How to implement lattice Chern number method for computing Z_2 invariants

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References

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[3] W. Feng, J. Wen, J. Zhou, D. Xiao, and Y. Yao, Comput. Phys. Commun. **183**, 1849 (2012).

[4] http://rhodia.ph.tsukuba.ac.jp/~hatsugai/modules/pico/PDF/workshopJuly2008/Fukui.pdf

Computing lattice Chern number

Z_2 invariant is written as

$$Z_2 = \frac{1}{2\pi}\left(\int_{\partial B} \mathbf{A}\cdot d\mathbf{k} - \int_B F_z dk_x dk_y\right)$$

$$\mathbf{A} = \frac{1}{i}\langle u_{\mathbf{k}}|\frac{\partial}{\partial \mathbf{k}}|u_{\mathbf{k}}\rangle \quad F_z = (\nabla \times \mathbf{A})_z$$

$$B = [-\frac{\mathbf{G}_1}{2}, \frac{\mathbf{G}_1}{2}] \otimes [0, \frac{\mathbf{G}_2}{2}]$$

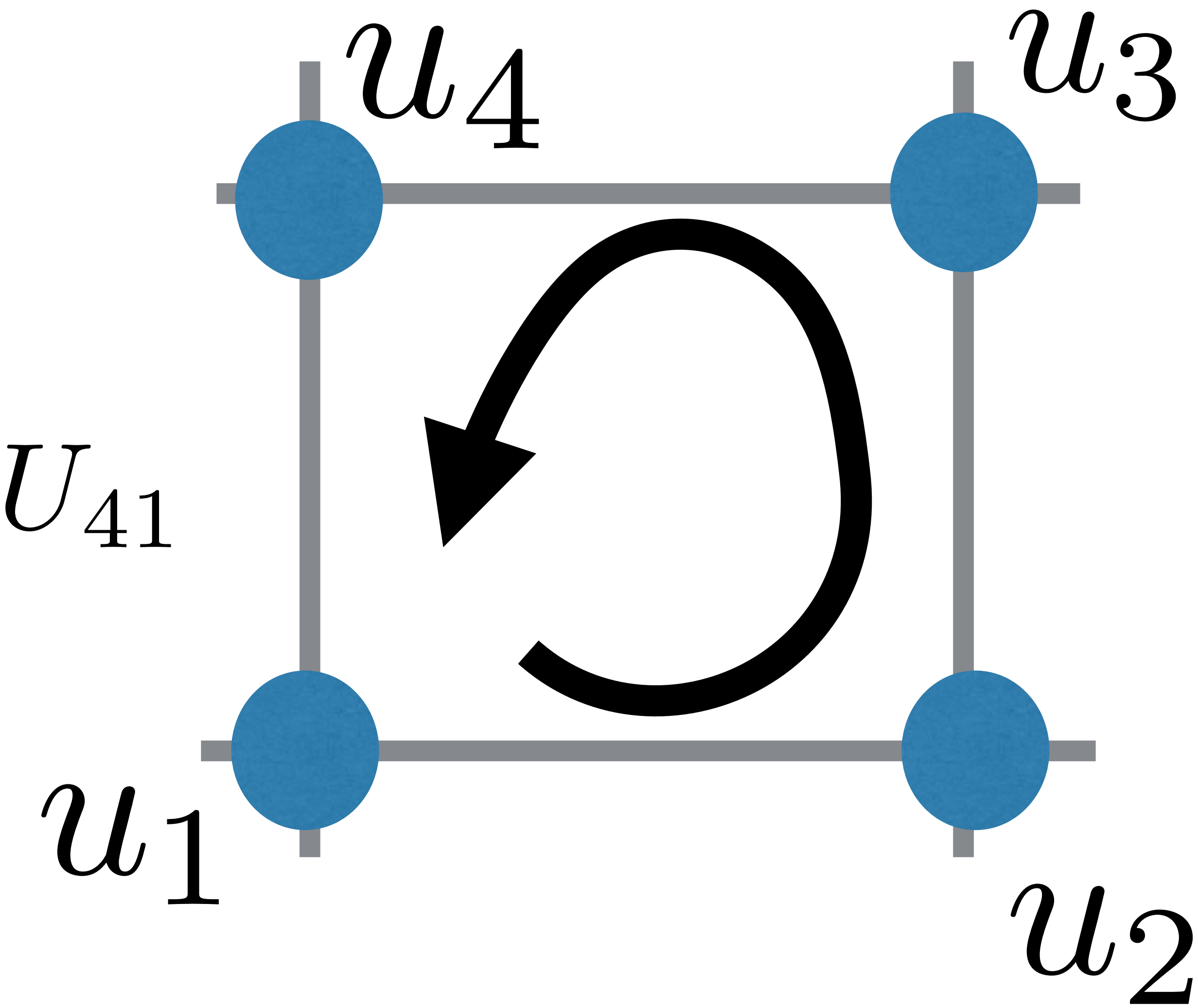
A is called "Berry connection",
F is called "Berry curvature"

We compute F and **A** on discritized BZ by Overlap matrix U

$$U_{ab} = \det\langle u_a | u_b \rangle$$

$$F_{\mathbf{k}} = \operatorname{Im}\log U_{12}U_{23}U_{34}U_{41}$$

$$A_{ab} = \operatorname{Im}\log U_{ab}$$



$$n(\mathbf{k}) = \frac{1}{2\pi}[A_{12} + A_{23} + A_{34} + A_{41} - F_{\mathbf{k}}]$$

n is called lattice Chern number (LCN)

We can obtain Z_2 invariant as

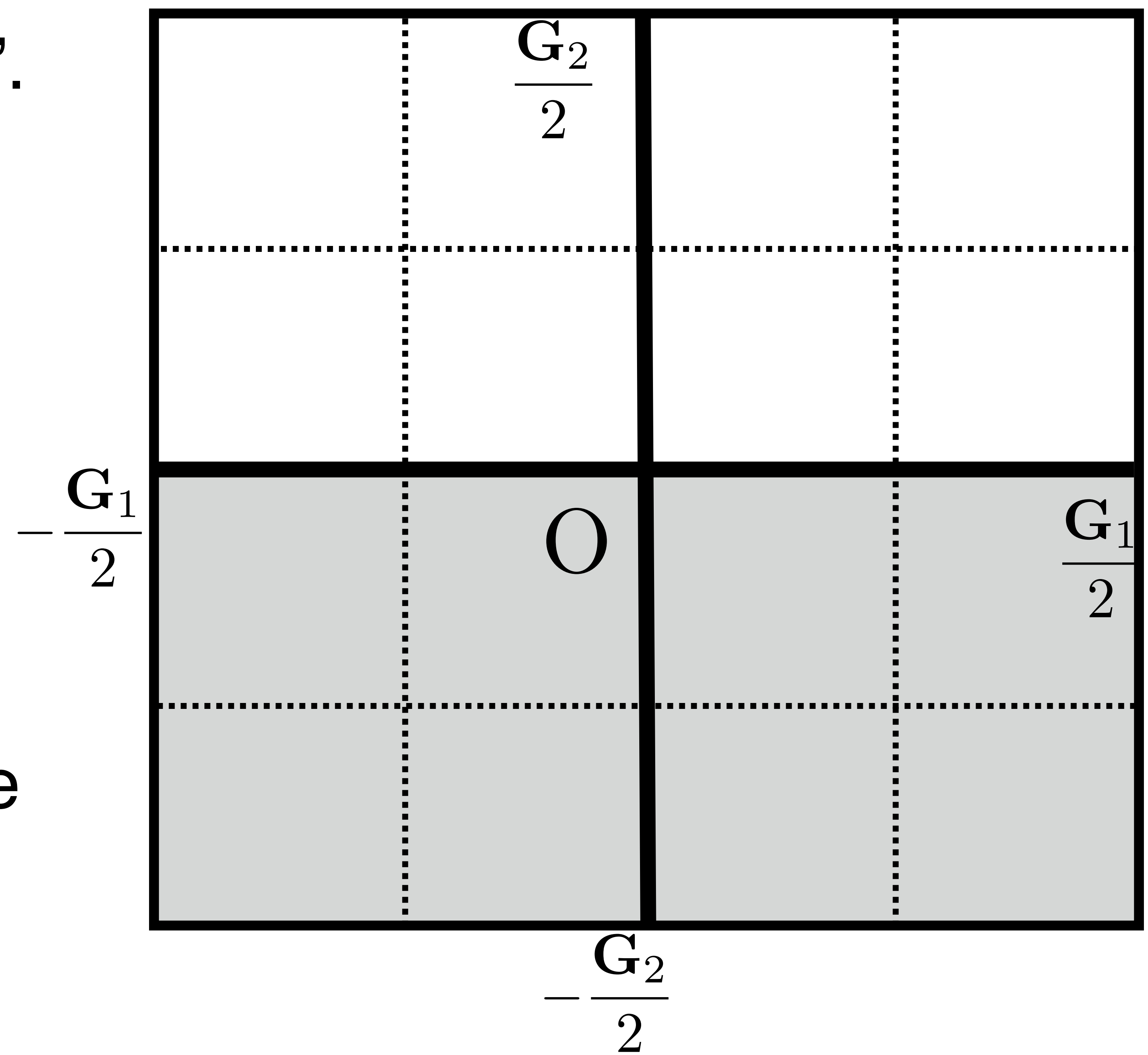
$$Z_2 = \sum_{\mathbf{k}}^{\text{Half BZ}} n(\mathbf{k}) \pmod 2$$

→we summate the LCN only on half BZ,
so **the summation depend on a gauge**.

Gauge Fix

You have to “gauge fix”.

1. Transition symmetric points
2. Time reversal symmetric points
3. Kramers degenerate points



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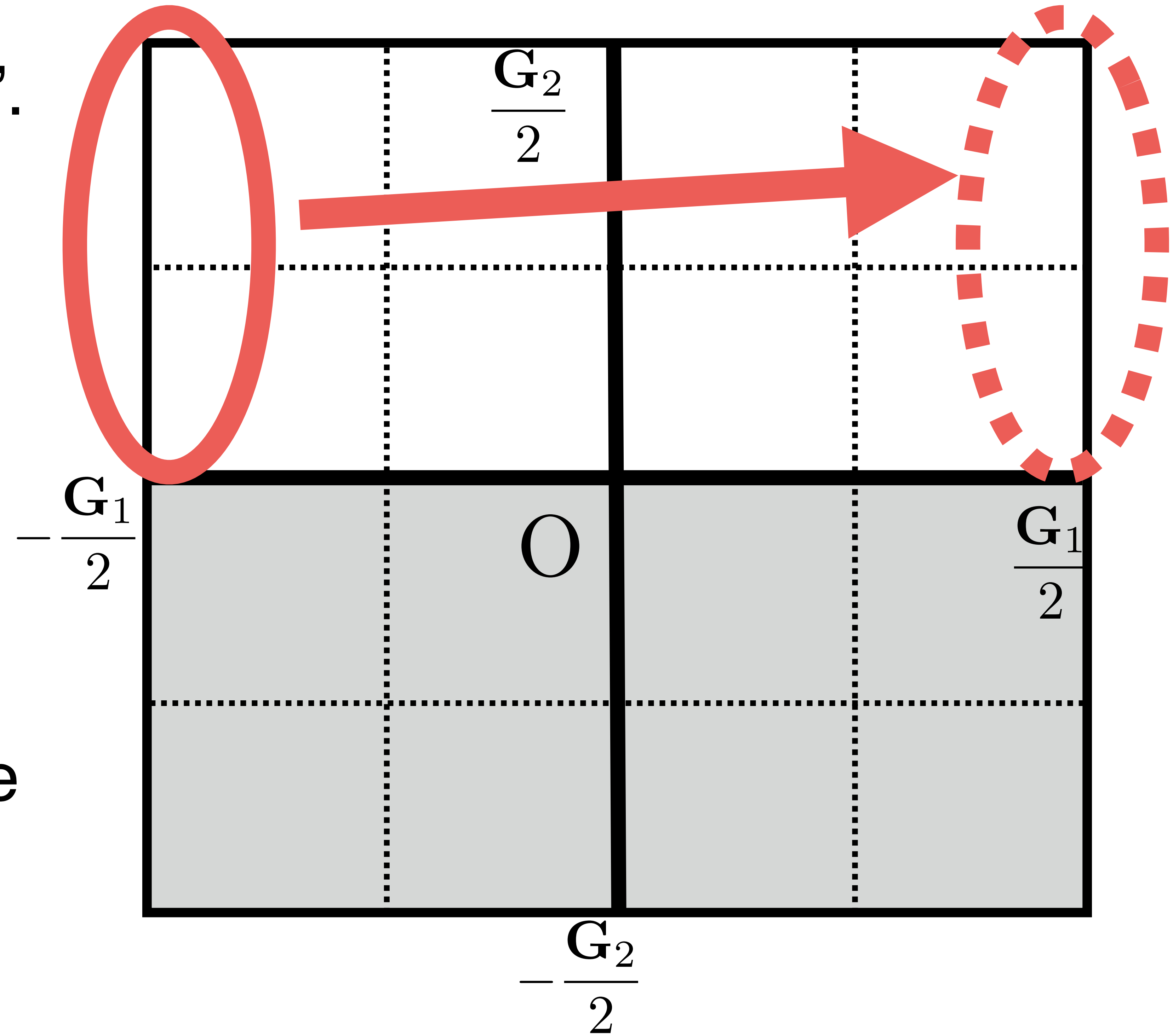

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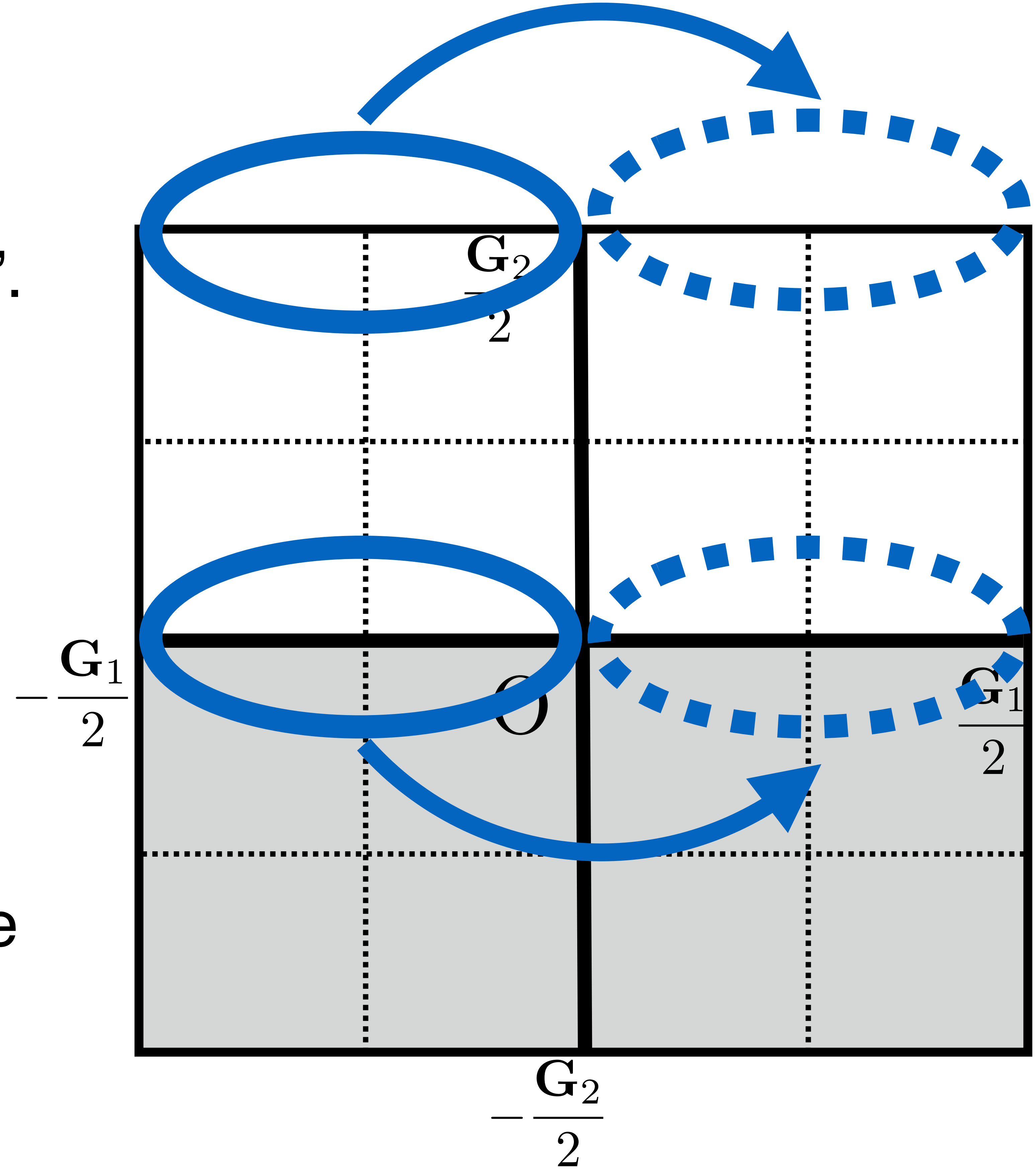

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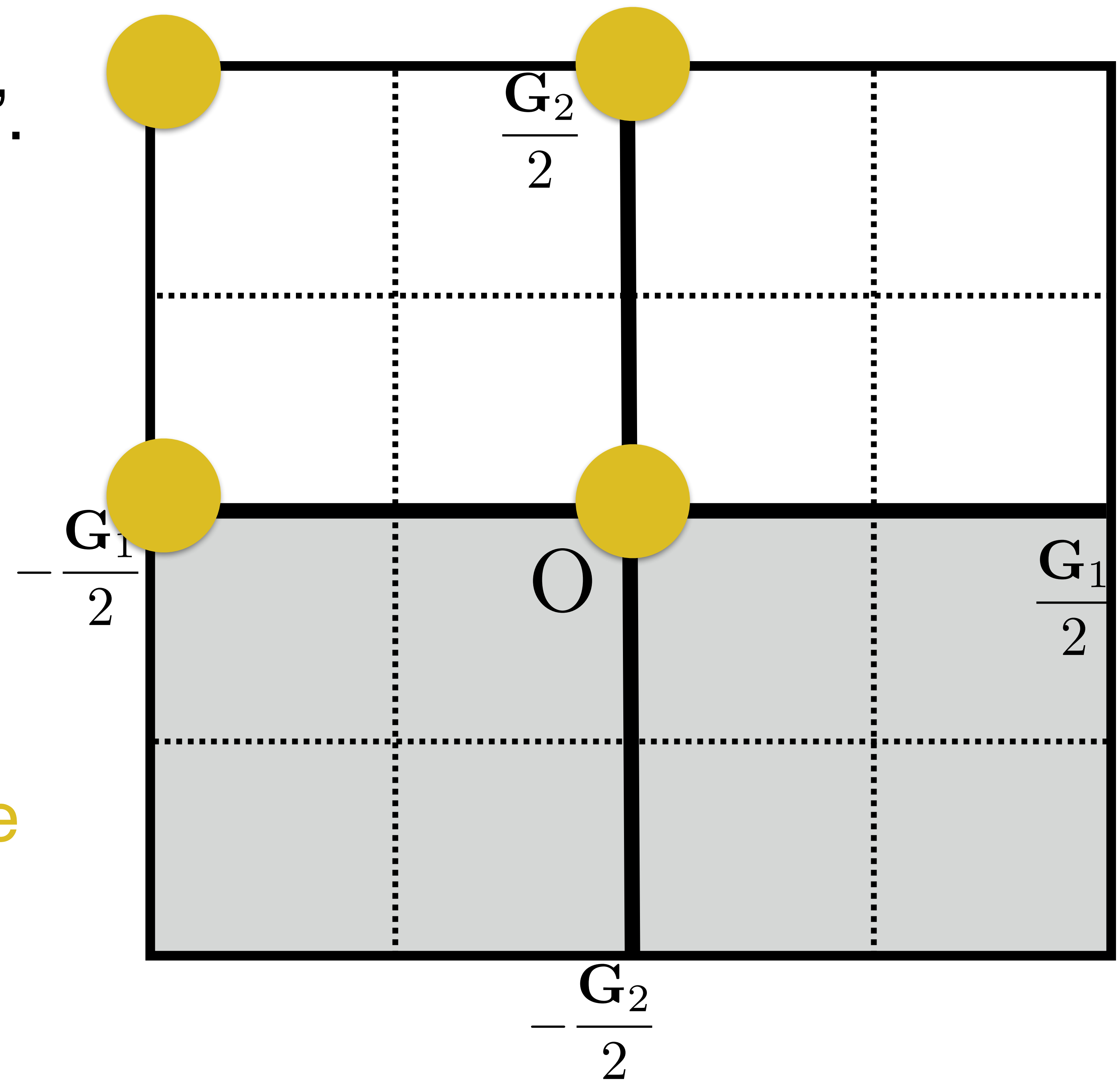


You have to “gauge fix”.

1. Transition symmetric points

$$|u_n(\mathbf{k}+\frac{\mathbf{G}_1}{2})\rangle = \mathrm{e}^{i\mathbf{G}_1\cdot\mathbf{r}}|u_n(\mathbf{k}-\frac{\mathbf{G}_1}{2}\rangle$$

You have to “gauge fix”.

2. Time reversal symmetric points

$$|u_n(\mathbf{k})\rangle = \Theta\,|u_n(-\mathbf{k})\rangle$$

$$\begin{aligned} |u_n(\mathbf{k})\rangle &= (S_+ - S_-)(|u_n^{*\uparrow}(-\mathbf{k})\rangle\,|\uparrow\rangle + |u_n^{*\downarrow}(-\mathbf{k})\rangle\,|\downarrow\rangle \\ &= |u_n^{*\downarrow}(-\mathbf{k})\rangle\,|\uparrow\rangle - |u_n^{*\uparrow}(-\mathbf{k})\rangle\,|\downarrow\rangle \end{aligned}$$

You have to “gauge fix”.

3. Kramers degenerate points

$$|u_{2n}(0)\rangle = \Theta\, |u_{2n-1}(0)\rangle$$

$$|u_{2n}(-\frac{\mathbf{G}_1}{2})\rangle = e^{i\mathbf{G}_1\cdot\mathbf{r}}\Theta\, |u_{2n-1}(-\frac{\mathbf{G}_1}{2})\rangle$$

$$|u_{2n}(\frac{\mathbf{G}_2}{2})\rangle = e^{-i\mathbf{G}_2\cdot\mathbf{r}}\Theta\, |u_{2n-1}(\frac{\mathbf{G}_2}{2})\rangle$$

$$|u_{2n}(\frac{\mathbf{G}_2}{2} - \frac{\mathbf{G}_1}{2})\rangle = e^{-i(\mathbf{G}_2-\mathbf{G}_1)\cdot\mathbf{r}}\Theta\, |u_{2n-1}(\frac{\mathbf{G}_2}{2} - \frac{\mathbf{G}_1}{2})\rangle$$

How to implement “gauge fix”

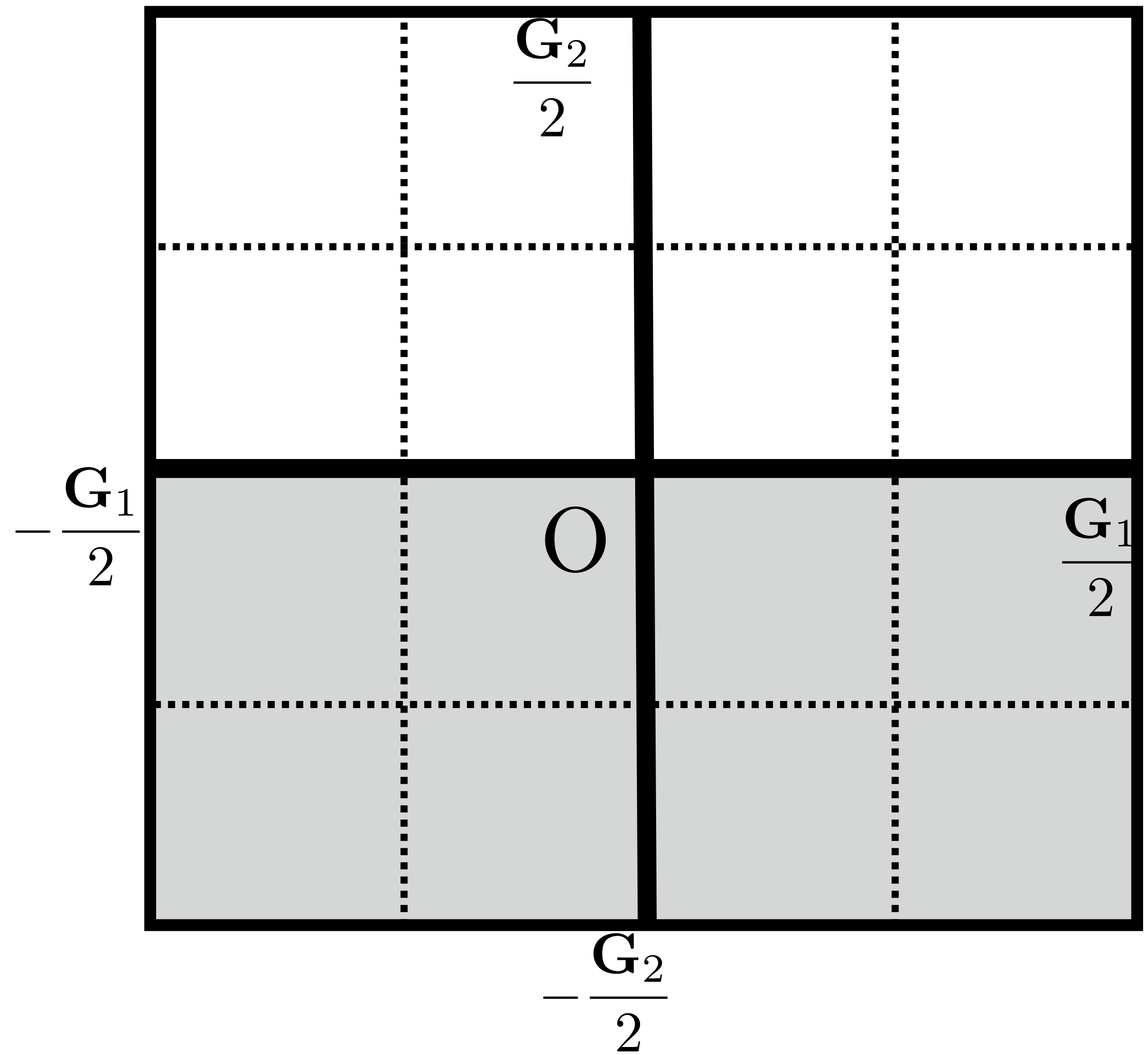
1. Fix gauge on "Kramers degenerate points"

2. Compute LCN on left BZ

3. Fix gauge on "Transition symmetric points" and "Time reversal symmetric points"

4. Compute LCN in right BZ

5. Summate LCN (mod 2)



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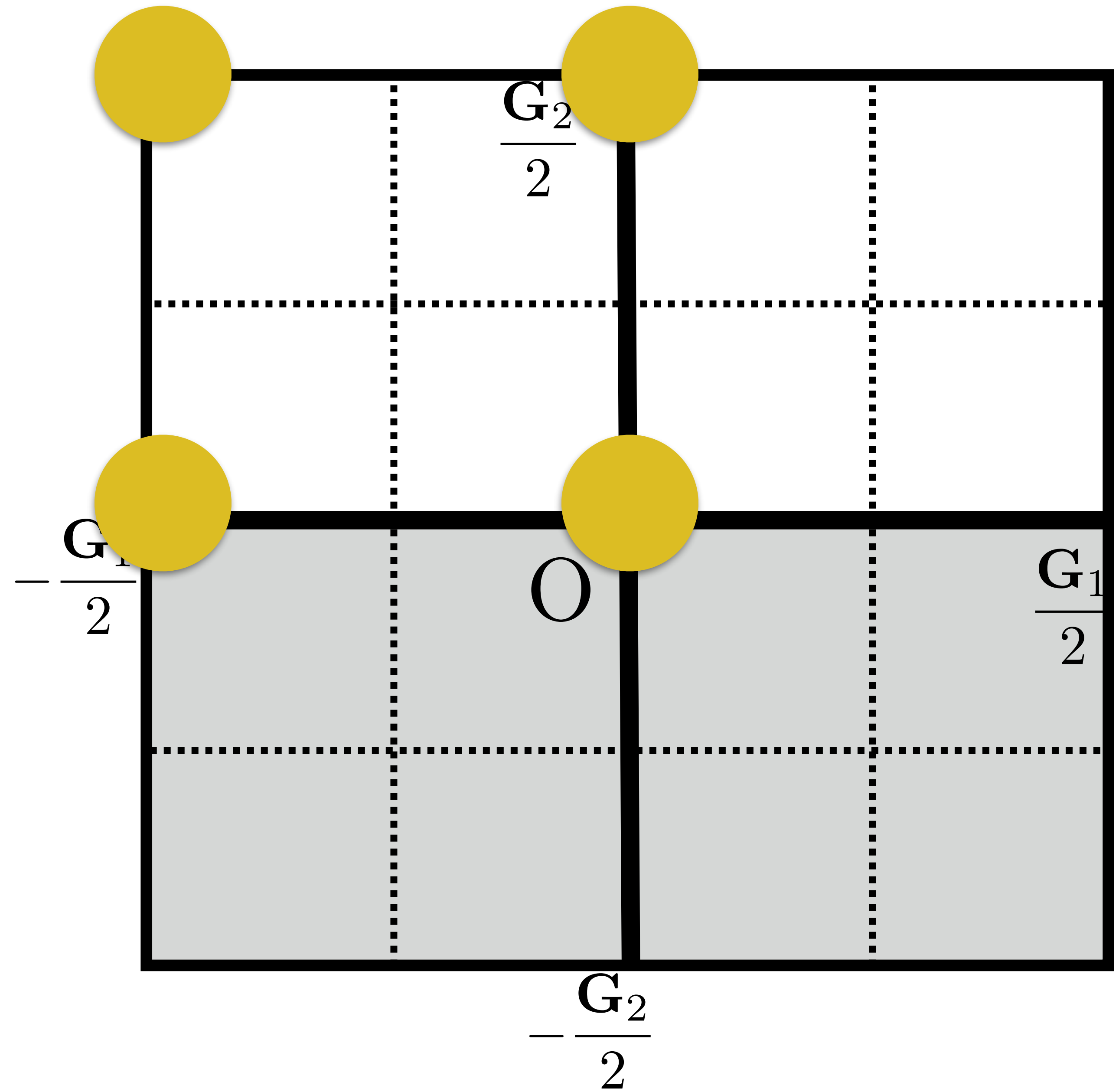

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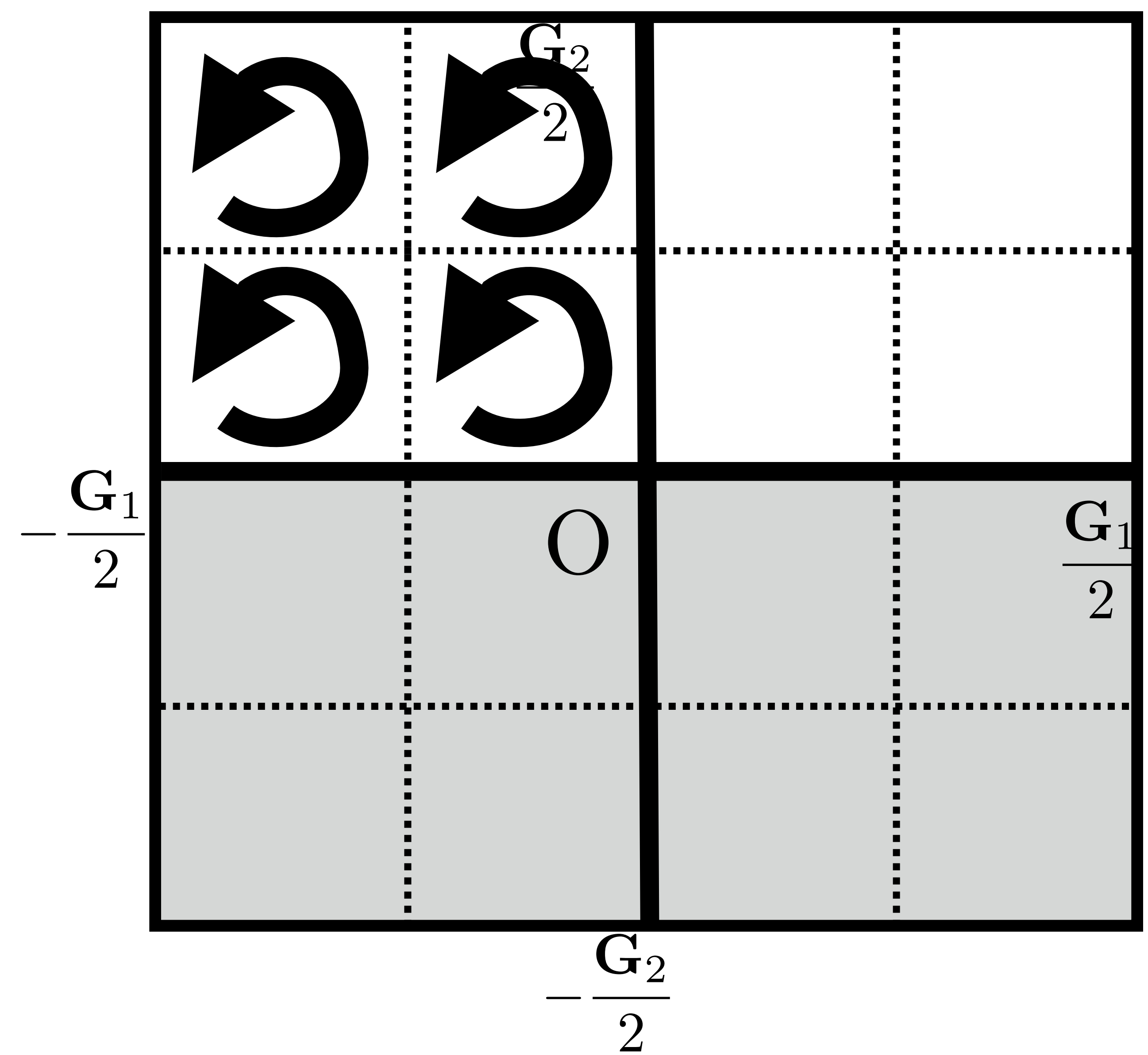

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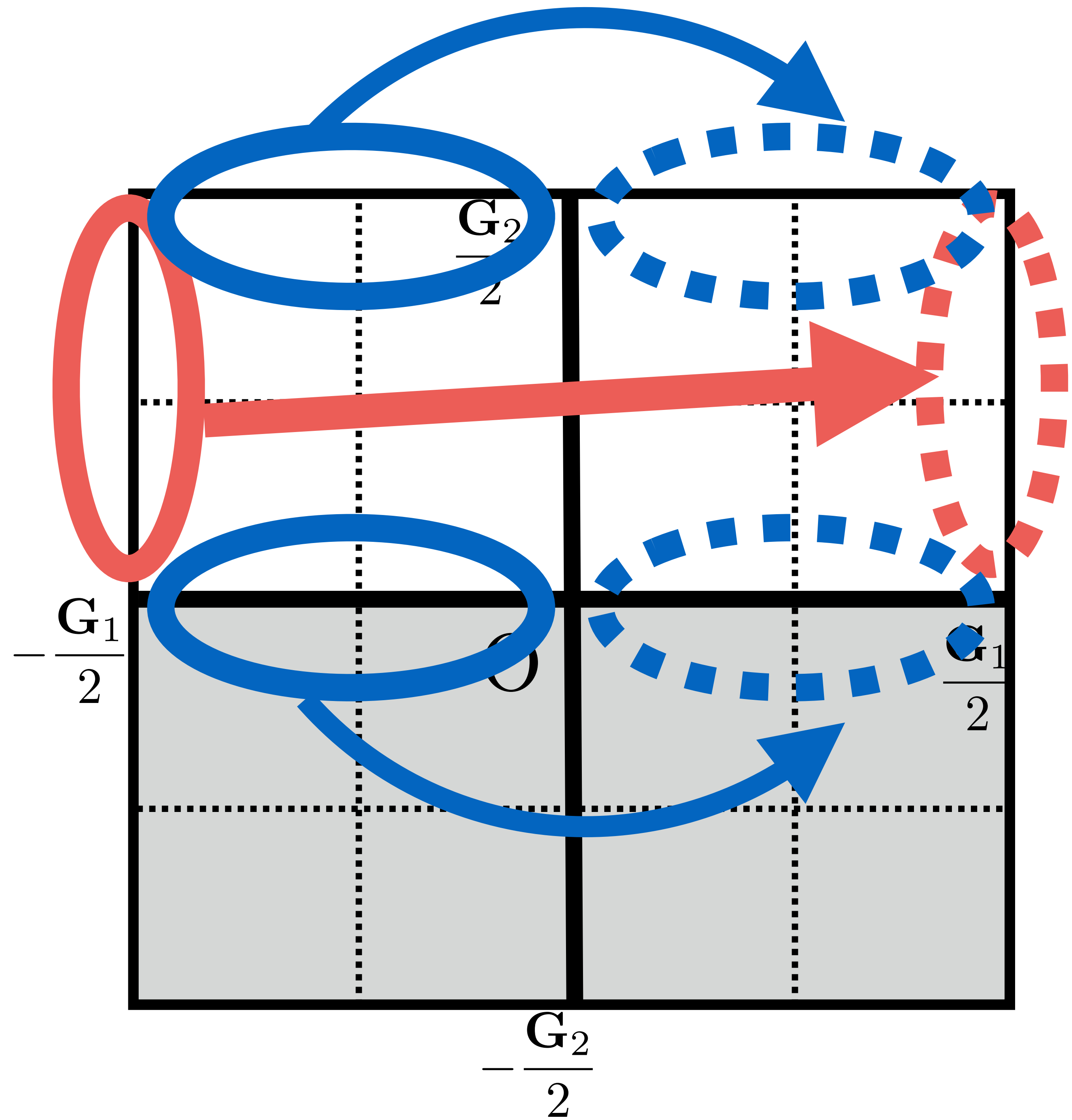

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4. **Compute LCN in right BZ**

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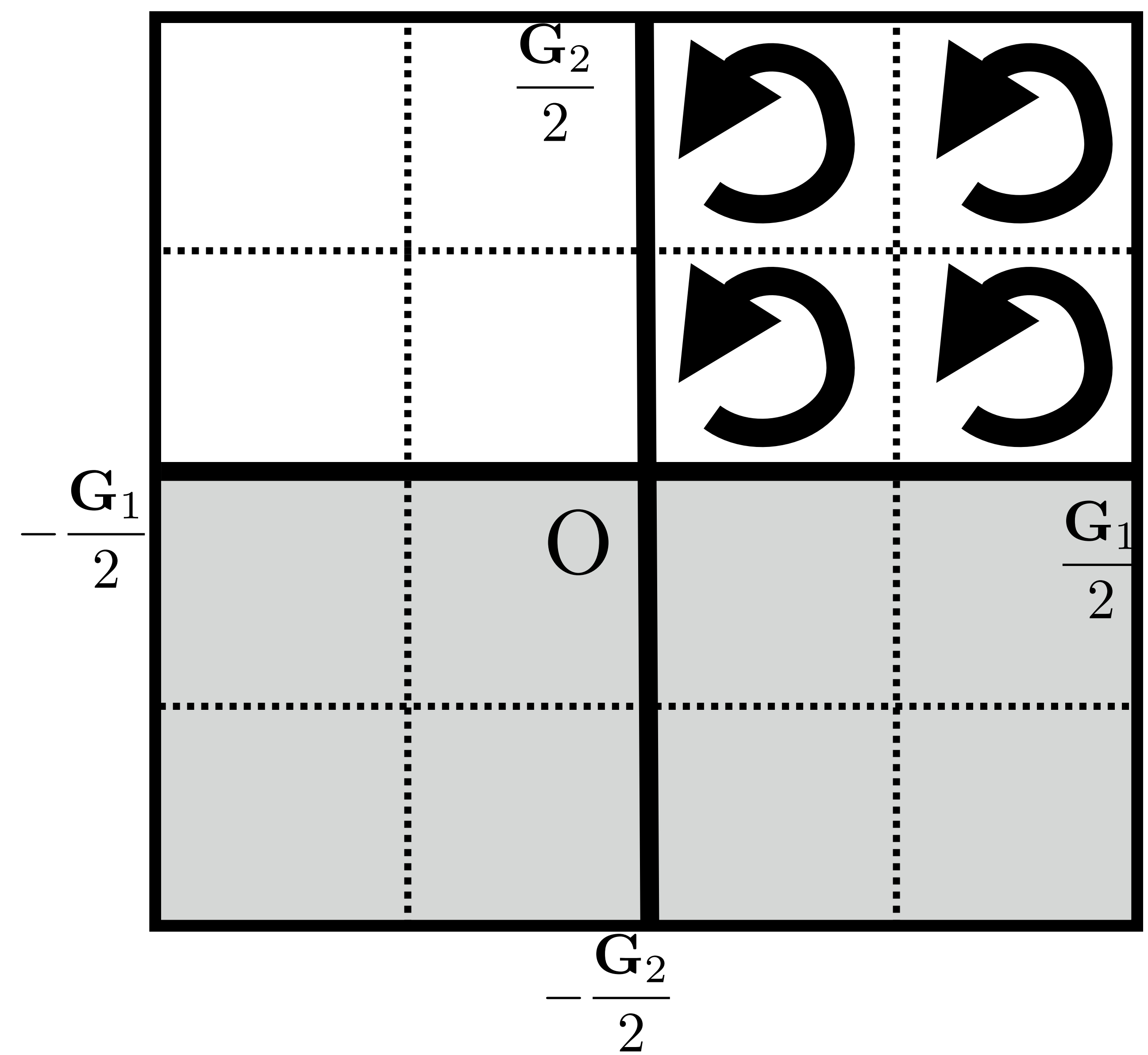

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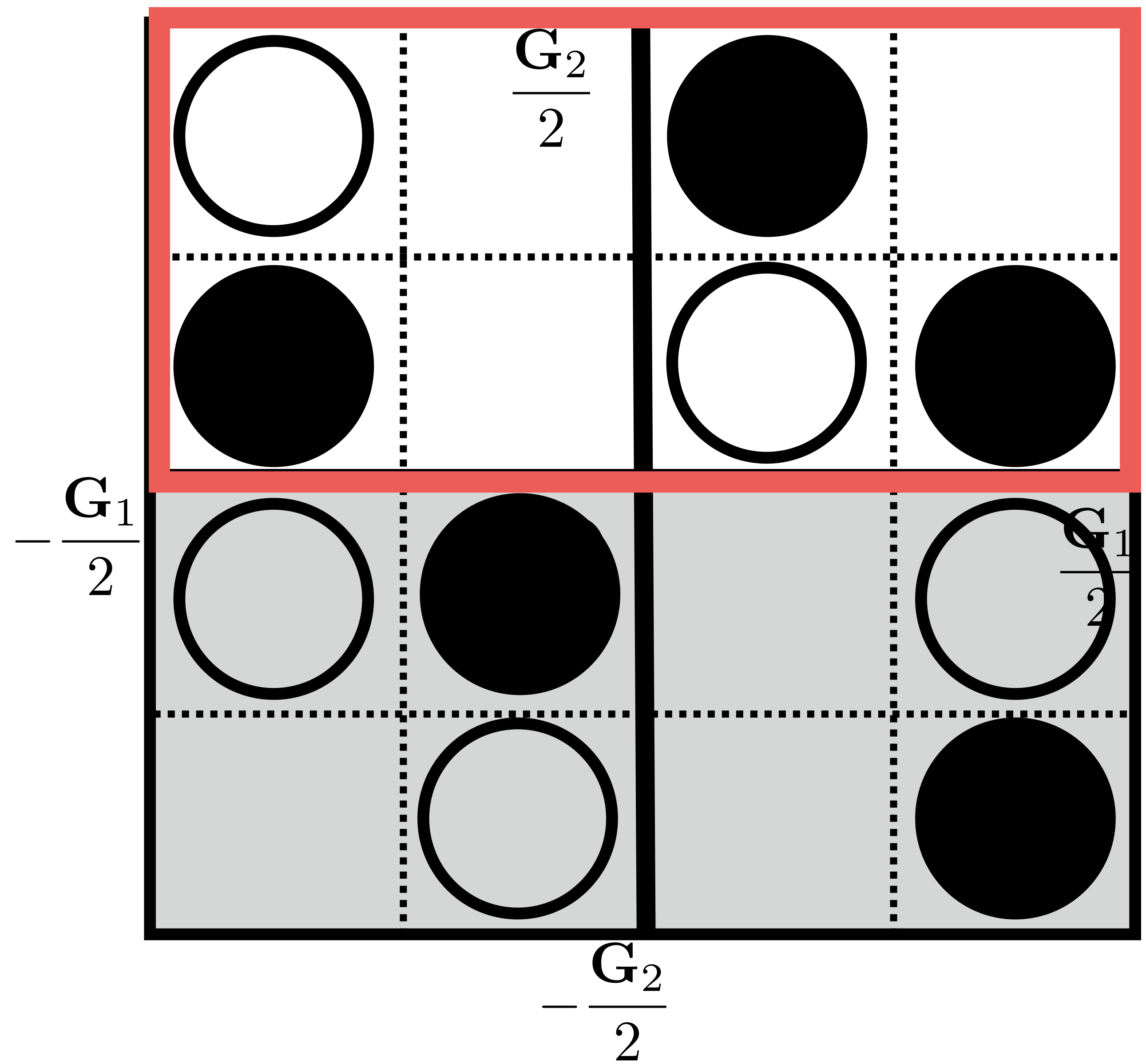
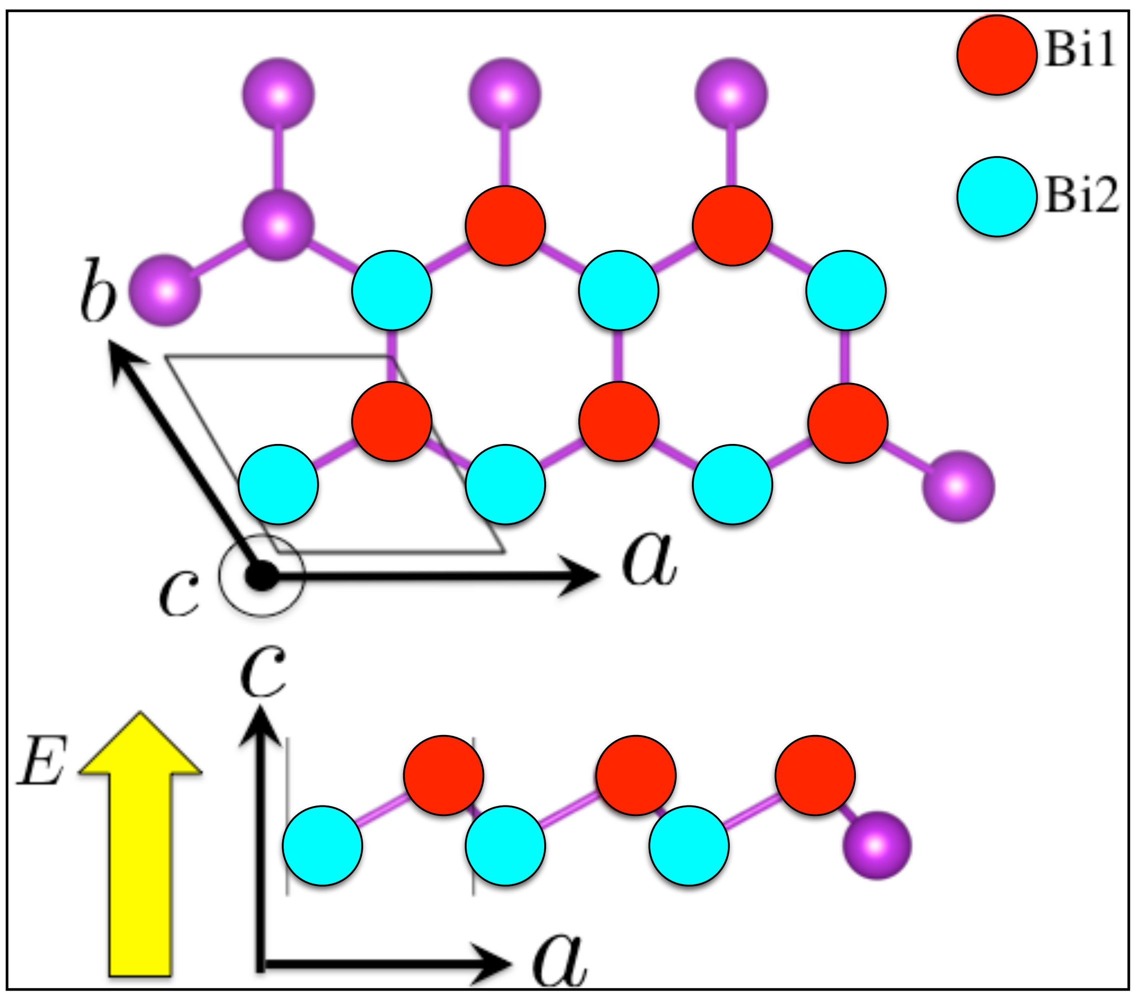


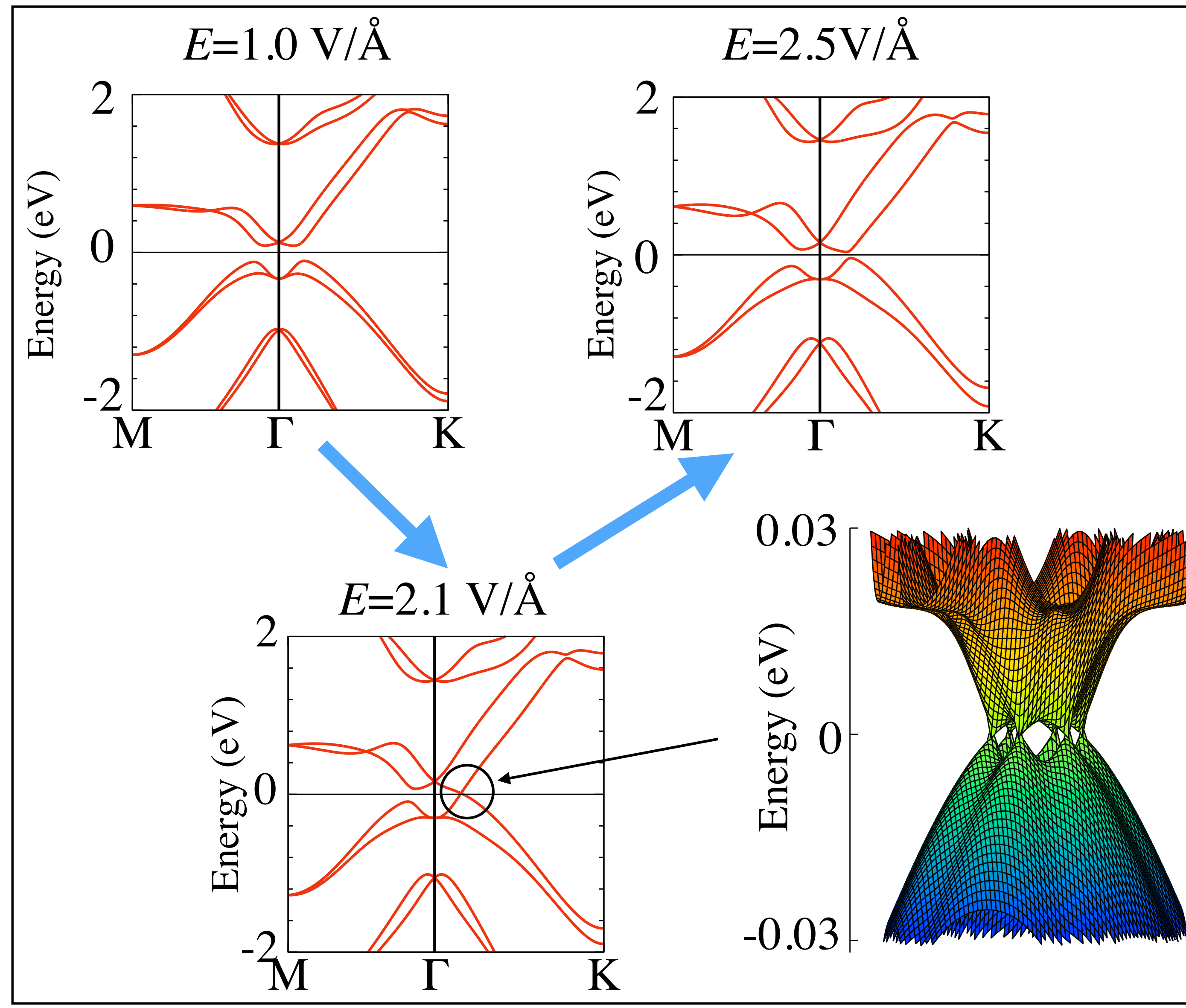
Application

We implement
to OpenMX

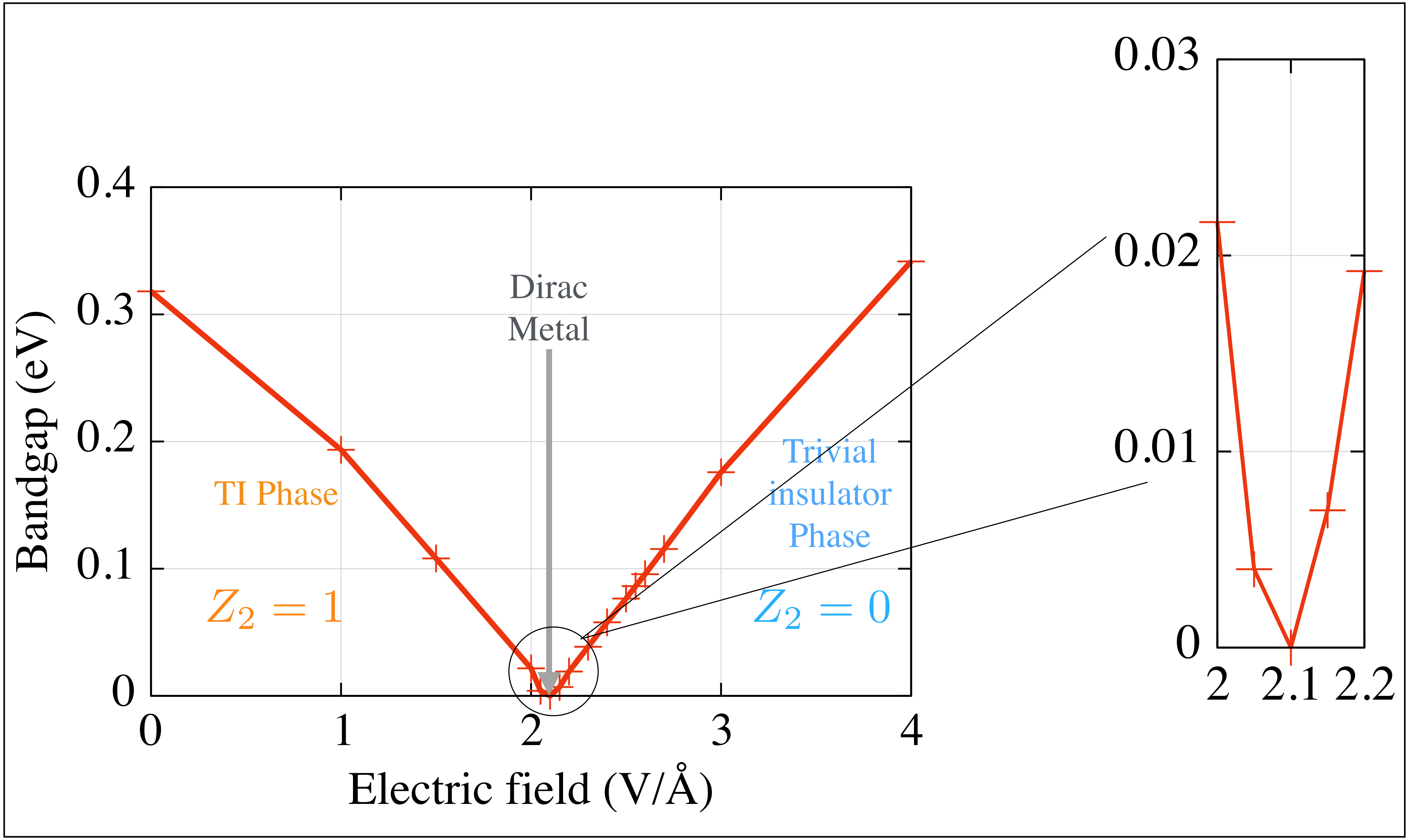
T. Ozaki et al., http://www.openmx-square.org/.

Electric-fields induced topological phase transition on one-bilayer Bi(111)





Topological phase diagram



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