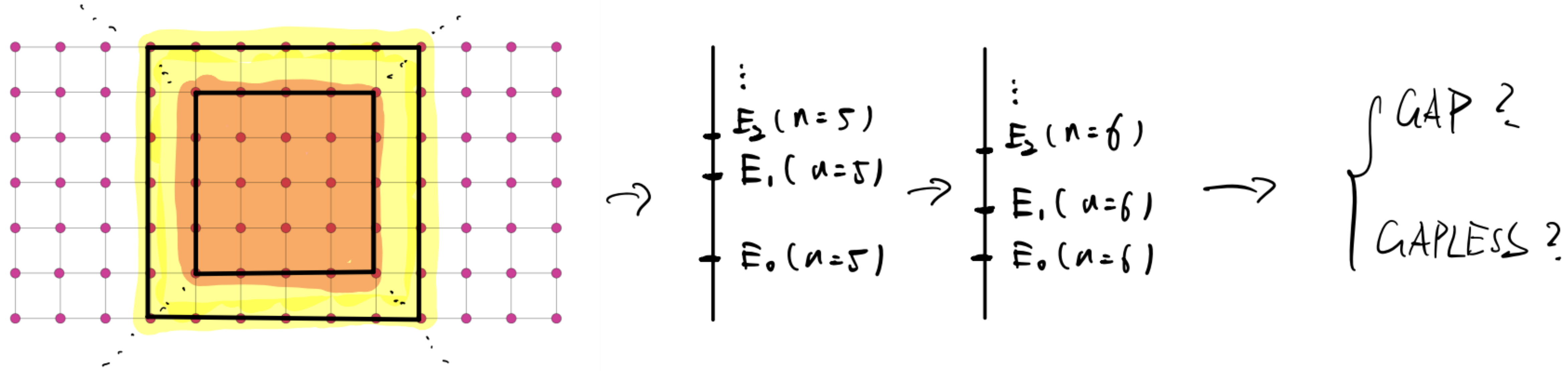

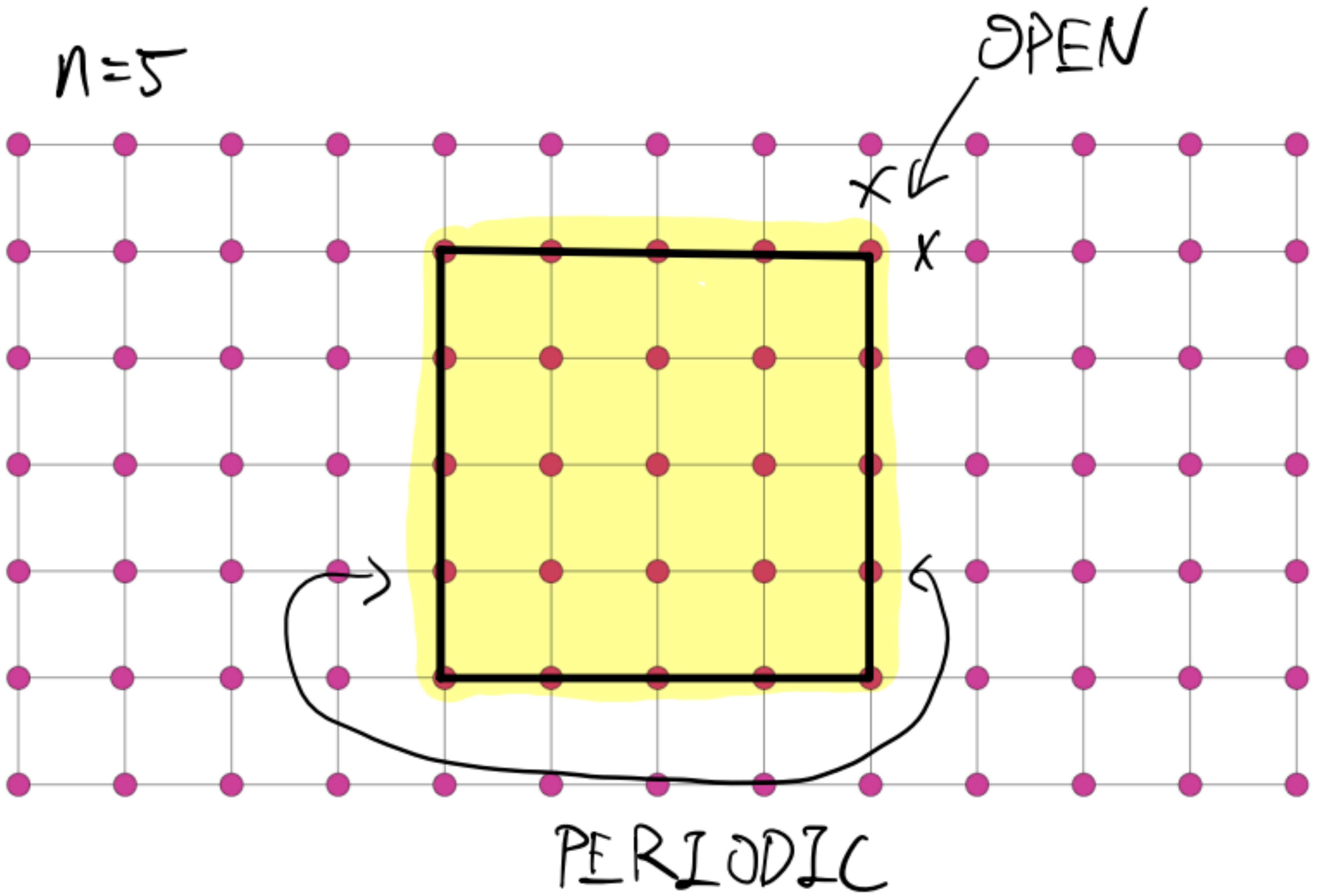

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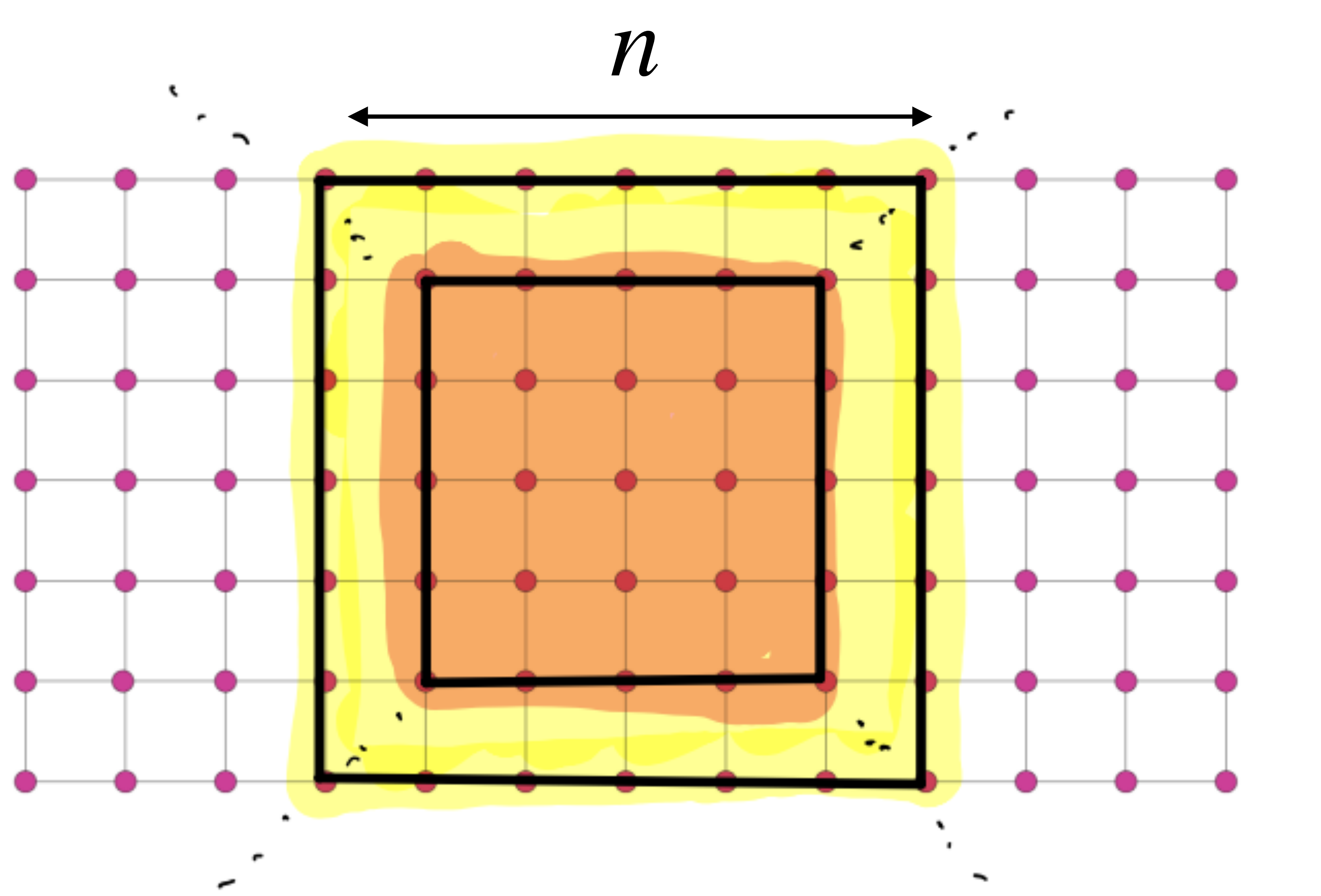
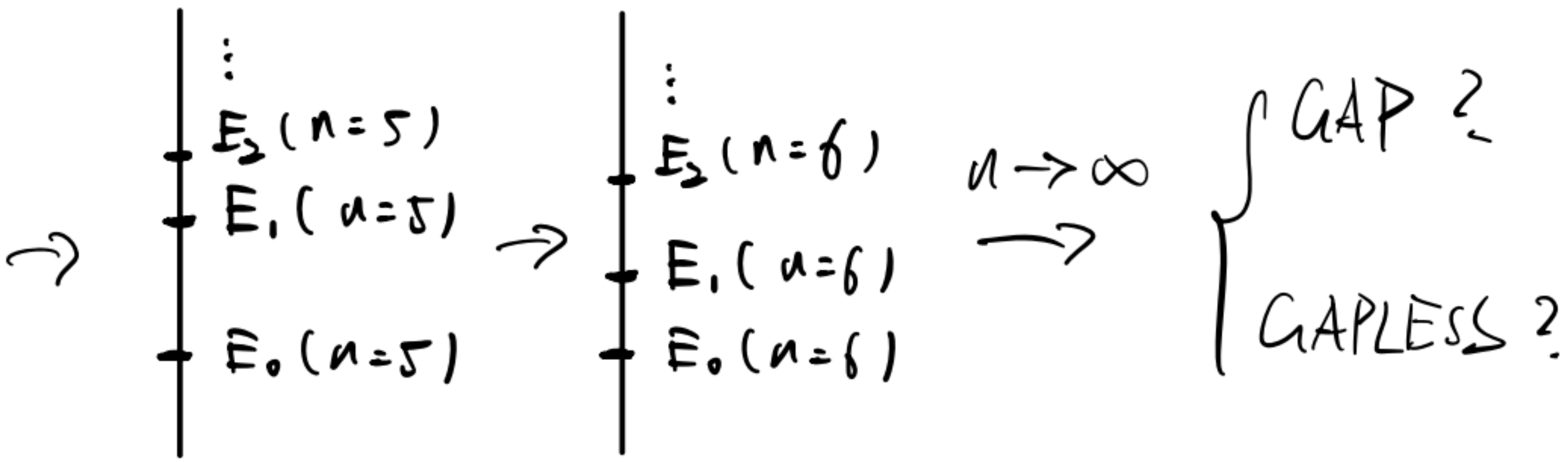
Different boundary conditions may change the properties of ρ^n_{GS} and $\Delta_n(H)$ as $n \to \infty$

Undecidability of spectral gap





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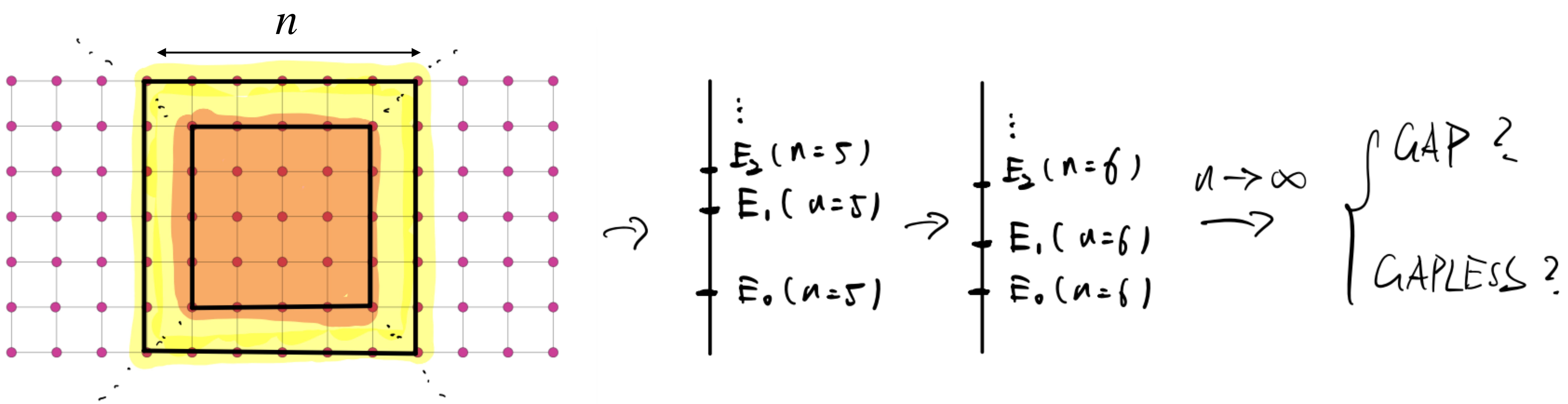

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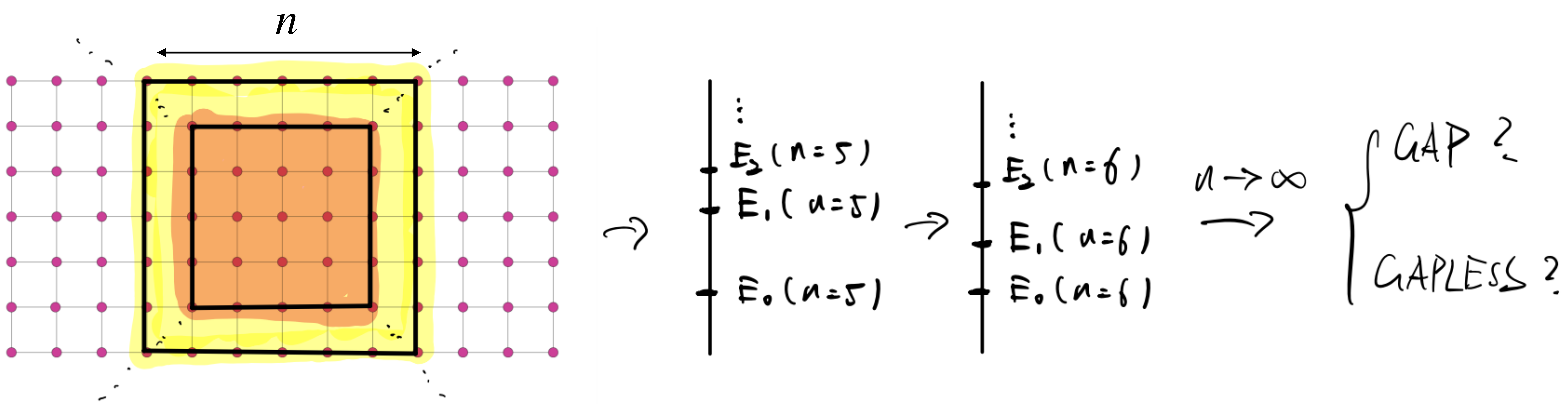

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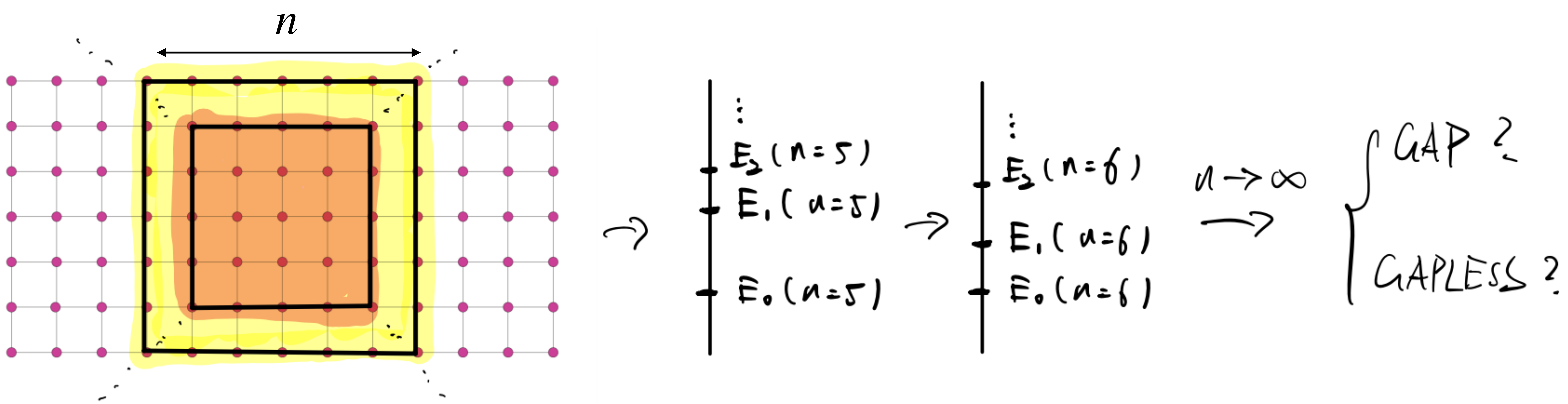

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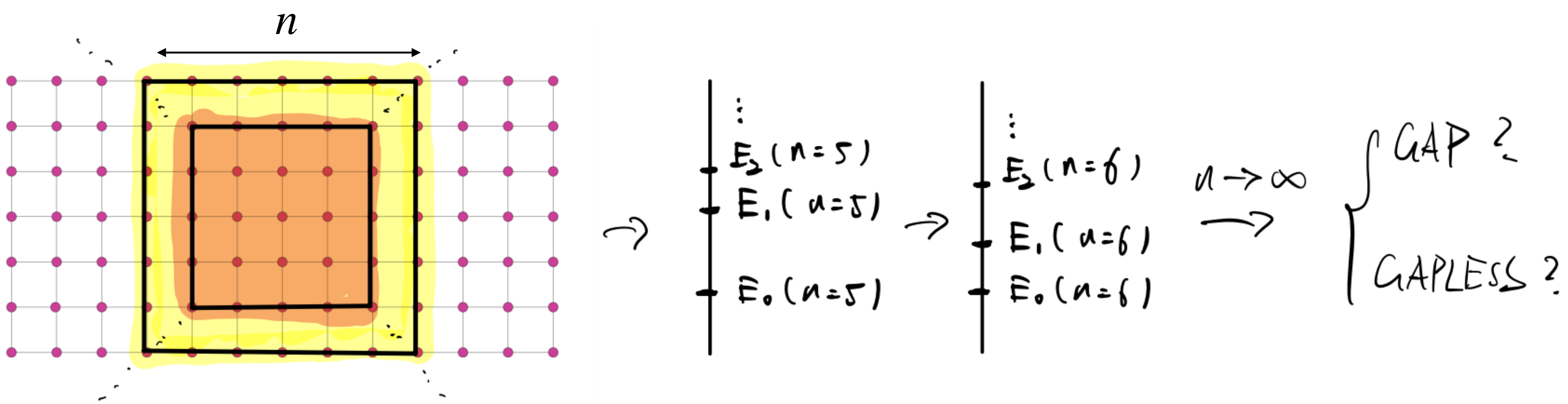

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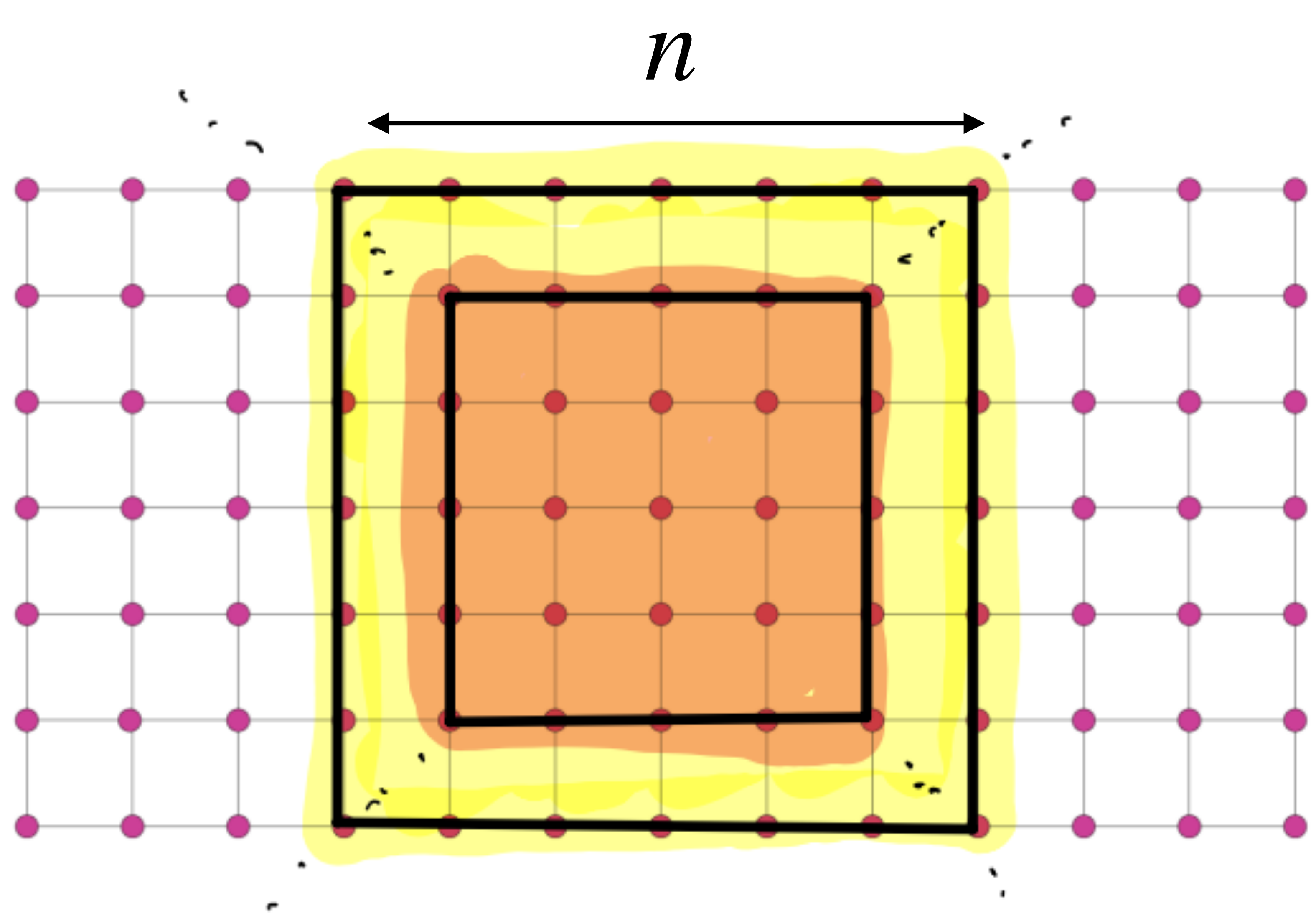

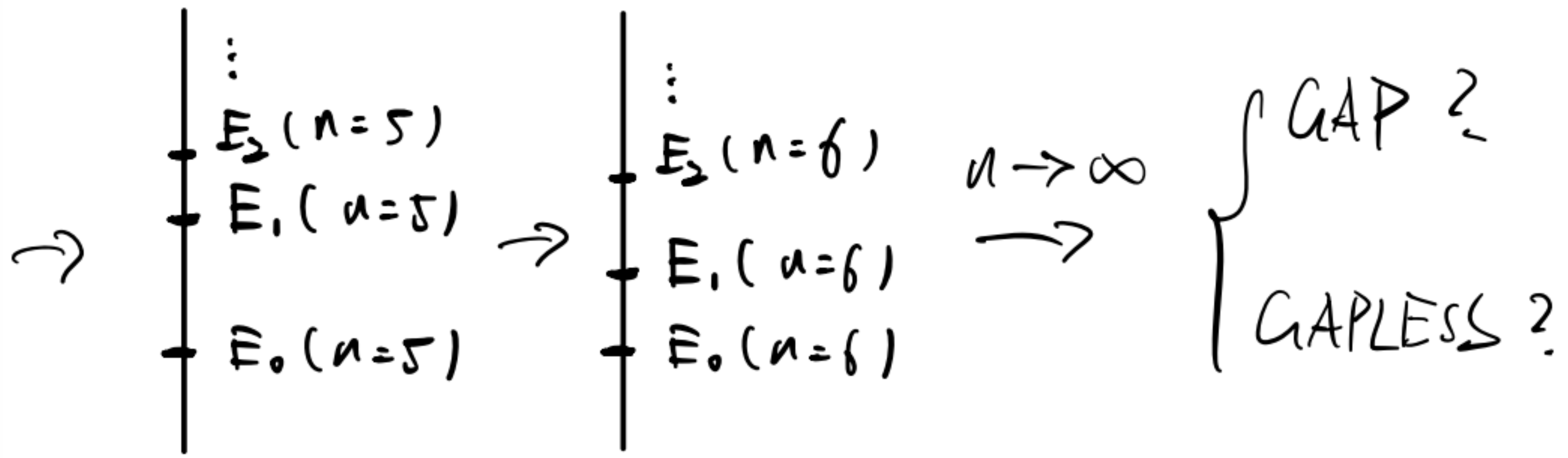

So thermodynamic limit does not even make sense for generic Hamiltonians?

• … $H) =$ …

• Difficult, as $E_0(n), E_1(n) \to \infty$

• CPW15: for H in $2D$ lattice with open boundary condition:

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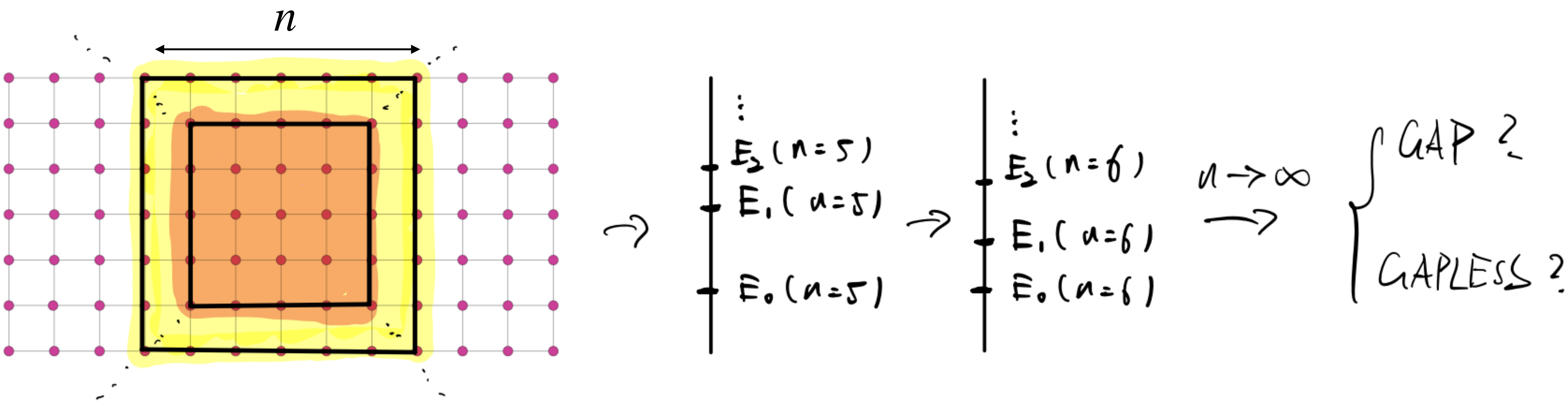
Thermodynamic limit with boundaries is a bad definition?



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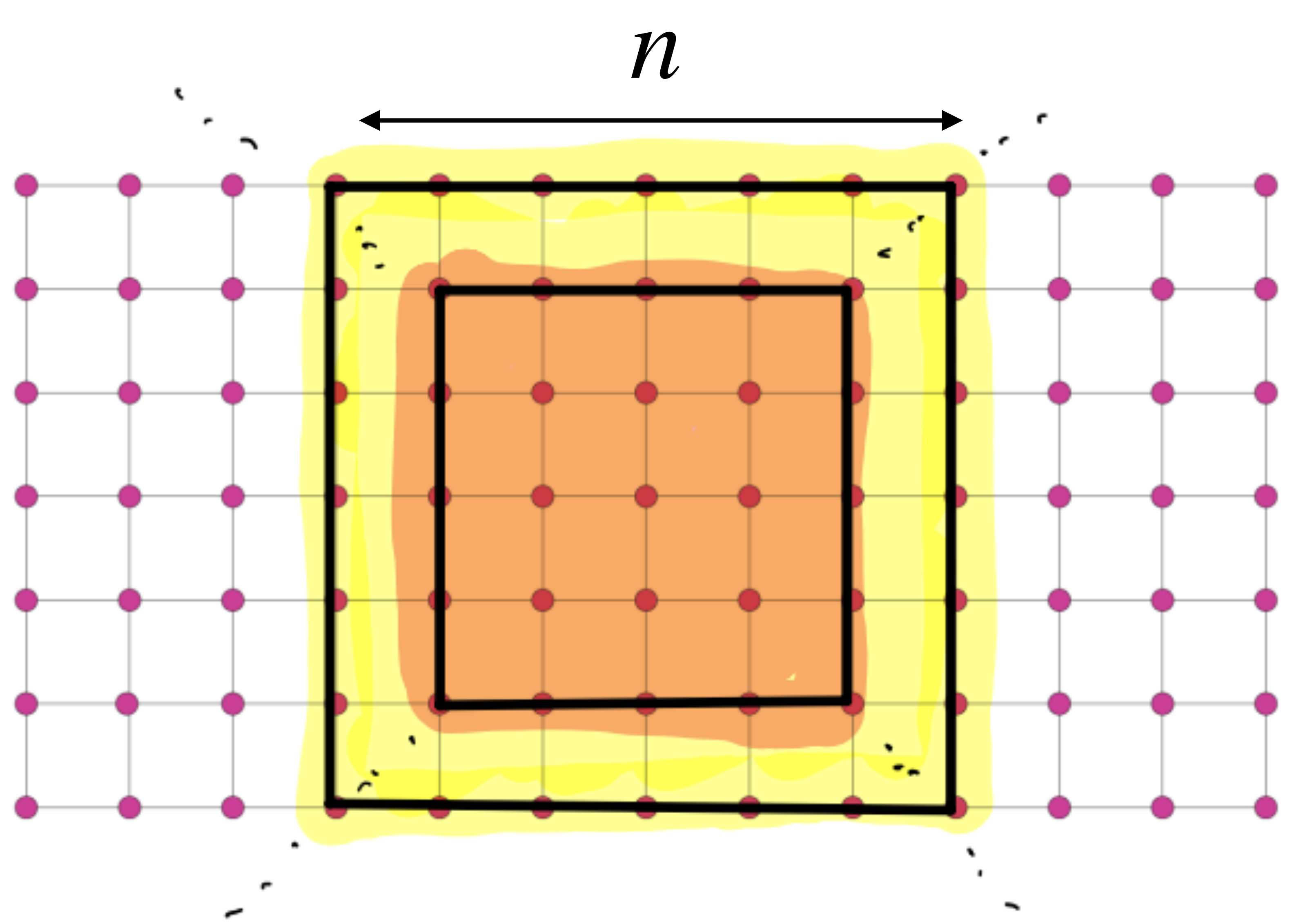
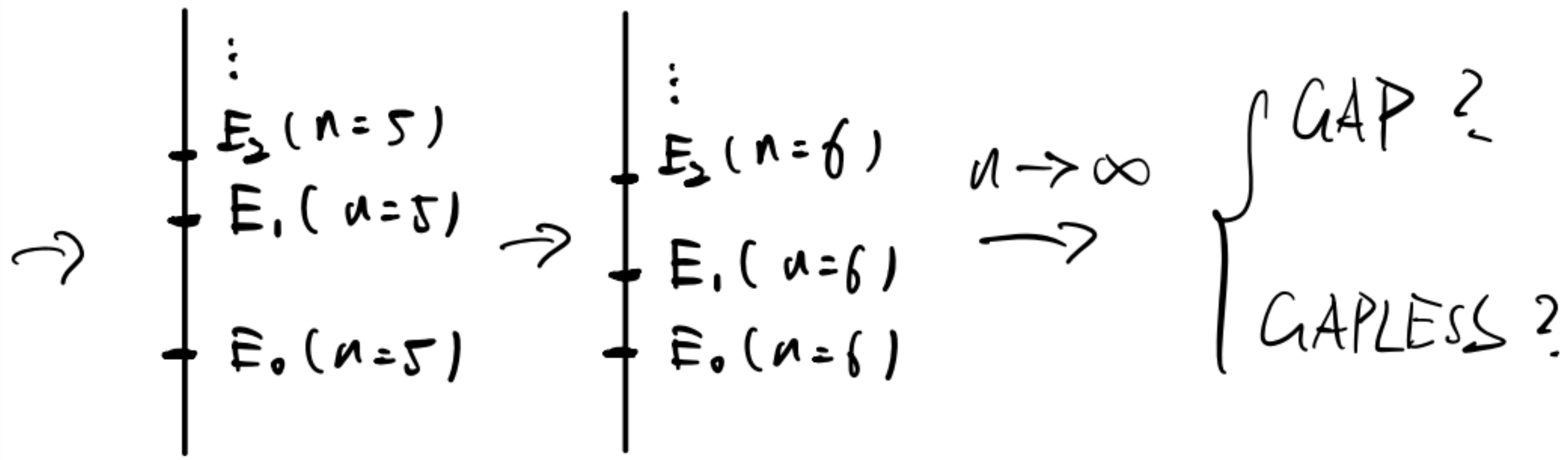
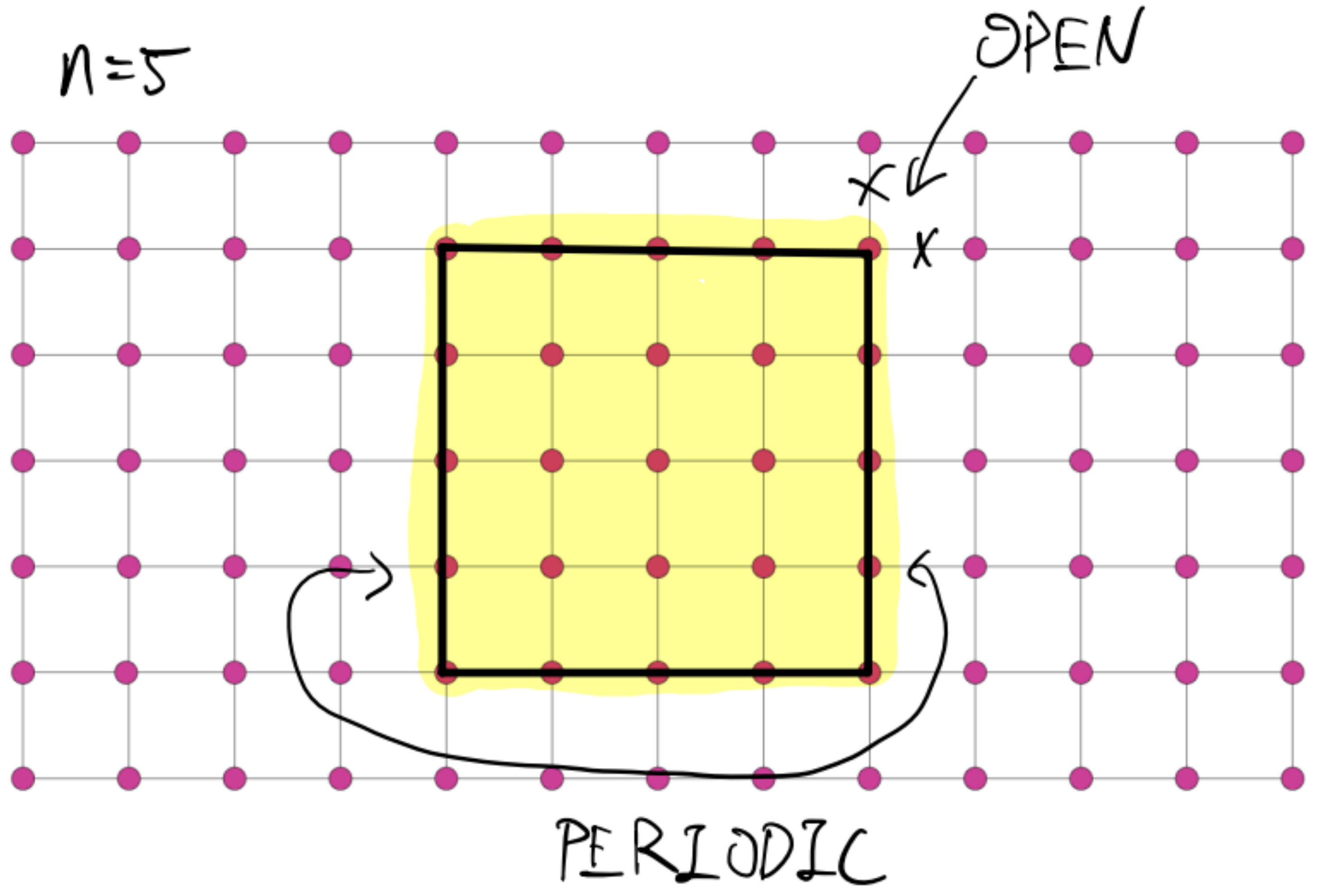




- Sensitive to boundary conditions:



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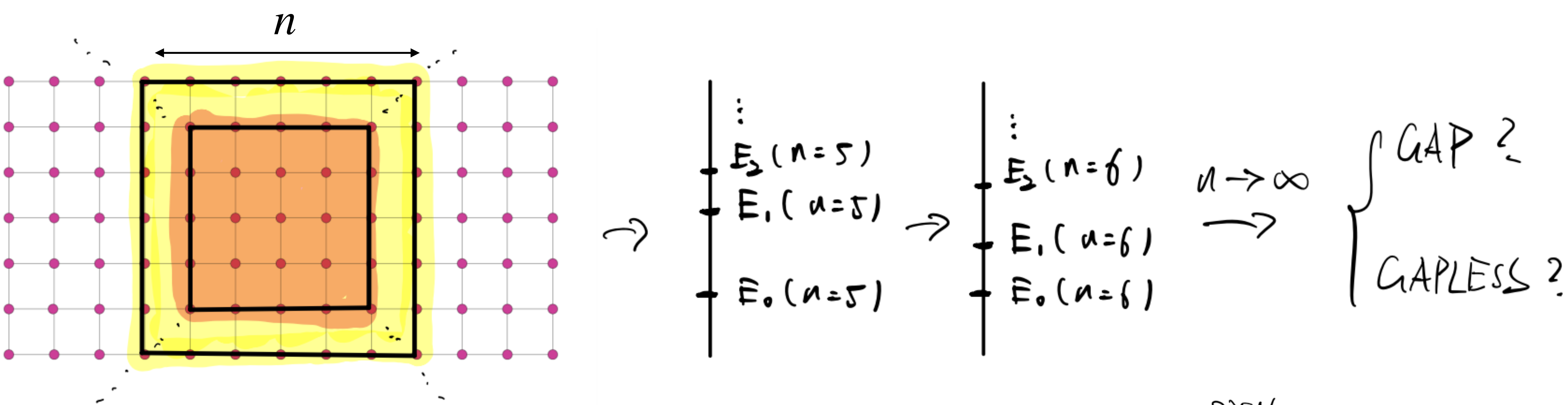
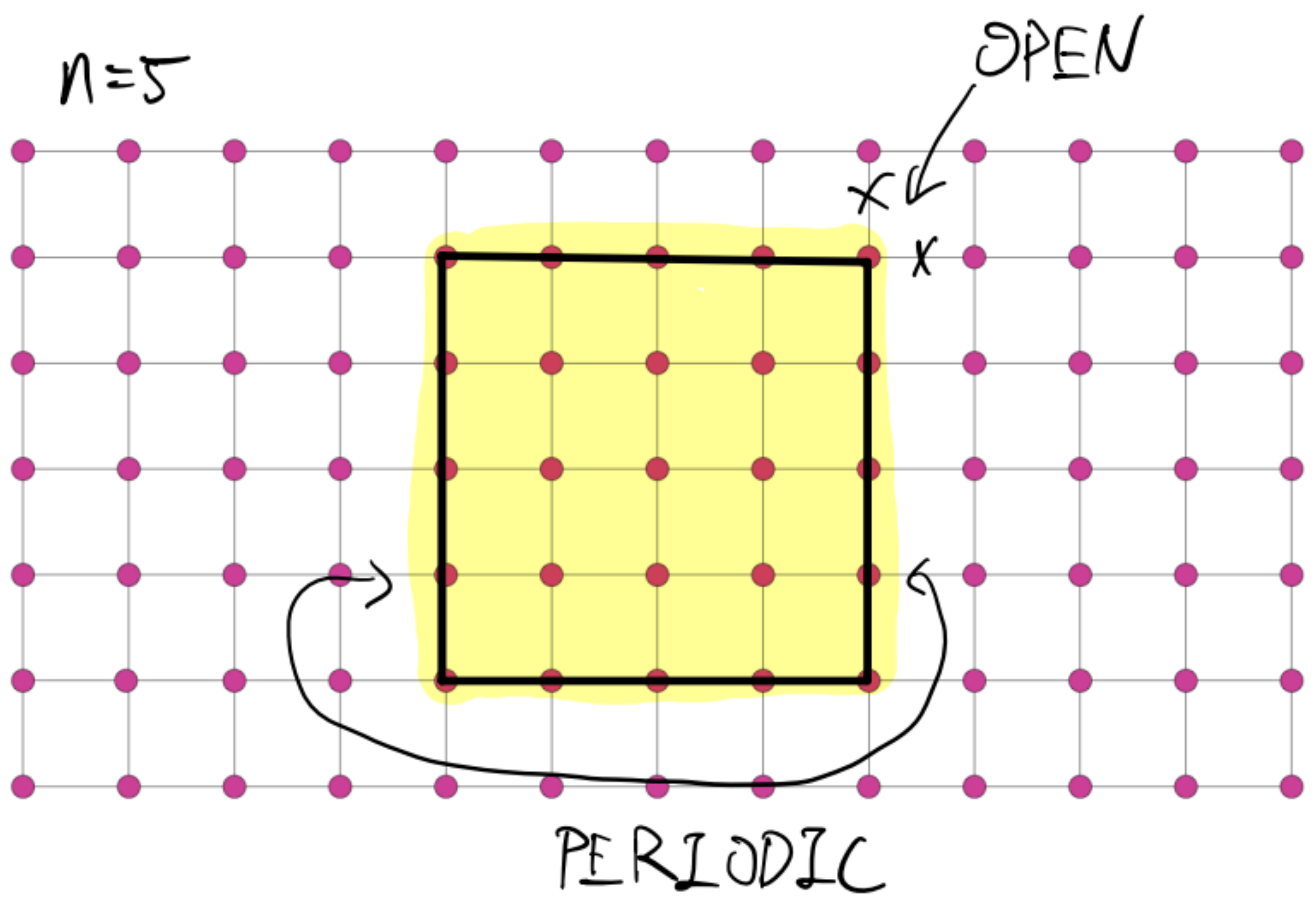


- Sensitive to boundary conditions:
- Can we capture only the *bulk* properties away from boundary?



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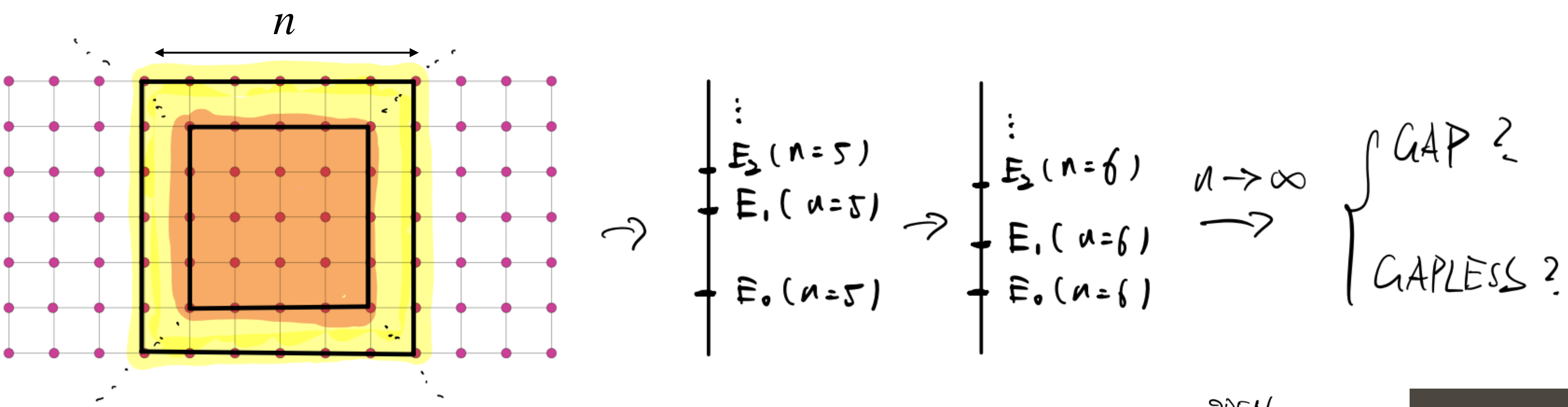

- Sensitive to boundary conditions:
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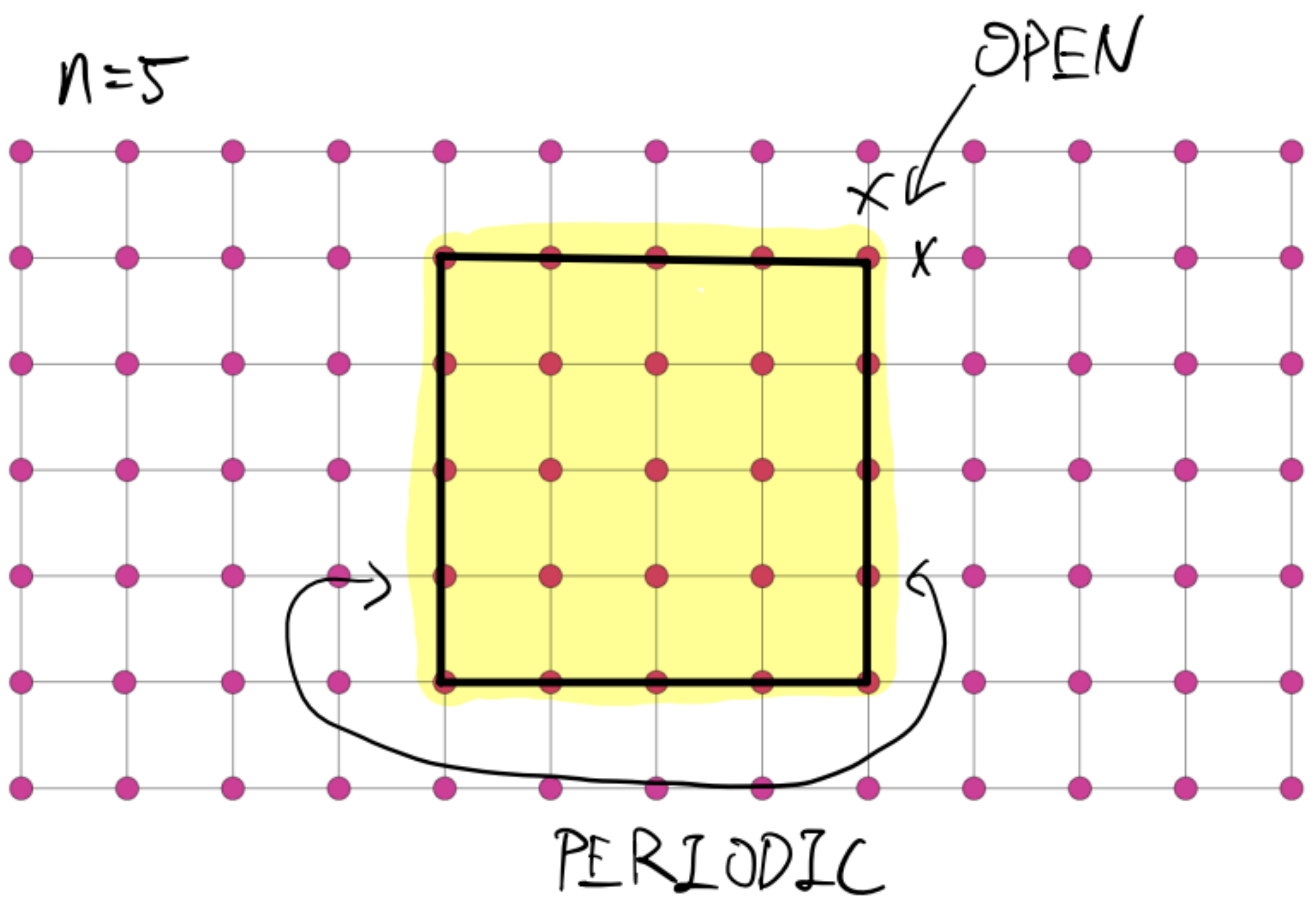
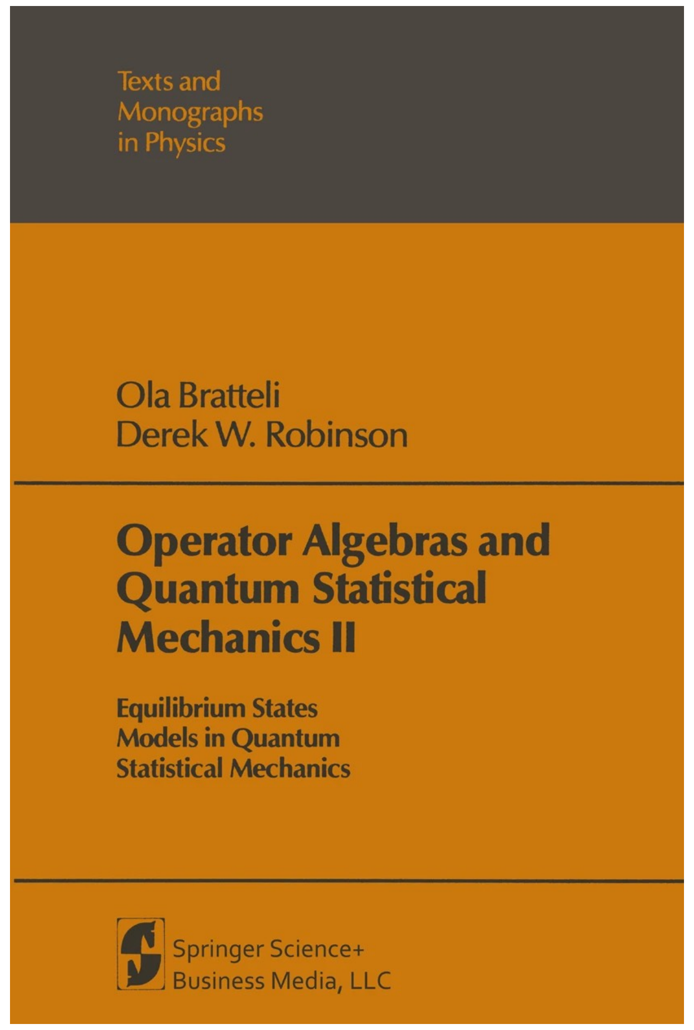
- Yes with operator algebras





Certifying ground-state properties of quantum many-body systems

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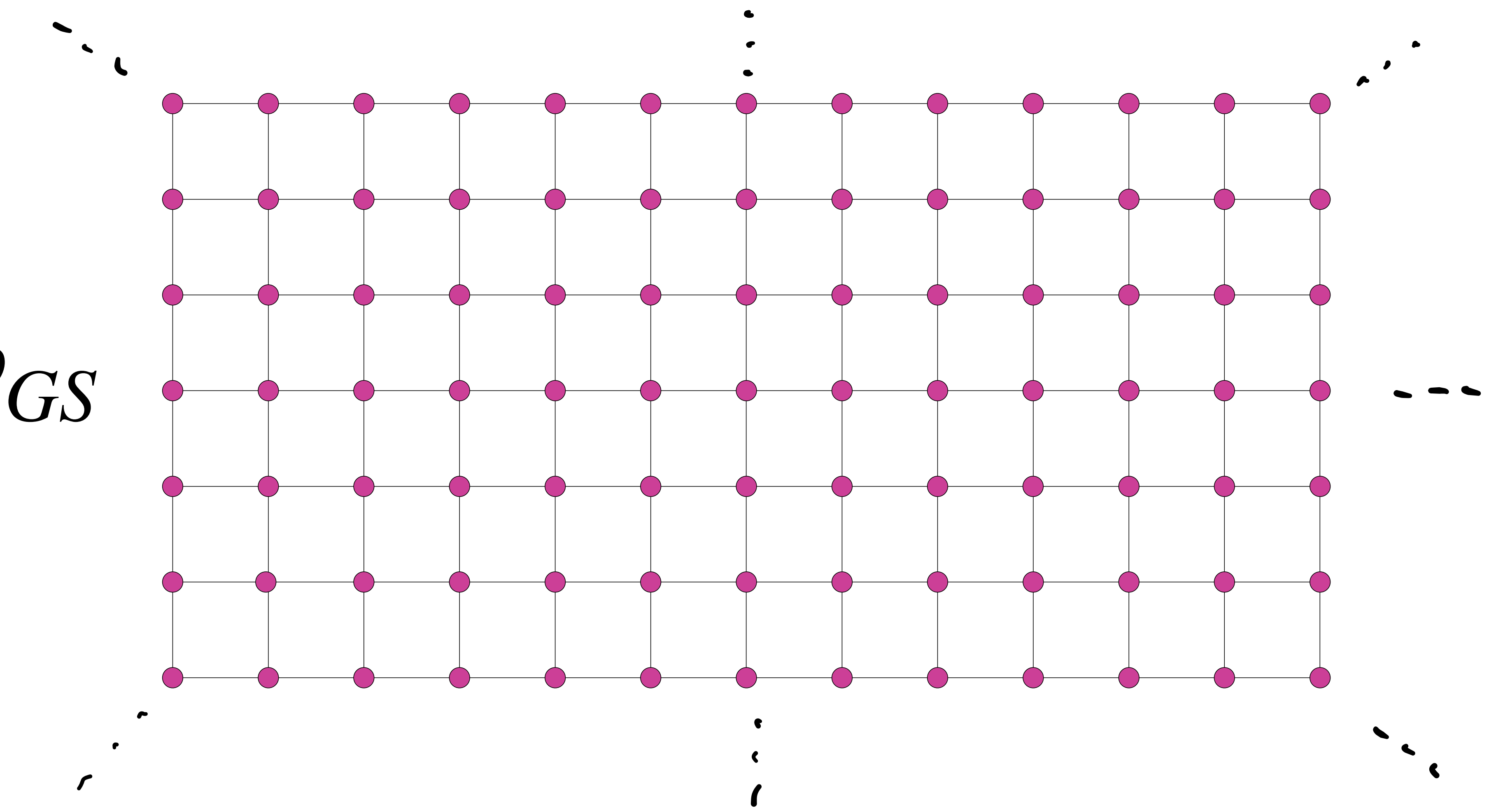
2. Finite systems
3. Thermodynamic limit with boundaries
4. **Thermodynamic limit: the bulk**

Alternative definition of ground states in thermodynamic limit

ρ_{GS}



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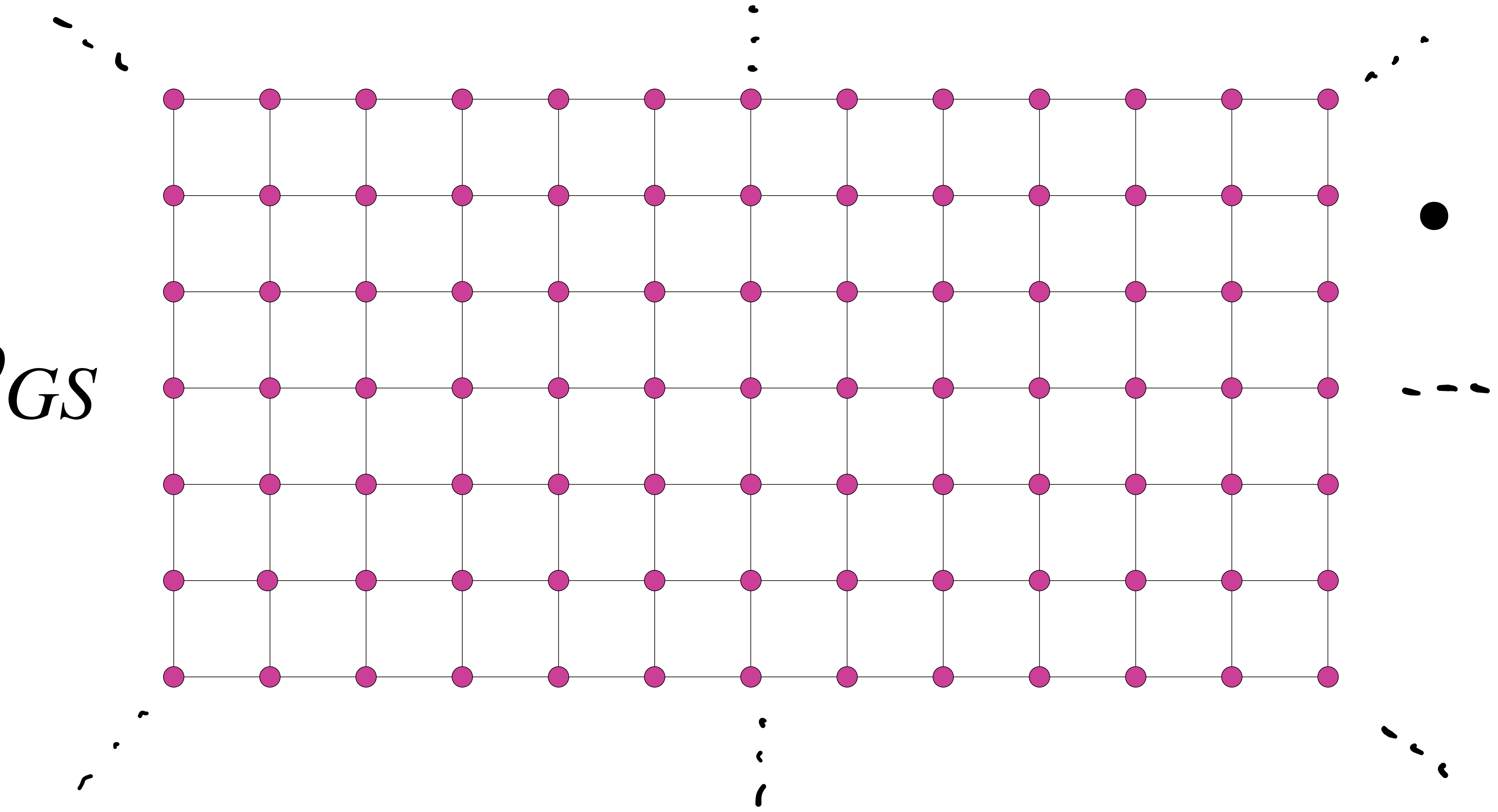

- A ground state ρ_{GS} must increase energy with any excitations

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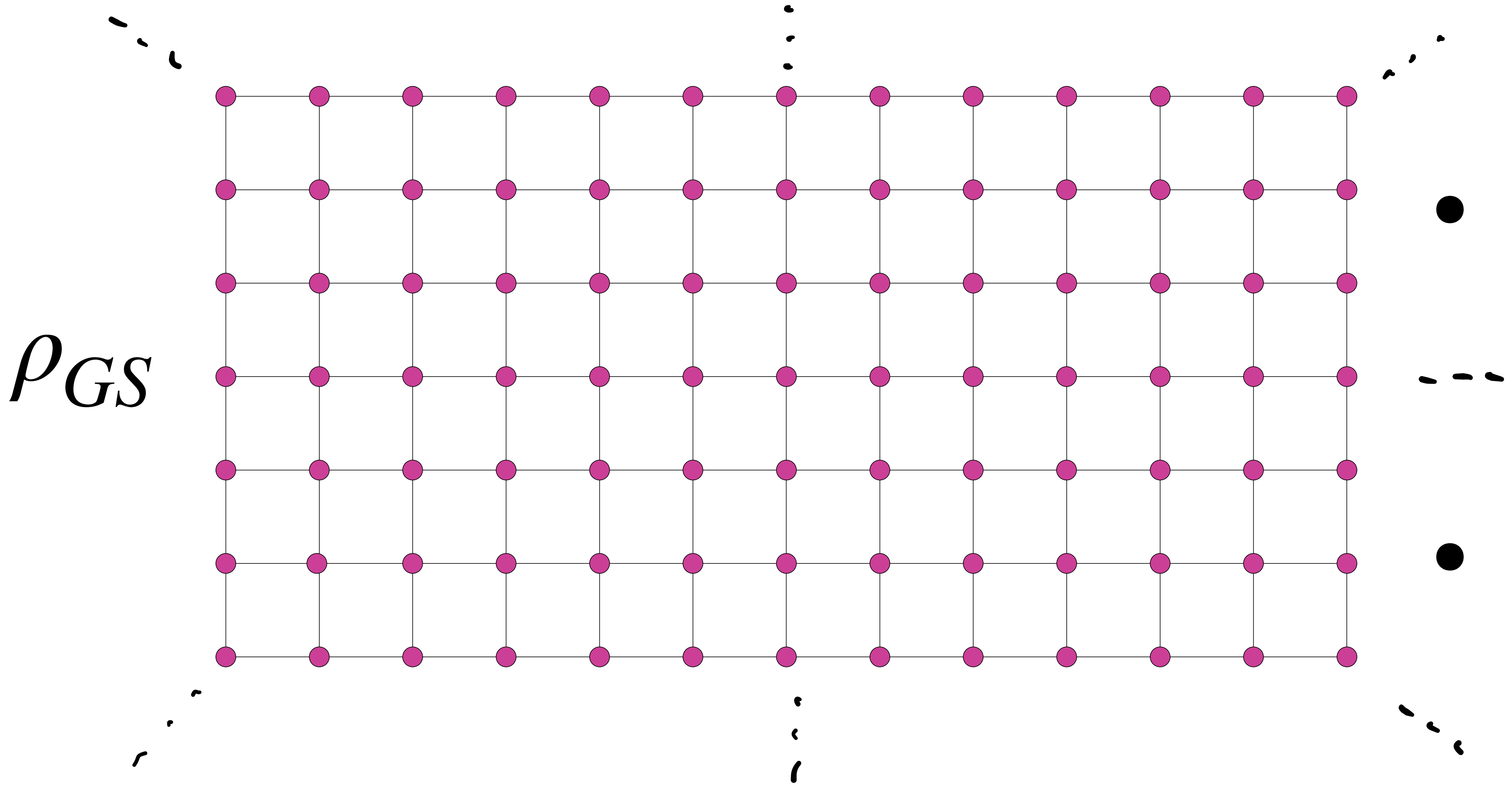

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$a = X_i Z_j, X_{i_1} Z_{i_2} \cdots Y_{i_d}, \ldots$

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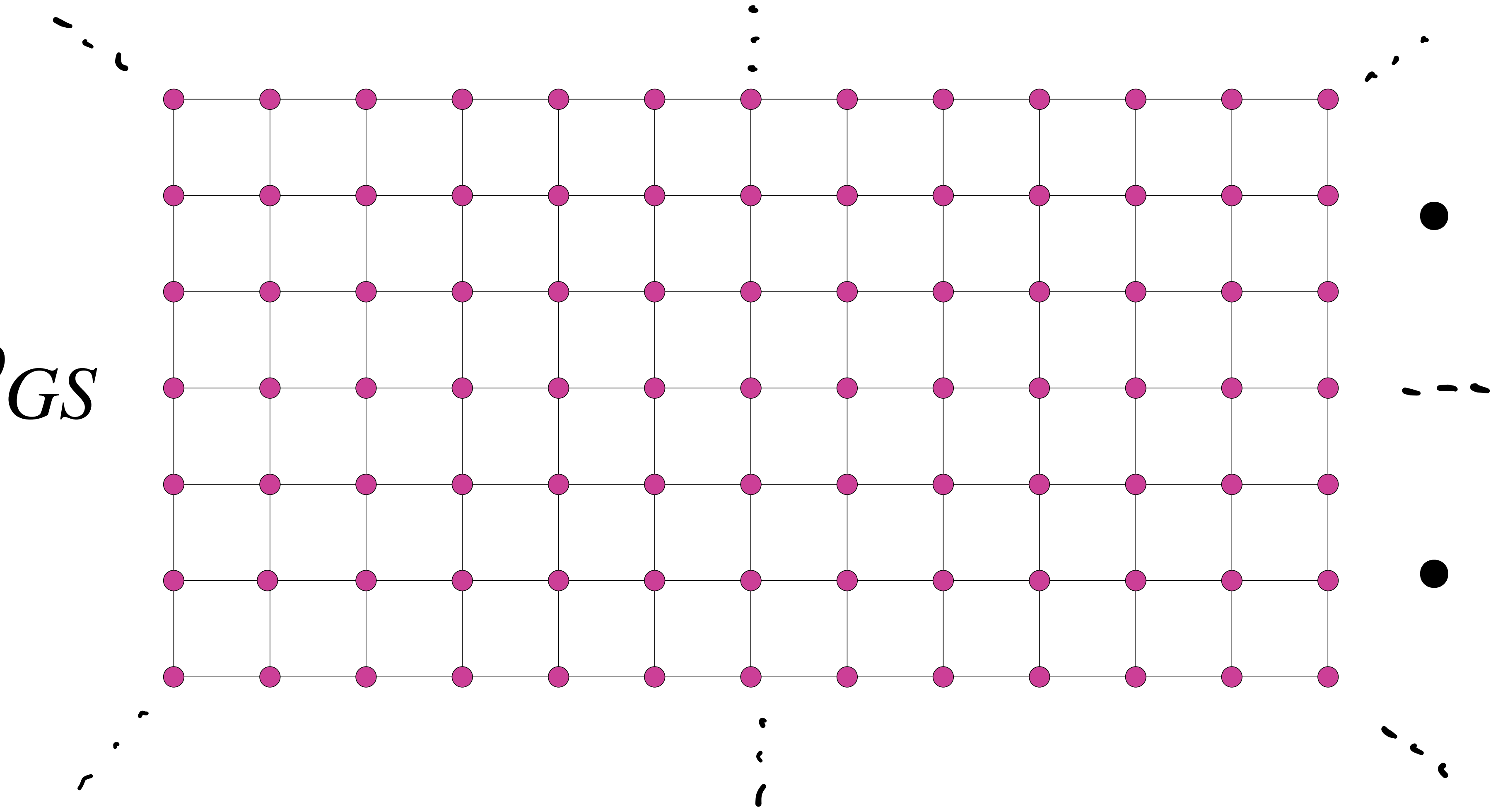
ρ_{GS} 

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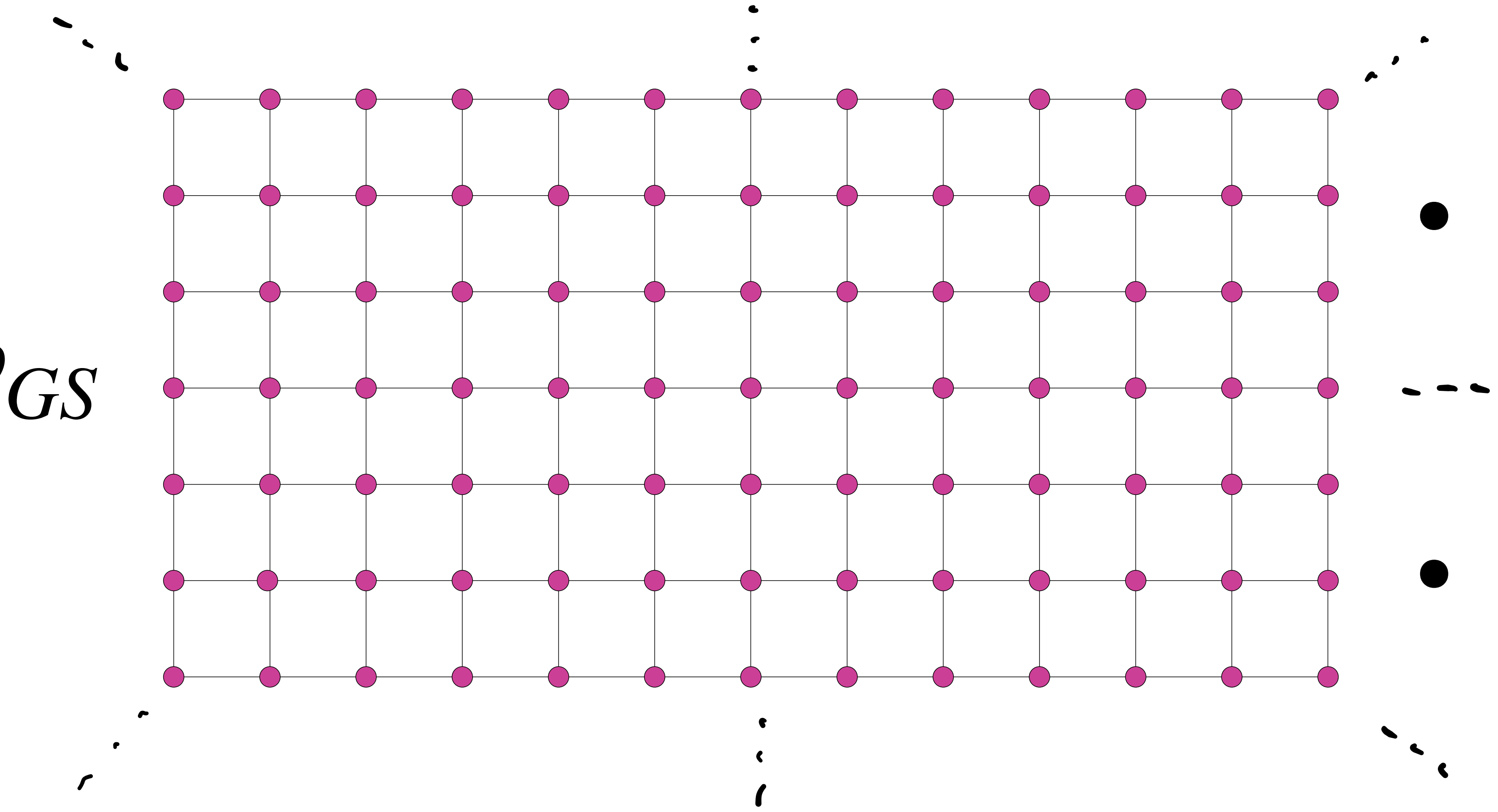

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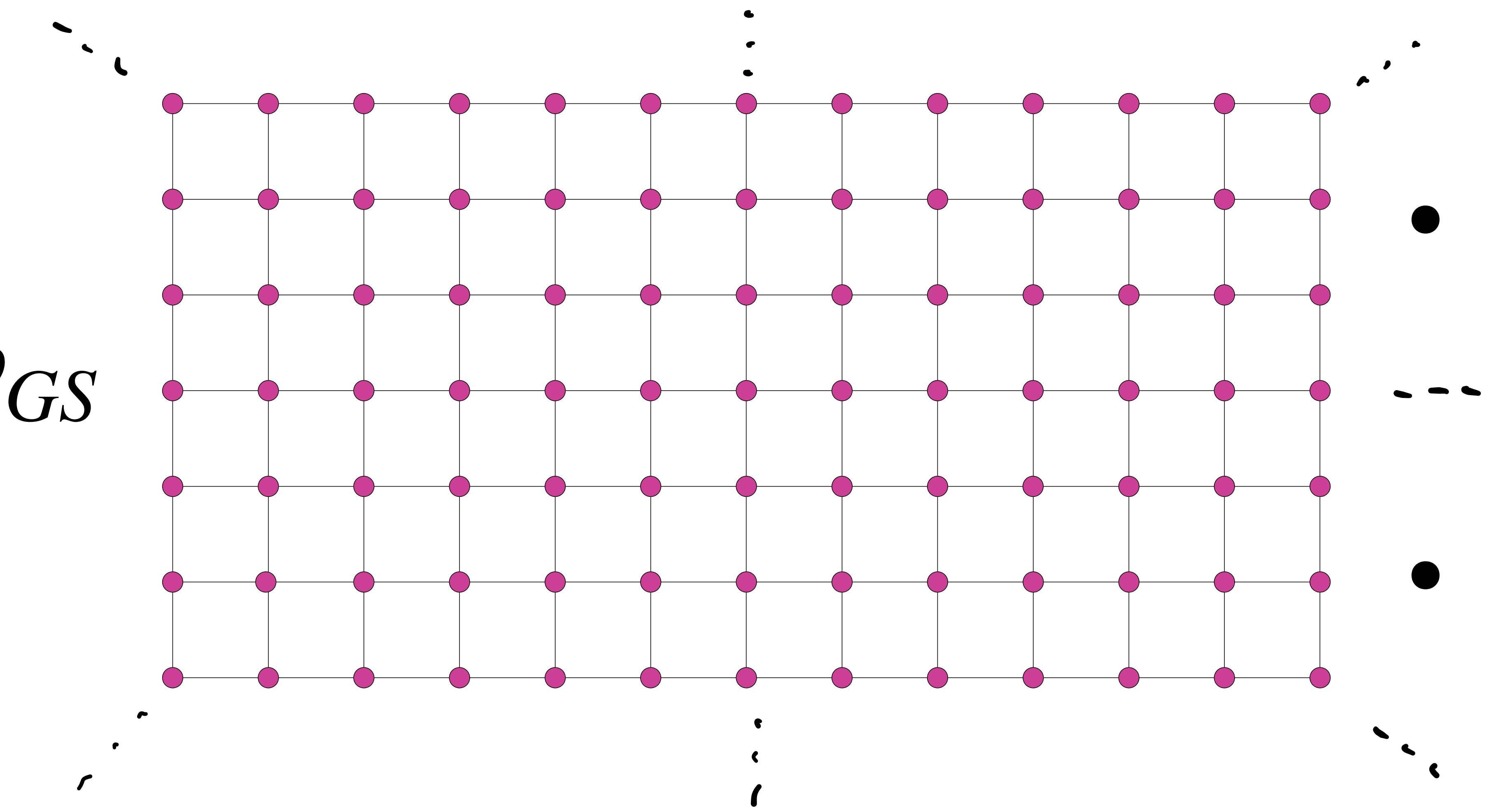

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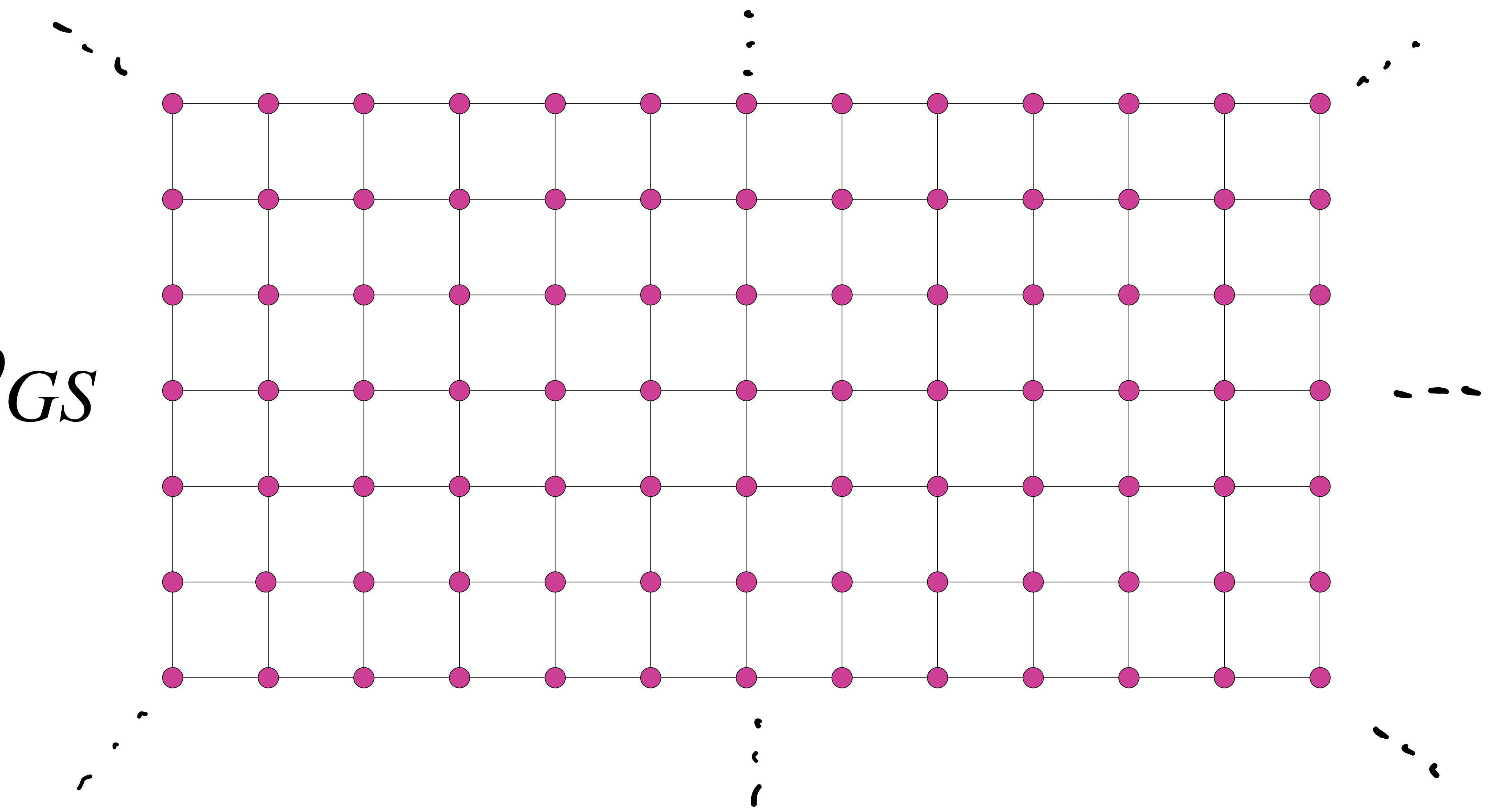
- Varying local $a \in \mathscr{A}$, $|\psi_a\rangle$ reaches all valid states

Bulk definition of ground states in thermodynamic limit

ρ_{GS}



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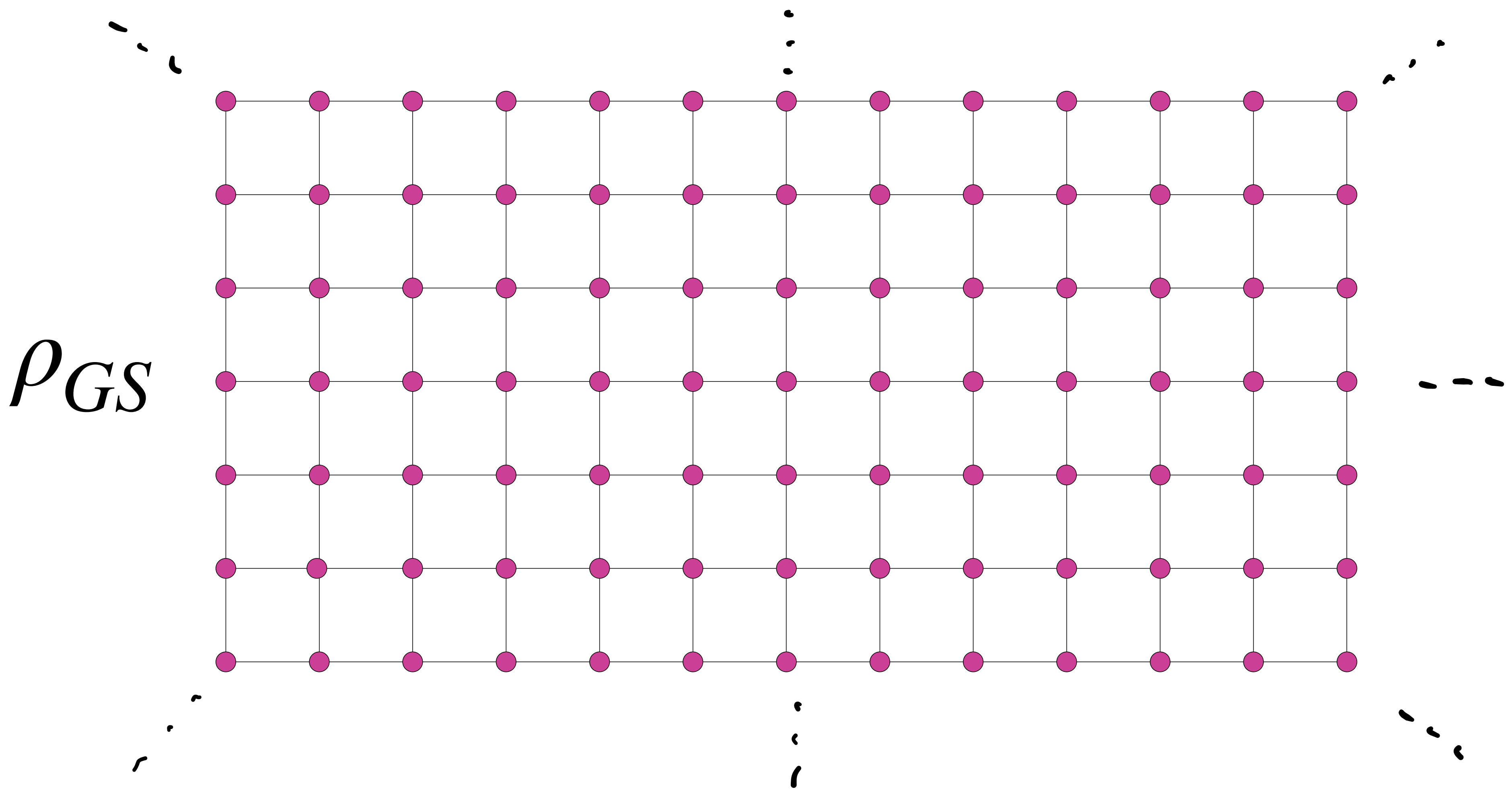

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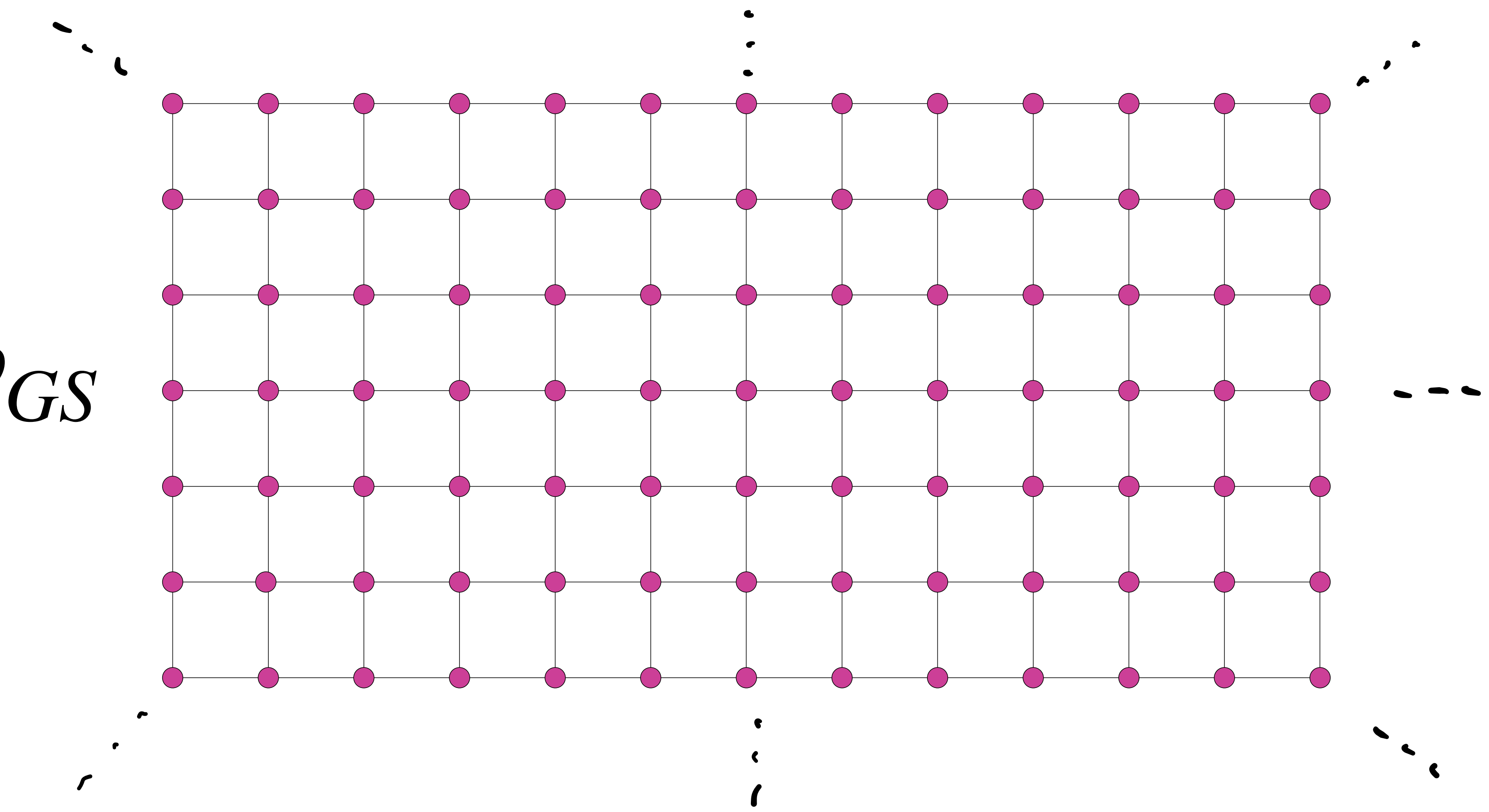

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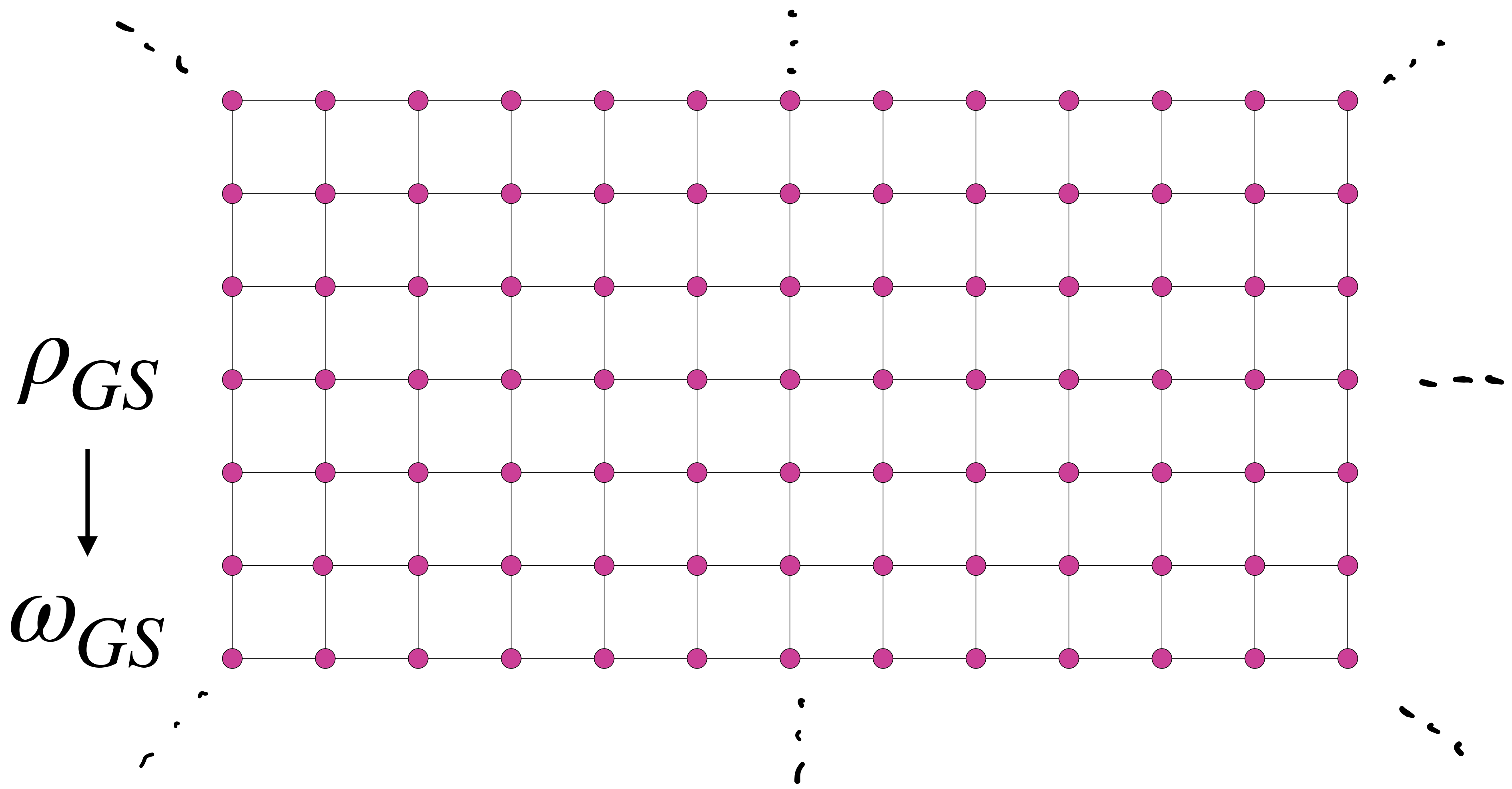

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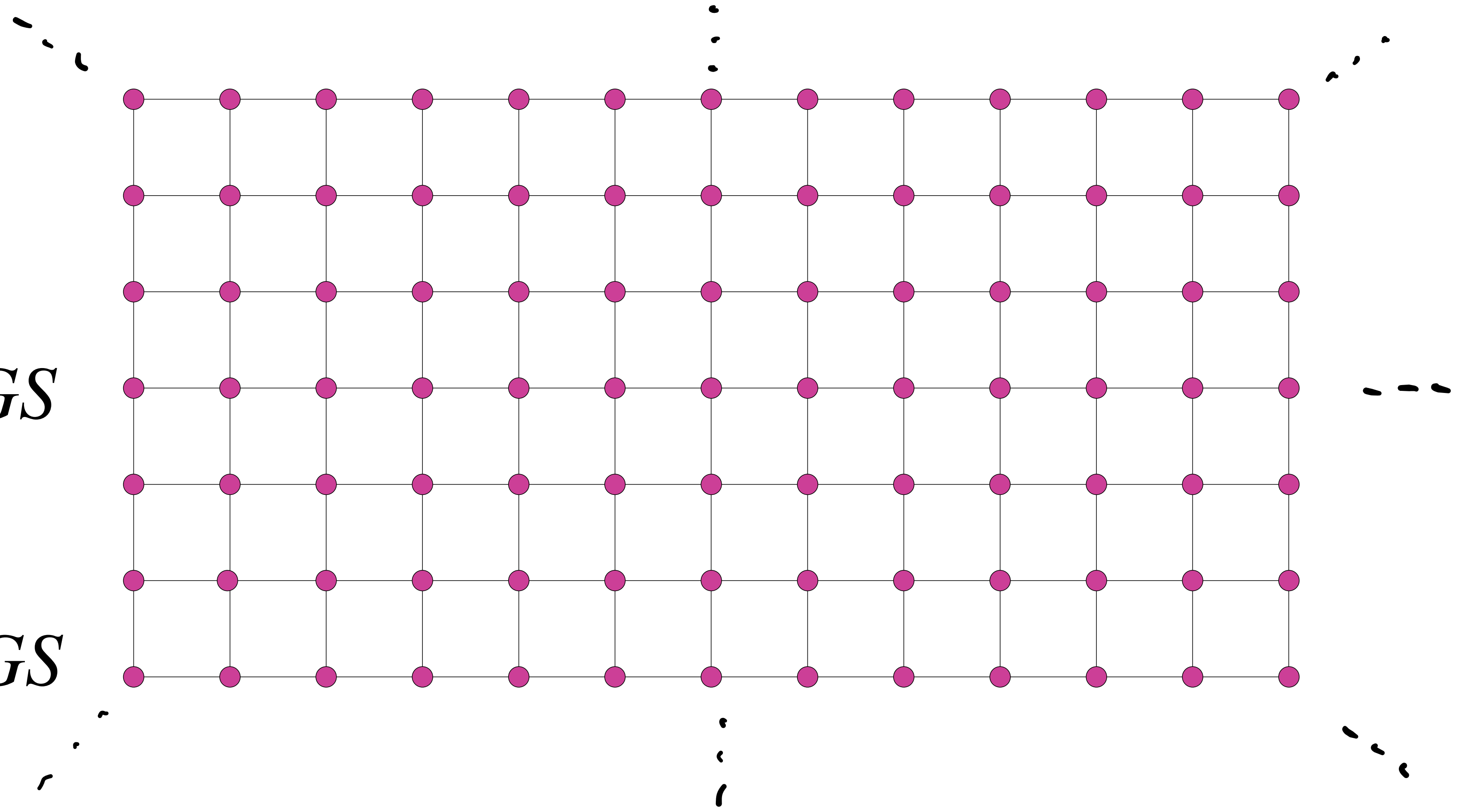

ρ_{GS}
$\downarrow$
ω_{GS}

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- Kubo-Martin-Schwinger (KMS) ground state

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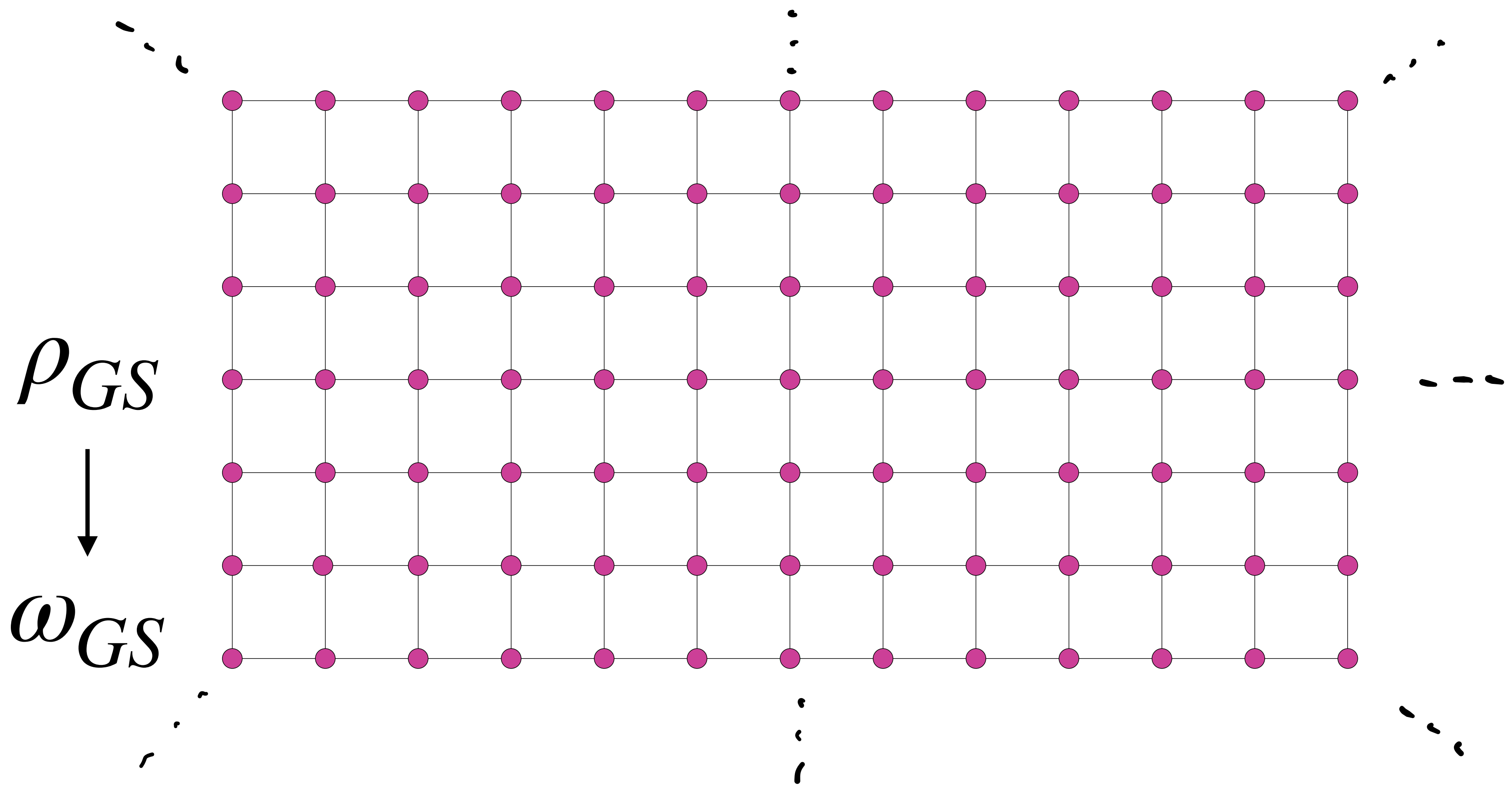

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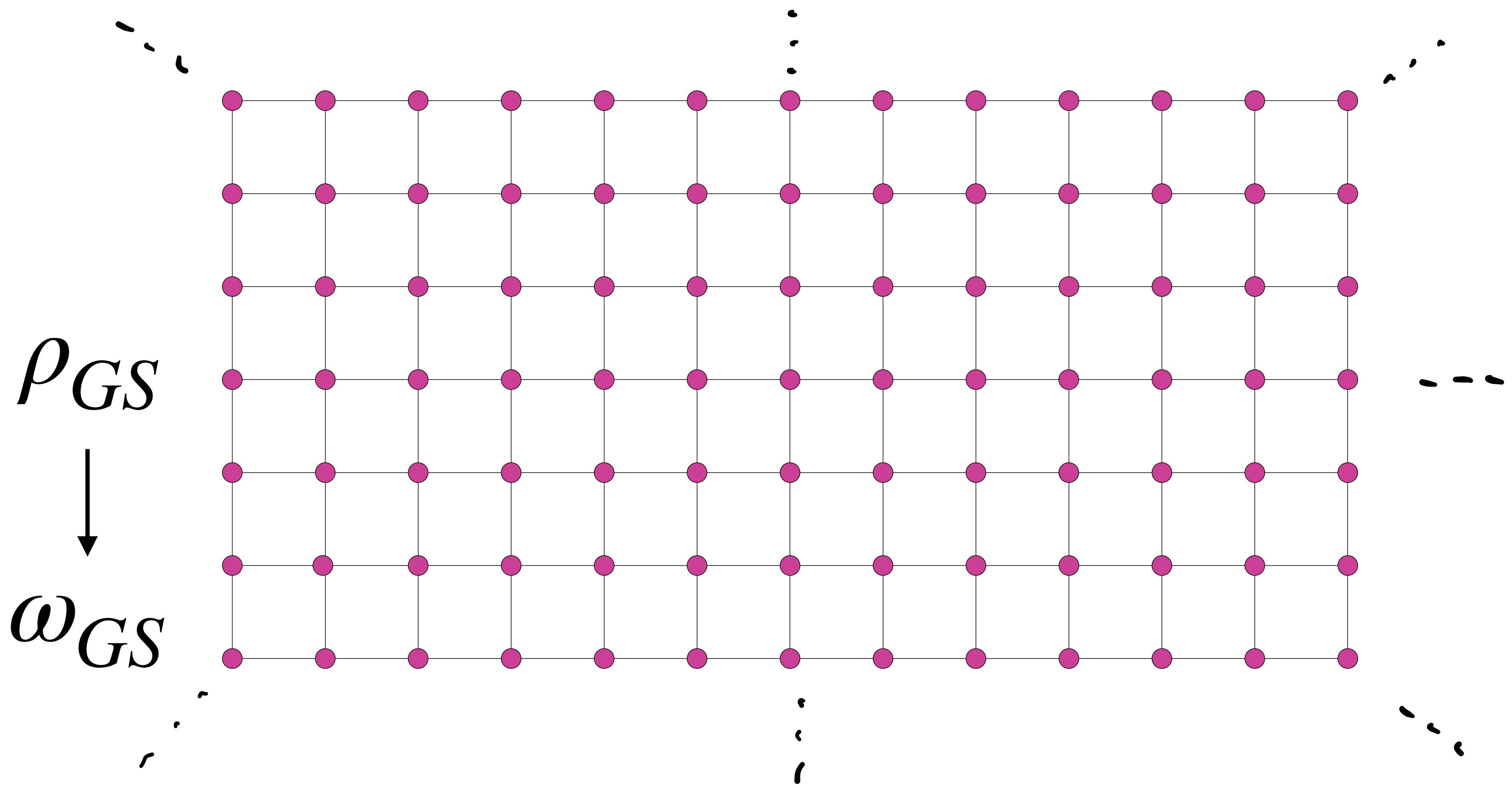

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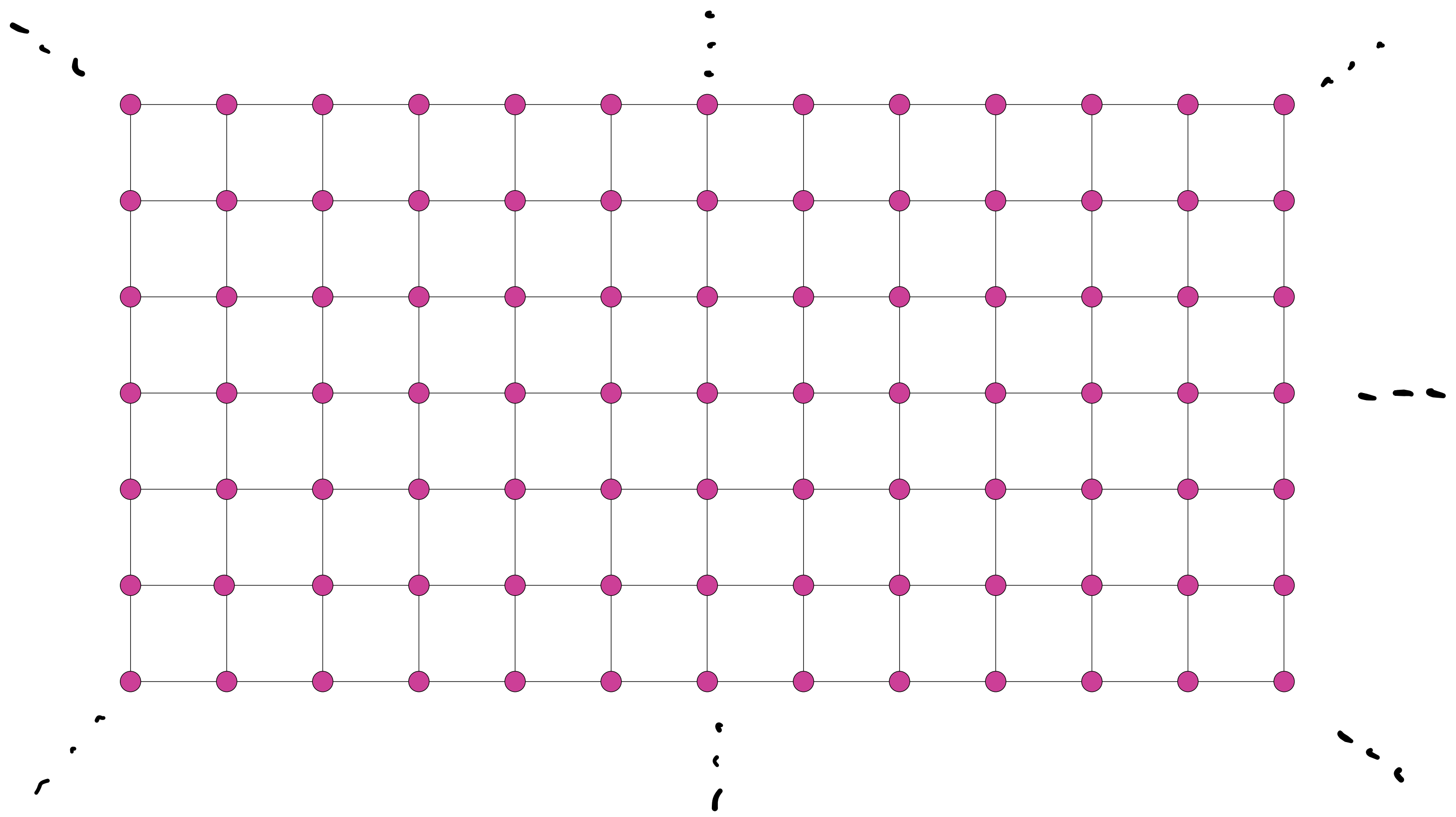
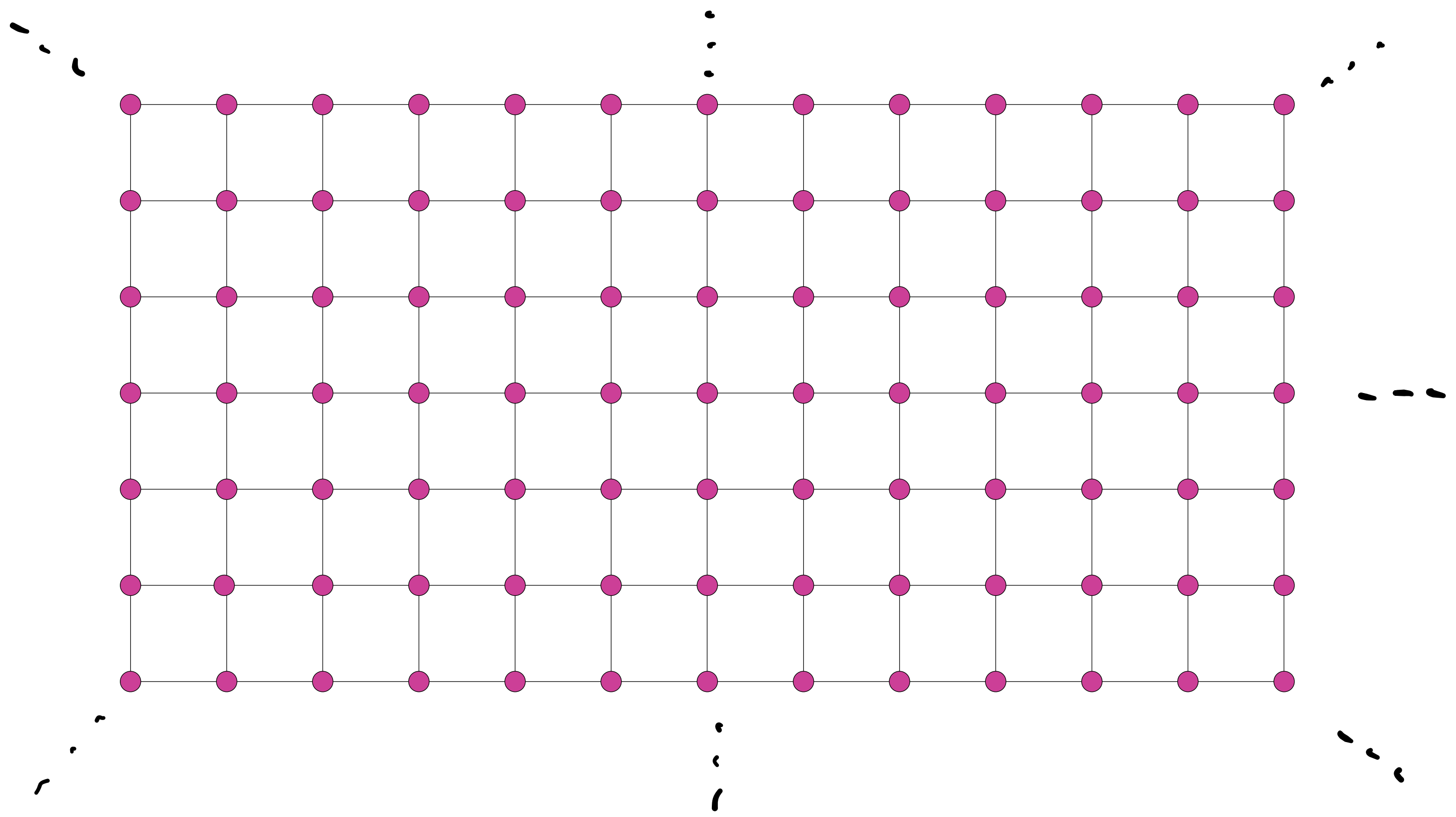
- ω_{GS} s.t. $\omega_{GS}(a^*[H, a]) \geq 0$, for all local $a \in \mathscr{A}$
- Directly in $n \to \infty$, no boundary term mentioned!

Bulk definition of spectral gaps in thermodynamic limit



Bulk definition of spectral gaps in thermodynamic limit



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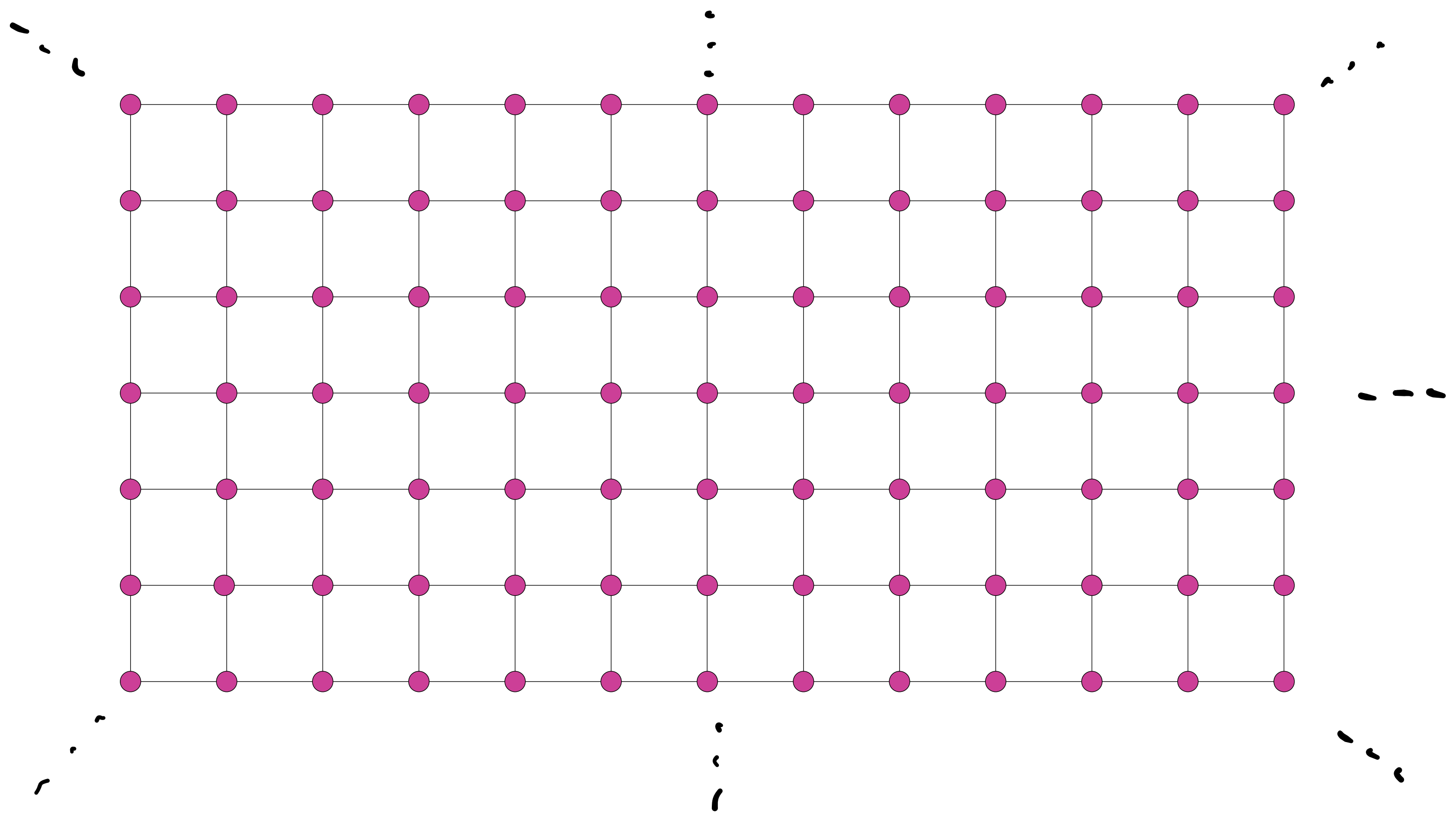

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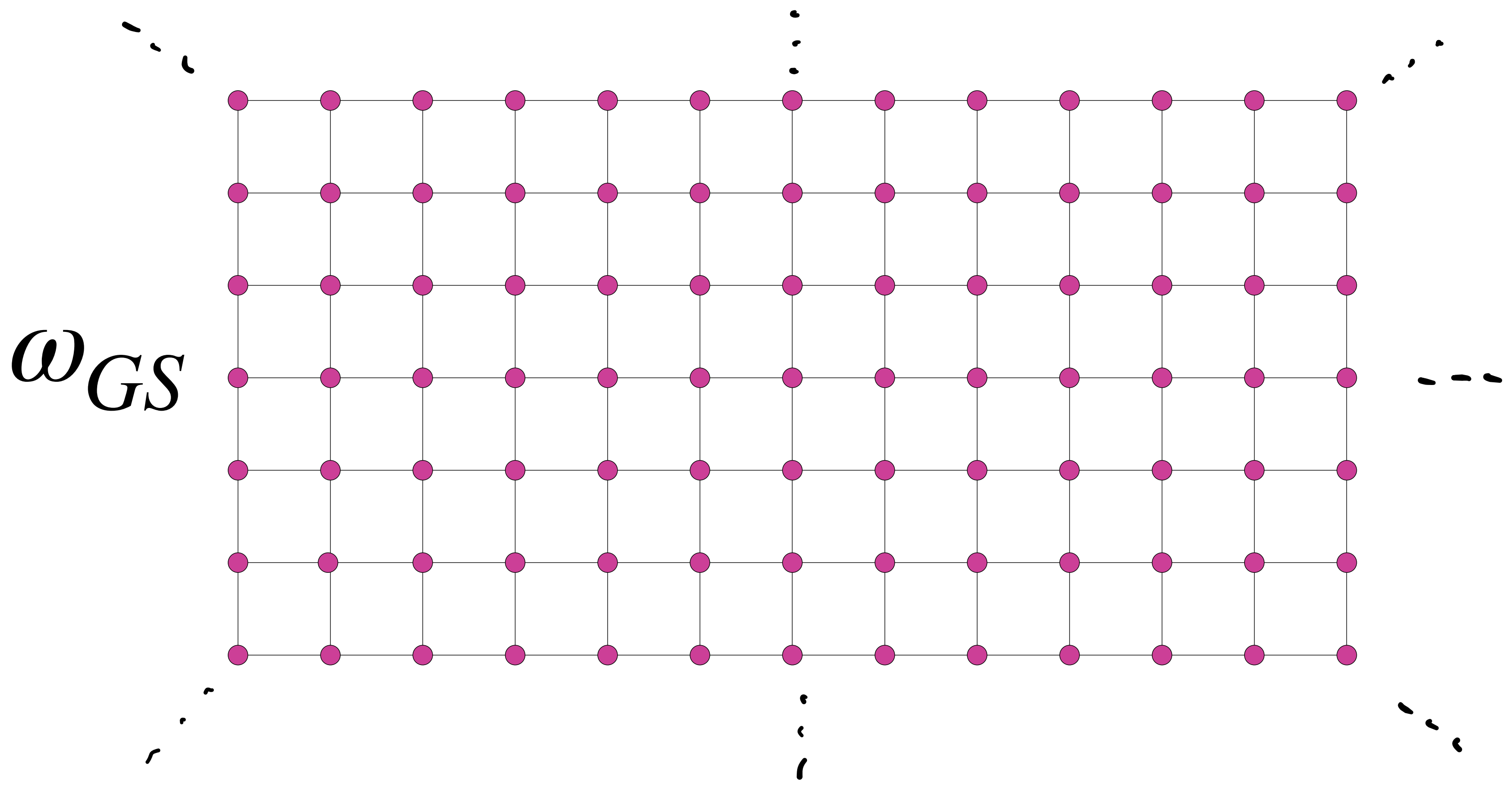

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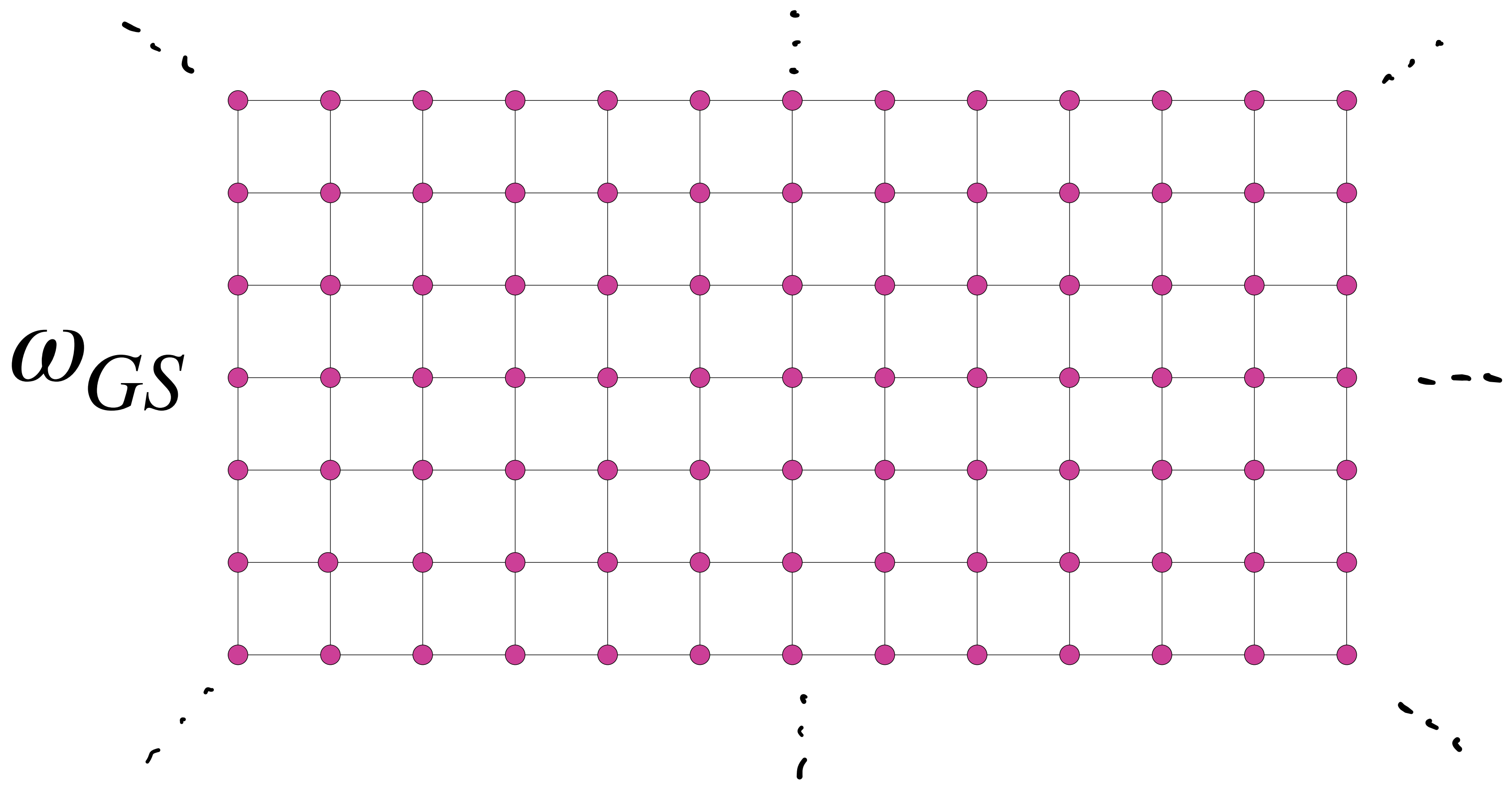

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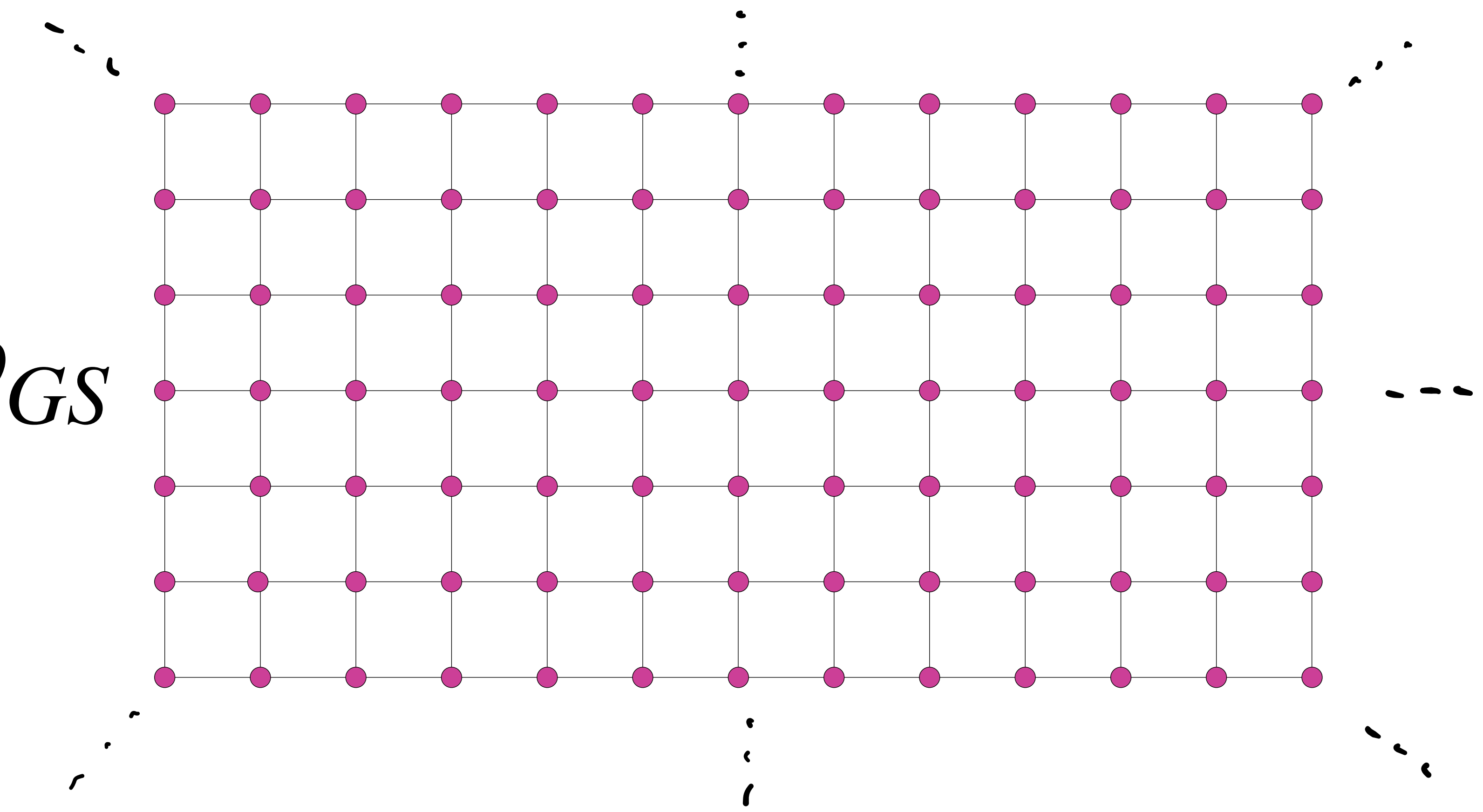

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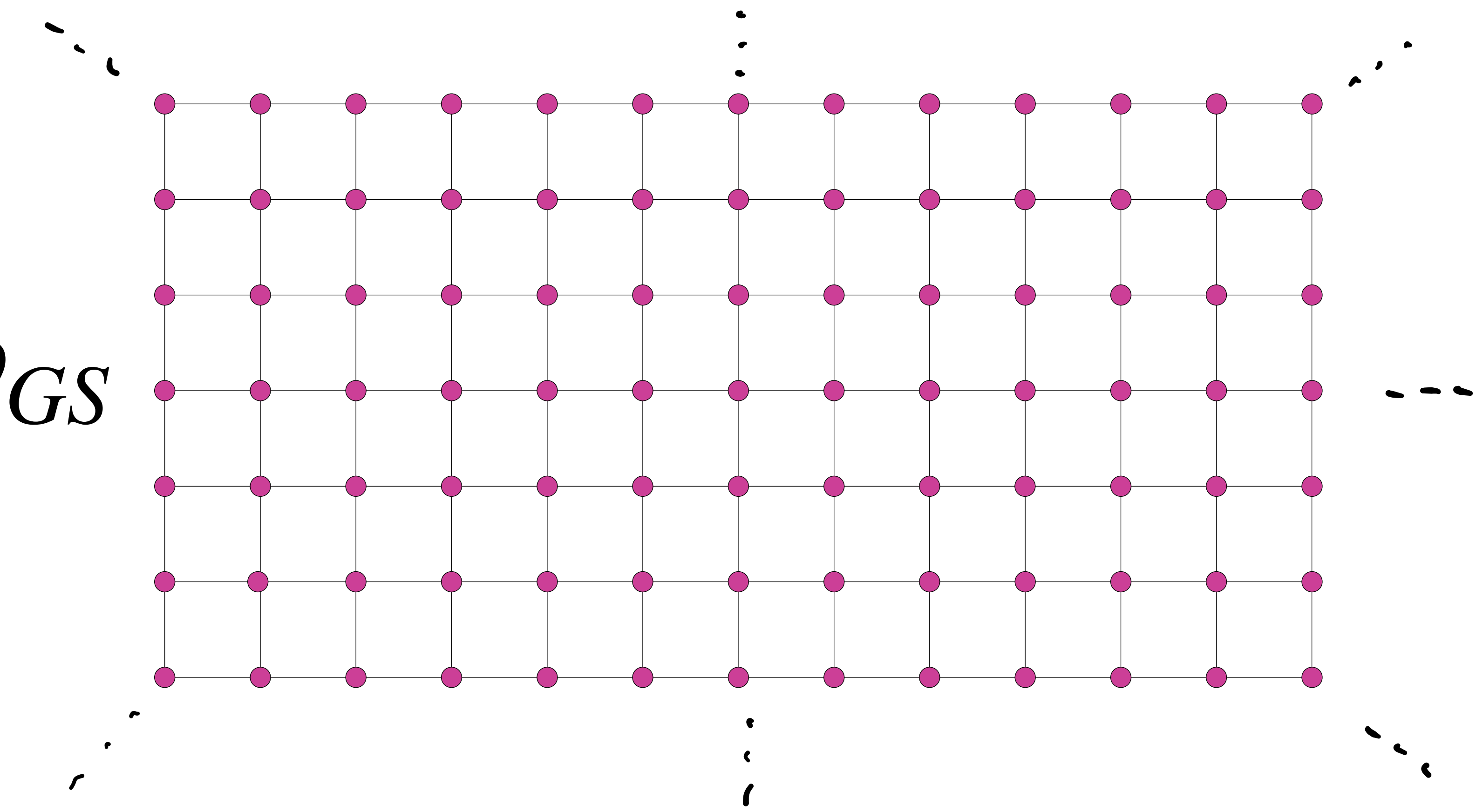

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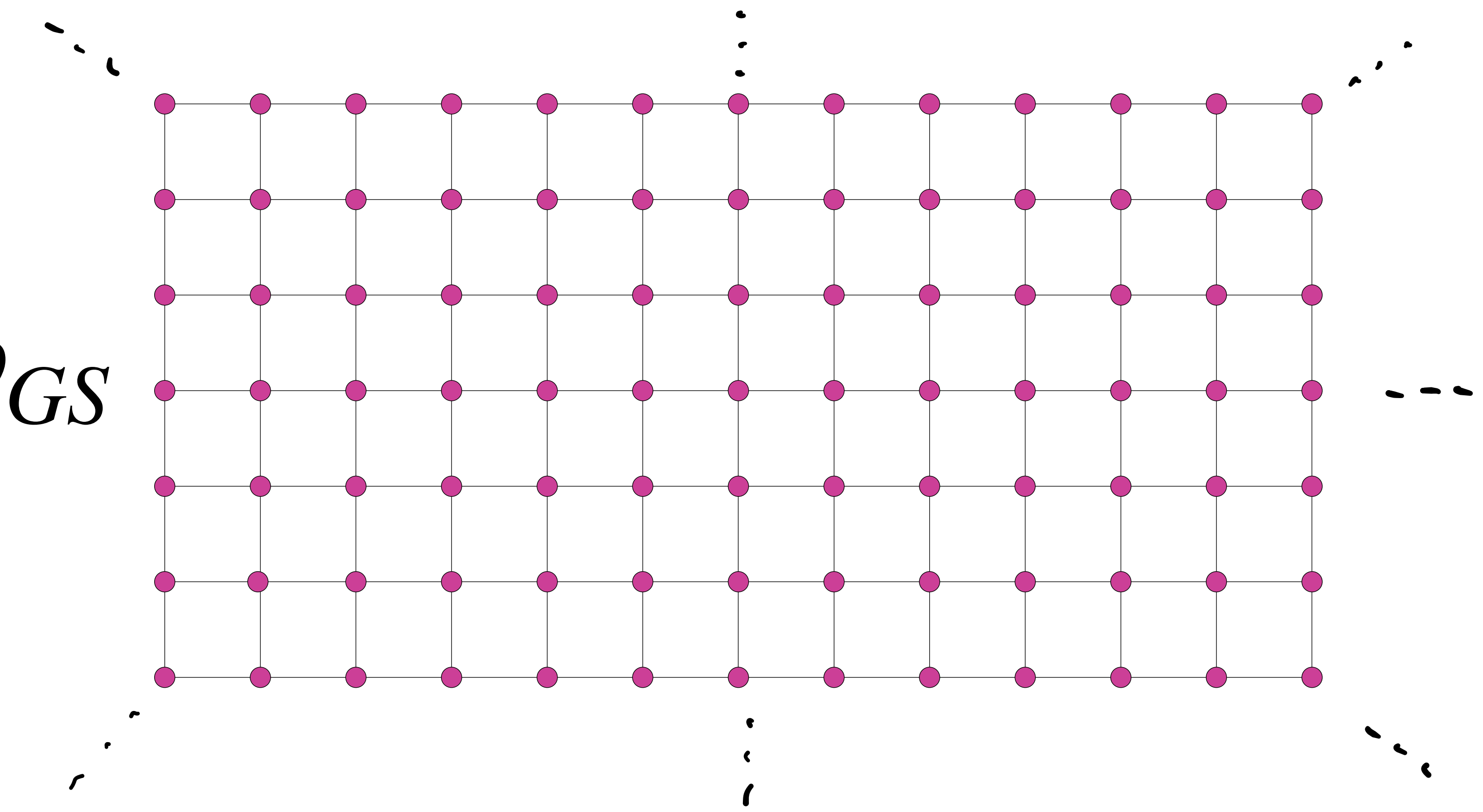

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- RHS = component of $|\psi_a\rangle$ orthogonal to GS subspace

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Idea: if candidate γ is too large, some finite SDP detect infeasibility

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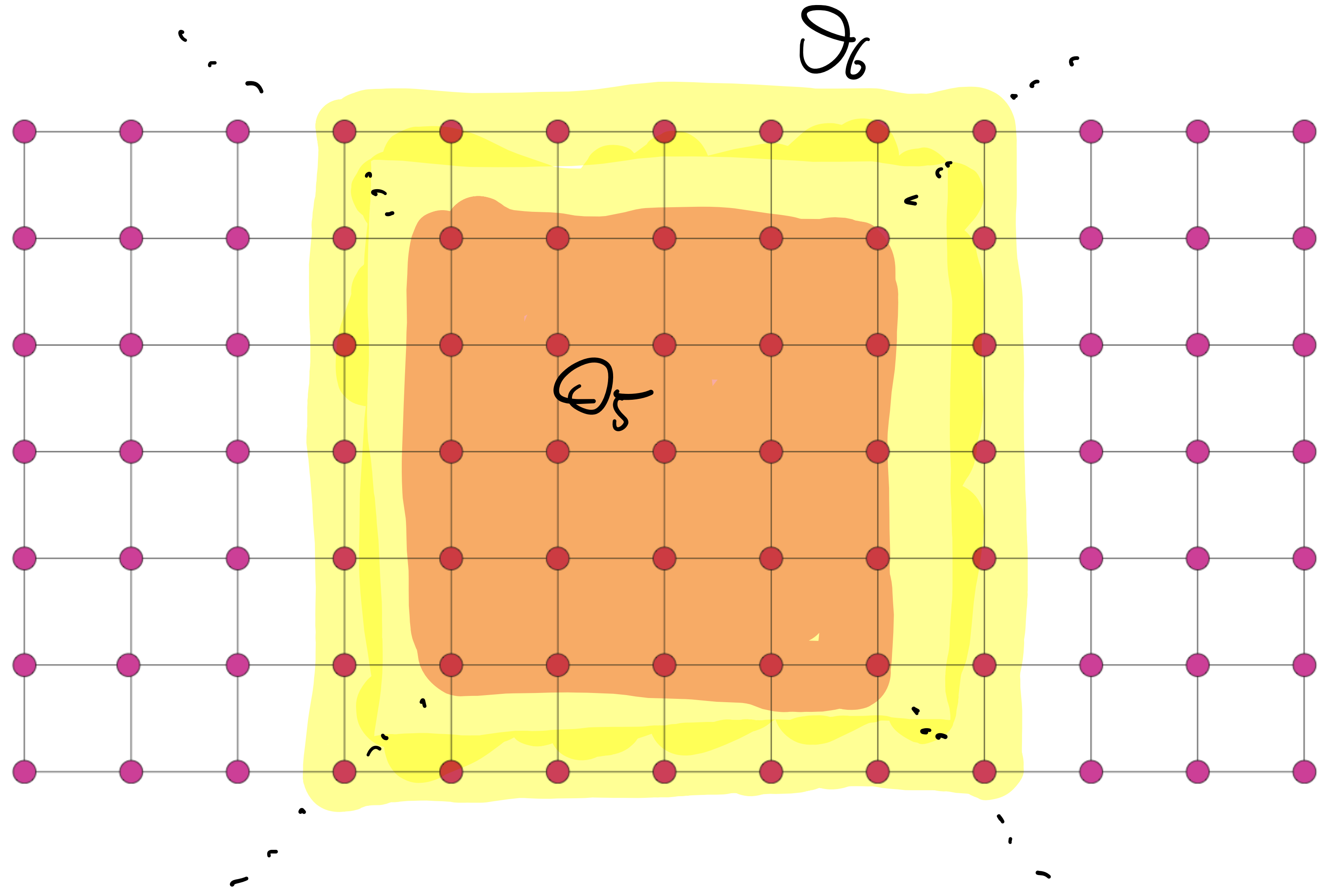

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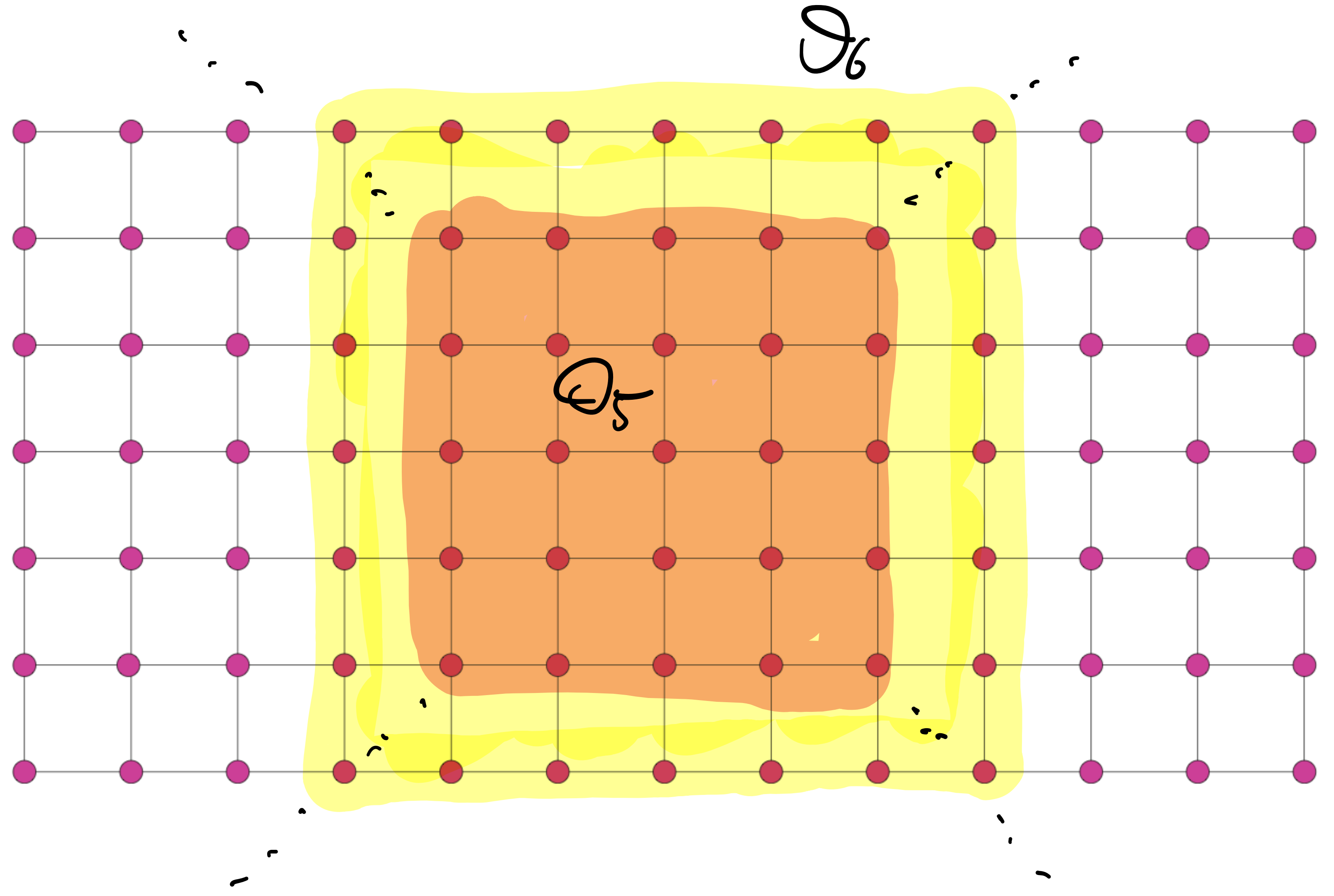

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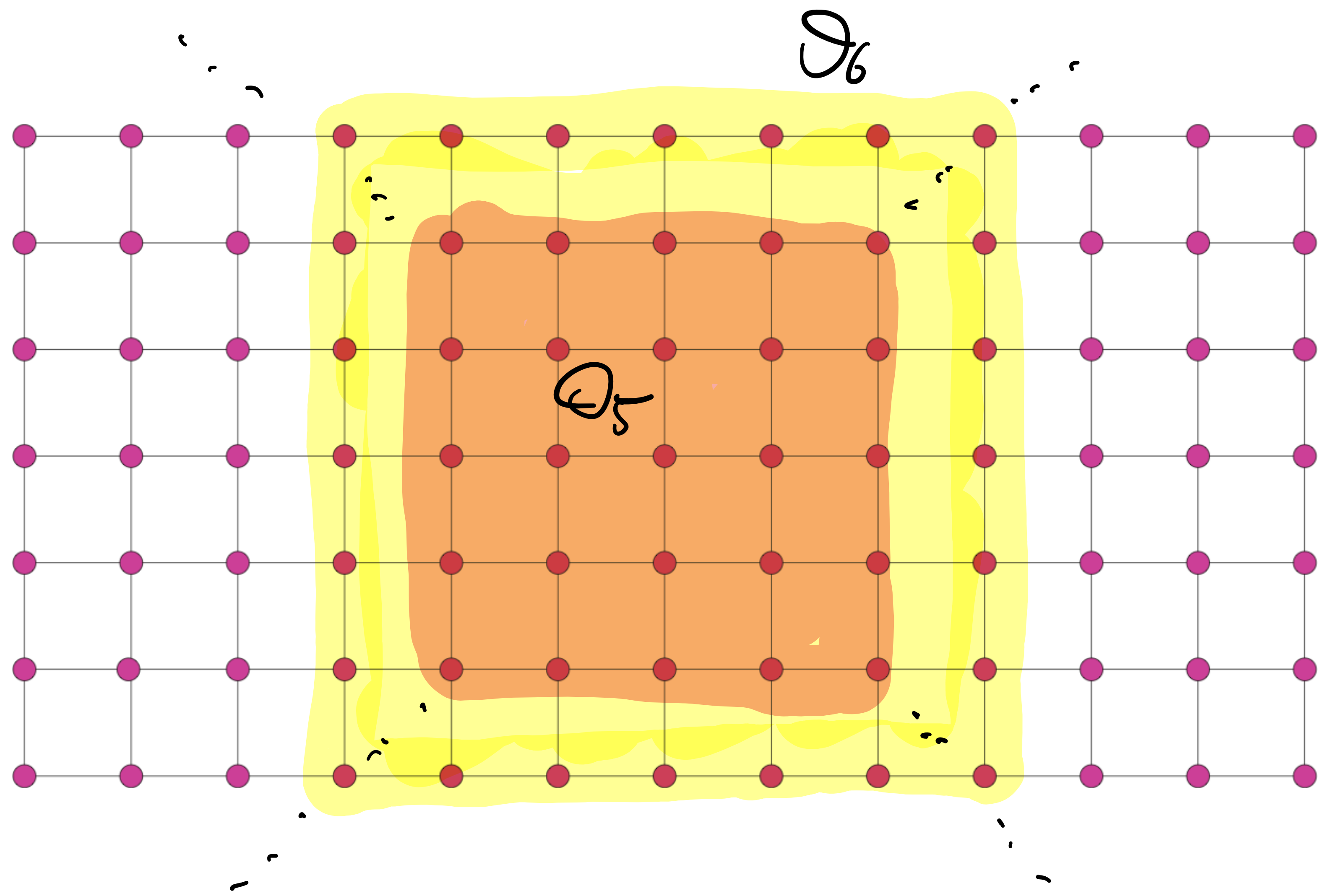

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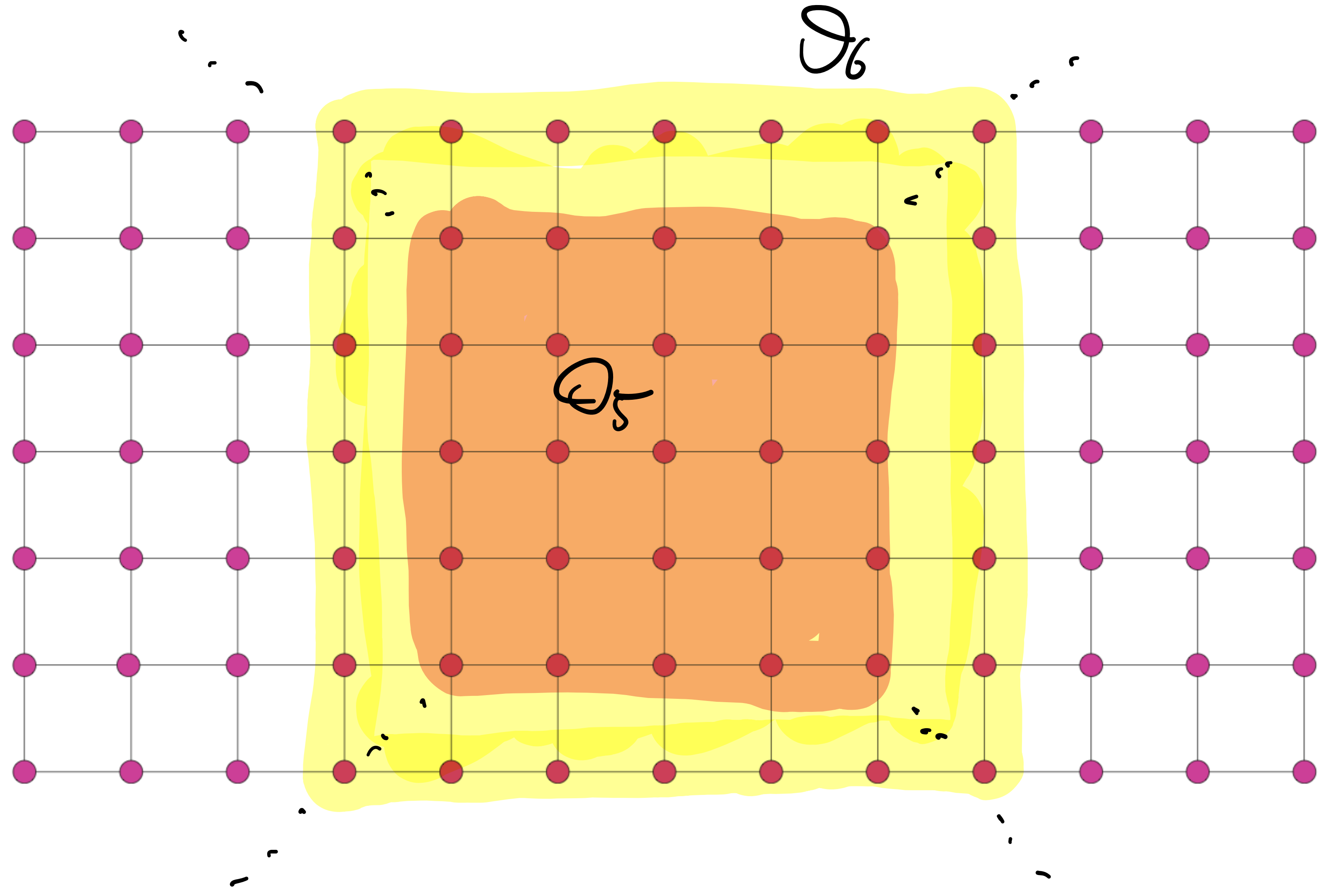

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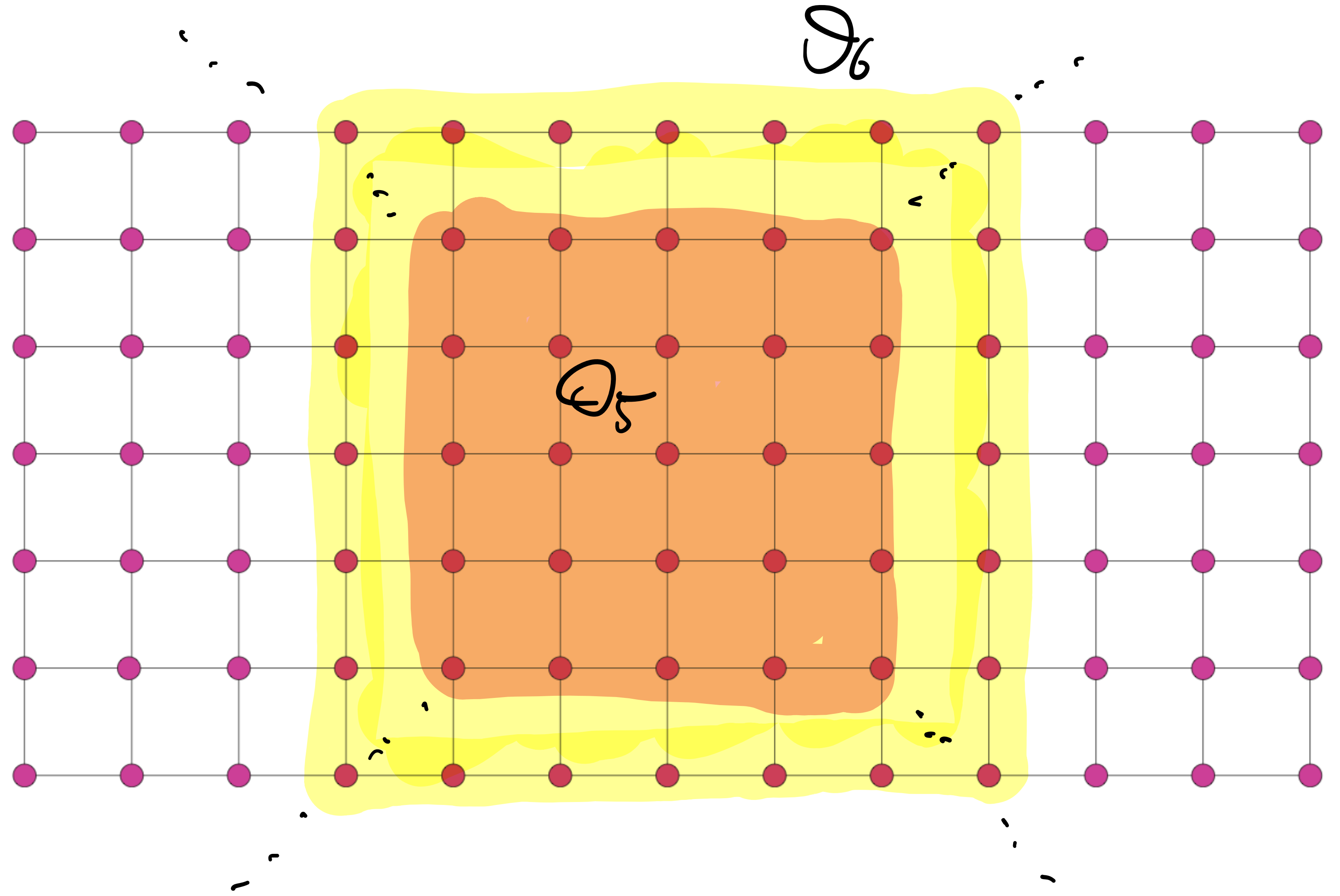

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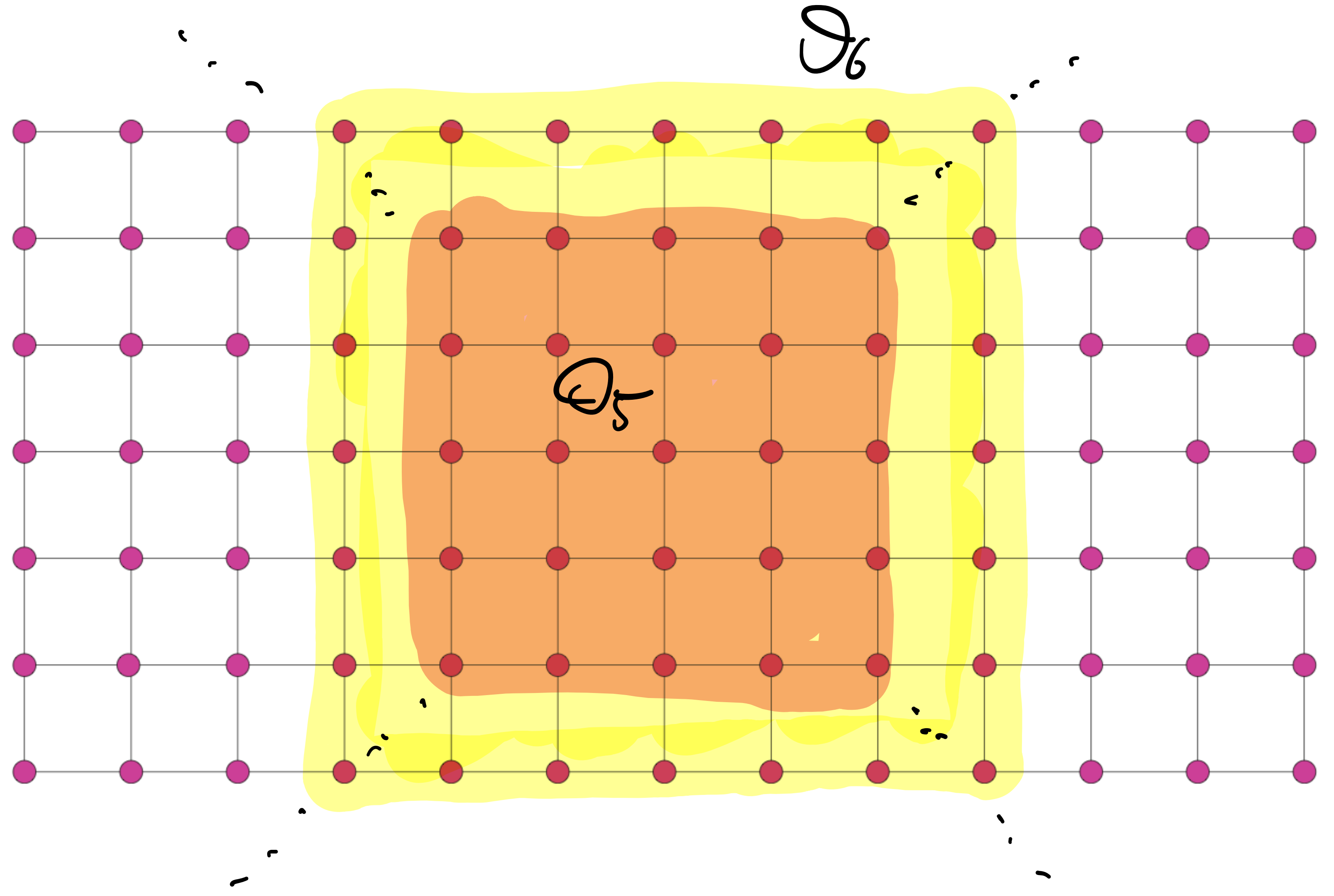

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If γ too big and L large enough, no ω satisfy the gap inequality

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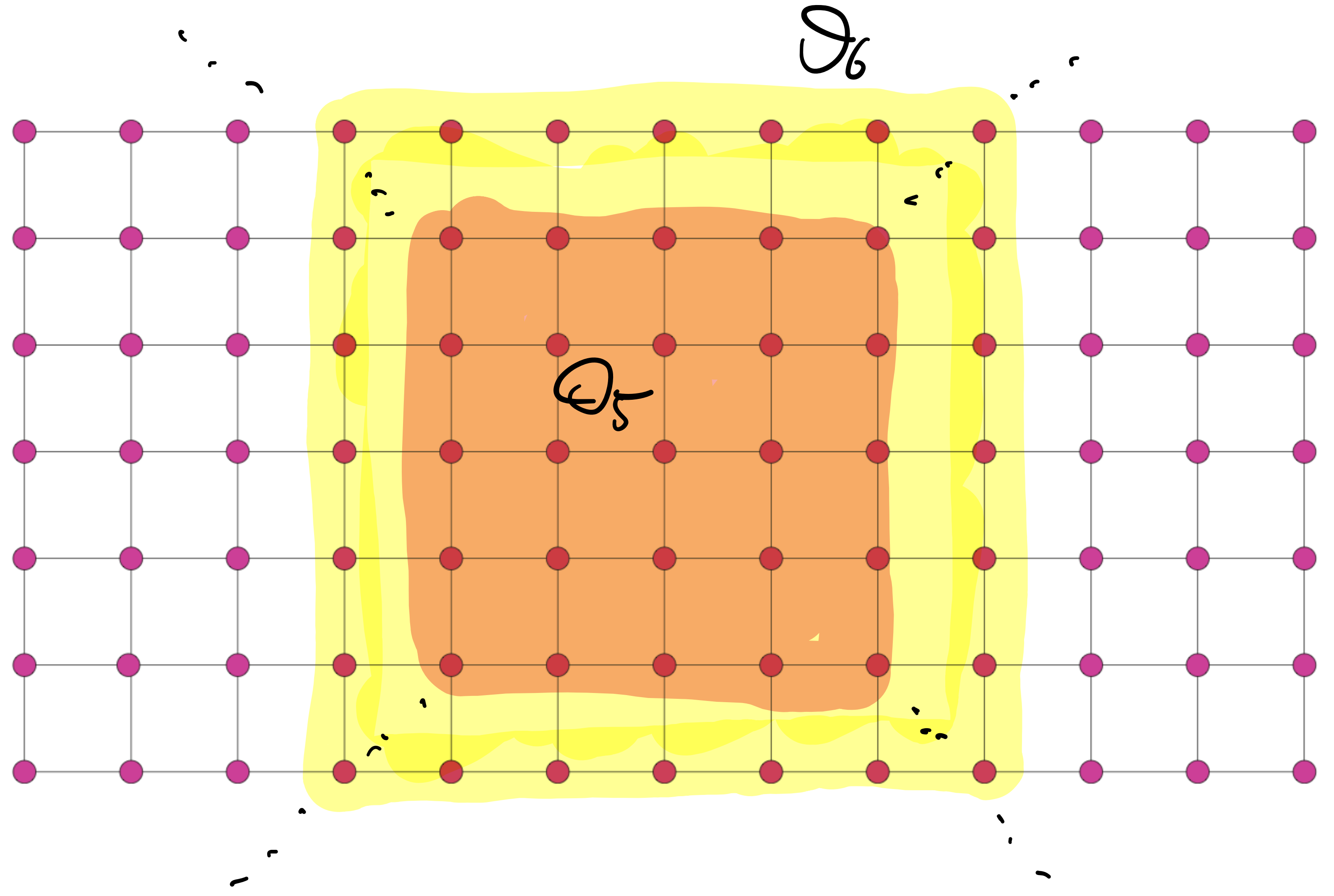

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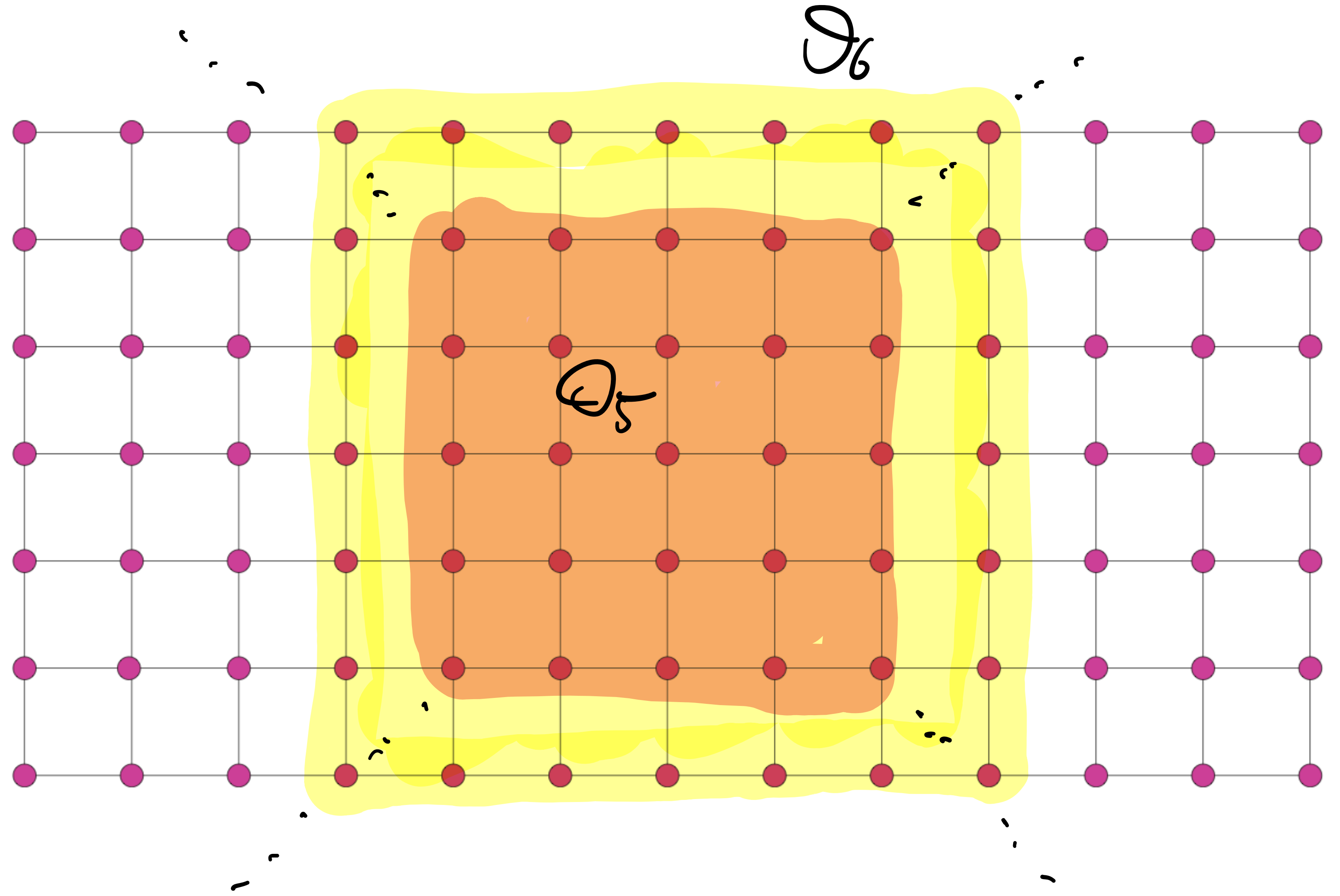

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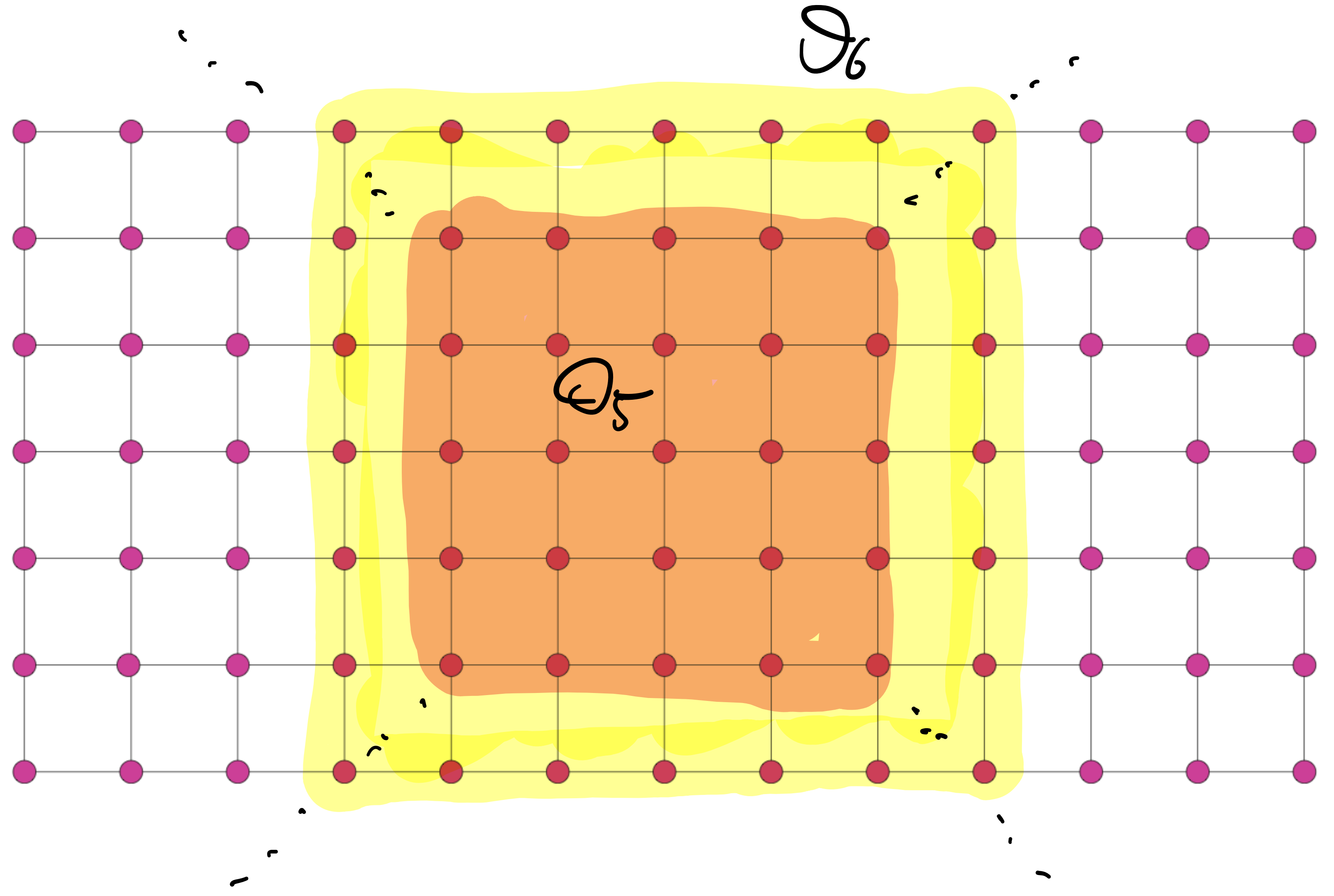

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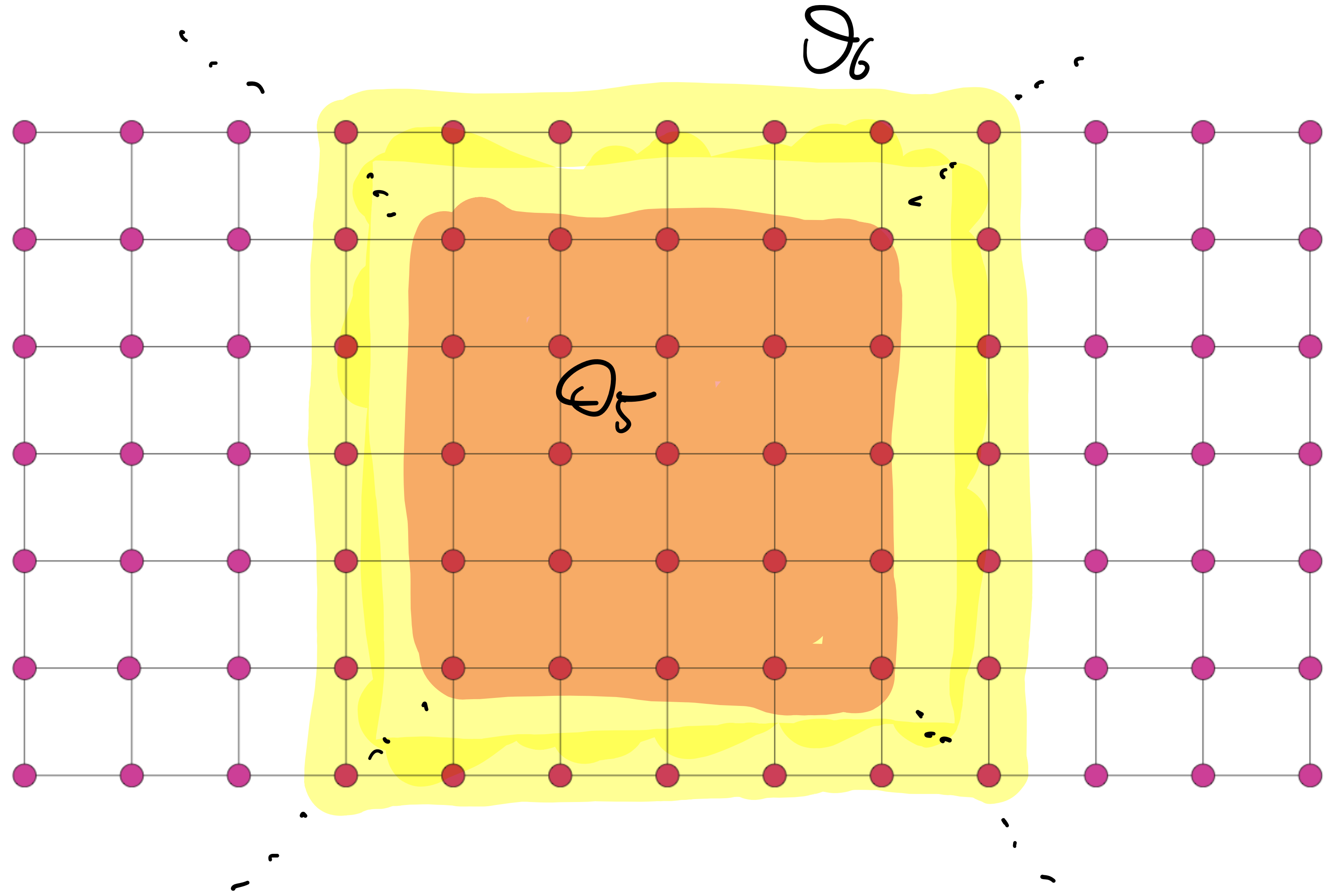

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Can be dealt with by state polynomial optimization — Klep, Magron, Volčič, Wang (Mathematical Programming, 2024)

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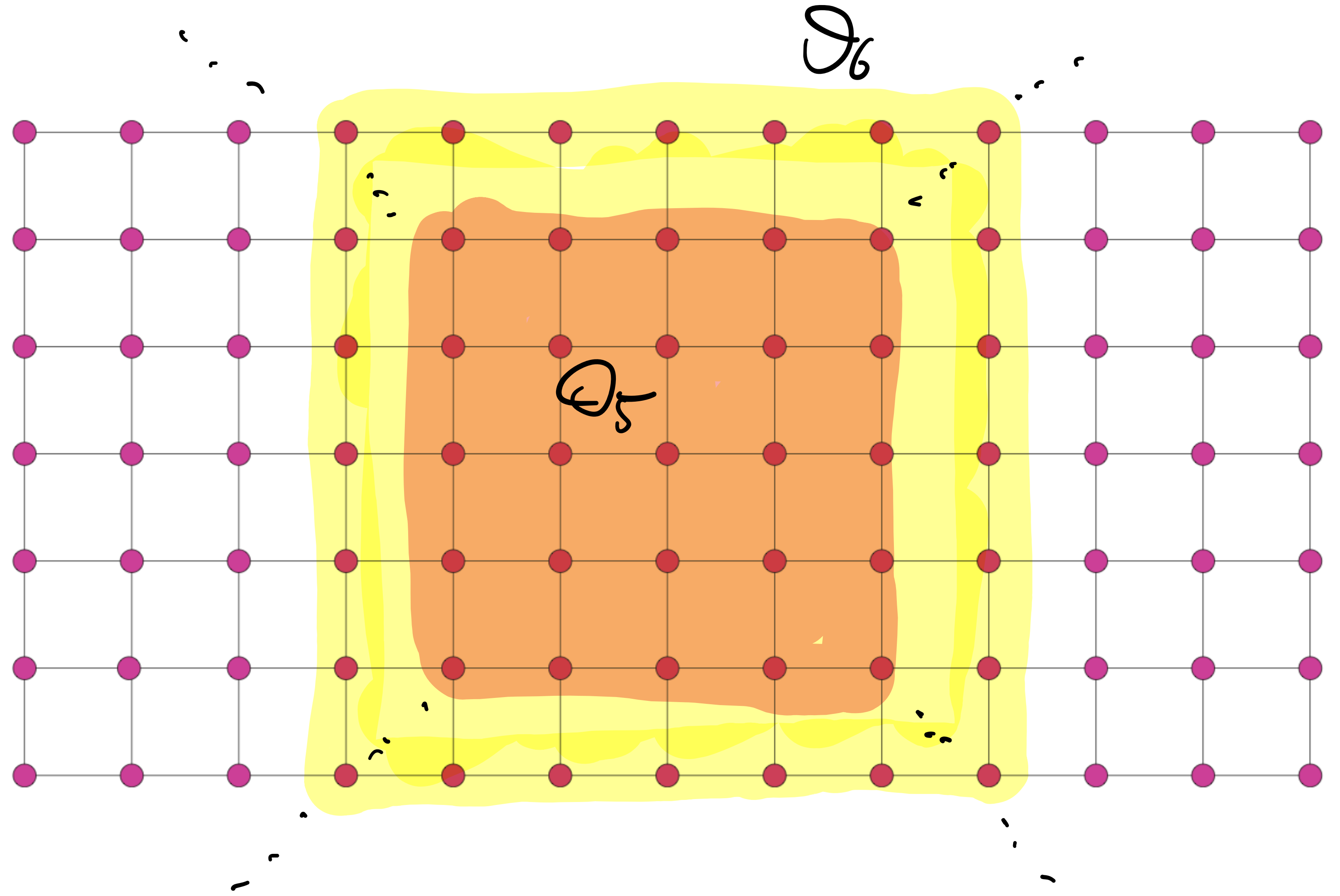

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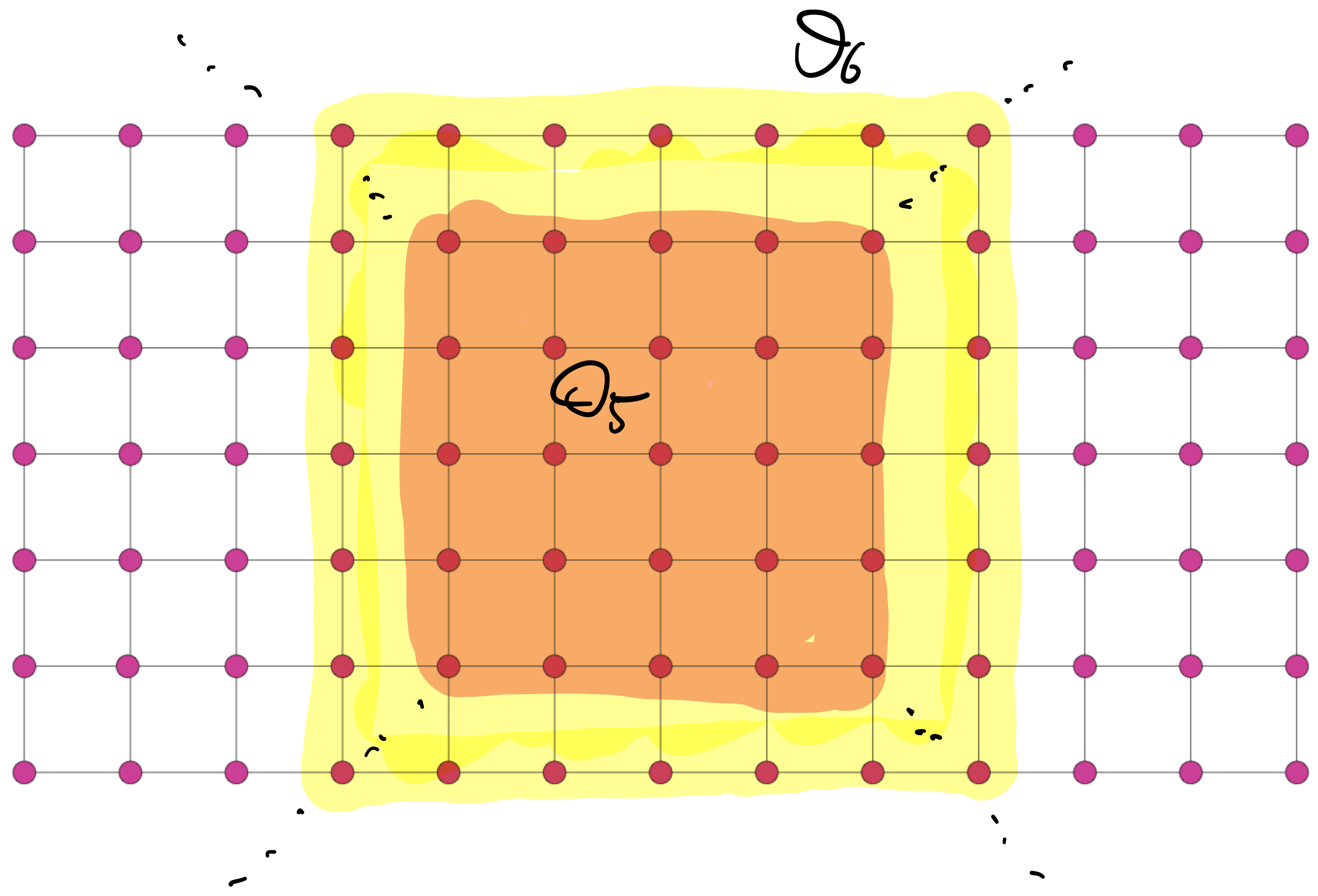

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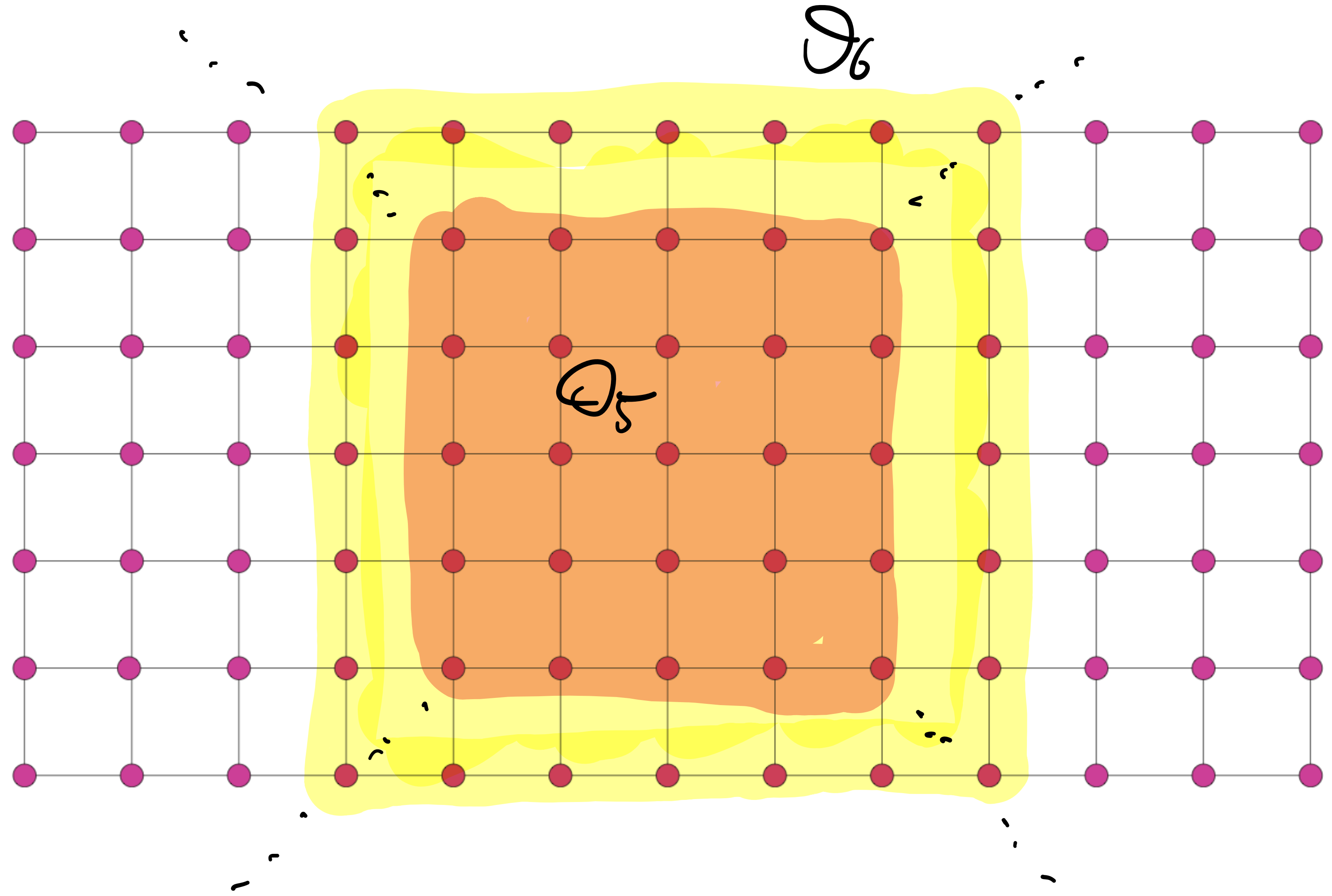

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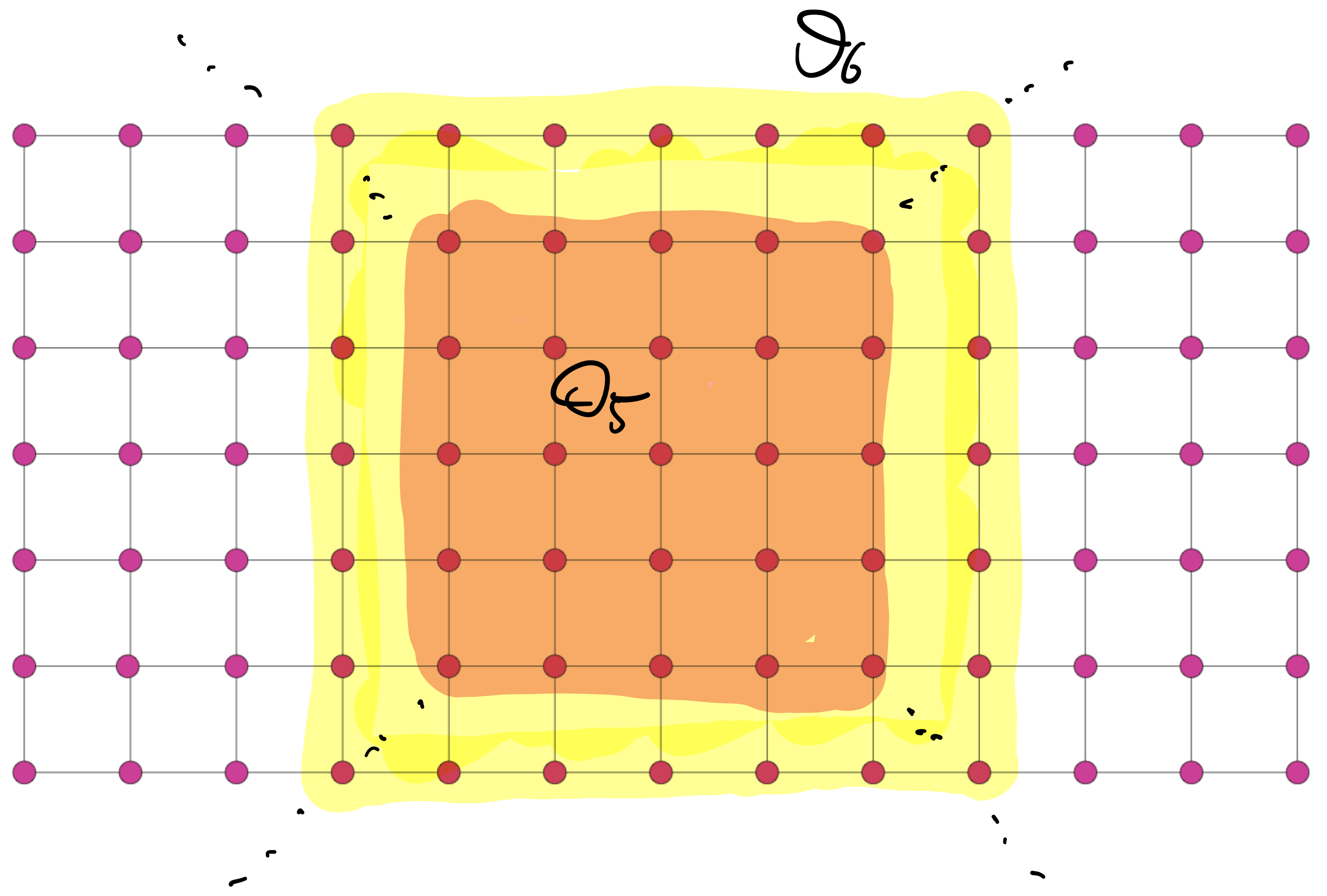

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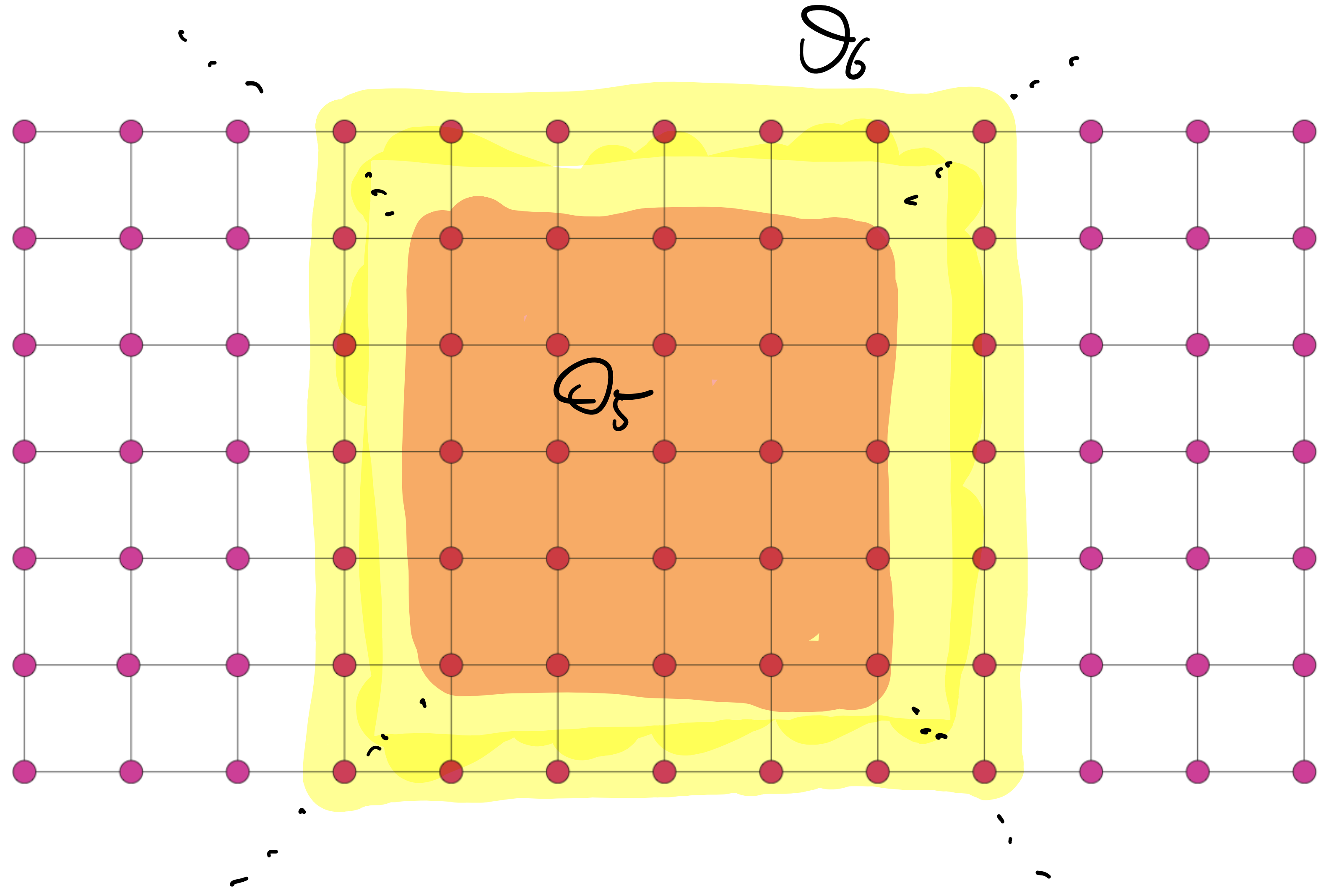

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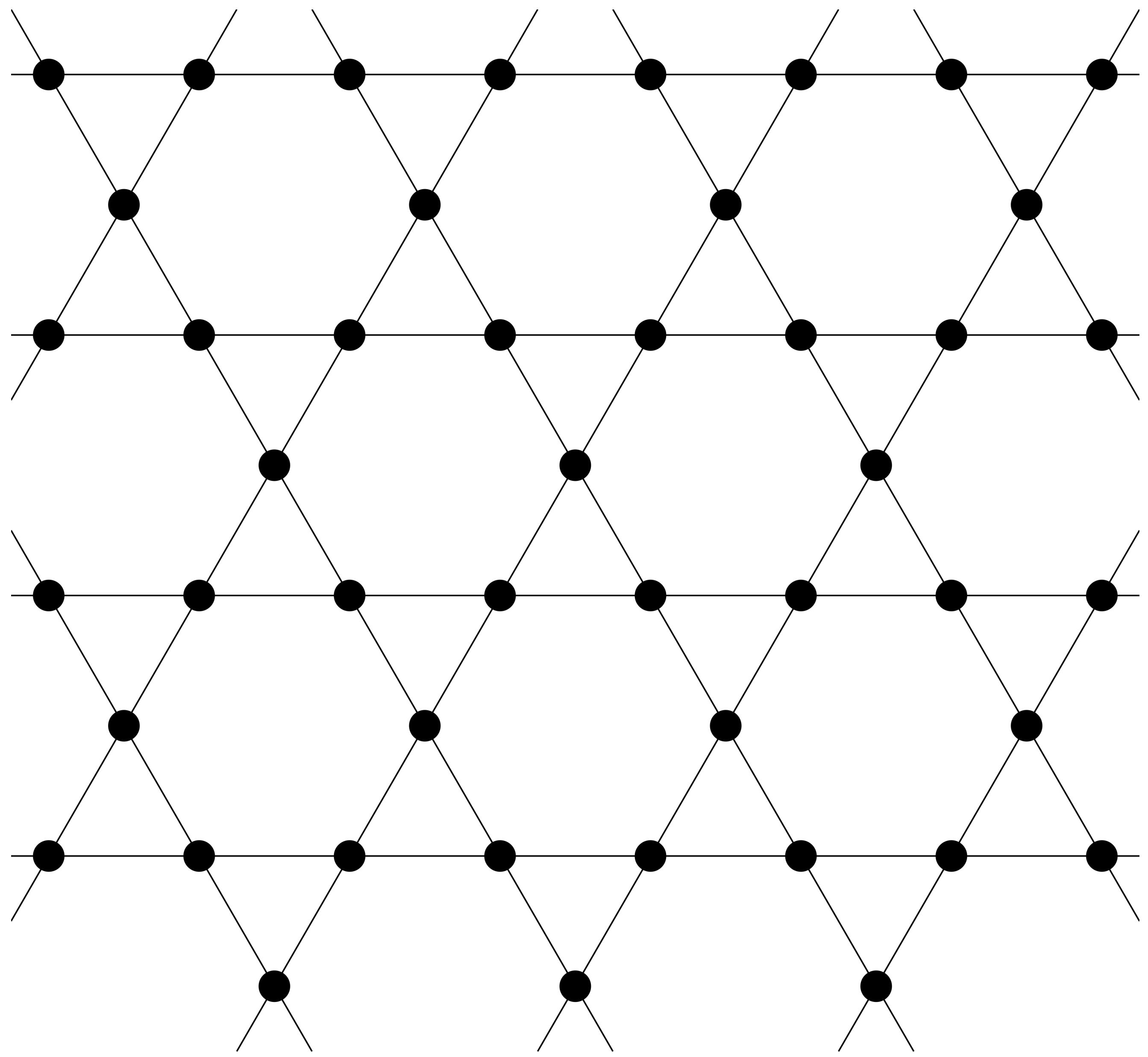
Application on spin-$1/2$ kagome lattice Heisenberg antiferromagnet



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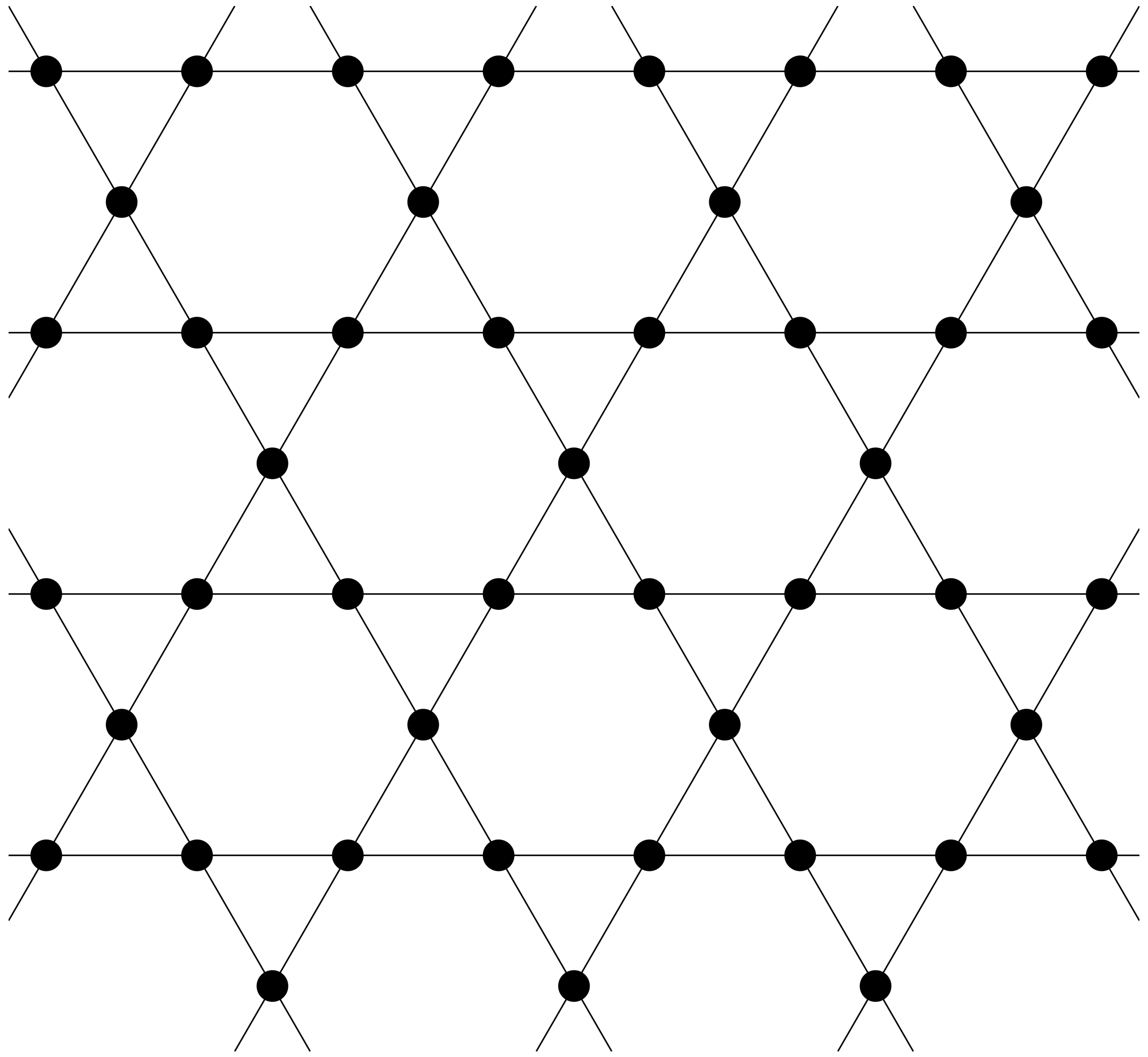

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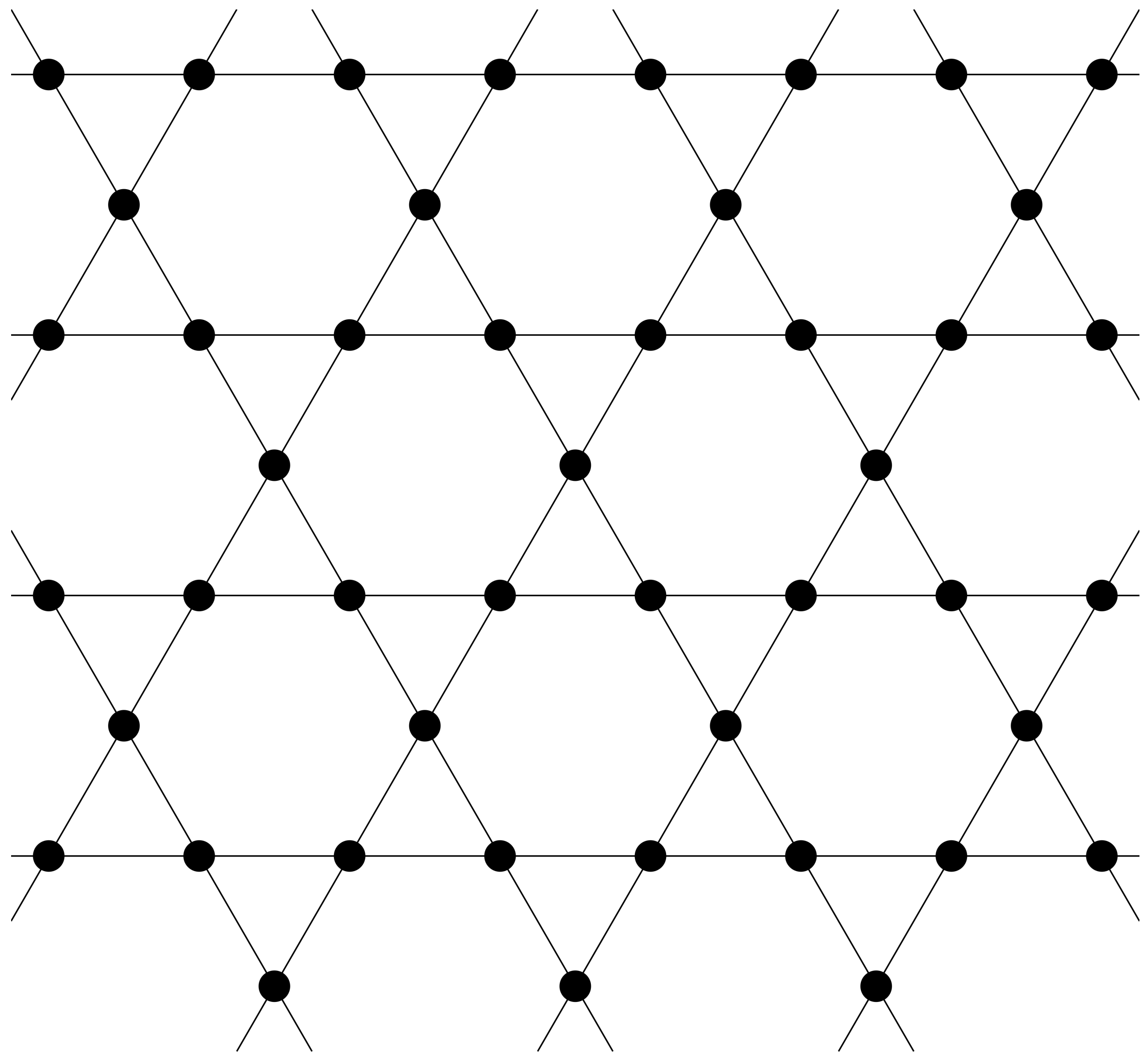

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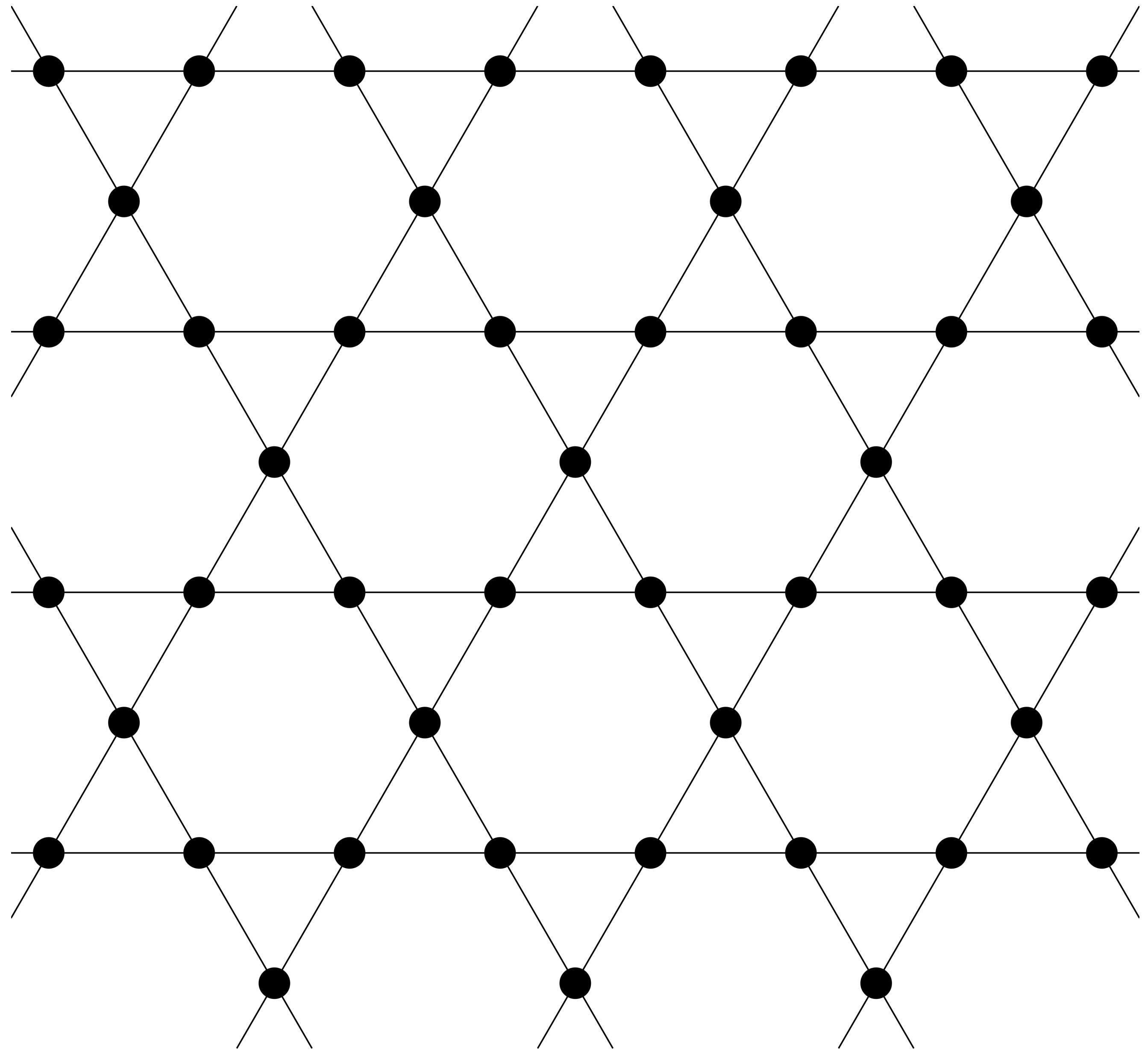

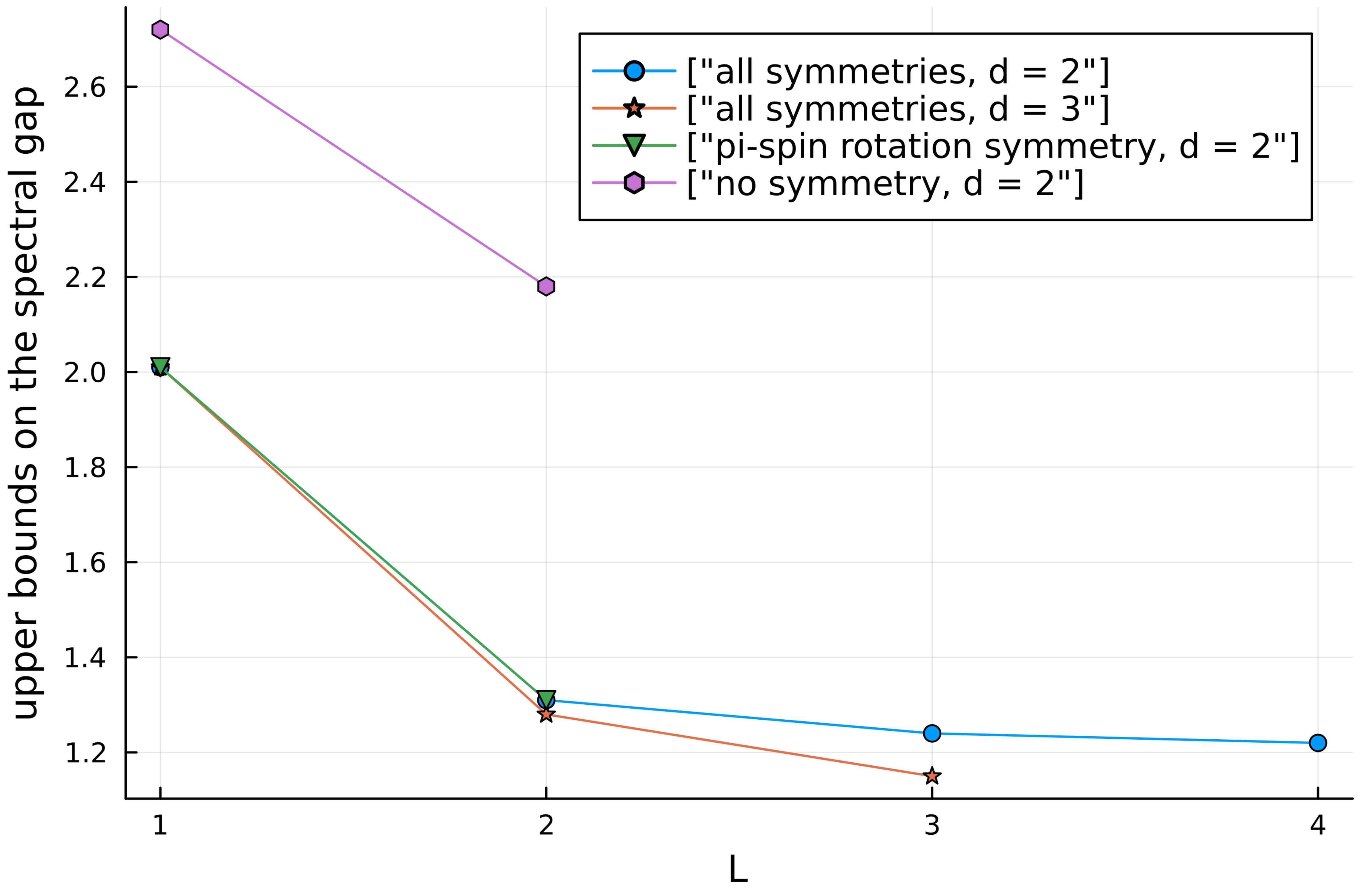

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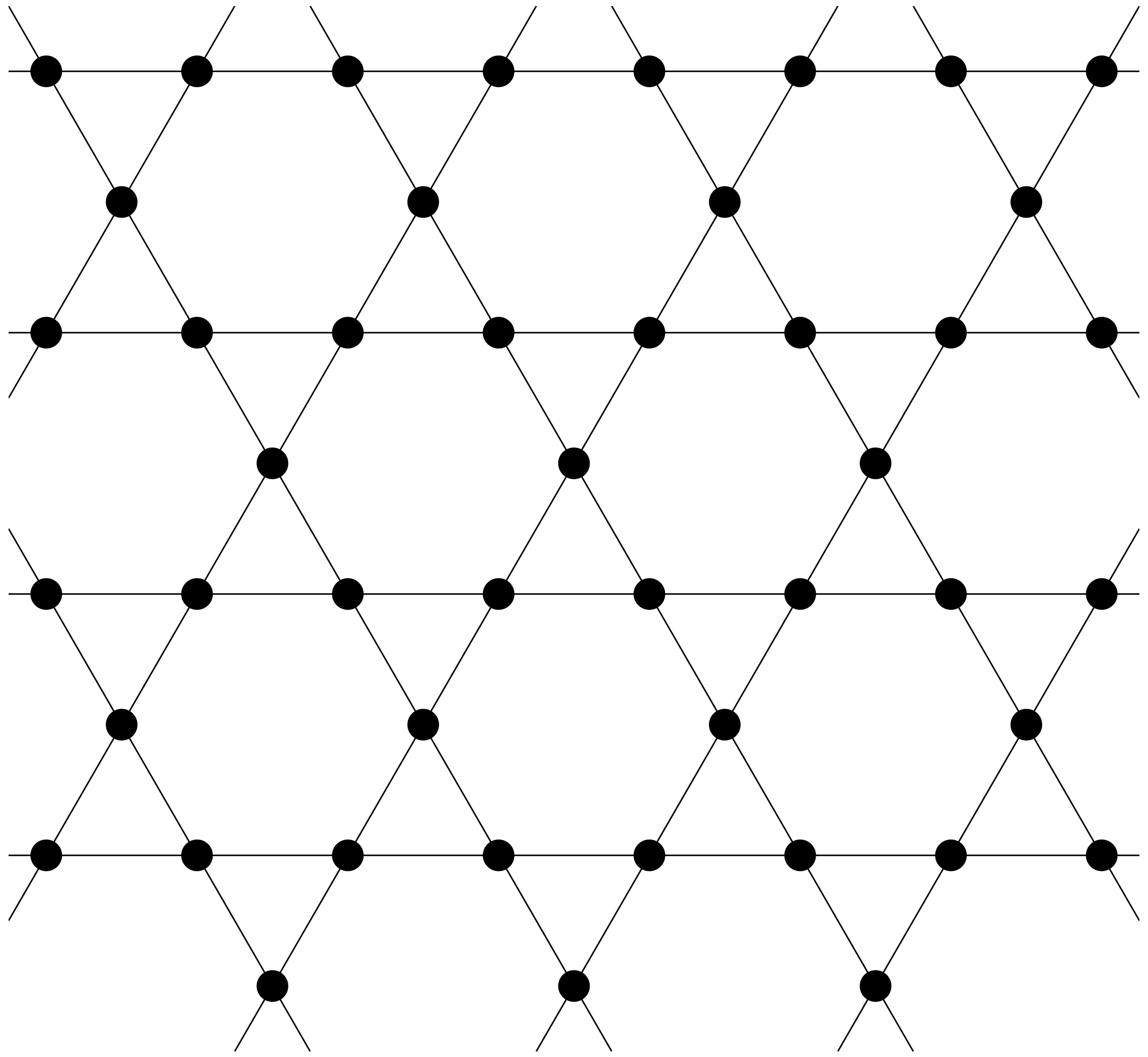

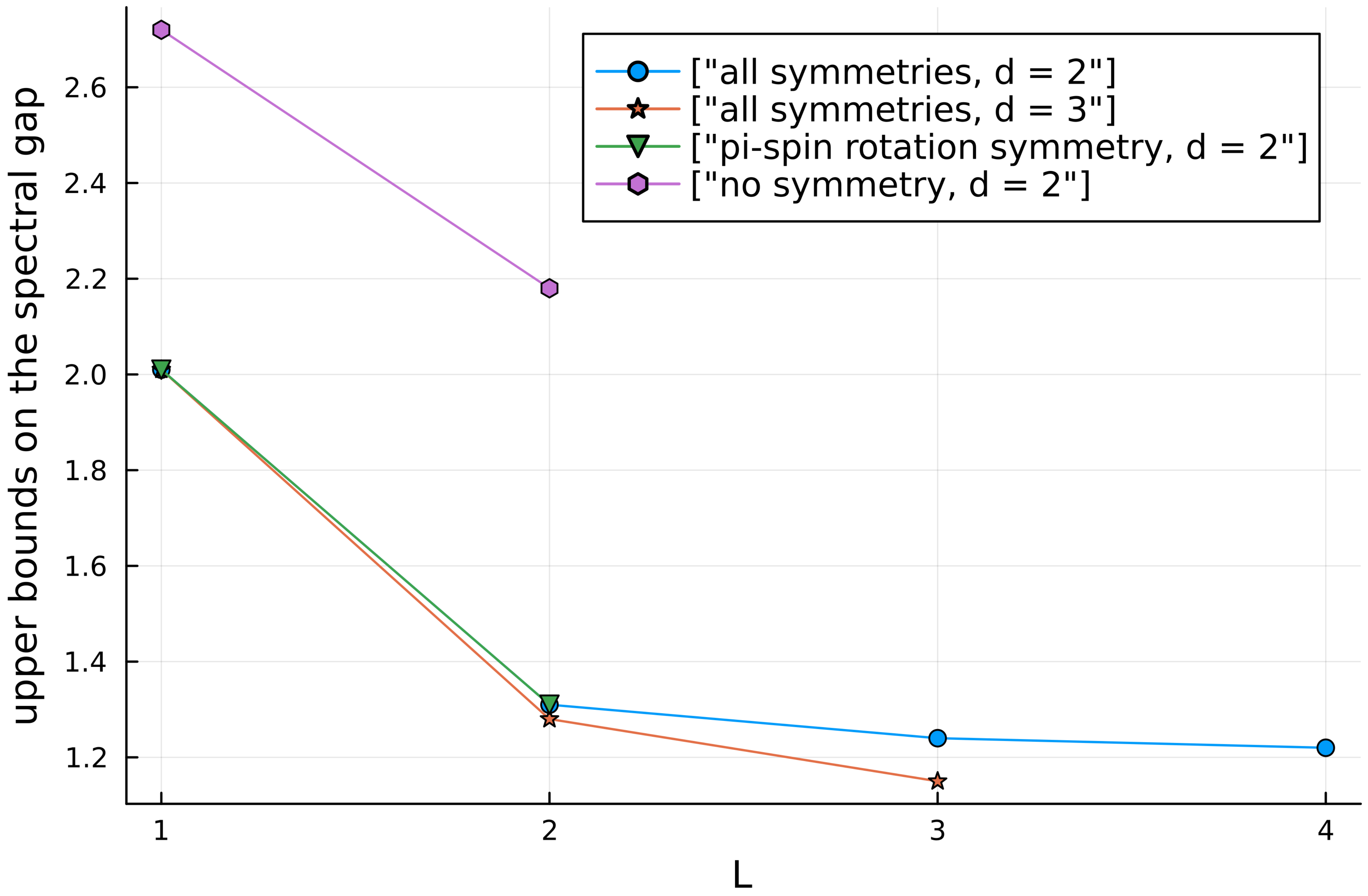

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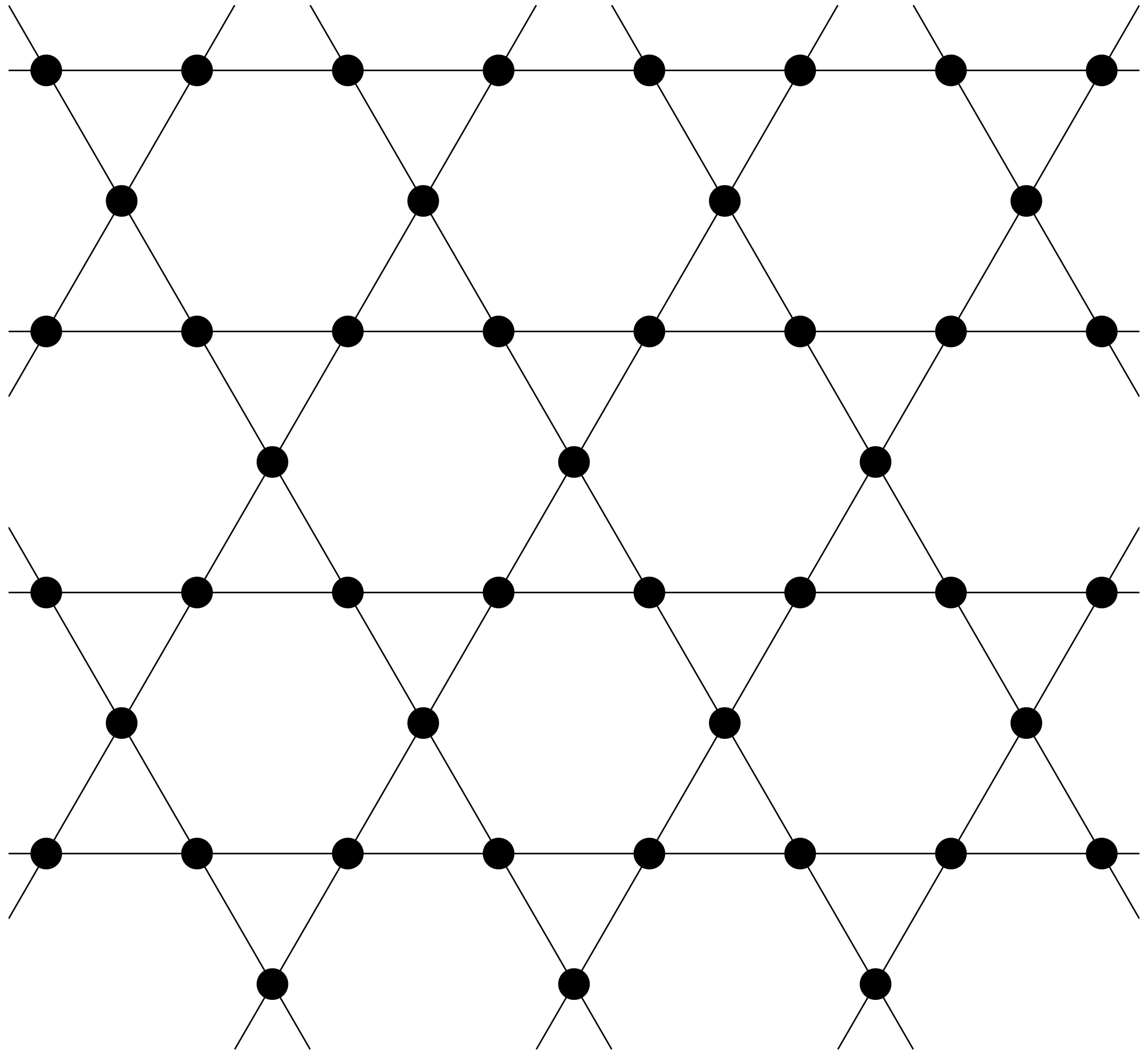

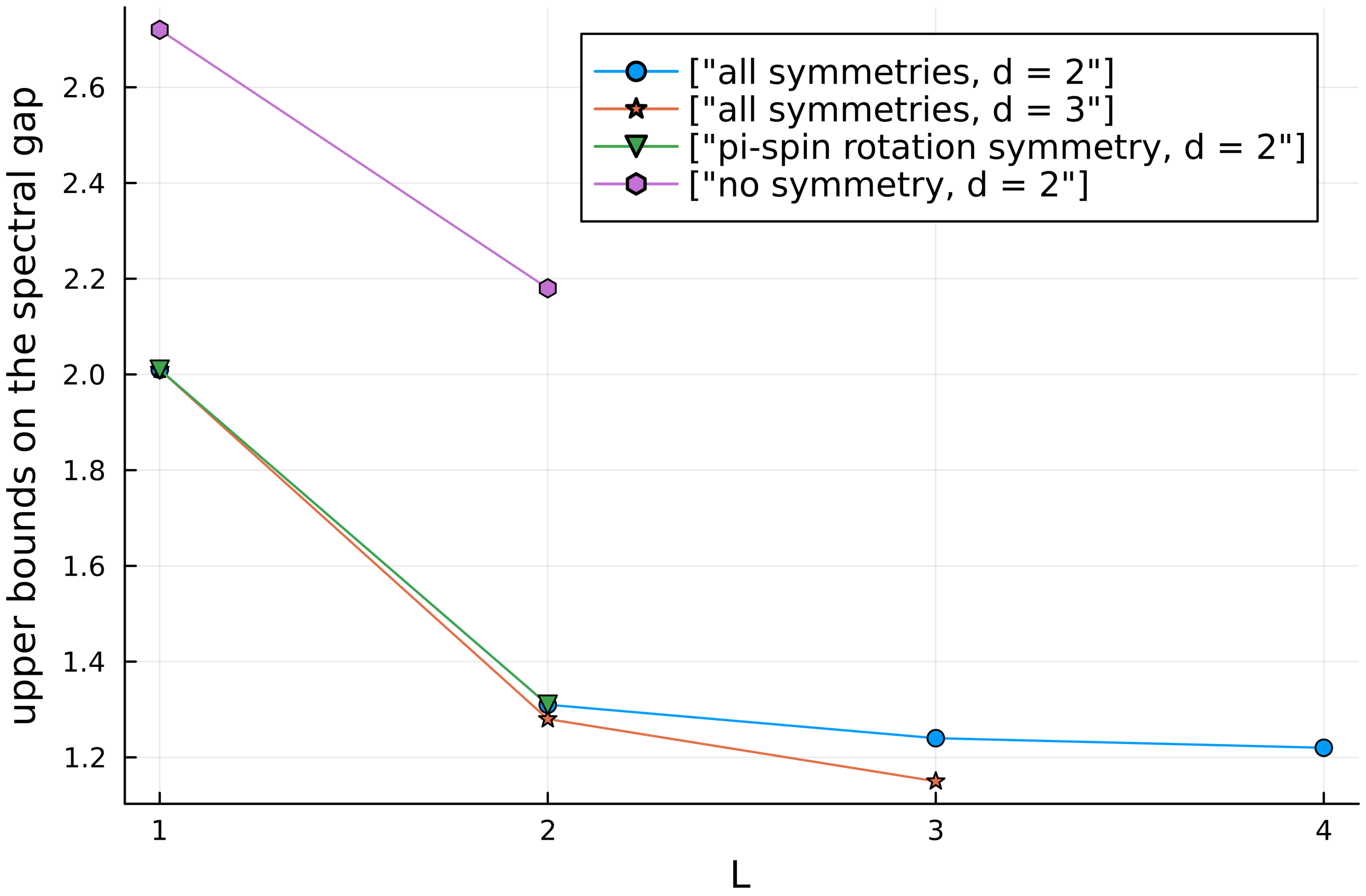

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- (Not competitive against variational estimates ~ 0.1)

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arXiv:2606.03836

Numerical on kagome

State restrictions	d	L=1	L=2	L=3	L=4
None	2	2.72	2.18	—	—
π spin rotations	2	2.00	1.31	—	—
Full symmetries	2	2.01	1.31	1.24	1.22
Full symmetries	3	2.01	1.28	1.15	—

d: polynomial degree. Patch: 5, 13, 27, 45 sites.

Full symmetries: π spin rotations, cyclic spin-component permutations, time reversal.

Numerical on spin-1/2 transverse-field Ising model