topology, oxidation states, and charge transport in ionic conductors

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invited talk given at the 2022 Psi-k conference, Lausanne, August 22-25, 2021

serious answers to three silly questions

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- how come the electric conductivity of non-ionic fluids vanishes, when the current fluctuations that determine it, do not?

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serious answers to three silly questions

- how come the electric conductivity of non-ionic fluids vanishes, when the current fluctuations that determine it, do not?
- how come the conductivity of (stoichiometric) electrolytes is correctly predicted when real-valued, time-dependent, tensor Born effective charges are replaced with integer-valued, time-independent, scalar atomic oxidation states?
- what are oxidation states, in the first place?

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charge transport

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energy transport

$$\boldsymbol{J}_{\mathcal{E}} = \sum_I e_I \boldsymbol{V}_I + \frac{1}{2} \sum_{I \neq J} (\boldsymbol{V}_I \cdot \boldsymbol{F}_{IJ})(\boldsymbol{R}_I - \boldsymbol{R}_J)$$

$$\boldsymbol{F}_{\mathcal{E}} = -\nabla T$$

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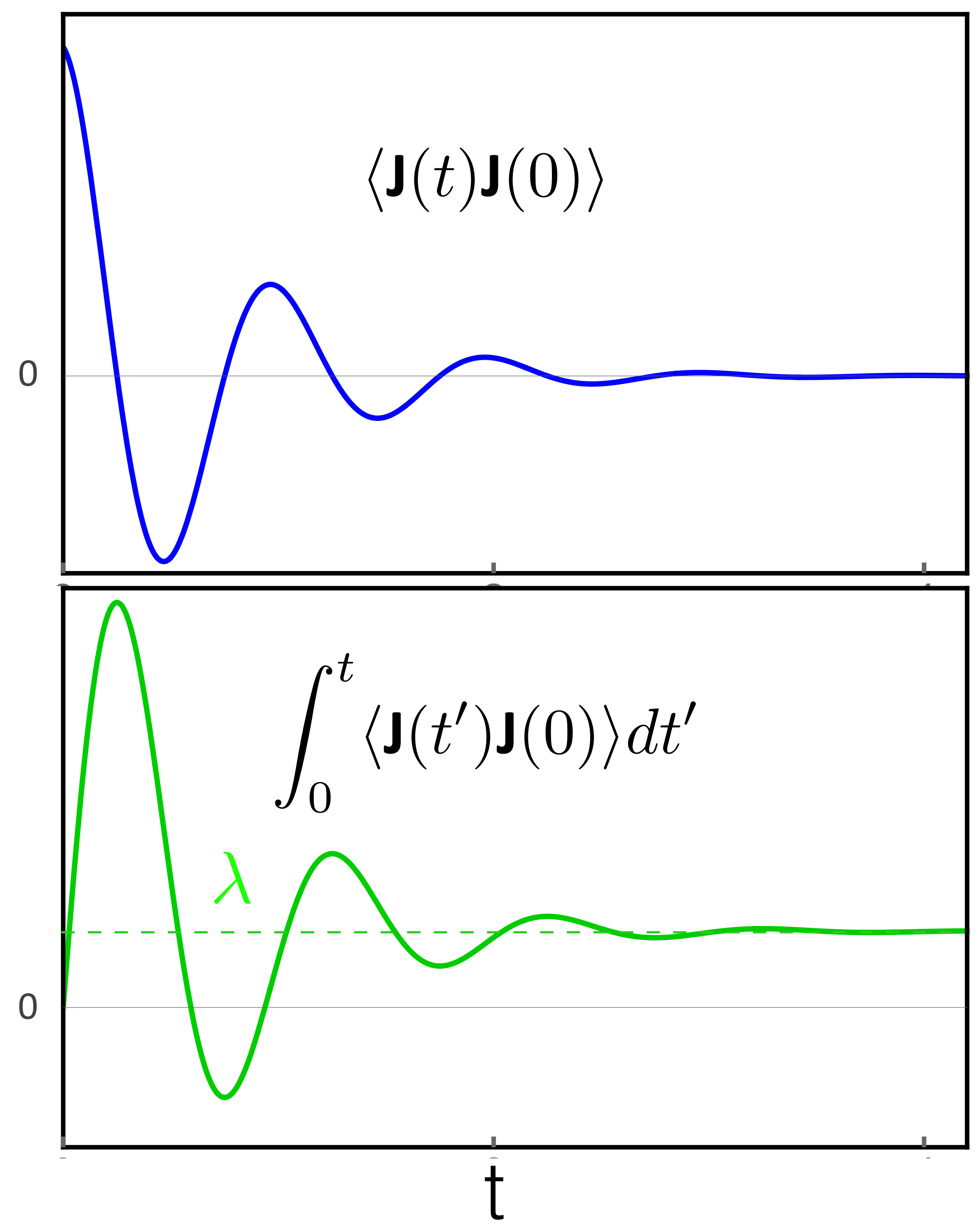

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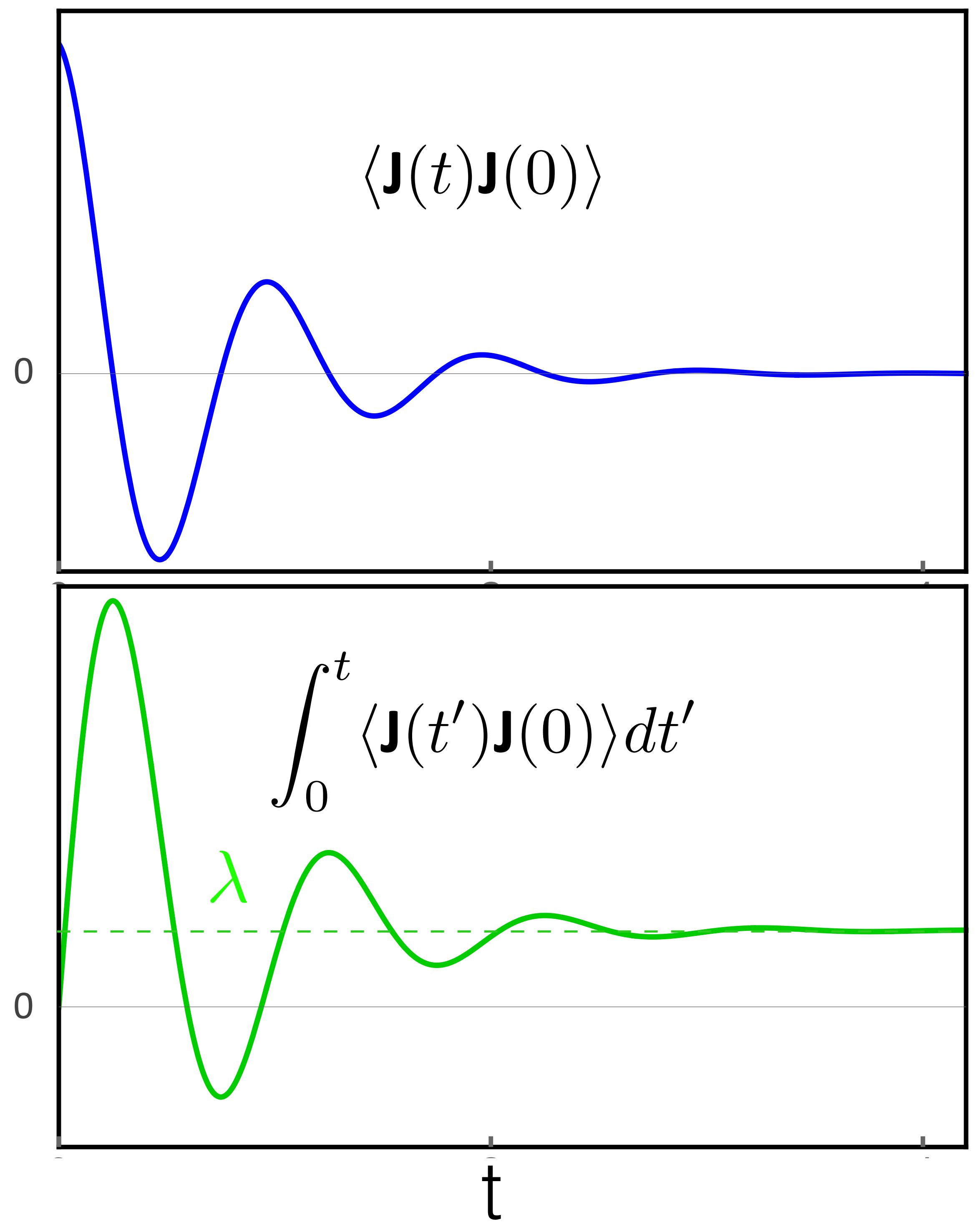
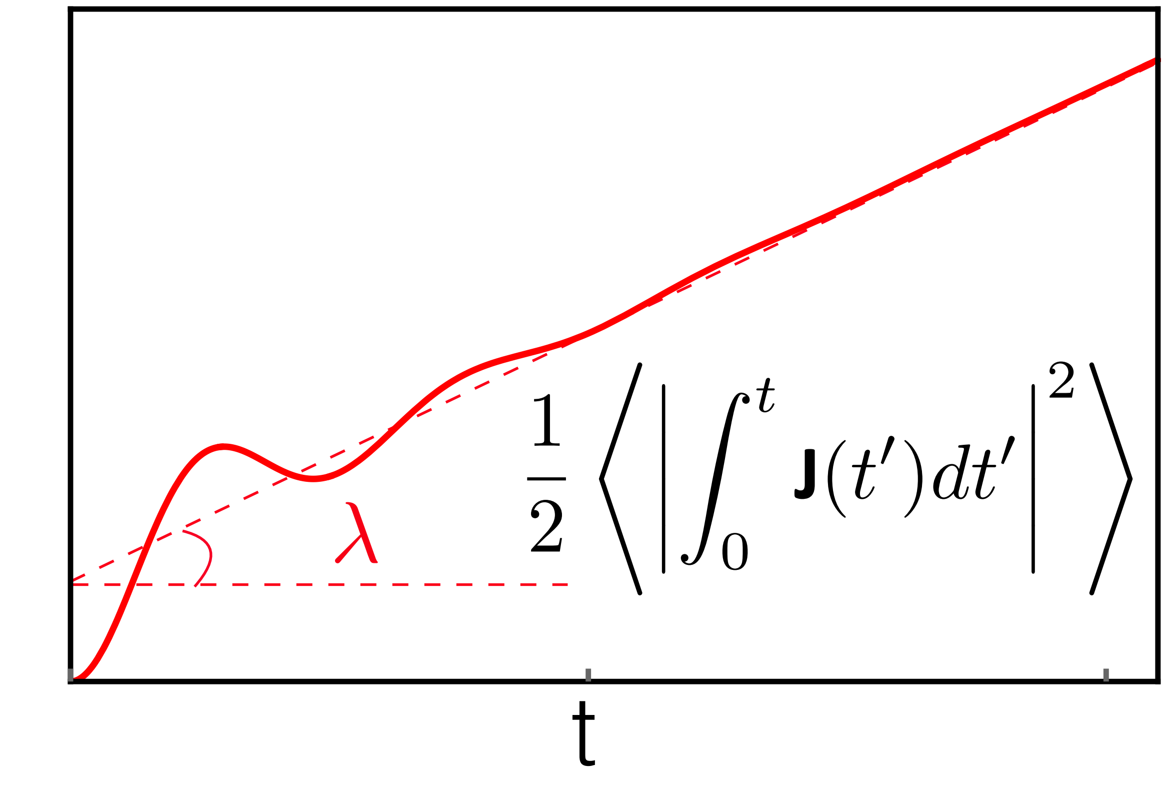
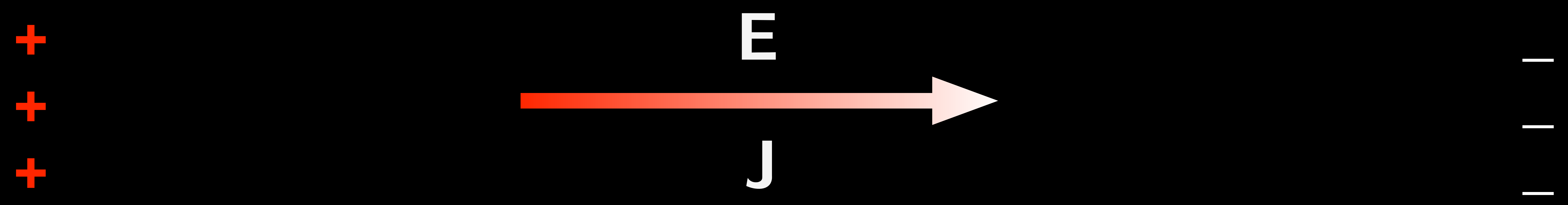


Einstein-Helfand

$$\lambda \propto \lim_{t\to\infty} \frac{1}{2t} \mathrm{var}\left[\int_0^t \boldsymbol{J}(t')dt'\right]$$



ionic transport



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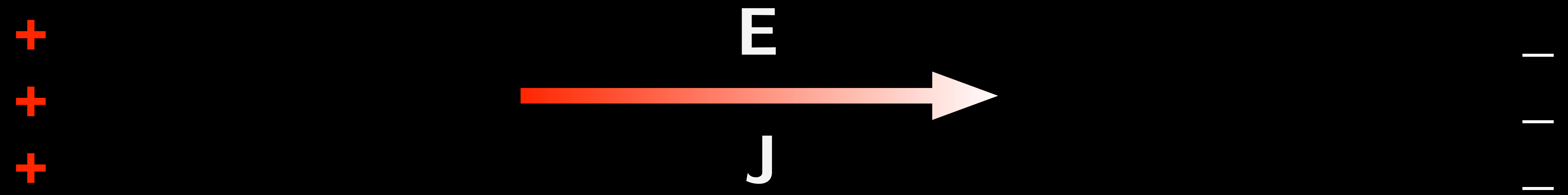

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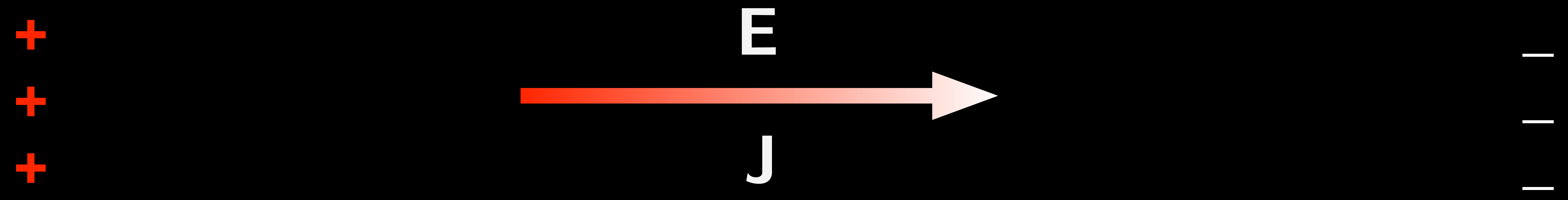

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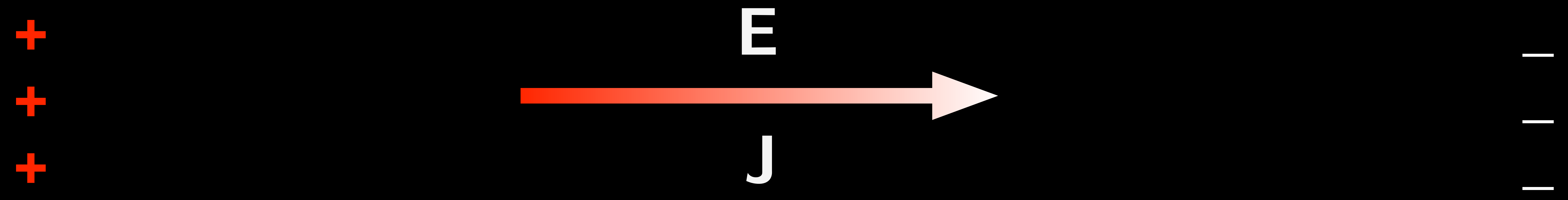

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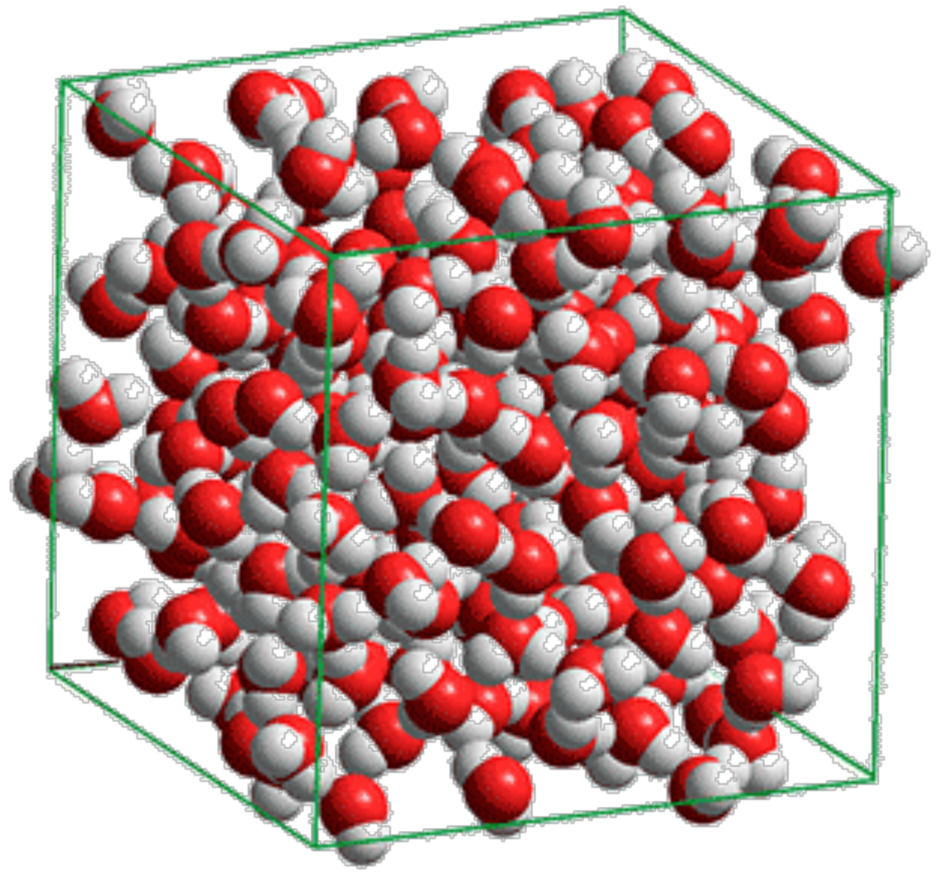
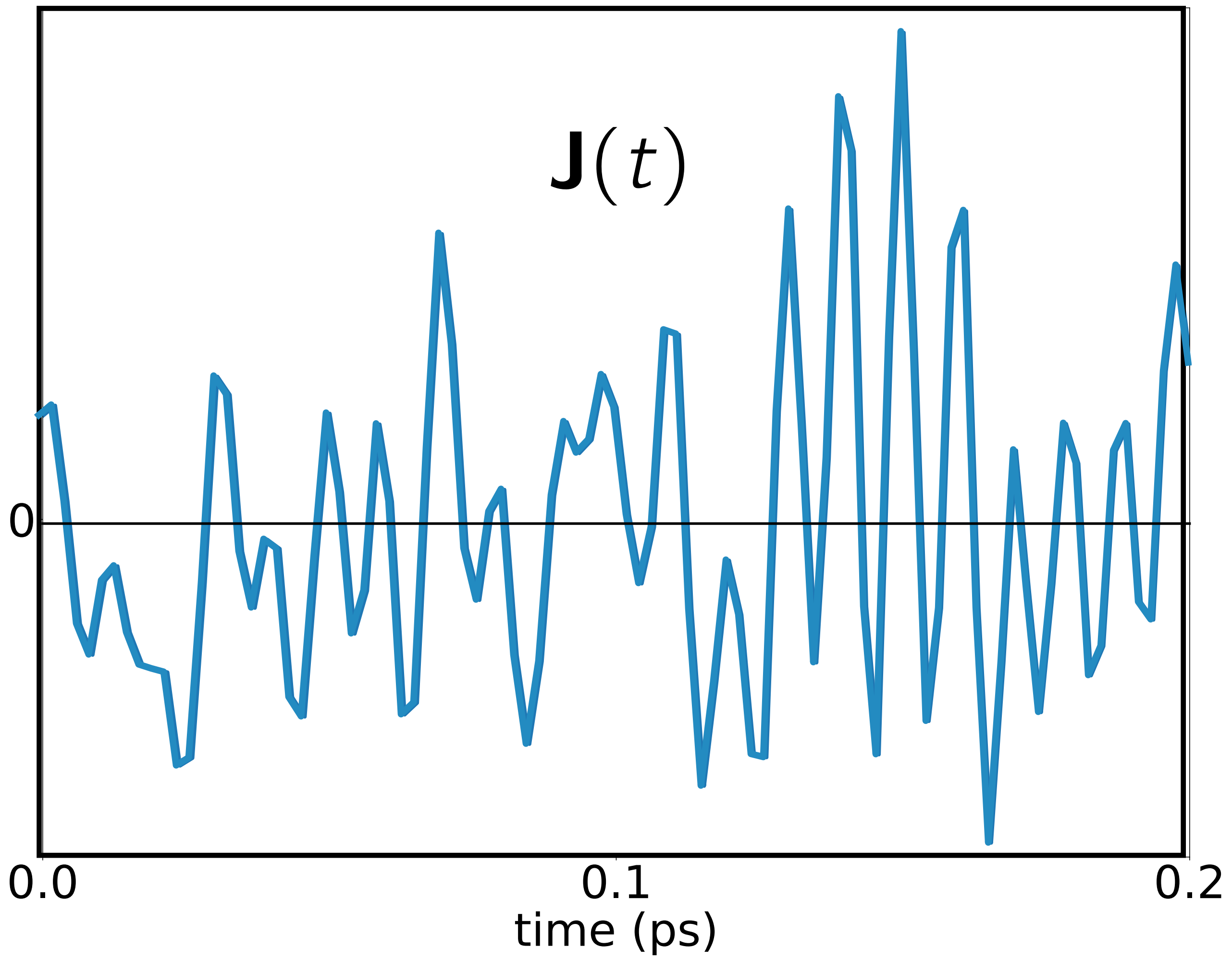
$$\sigma = \frac{\Omega}{3k_BT}\left\langle |\mathbf{J}|^2 \right\rangle \times \tau_J$$

the conundrum

molecular H_2O





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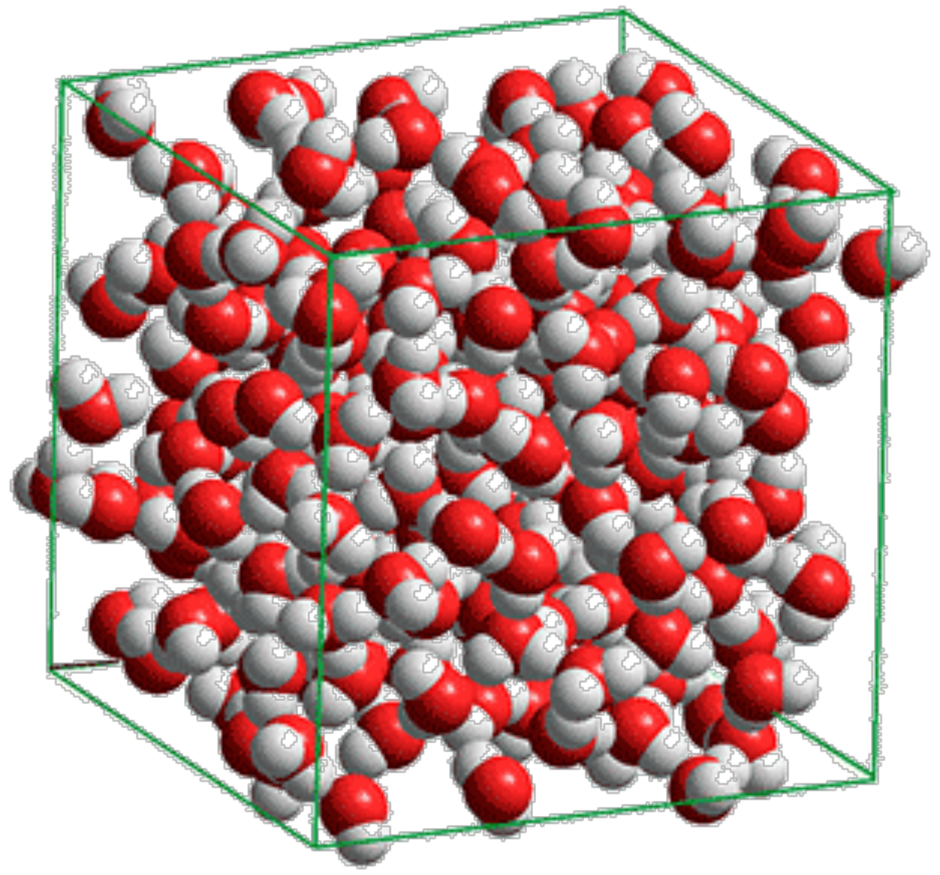

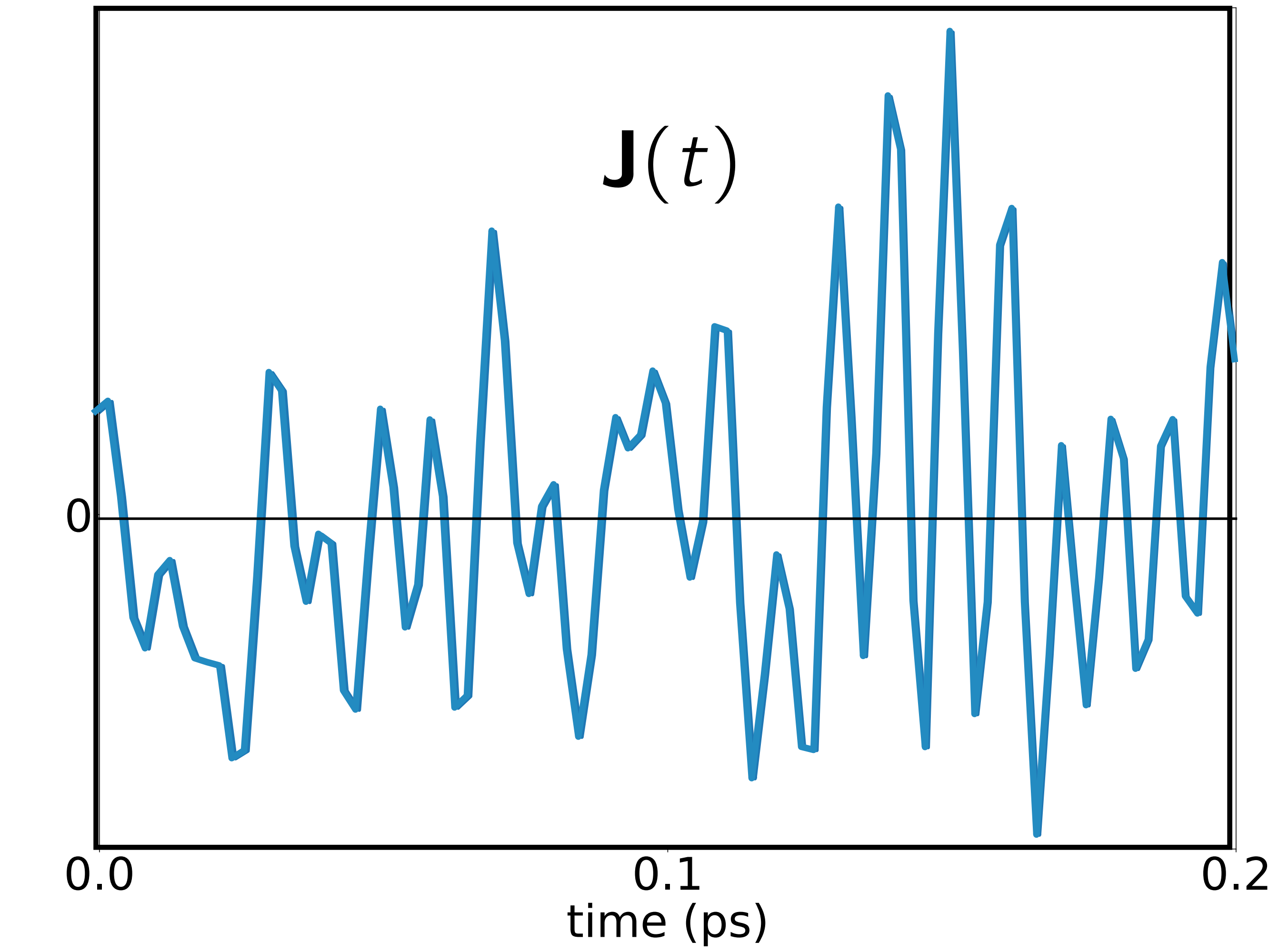

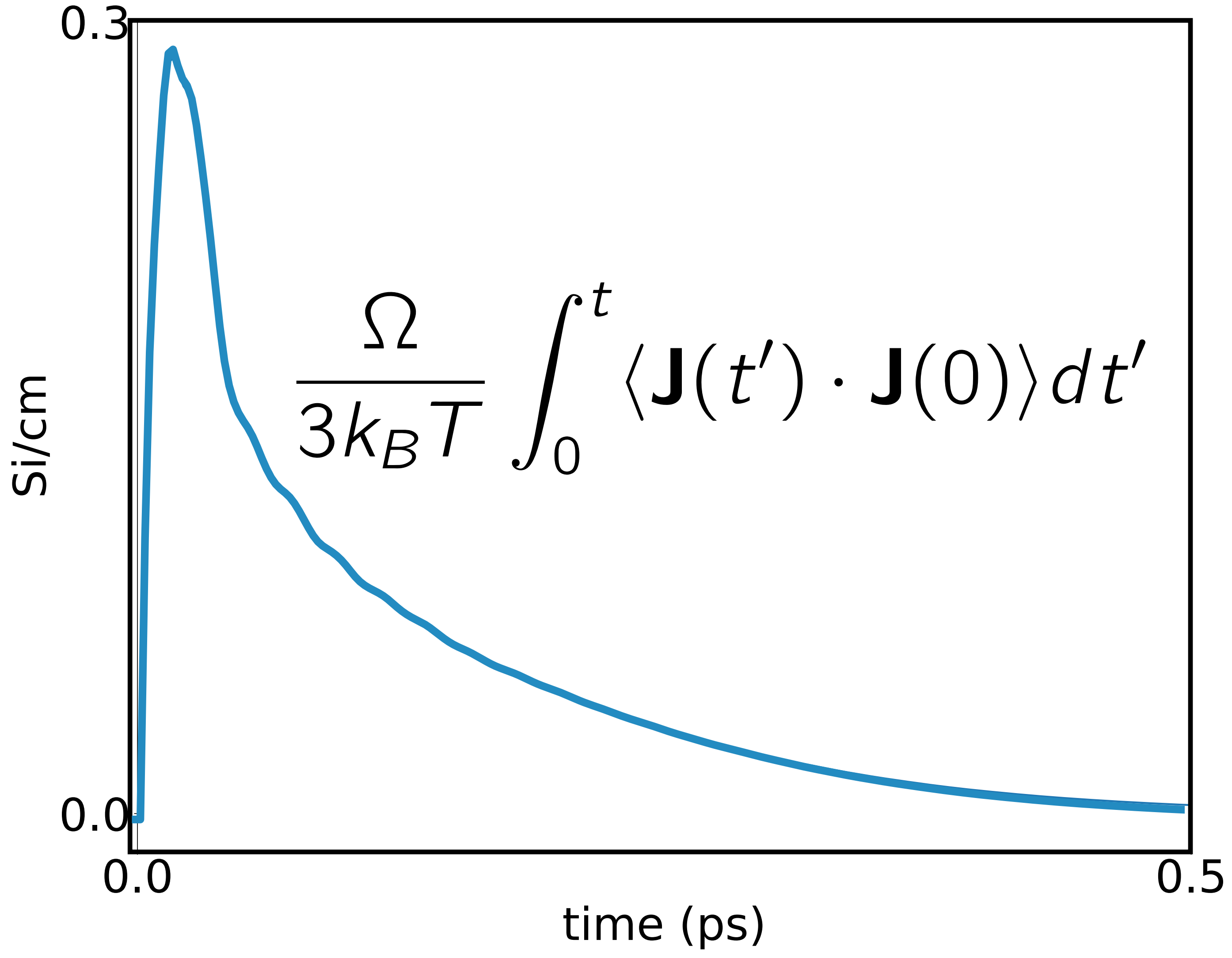

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PRL **107,** 185901 (2011) PHYSICAL REVIEW LETTERS week ending 28 OCTOBER 2011

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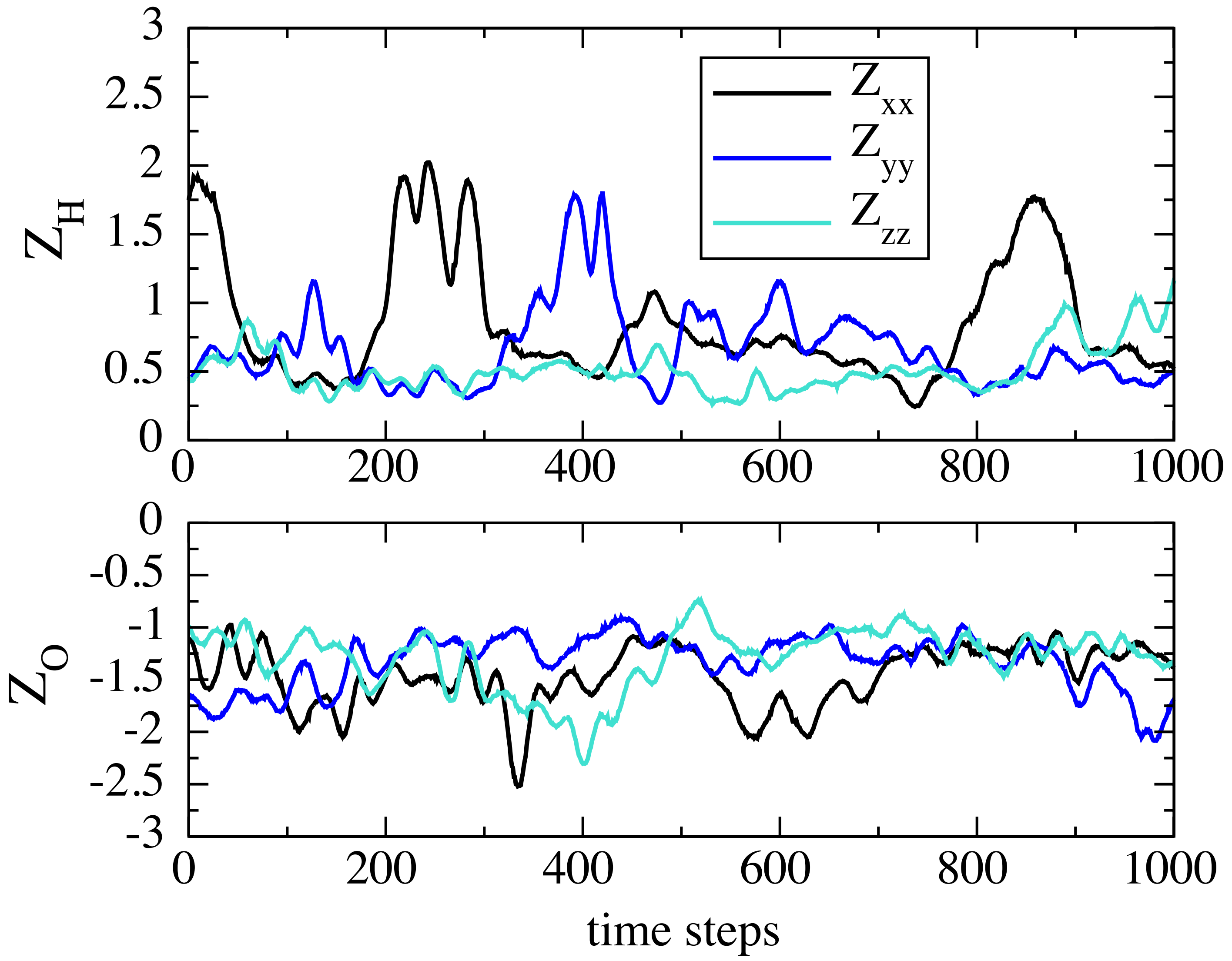
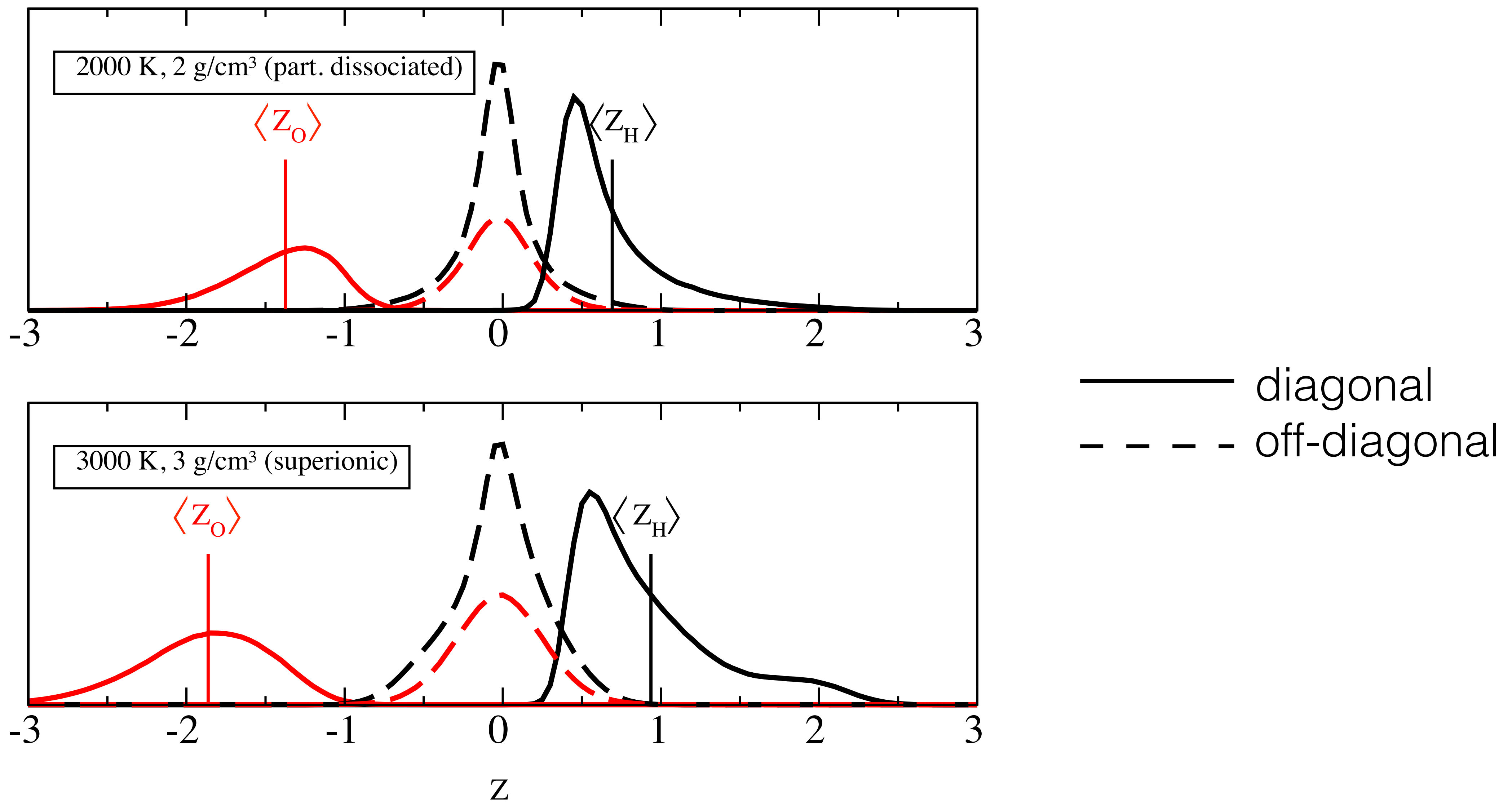
Martin French,[1] Sebastien Hamel,[2] and Ronald Redmer[1]





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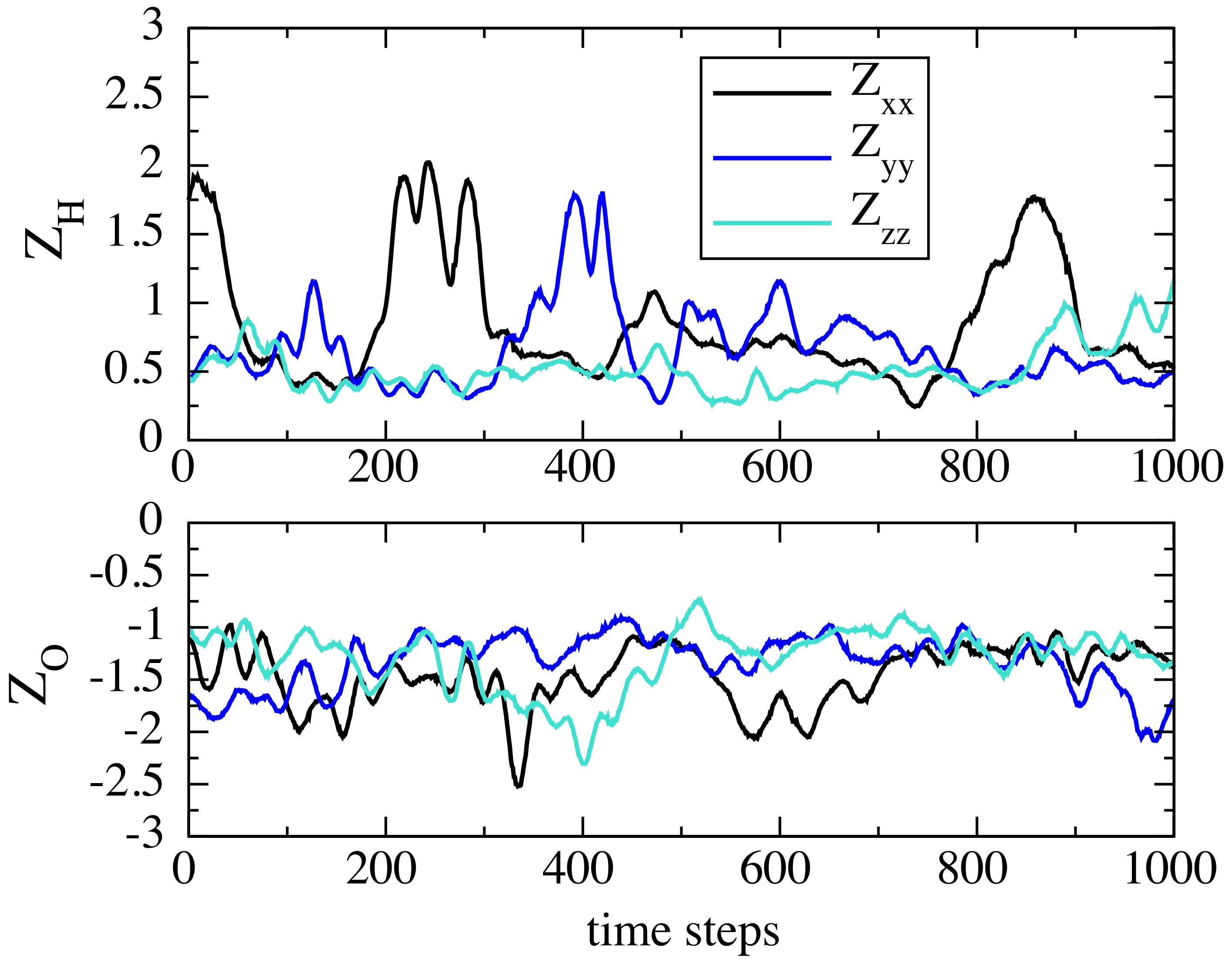

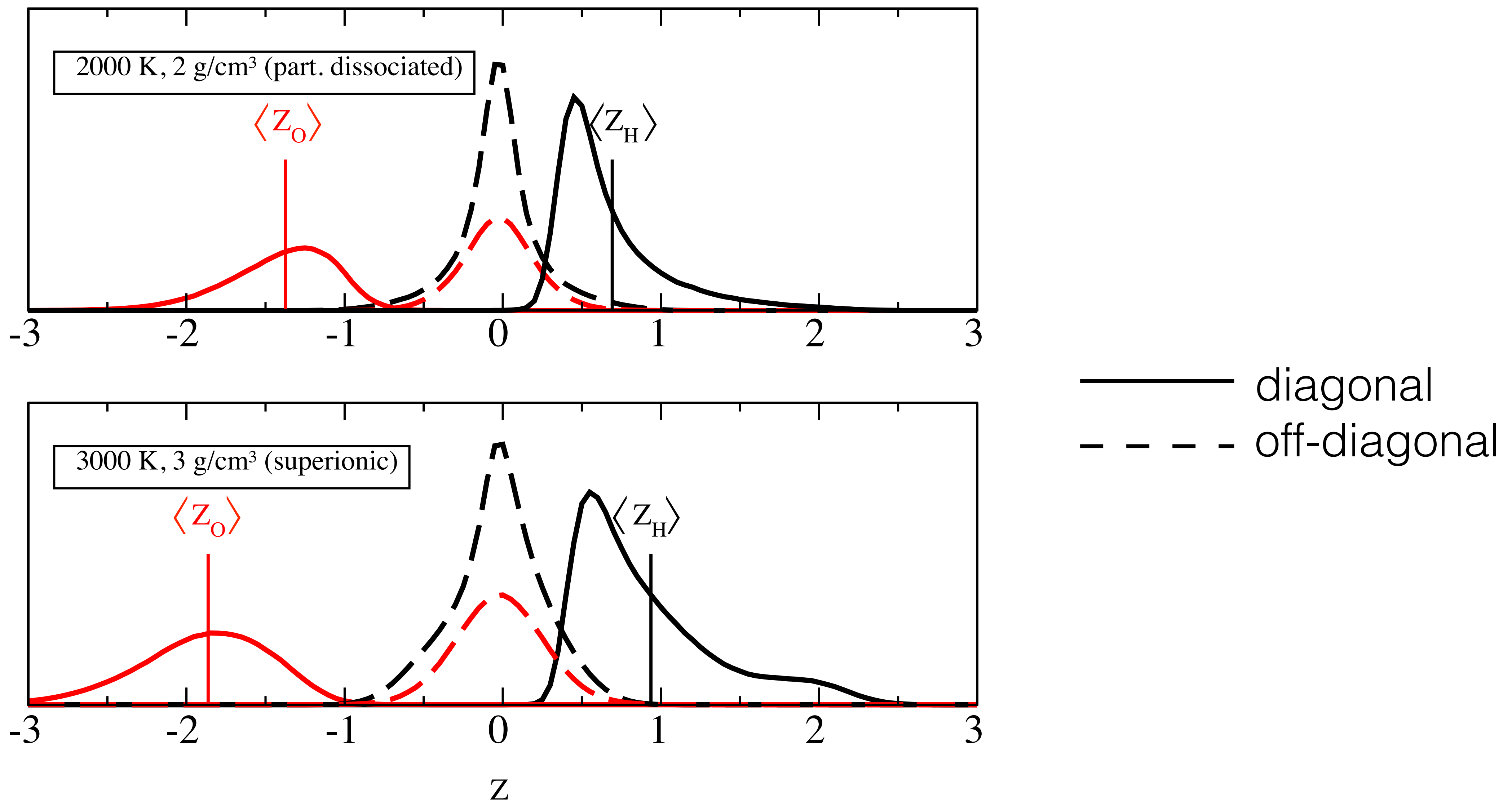

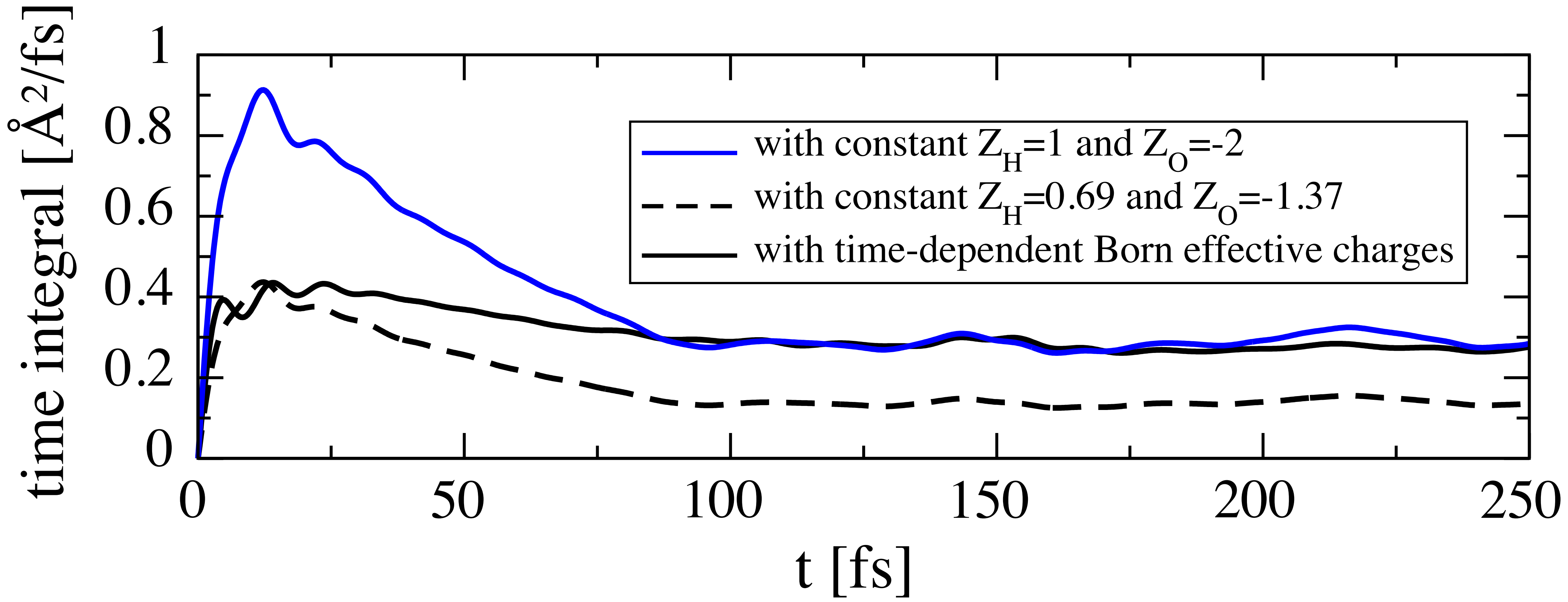

$$\int_0^t \langle \boldsymbol{J}(t')\boldsymbol{J}(0)\rangle dt'$$

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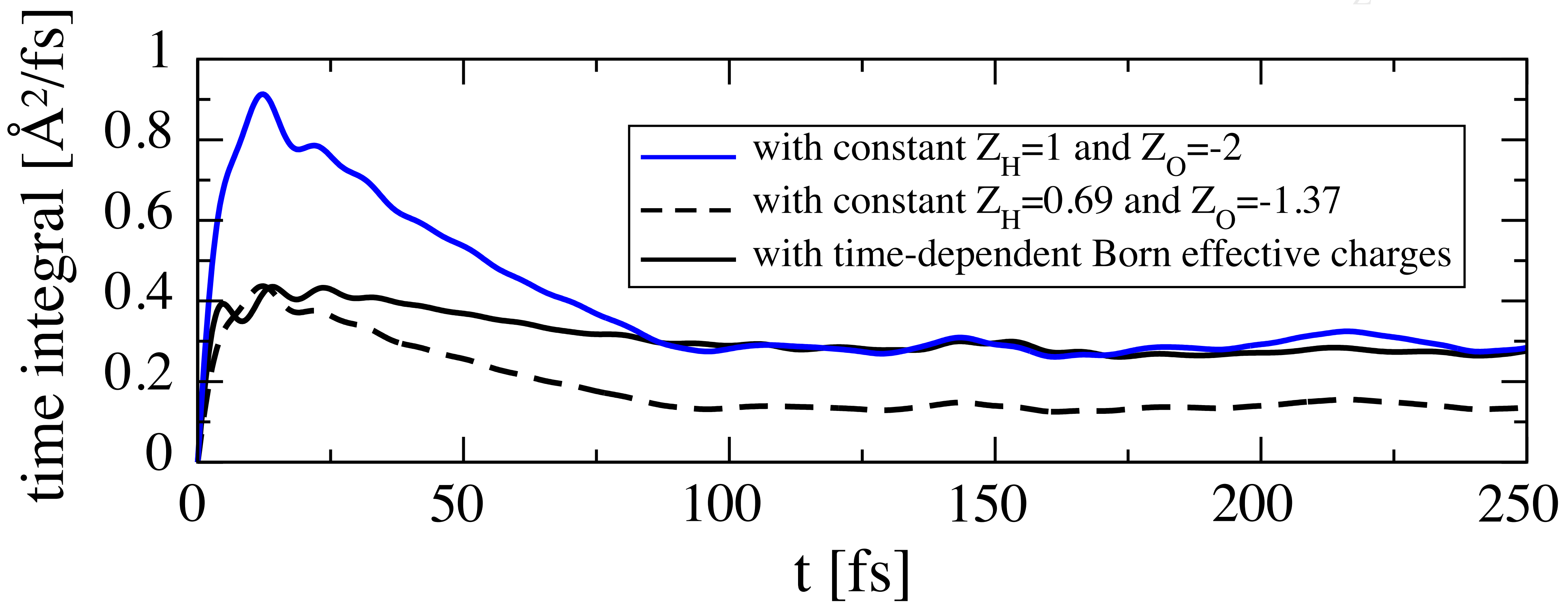

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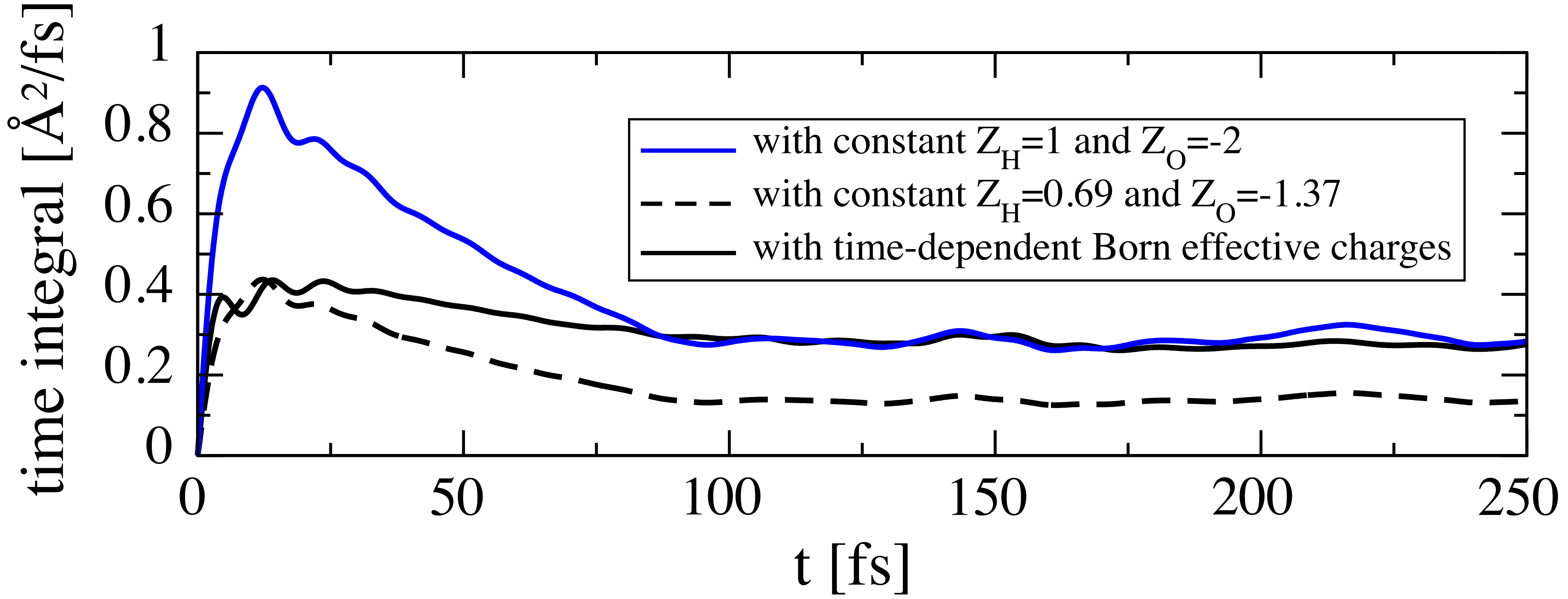
atomic *"oxidation states"*



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how come?

and what are oxidation states, in the first place?

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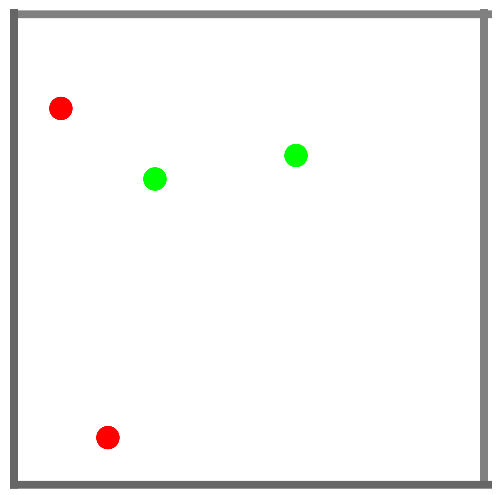

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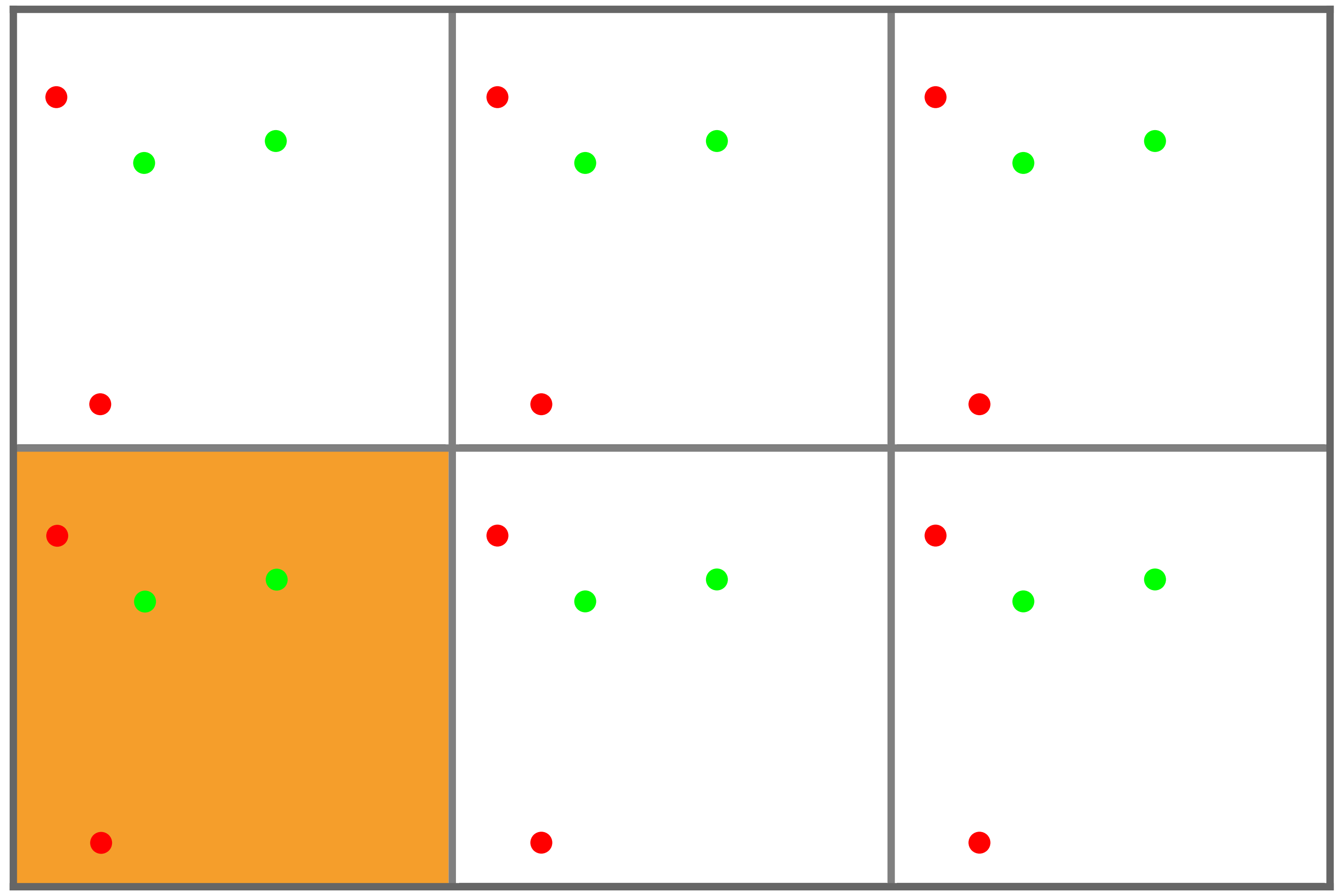

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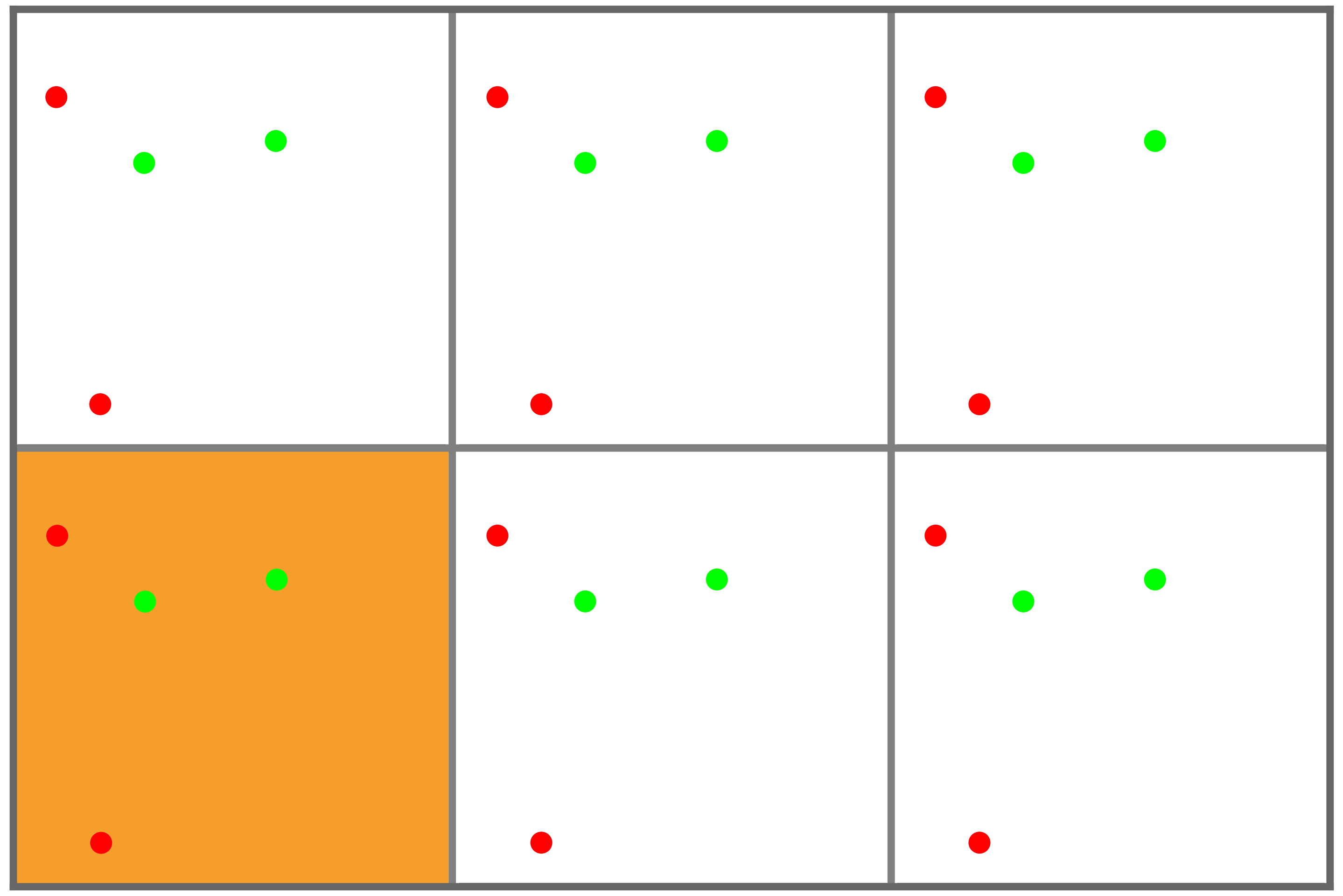
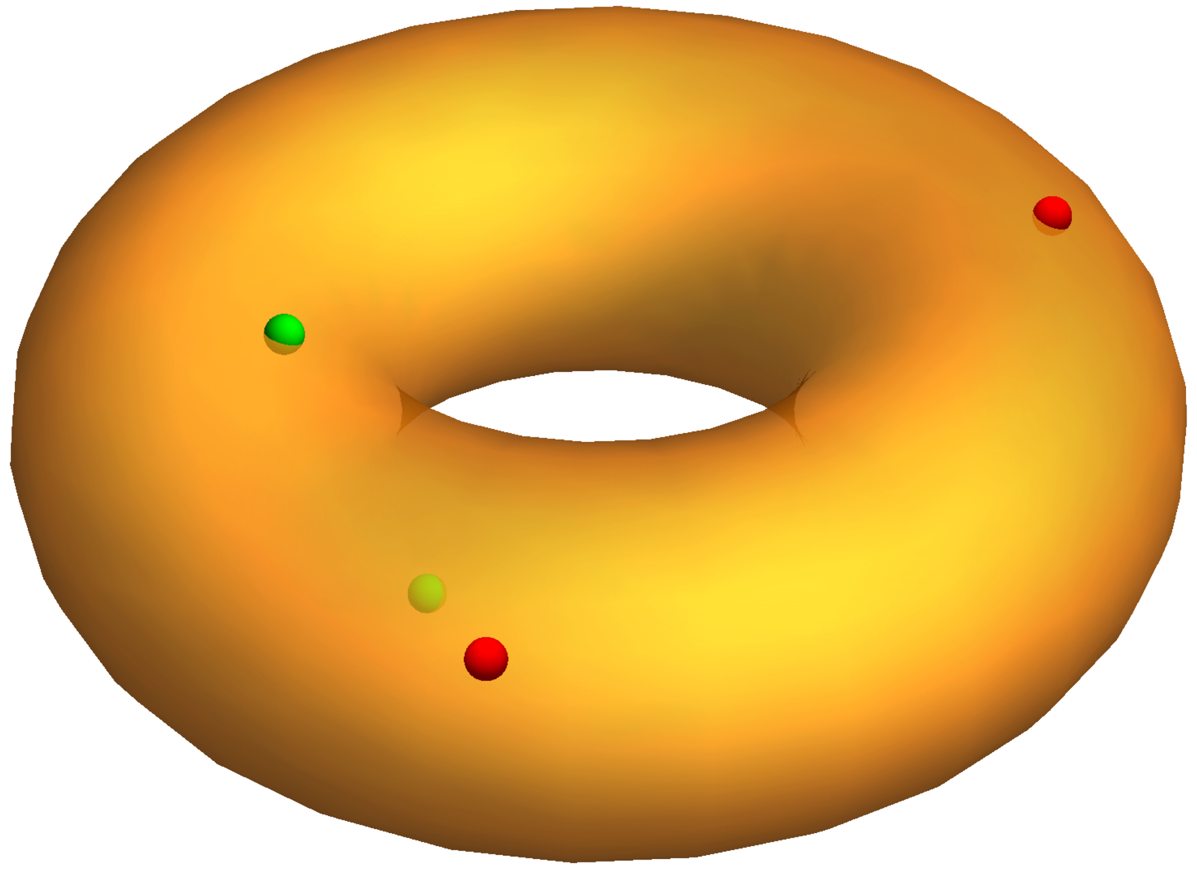
$$[0, L]^{3N} \xrightarrow{\text{PBC}} \mathbb{T}^{3N}$$





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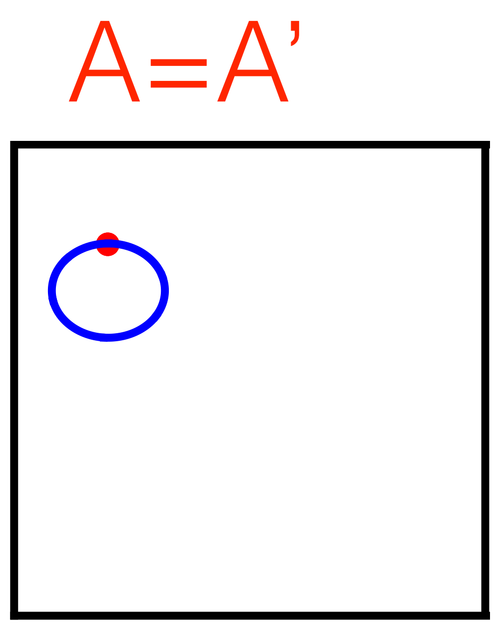

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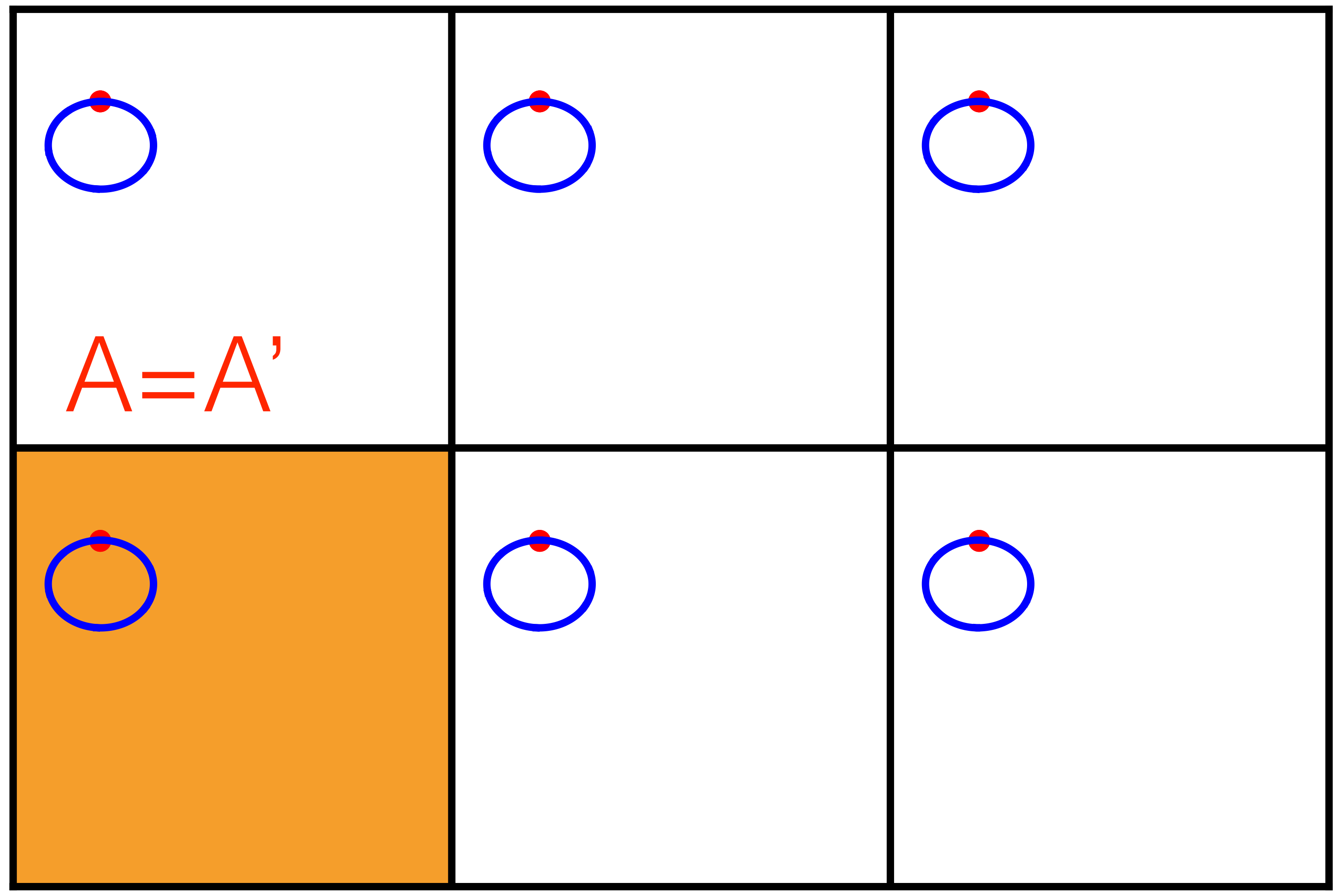

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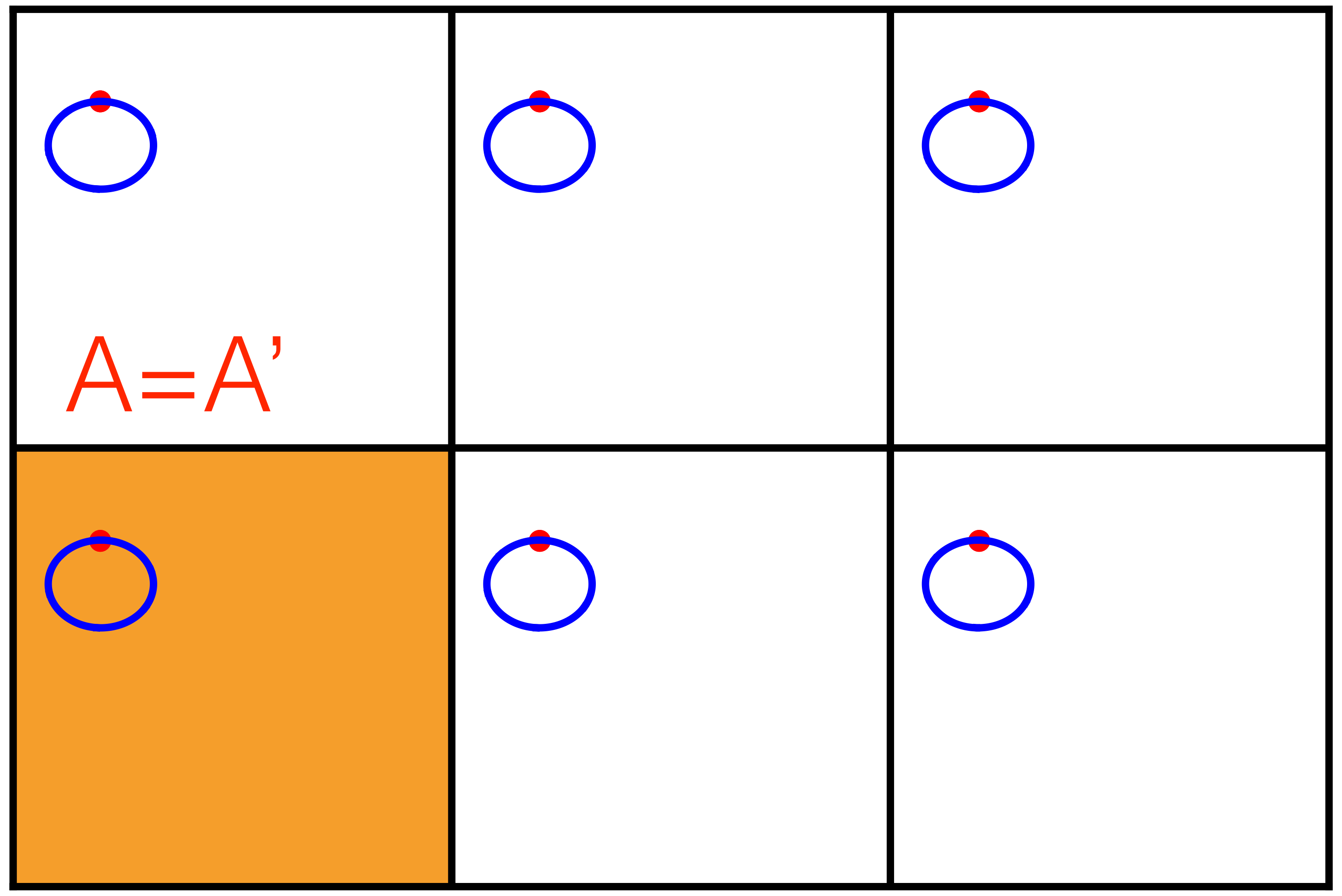

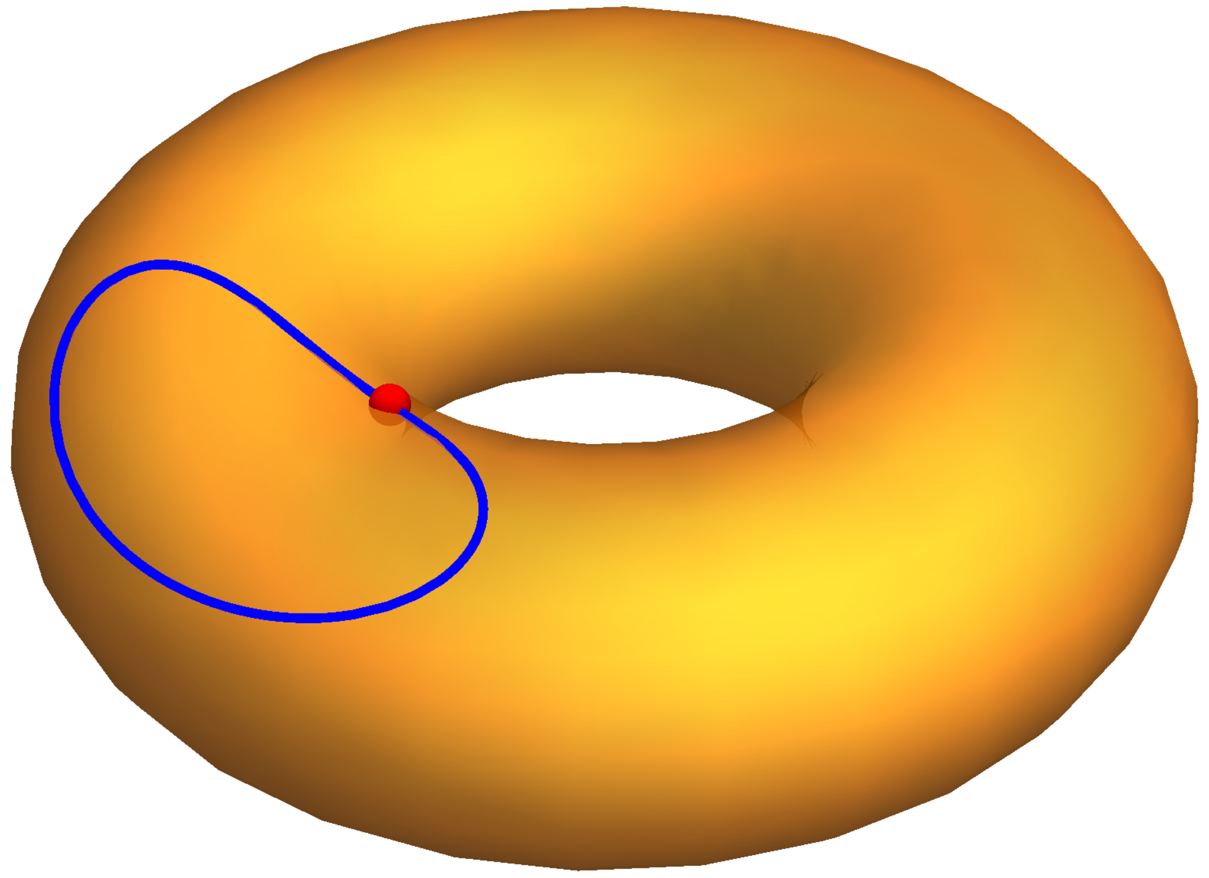

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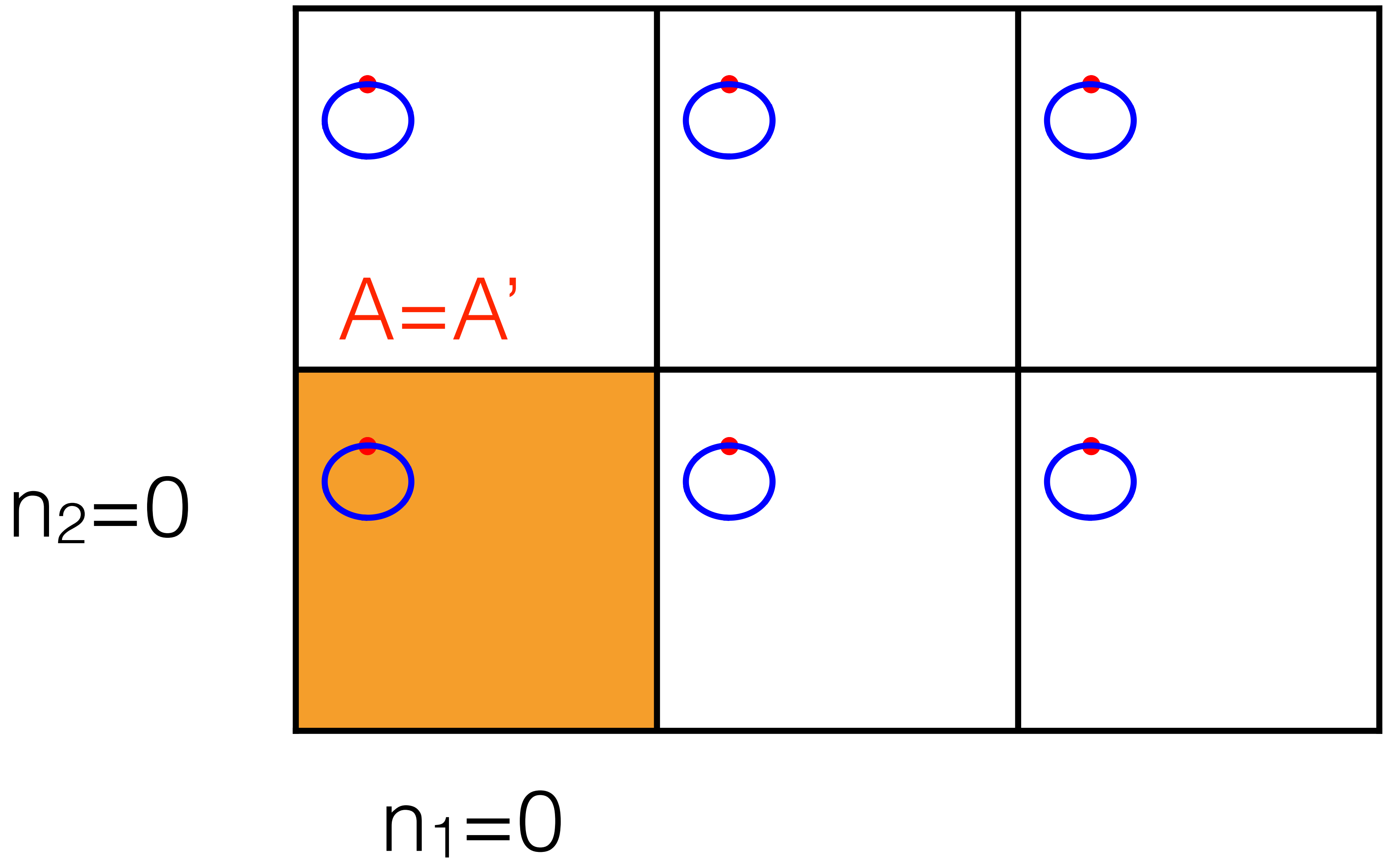

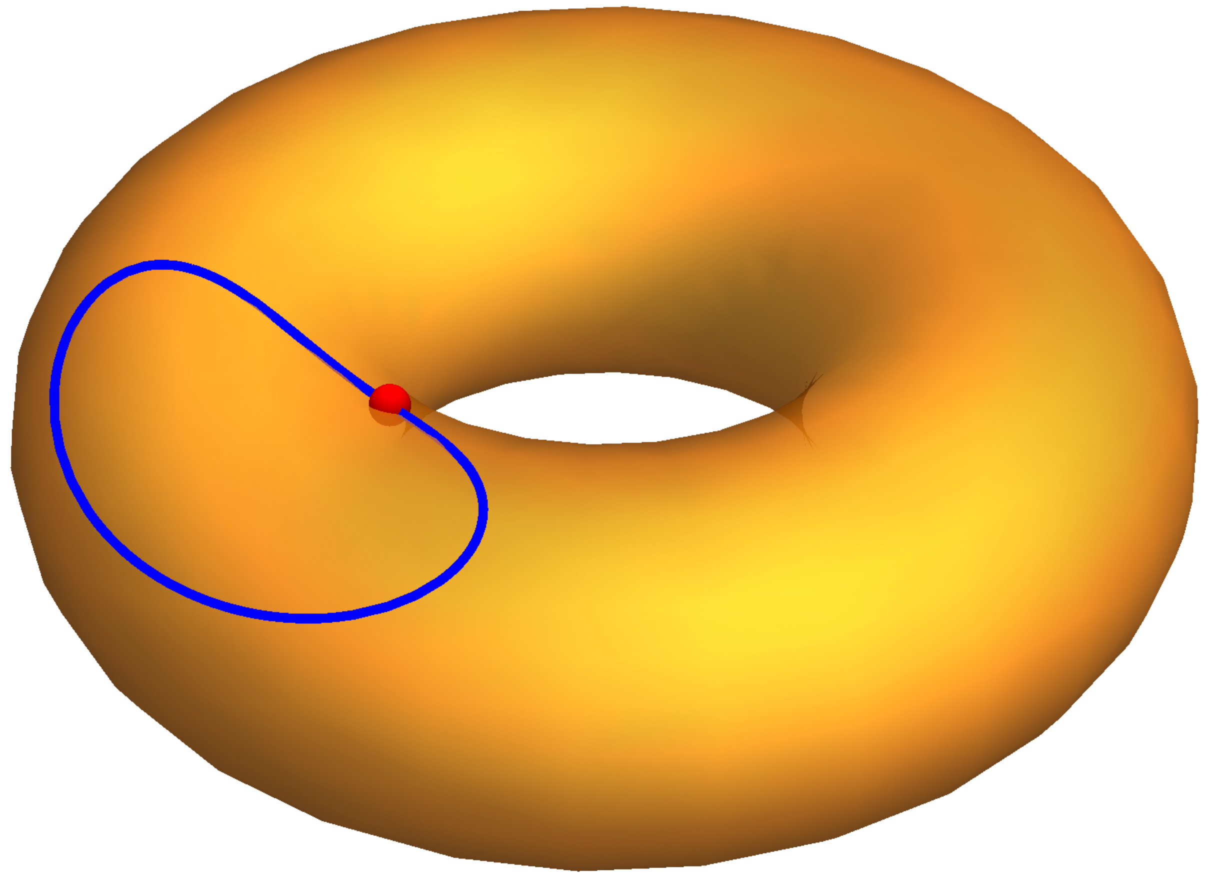

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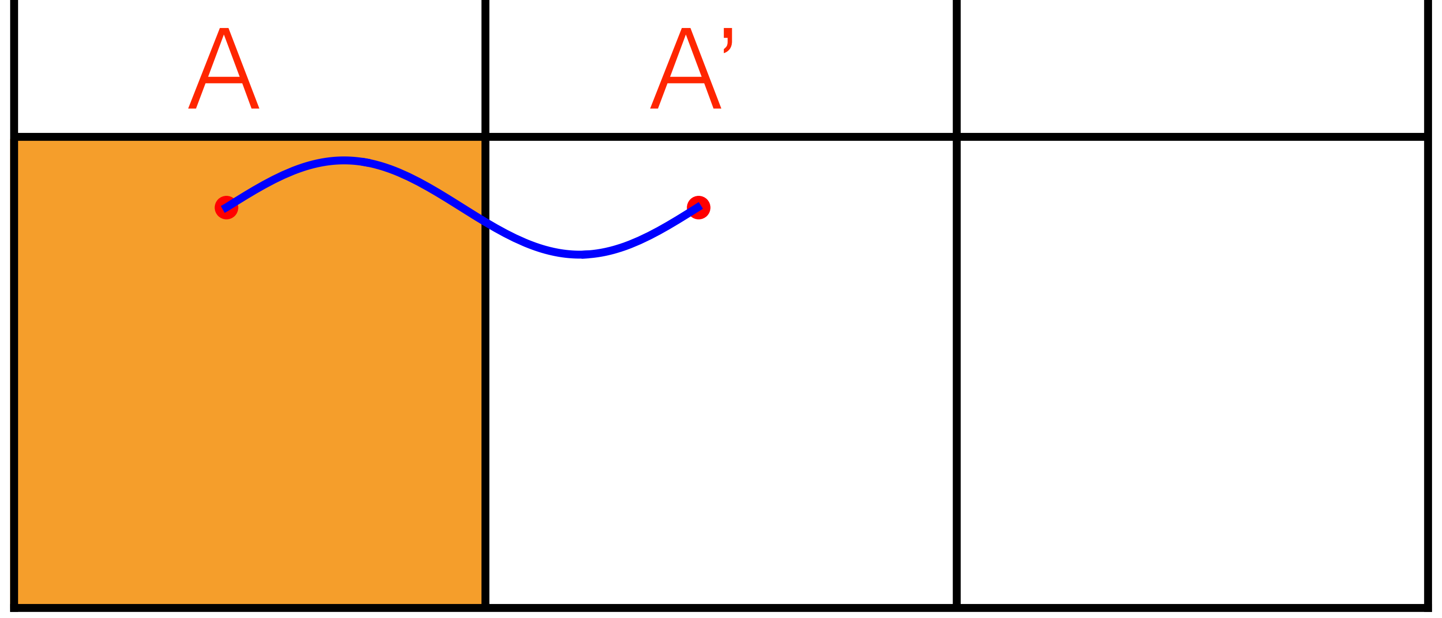

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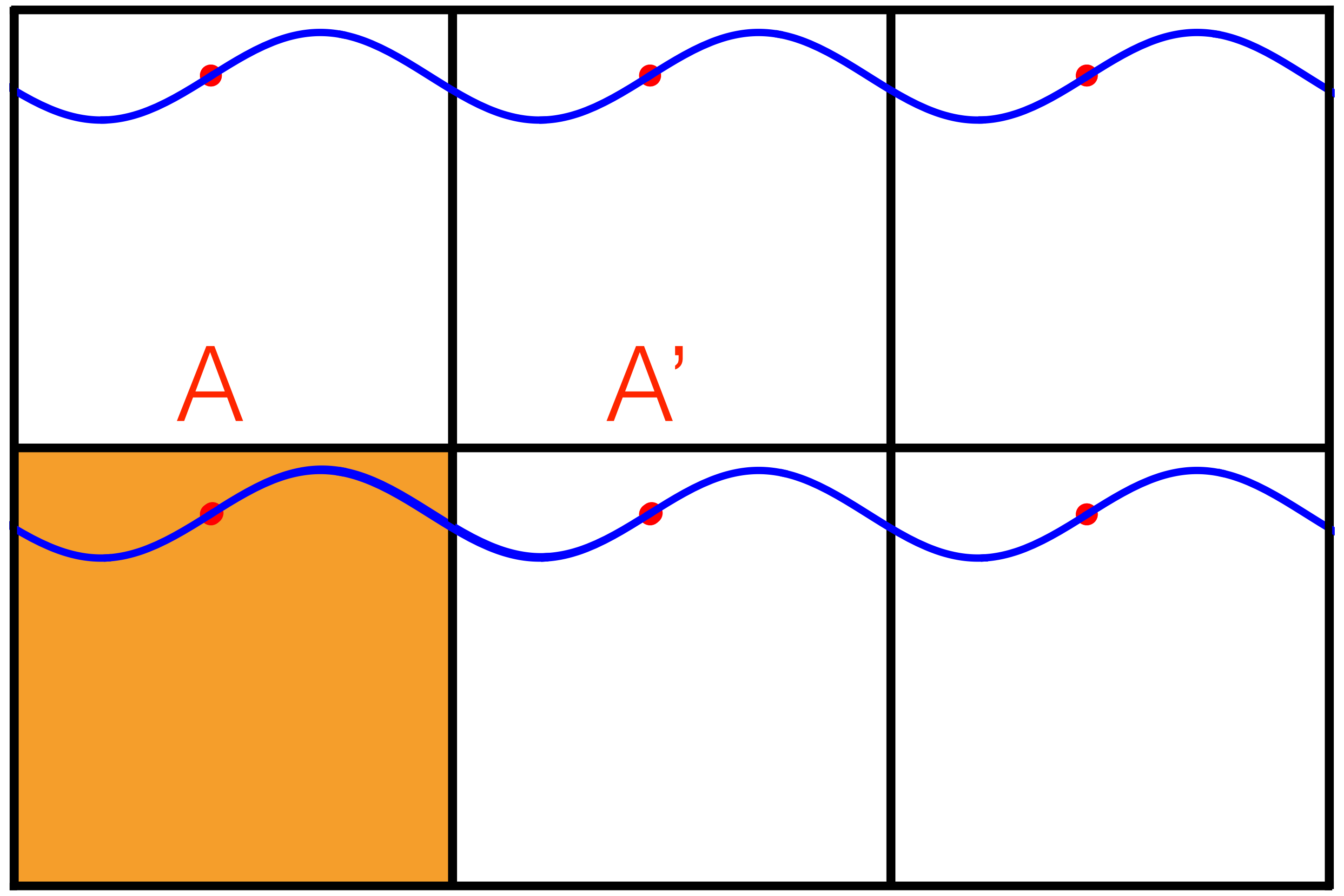

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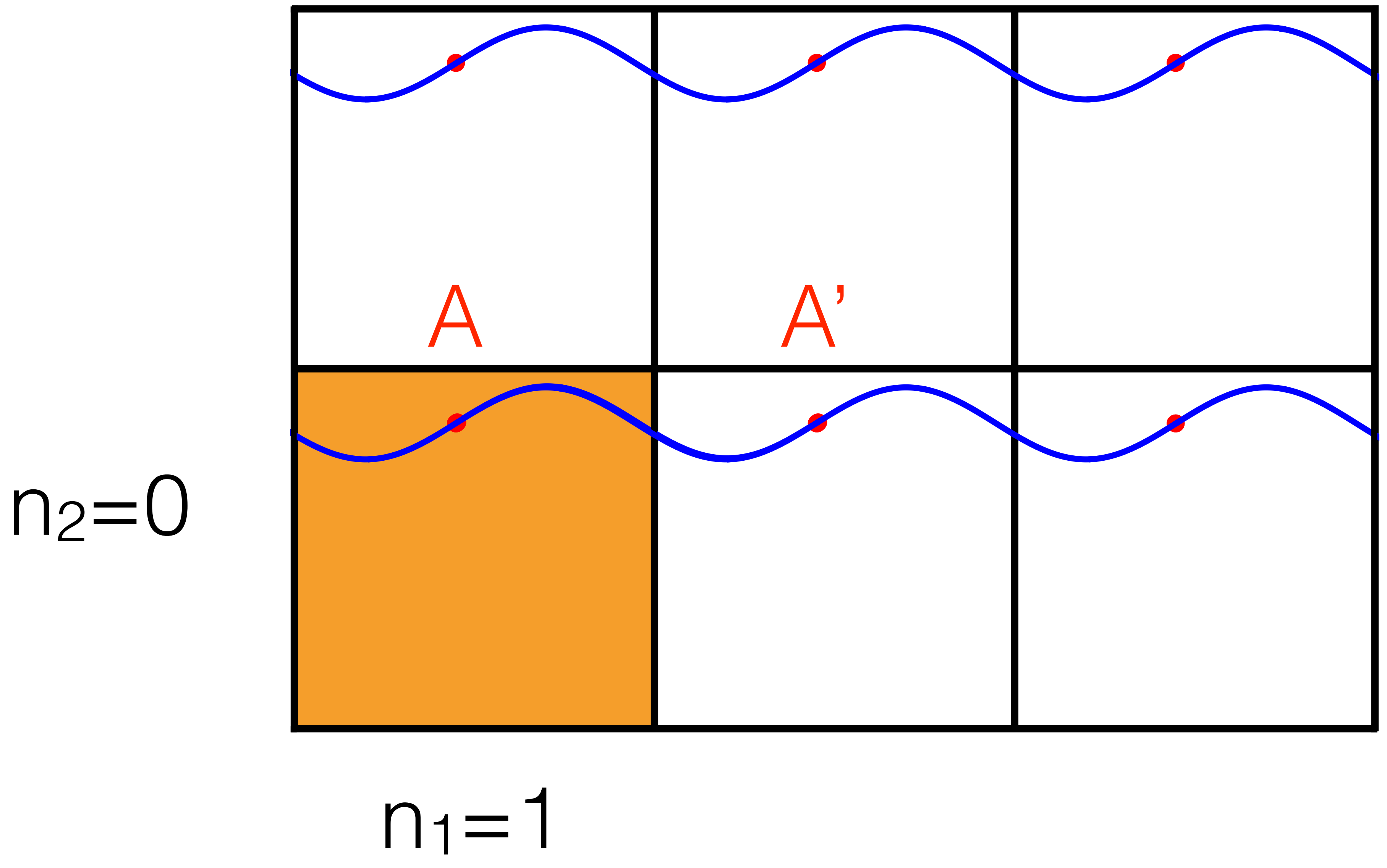

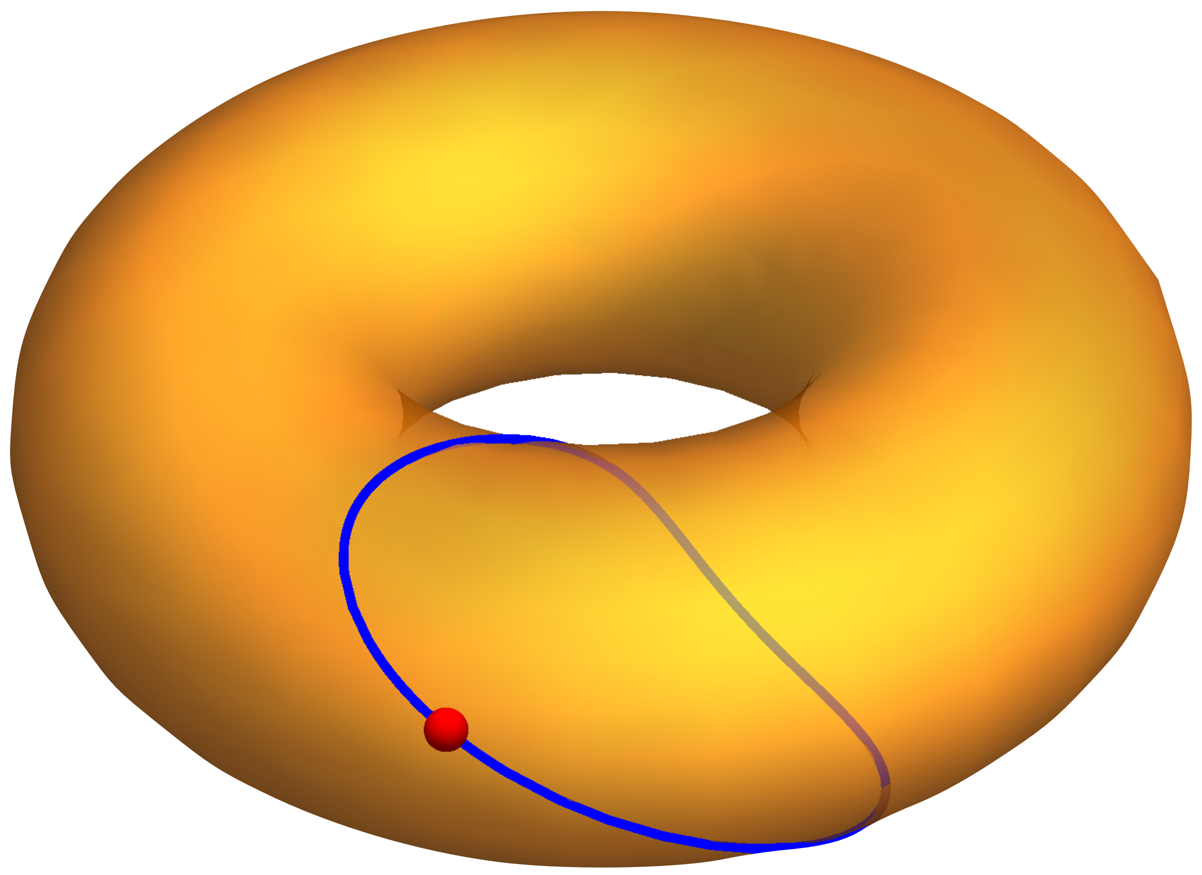

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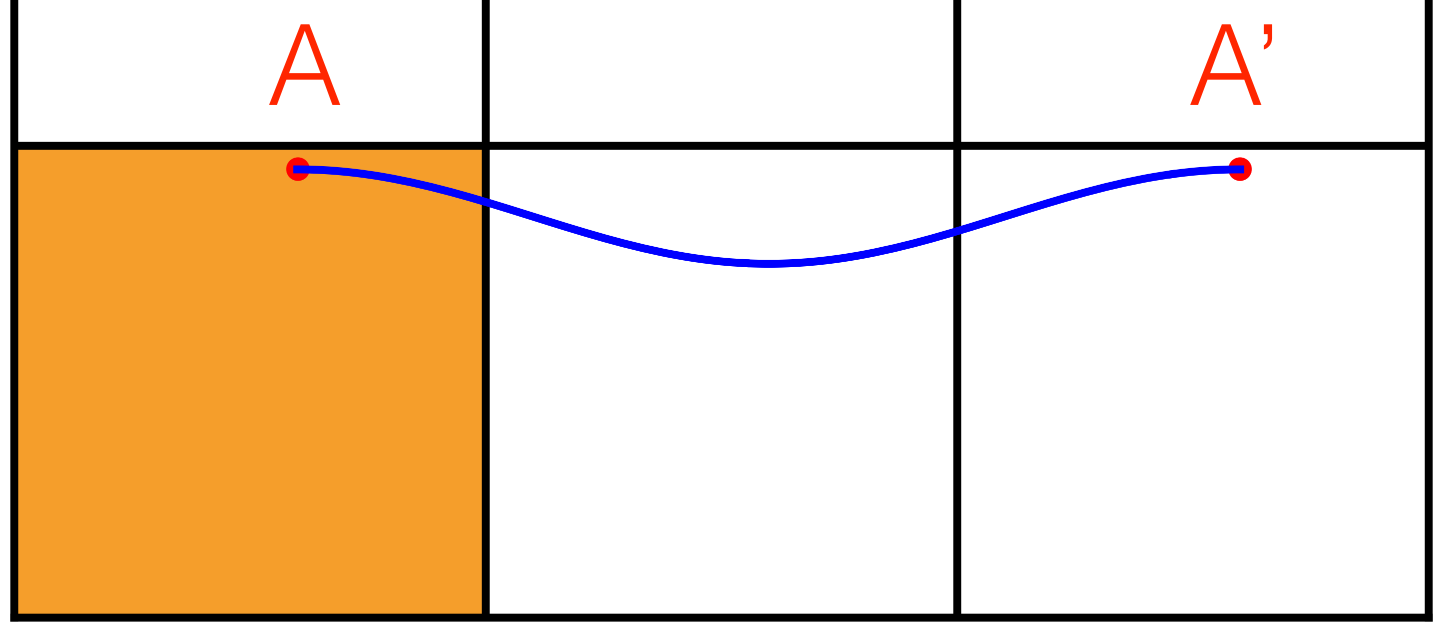

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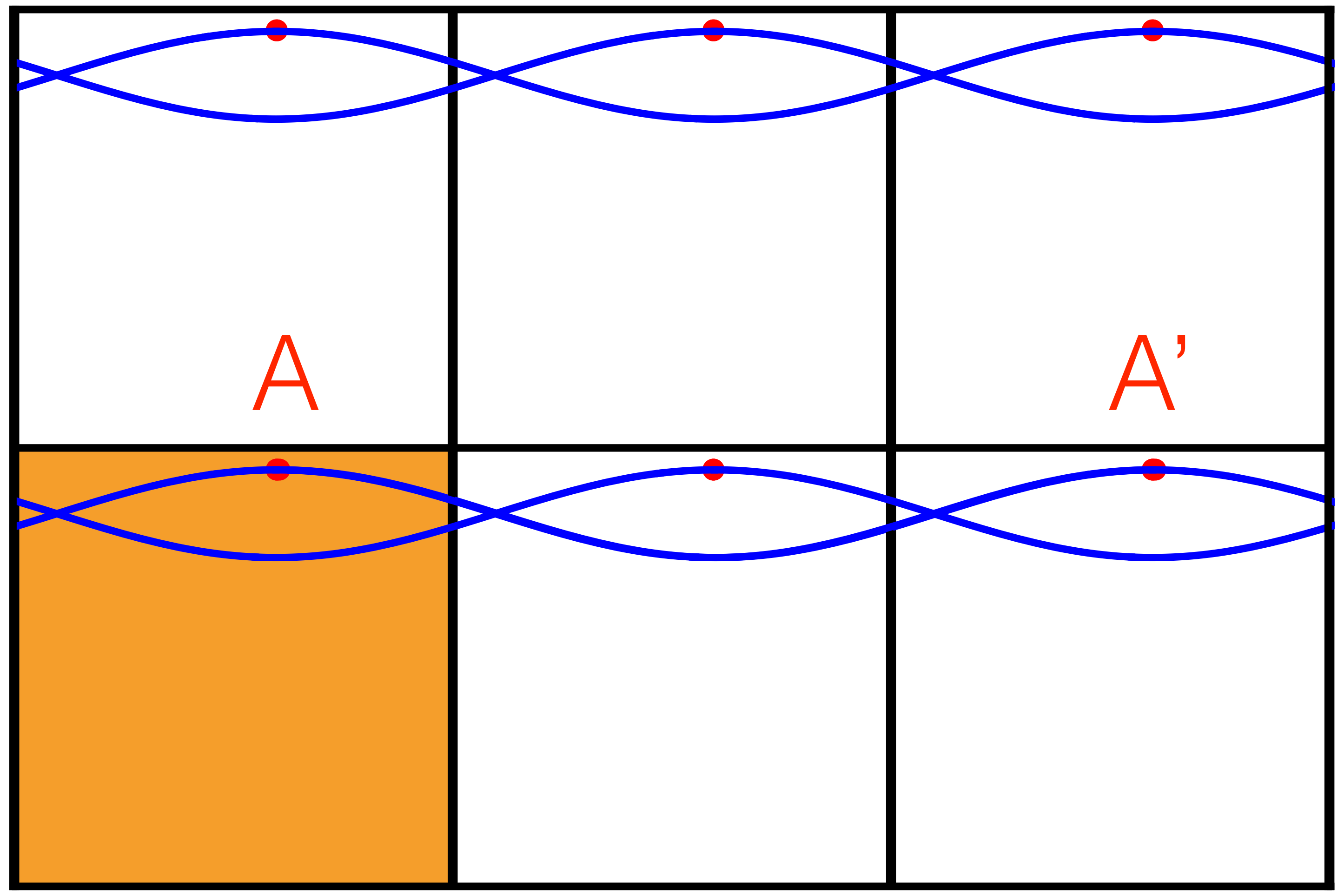

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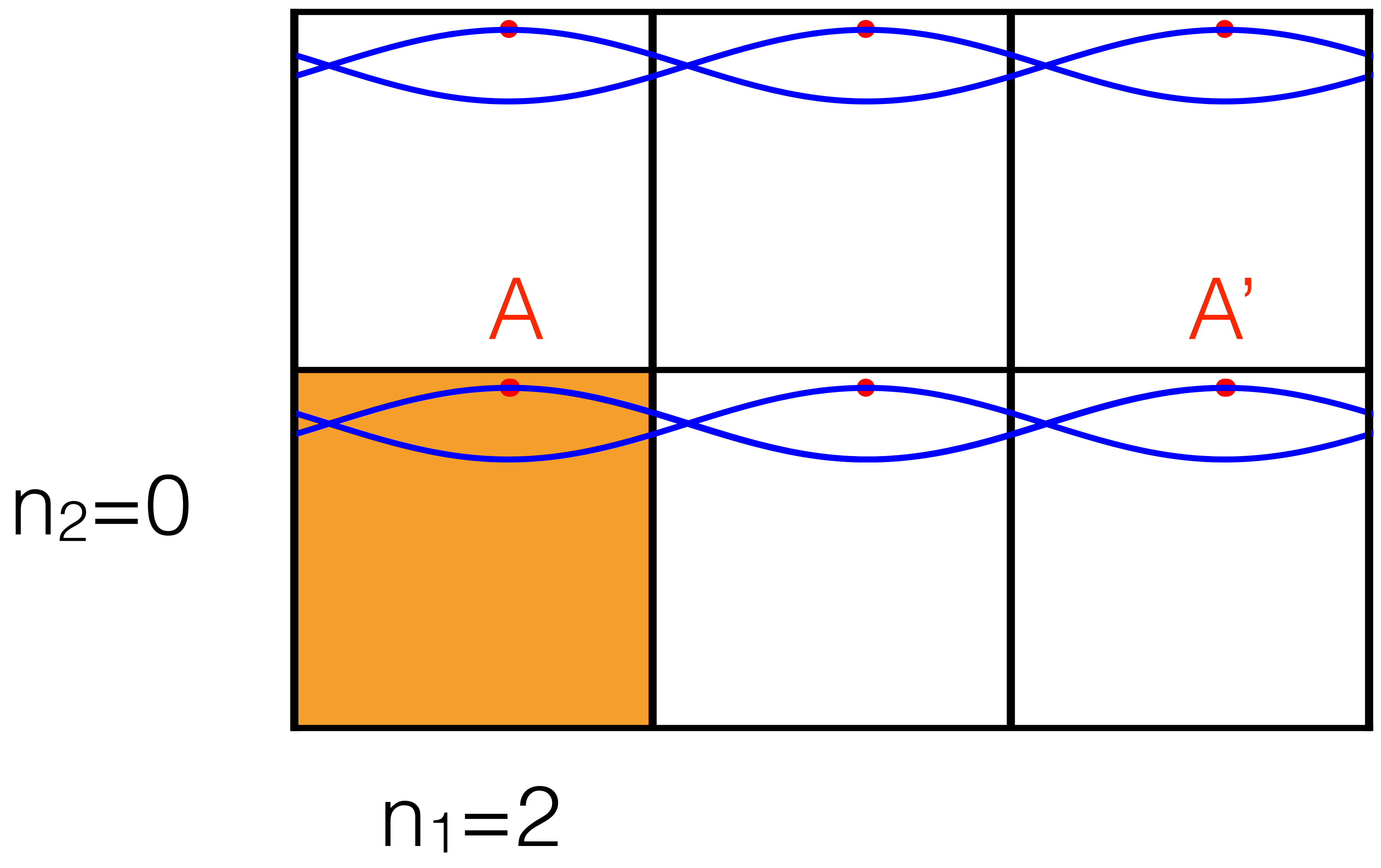

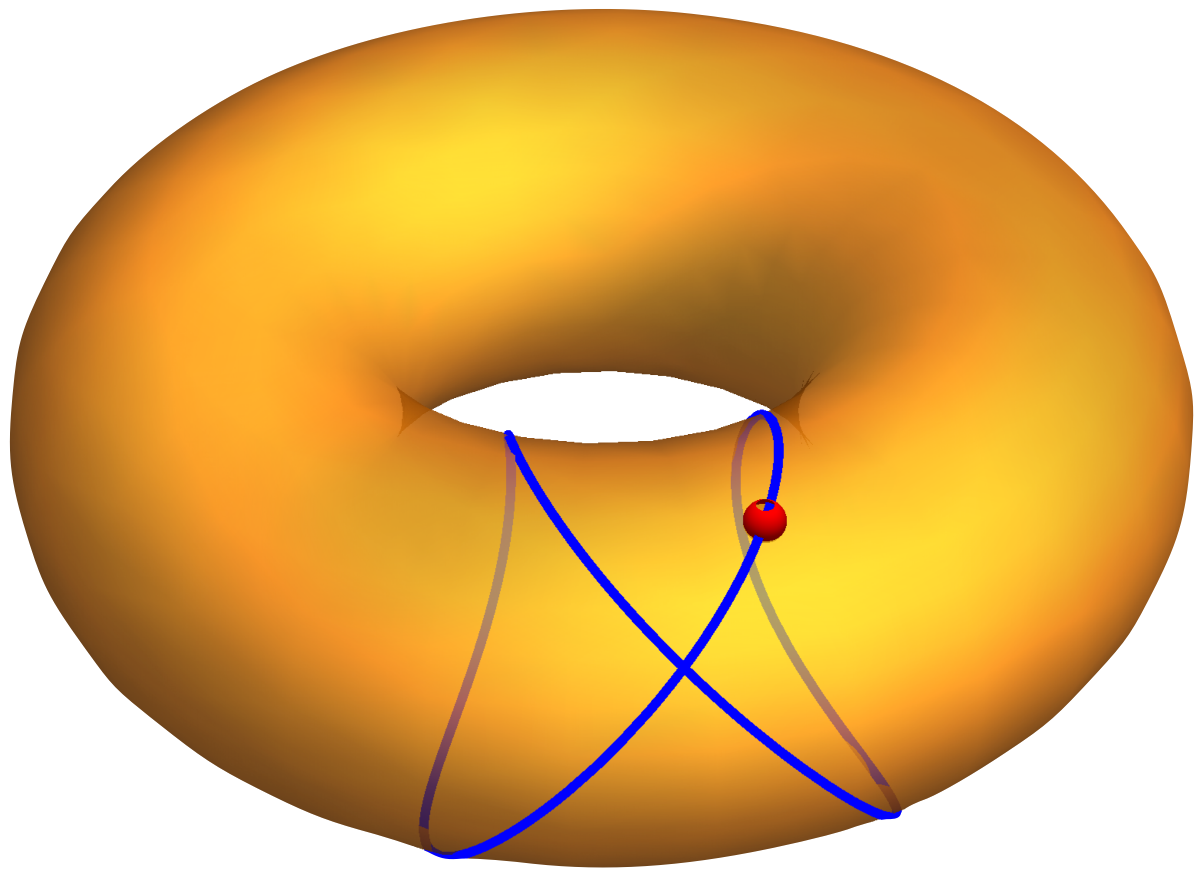

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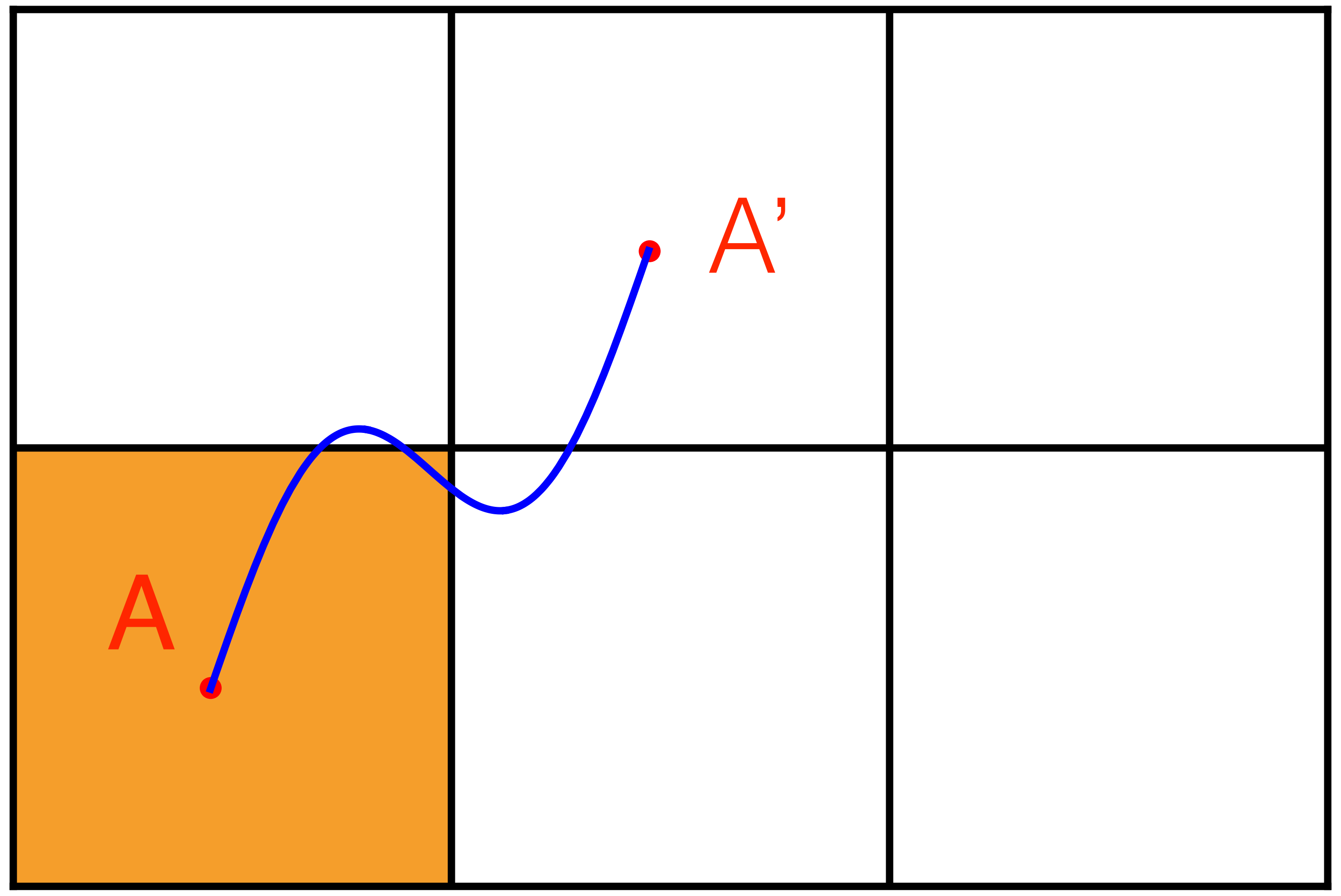

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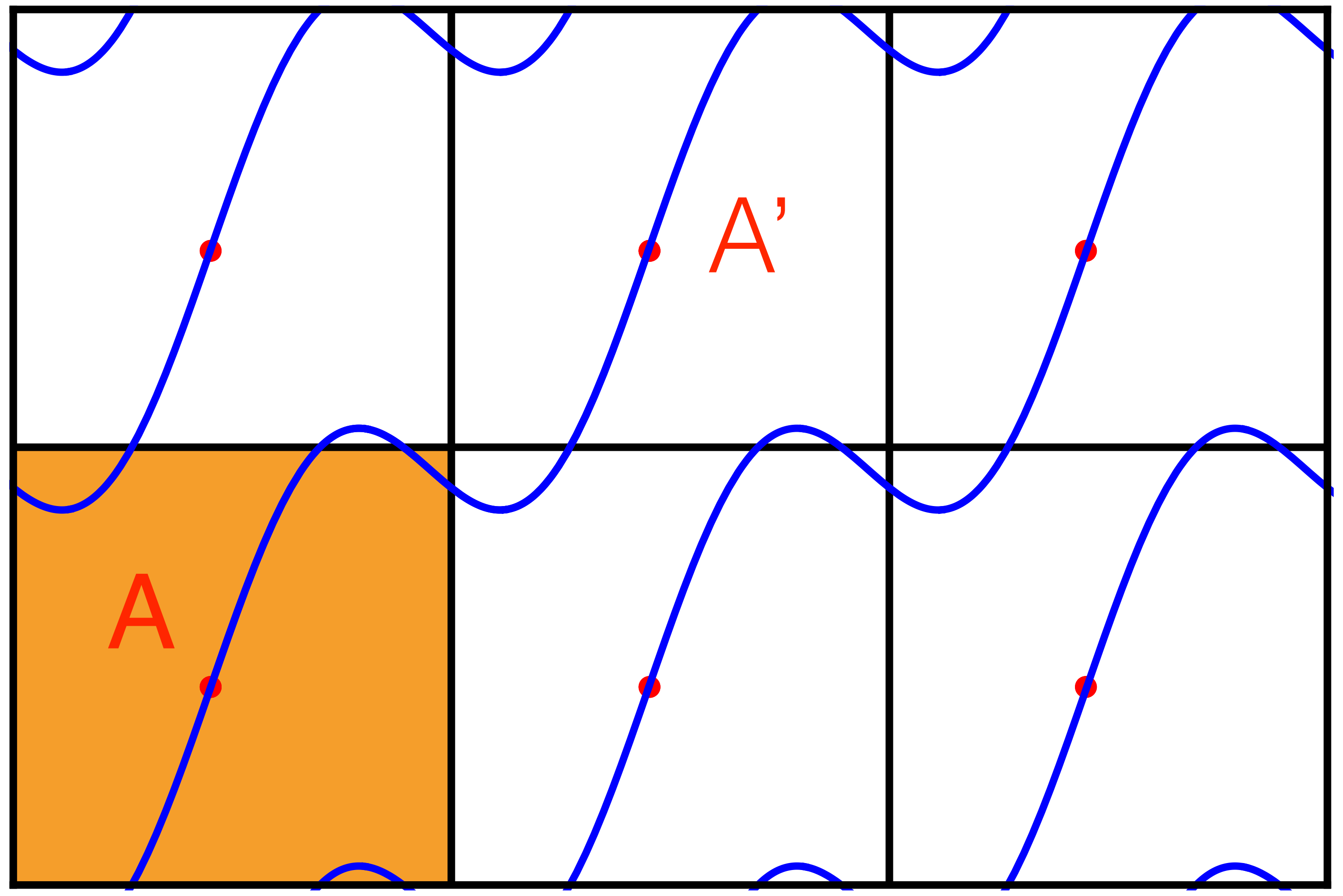

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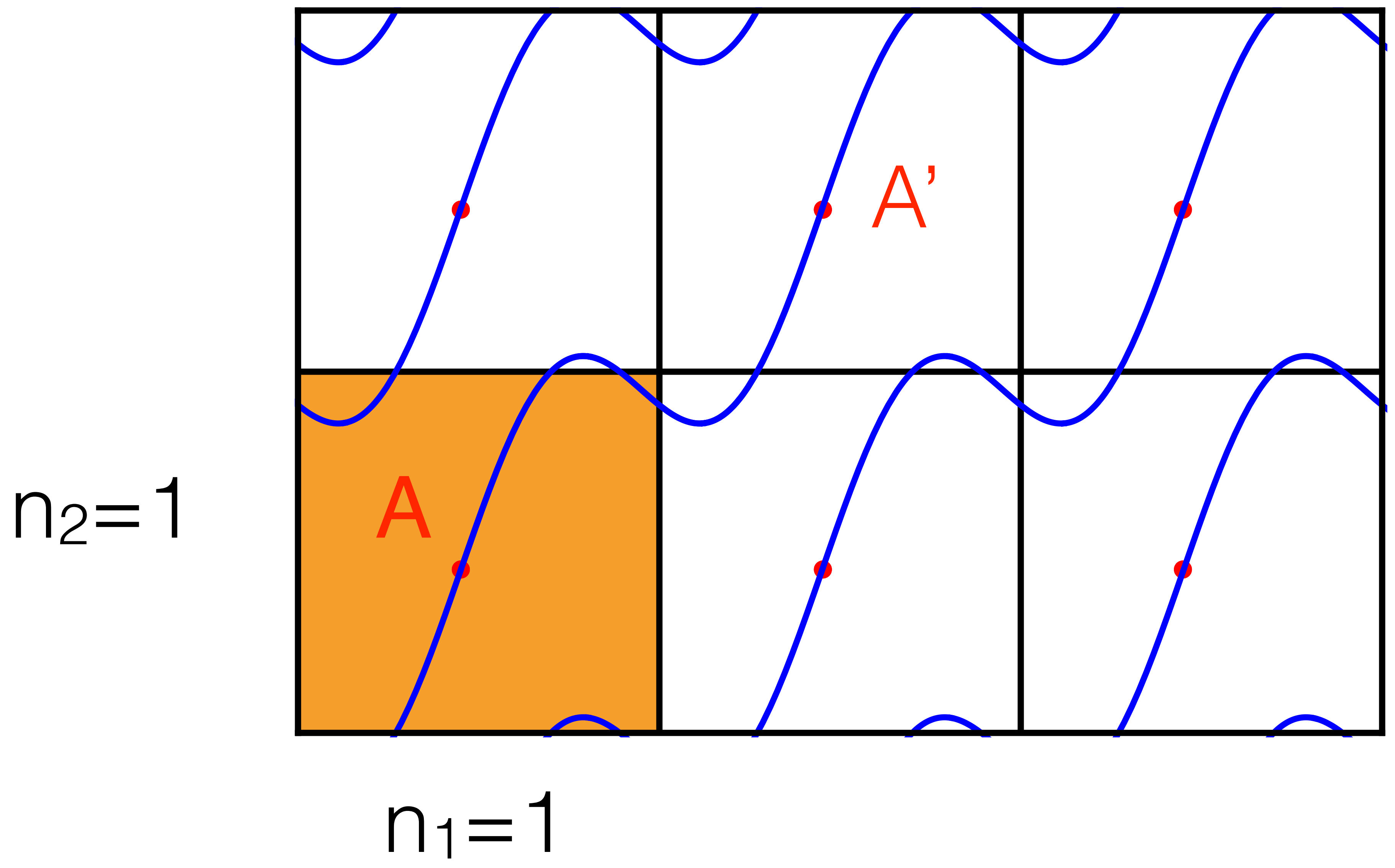

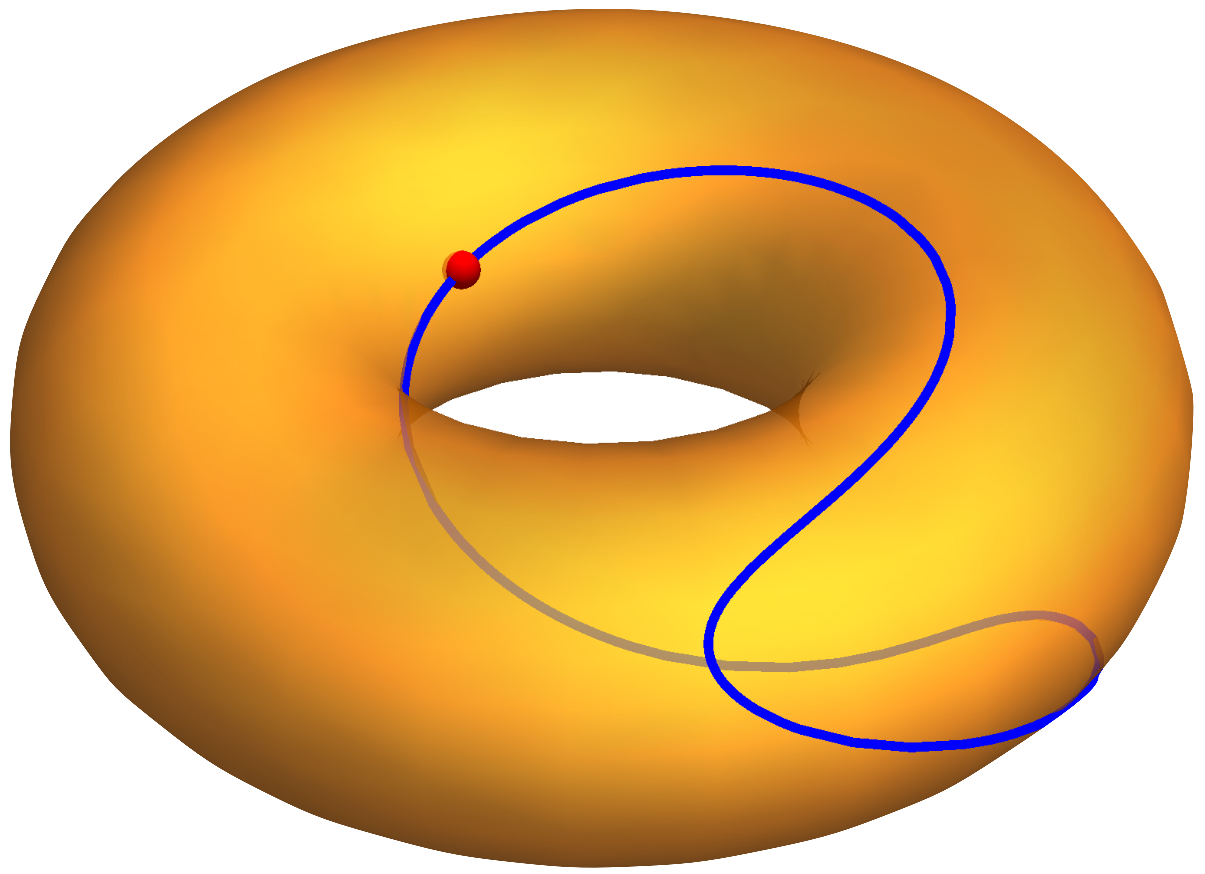

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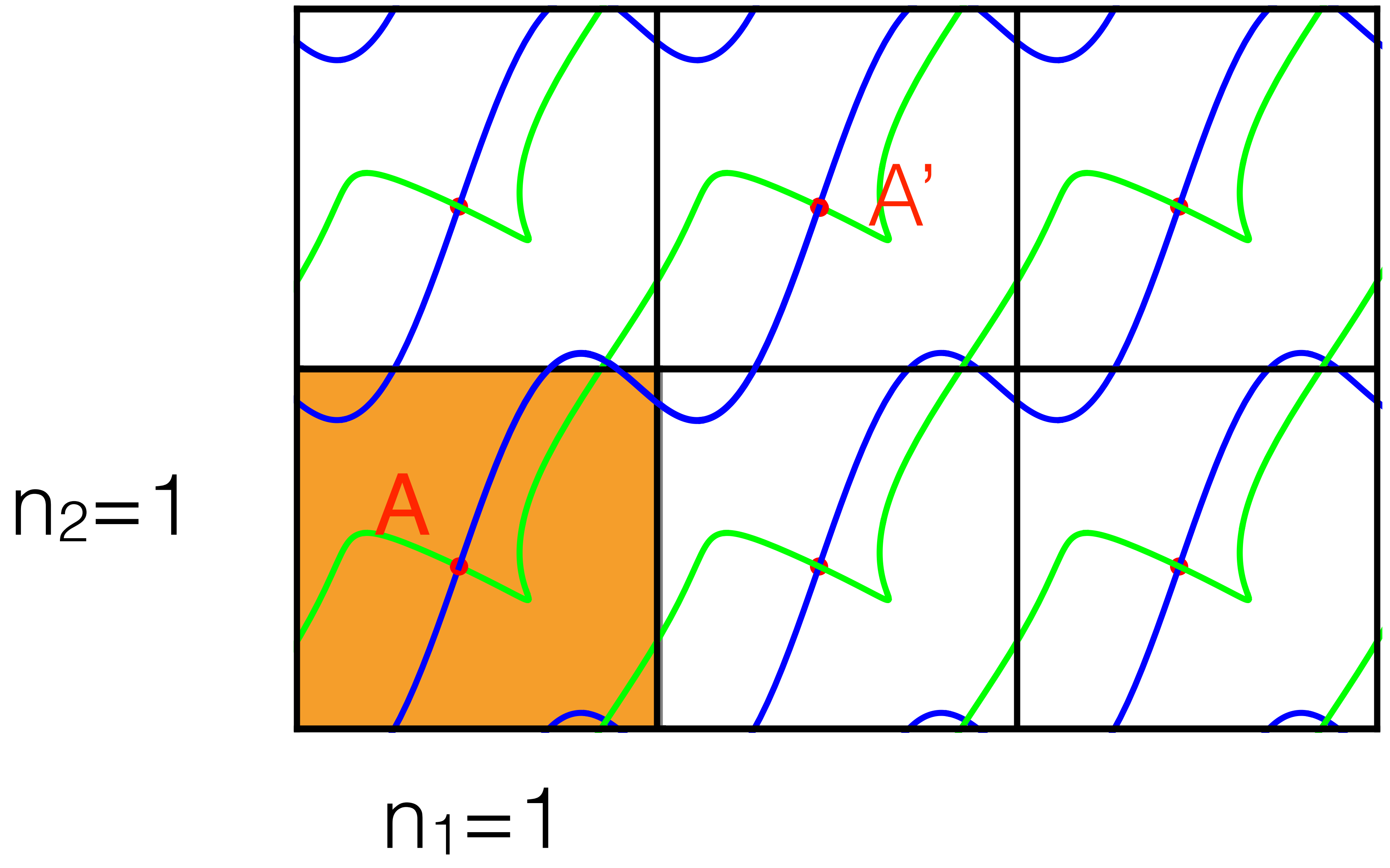

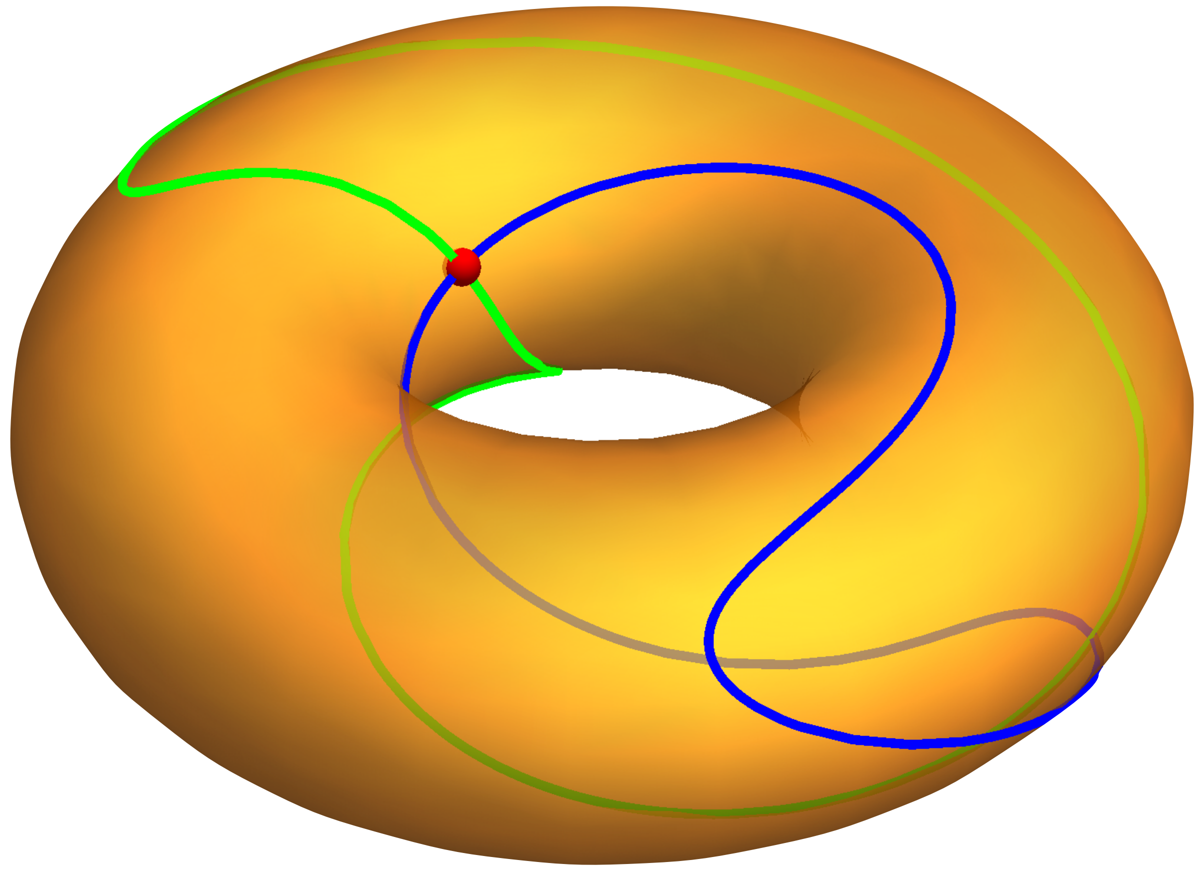

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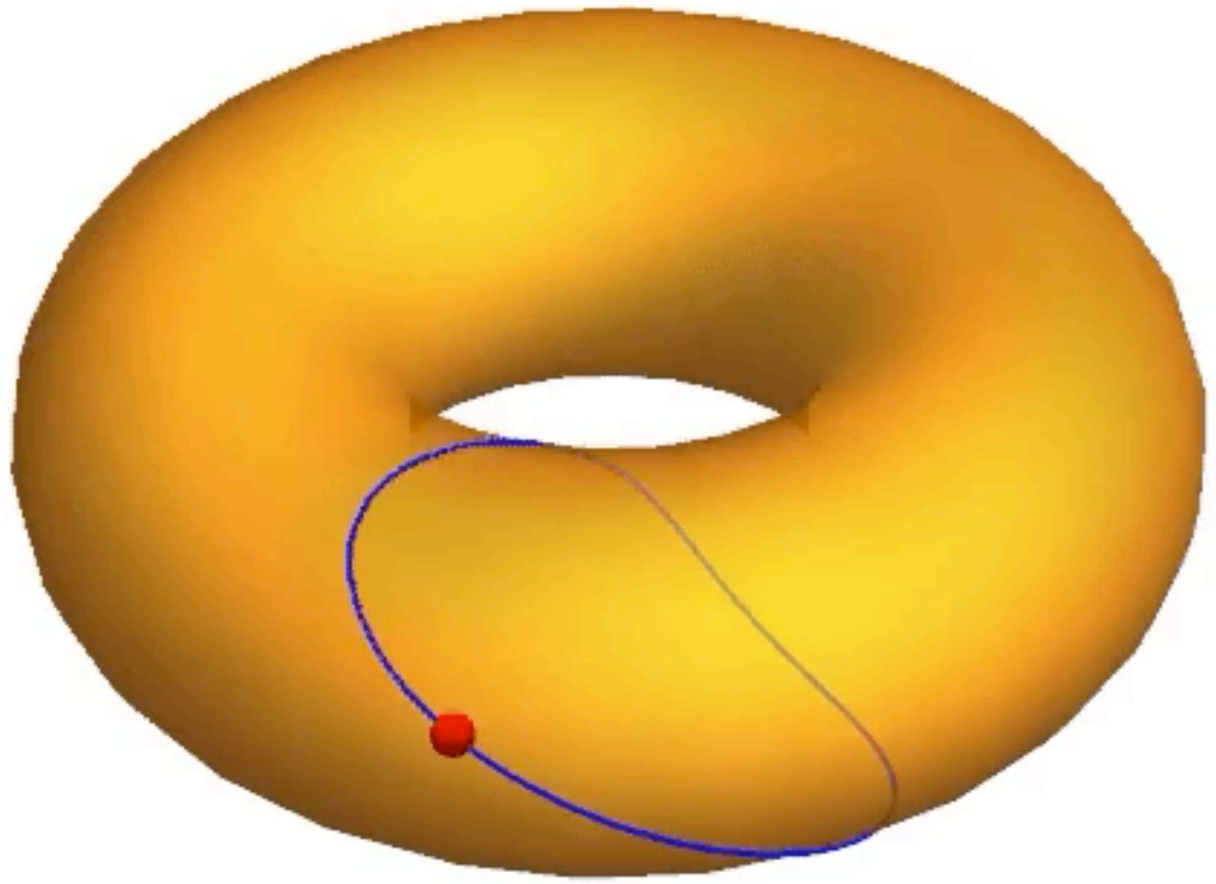

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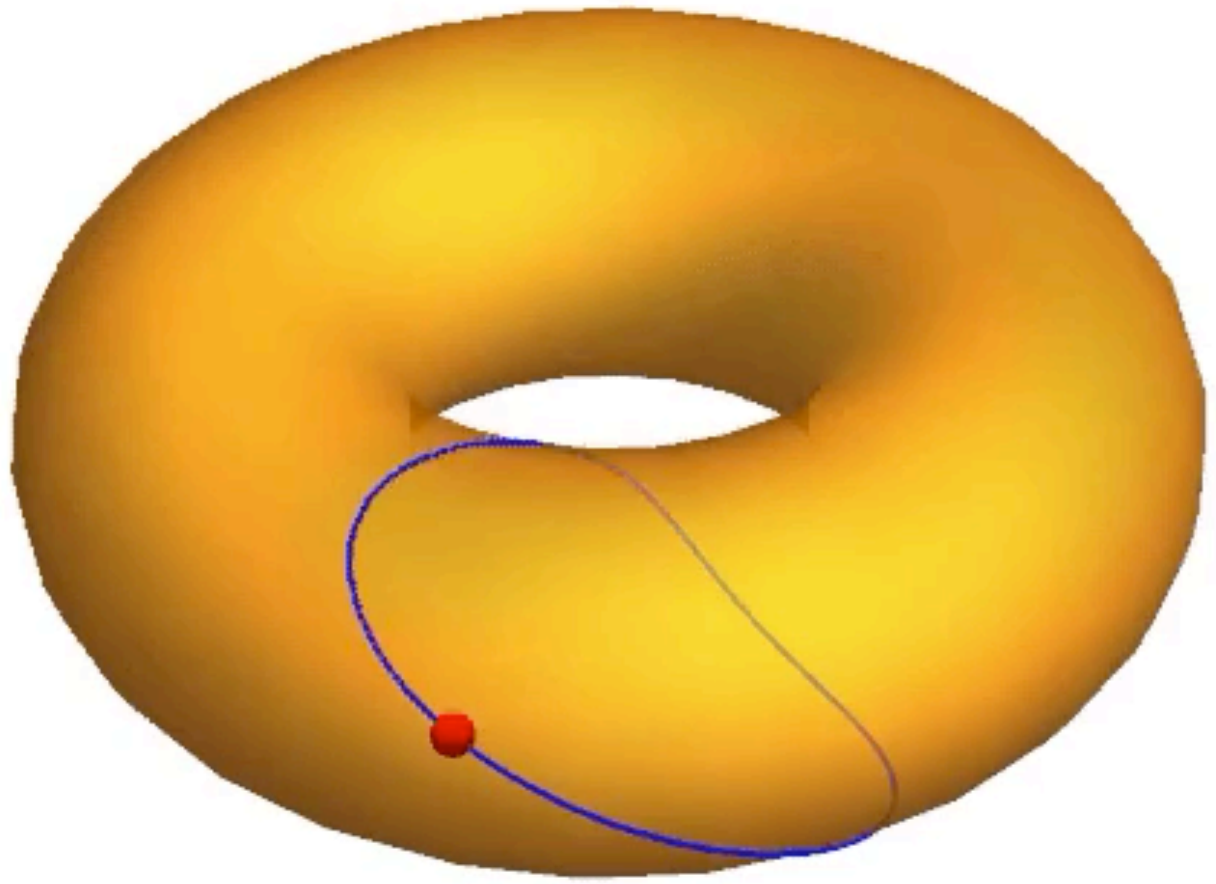

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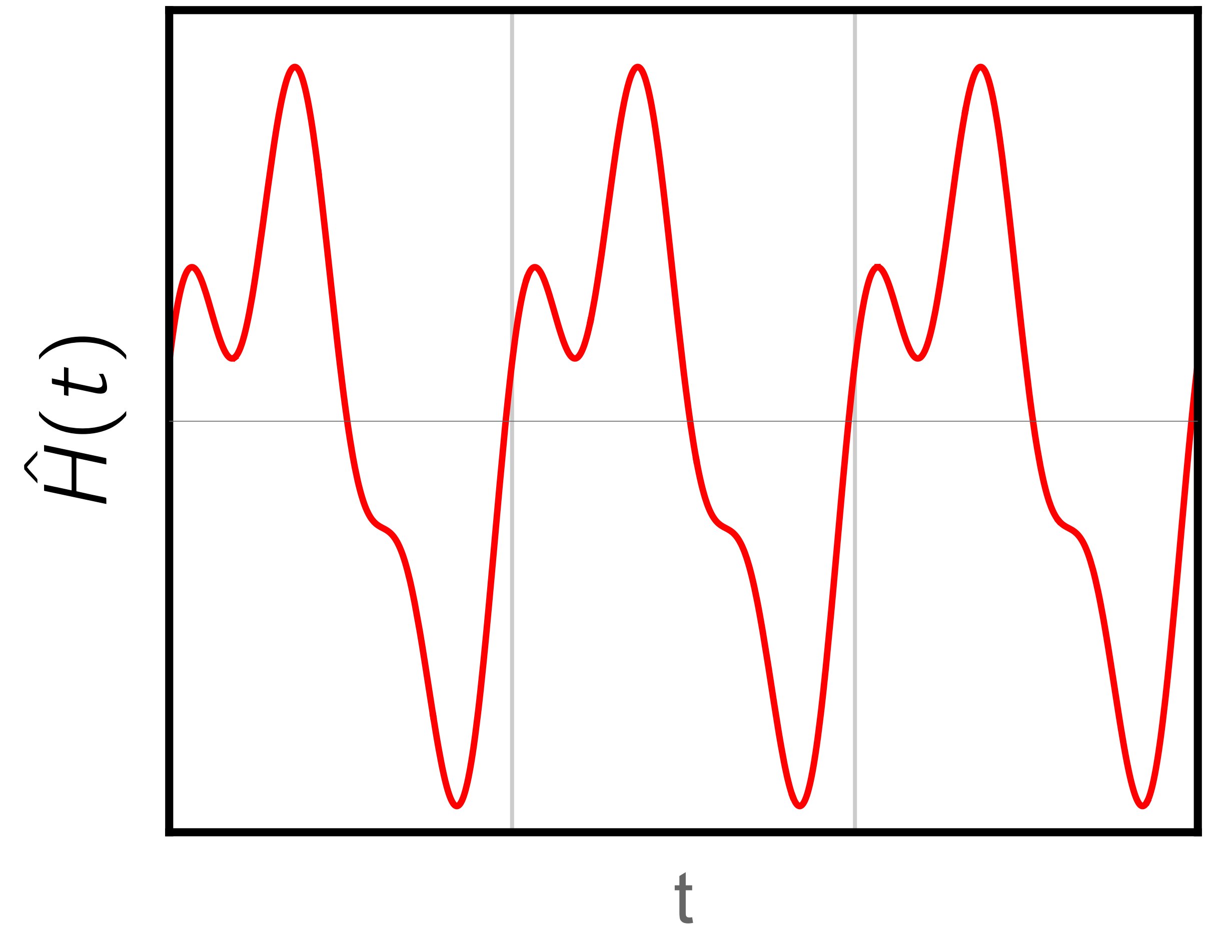
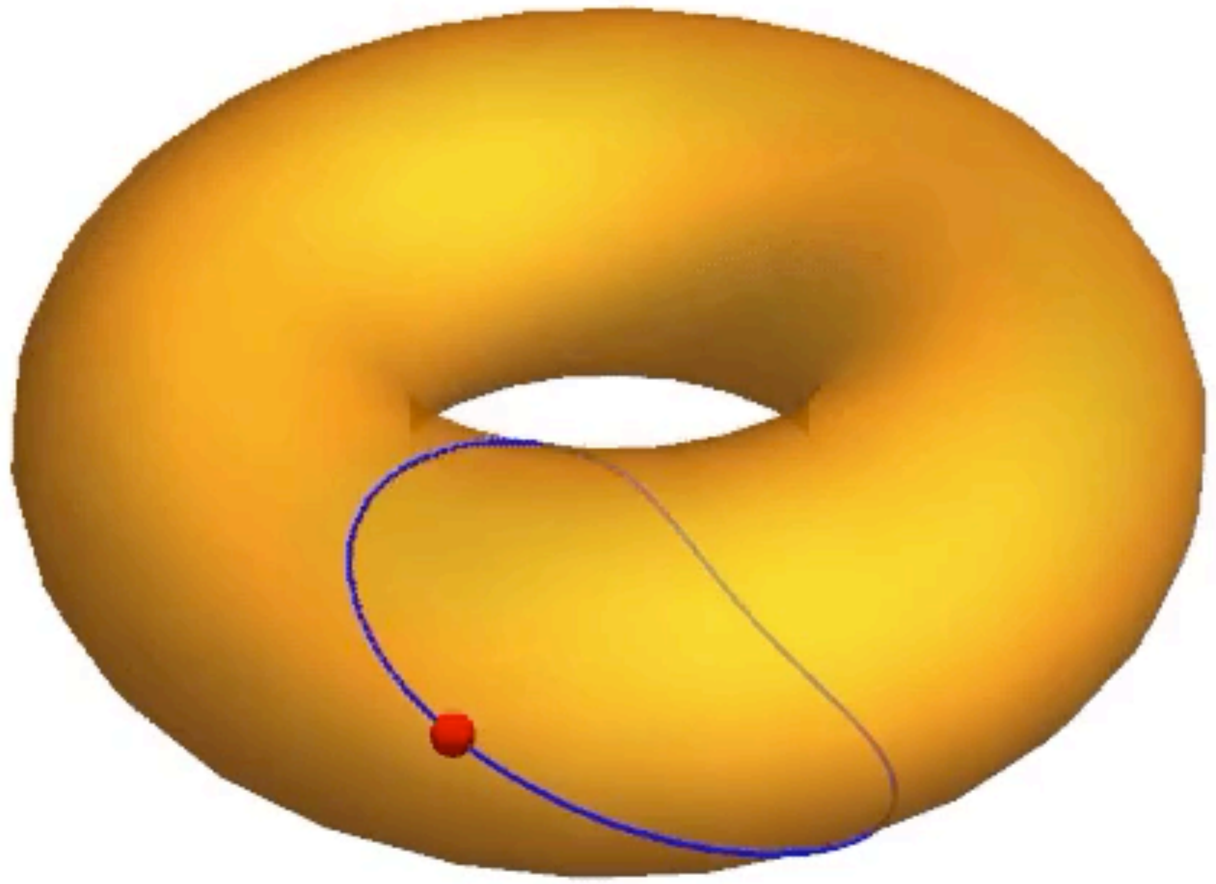


$$\hat{H}(t+T) = \hat{H}(t)$$



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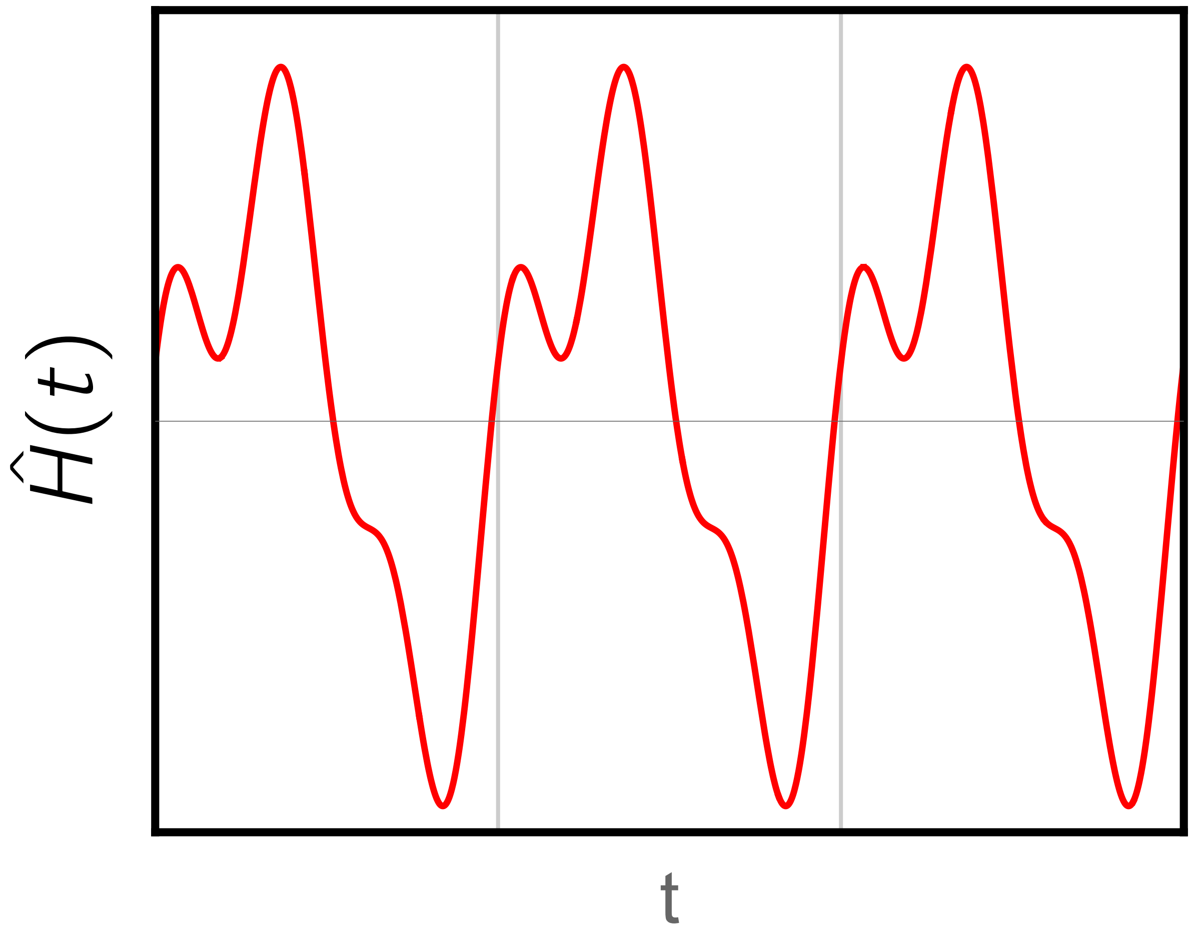

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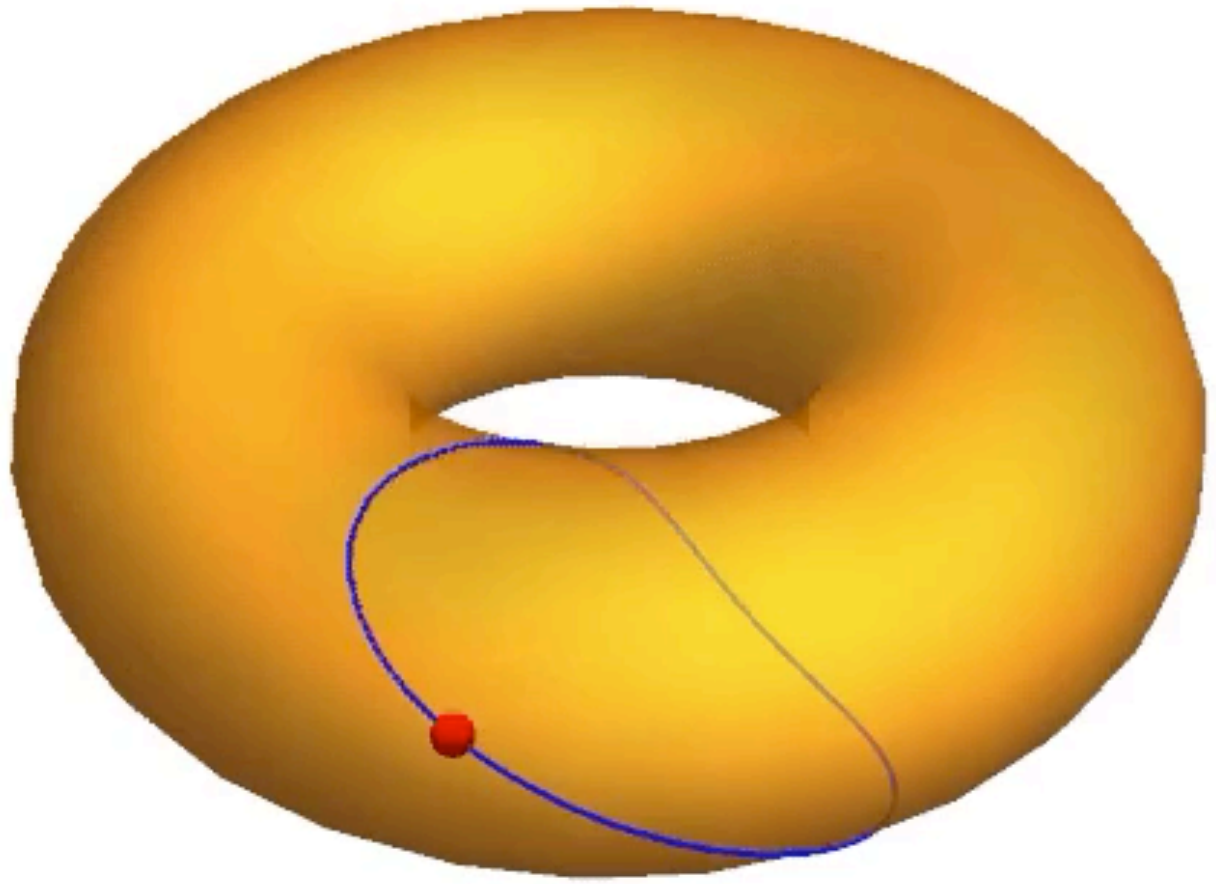
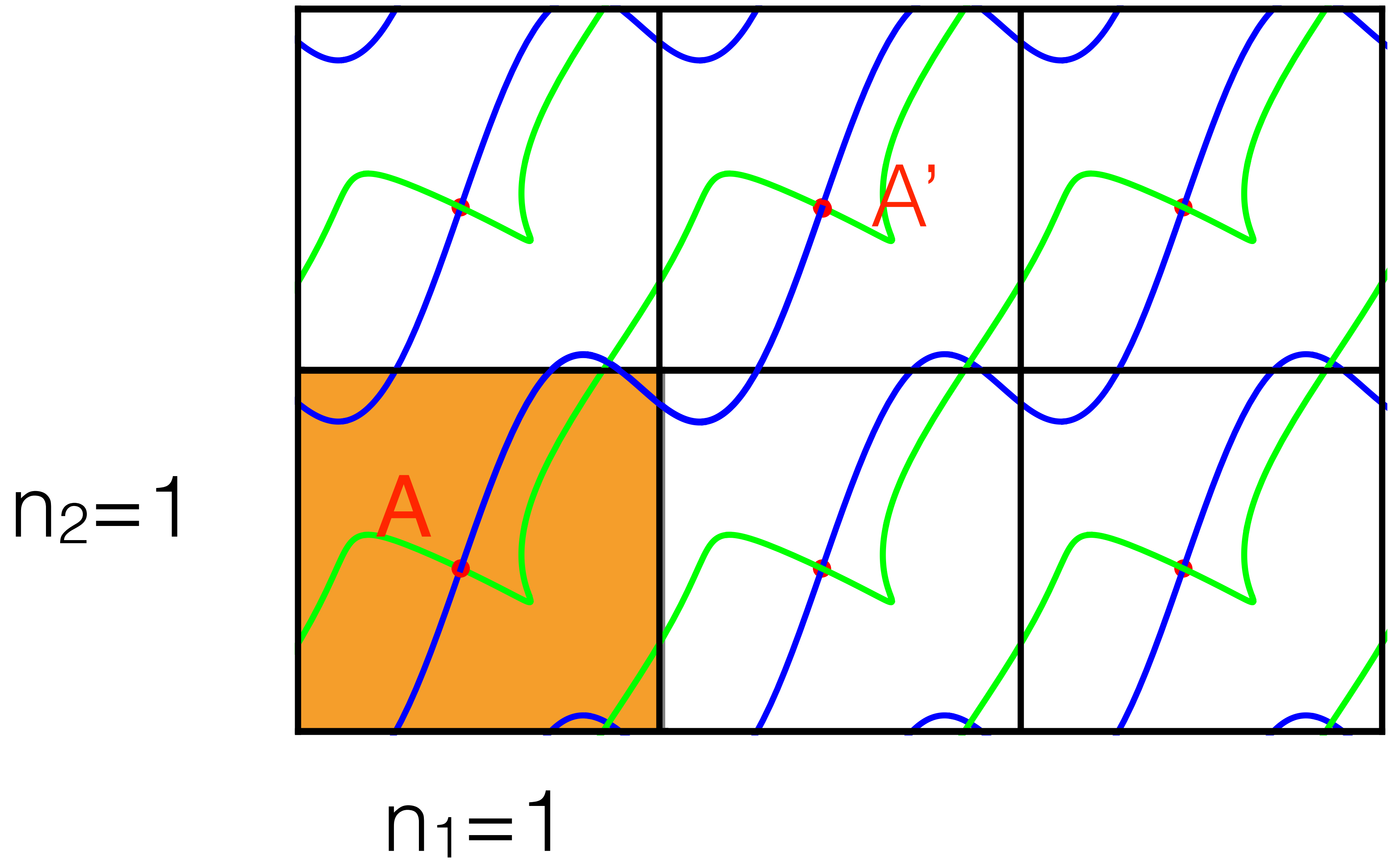
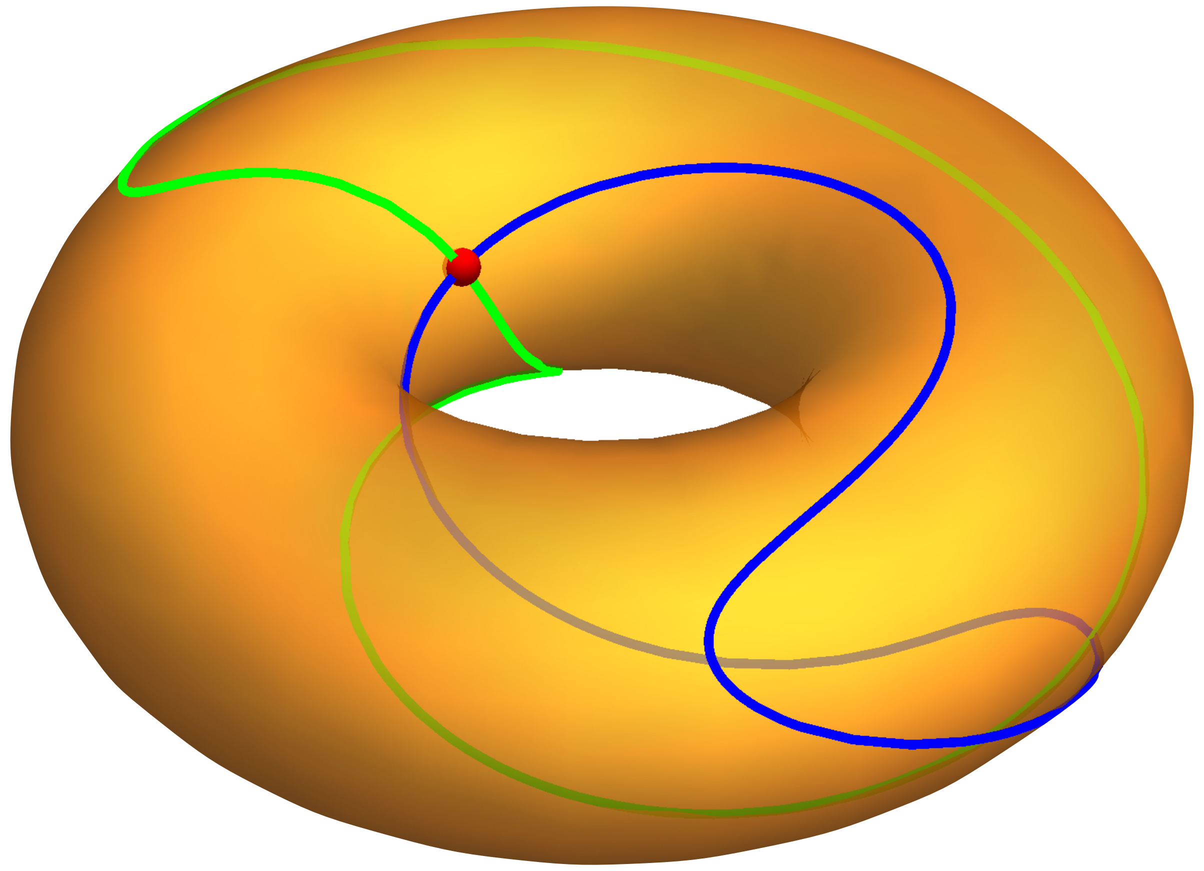


$$\frac{L^2}{e}\int_0^T J_\alpha(t)dt = \frac{1}{Le}\int d\mu_\alpha[X] = Q_\alpha \in \mathbb{Z}$$

D.J. Thouless, *Quantization of particle transport*, Phys. Rev. B **27**, 2083 (1983)

… they are topological invariants!





$$Q_\alpha(AA') = Q_\alpha(AA') = Q_\alpha[n_1 = 1, n_2 = 1]$$

atomic oxidation states

$$Q_\alpha[\mathcal{C}] = \frac{1}{\ell}\mu_\alpha[\mathcal{C}]$$

atomic oxidation states

$$
\begin{aligned}
Q_\alpha[\mathcal{C}] &= \frac{1}{\ell}\mu_\alpha[\mathcal{C}] \\
&= Q_\alpha(n_{1x}, n_{1y}, n_{1z}, \cdots n_{Nz})
\end{aligned}
$$

atomic oxidation states

$$Q_\alpha[\mathcal{C}] = \frac{1}{\ell}\mu_\alpha[\mathcal{C}]$$
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$$Q_\alpha[\mathcal{C}_1 \circ \mathcal{C}_2] = Q_\alpha[\mathcal{C}_1] + Q_\alpha[\mathcal{C}_2]$$

atomic oxidation states

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- All loops can be shrunk to a point without closing the gap (*strong adiabaticity*);
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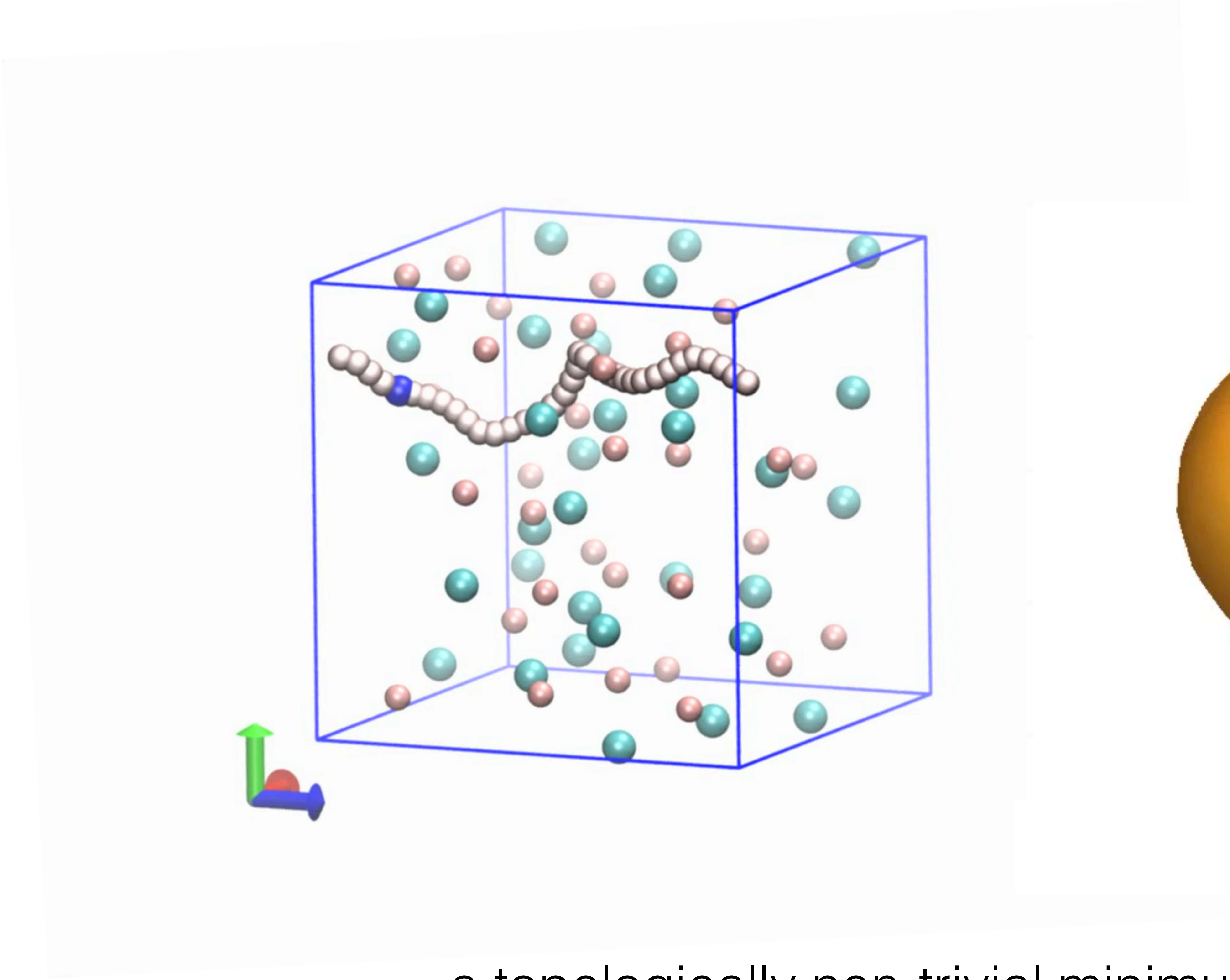
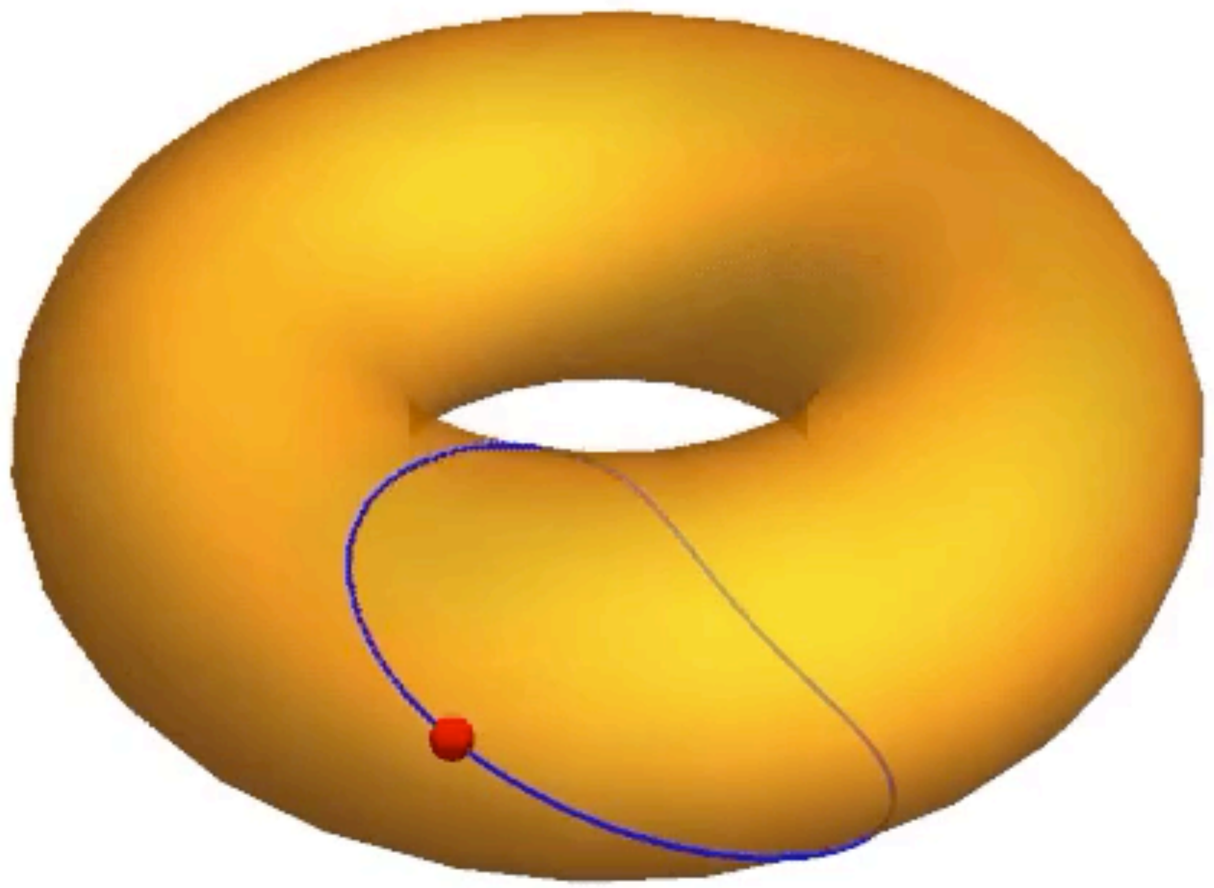
$$q_{i\alpha\beta} = q_{S(i)}\delta_{\alpha\beta}$$

atomic oxidation state

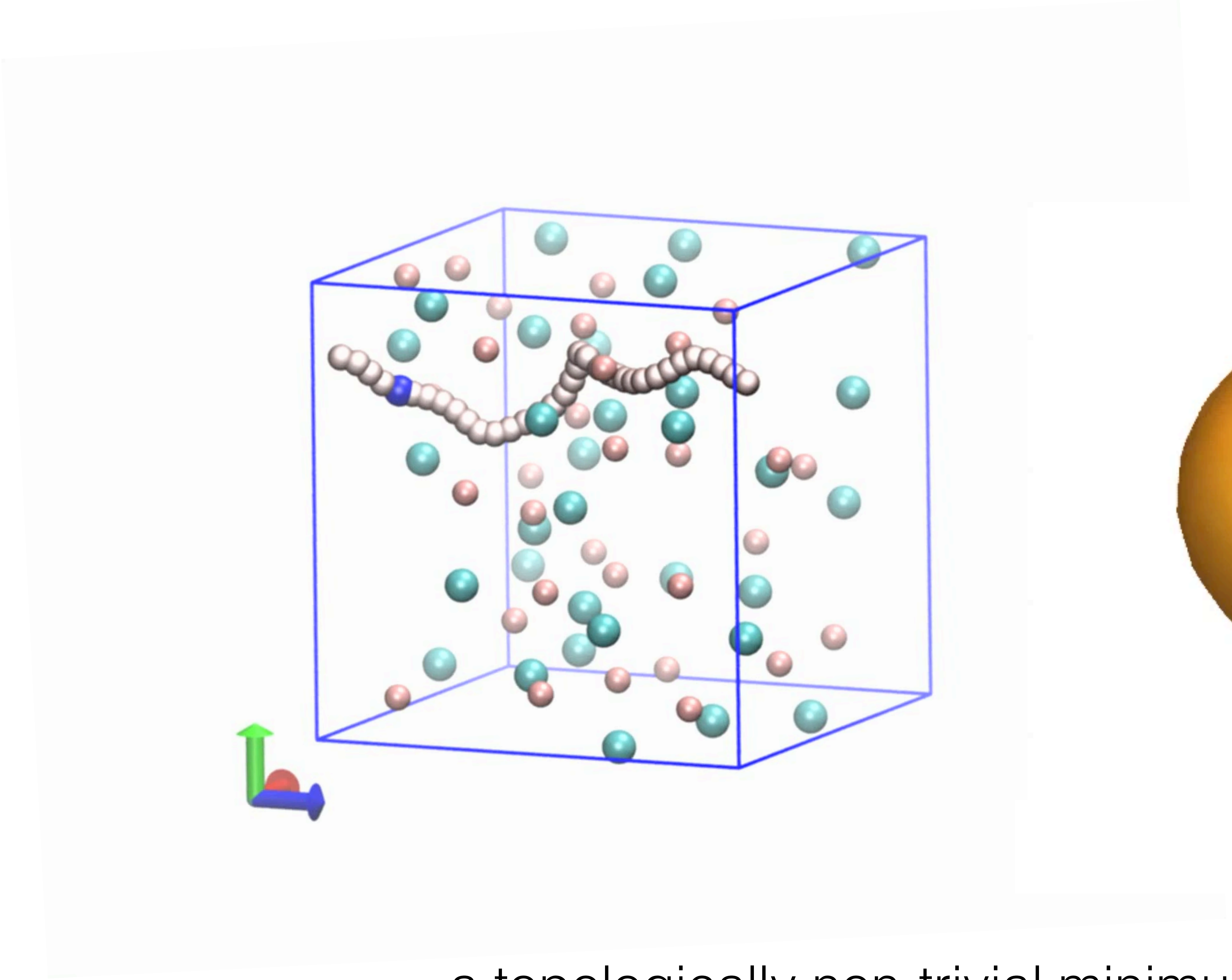
a numerical experiment on molten KCl

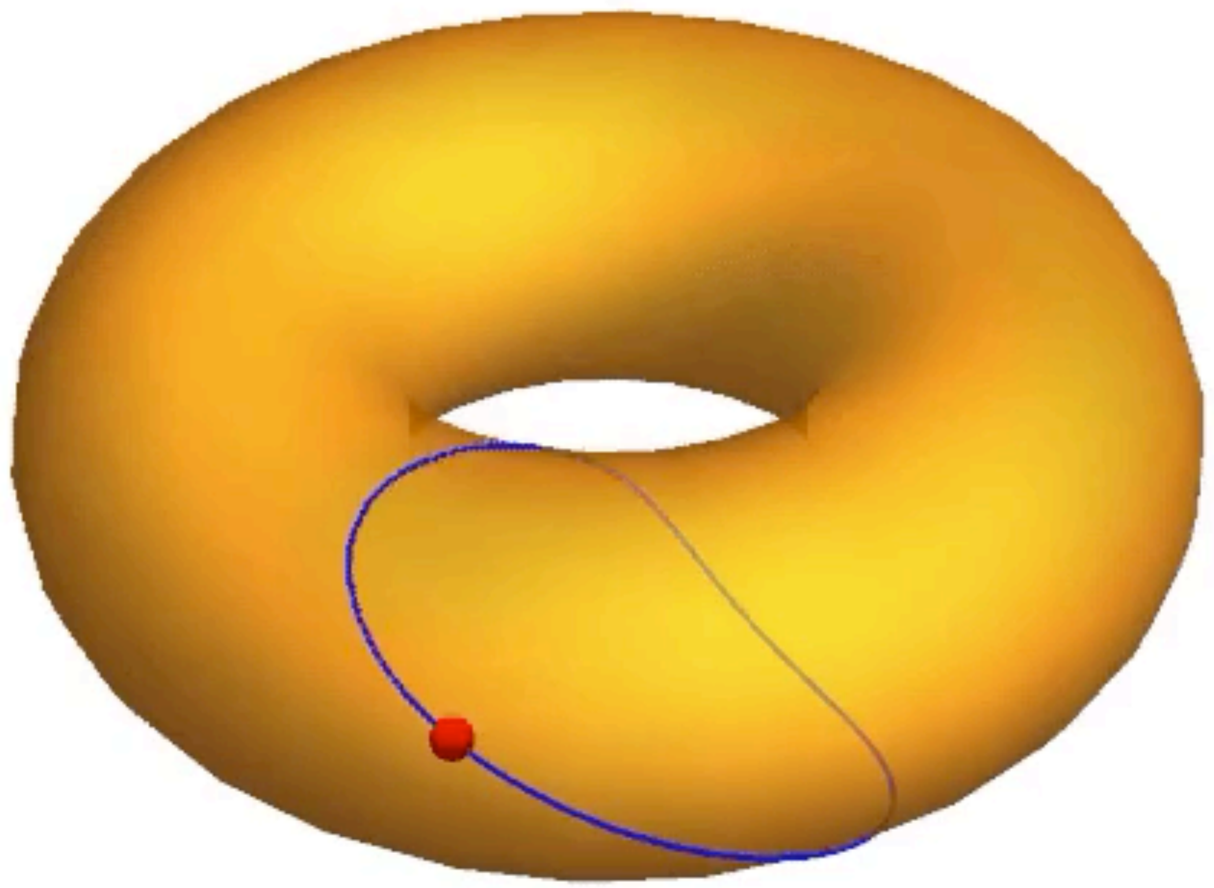




a topologically non-trivial minimum-energy path
connecting two identical configurations of a ionic melt

a numerical experiment on molten KCl





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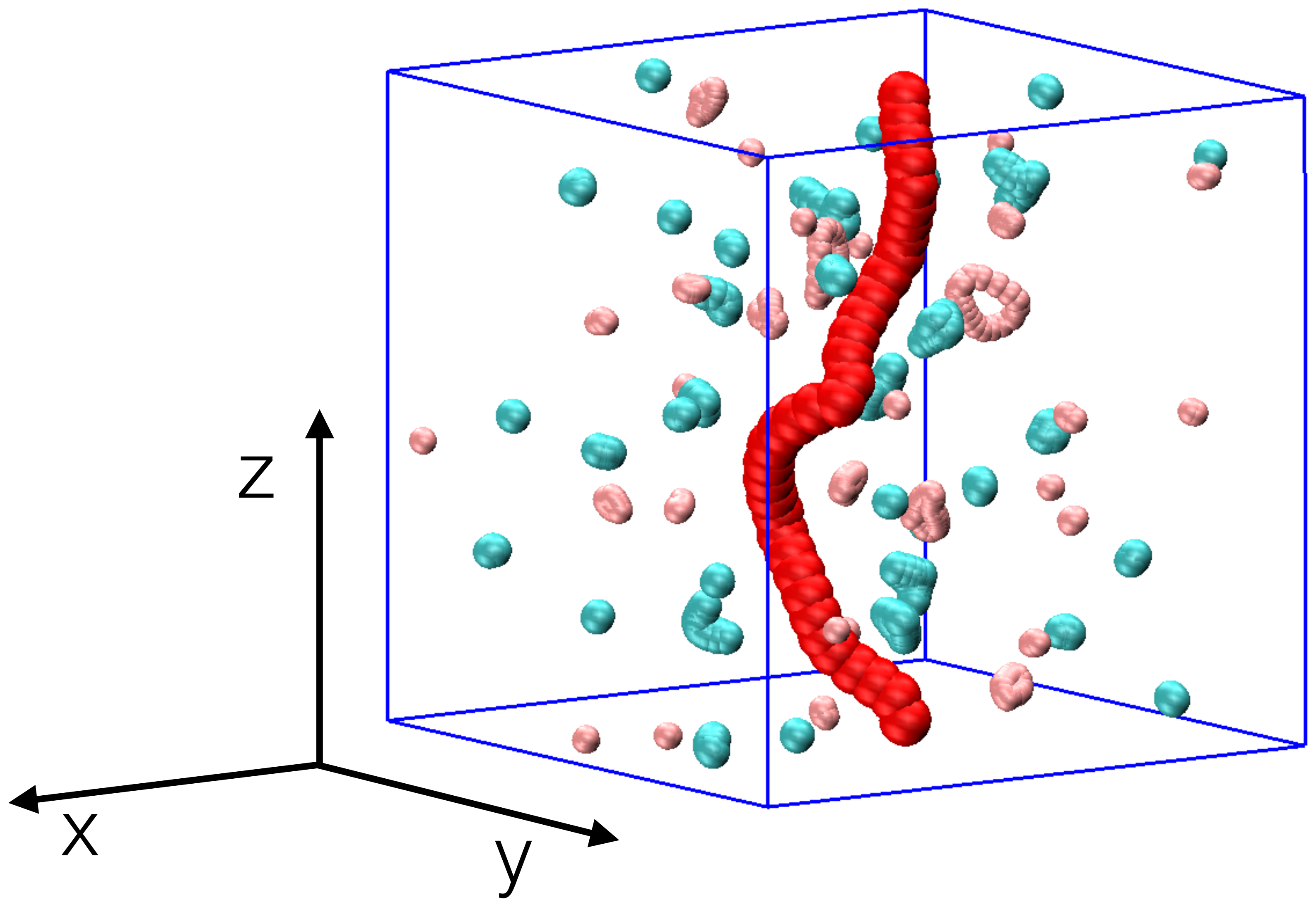

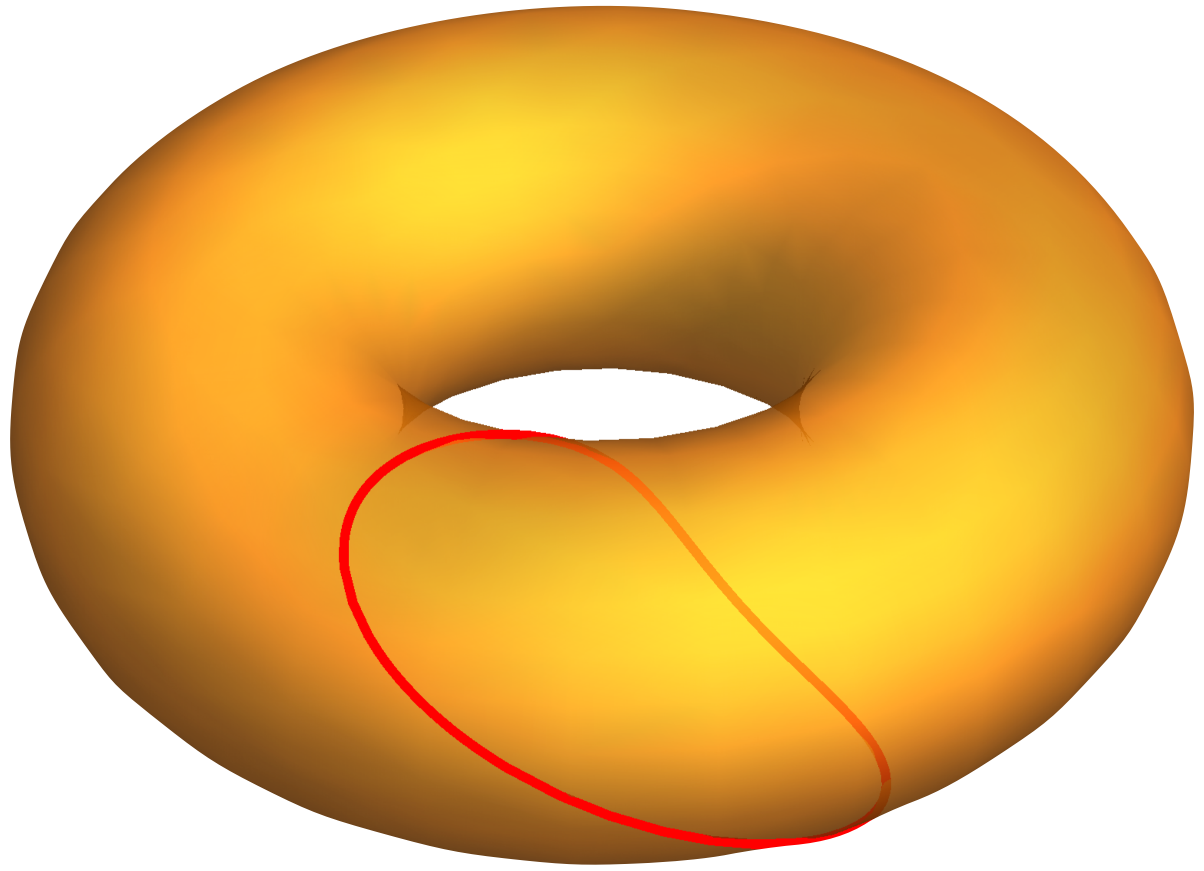

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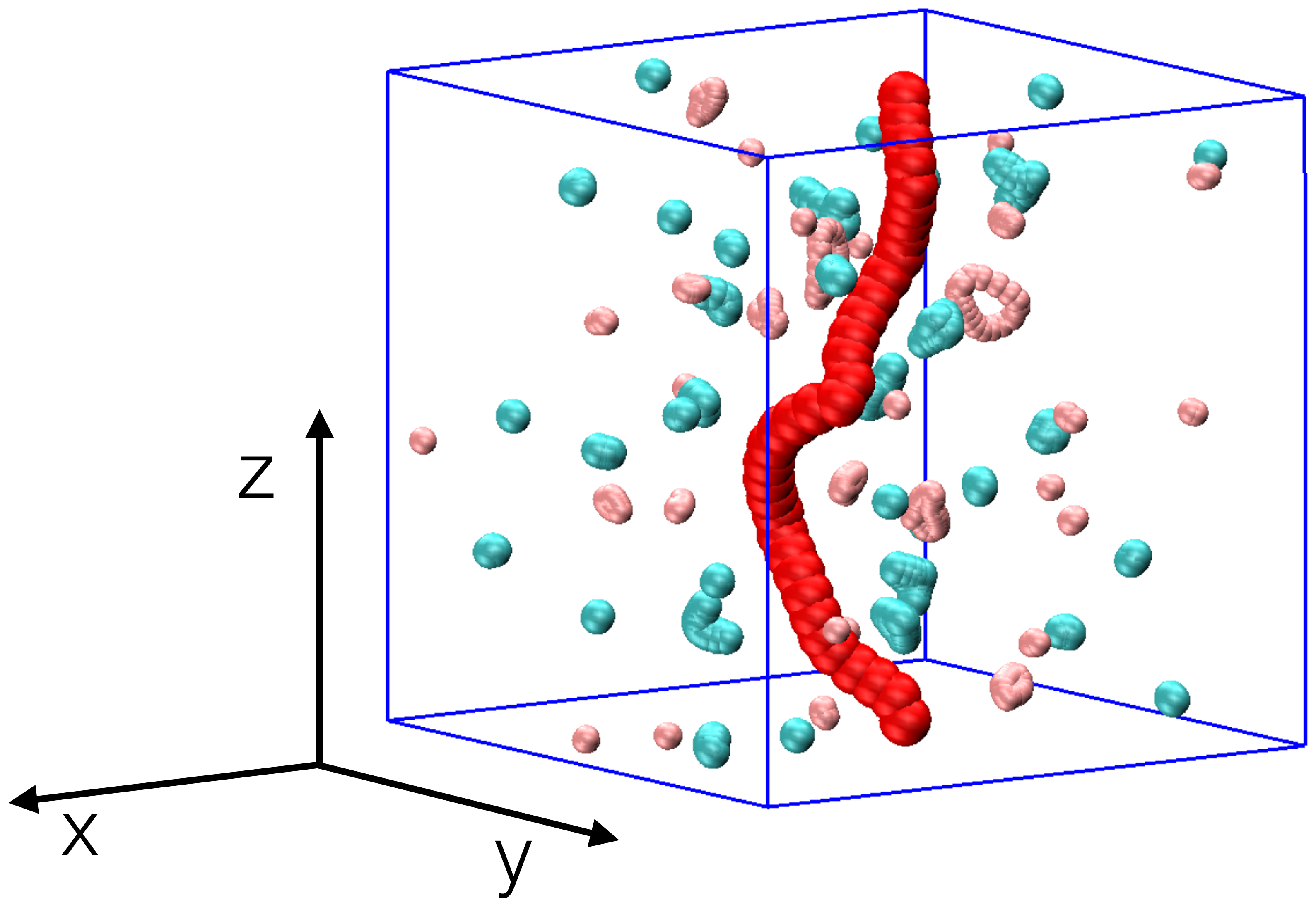
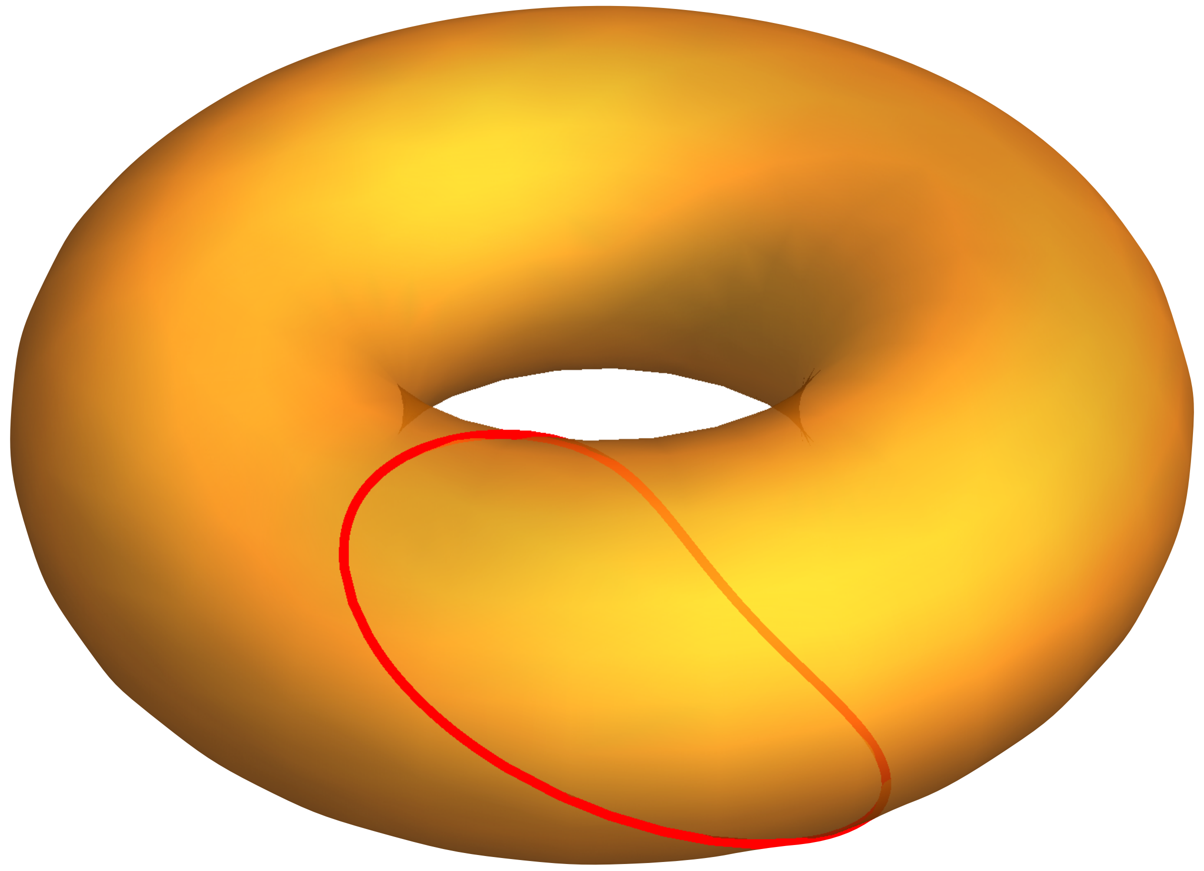
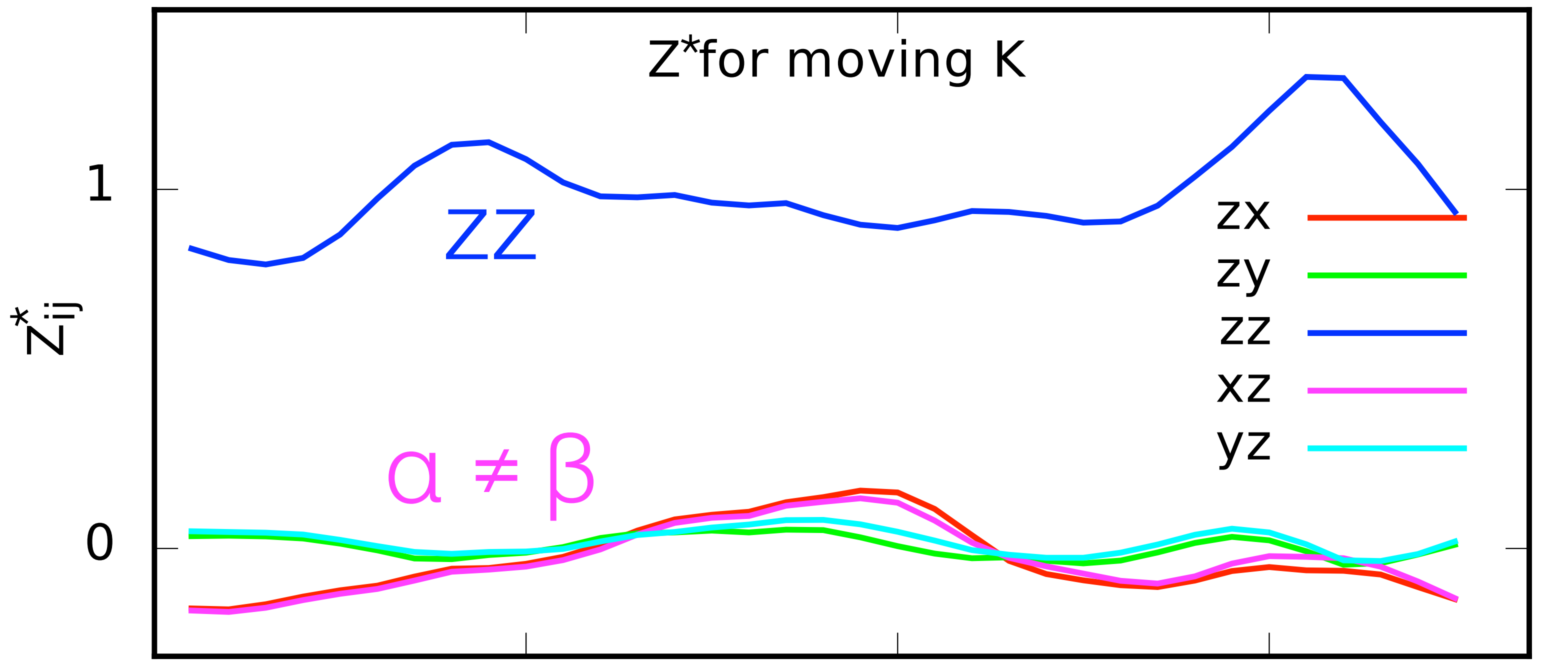
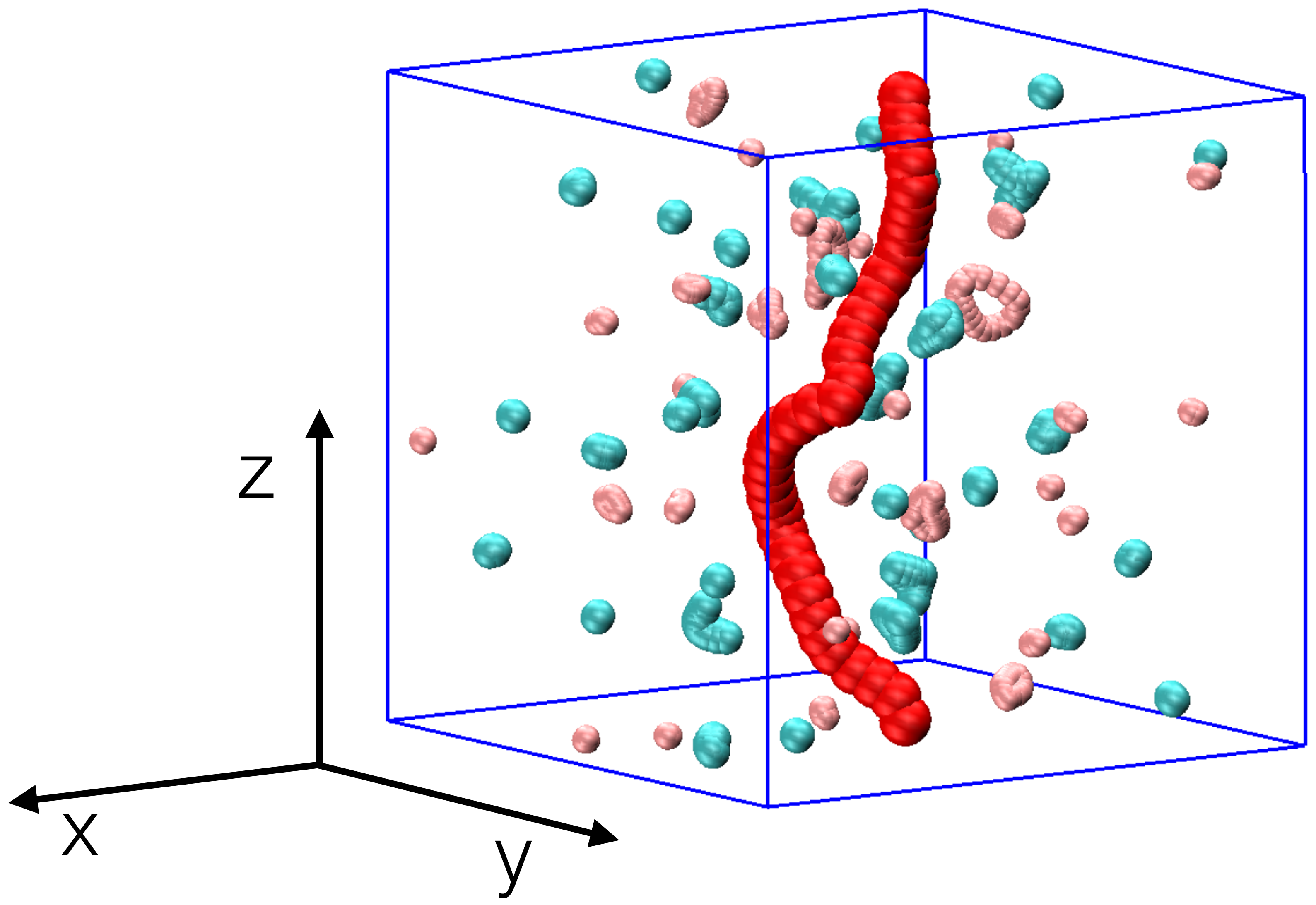


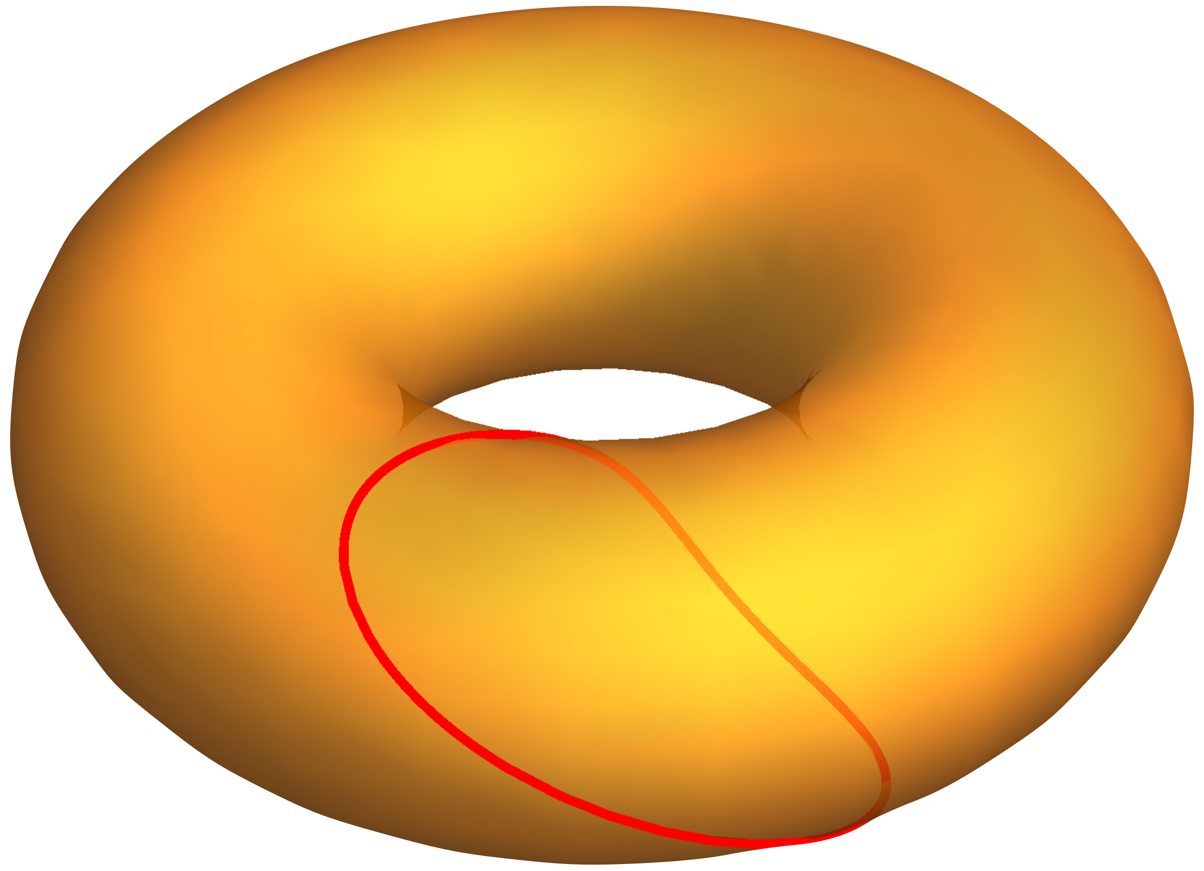


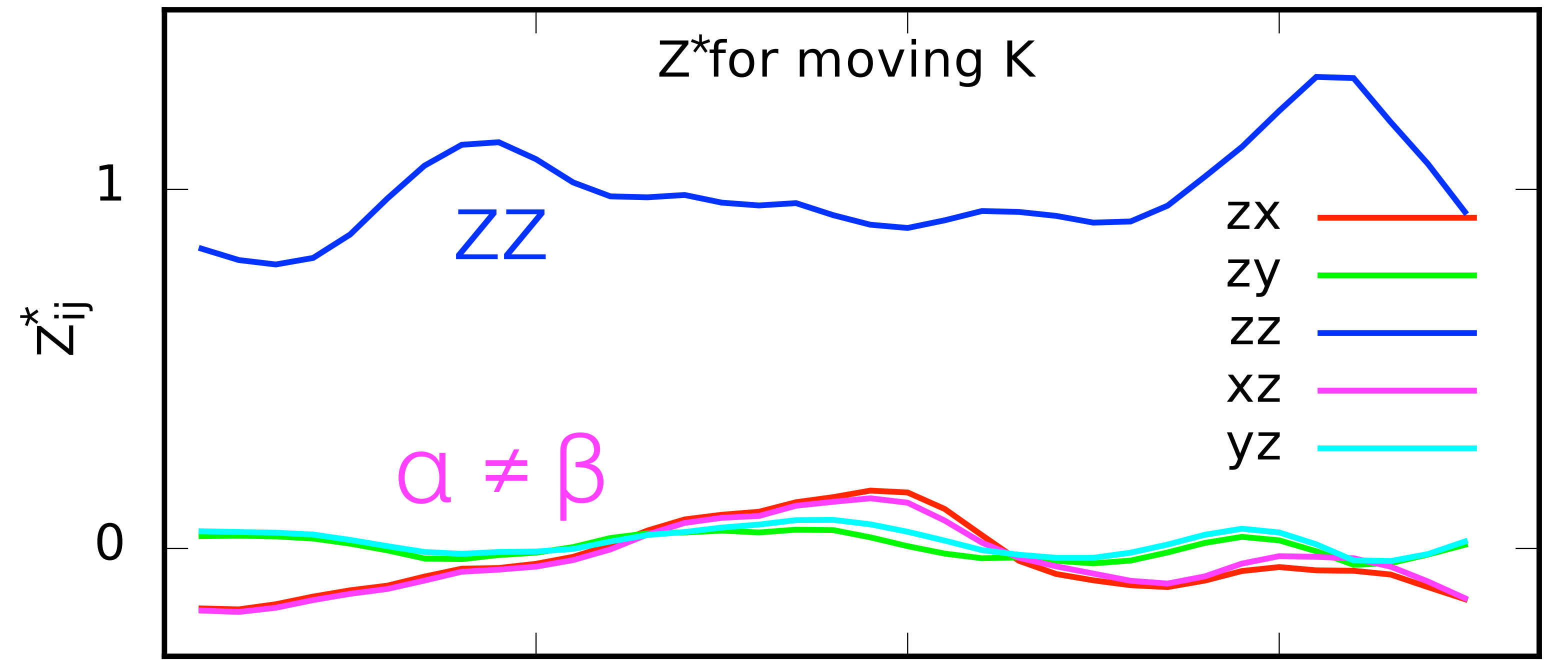


effective charge

a numerical experiment on molten KCl







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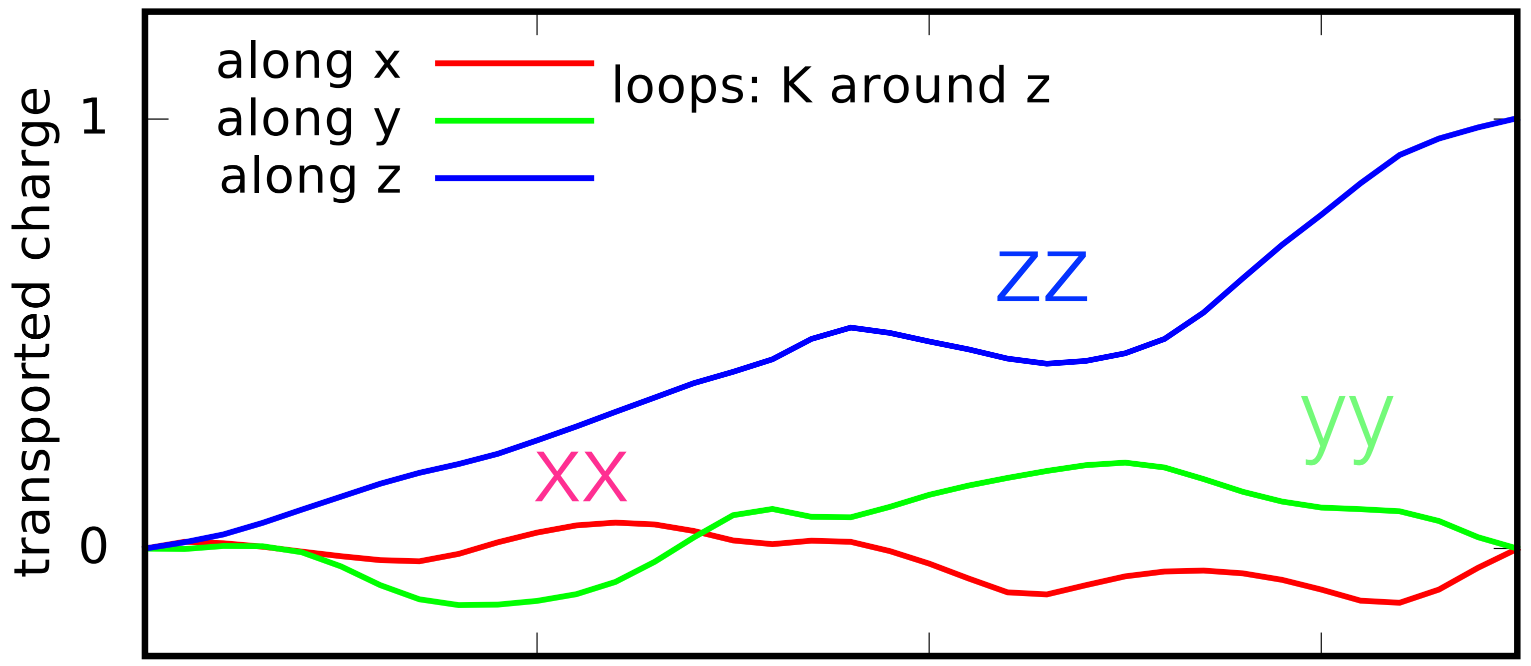
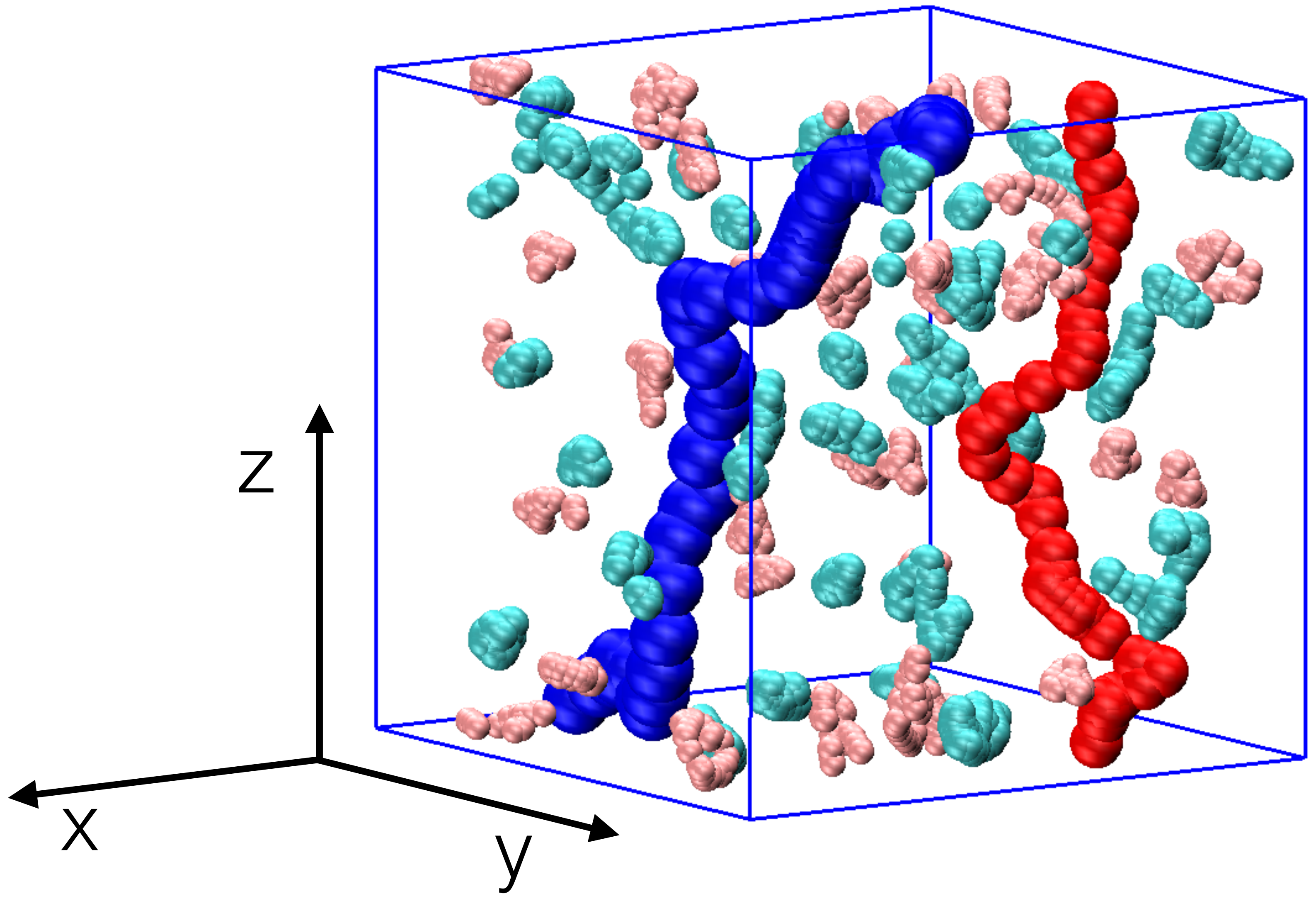
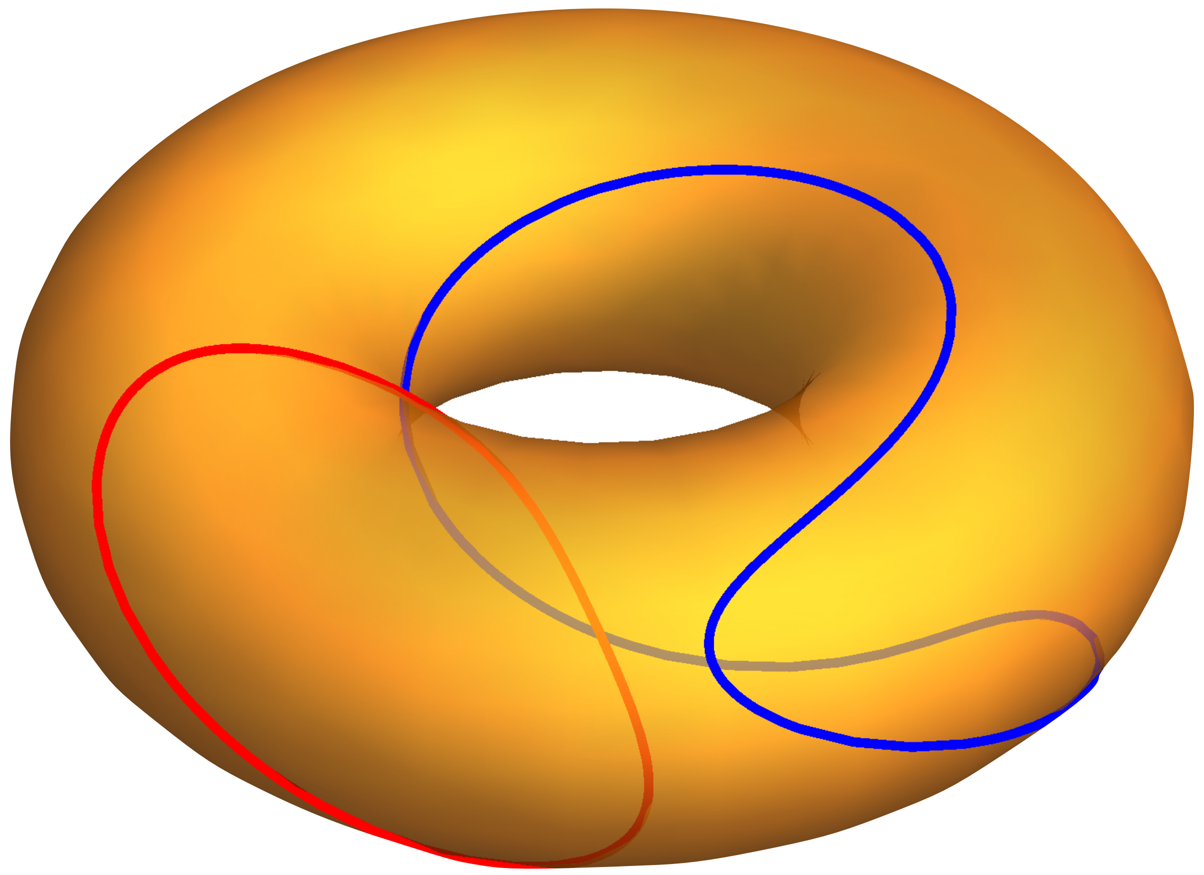


topological charge

Q_x = =-0.000(6); Q_y = 0.000(2); Q_z = 1.00(18)

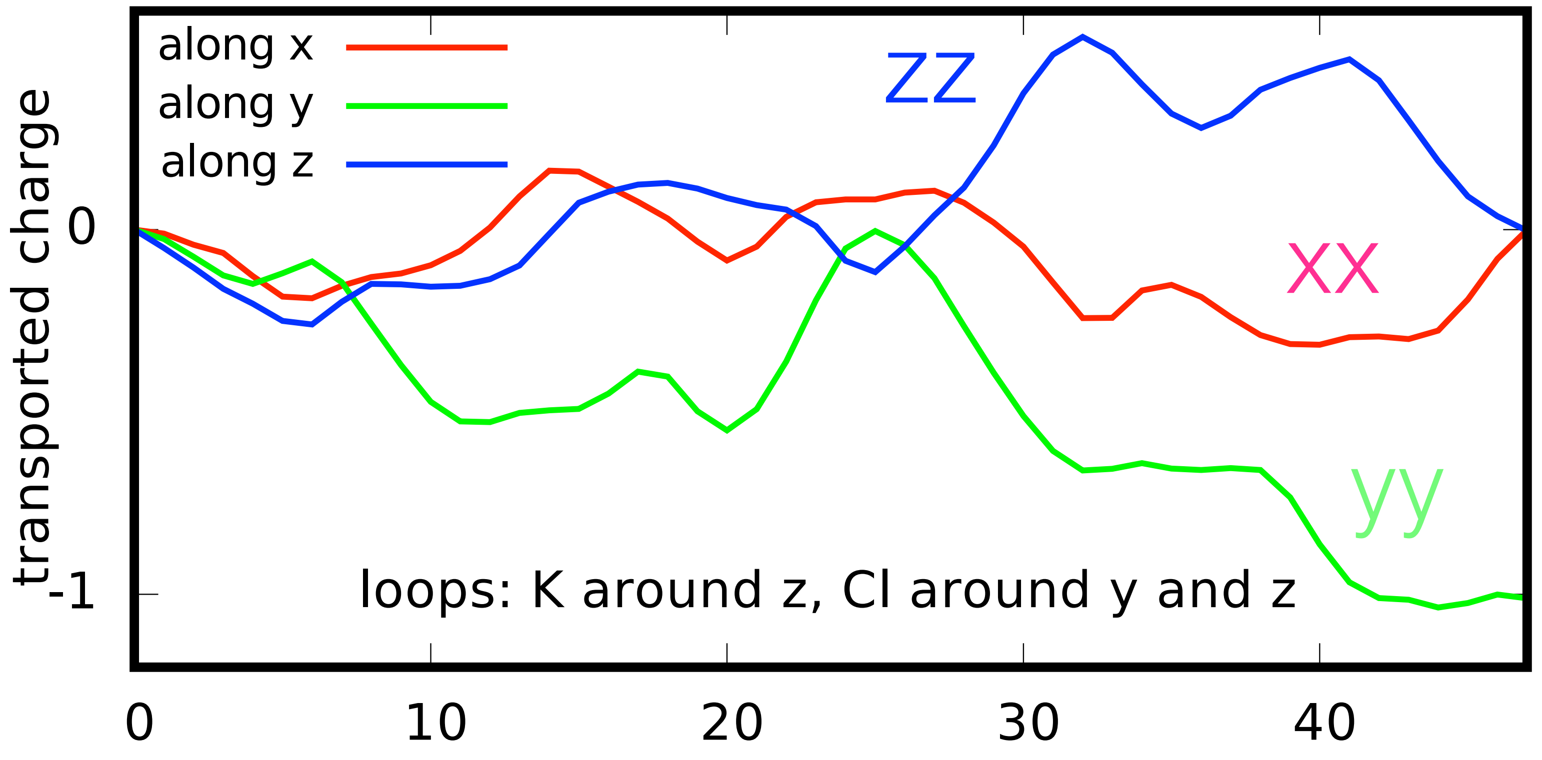
a numerical experiment on molten KCl





$Q_z[Cl]=-1$ $Q_y[Cl]=-1$

$Q_z[K] = 1$ $Q_z[K] = 0$



the charges transported by K and Cl
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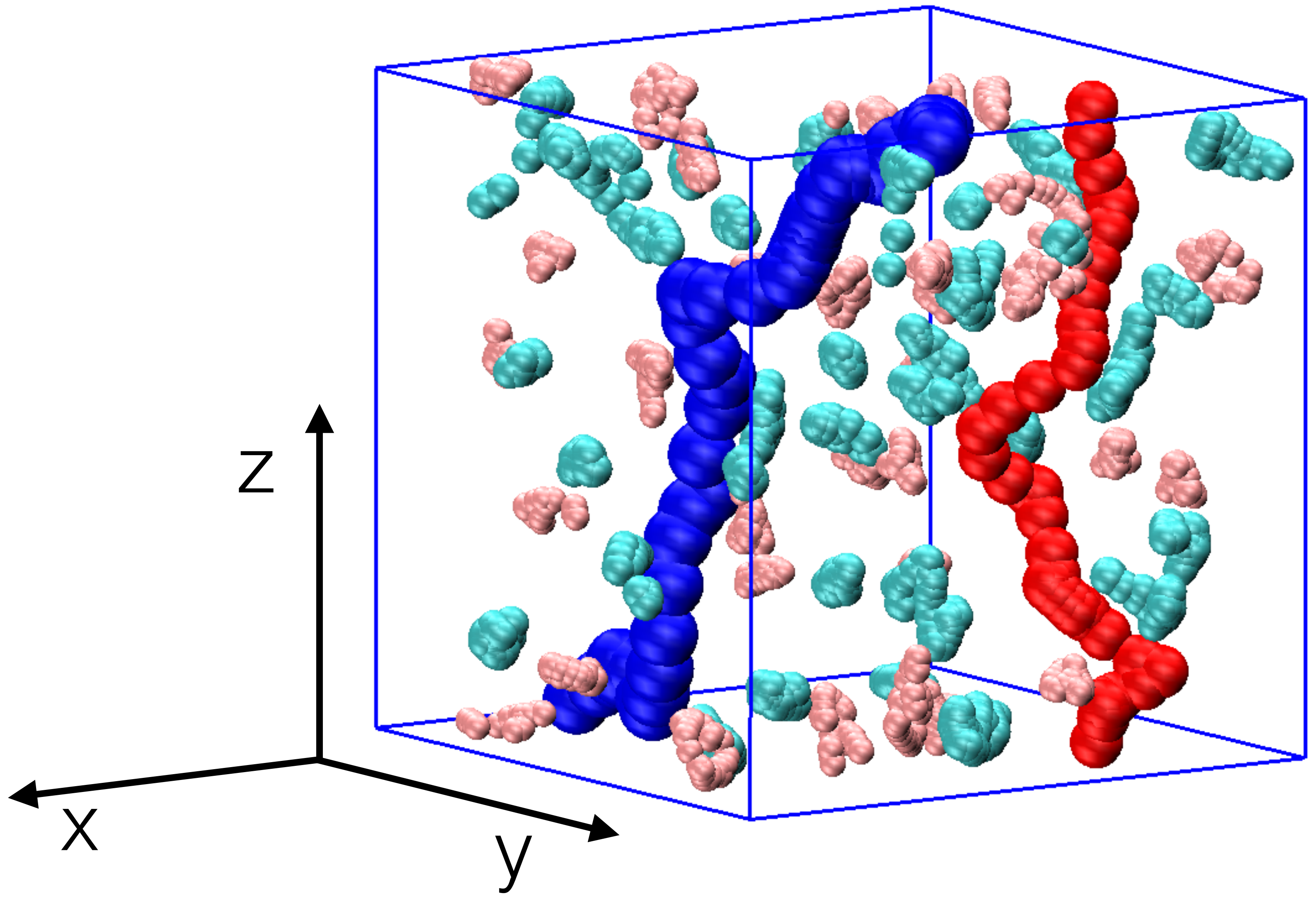
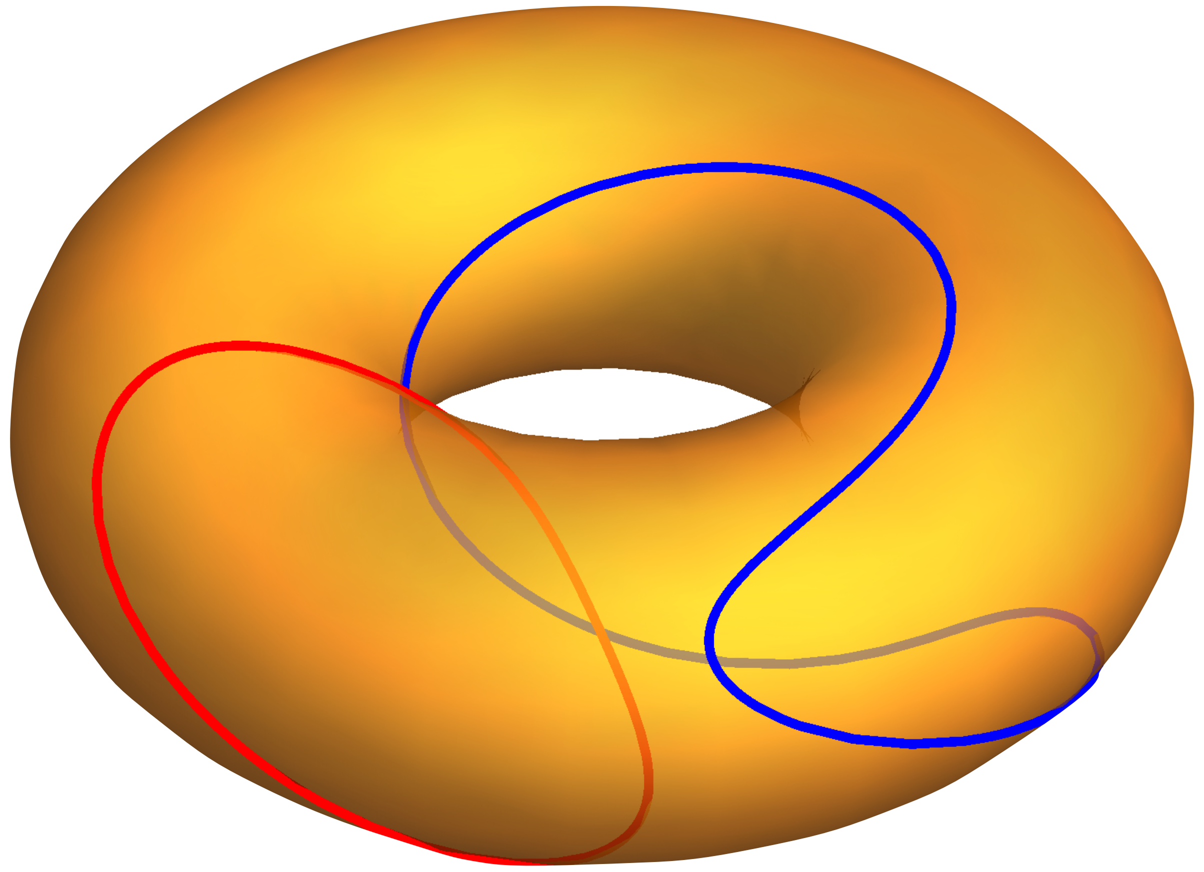
a numerical experiment on molten KCl





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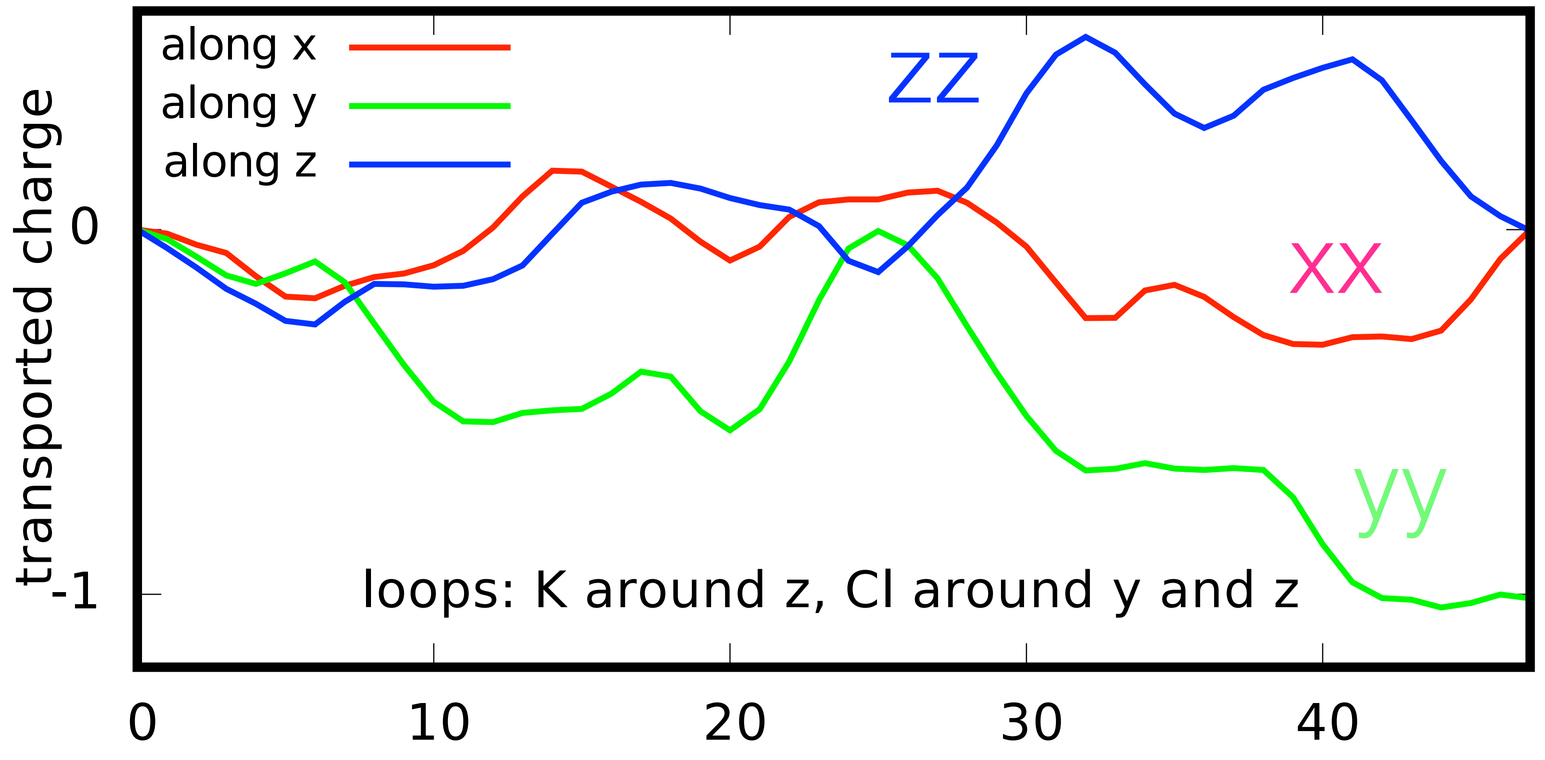

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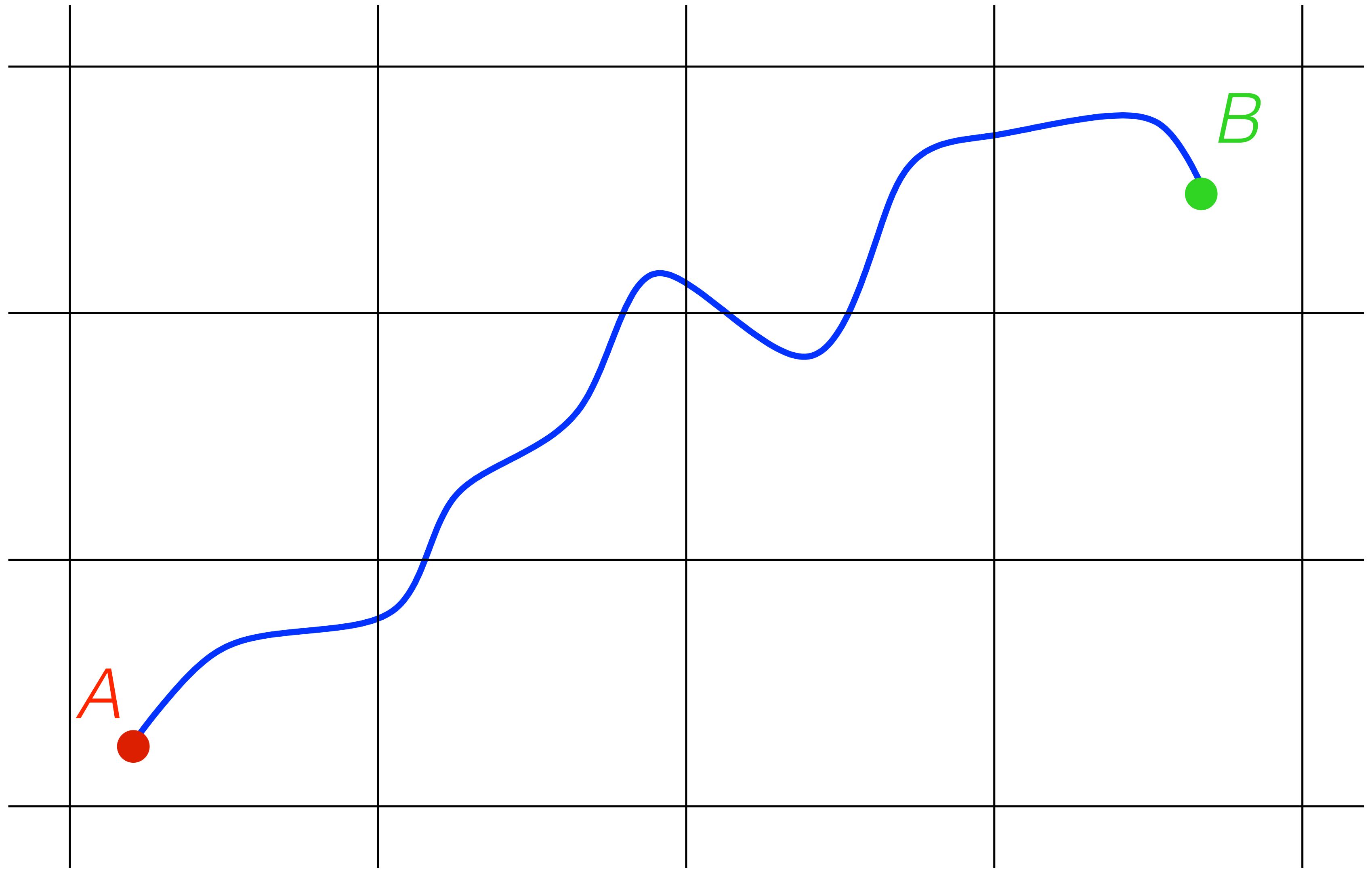
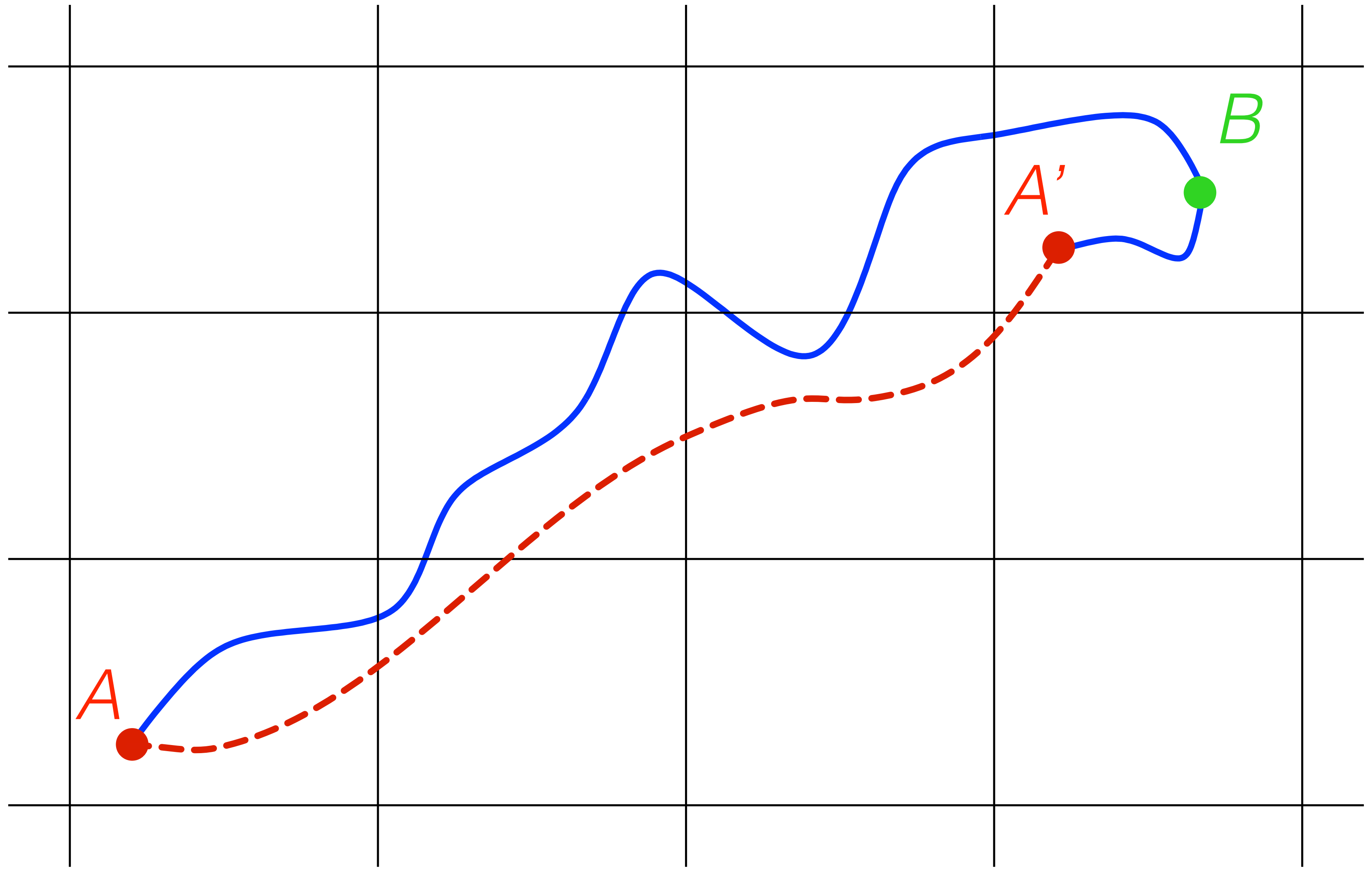
gauge invariance of charge transport



$$\sigma \propto \lim_{t\to\infty} \frac{1}{2t} \mathrm{var}\left[\mu_{AB}(t)\right]$$

$$\mu_{AB}(t) = \int_0^t J(t')dt'$$

gauge invariance of charge transport



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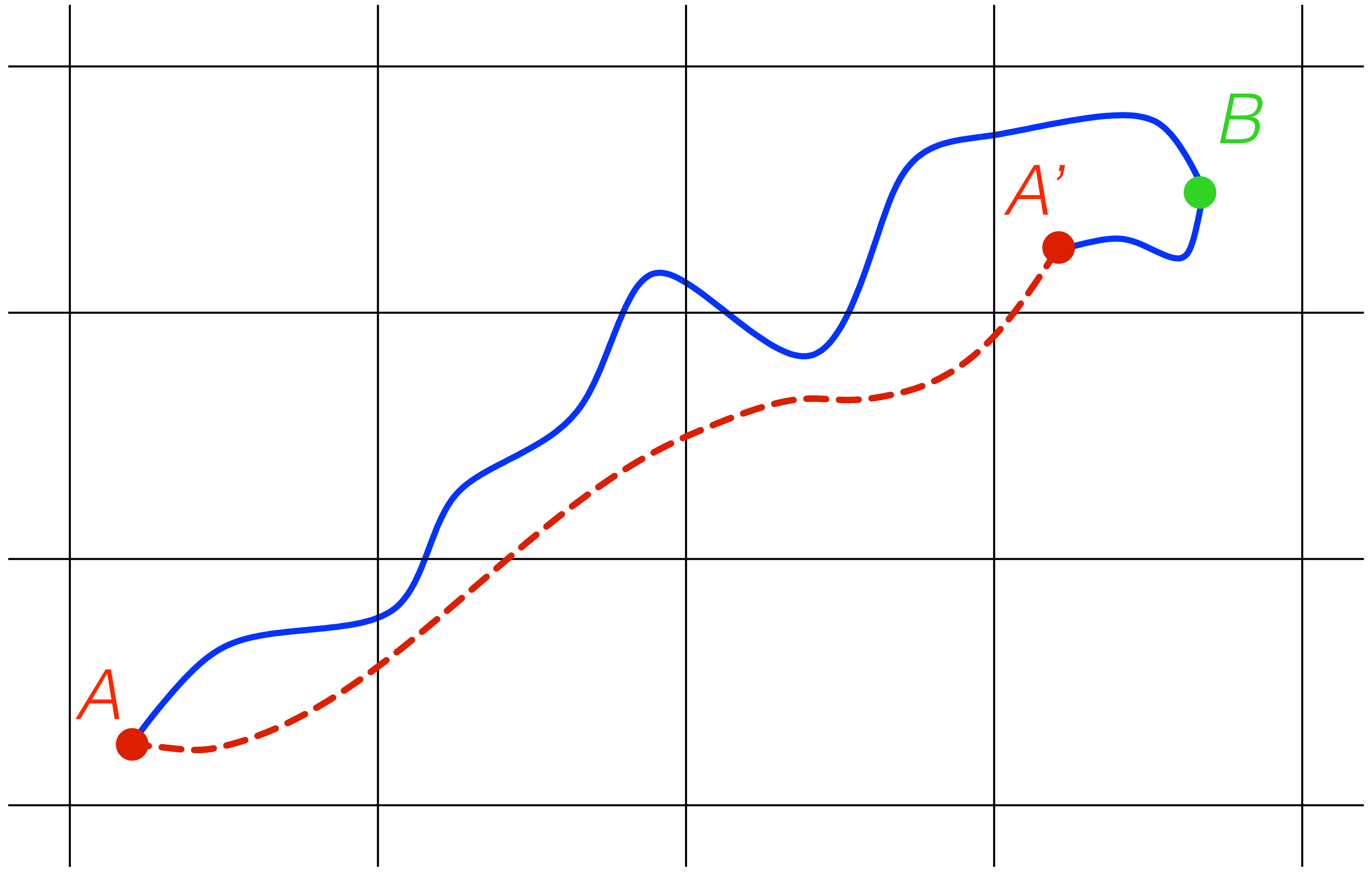

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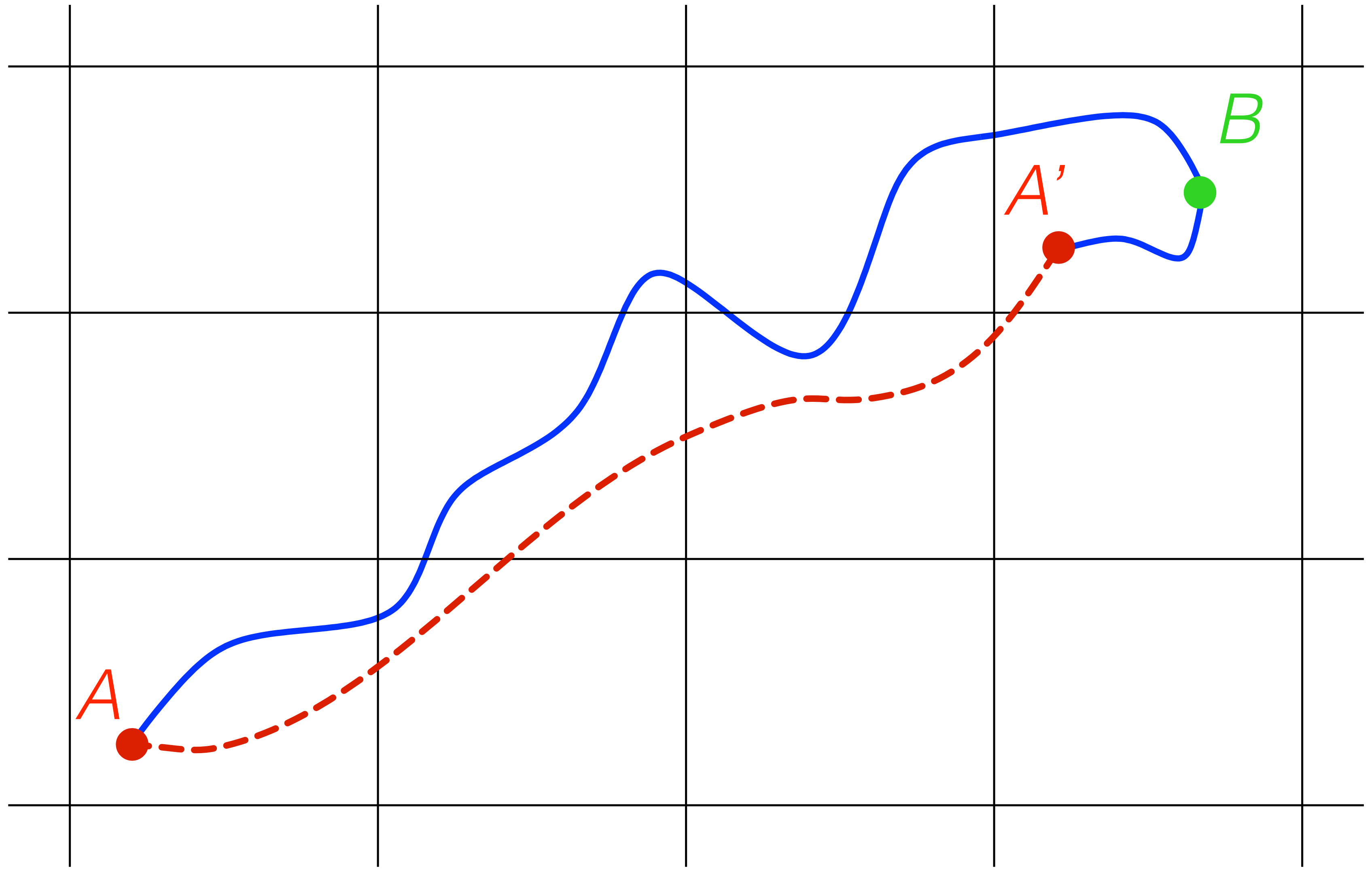

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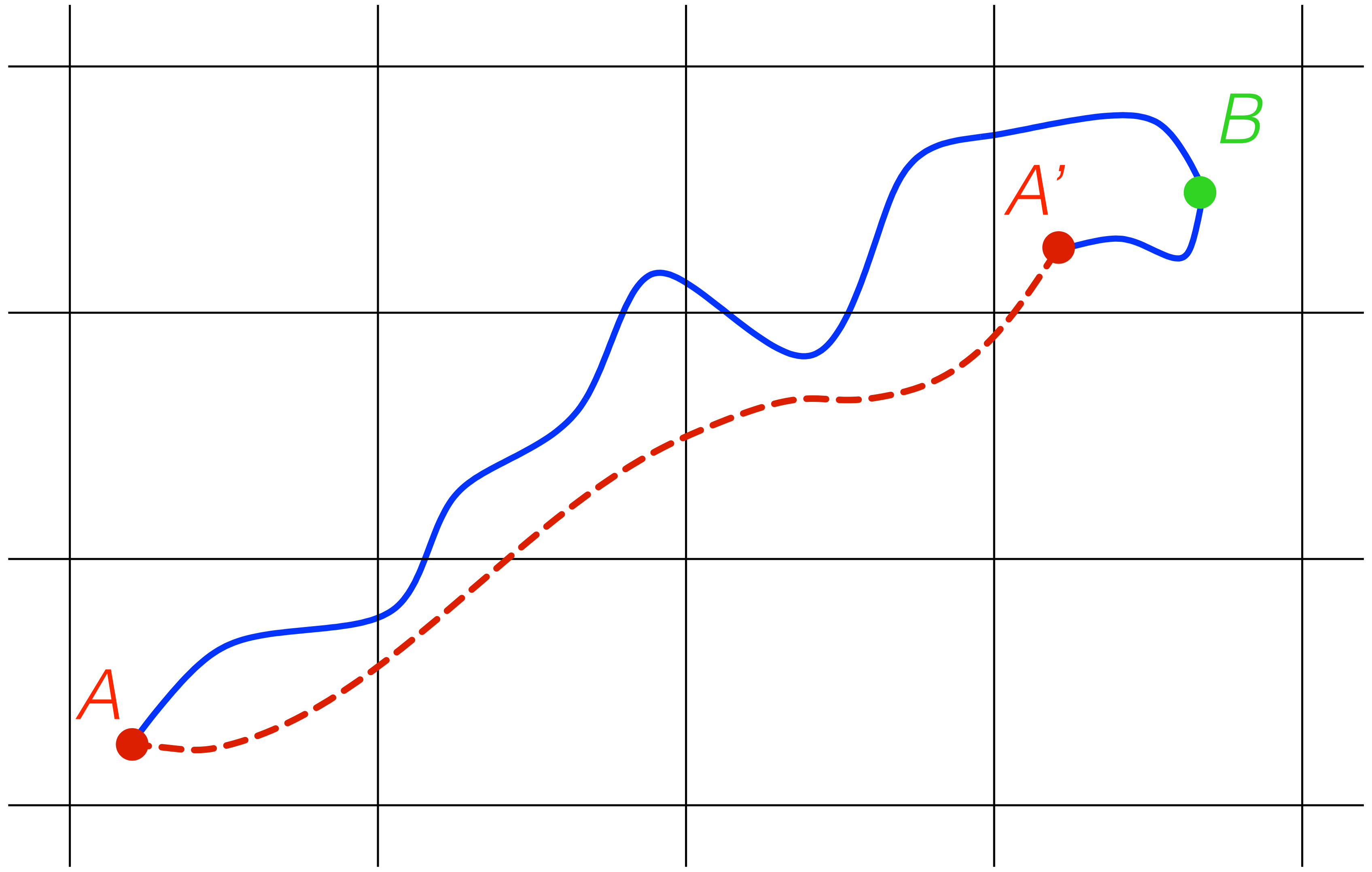

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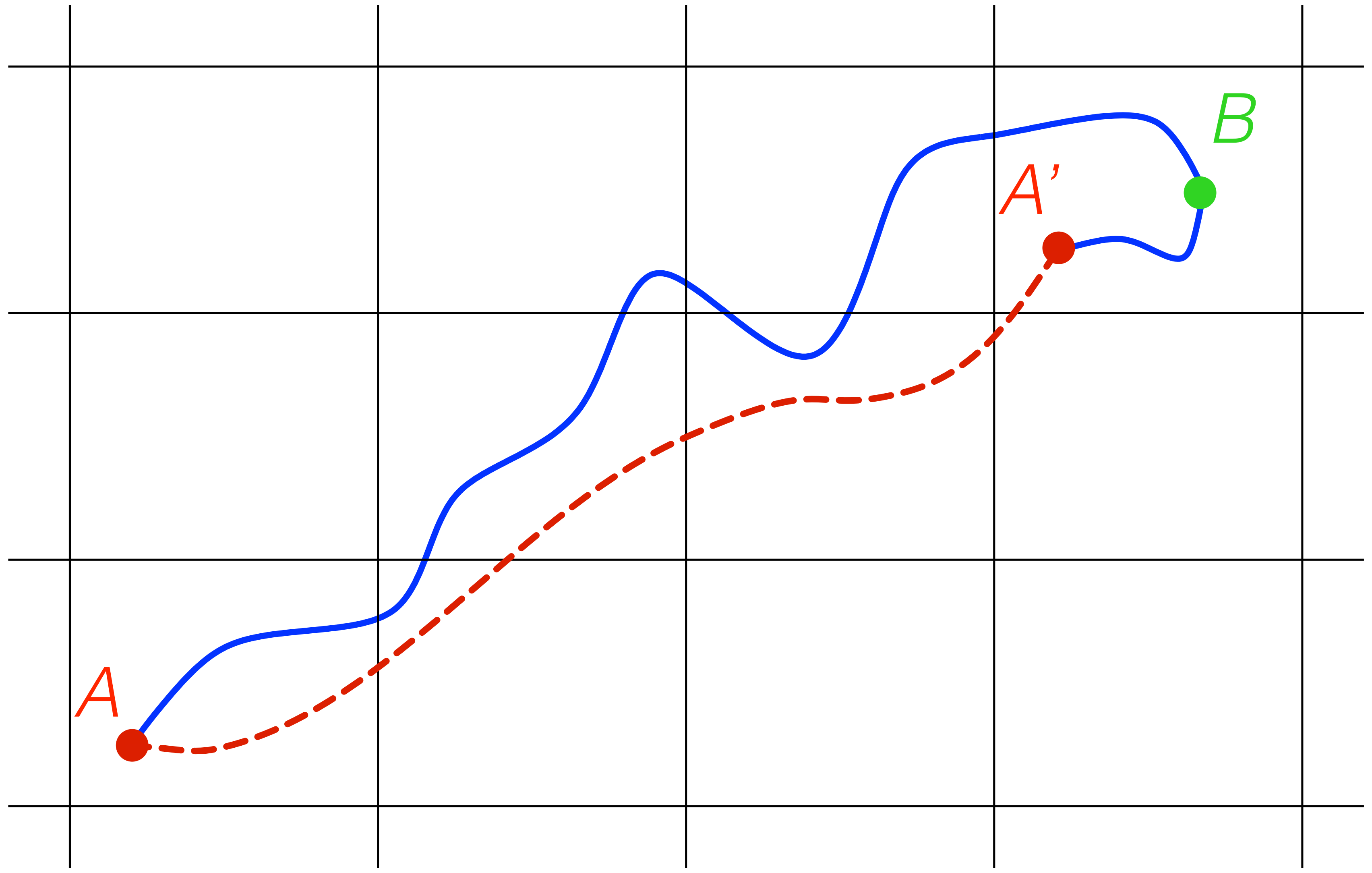
gauge invariance of charge transport



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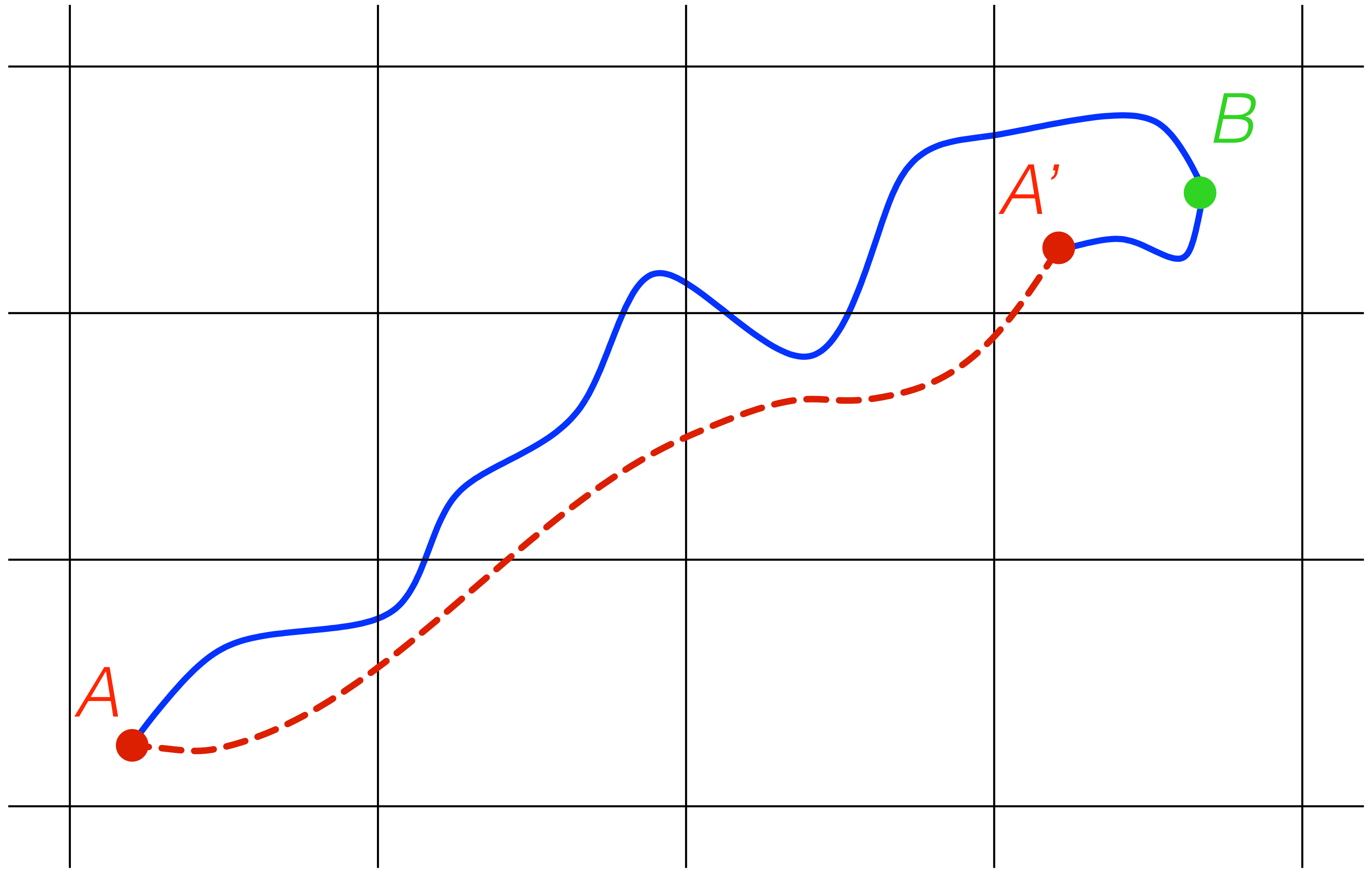

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$$Q(AA') = \frac{1}{\ell} \int_A^{A'} d\mu(X)$$

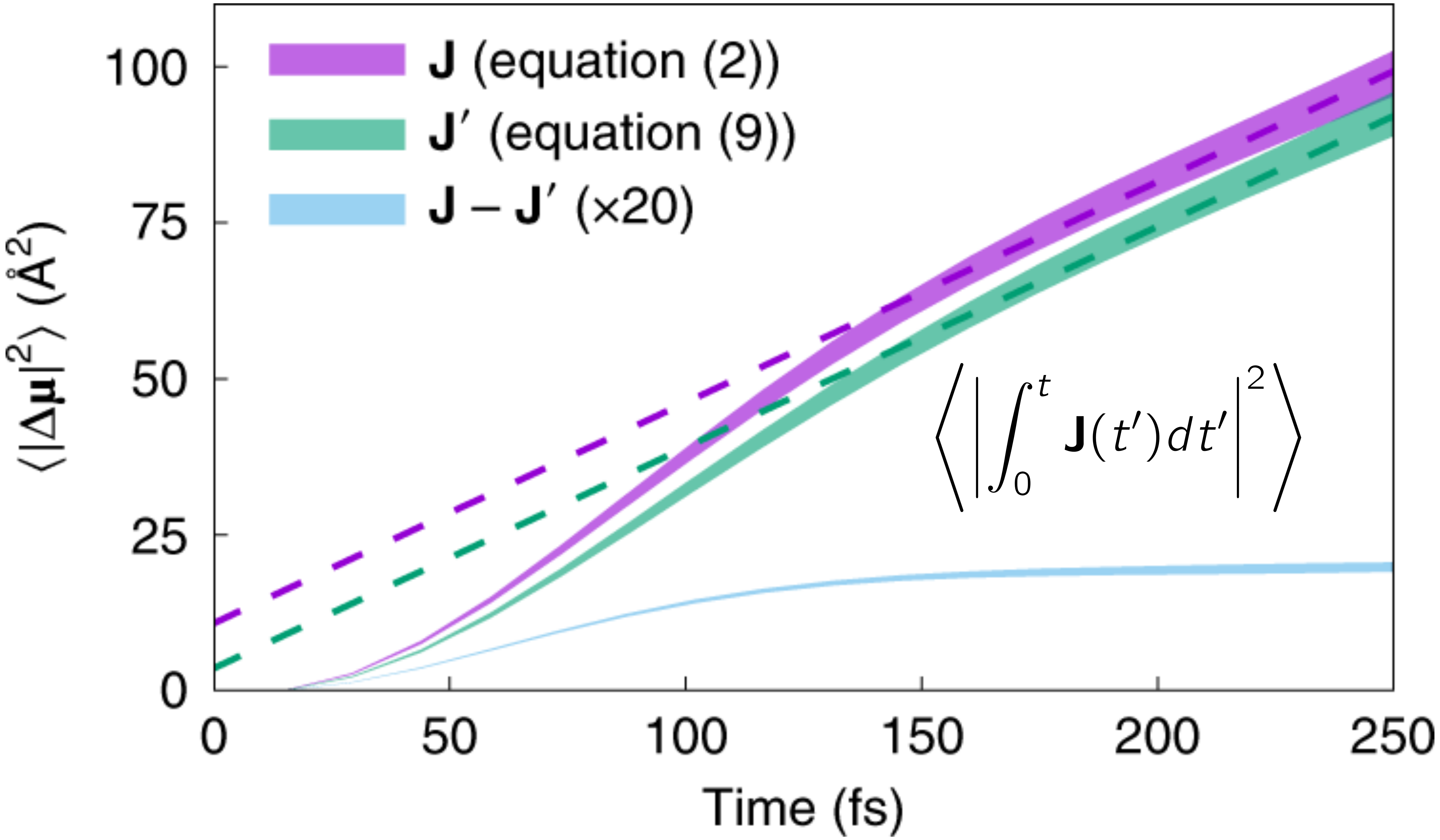
$$\in \mathbb{Z}$$

D.J. Thouless, *Quantization of particle transport*, Phys. Rev. B **27**, 2083 (1983)

currents from atomic oxidation numbers

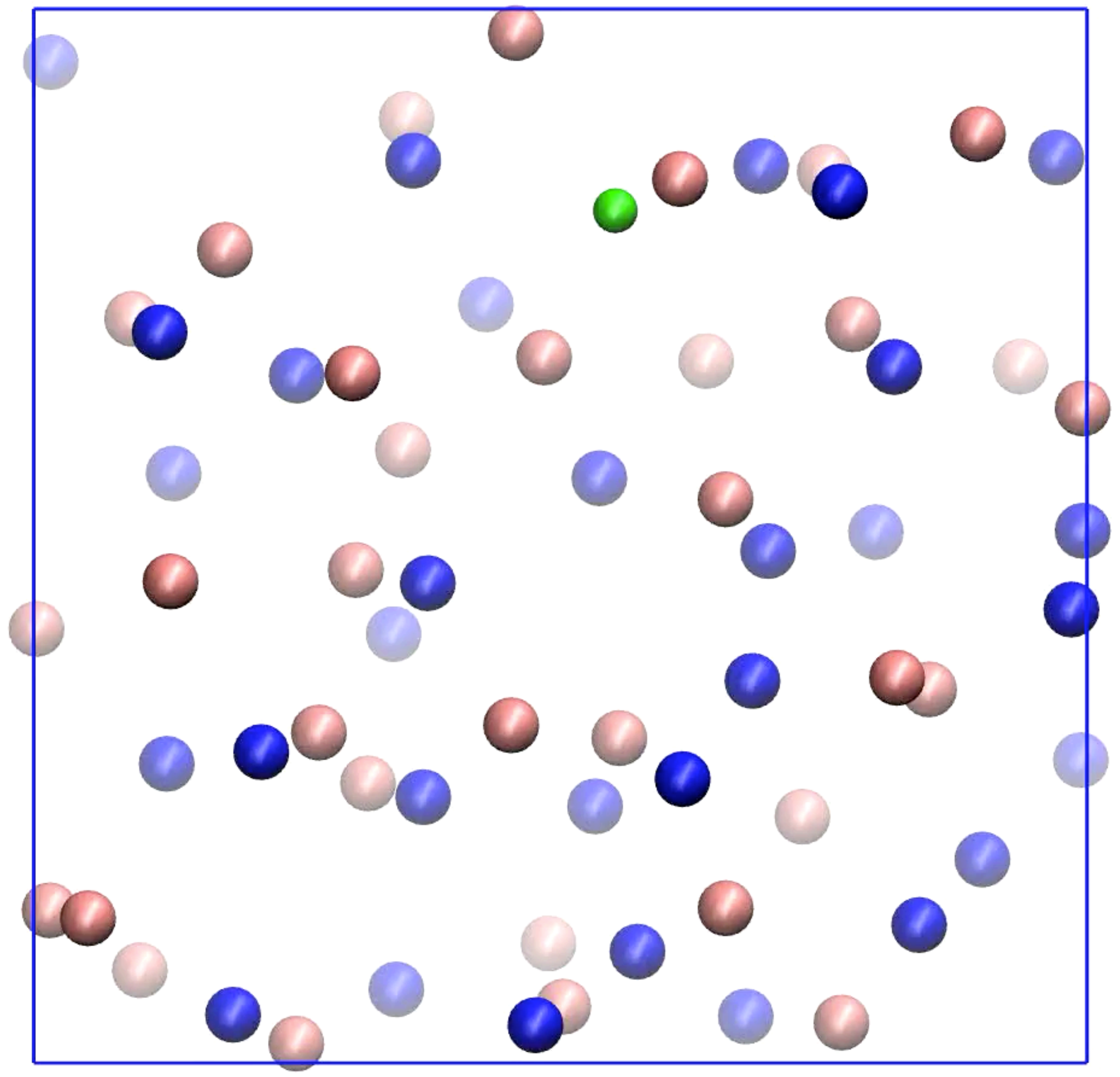
(2) $$J_\alpha = \sum_{i\beta} Z^*_{i\alpha\beta} v_{i\beta}$$

(9) $$J'_\alpha = \sum_{i} q_{S(i)} v_{i\alpha}$$



non-stoichiometric melts

$K_x(KCl)_{1-x}$



$K_{33}Cl_{31}$

$x \approx 0.06$

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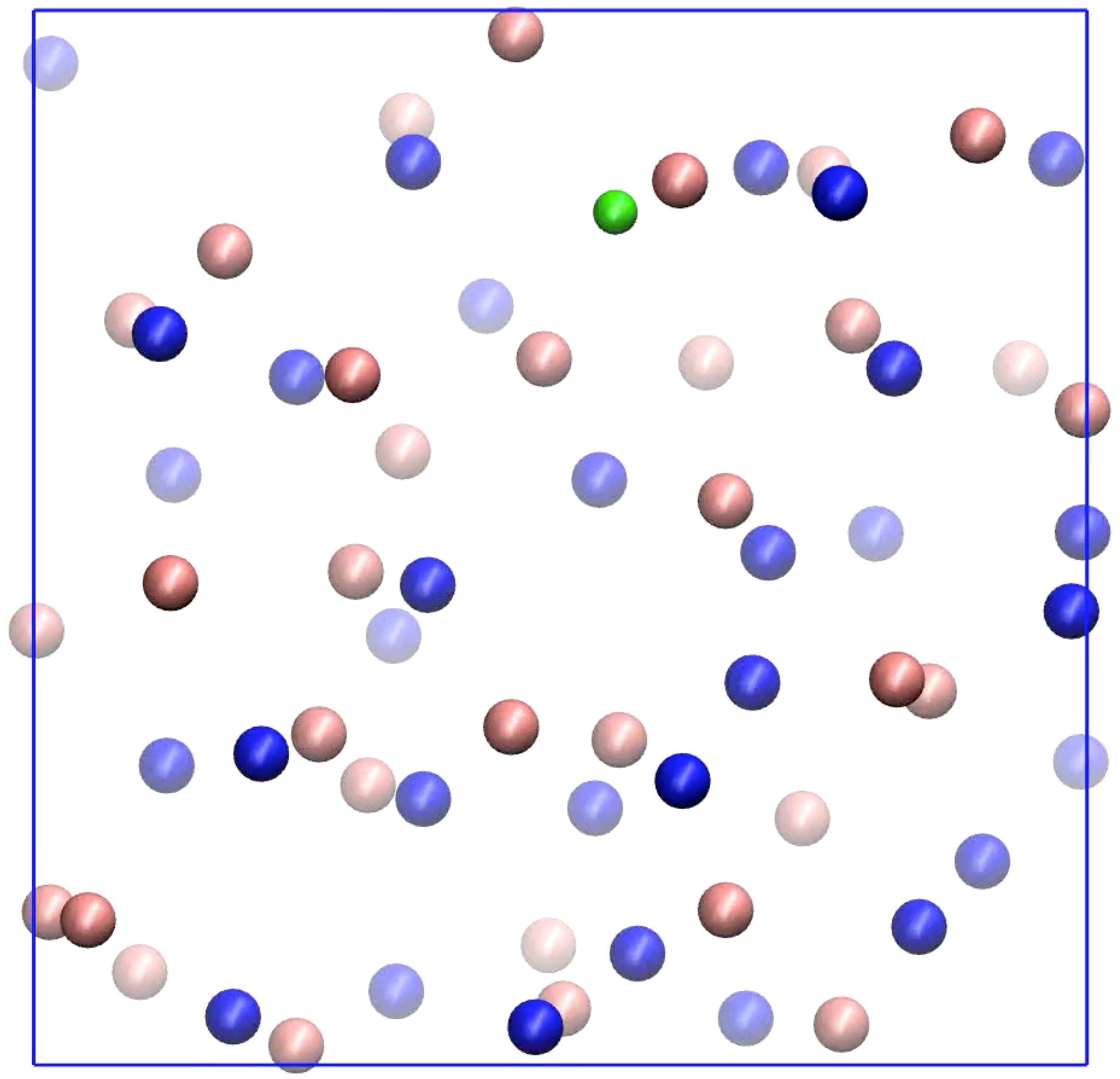

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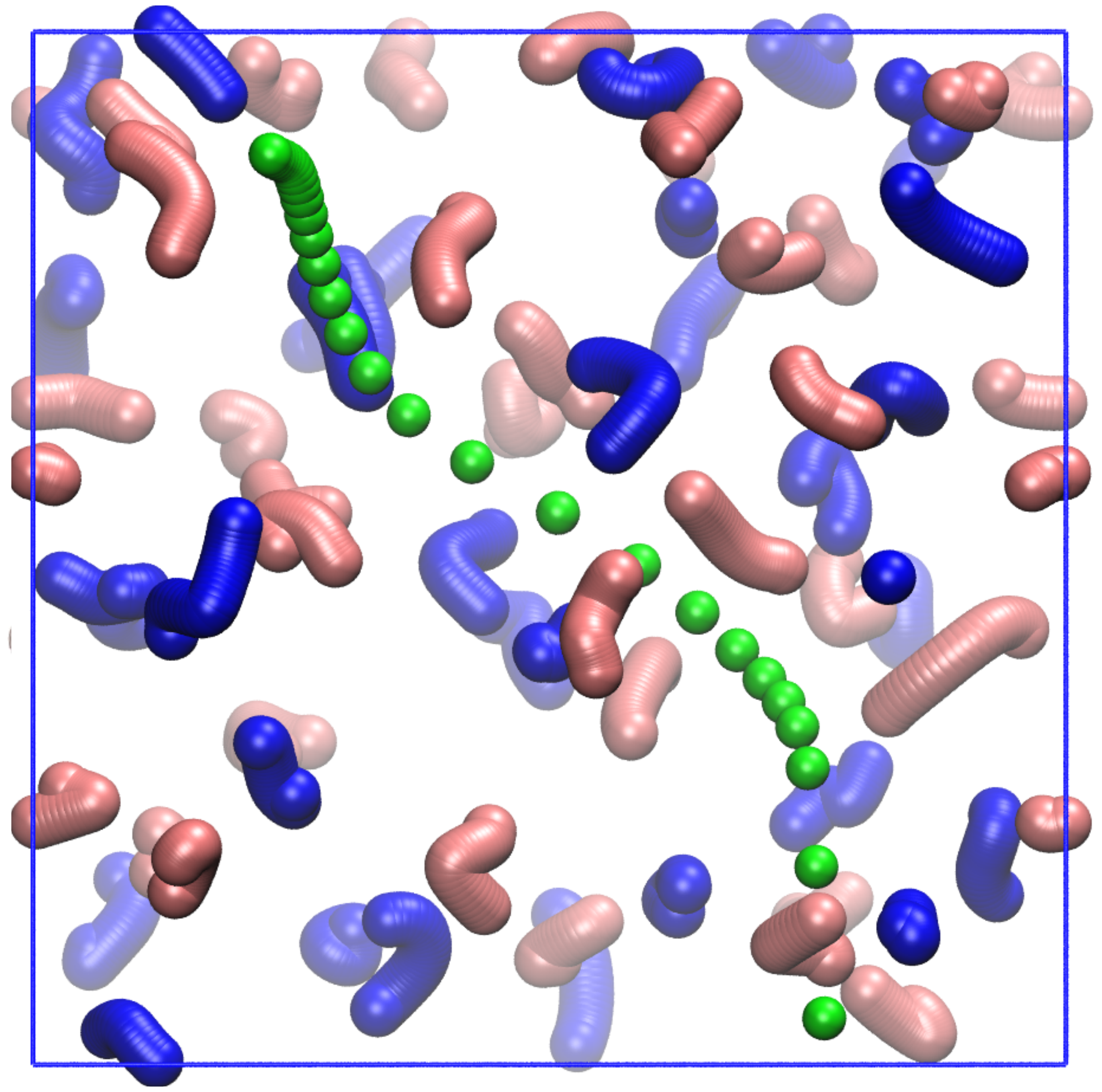

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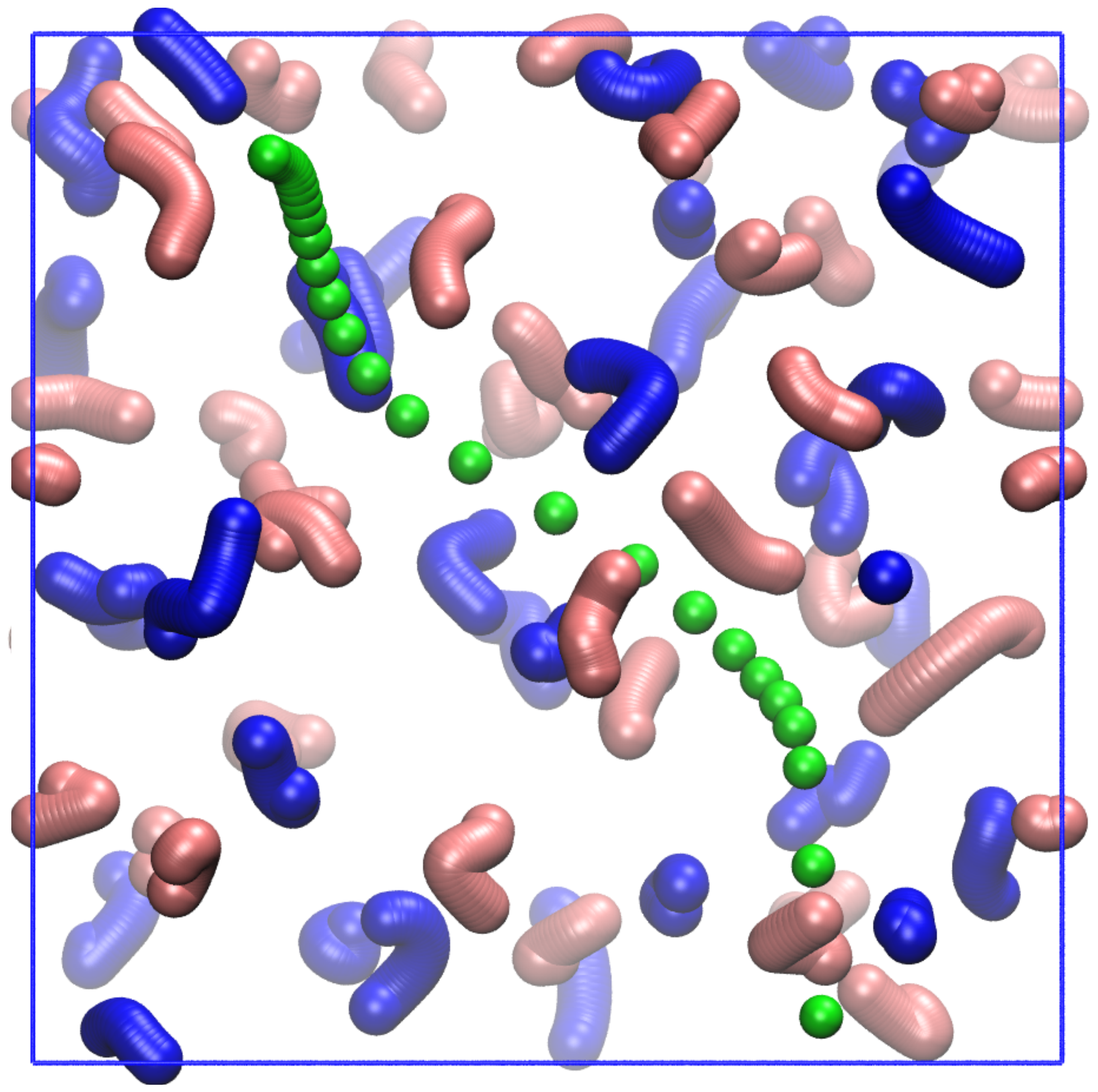
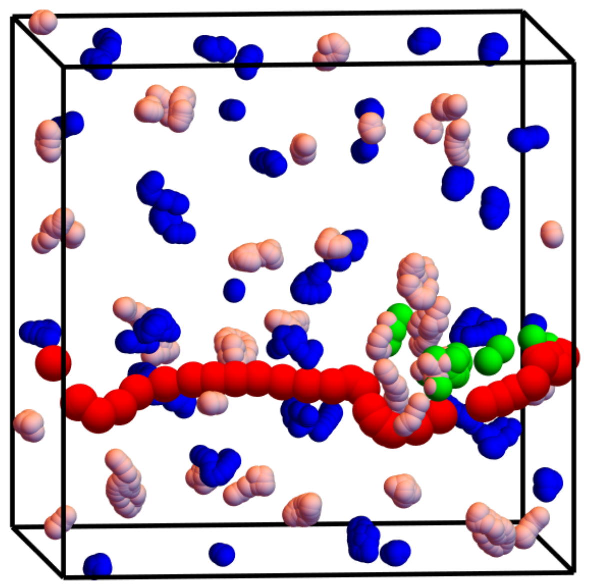
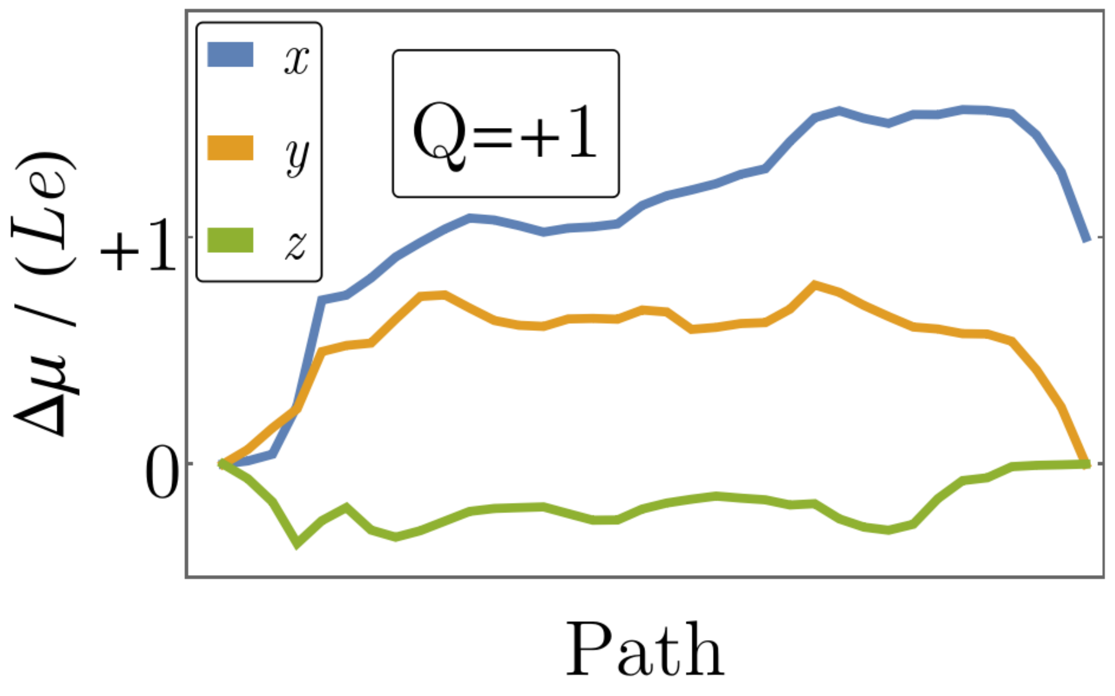


$K_{33}Cl_{31}$

x≈0.06





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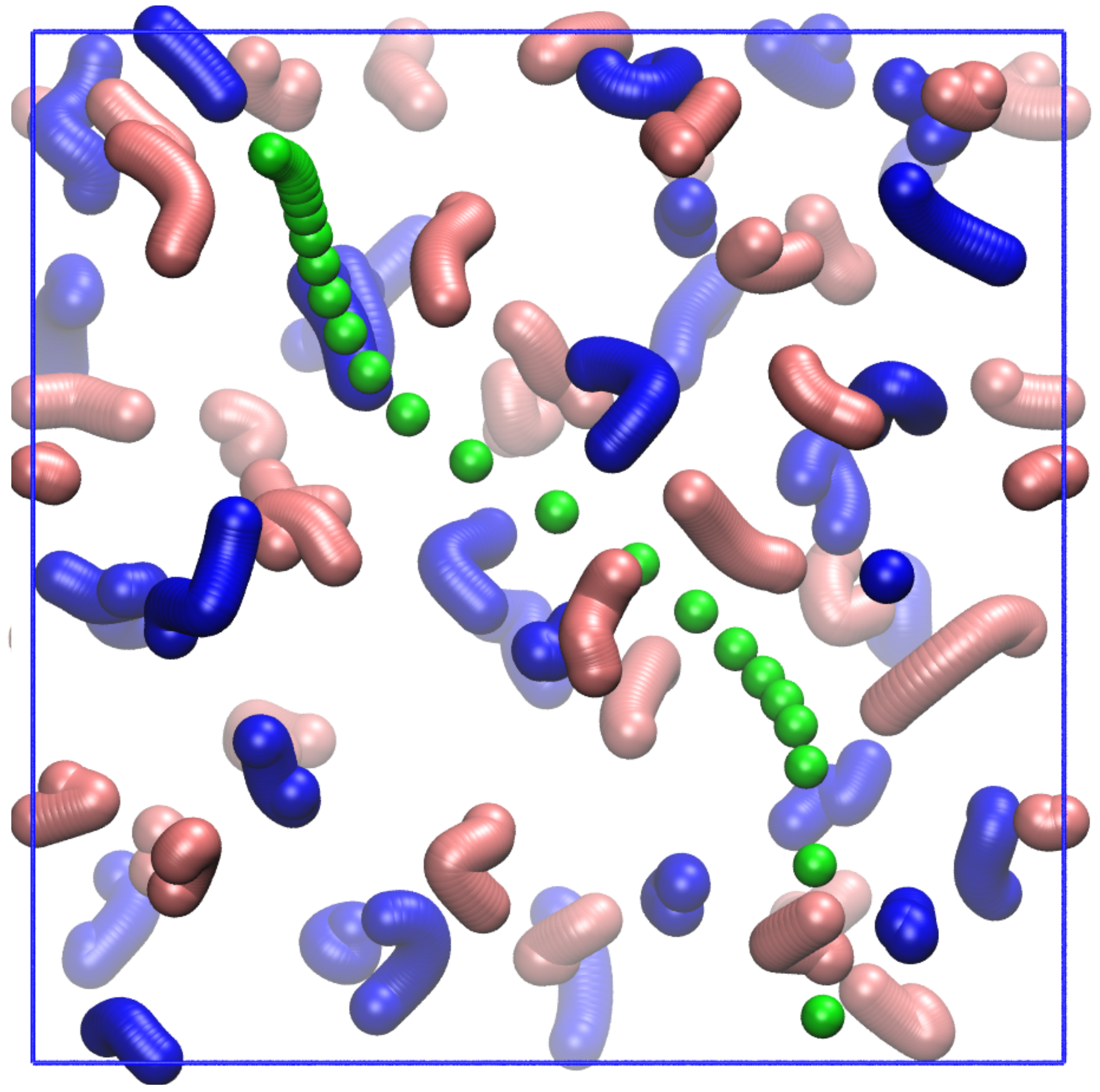

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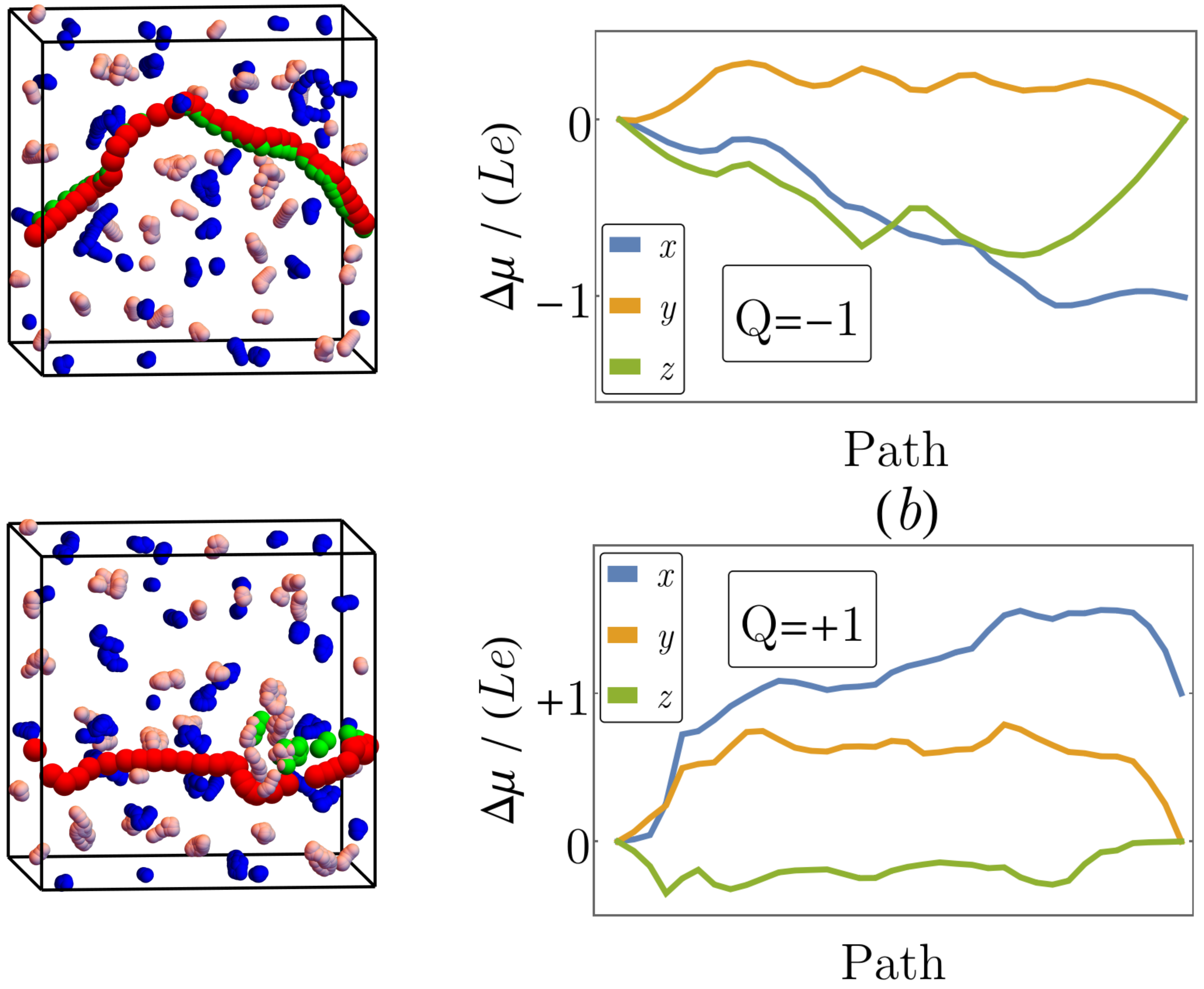
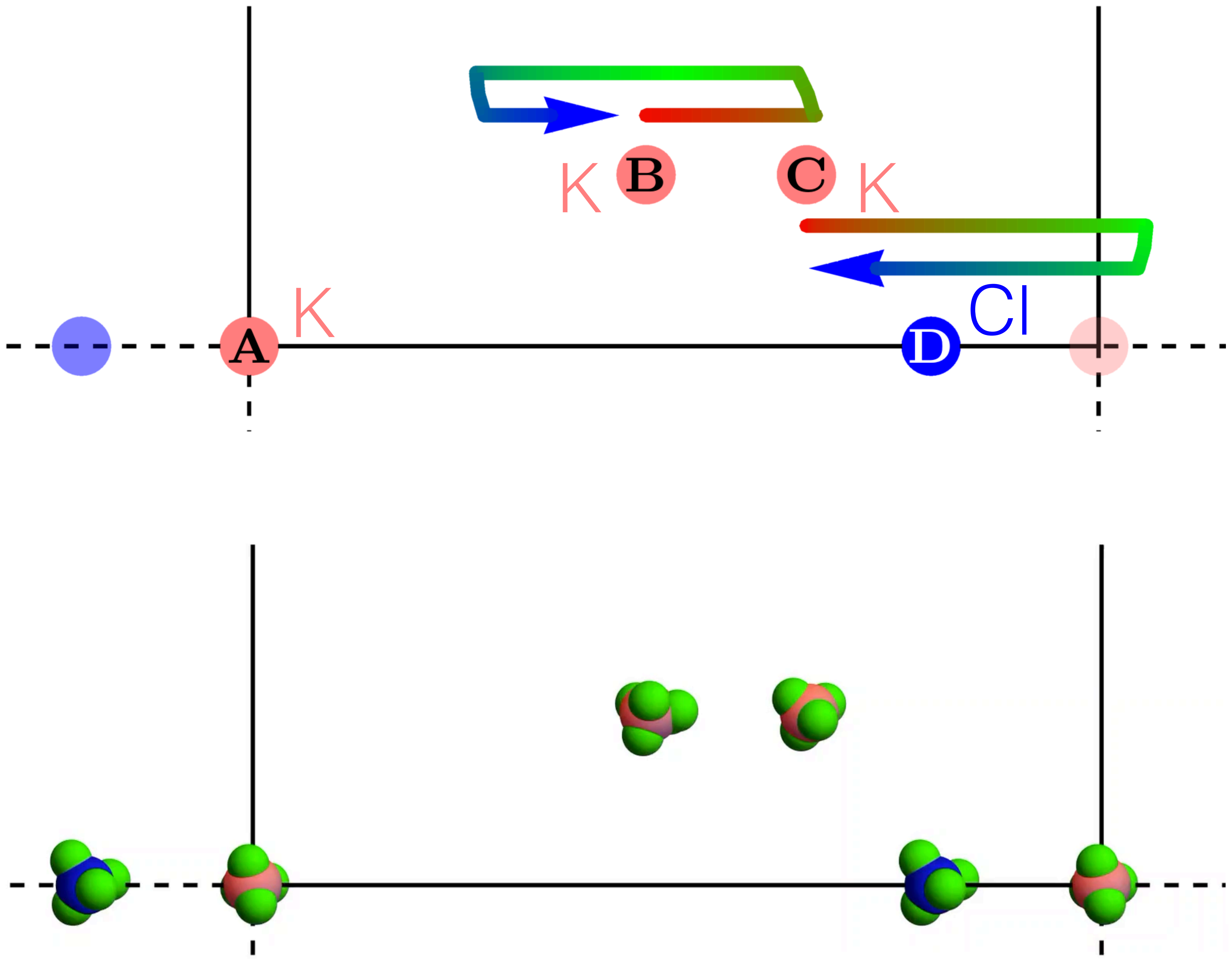
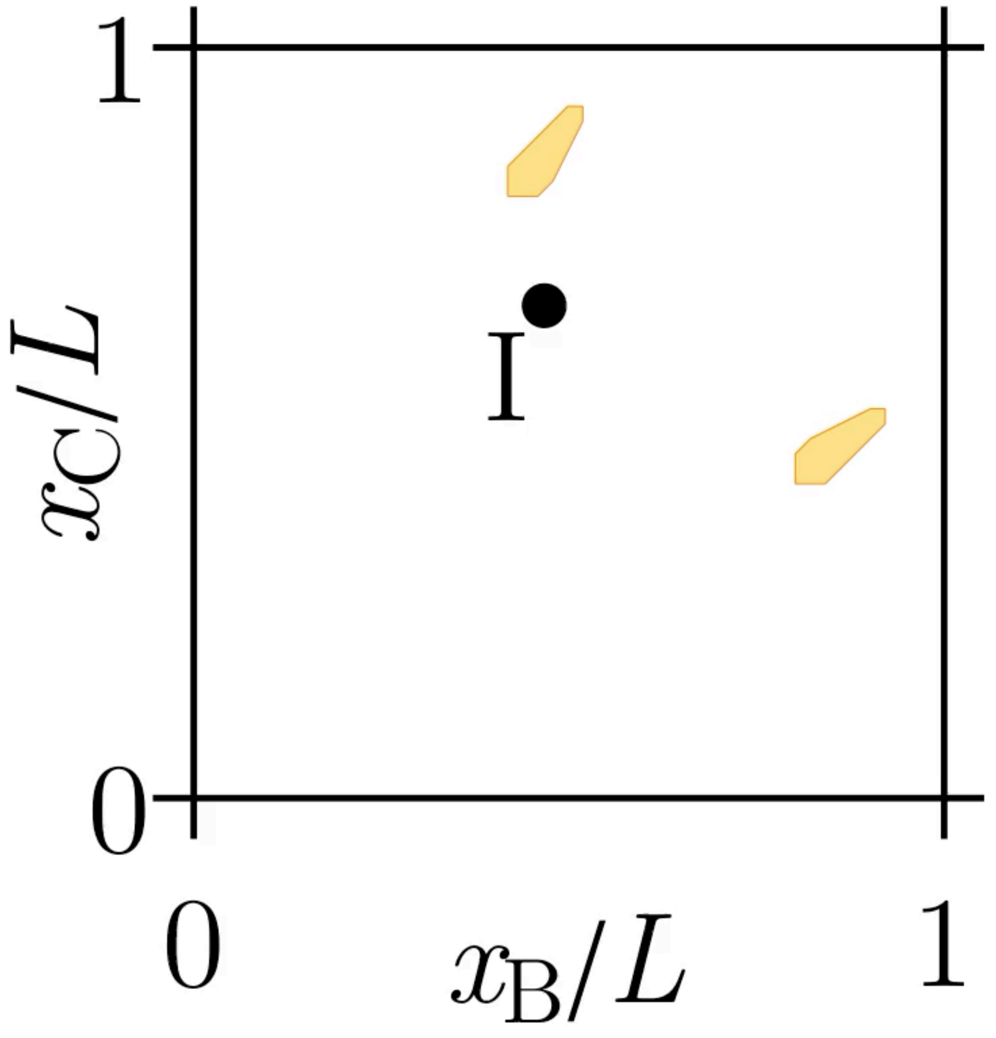


non-trivial particle transport





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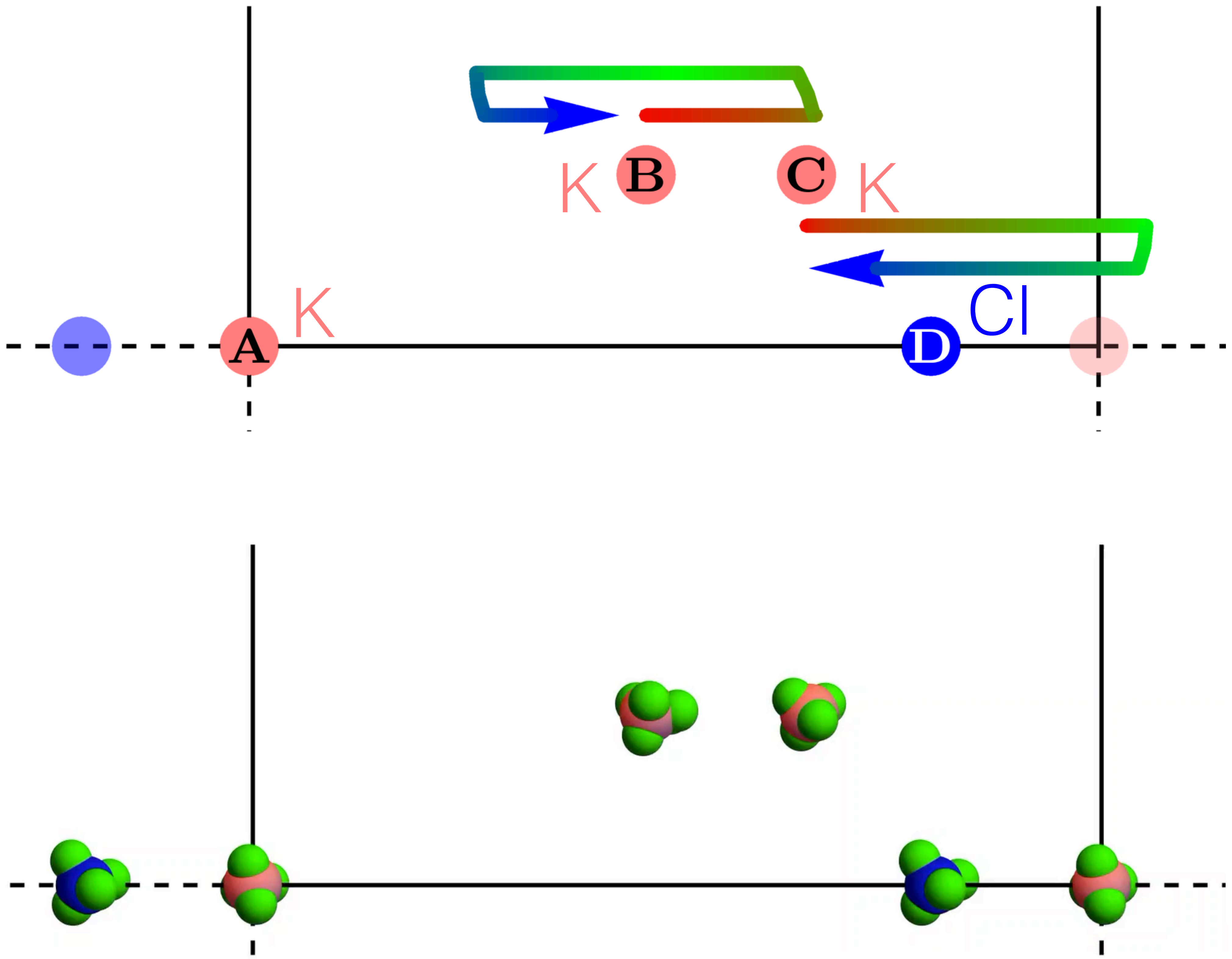

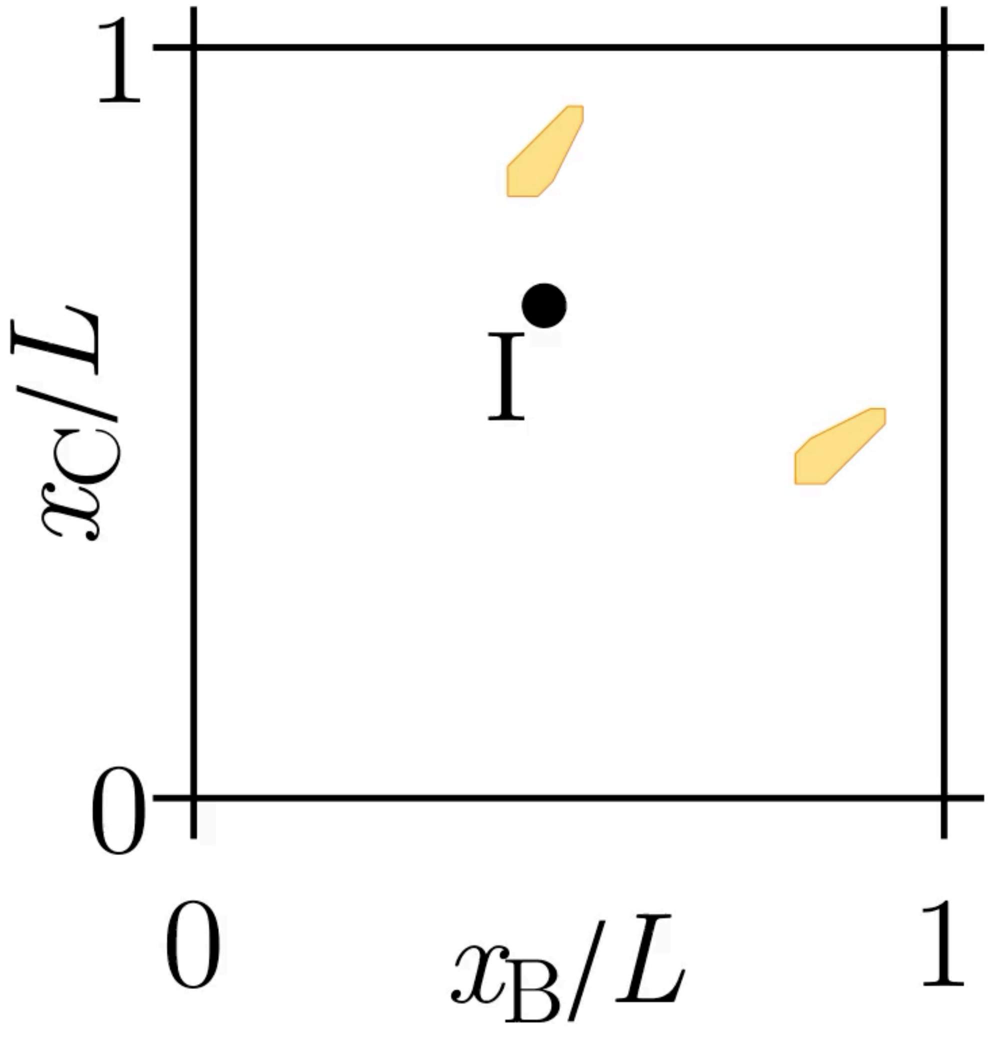

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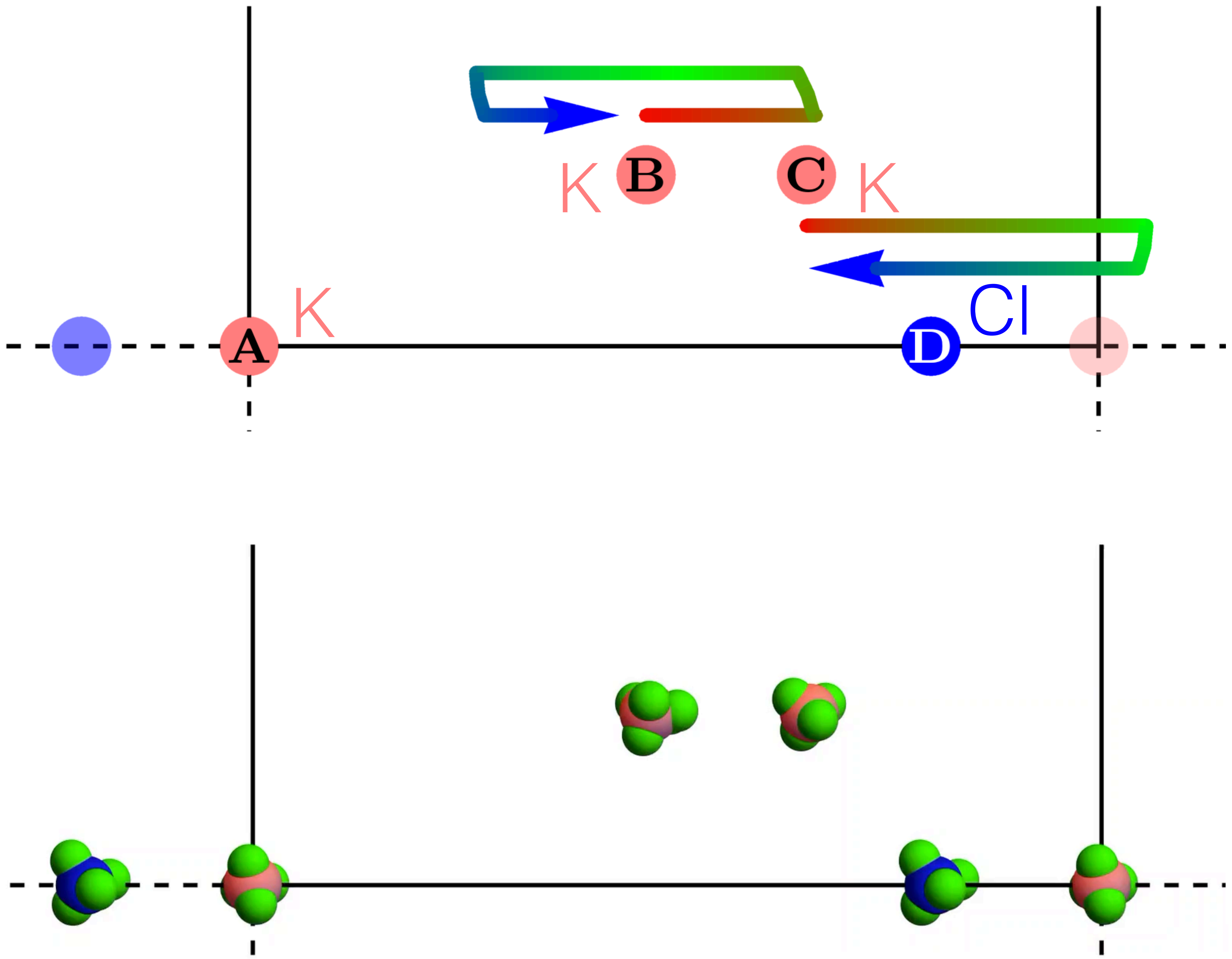
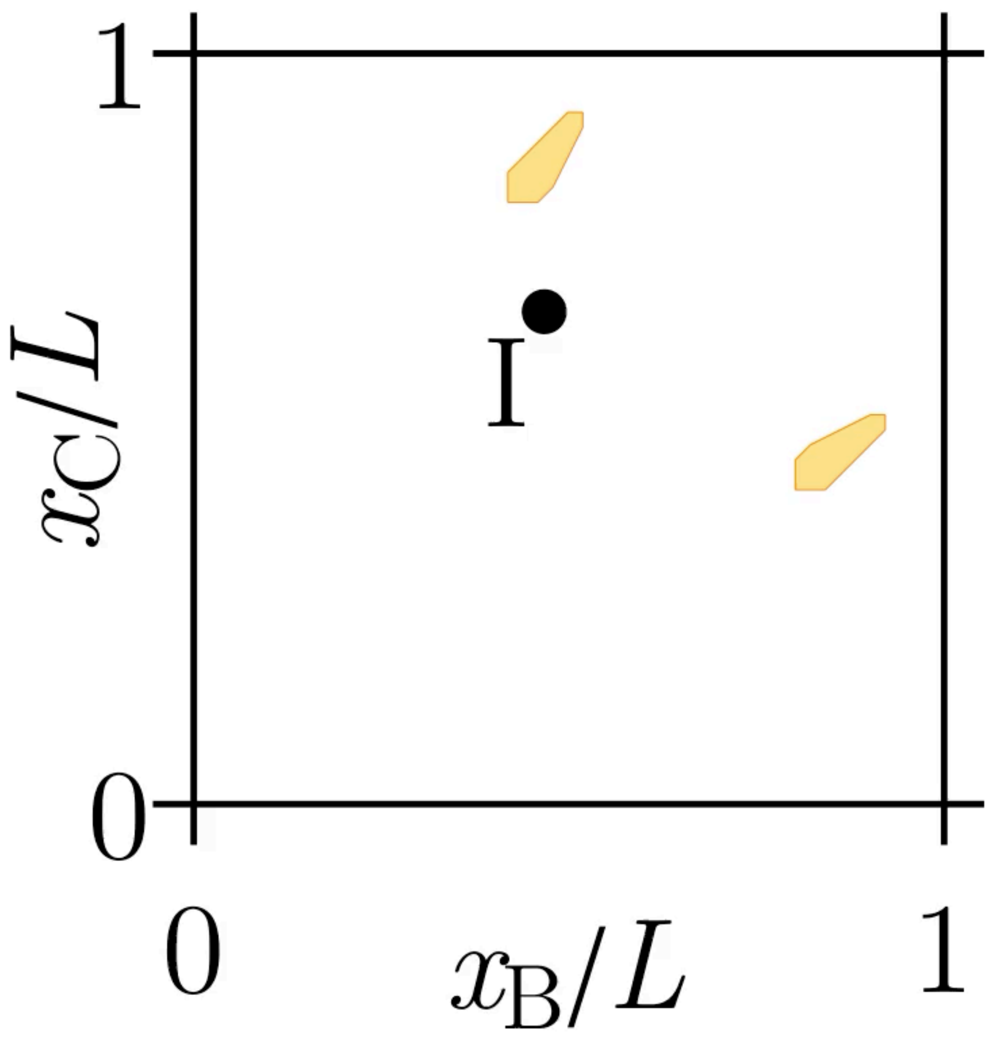
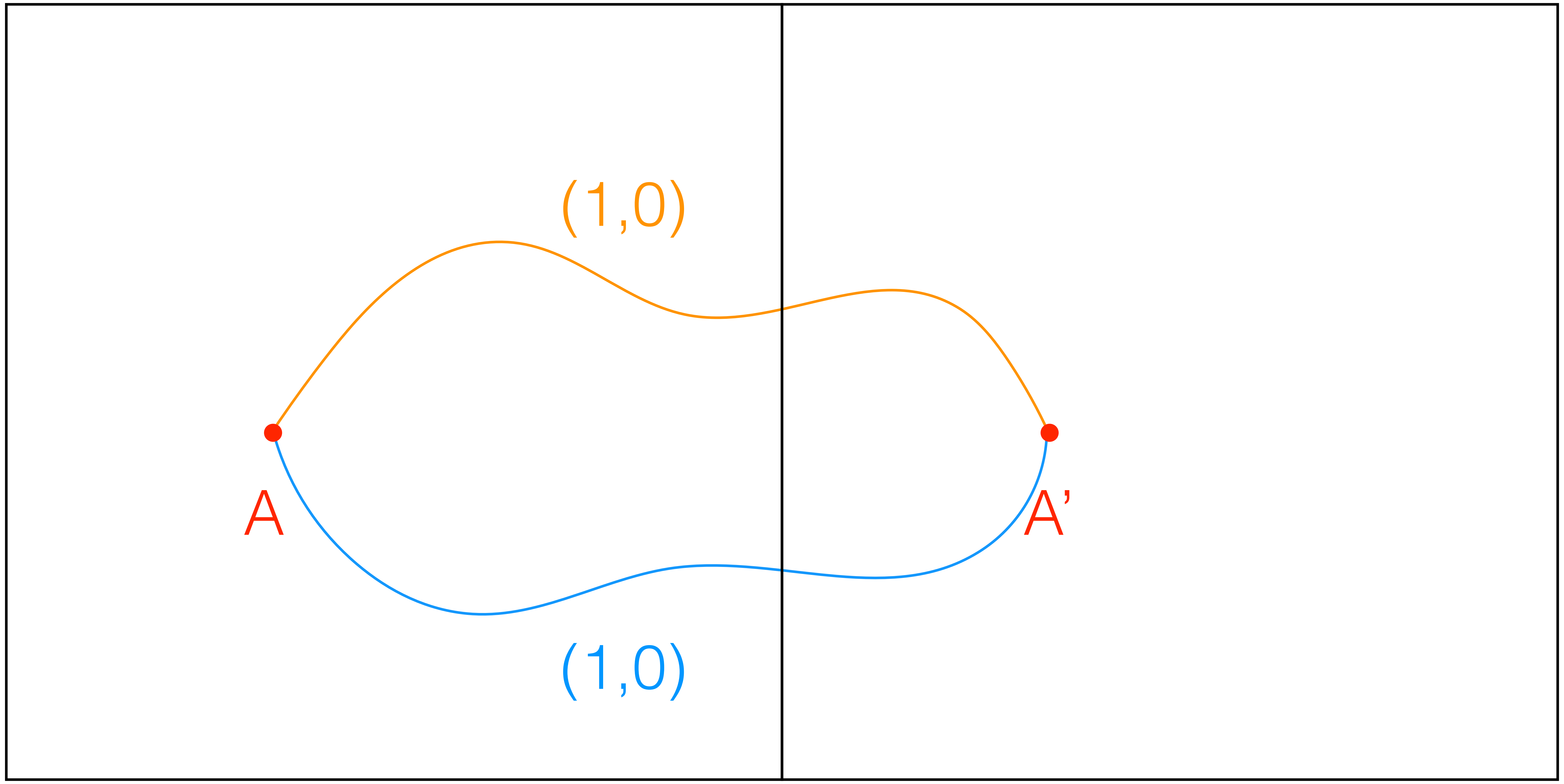




breach of strong adiabaticity



$$\mu = \mu^*$$

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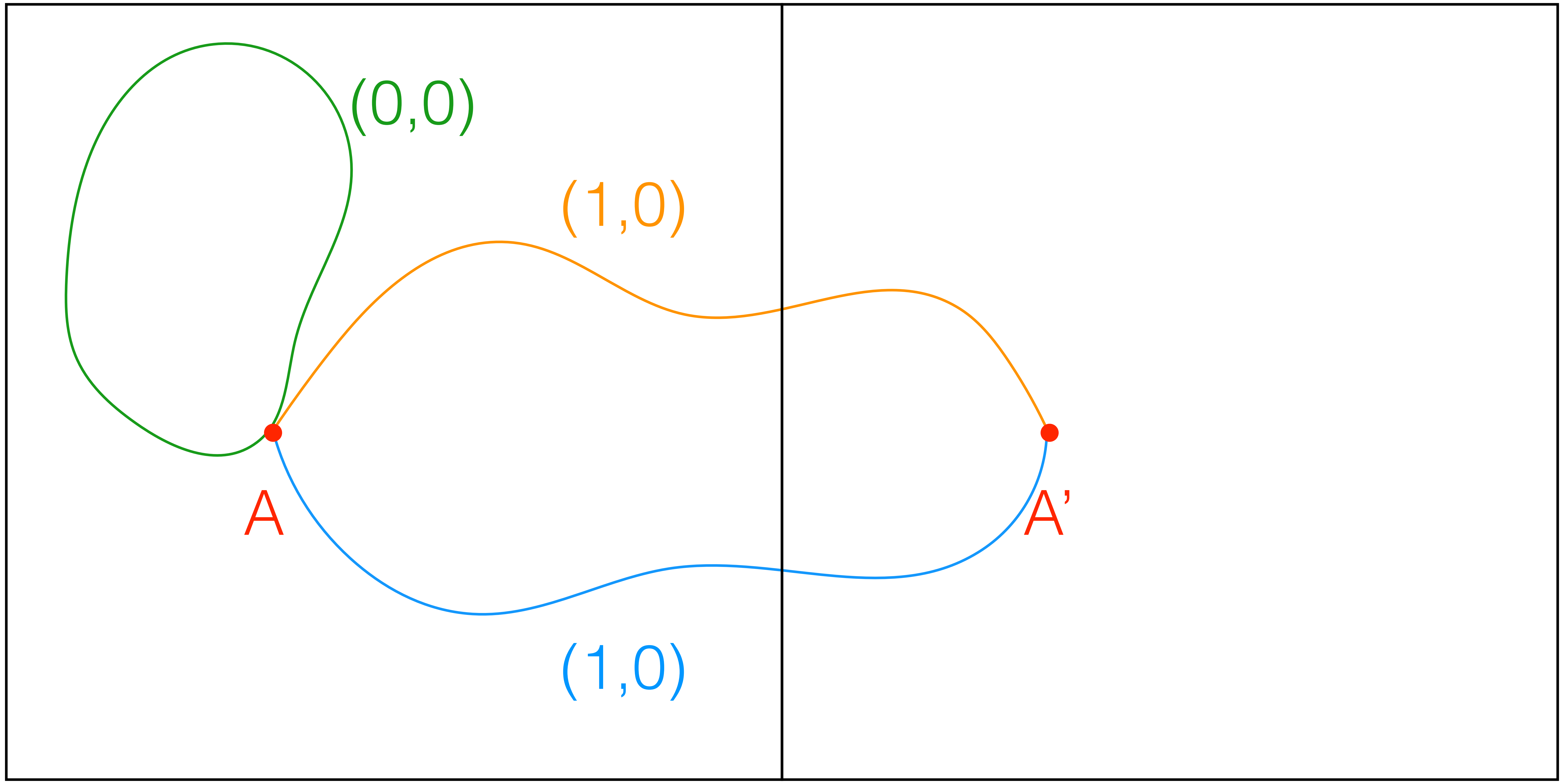

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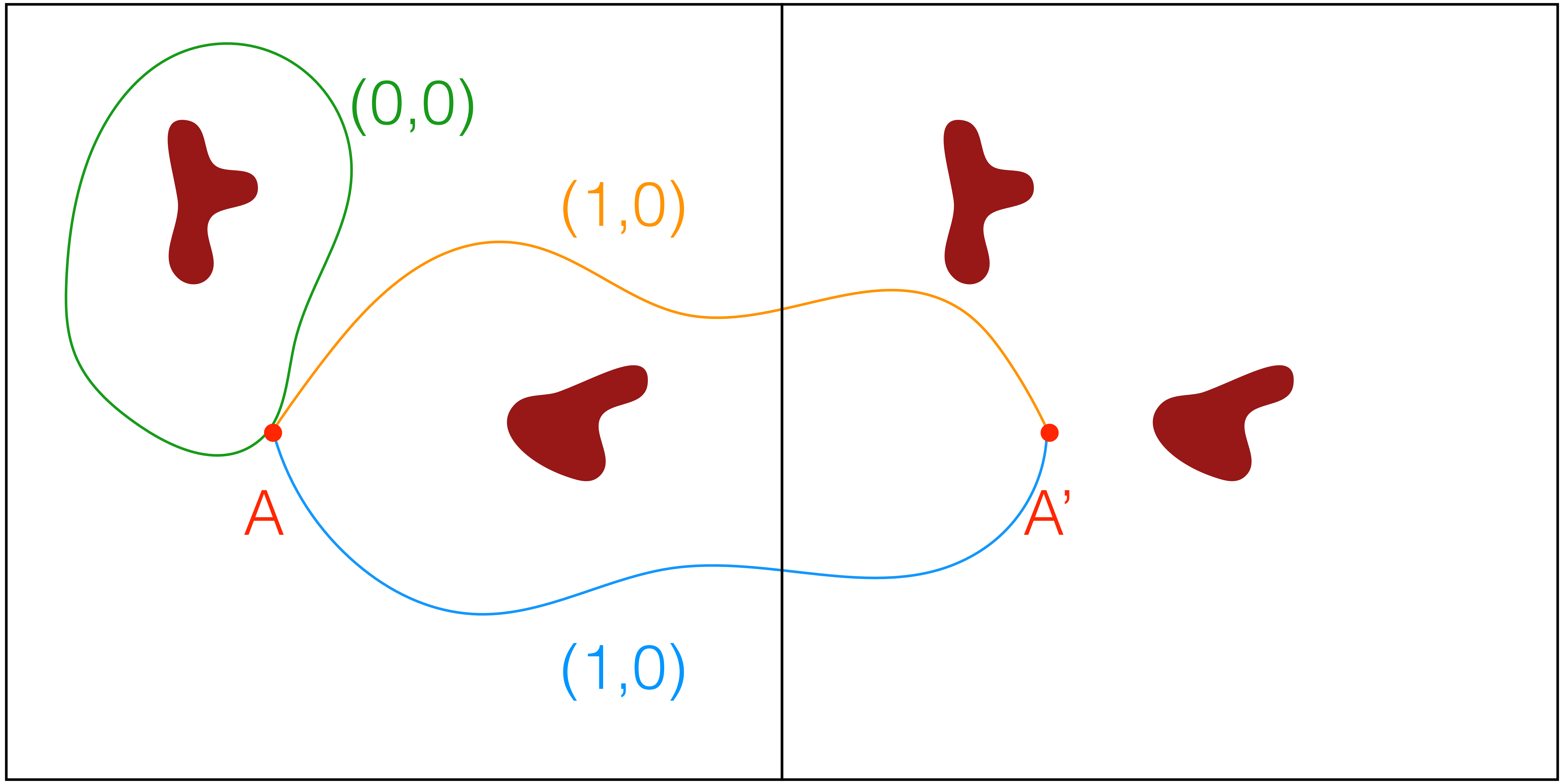
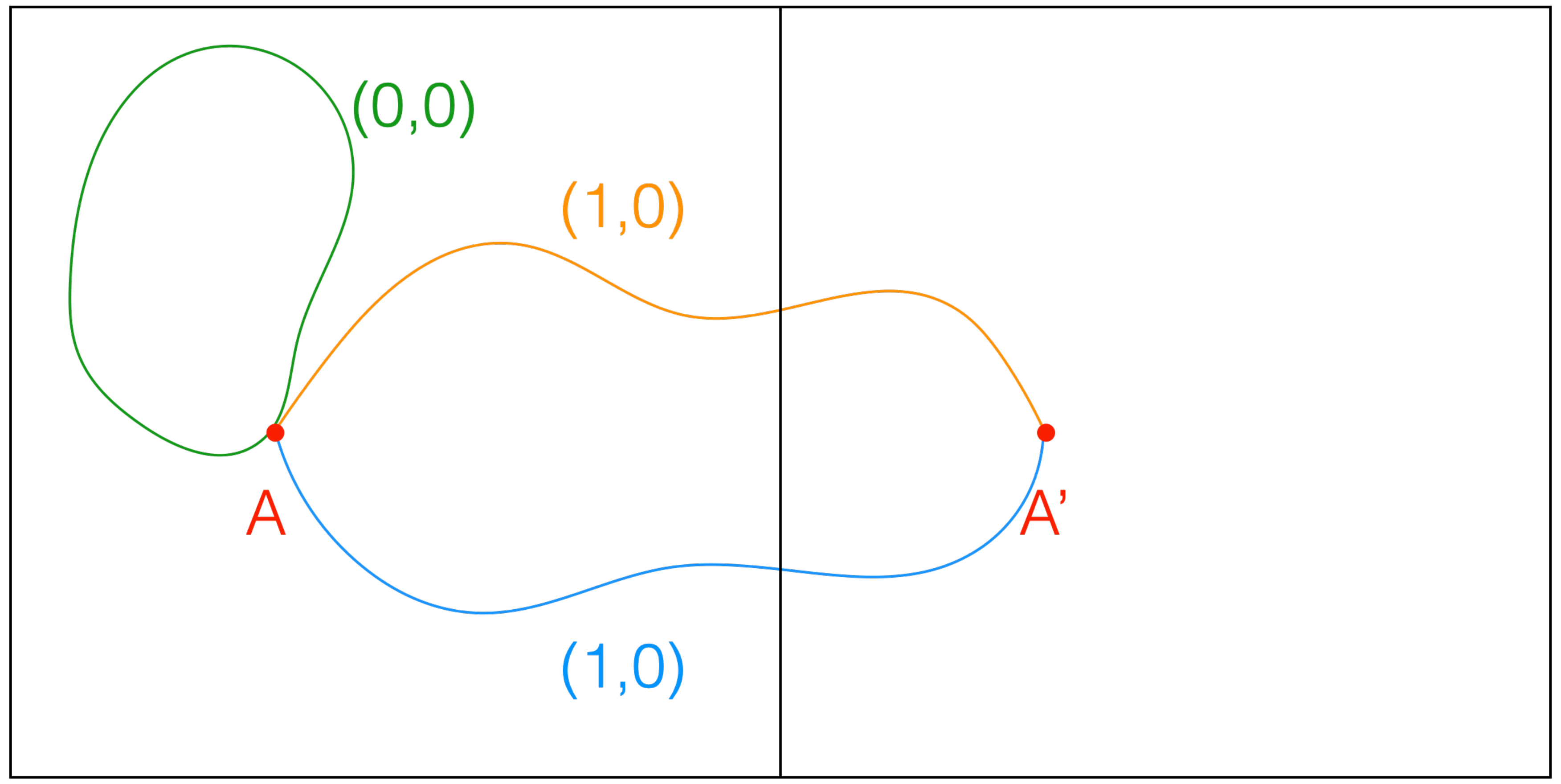


$\mu \neq \mu^*$

$\mu \neq 0$

strongly adiabatic transport



$$\mu = \mu^*$$
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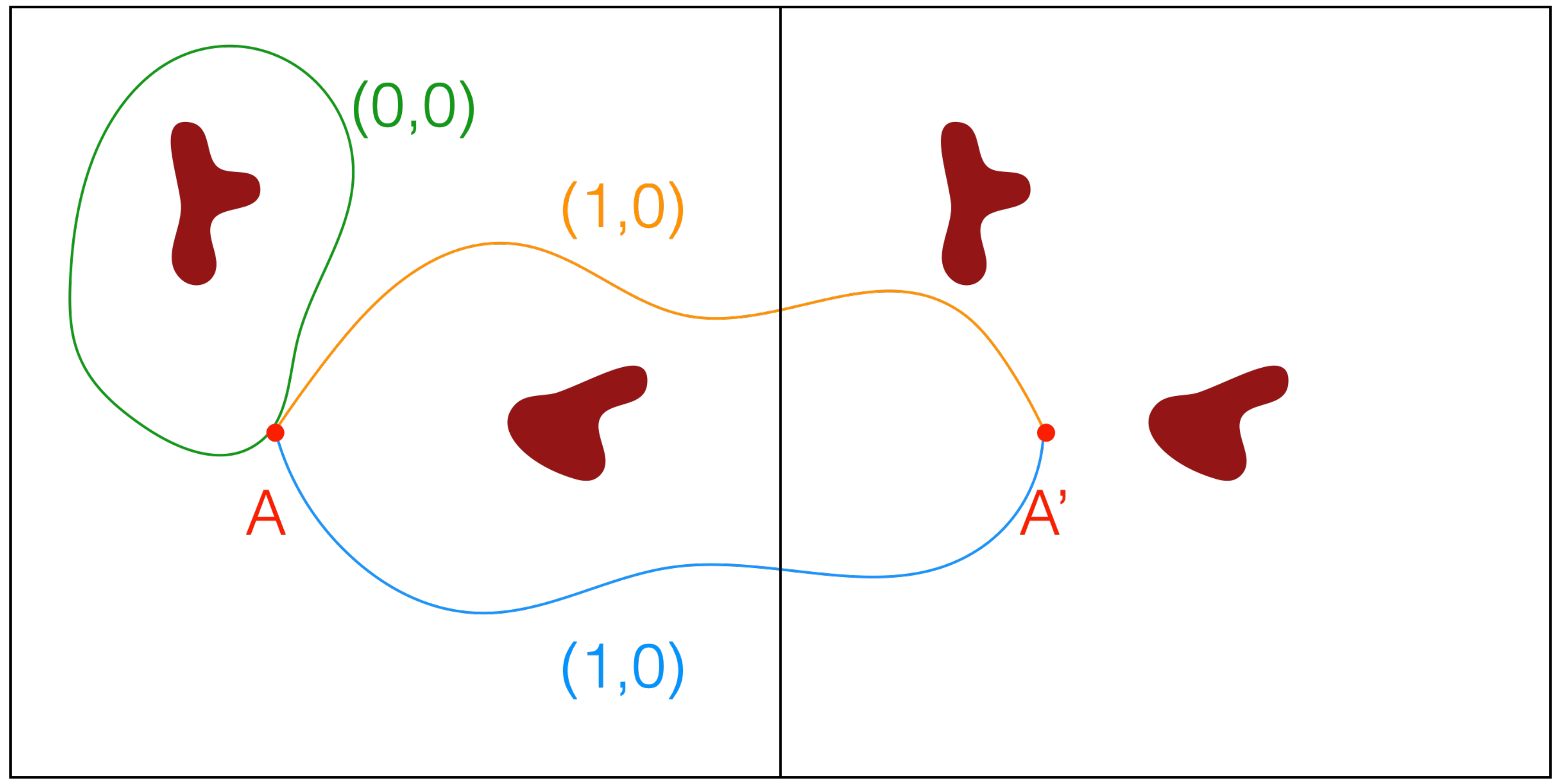
weakly adiabatic transport



$$\mu \neq \mu^*$$
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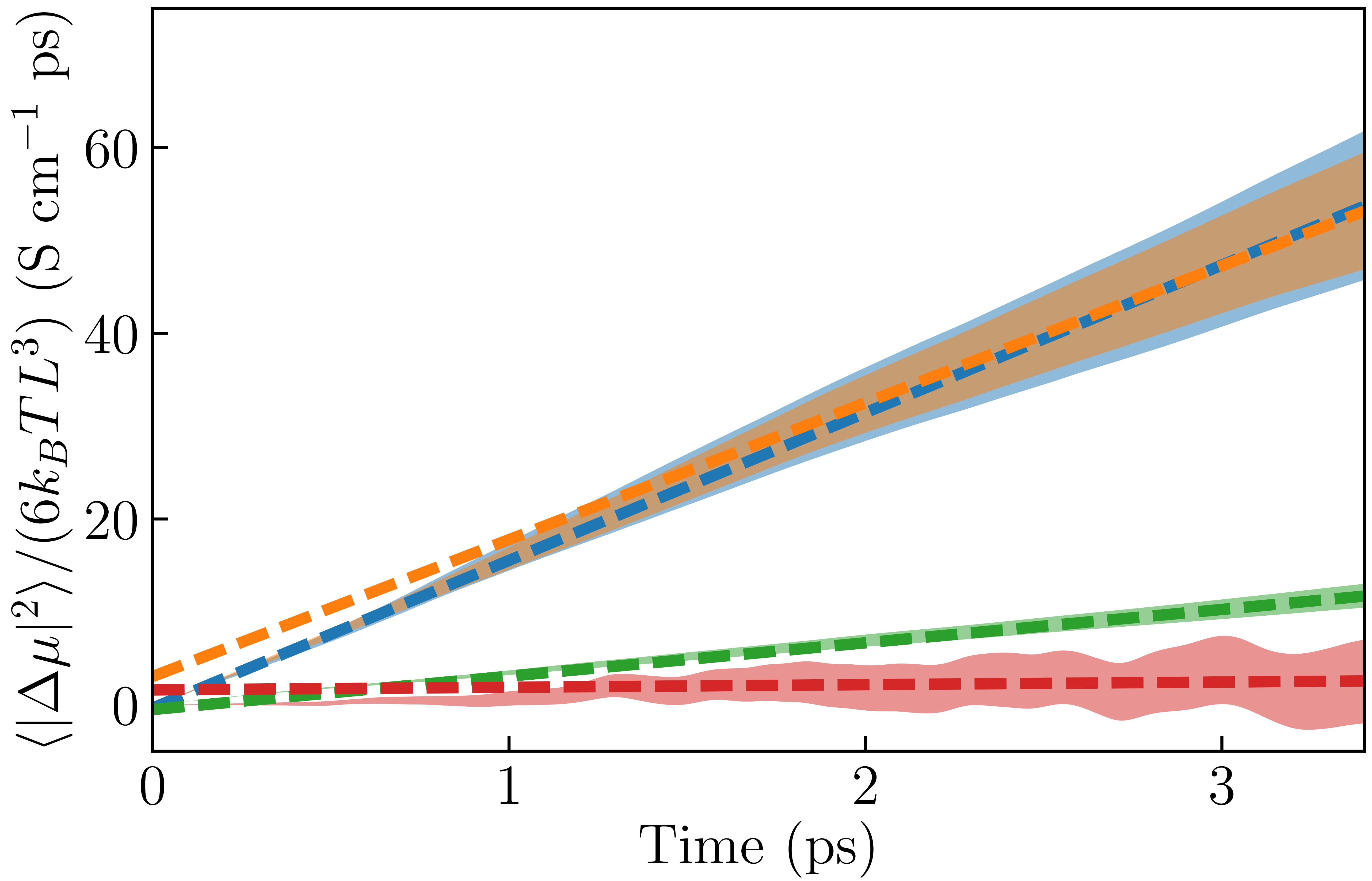
not trivial weakly adiabatic conductivity



$$\Delta\boldsymbol{\mu} = e\int_0^t \mathbf{J}(t')dt'$$

$$J_\alpha(t) = \sum_{i\beta} Z^*_{i\alpha\beta}(t)v_{i\beta}(t)$$

$$J_\alpha(t) = \sum_i q_{S(i)}v_{i\alpha}(t) - 2v^{lp}_\alpha(t)$$

cross term

conclusions

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- topological quantisation of adiabatic charge transport allows for a rigorous definition of the atomic oxidation states;

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- gauge invariance and quantisation of charge transport make the electric conductivity of stoichiometry electrolytes depend on the formal oxidation numbers of the ionic species, via the Green-Kubo formula;

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conclusions

- topological quantisation of adiabatic charge transport allows for a rigorous definition of the atomic oxidation states;
- gauge invariance and quantisation of charge transport make the electric conductivity of stoichiometry electrolytes depend on the formal oxidation numbers of the ionic species, via the Green-Kubo formula;
- breach of strong adiabaticity in non-stoichiometric electrolytes triggers an anomalous transport regime, intermediate between metallic and ionic, whereby charge may be transported without any concurrent mass displacement.

thanks to:

Federico Grasselli

Paolo Pegolo

nature physics ARTICLES
PUBLISHED ONLINE: 19 OCTOBER 2015 | DOI: 10.1038/NPHYS3509

Microscopic theory and quantum simulation of atomic heat transport

Aris Marcolongo[1], Paolo Umari[2] and Stefano Baroni[1*]

nature physics ARTICLES
https://doi.org/10.1038/s41567-019-0562-0

Topological quantization and gauge invariance of charge transport in liquid insulators

Federico Grasselli[1] and Stefano Baroni[1,2*]

PHYSICAL REVIEW X

Oxidation States, Thouless' Pumps, and Nontrivial Ionic Transport in Nonstoichiometric Electrolytes

Paolo Pegolo, Federico Grasselli, and Stefano Baroni
Phys. Rev. X **10**, 041031 – Published 12 November 2020

adp annalen der physik

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Topology, Oxidation States, and Charge Transport in Ionic Conductors

Paolo Pegolo, Stefano Baroni, Federico Grasselli

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