topological quantisation and gauge invariance of charge transport in liquid insulators

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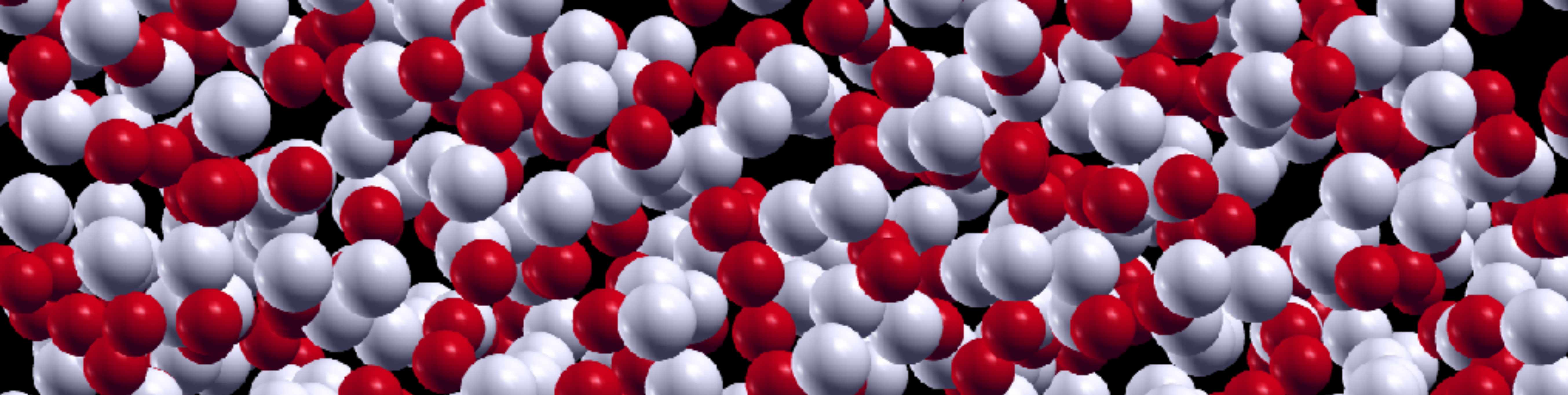

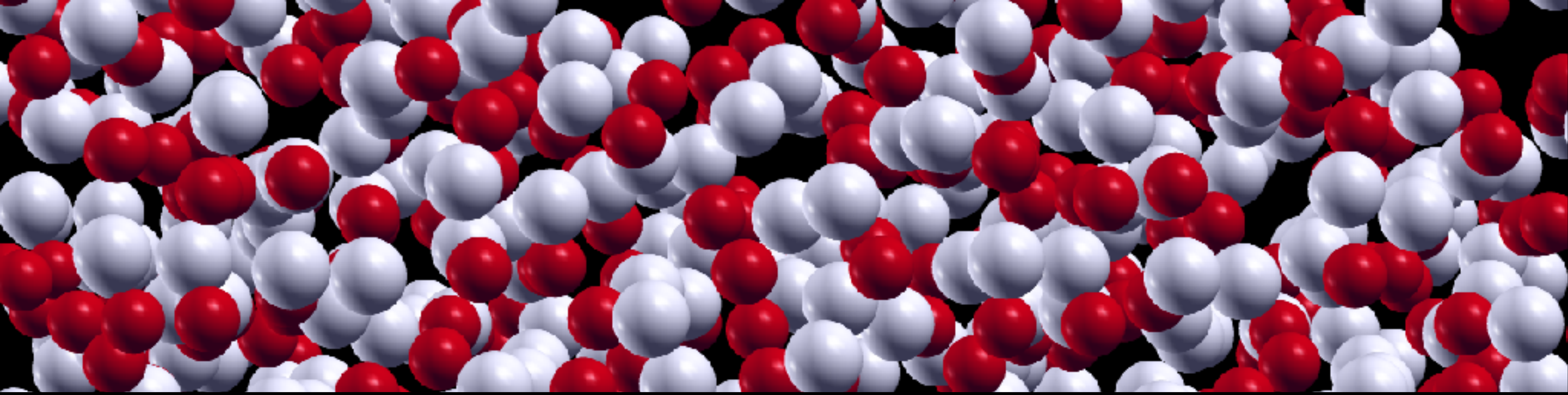

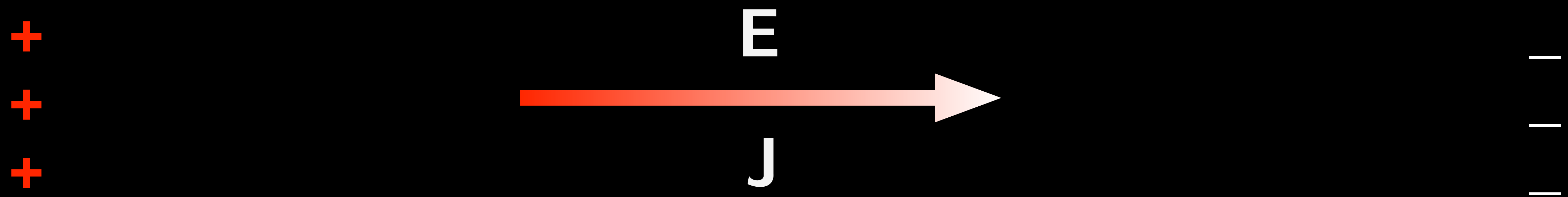
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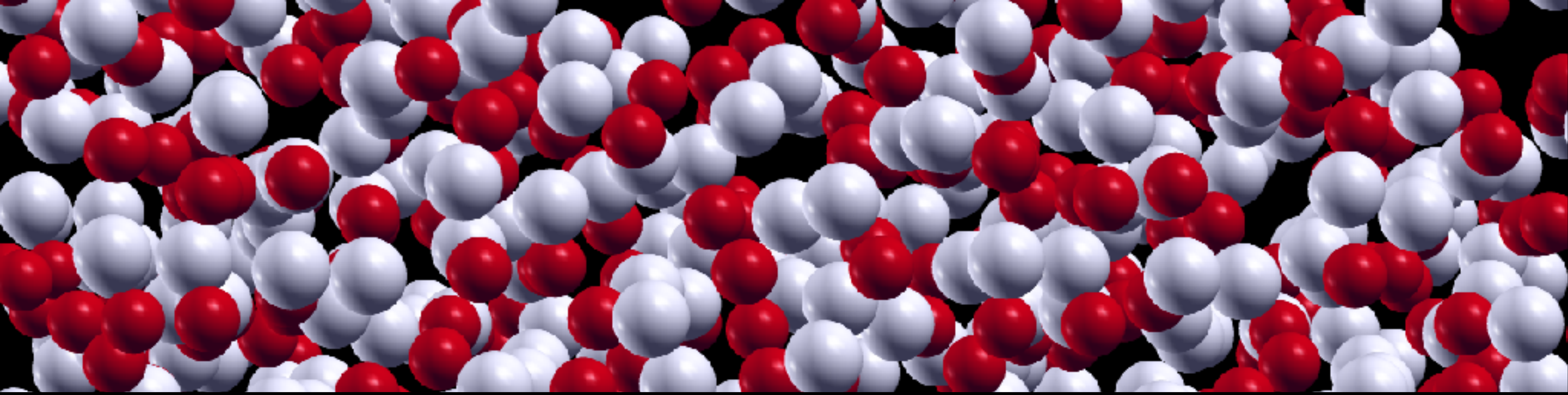
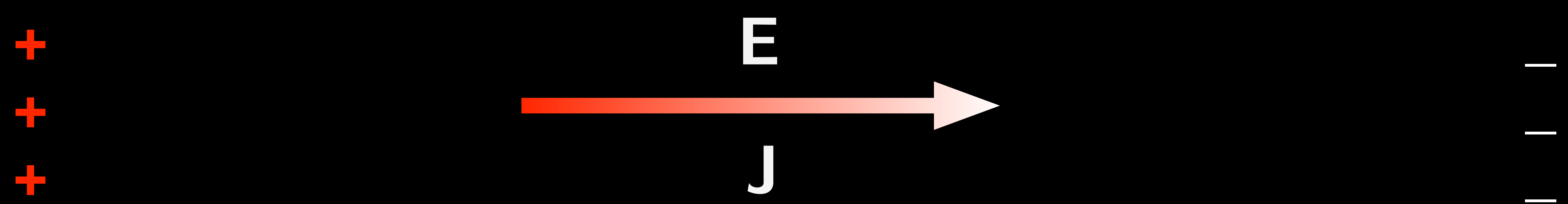
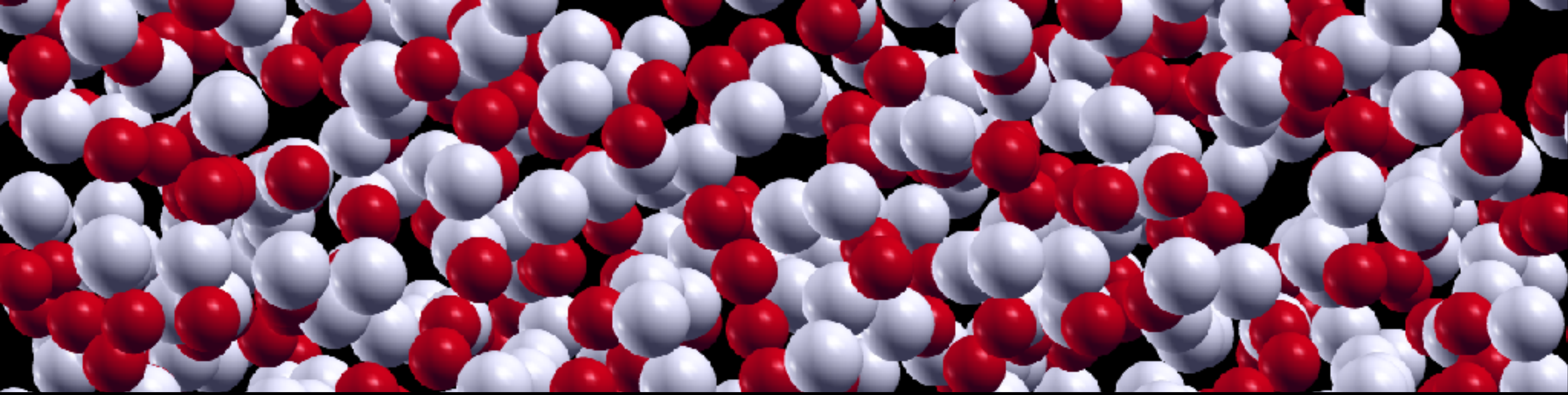


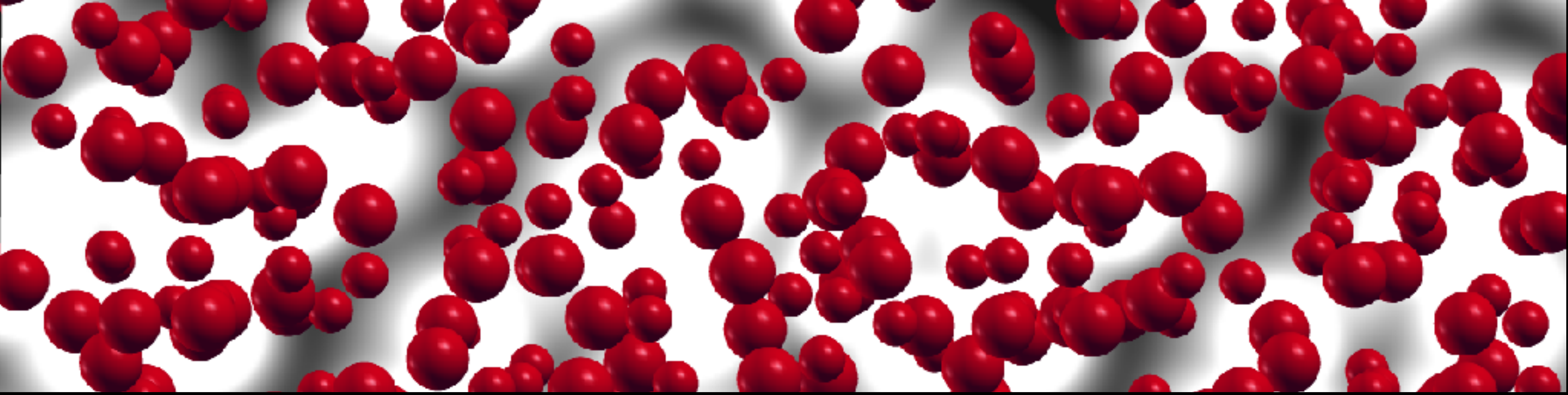


$$\mathbf{J} = \sigma \mathbf{E}$$



$$\mathbf{J} = \sigma \mathbf{E}$$

$$\mathbf{J} = \sum_i q_i \mathbf{v}_i$$



+ + +

$\mathbf{E}$

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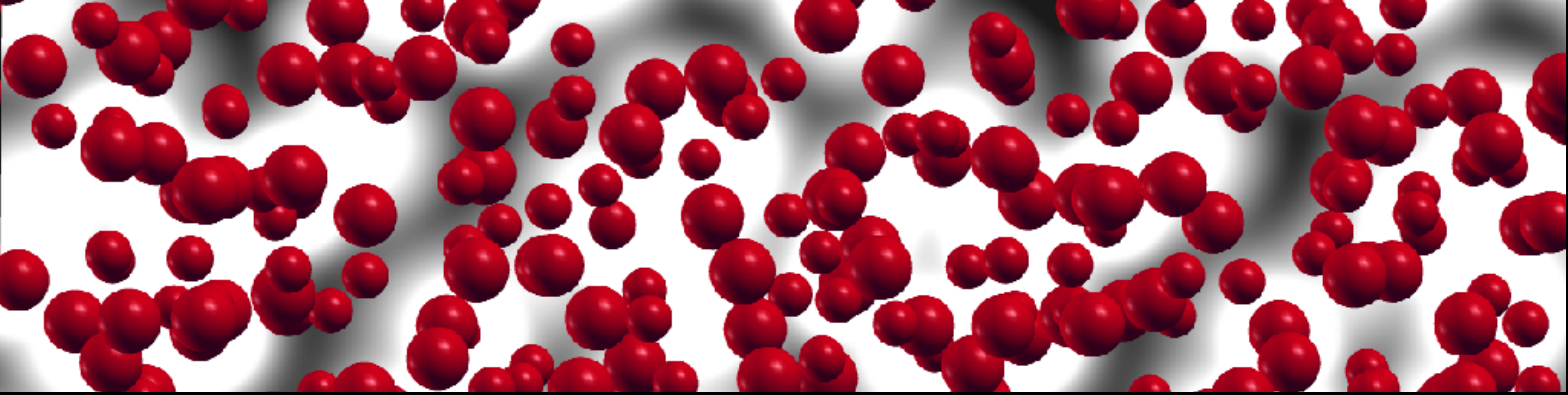
$$\mathbf{J} = \sigma \mathbf{E}$$

$$\mathbf{J} = ???$$



$$\mathbf{J} = \sigma \mathbf{E}$$

$$\begin{aligned}\mathbf{J} = \dot{\mathbf{P}} &= \frac{1}{\Omega}\dot{\boldsymbol{\mu}} \\ &= \frac{1}{\Omega}\sum_i \mathbf{Z}_i^* \cdot \mathbf{v}_I\end{aligned}$$

$$Z^*_{i\alpha\beta} = \frac{\partial \mu_\alpha}{x_{i\beta}}$$

the Green-Kubo theory transport

A is extensive

$$A = \int_\Omega a(\mathbf{r}) d\mathbf{r}$$

the Green-Kubo theory transport

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A is conserved

$$\dot{a}(\mathbf{r}, t) = -\nabla \cdot \mathbf{j}_a(\mathbf{r}, t)$$

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$$\mathbf{J} = \lambda \mathbf{F} \qquad \begin{cases} \mathbf{J} = \dfrac{1}{\Omega}\displaystyle\int_\Omega \mathbf{j}(\mathbf{r}) d\mathbf{r} \\ \mathbf{F} = \dfrac{1}{\Omega}\displaystyle\int_\Omega \nabla x(\mathbf{r}) d\mathbf{r} \\ x = \dfrac{\partial S}{\partial A} \end{cases}$$

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$$\boxed{\lambda = \frac{\Omega}{k_B T} \int_0^\infty \langle J(t) J(0) \rangle dt}$$

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the Green-Kubo theory transport

$$\lambda = \frac{\Omega}{k_B T} \int_0^\infty \langle J(t) J(0) \rangle dt$$

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$$J_{\mathcal{E}} = -\kappa \nabla T$$

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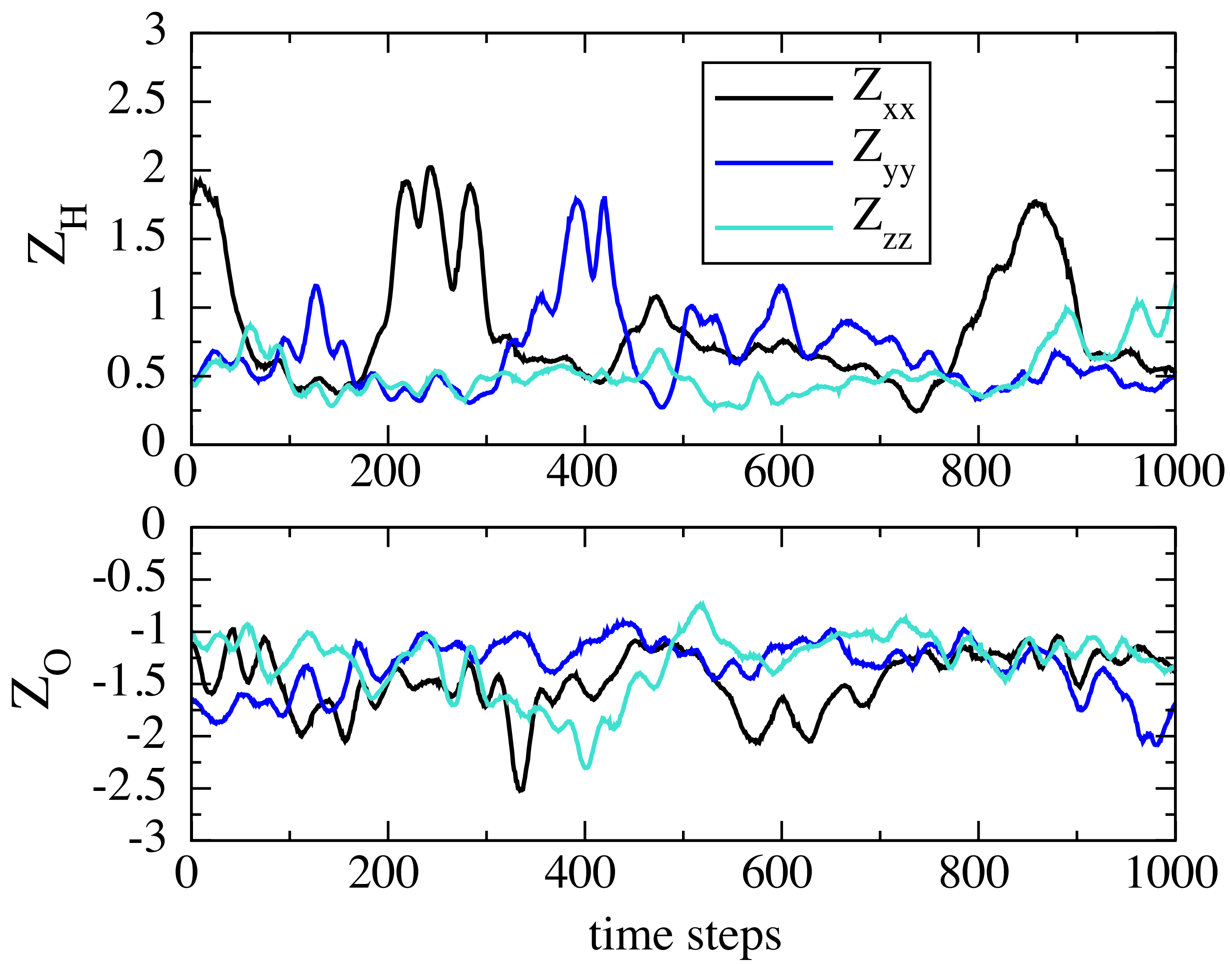
Q = charge

$$J_\mathcal{Q} = \sigma E$$

$$\sigma = \frac{\Omega}{k_B T} \int_0^\infty \langle J_\mathcal{Q}(t) J_\mathcal{Q}(0) \rangle dt$$

the conundrum



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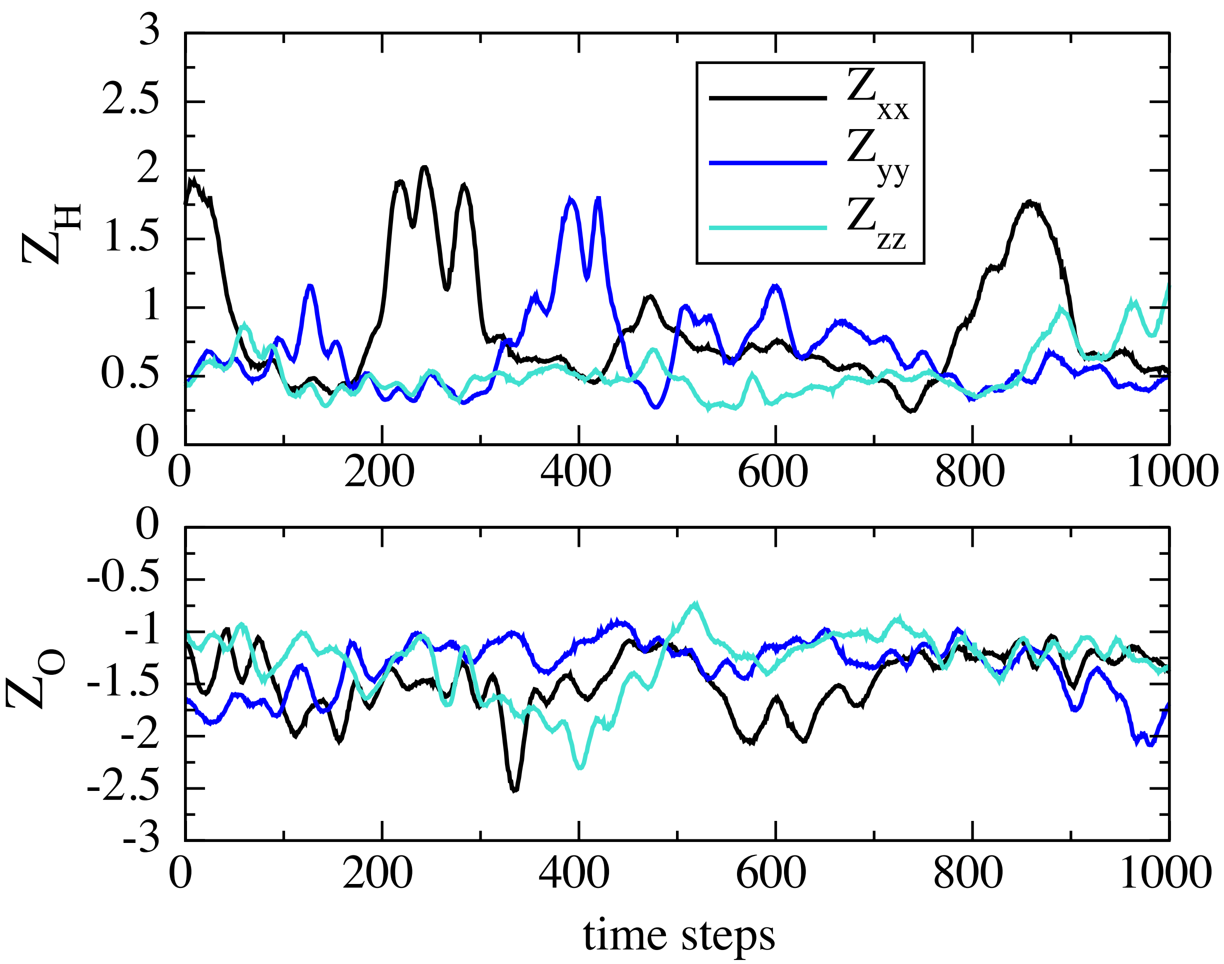

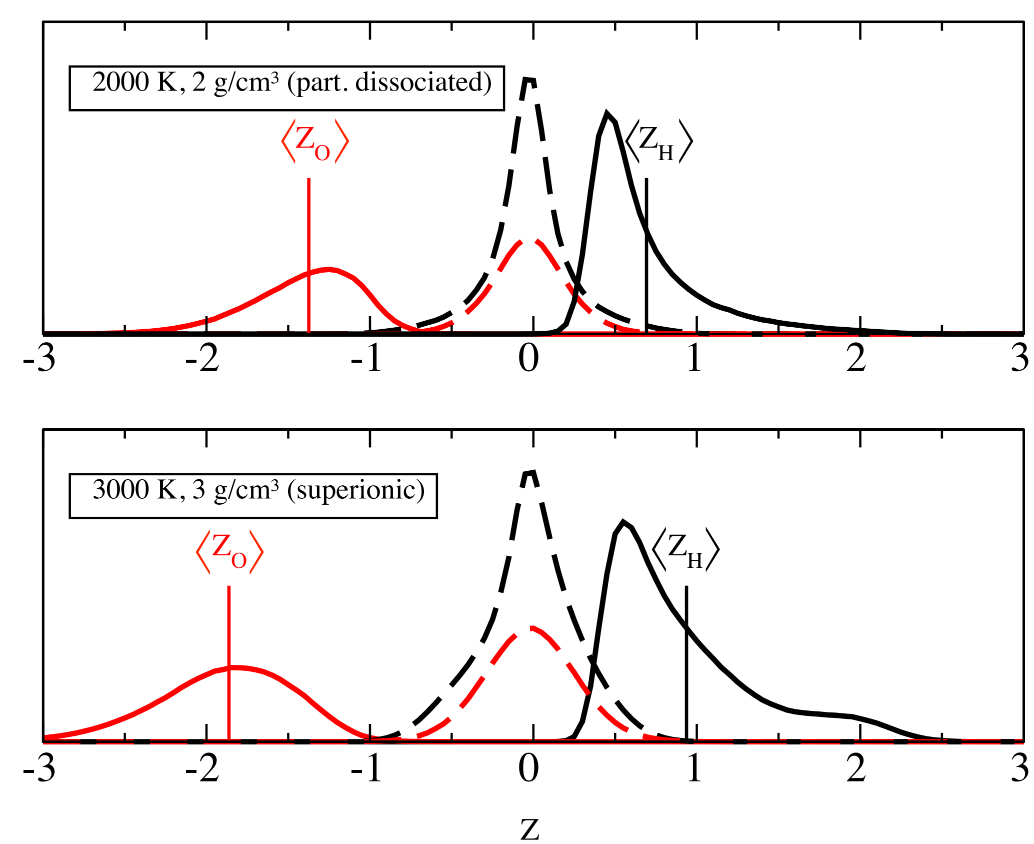

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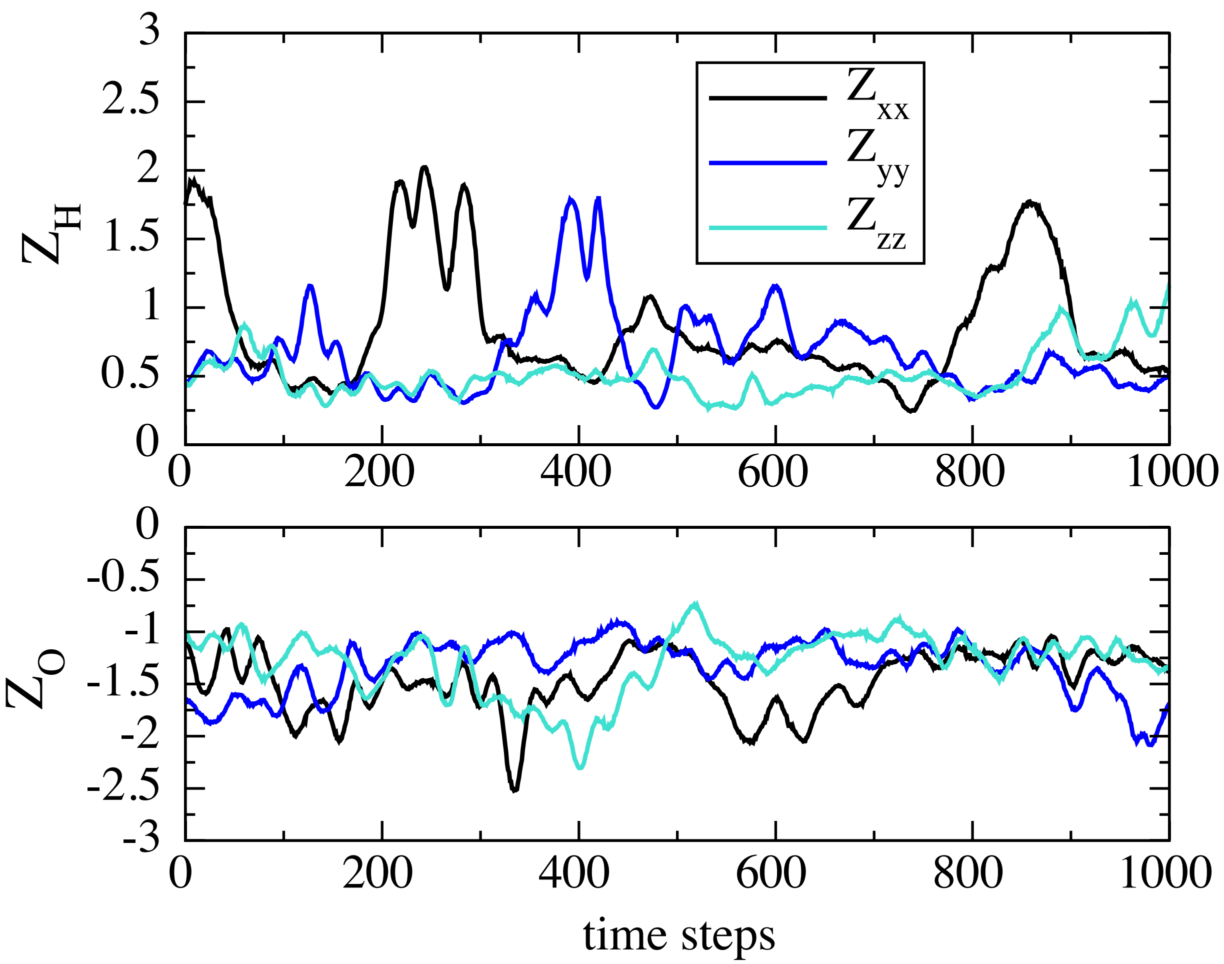

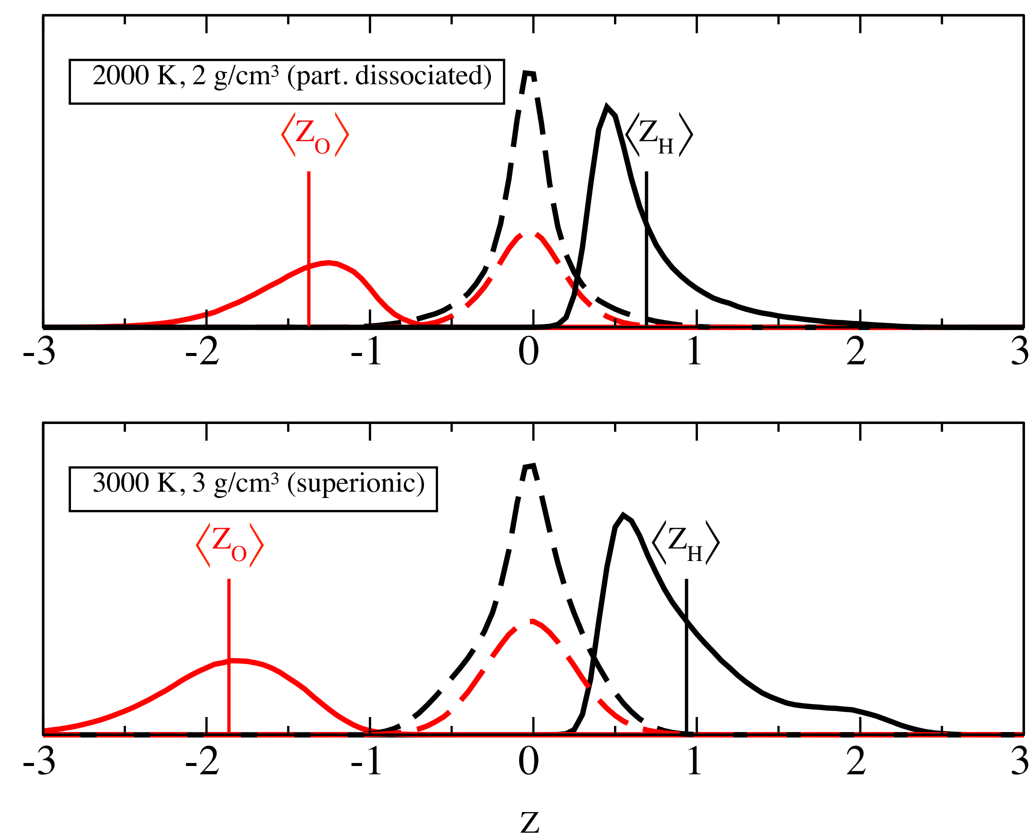

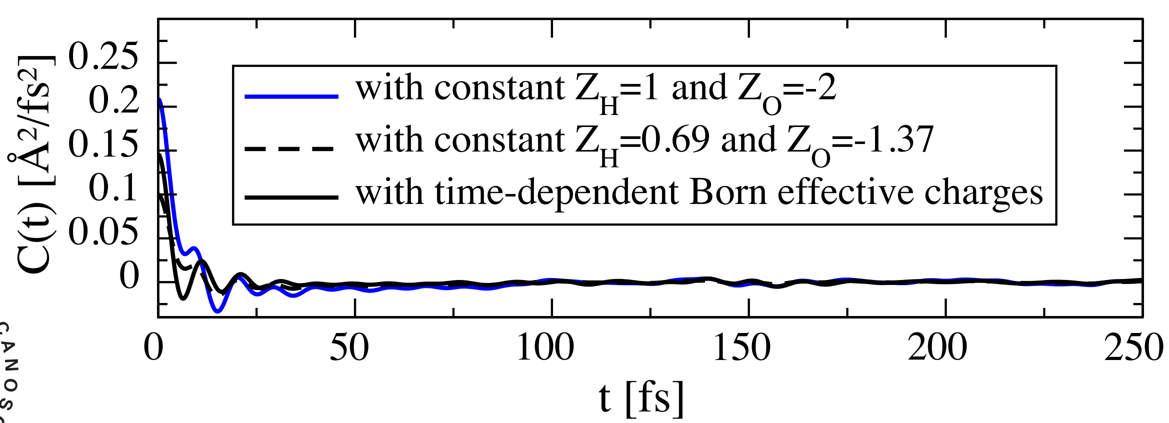

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PRL **107,** 185901 (2011) PHYSICAL REVIEW LETTERS week ending 28 OCTOBER 2011

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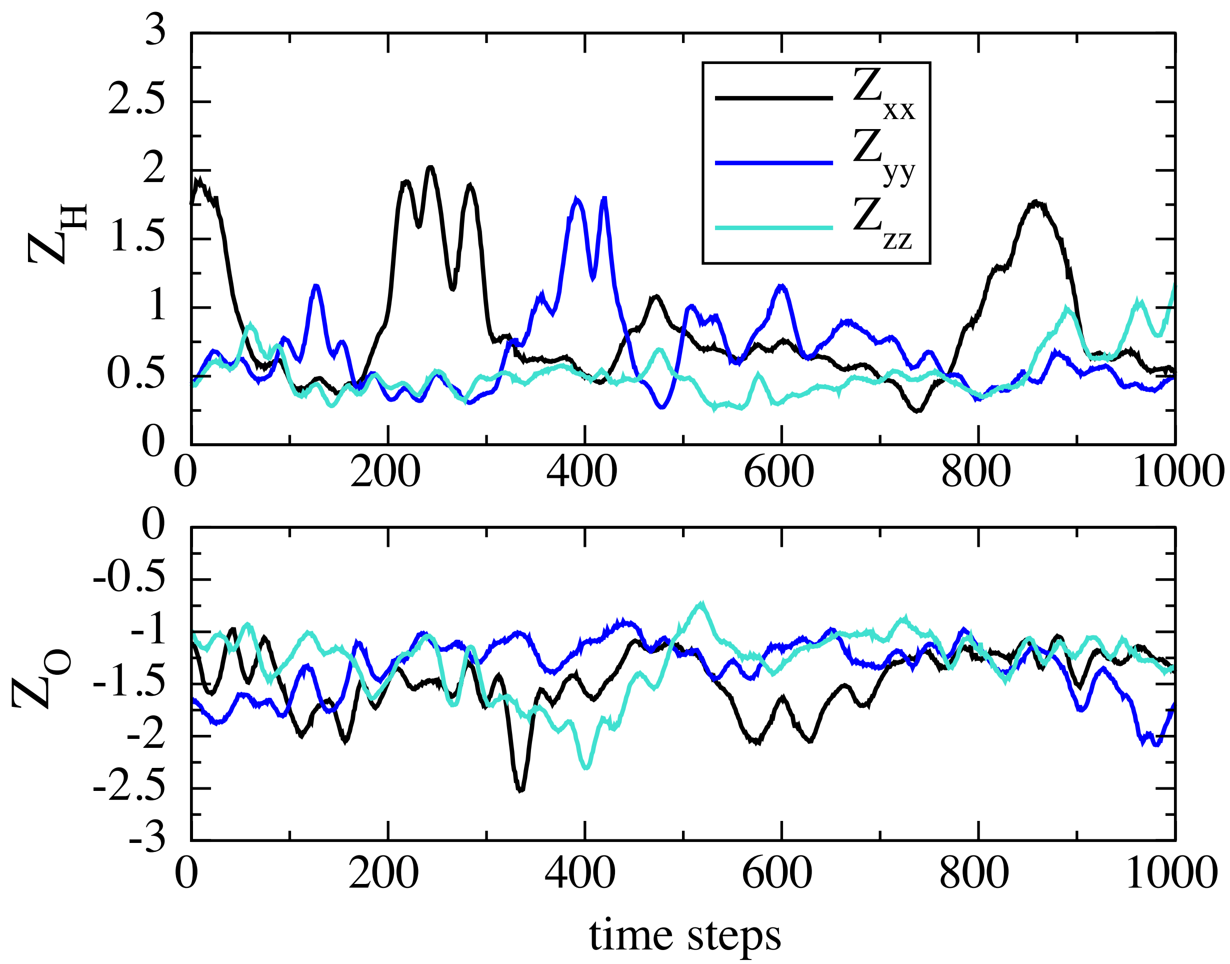
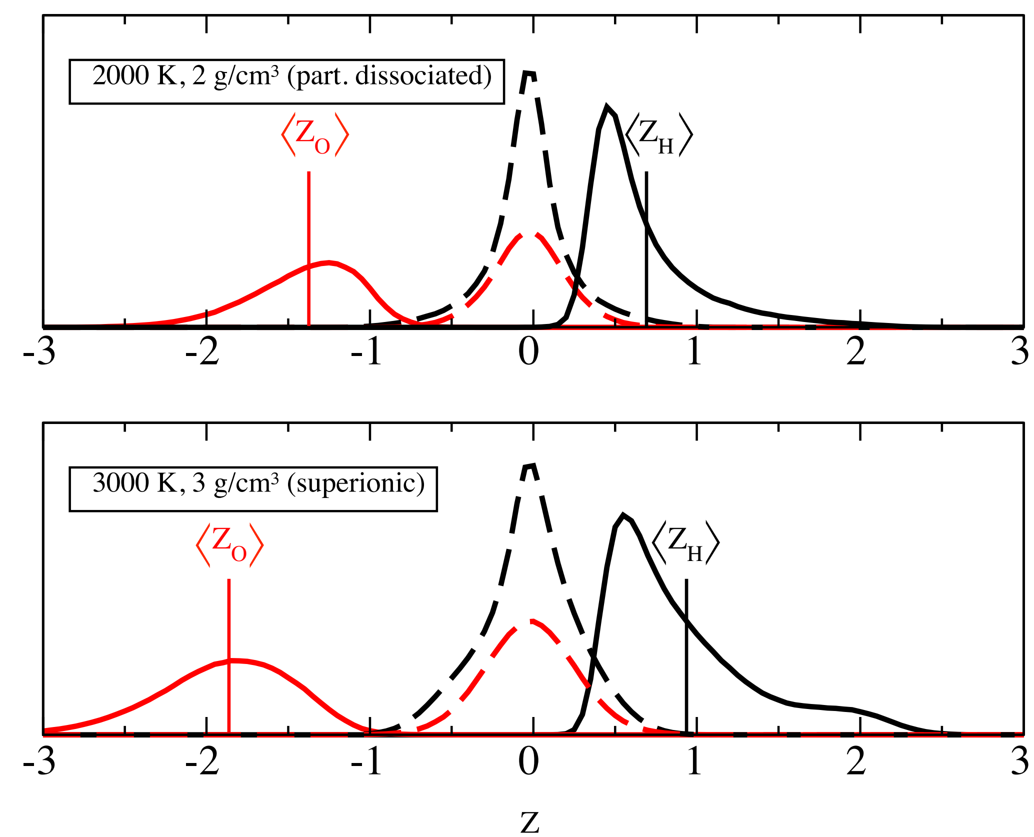
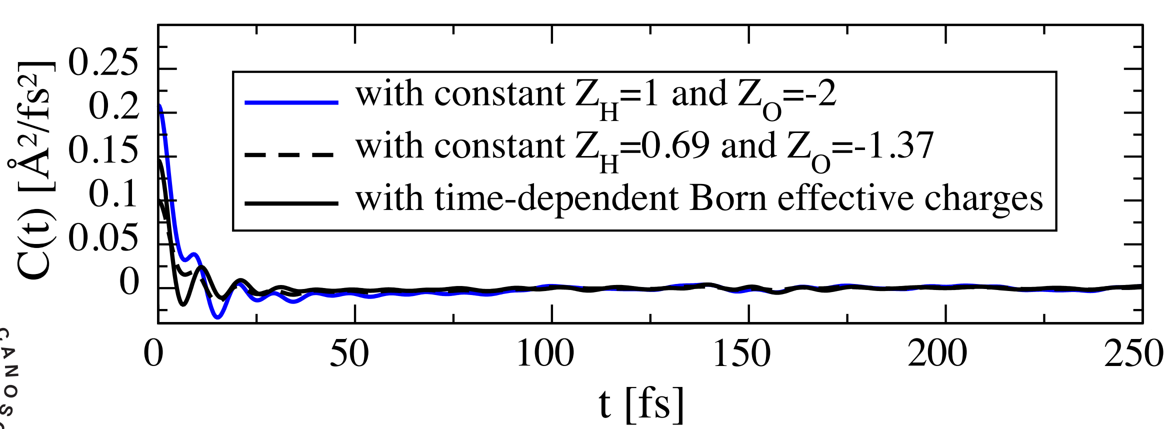
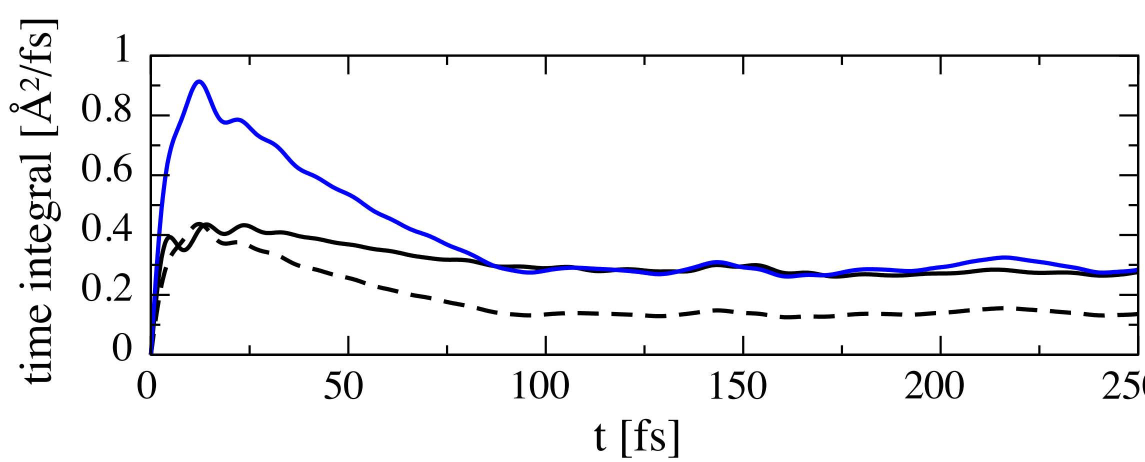
Martin French,[1] Sebastien Hamel,[2] and Ronald Redmer[1]









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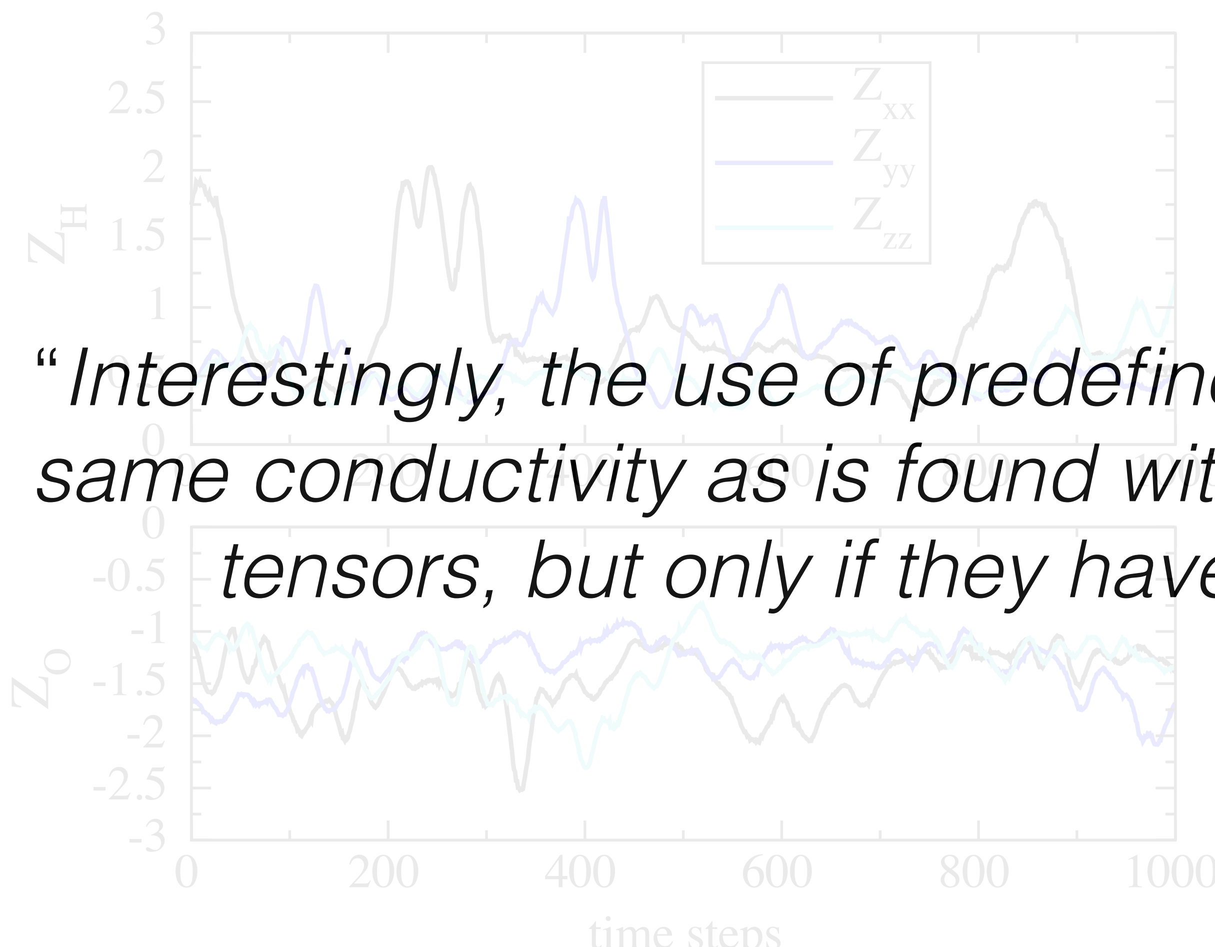
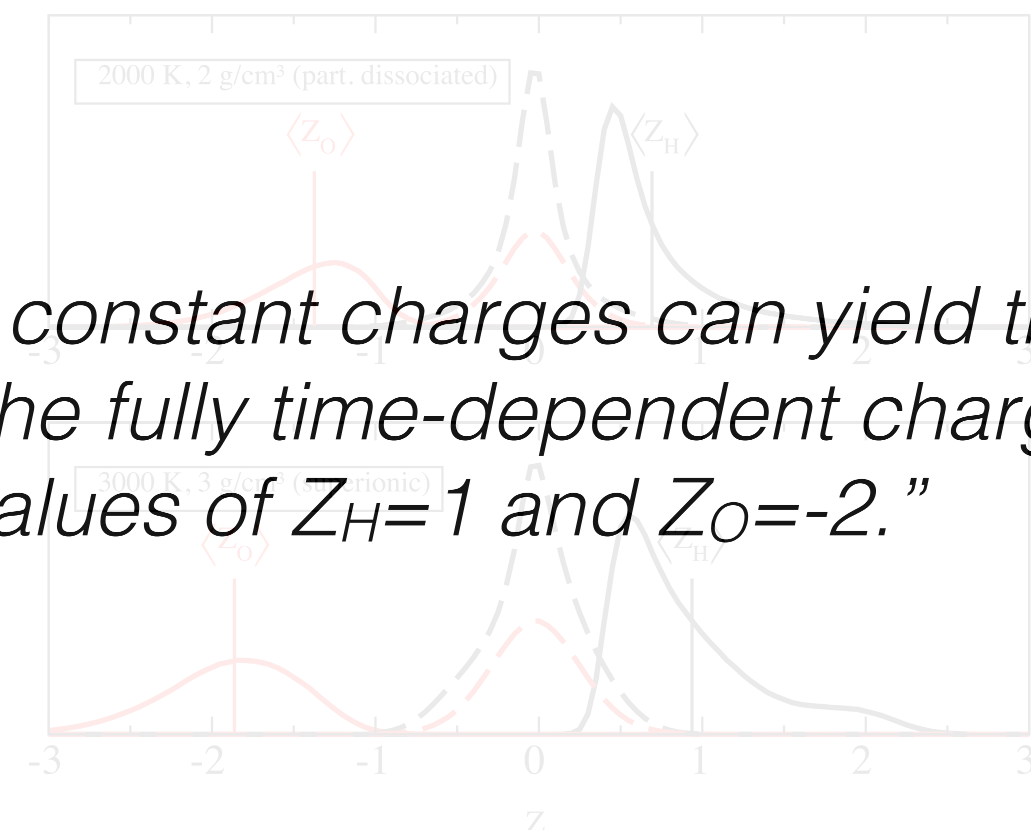
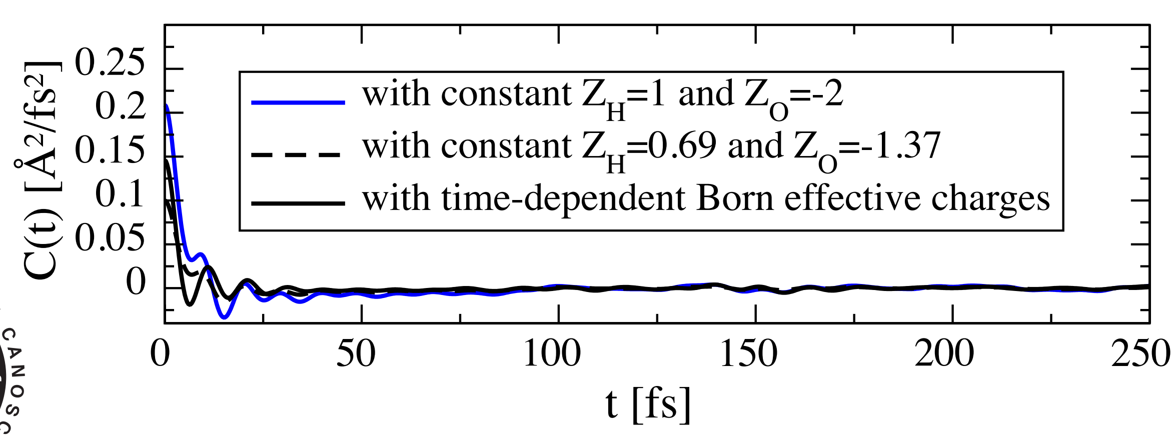
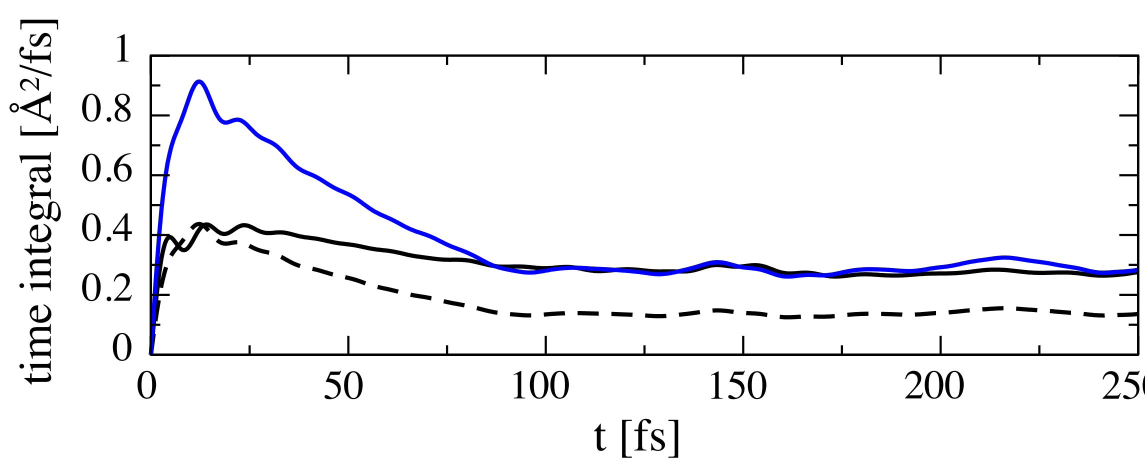




"Interestingly, the use of predefined constant charges can yield the same conductivity as is found with the fully time-dependent charge tensors, but only if they have values of Z_H=1 and Z_O=-2."





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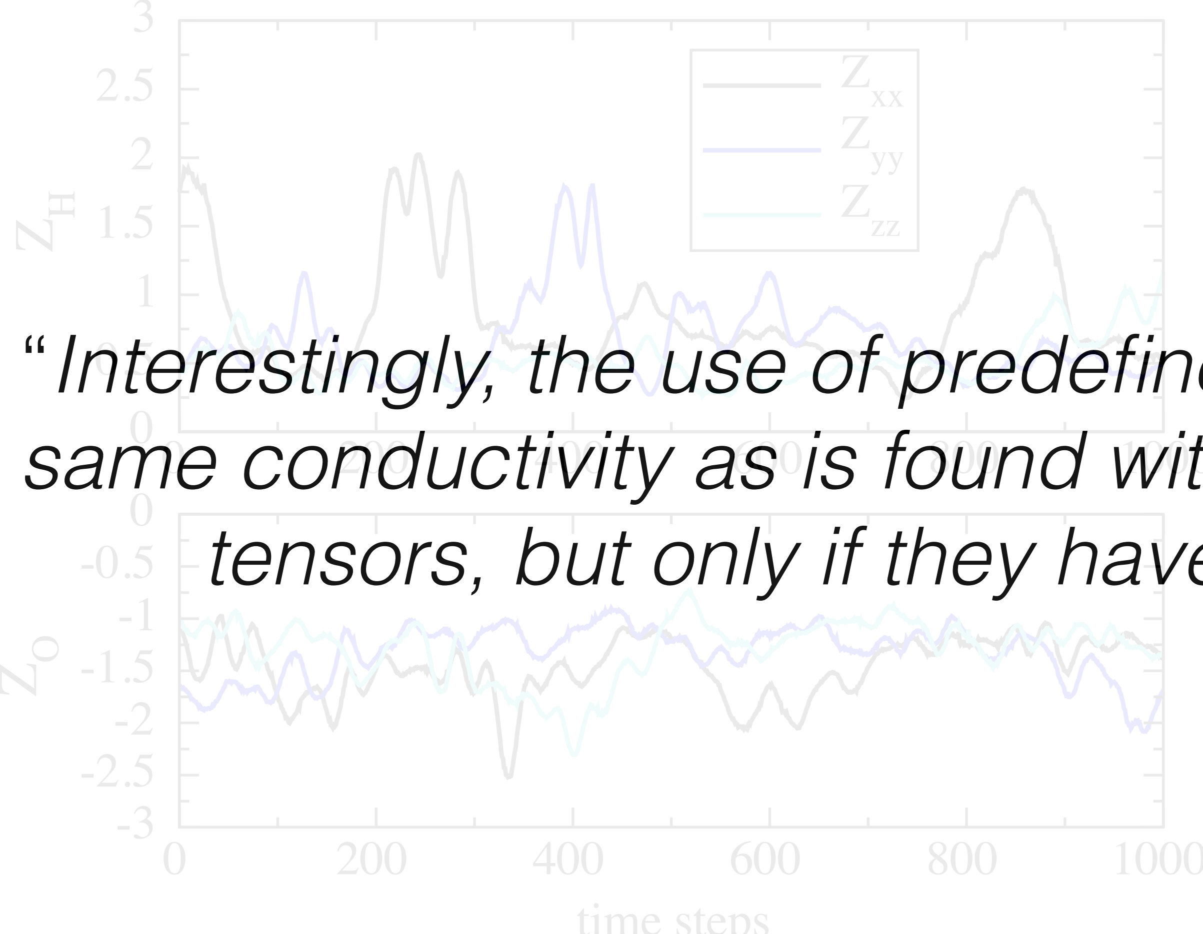
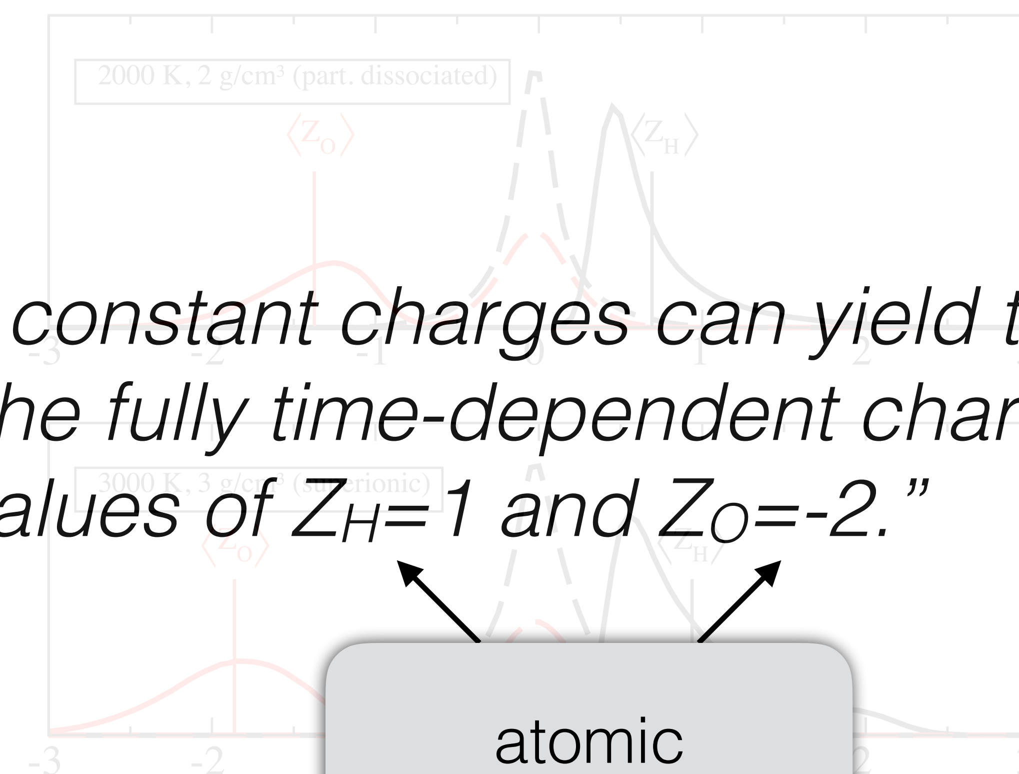
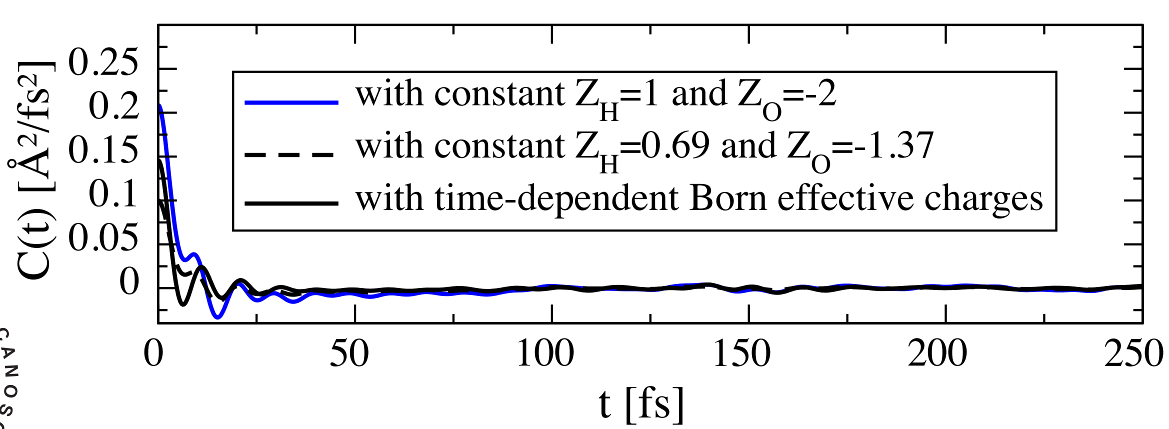
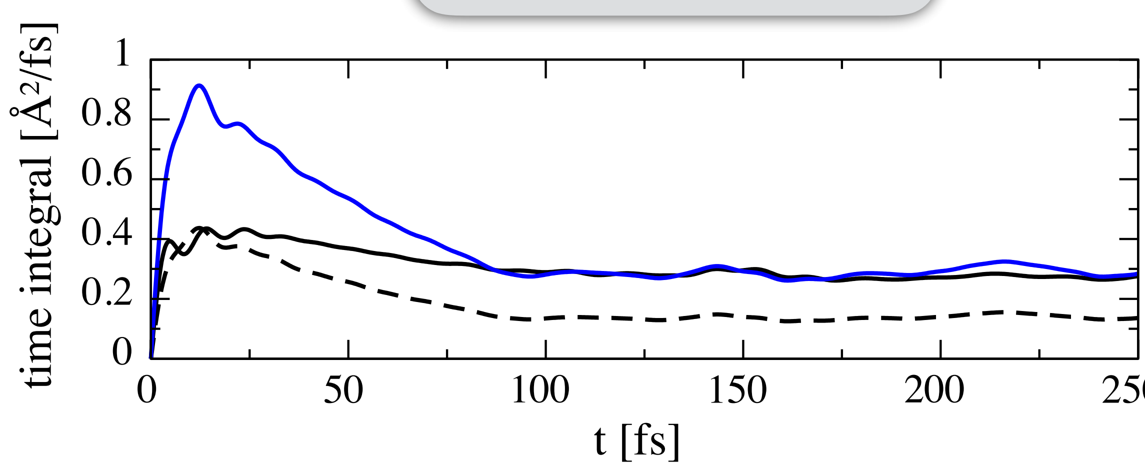




"*Interestingly, the use of predefined constant charges can yield the same conductivity as is found with the fully time-dependent charge tensors, but only if they have values of Z_H=1 and Z_O=-2.*"

atomic "oxidation states"





how come?

the Einstein-Helfand relations

Einstein (1905)

$$\left\langle |x(t)-x(0)|^2 \right\rangle = \left\langle \left| \int_0^t v(t')dt' \right|^2 \right\rangle$$

$$\approx 2t \underbrace{\int_0^\infty \langle v(t)v(0)\rangle dt}_{D}$$

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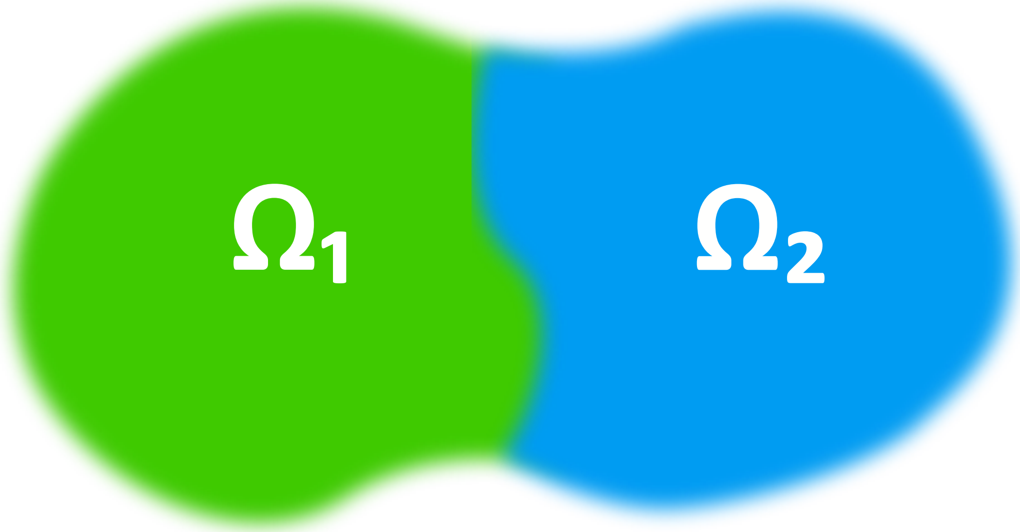
Helfand (1960)

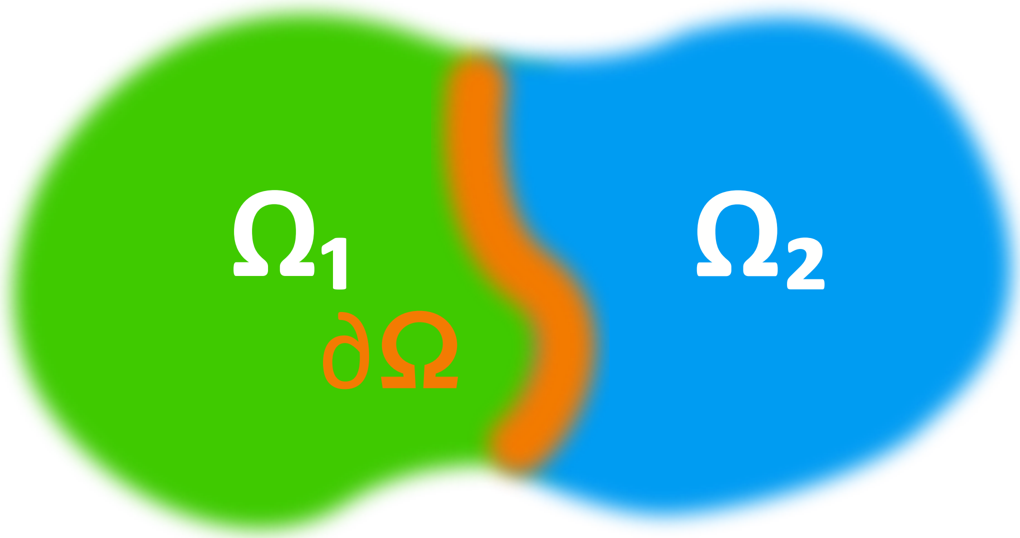
$$\left\langle \left| \int_0^t J(t')dt' \right|^2 \right\rangle \approx 2t \underbrace{\int_0^\infty \langle J(t)J(0)\rangle dt}_{\frac{k_B T}{\Omega}\lambda}$$

gauge transformation of conserved currents



$$E[\Omega_1 \cup \Omega_2] = E[\Omega_1] + E[\Omega_2]$$

gauge transformation of conserved currents



$$E[\Omega_1 \cup \Omega_2] = E[\Omega_1] + E[\Omega_2] + W[\partial\Omega]$$

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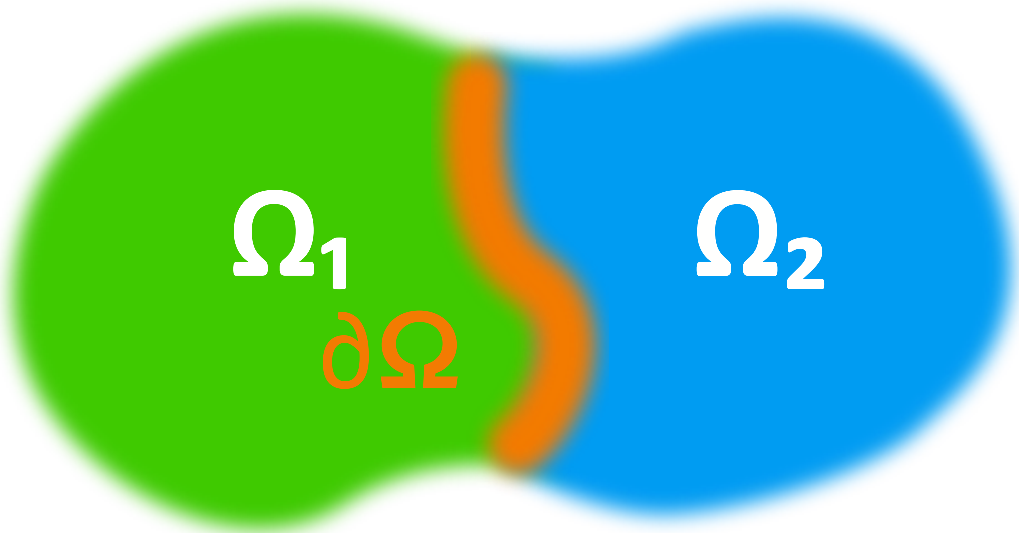

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extensivity

$$\mathcal{E}[\Omega] = \int_\Omega e(\mathbf{r})\,d\mathbf{r}$$

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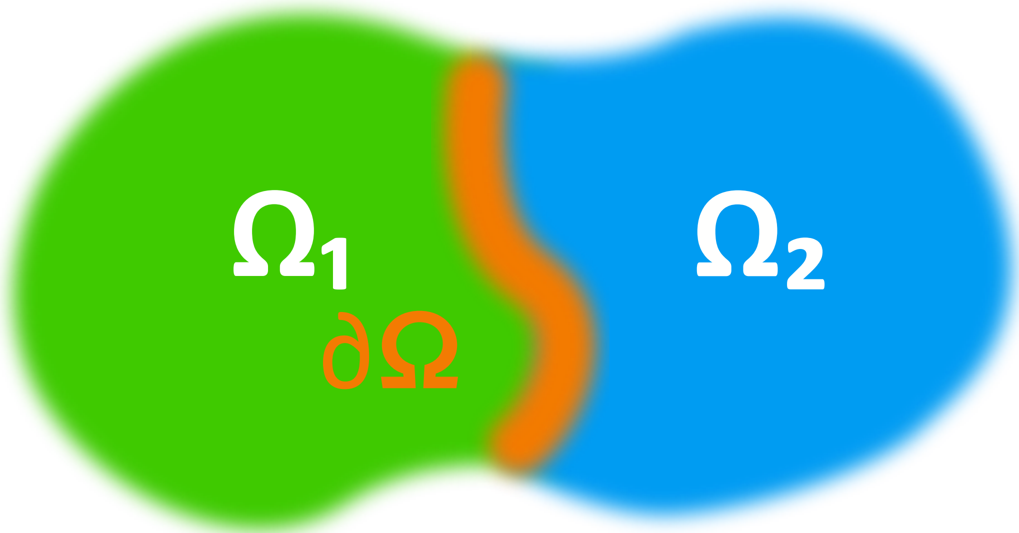

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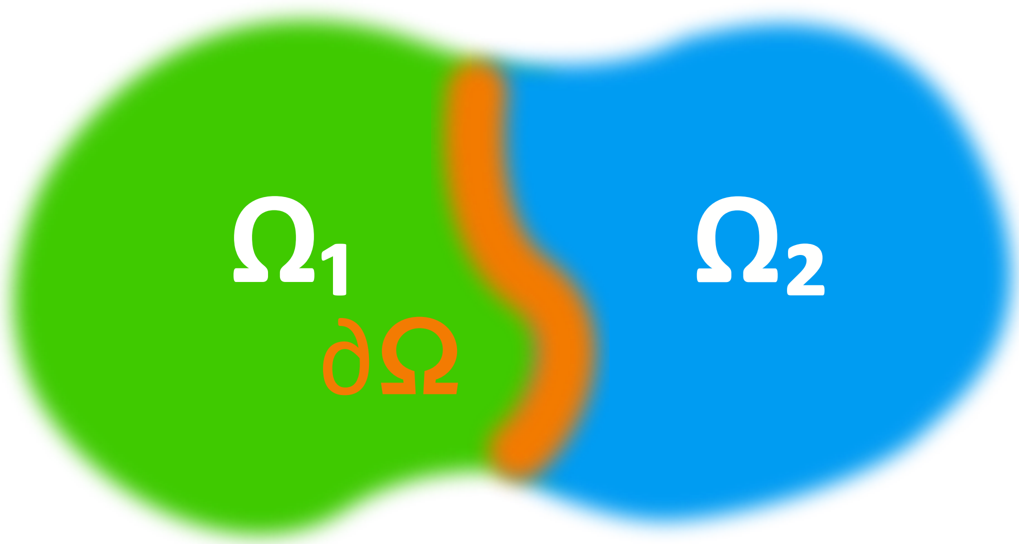

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gauge invariance $\mathcal{E}'[\Omega] = \mathcal{E}[\Omega] + \mathcal{O}[\partial\Omega]$

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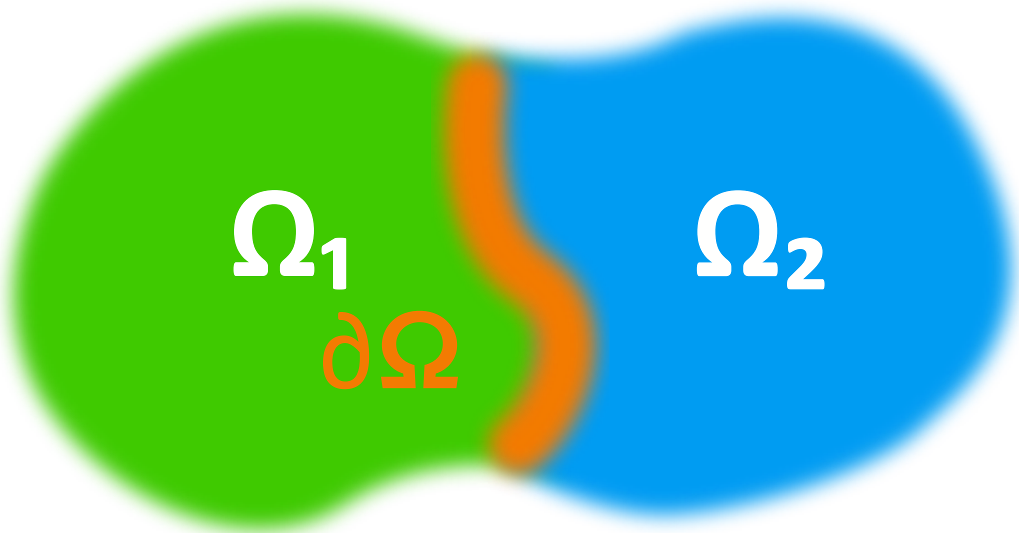

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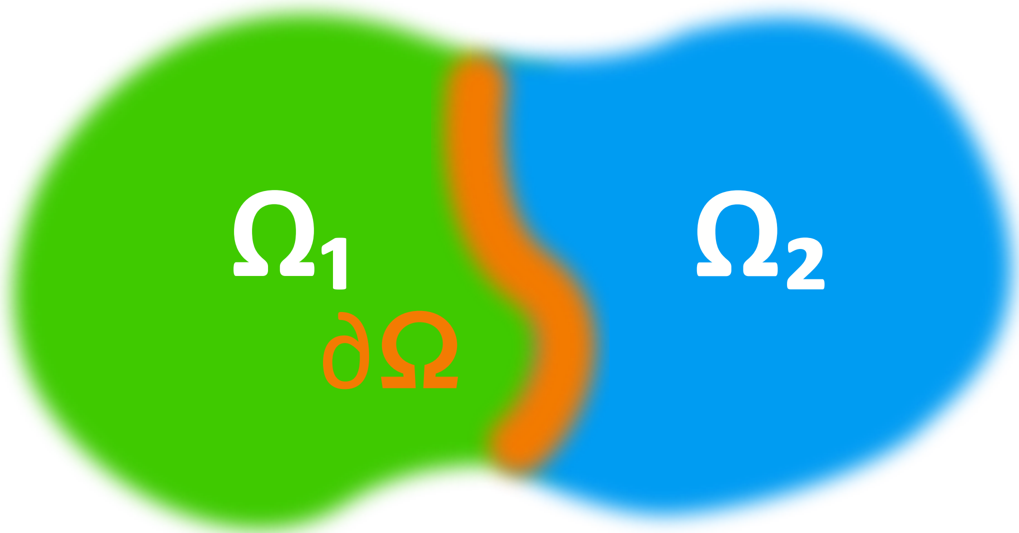

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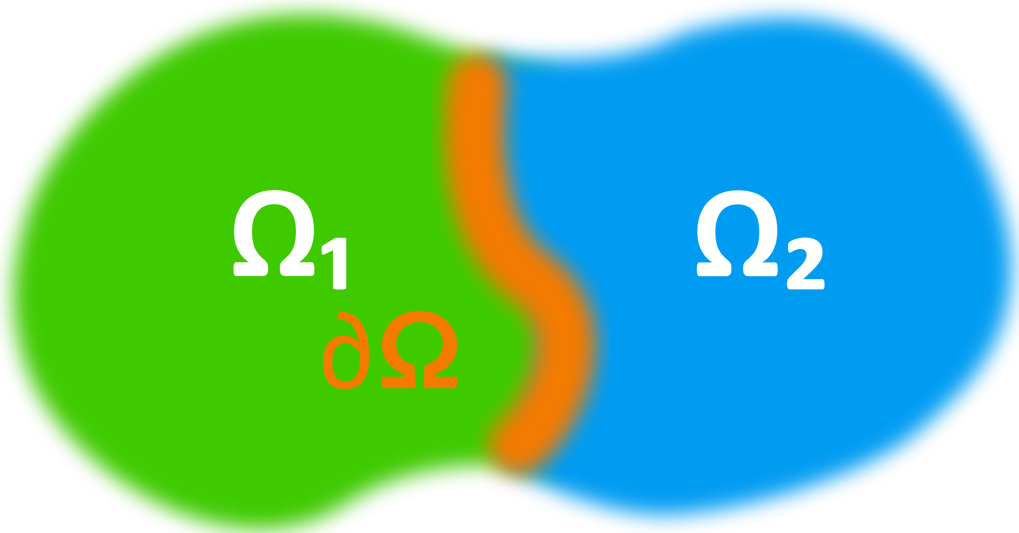

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gauge invariance of transport coefficients

$$J' = J + \dot{P}$$

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gauge invariance of transport coefficients

$$J' = J + \dot{P}$$

any two conserved densities that differ by the divergence of a (bounded) vector field are physically equivalent

$$\lambda \sim \frac{1}{2t}\mathrm{var}\left[D(t)\right] \qquad D(t) = \int_0^t J(t')\,dt'$$

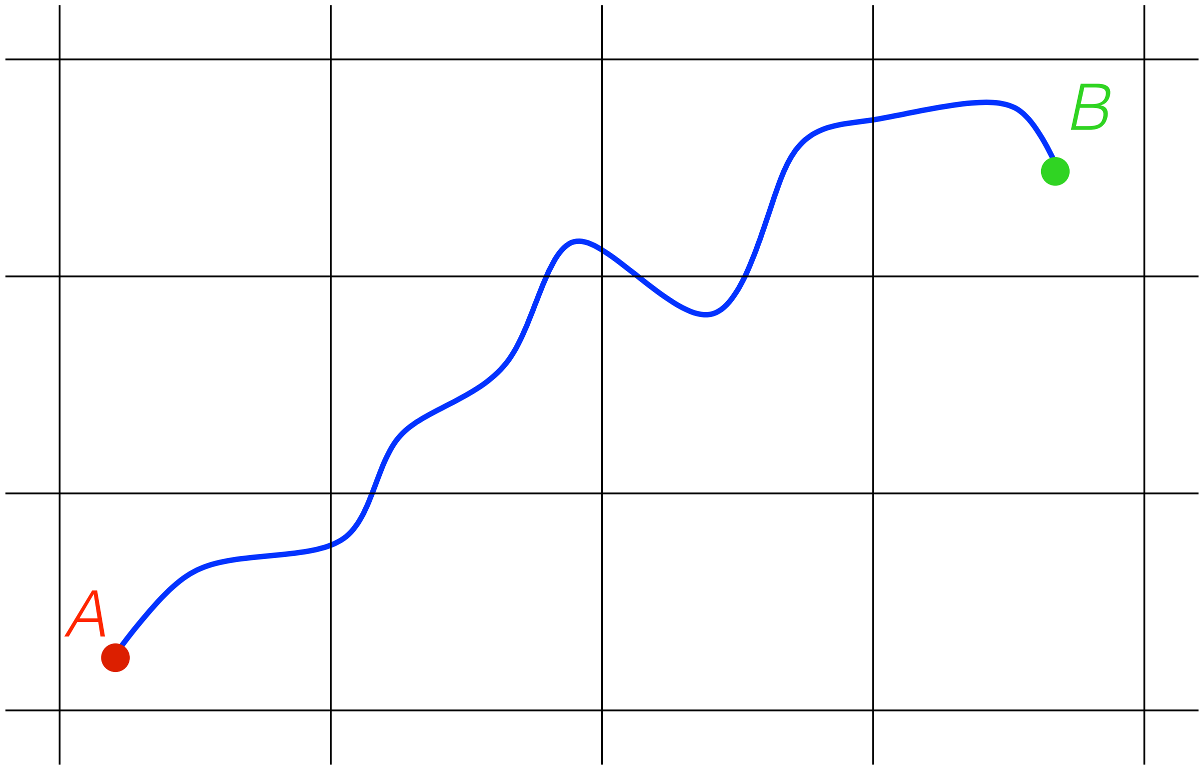
the corresponding conserved fluxes differ by a total time derivative, and the transport coefficients coincide

$$D'(t) = D(t) + P(t) - P(0)$$

$$\lambda' = \lambda$$

$$\mathrm{var}\left[D'(t)\right] = \underbrace{\mathrm{var}\left[D(t)\right]}_{\mathcal{O}(t)} + \underbrace{\cancel{\mathrm{var}\left[\Delta P(t)\right]} + \cancel{2\mathrm{cov}\left[D(t)\cdot\Delta P(t)\right]}}_{\mathcal{O}(t^{\frac{1}{2}})}$$

gauge invariance of charge transport



$$\sigma \propto \lim_{t\to\infty} \frac{1}{2t} \left\langle |\mu_{AB}|^2 \right\rangle$$

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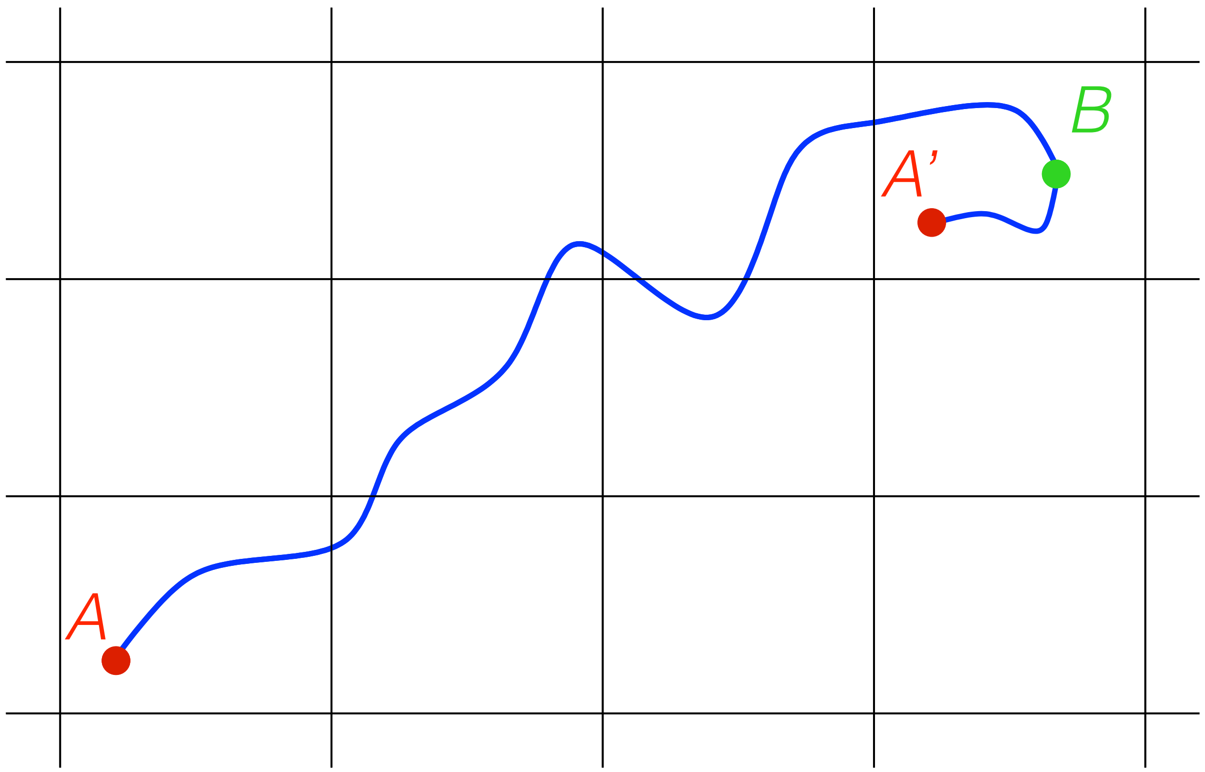
gauge invariance of charge transport



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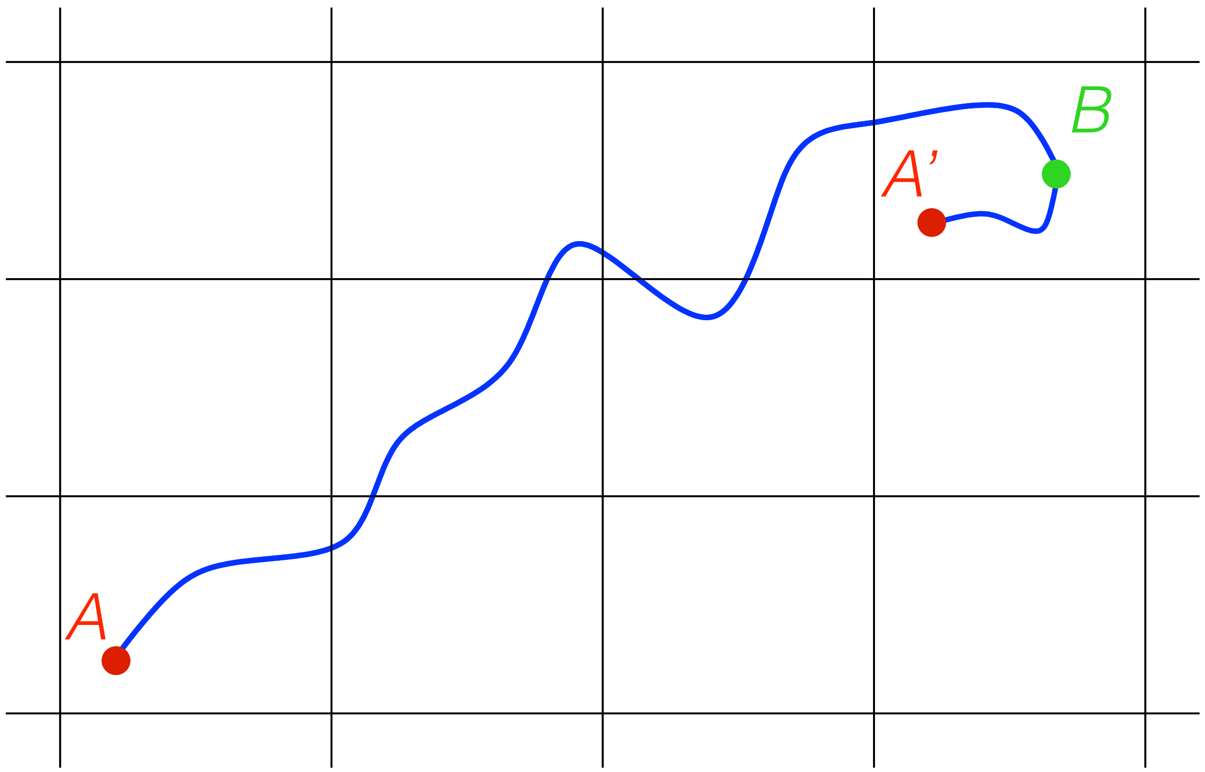
$$= \mu_{AA'} + \mu_{A'B}$$

gauge invariance of charge transport



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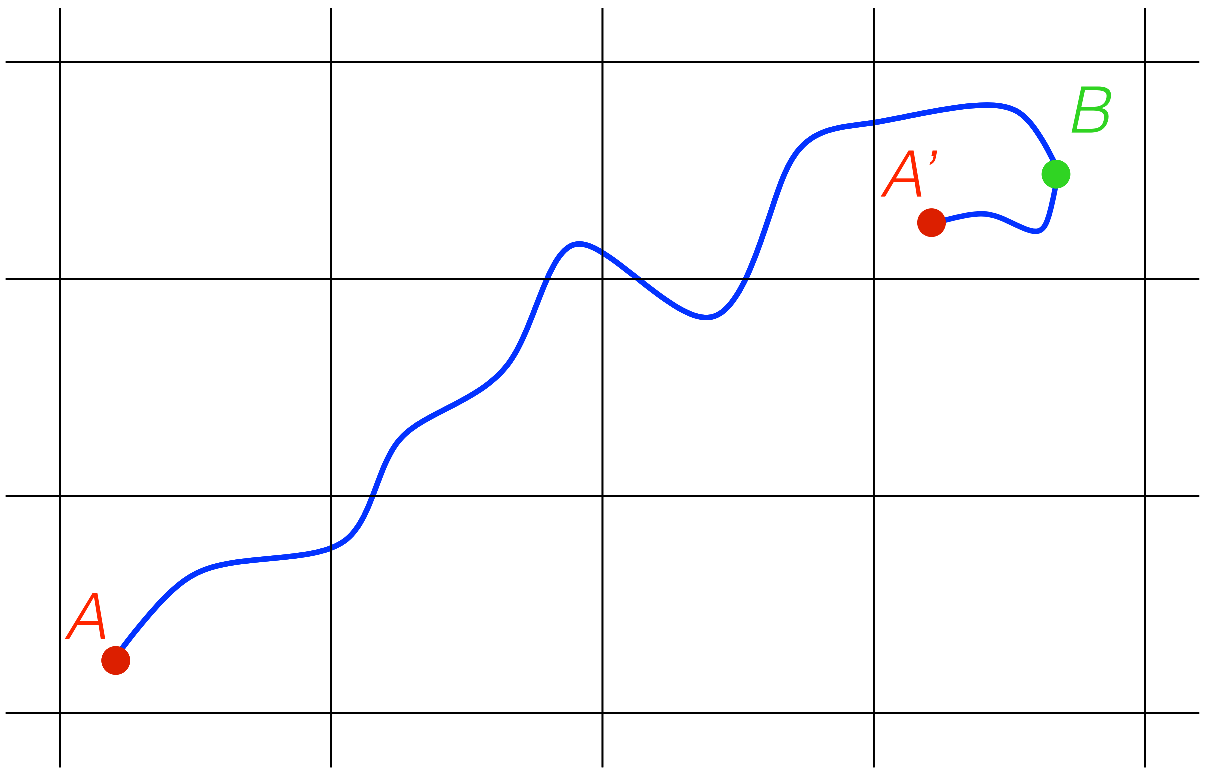
$$\mathrm{var}\left[\mu_{AB}\right] = \mathrm{var}\left[\mu_{AA'}\right] + \underbrace{\mathrm{var}\left[\mu_{A'B}\right]}_{bounded} + 2\mathrm{cov}\left[\mu_{AA'} \cdot \mu_{A'B}\right]$$

gauge invariance of charge transport



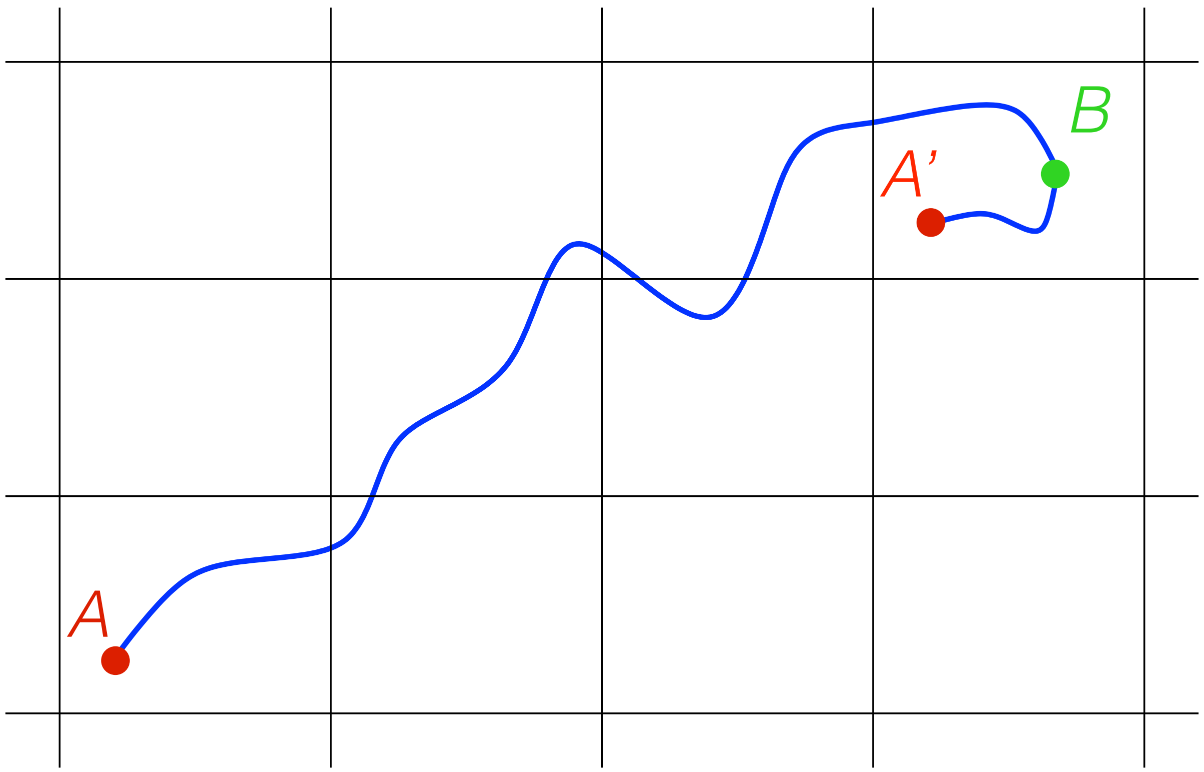
$$\sigma \propto \lim_{t\to\infty} \frac{1}{2t} \langle |\mu_{AB}|^2 \rangle$$

$$\mu_{AB} = \int_0^t J(t')dt'$$
$$= \mu_{AA'} + \mu_{A'B}$$

$$\mathrm{var}[\mu_{AB}] = \mathrm{var}[\mu_{AA'}] + \underbrace{\cancel{\mathrm{var}[\mu_{A'B}]}}_{\textit{bounded}} + \cancel{2\mathrm{cov}[\mu_{AA'} \cdot \mu_{A'B}]}$$

$$\boxed{\sigma \propto \lim_{t\to\infty} \frac{1}{2t} \langle |\mu_{AA'}|^2 \rangle}$$

Thouless' quantisation of particle transport



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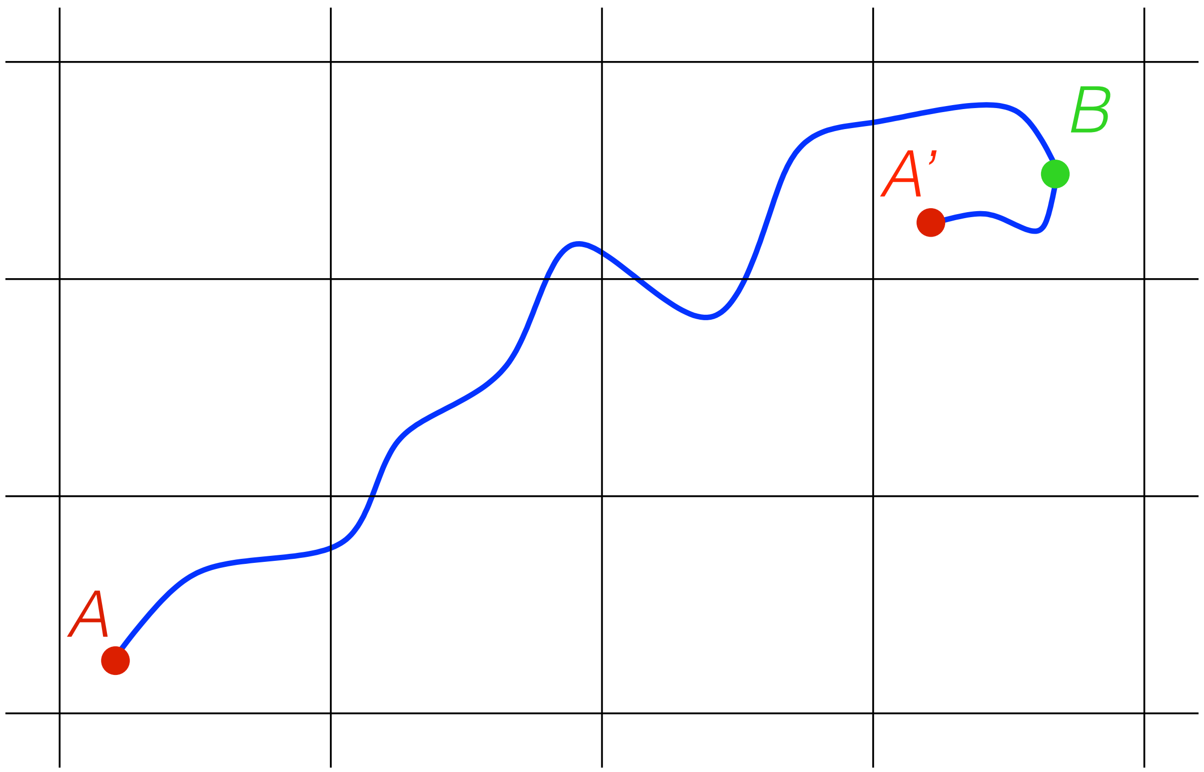


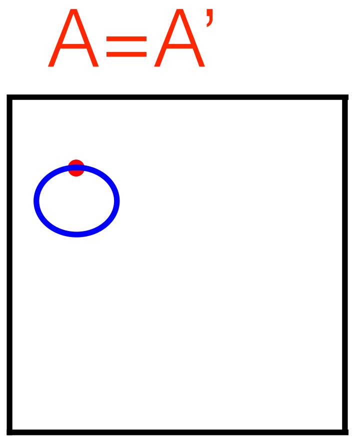
$$\sigma \propto \lim_{t\to\infty} \frac{1}{2t} \left\langle |\mu_{AA'}|^2 \right\rangle$$

$$\hat{H}(B) \neq \hat{H}(A)$$
$$\hat{H}(A') = \hat{H}(A)$$

$$\begin{aligned} \mu_{AA'} &= \int_A^{A'} d\mu(X) \\ &= \ell Q(AA') \end{aligned}$$
$$Q(AA') \in \mathbb{Z}$$

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

topological invariants



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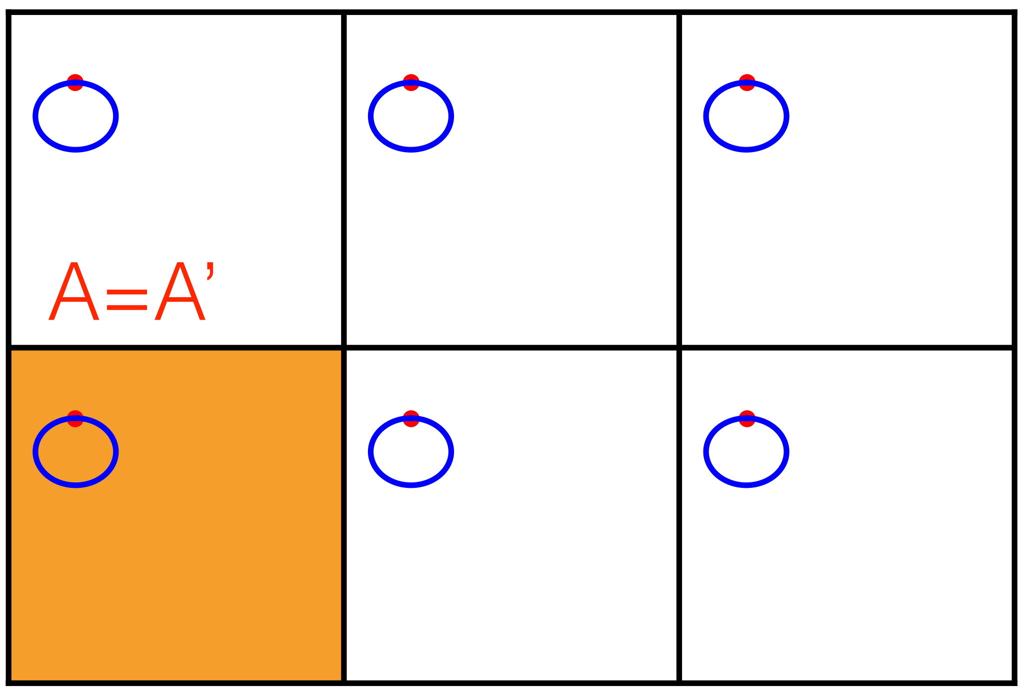
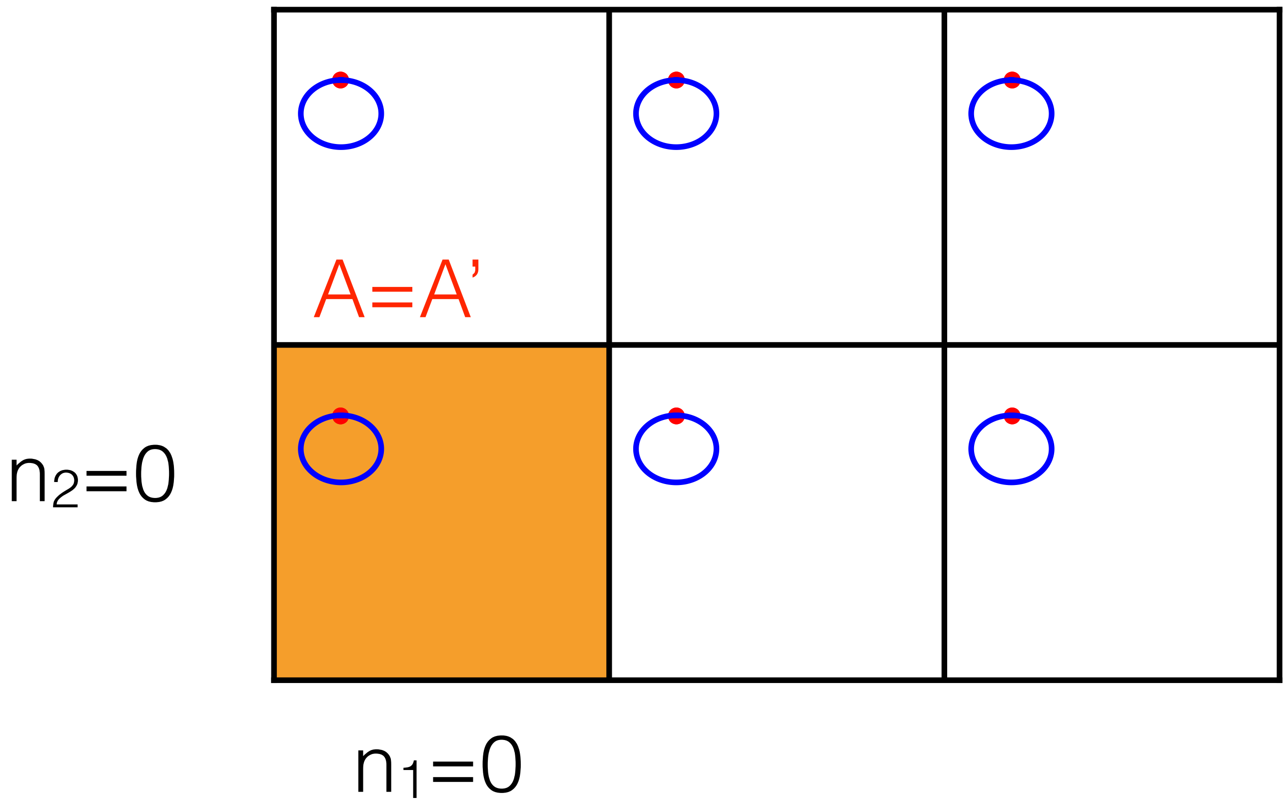
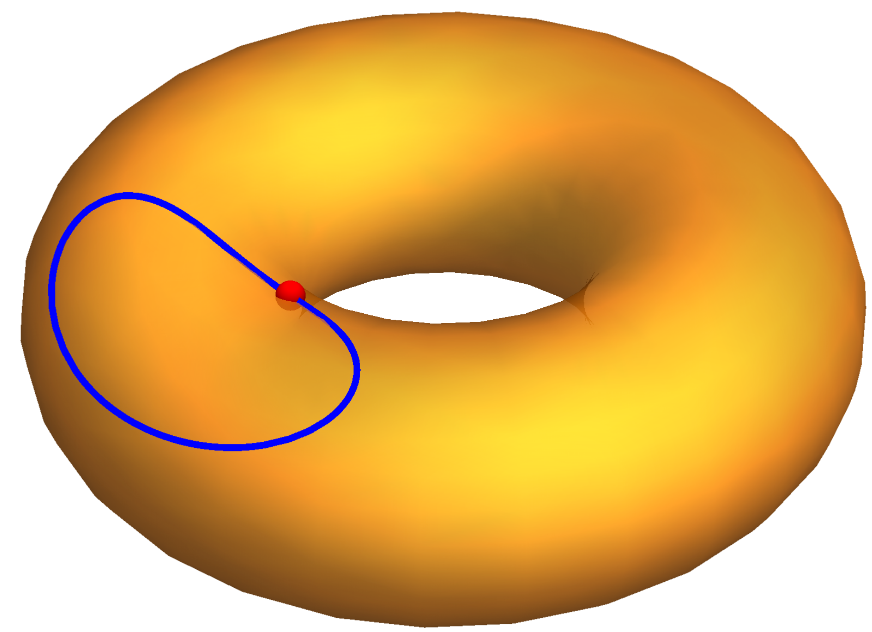


topological invariants





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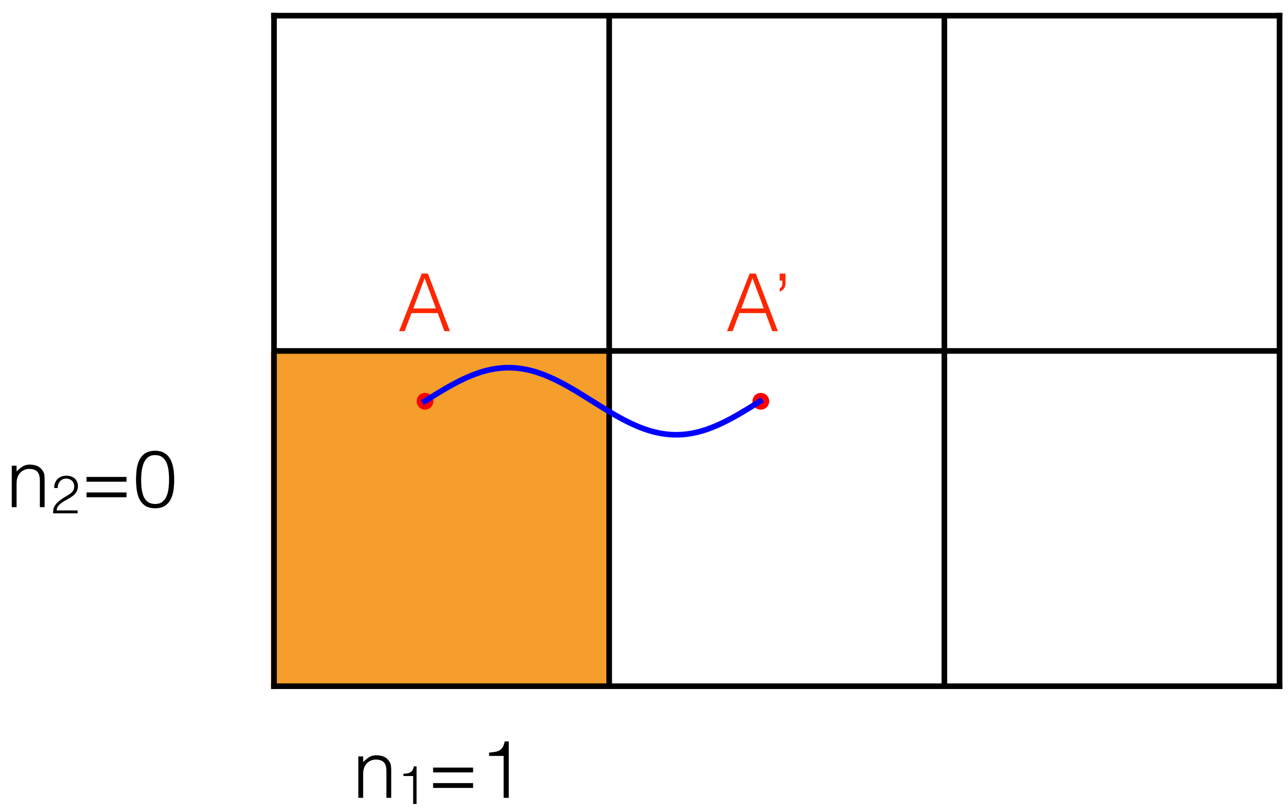

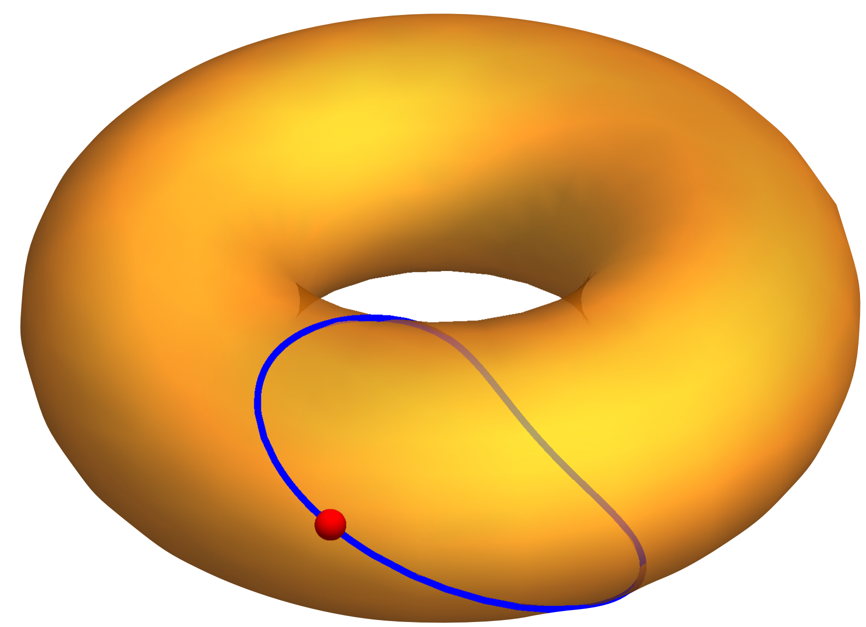

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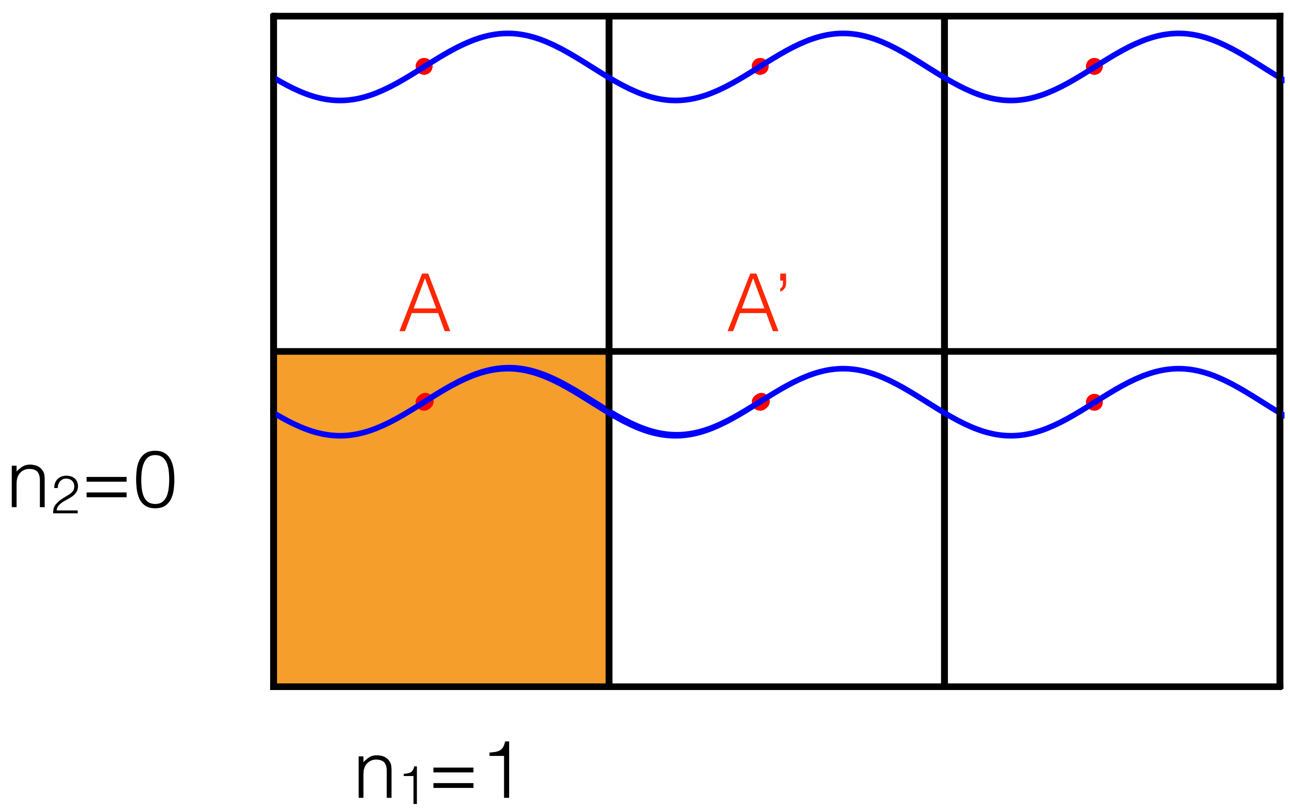

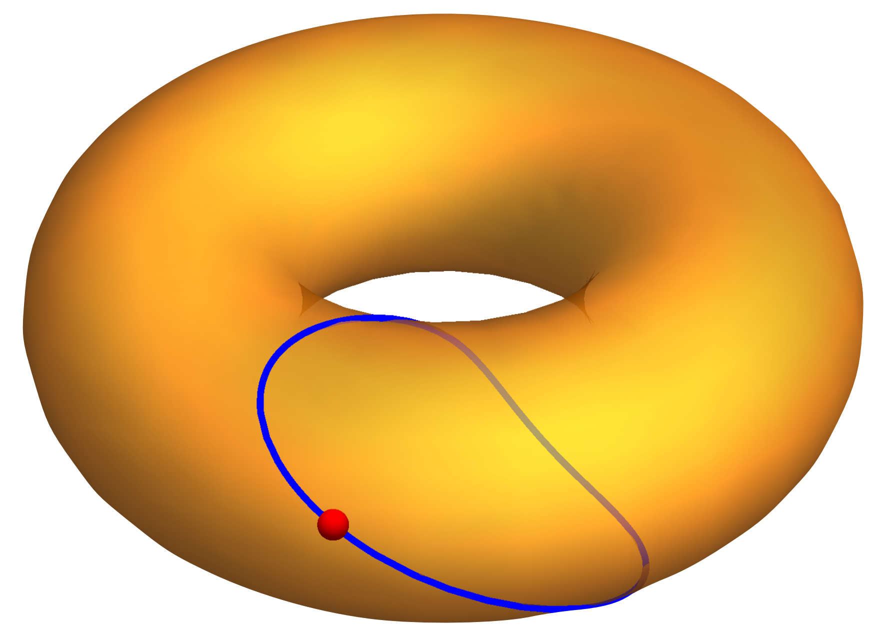

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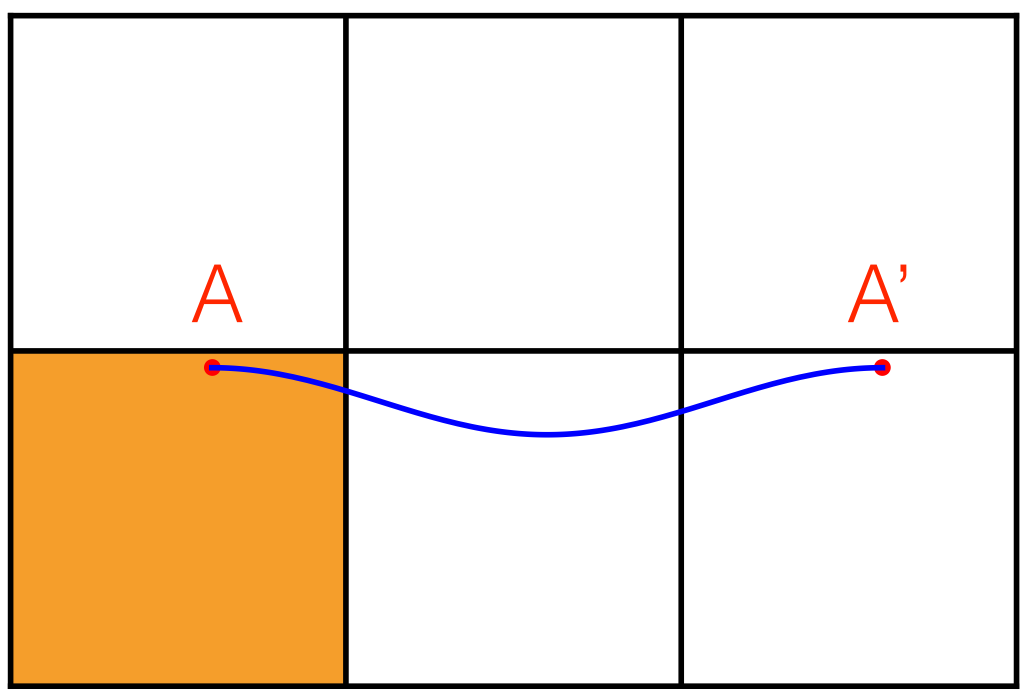
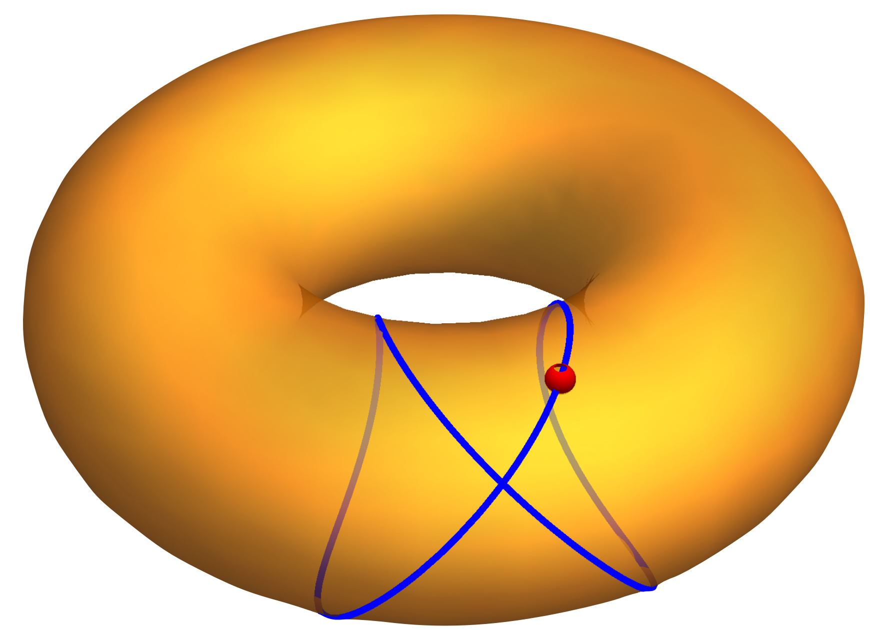


$n_2=0$

$n_1=2$



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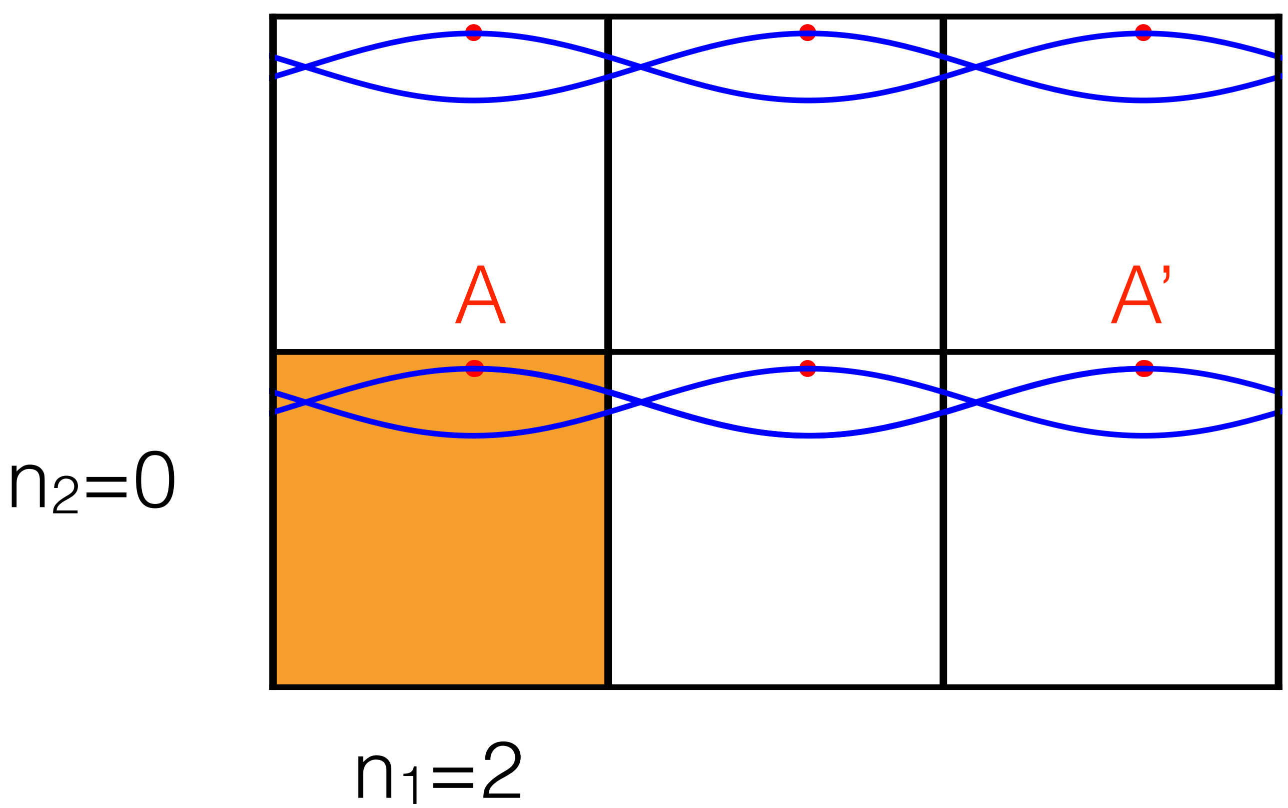

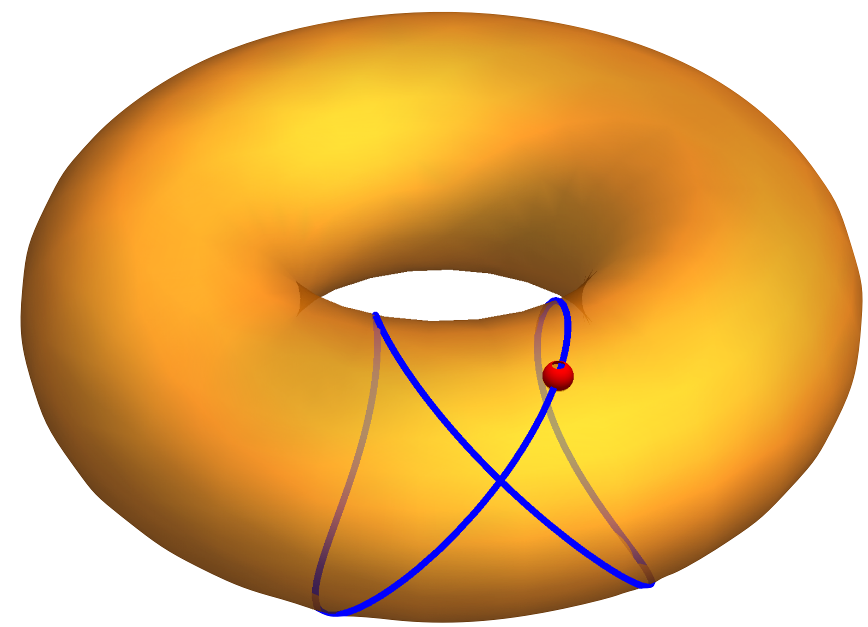

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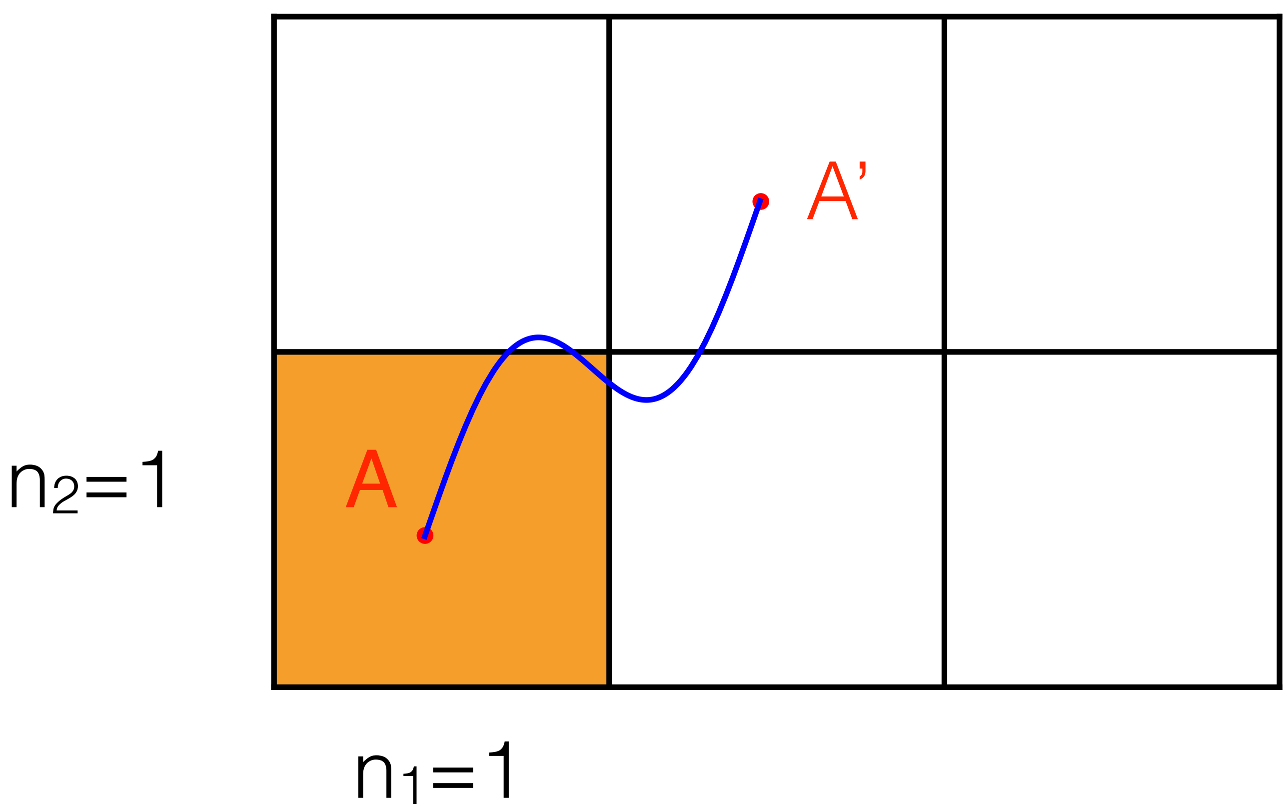
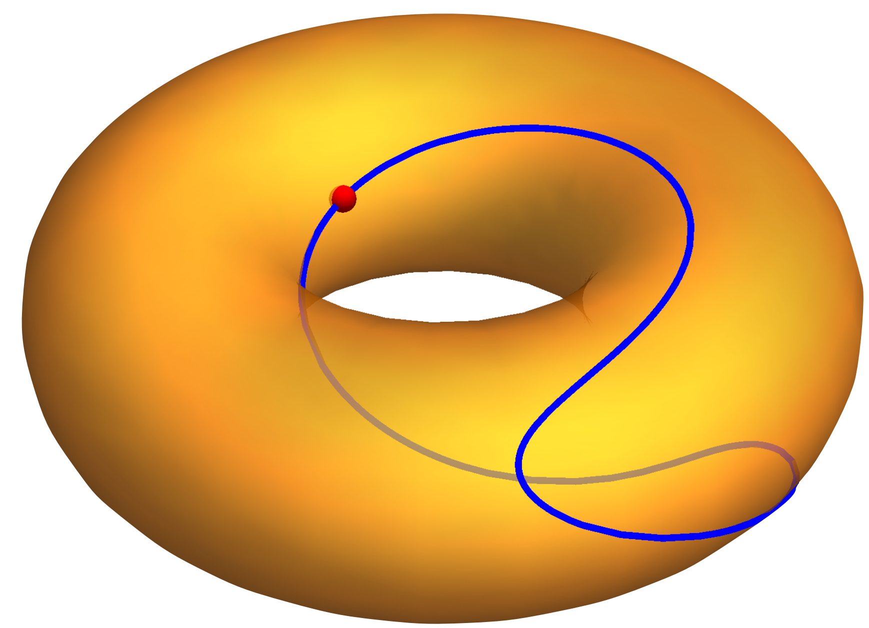
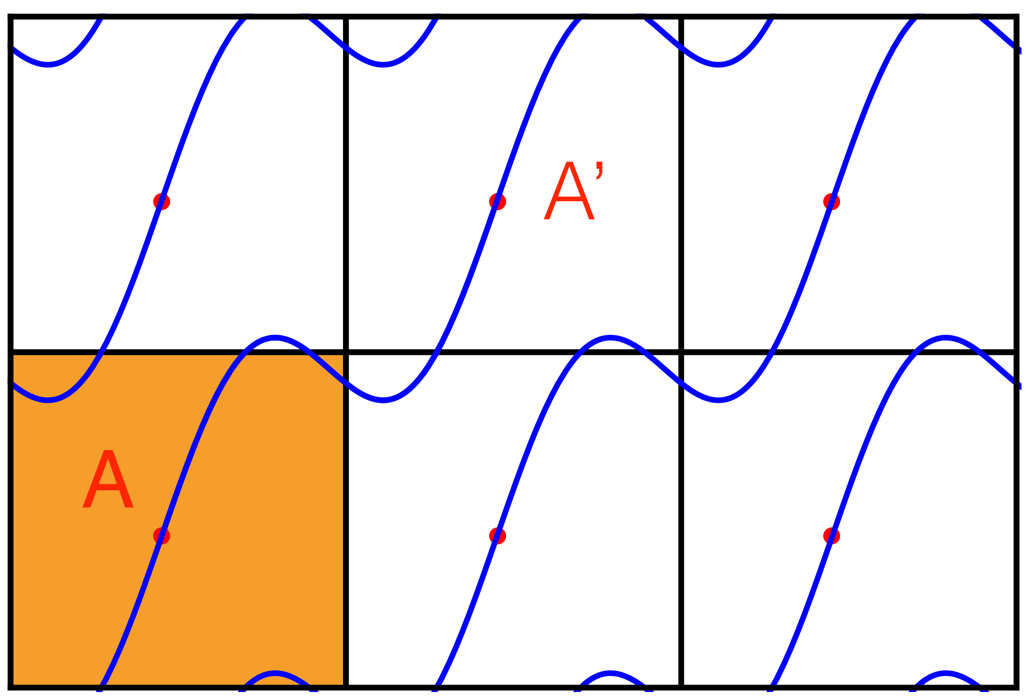


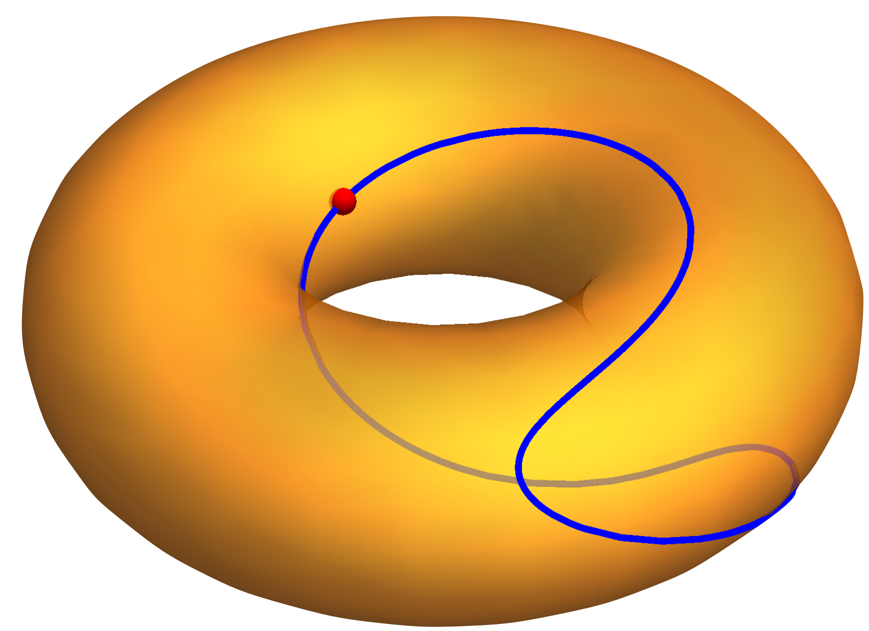


topological invariants

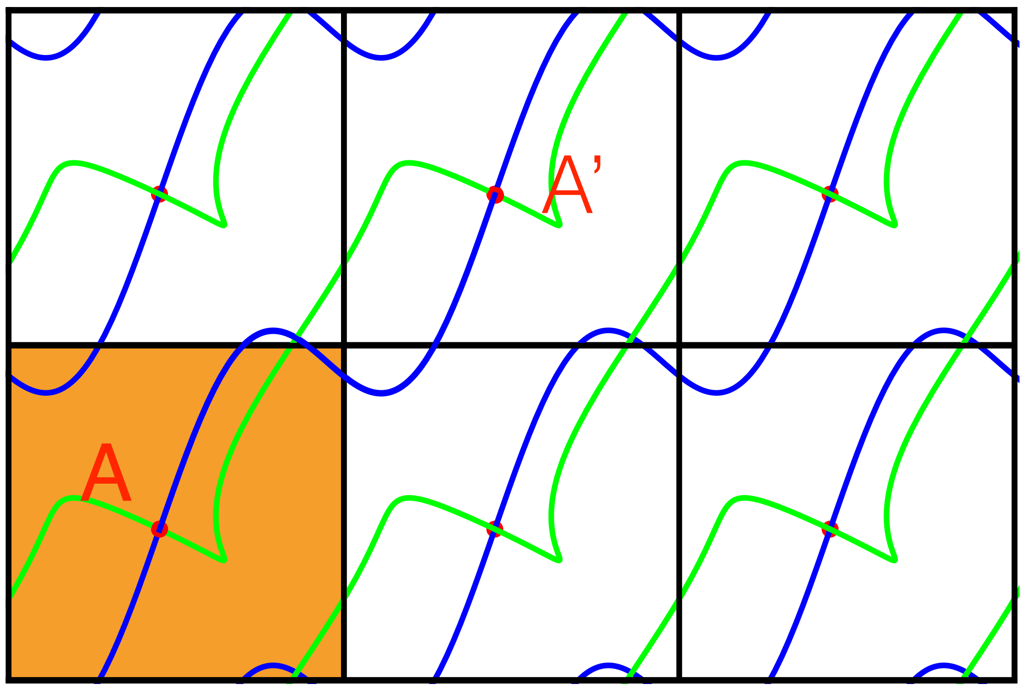


$n_2=1$

$n_1=1$



topological invariants



$n_2=1$

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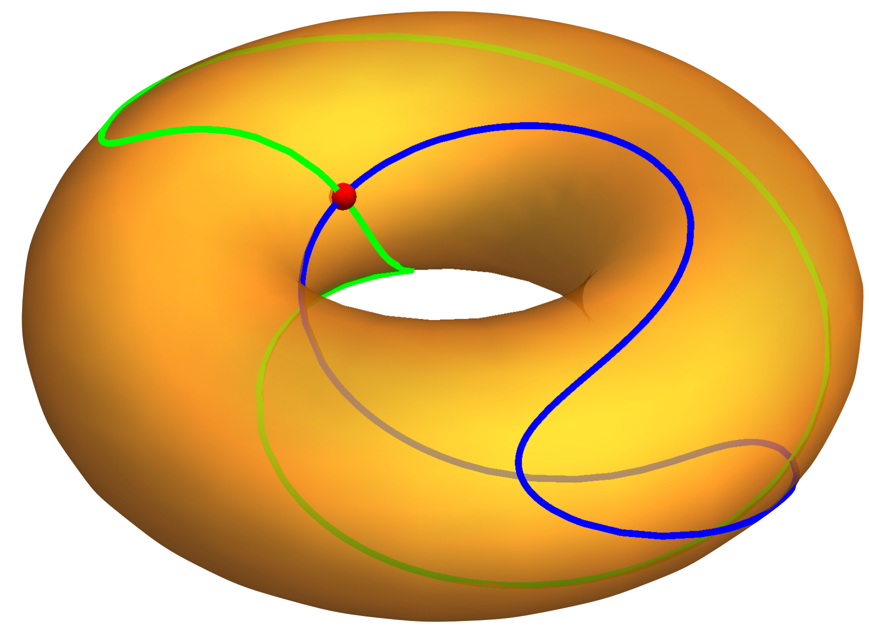
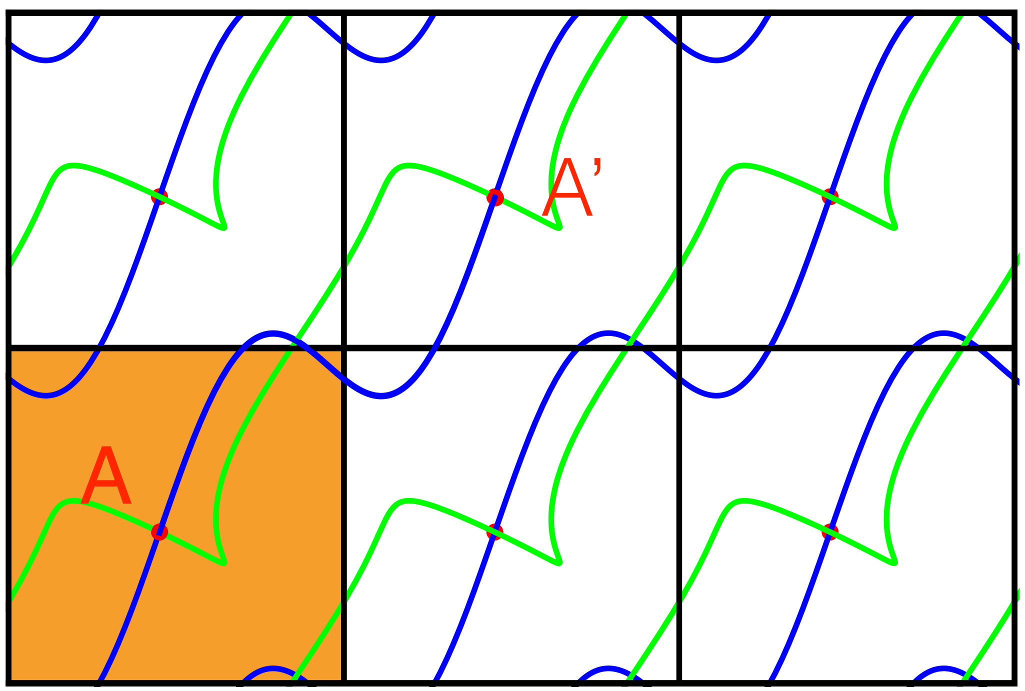
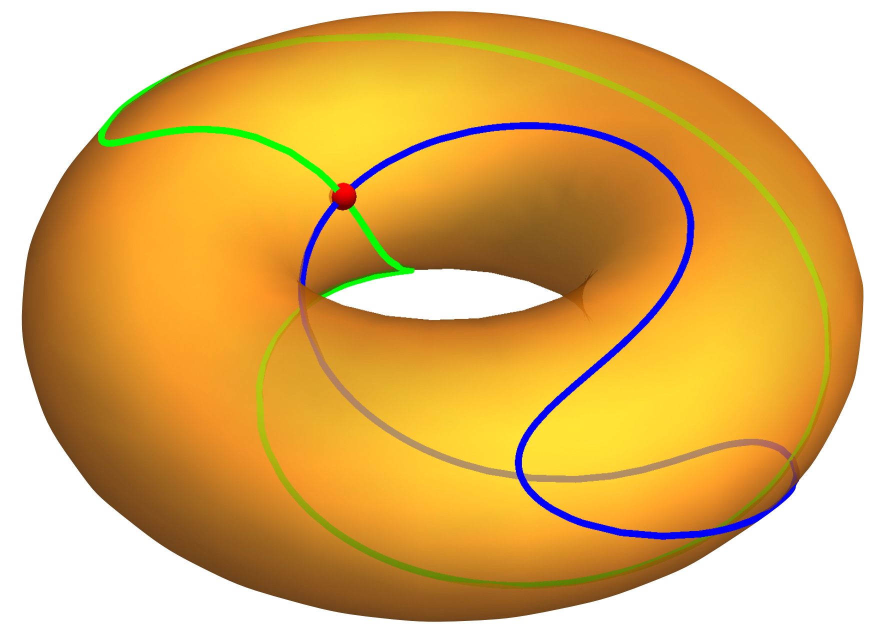


topological invariants



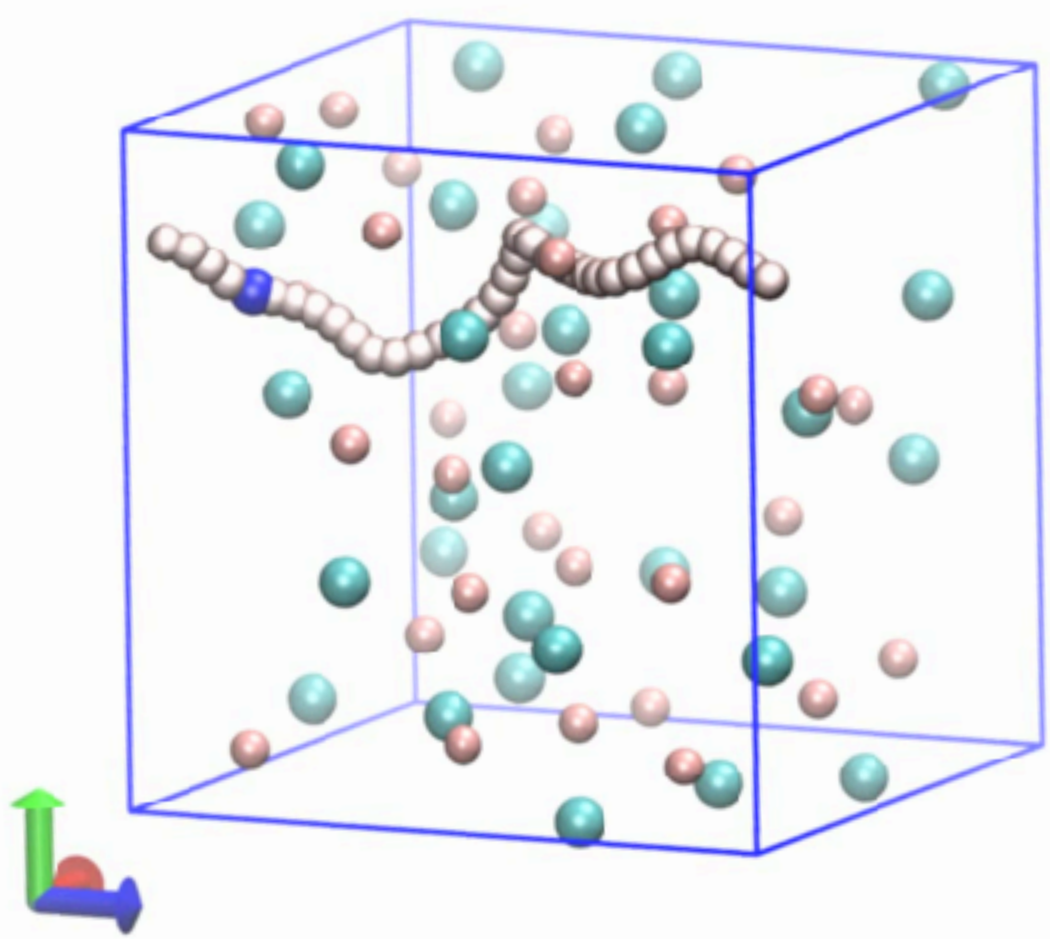
n_2=1

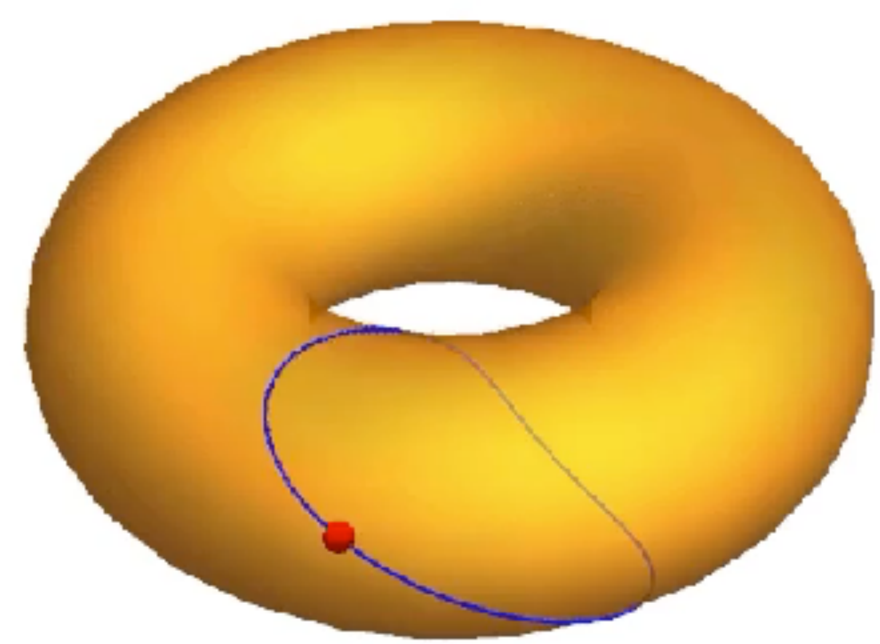
n_1=1



$$Q(AA') = Q(AA') = Q[n_1 = 1, n_2 = 1]$$

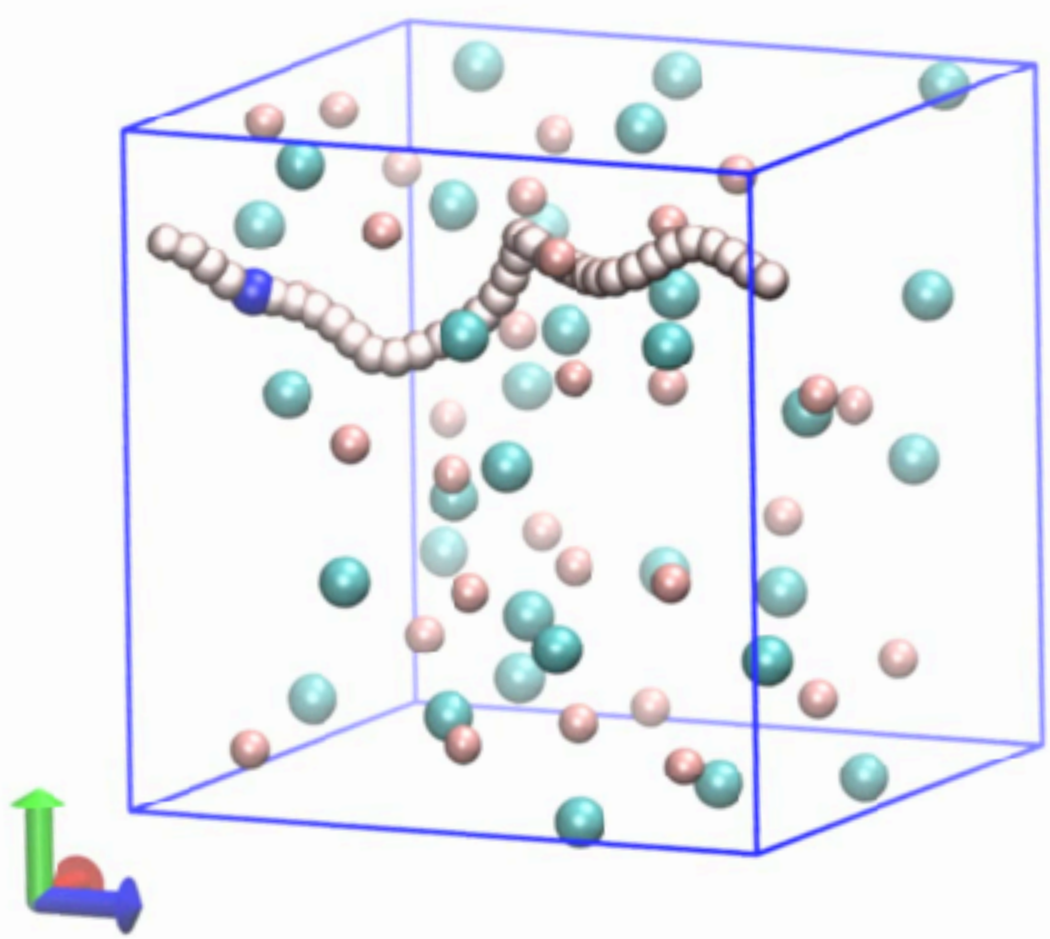
a numerical experiment on molten KCl

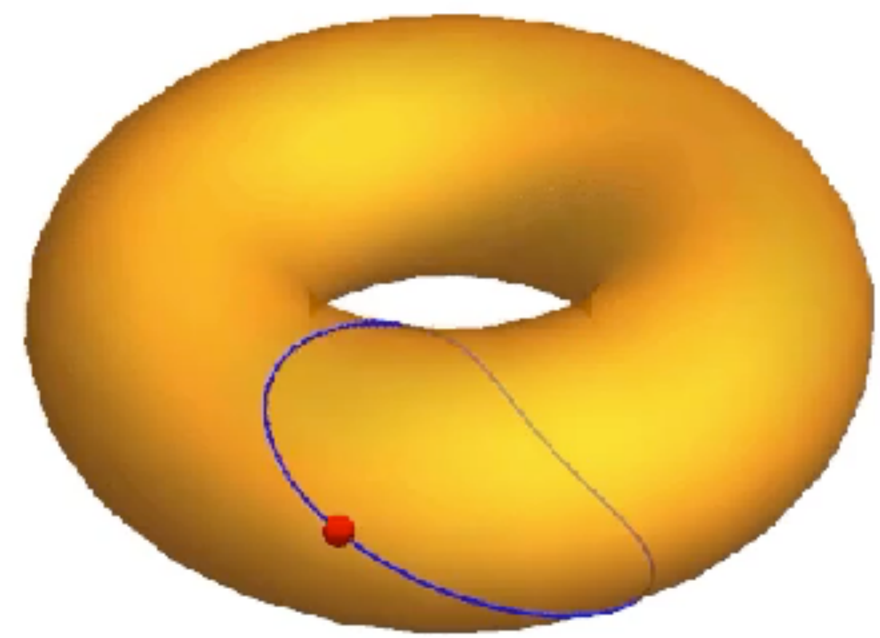




a topologically non-trivial minimum-energy path
connecting two identical configurations of a ionic fluid

a numerical experiment on molten KCl





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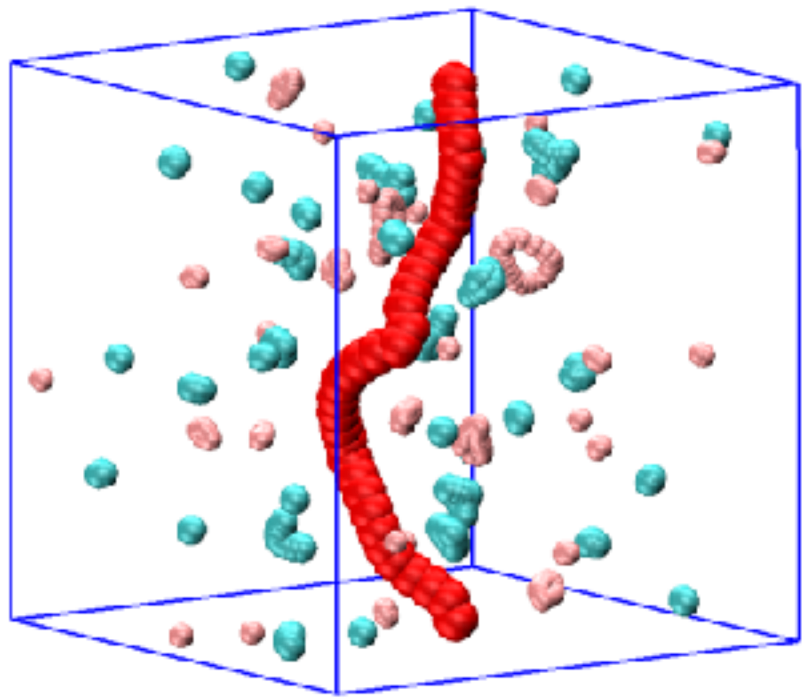

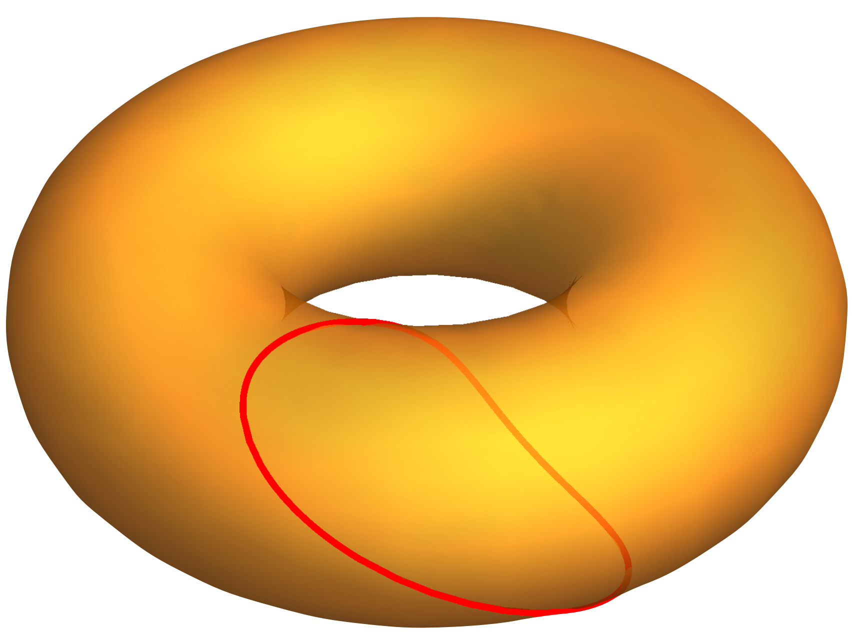

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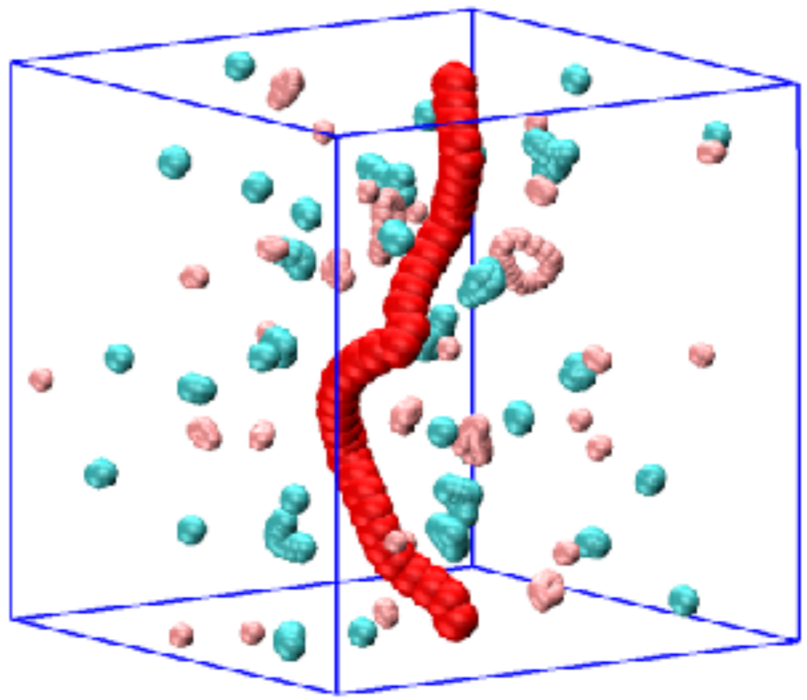

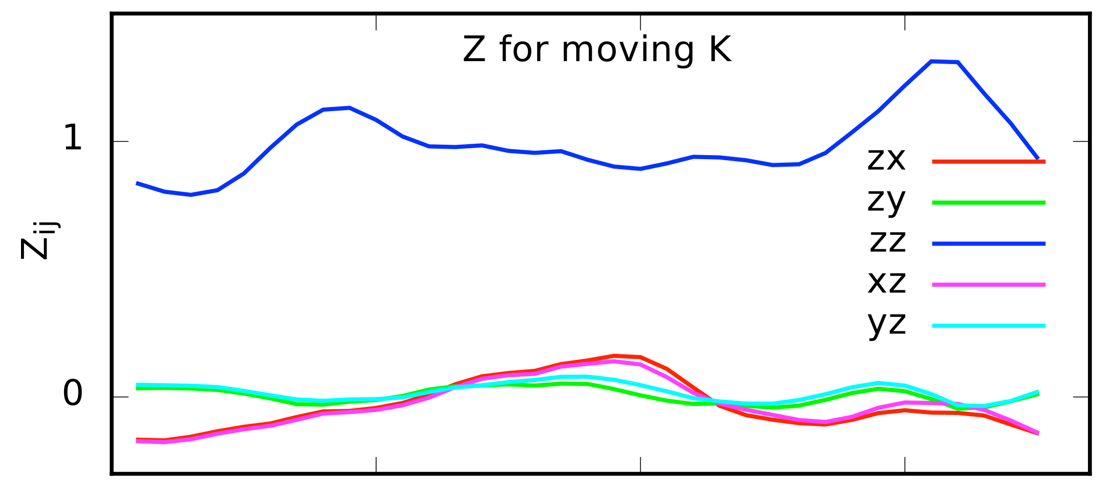

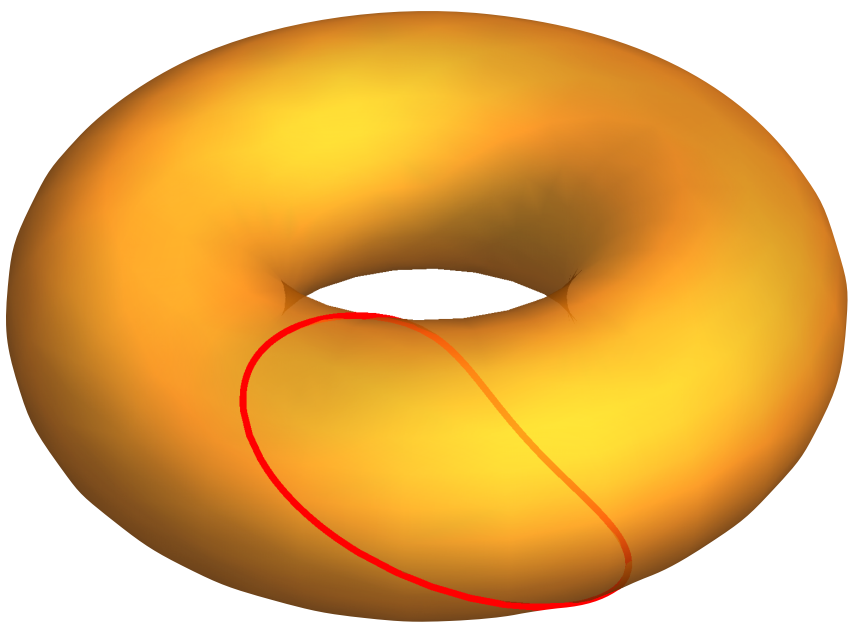

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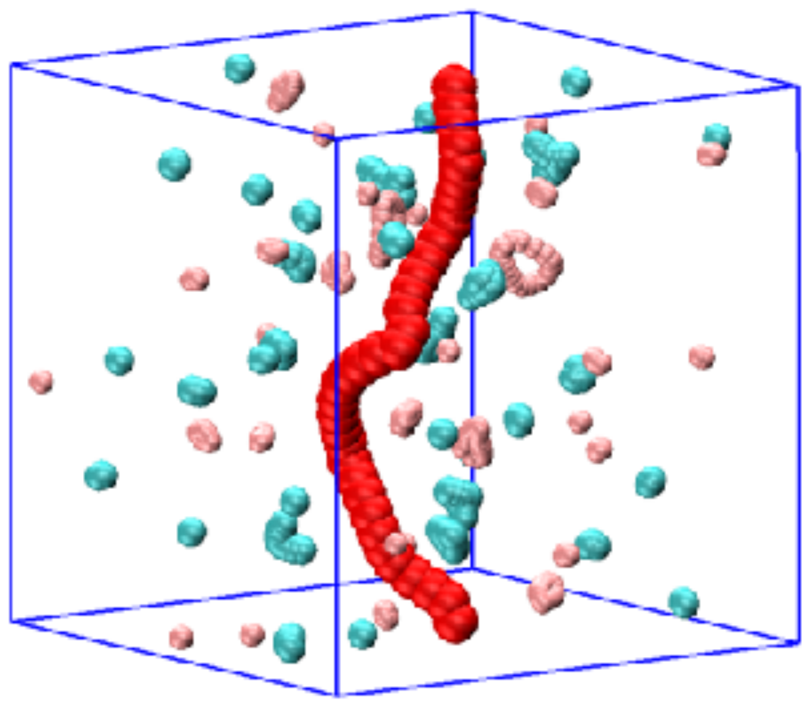
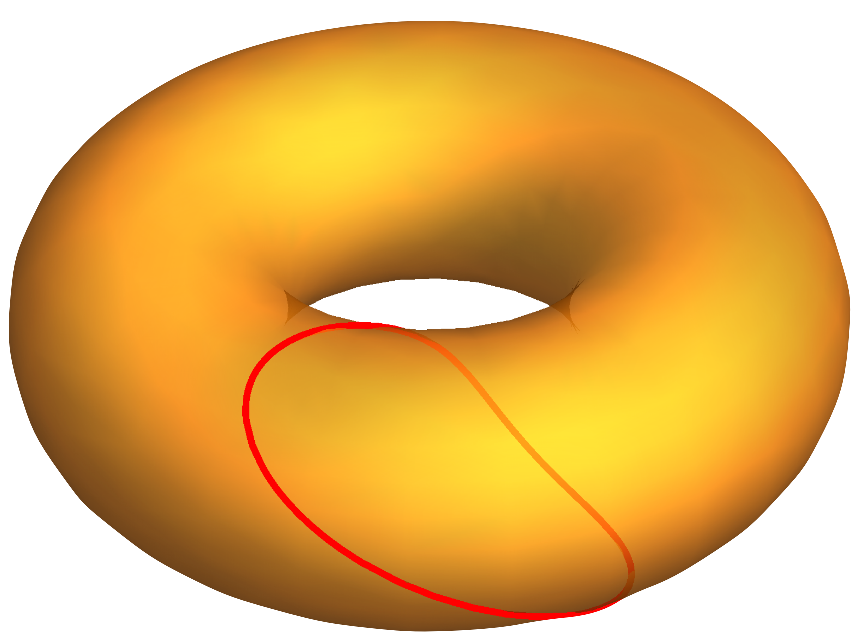
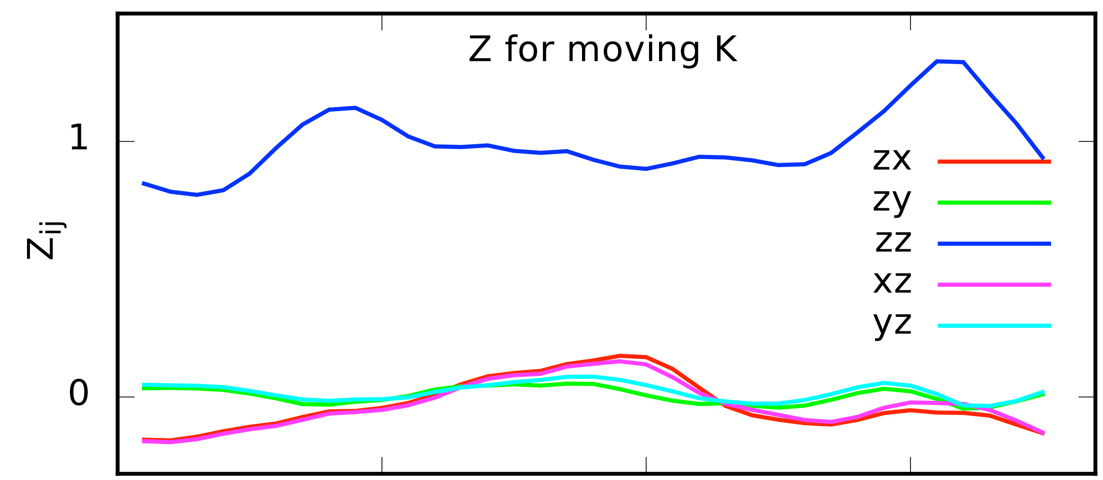
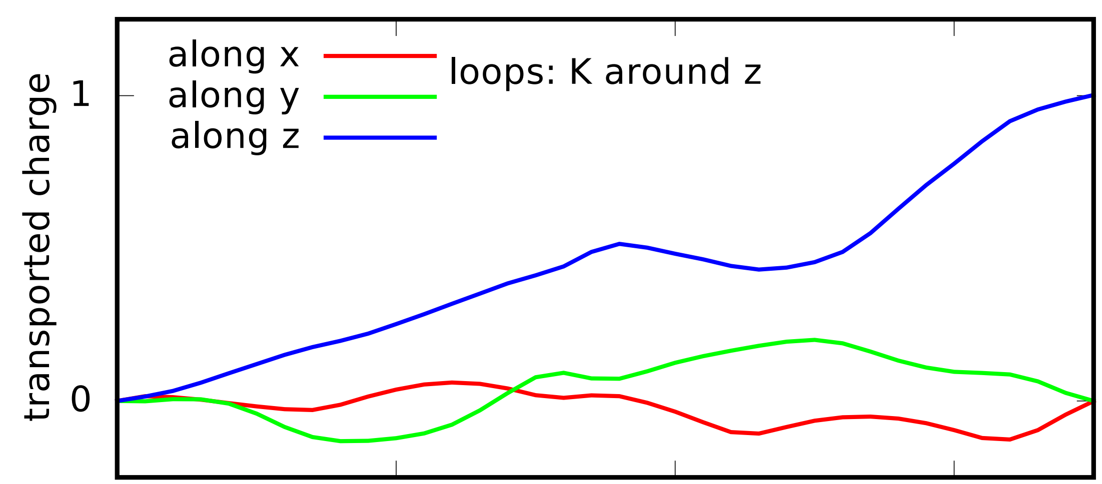


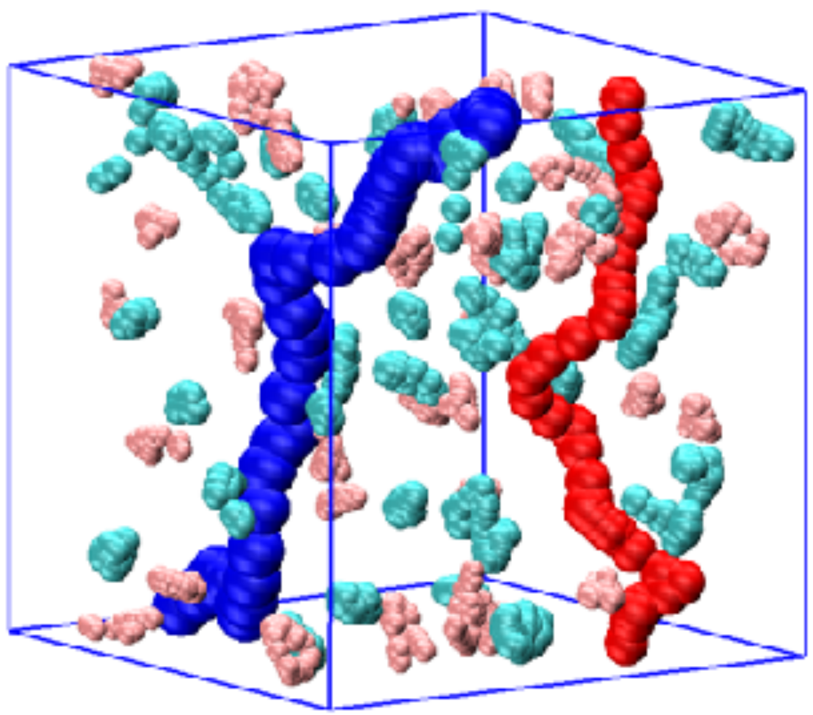


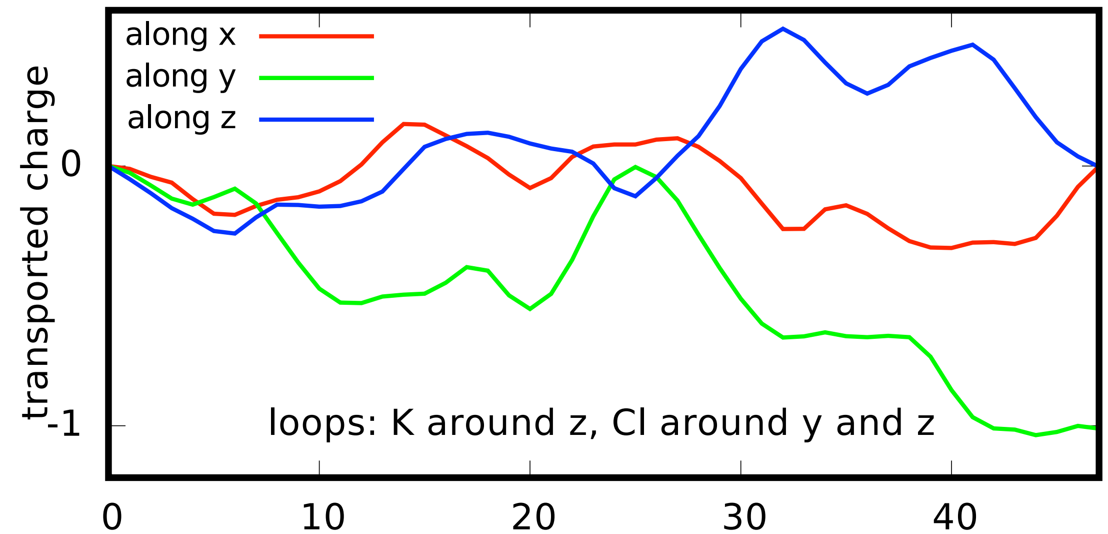


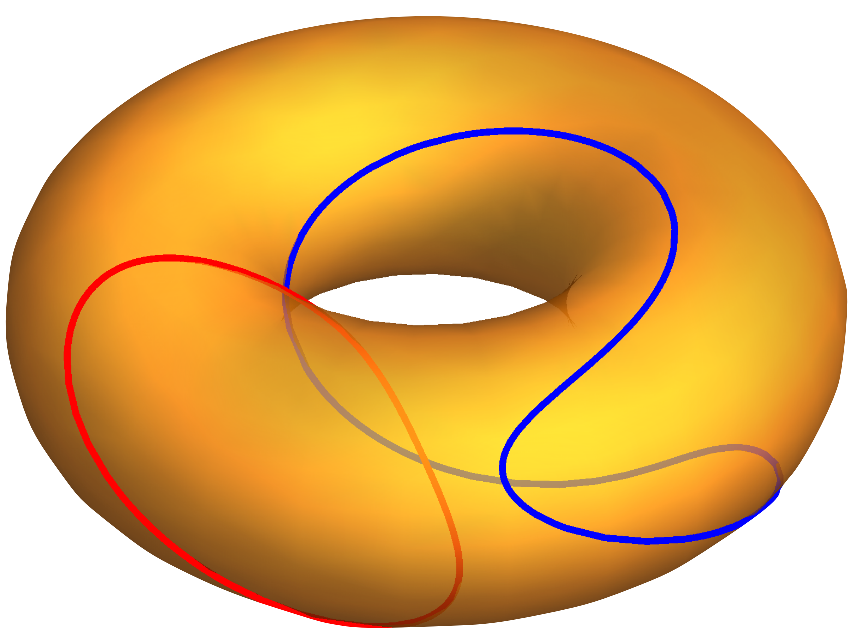


qx = =-0.000(6); qy = 0.000(2); qz = 1.00(18)

a numerical experiment on molten KCl

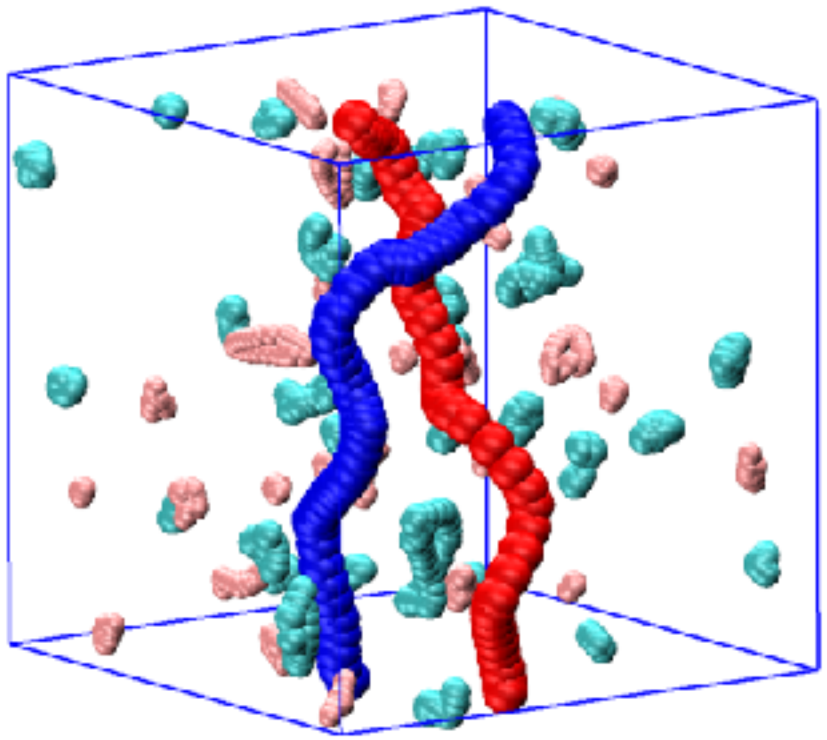


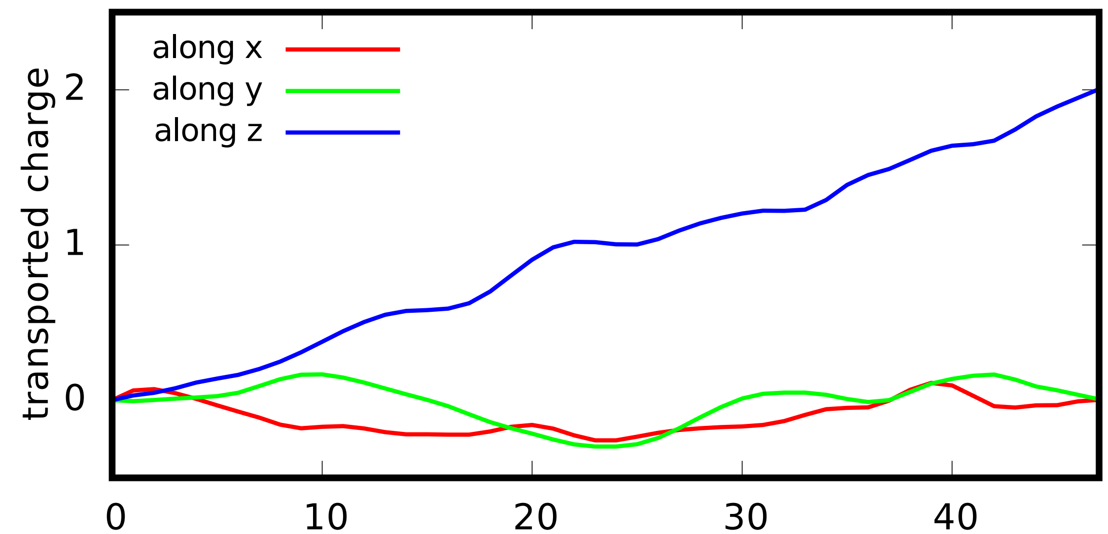


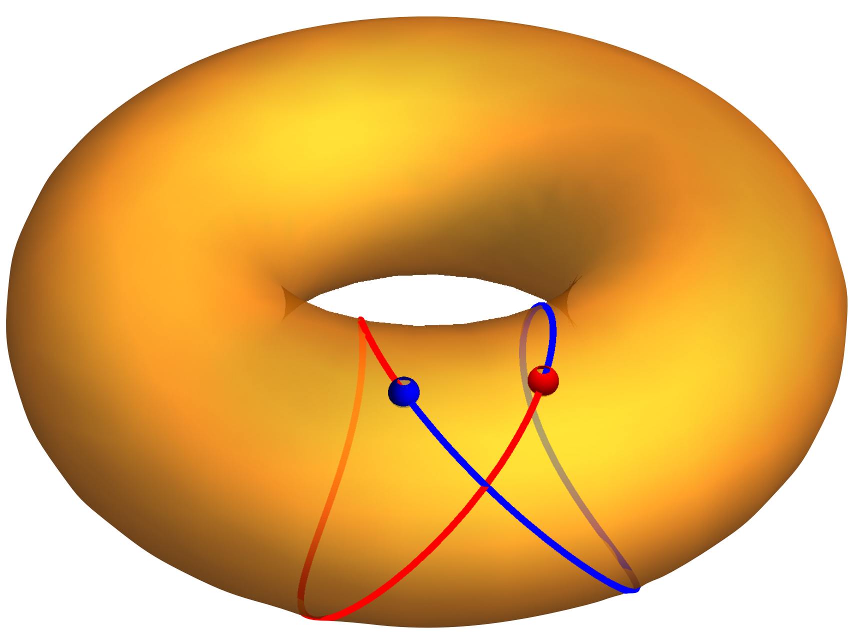


the charges transported by K and Cl around z cancel exactly

a numerical experiment on molten KCl







the exchange of two cations
transports a net charge equal to +2

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}
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- All loops can be shrunk to a point without closing the gap (*strong adiabaticity*);

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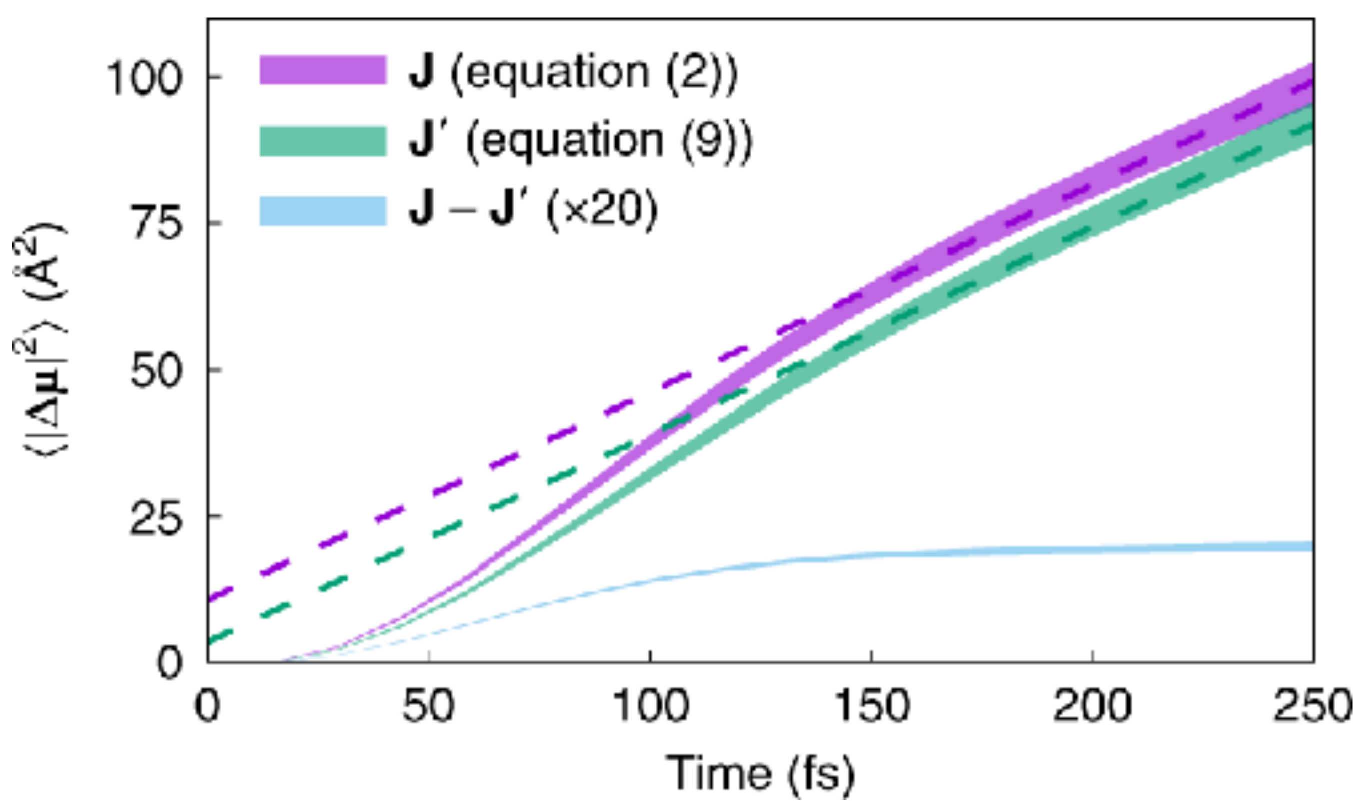
$$q_{i\alpha\beta} = q_{S(i)}\delta_{\alpha\beta}$$

atomic oxidation state

currents from atomic oxidation numbers

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

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



$$\left\langle \left| \int_0^t \mathbf{J}(t')dt' \right|^2 \right\rangle$$

conclusions

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- gauge invariance and topological quantization of charge transport make the electric conductivity of ionic fluids depend on the formal oxidation numbers of the ionic species, via the Green-Kubo formula.

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Topological quantization and gauge invariance of charge transport in liquid insulators

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

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Microscopic theory and quantum simulation of atomic heat transport

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

Federico Grasselli
SISSA

Aris Marcolongo
SISSA, now @IBM Zürich

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