linear-response theory (and numerical simulation) of transport in condensed matter

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Trieste — Italy

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the linear-response theory of transport

$$\mathcal{A} \begin{cases} \text{extensive:} & \mathcal{A} = \int a(\boldsymbol{r})\, d\boldsymbol{r} \\ \text{conserved:} & \dot{a}(\boldsymbol{r}, t) + \nabla \cdot \boldsymbol{j}(\boldsymbol{r}, t) = 0 \end{cases}$$

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$$\boldsymbol{J} = \frac{1}{\Omega} \int \boldsymbol{j}(\boldsymbol{r}) d\boldsymbol{r} \qquad \boldsymbol{F} = \frac{1}{\Omega} \int \nabla \frac{\partial S}{\partial A} d\boldsymbol{r}$$

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$$\boldsymbol{J} = \lambda \boldsymbol{F}$$

charge transport

$$\boldsymbol{J}_{\mathcal{Q}} = \sum_{I} q_I \boldsymbol{V}_I$$

$$\boldsymbol{F}_{\mathcal{Q}} = -\nabla \phi$$

λ = electric conductivity

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$$\boldsymbol{J}_{\mathcal{P}} = \frac{1}{m}\sum_I \mathbf{p}_I \mathbf{p}_I + \frac{\partial E}{\partial \boldsymbol{\epsilon}} + p\boldsymbol{\delta}$$

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$$\lambda \propto \int_0^\infty \langle \boldsymbol{J}(t)\boldsymbol{J}(0)\rangle dt$$

Green-Kubo

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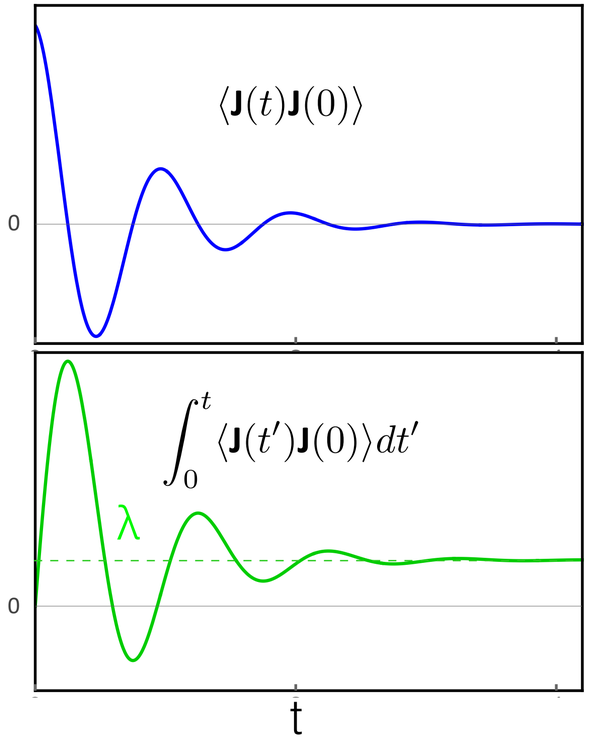
Green-Kubo

$$\lambda \propto \underbrace{\int_0^\infty \langle \boldsymbol{J}(t)\boldsymbol{J}(0)\rangle dt}_{\langle \boldsymbol{J}^2\rangle \tau}$$



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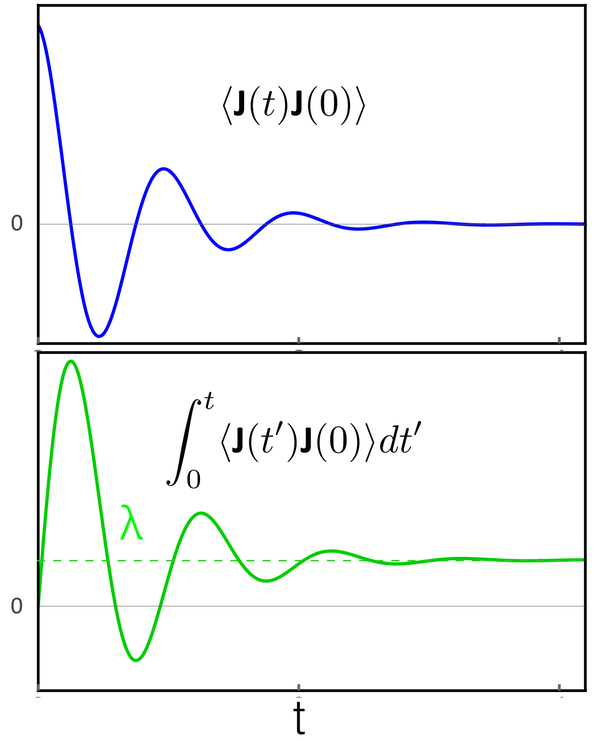
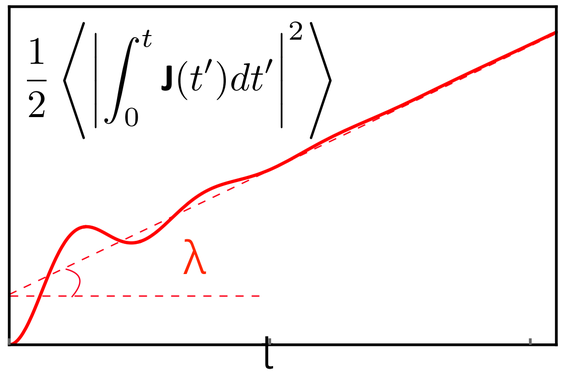


Einstein-Helfand

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



correlation functions from molecular dynamics

$$\lambda \propto \int_0^\infty \langle \boldsymbol{J}(t)\boldsymbol{J}(0)\rangle dt$$

$$\boldsymbol{J}(t) = \boldsymbol{J}(\Gamma_t)$$

$$\Gamma_t = \{q_t, p_t\}$$

$$\dot{q} = \frac{\partial H}{\partial p}$$

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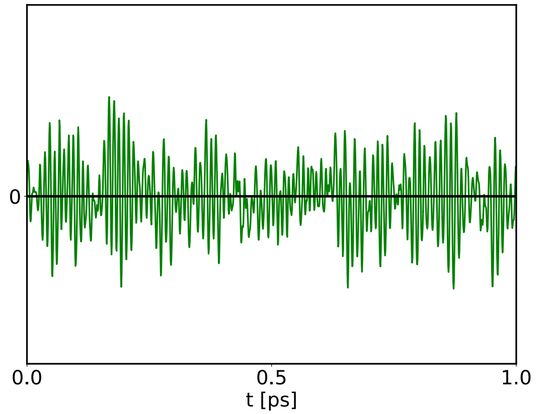

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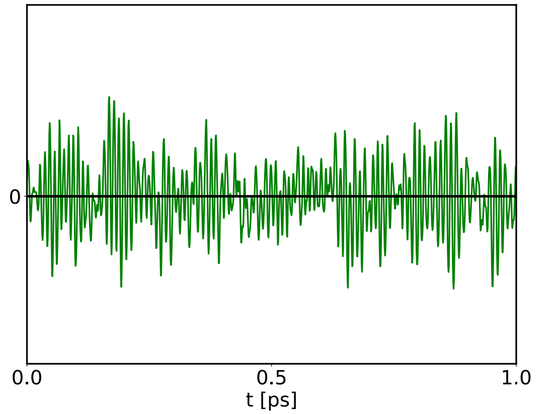
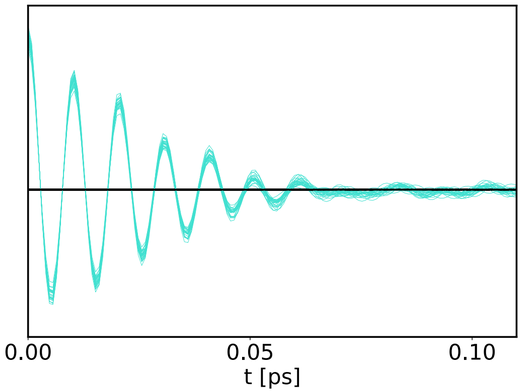


$$\langle \boldsymbol{J}(t)\boldsymbol{J}(0)\rangle = \frac{1}{T-t}\int_0^{T-t} \boldsymbol{J}(t+t')\boldsymbol{J}(t')dt'$$



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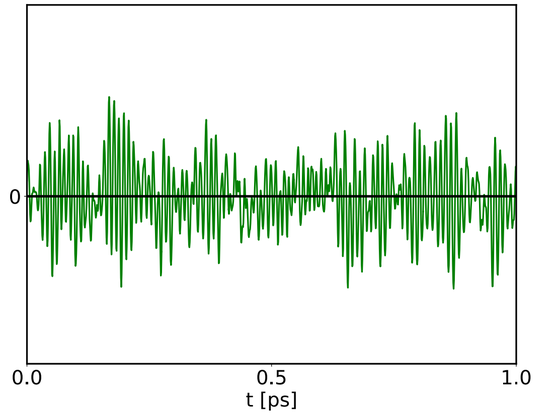

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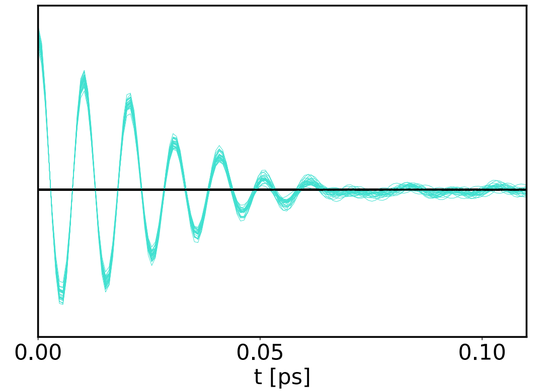
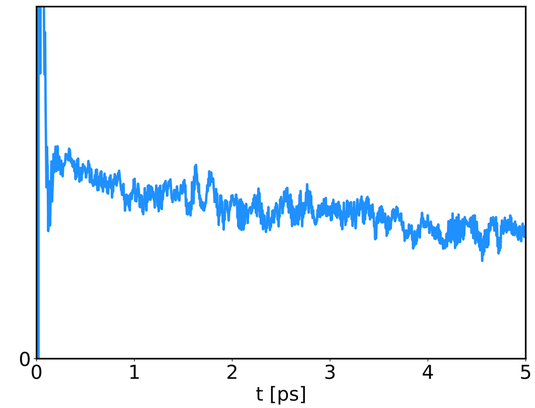


$$\lambda(\tau) = \int_0^\tau \langle \boldsymbol{J}(t)\boldsymbol{J}(0)\rangle dt$$



spectral analysis

$$\boldsymbol{J} = \int_V \boldsymbol{j}(\boldsymbol{r})\, d\boldsymbol{r}$$

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stationarity implies:

$$\langle \tilde{\boldsymbol{J}}_T(\omega)\tilde{\boldsymbol{J}}_T(-\omega')\rangle \sim \begin{cases} 1/T & \text{for } \omega \neq \omega' \\ TS(\omega) & \text{for } \omega = \omega' \end{cases}$$

spectral analysis

$$\lambda = \int_0^\infty \langle \boldsymbol{J}(t)\boldsymbol{J}(0)\rangle dt \qquad S(\omega)$$

$$= \frac{1}{2}\int_{-\infty}^{\infty} \langle \boldsymbol{J}(t)\boldsymbol{J}(0)\rangle e^{i\omega t} dt \Big|_{\omega=0}$$

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sample spectrum
aka "*periodogram*"

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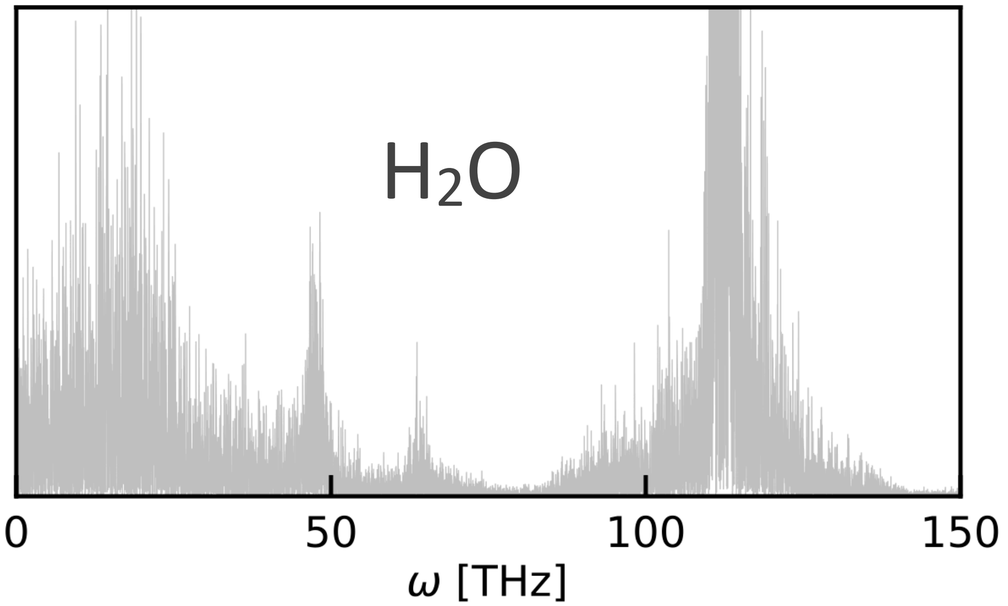

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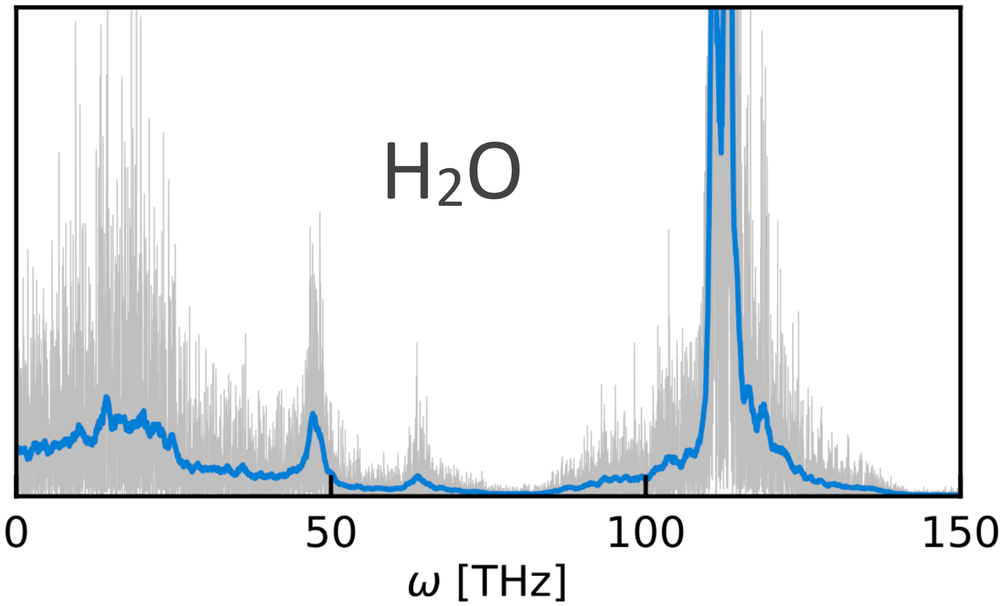

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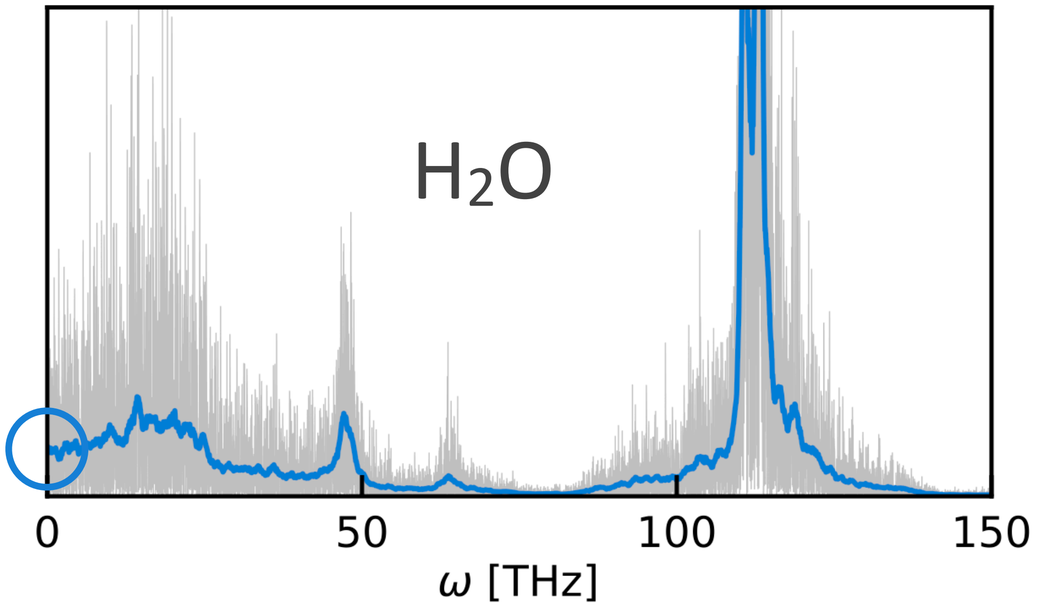

separating flour from bran

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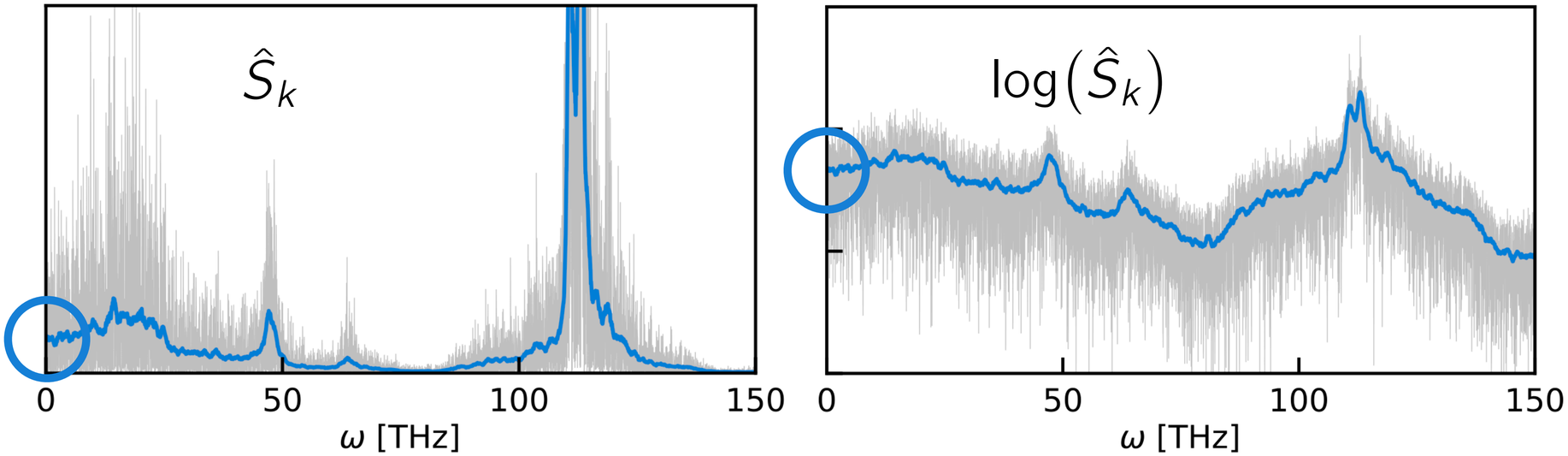

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"cepstral coefficients"
(J.W. Tukey, 1963)

$$\hat{C}_n \doteq \frac{1}{N}\sum_{k=0}^{N-1} \log\left(\hat{S}_k\right) \mathrm{e}^{2\pi i \frac{kn}{N}}$$

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$$\sum_{n=-P^*+1}^{P^*-1} \hat{C}_n e^{2\pi i \frac{kn}{N}} = \log\left(S(\omega_k)\right) + \lambda + \widehat{W}_k$$

$$\widehat{W} \sim \mathcal{N}\left(0, \frac{4P^* - 2}{N}\sigma^2\right)$$

the cepstral cavobulary

The Quefrency Alanysis of Time Series for Echoes: Cepstrum, Pseudo-Autocovariance, Cross-Cepstrum and Saphe Cracking

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spectrum	.....	cepstrum
frequency	.....	quefrency
analysis	.....	alansys
period	.....	repiod
filtering	.....	liftering
phase	.....	saphe

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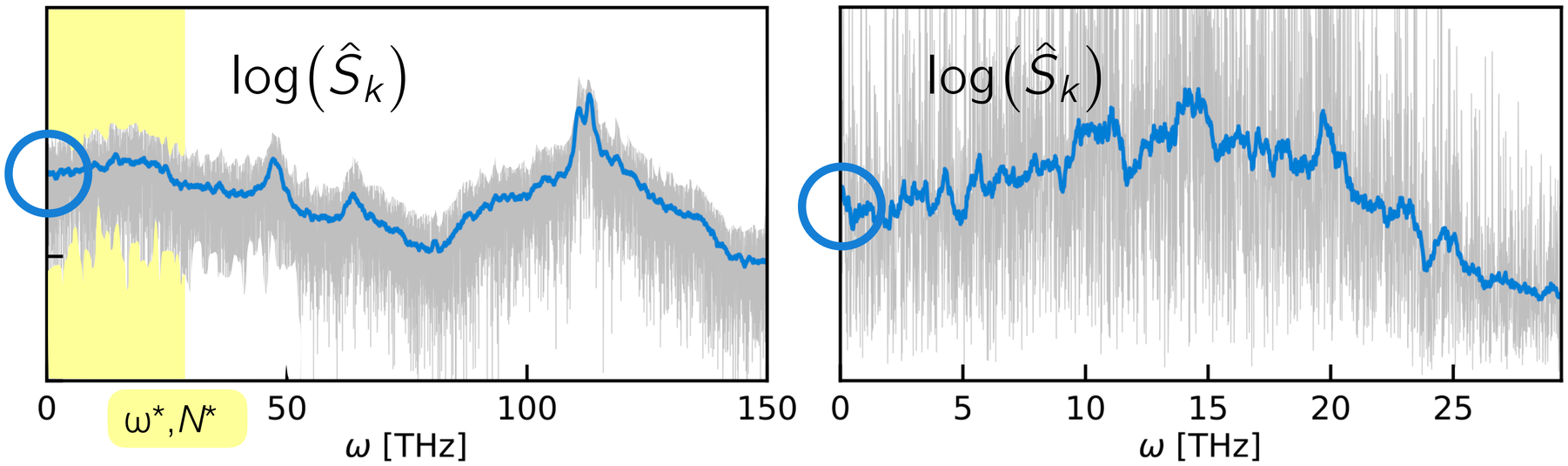

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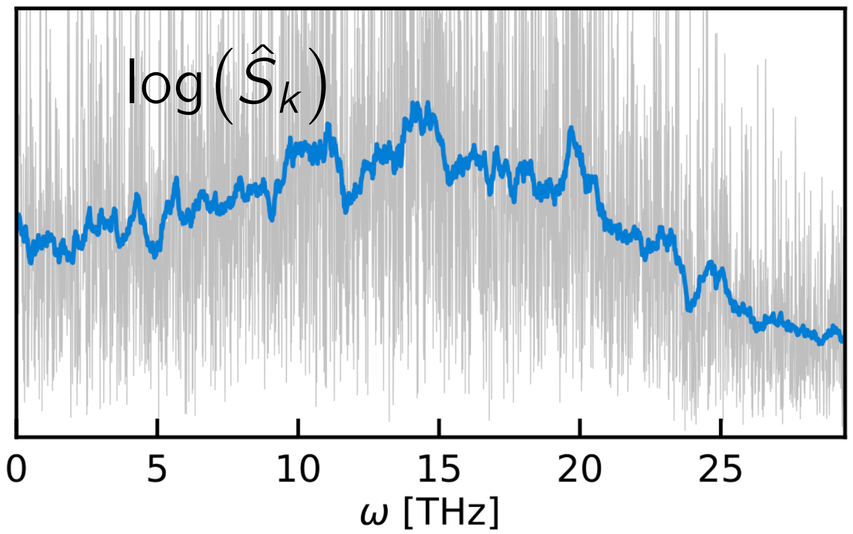

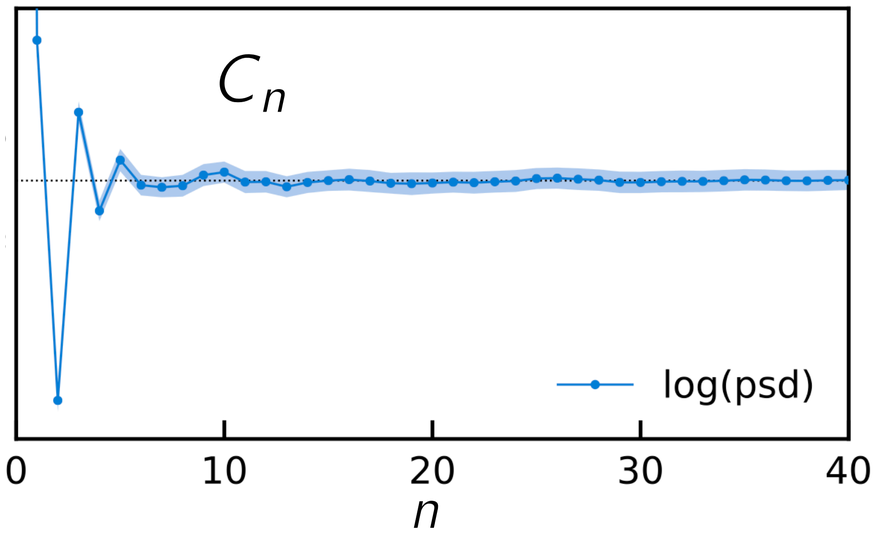

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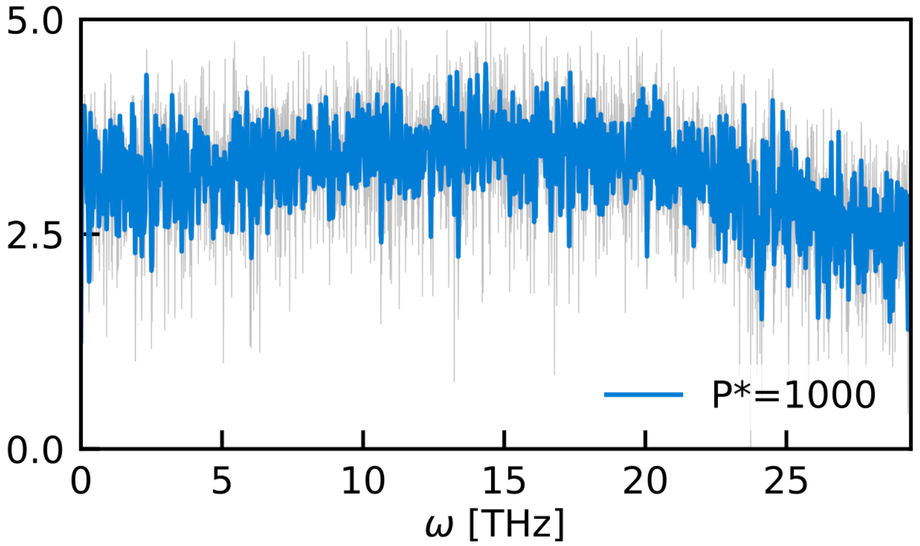

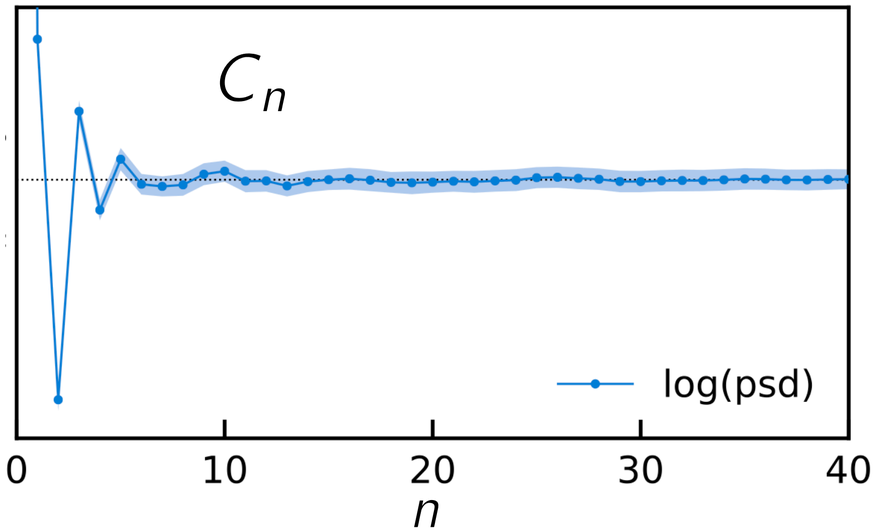

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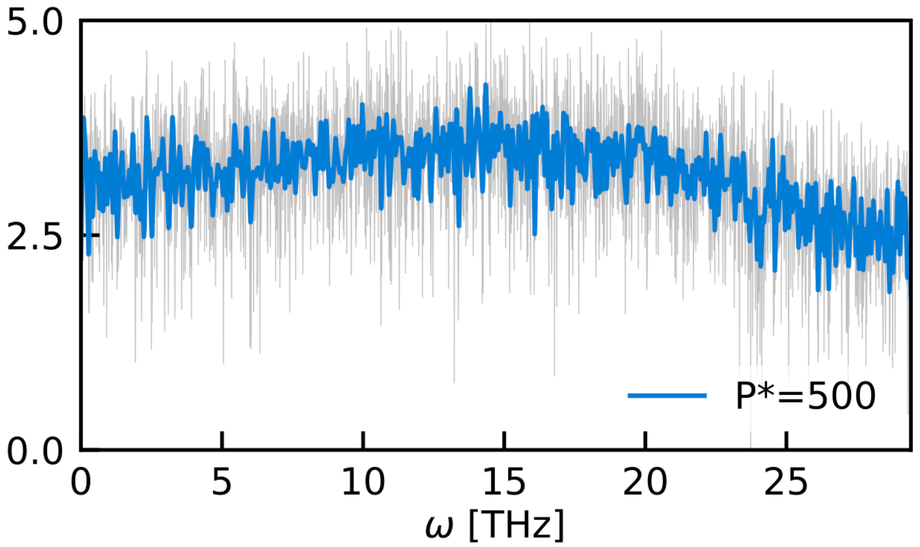

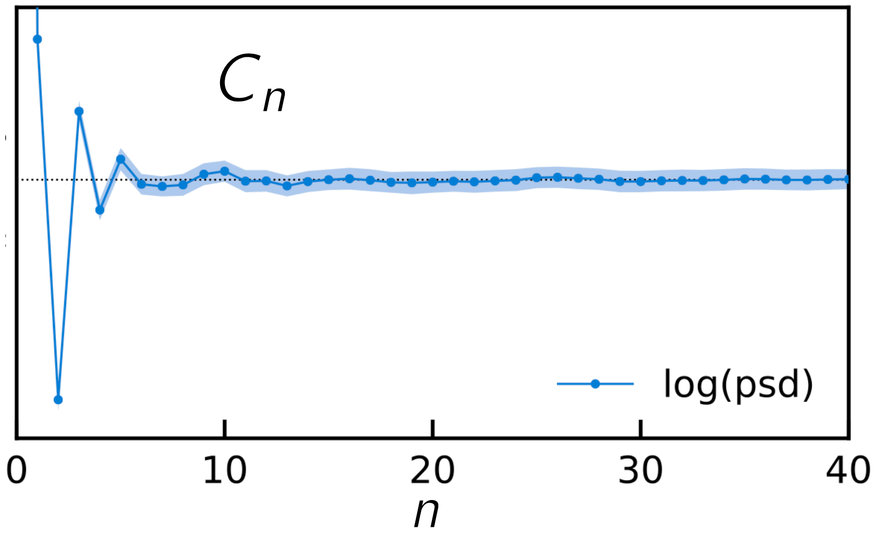

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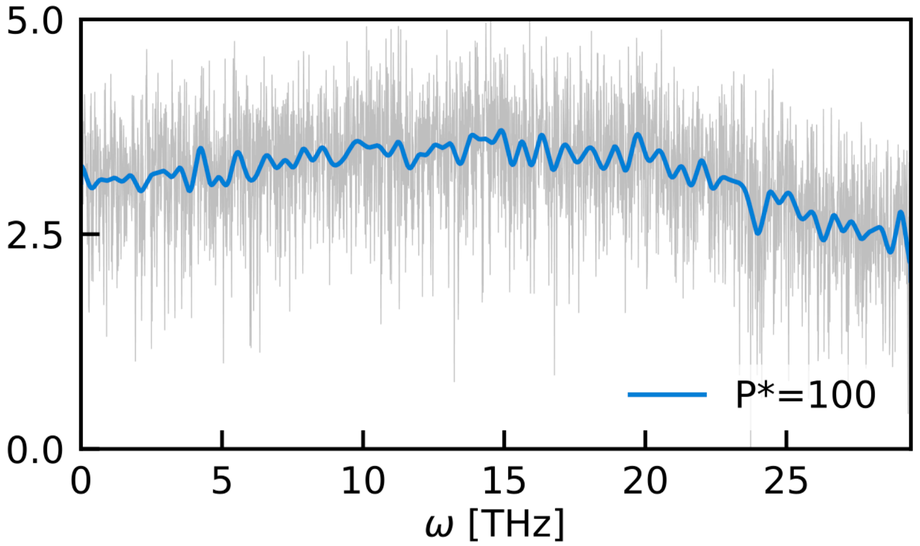

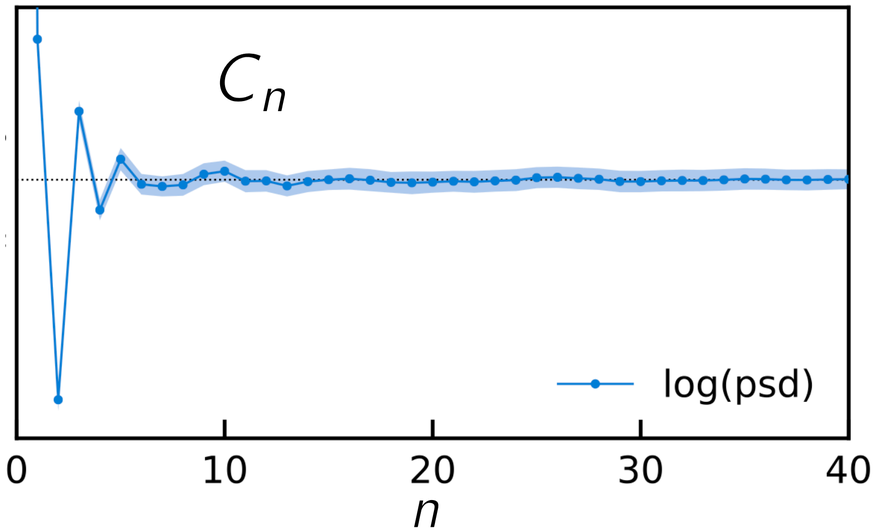

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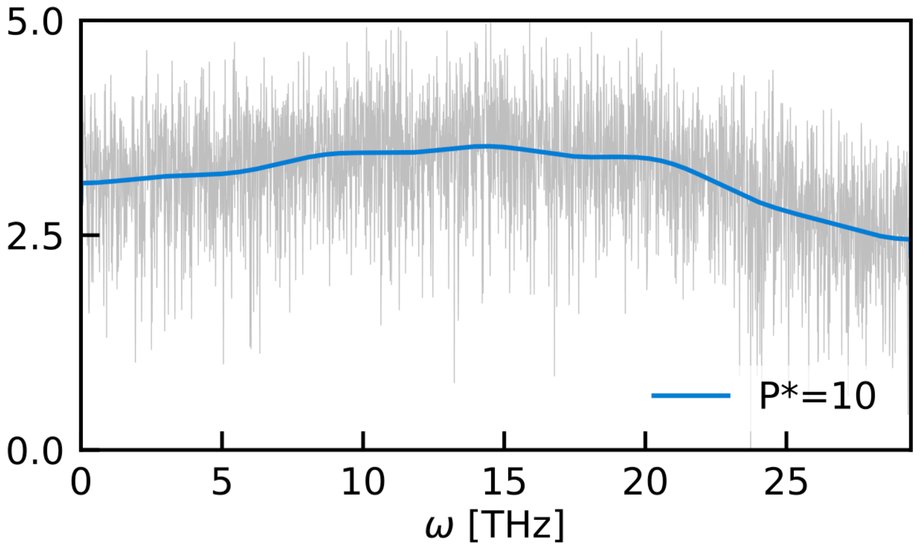

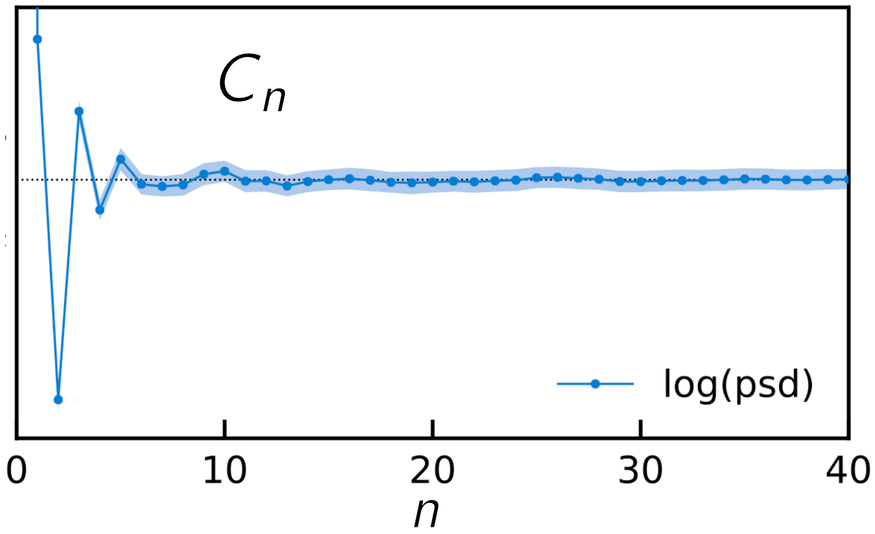

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$$\log\big(S(0)\big) = -\lambda + C_0 + 2\sum_{n=1}^{P^*-1} C_n \pm \sigma\sqrt{\frac{4P^* - 2}{N^*}}$$

constants independent of the time series being sampled

determining the optimal number of cepstral coefficients

cepstral analysis amounts to assuming that the logarithm of the power spectrum can be modelled by a smooth Fourier series:

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AIC: $\alpha = 2$

checking normality

$$\eta = \frac{V}{k_B T} \int_0^\infty \langle \sigma_s(t) \sigma_s(0) \rangle dt$$

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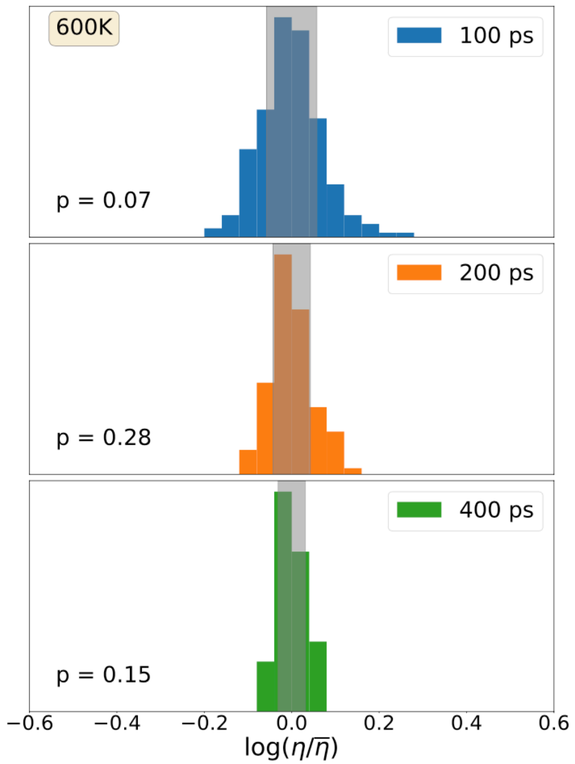
viscosity of DeepMD water computed for different temperatures and using trajectory segments of different lengths



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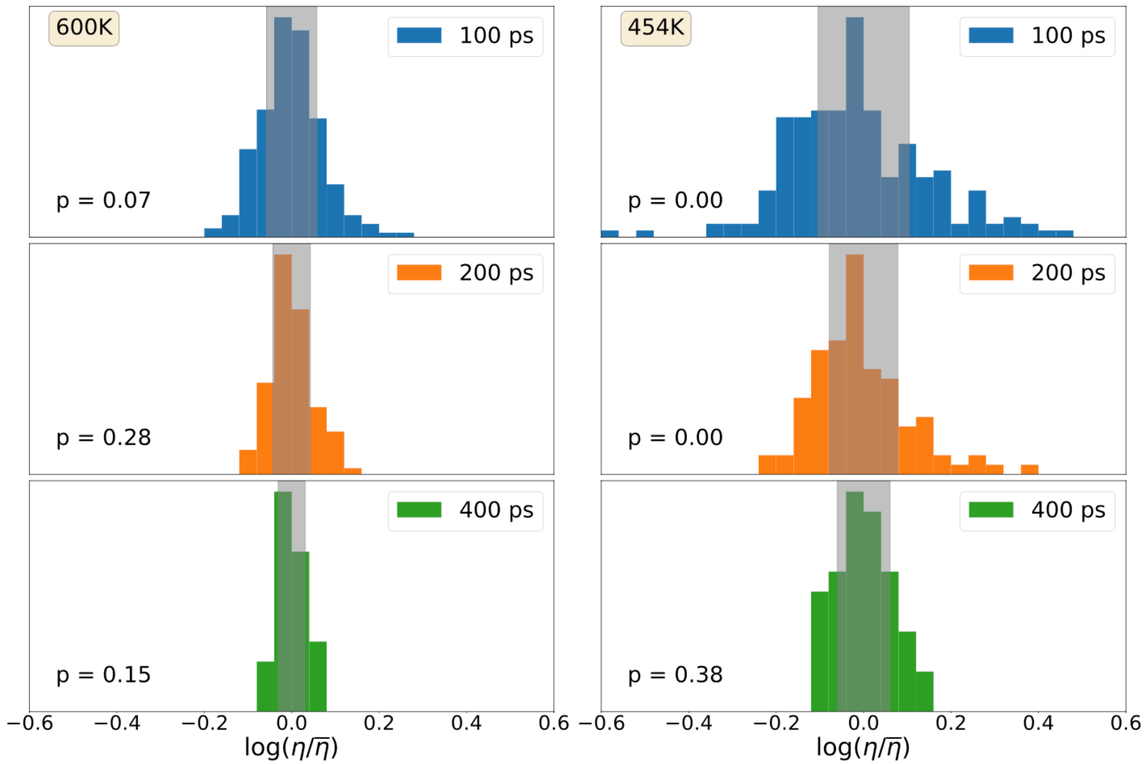

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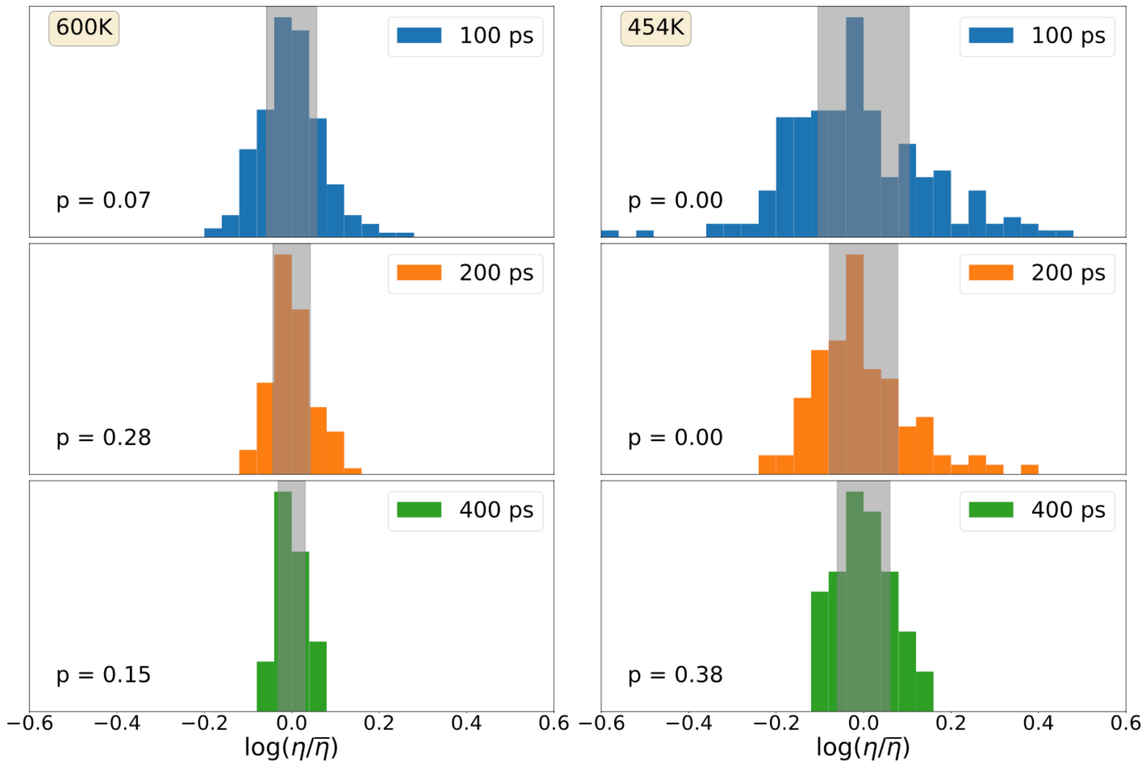

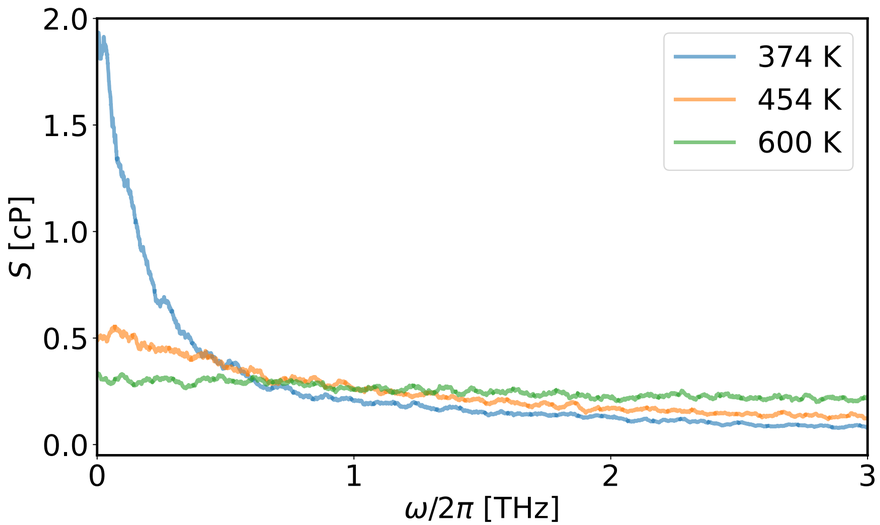

hurdles toward an ab initio Green-Kubo theory

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

PRL **104,** 208501 (2010) PHYSICAL REVIEW LETTERS week ending 21 MAY 2010

Thermal Conductivity of Periclase (MgO) from First Principles

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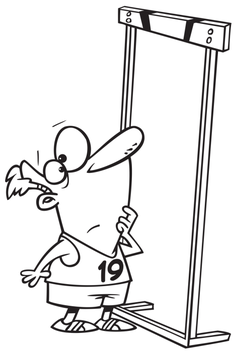

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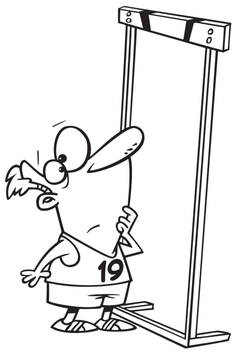

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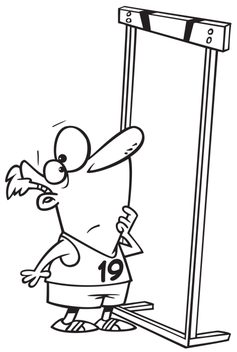
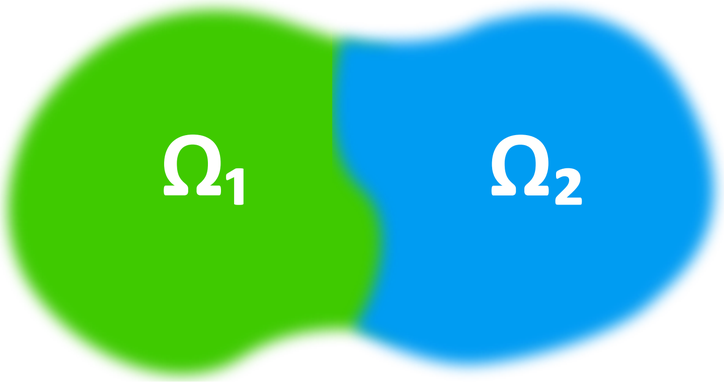


how is it that a formally exact theory of
the electronic ground state cannot predict
all measurable adiabatic properties?

gauge invariance of transport coefficients

energy is extensive



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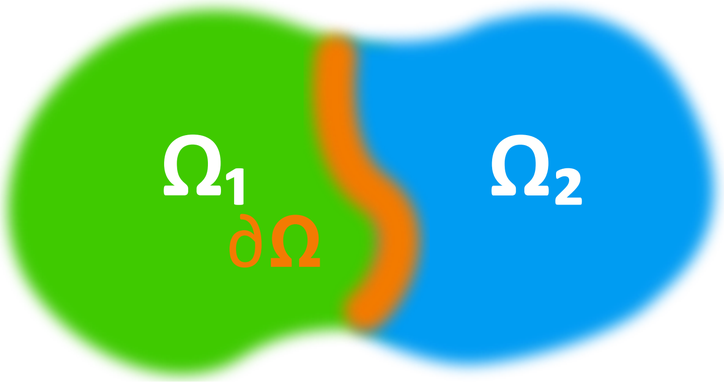

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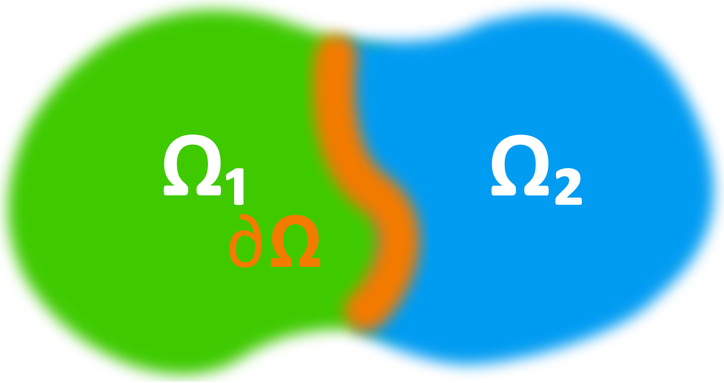

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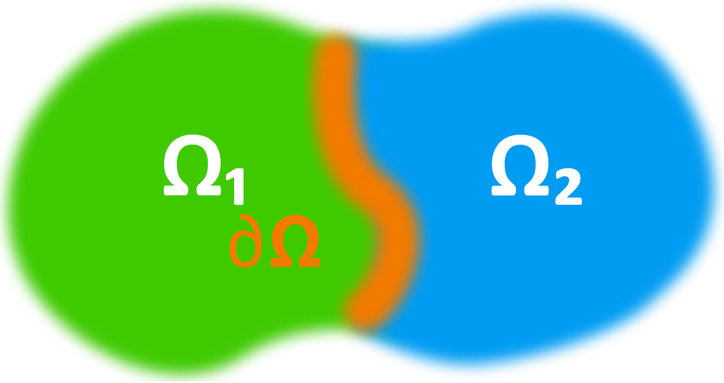

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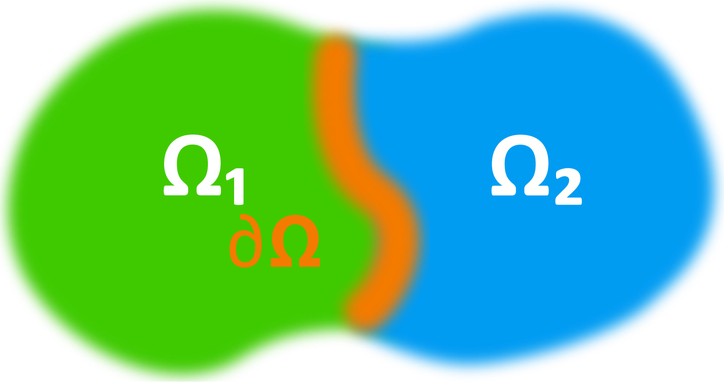

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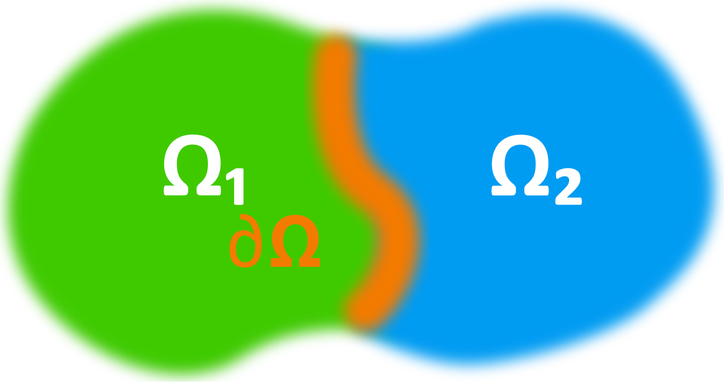

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gauge invariance $\quad e'(\mathbf{r}) = e(\mathbf{r}) - \nabla \cdot \mathbf{p}(\mathbf{r})$

energy conservation $\quad \dot{e}(\mathbf{r}, t) = -\nabla \cdot \mathbf{j}(\mathbf{r}, t)$

gauge invariance of transport coefficients

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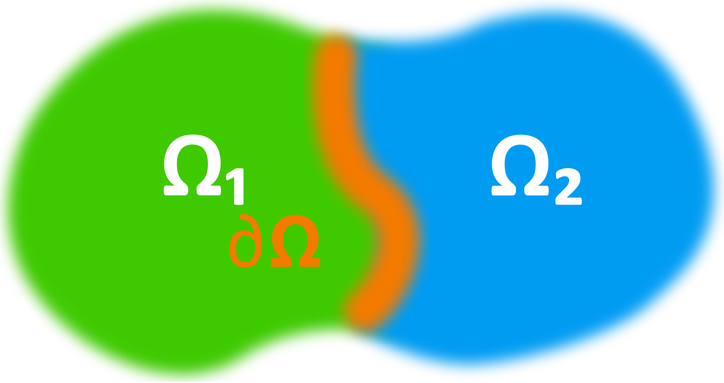

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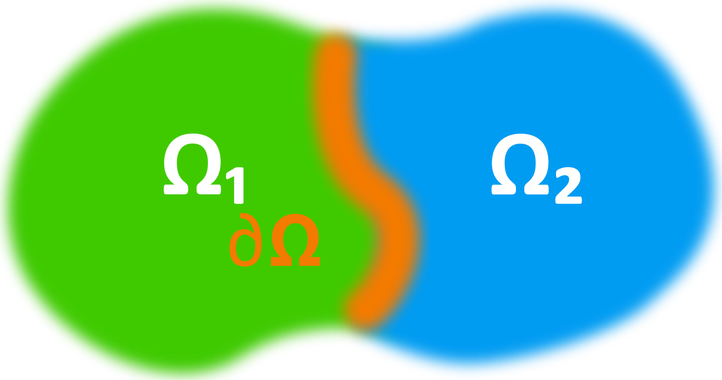

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gauge invariance of transport coefficients

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

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

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Microscopic theory and quantum simulation of atomic heat transport

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

gauge invariance of heat transport

PRL **104,** 208501 (2010) PHYSICAL REVIEW LETTERS week ending 21 MAY 2010

Thermal Conductivity of Periclase (MgO) from First Principles

Stephen Stackhouse*
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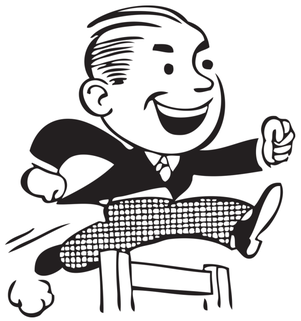
sensitive to the form of the potential. The widely used Green-Kubo relation [14] does not serve our purposes, because in first-principles calculations it is impossible to uniquely decompose the total energy into individual contributions from each atom.

solution:

choose *any* local representation of the energy that integrates to the correct value and whose correlations decay at large distance — the conductivity computed from the resulting current will be *independent* of the chosen representation.



gauge invariance and neural-network potentials

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

$$\sum_I e_I = E \qquad\qquad \boldsymbol{F}_{IJ} = -\frac{\partial e_I}{\partial \boldsymbol{R}_J} = 0 \text{ for } |\boldsymbol{R}_I - \boldsymbol{R}_J| \geq R^*$$

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how come that two currents, ***J*** and ***J'***, derived from different (and *not measurable*) local partitions of the total energy, $\{e_I\}$ and $\{e'_I\}$, both satisfying the above conditions, and hence equally acceptable, result in the same *measurable* value of the heat conductivity?

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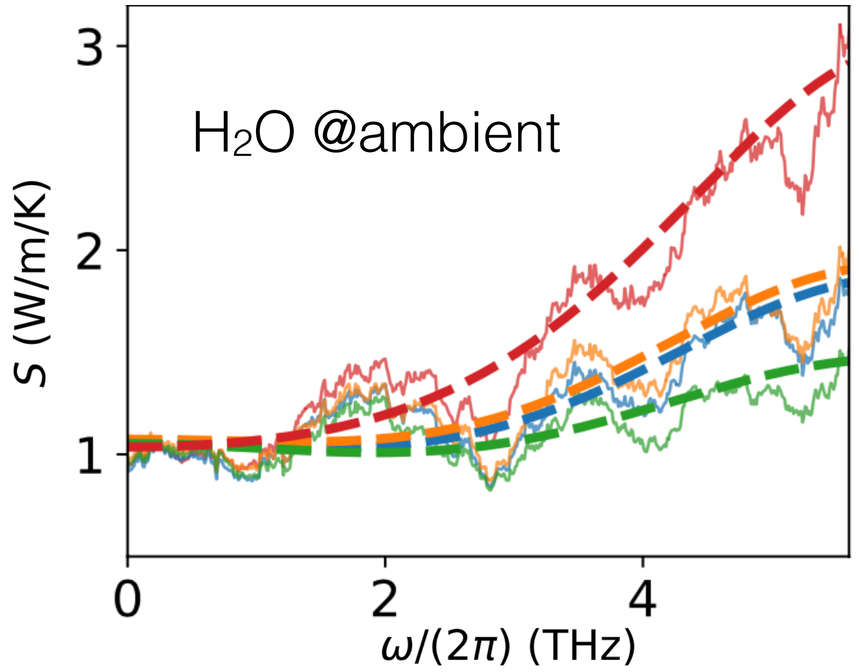

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- the straightforward application of the Green-Kubo theory of linear response to *ab initio* molecular dynamics is numerically challenging, in that it would require sampling trajectories of several nano-seconds;
- cepstral analysis provides a rigorous and practical means of exploiting the information on the spectral properties of the current being sampled, to evaluate transport coefficients and their statistical uncertainties with MD simulations of the order of a few hundred ps.

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PHYSICAL REVIEW LETTERS 122, 255901 (2019)

Theory and Numerical Simulation of Heat Transport in Multicomponent Systems

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PHYSICAL REVIEW B

covering condensed matter and materials physics

Heat transport in liquid water from first-principles and deep neural network simulations

Davide Tisi, Linfeng Zhang, Riccardo Bertossa, Han Wang, Roberto Car, and Stefano Baroni

Phys. Rev. B **104**, 224202 – Published 13 December 2021

npj | computational materials

Viscosity in water from first-principles and deep-neural-network simulations

Cesare Malosso, Linfeng Zhang, Roberto Car, Stefano Baroni ✉ & Davide Tisi

npj Computational Materials **8**, Article number: 139 (2022) | Cite this article

SCIENTIFIC REPORTS

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Accurate thermal conductivities from optimally short molecular dynamics simulations

Loris Ercole[1], Aris Marcolongo[2] & Stefano Baroni[1]

Heat Transport in Insulators from Ab Initio Green-Kubo Theory

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Stefano Baroni, Riccardo Bertossa, Loris Ercole, Federico Grasselli, and Aris Marcolongo

W. Andreoni, S. Yip (eds.), *Handbook of Materials Modeling*,
https://doi.org/10.1007/978-3-319-44680-6_12

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arXiv > physics > arXiv:2202.11571

Physics > Computational Physics

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SporTran: a code to estimate transport coefficients from the cepstral analysis of (multivariate) current time series

Loris Ercole, Riccardo Bertossa, Sebastiano Bisacchi, Stefano Baroni

Computer Physics Communications, in press

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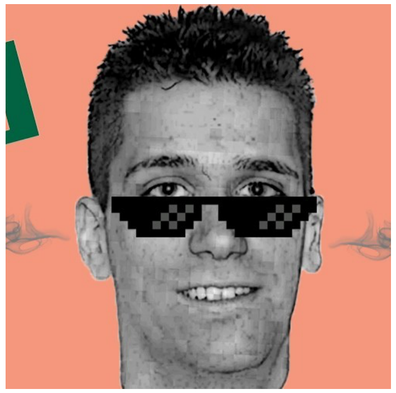

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