Power spectra and the Fourier Transform

Lecture at the Pencil Code School, CERN

Isak Stomberg, Oct. 21, 2025

Overview

Continuum

Intro

Two-point correlation function $\xi(\mathbf{r})$

Fourier transform

Power Spectrum $P(\mathbf{k})$

Power Spectral density $\mathscr{P}(k)$

Variance

A “formal” estimator for $P(\mathbf{k})$

Lattice

Consequences of lattice discretization and periodic boundary conditions

Discrete Fourier Transform

Power Spectrum on the lattice

Introduction

- A large number of physical **systems exhibit stochasticity** and **are random realizations:** Examples include turbulent fluids, density perturbations, gravitational wave backgrounds, and acoustic noise fields.

- To quantify such seemingly random systems, it is generally **not meaningful** to **study individual realizations** (i.e., specific field configurations), **but** rather their **statistical properties**.

- In particular, we are often interested in **understanding** how a statistical **quantity** depends on the **scale** of interest - for instance, a **length** scale r or wavenumber k, or a time **duration** τ or frequency f.

- This allows us to answer **questions** such as *"on what scale are density perturbations largest?"* or *"at what slope does the noise power decay at high frequencies?"*

- The aim of this lecture is to build up the concept of a **power spectrum**: starting from **real-space correlations**, moving to their **Fourier-space representation**, and finally to the **discrete periodic lattice** relevant for numerical simulations.

Continuum

Two-point Correlation Function

- Consider a **statistically homogeneous** and **stochastic scalar field** $f(\mathbf{x})$ with zero mean, $\langle f(\mathbf{x}) \rangle = 0$
- The most basic **statistical measure** of **correlations** is the **two-point correlation function:**

$$\xi(\mathbf{r}) = \langle f(\mathbf{x}) f(\mathbf{x} + \mathbf{r}) \rangle$$

  where $\langle \cdot \rangle$ denotes **ensemble average**, i.e. an average over all realizations, and ξ depends only on $\mathbf{r}$ from homogeneity.

- Note that we usually do **not have access** to an **ensemble** of universes or simulations.
- If the system is assumed to be **statistically homogeneous** (translation invariant), we can **replace** the **ensemble average by** a **spatial average** over the simulation domain (ergodicity):

$$\xi(\mathbf{r}) = \frac{1}{V} \int_V d^3x \, f(\mathbf{x}) f(\mathbf{x} + \mathbf{r})$$

- For **isotropic statistics**, the correlation function **depends** only on the **magnitude** $r = |\mathbf{r}|$, $\xi(\mathbf{r}) = \xi(r)$

Fourier Transform

Fourier transform

$$\tilde{f}(\mathbf{k}) = \int_{\mathbb{R}^3} d^3x\, f(\mathbf{x})\, e^{-i\mathbf{k}\cdot\mathbf{x}},$$

Inverse Fourier transform

$$f(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3}\, \tilde{f}(\mathbf{k})\, e^{+i\mathbf{k}\cdot\mathbf{x}}$$

We will use this to obtain a definition of the power spectrum.

Power Spectrum

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- Consider the ensemble average $\langle \tilde{f}(\mathbf{k}) \tilde{f}^*(\mathbf{k}') \rangle$

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Power Spectrum

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Change of variables:
set $\mathbf{r} = \mathbf{x}' - \mathbf{x},\ \mathbf{x}' = \mathbf{x} + \mathbf{r}$

$$= \int d^3x \int d^3r\, e^{-i\mathbf{k}\cdot\mathbf{x}}\, e^{+i\mathbf{k}'\cdot(\mathbf{x}+\mathbf{r})}\, \xi(\mathbf{r})$$

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Identify delta, use that $\xi(-\mathbf{r}) = \xi(\mathbf{r})$, define $P(\mathbf{k})$ as Fourier transform of $\xi(\mathbf{r})$

$$= (2\pi)^3 \delta^{(3)}(\mathbf{k} - \mathbf{k}') \underbrace{\int d^3r \, e^{-i\mathbf{k}\cdot\mathbf{r}} \xi(\mathbf{r})}_{P(\mathbf{k})} .$$

Different modes are uncorrelated

Power Spectrum

Fourier transform

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- Define the Power Spectrum: $\left\langle \tilde{f}(\mathbf{k})\tilde{f}^*(\mathbf{k}')\right\rangle = (2\pi)^3 \delta^{(3)}(\mathbf{k}-\mathbf{k}')\, P(\mathbf{k})$

Interpretation and Variance

- The **two-point function** and **Power spectrum** are **Fourier pairs:**

$$\langle f(\mathbf{x}) f(\mathbf{x}+\mathbf{r})\rangle = \xi(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} P(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{r}}, \quad P(\mathbf{k}) = \int d^3r\, \xi(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}}$$

- At zero separation $\mathbf{r} = \mathbf{0}$: $\langle f^2\rangle \equiv \xi(0) = \int \frac{d^3k}{(2\pi)^3} P(\mathbf{k})$

- **Interpretation**:
  The power spectrum measures the contribution to the total variance per 3D Fourier element.

Power spectral density

- If the **statistics** of the field are **isotropic**, then the power spectrum depends only on the **magnitude** of the wavevector: $P(\mathbf{k}) = P(k), \qquad k = |\mathbf{k}|$

- Switch to spherical coordinates in k-space: $d^3k = k^2\, dk\, d\Omega\,, \quad \int d\Omega \;=\; 4\pi$

- At zero separation $\mathbf{r} = 0$:

$$\begin{aligned}\langle f^2 \rangle &= \int \frac{d^3k}{(2\pi)^3} P(k) \\ &= \int_0^\infty \int d\Omega \, \frac{k^2\, dk}{(2\pi)^3} P(k) \\ &= \int_0^\infty \frac{4\pi k^2}{(2\pi)^3} P(k)\, dk. \equiv \int_0^\infty \mathcal{P}(k)\, dk.\end{aligned}$$

Power Spectral Density

$$\mathcal{P}(k) = \frac{k^2}{2\pi^2} P(k)$$

- **Interpretation of the Power Spectral Density**:

  The power spectral density measures the contribution to the total variance per k.

  This is a more natural quantity, since it *tells us something about the variance at a certain scale.*

A formal estimator

- Suppose we set $\mathbf{k} = \mathbf{k}'$ (ill-defined): $\left\langle |\tilde{f}(\mathbf{k})|^2 \right\rangle = (2\pi)^3 \delta^{(3)}(0)\, P(\mathbf{k})$
- We may "**interpret**" this using that, **formally**, $\delta^{(3)}(0) = \frac{V_{\mathbb{R}}}{(2\pi)^3}$ so that: $P(\mathbf{k}) \sim \frac{\left\langle |\tilde{f}(\mathbf{k})|^2 \right\rangle}{V_{\mathbb{R}}}$
- If we assume **isotropy**, then $P(\mathbf{k}) = P(k)$, and we can construct an **estimator** for $P(k)$ by computing the **average over infinitesimal spherical shells** of radius k:

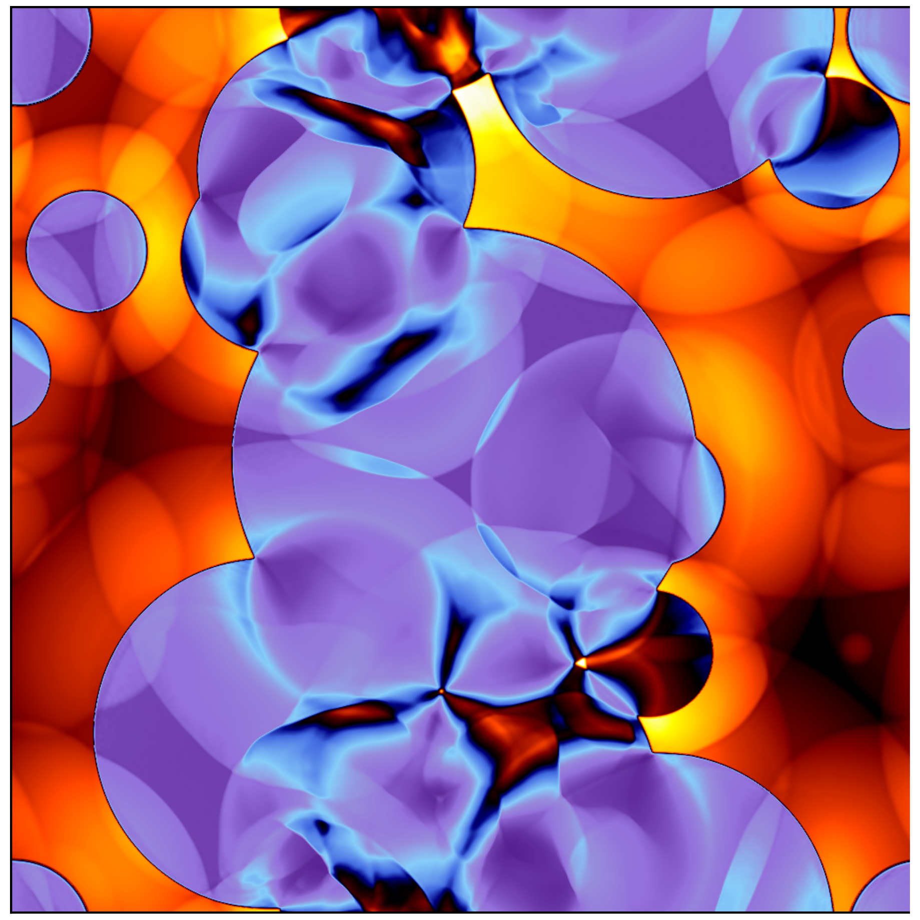
$$P(k) \;\approx\; \frac{1}{4\pi} \int d\Omega_{\hat{\mathbf{k}}} \, \frac{|\tilde{f}(\mathbf{k})|^2}{V_{\mathbb{R}}} \Bigg|_{|\mathbf{k}|=k} .$$

- *This expression is not well defined due to the infinite volume factor $V_{\mathbb{R}}$, but it is structurally interesting, since, as we shall soon see, we will be able to replace it with the finite simulation volume V when moving to the lattice.*

Simulations and the Lattice

Typical simulation

Finite simulation domain
$V = L^3$



Discretized lattice.
N^3 sites, $\mathbf{x}_\mathbf{m} = \Delta x\, \mathbf{m}$

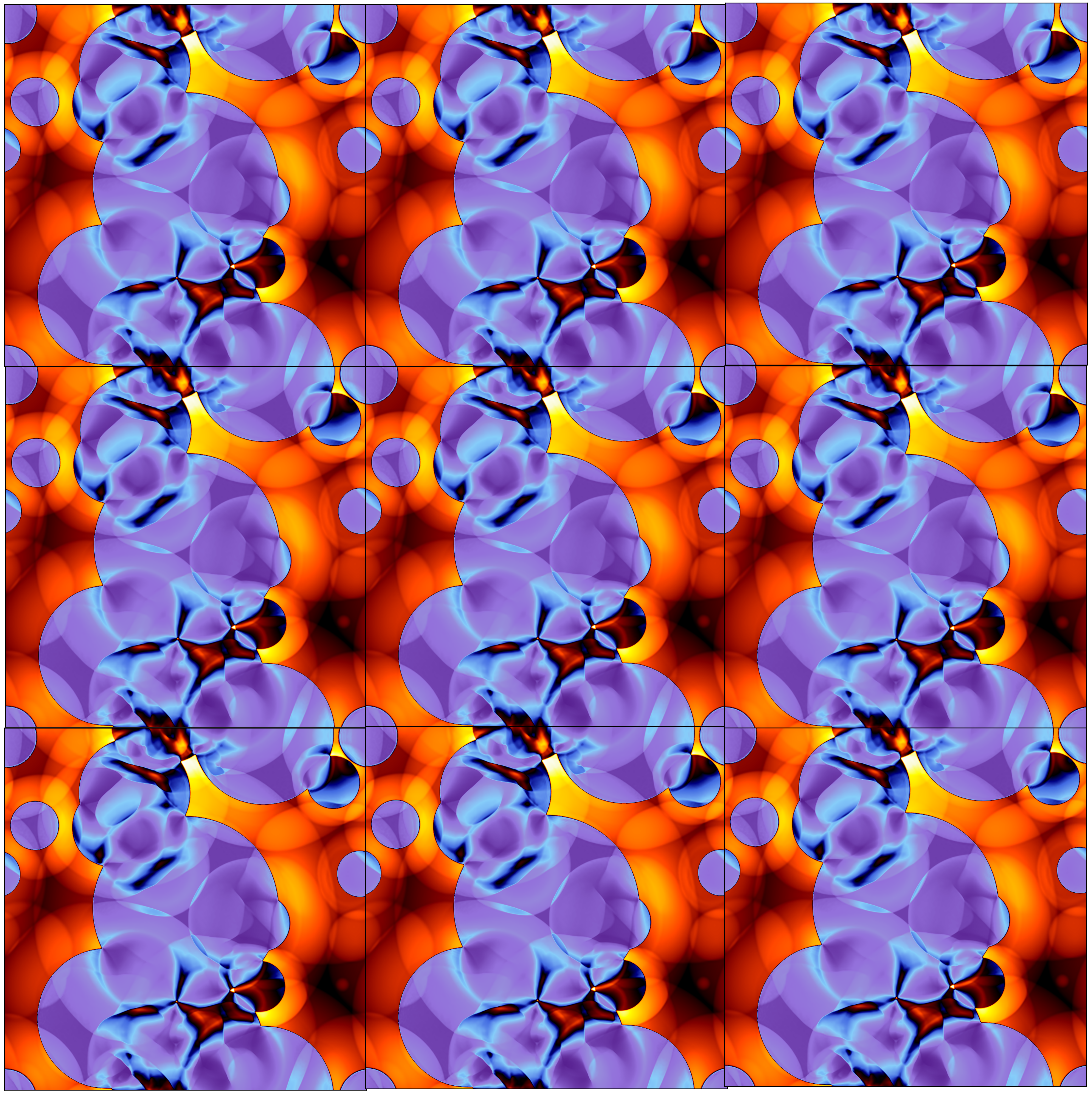
Periodic boundary conditions

The full universe is

an infinite space

of discretized

periodic domains



Consequences?

Consequences of lattice discretization

- Simulations: consider periodic cubic domains $V = [0, L)^3$ with N^3 lattice sites
- Lattice sites are reached as: $\mathbf{x}_\mathbf{m} = \Delta x\, \mathbf{m}, \qquad m_i = 0, 1, \ldots, N-1$

- **Periodicity**: $e^{i\mathbf{k}\cdot(\mathbf{x}+L\mathbf{e}_i)} = e^{i\mathbf{k}\cdot\mathbf{x}} \quad \forall\, i,$ which means $e^{ik_iL} = 1 \quad \Rightarrow \quad k_iL = 2\pi n_i, \qquad n_i \in \mathbb{Z}$

  Hence, *allowed wave vectors are discrete:* $\mathbf{k}_\mathbf{n} = \frac{2\pi}{L}\mathbf{n}, \qquad \mathbf{n} = (n_x, n_y, n_z) \in \mathbb{Z}^3$ $\quad \Delta k = \frac{2\pi}{L}$

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- **Discrete sampling on lattice sites:** Two Fourier modes $\mathbf{k}$ and $\mathbf{k}'$ are **indistinguishable** on this **sampling** if $\quad e^{i\mathbf{k}'\cdot\mathbf{x_m}} = e^{i\mathbf{k}\cdot\mathbf{x_m}} \quad \forall\, \mathbf{m}$
- Satisfied when $\quad e^{i(\mathbf{k}'-\mathbf{k})\cdot(\Delta x\,\mathbf{m})} = 1 \quad \forall\, \mathbf{m}$

$$\Rightarrow \quad (\mathbf{k}' - \mathbf{k}) \cdot (\Delta x\, \mathbf{m}) = 2\pi\, (\boldsymbol{\ell} \cdot \mathbf{m}), \qquad \boldsymbol{\ell} \in \mathbb{Z}^3$$

- **Hence**, *the discretely sampled field cannot distinguish between wavevectors separated by integer multiples of* $2\pi/\Delta x = N\Delta k$ *along any axis, and it is sufficient to restrict to* ***one unique set*** *of* N ***independent modes per direction****, for instance* $\quad k_i \in \left[-\frac{\pi}{\Delta x}, \frac{\pi}{\Delta x}\right)$

which can be implemented as

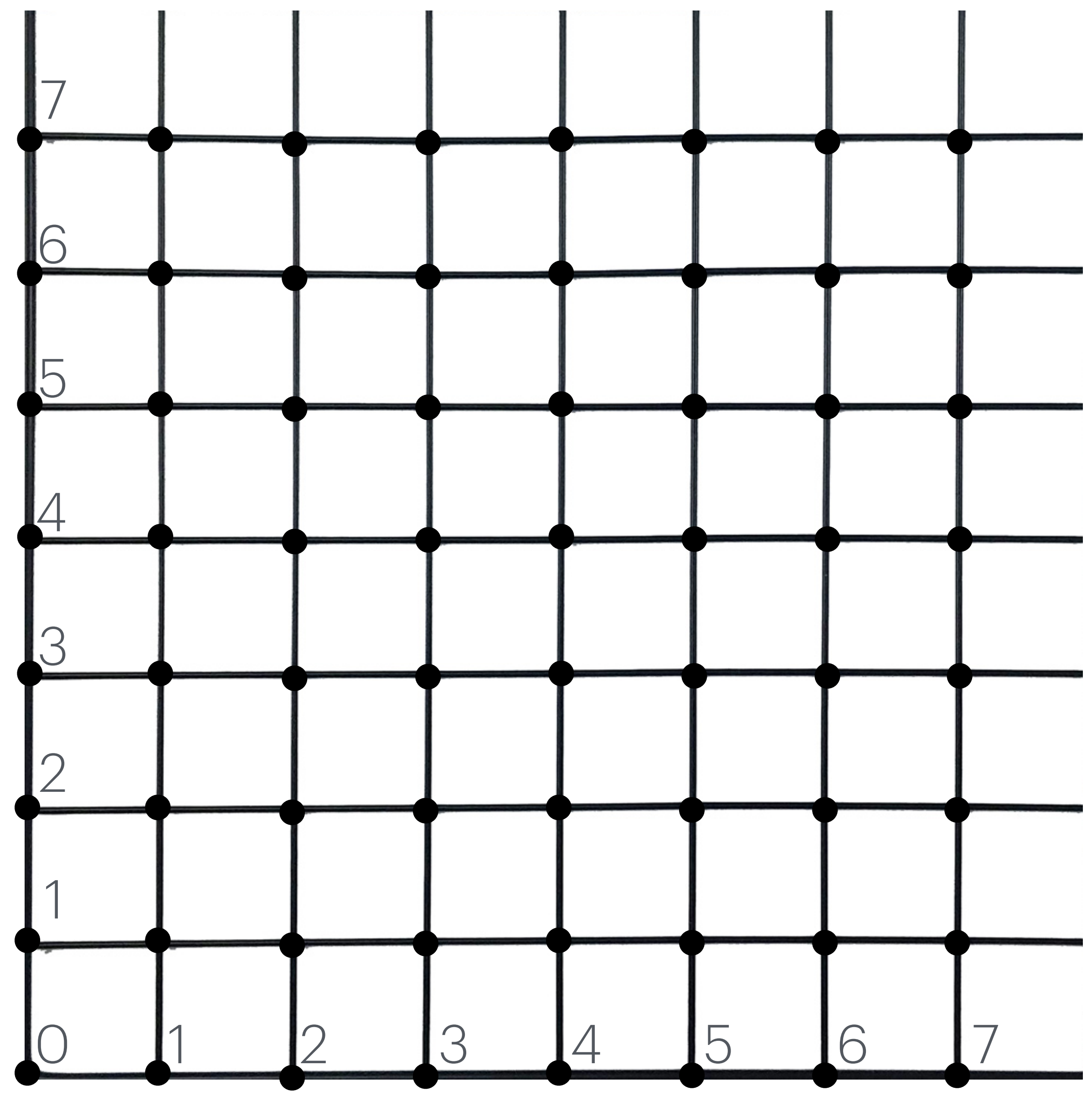
$$k_i(\mathbf{n}) = \frac{2\pi}{L} \times \begin{cases} n_i, & 0 \le n_i \le \lfloor \frac{N}{2} \rfloor, \\ n_i - N, & \lfloor \frac{N}{2} \rfloor < n_i \le N-1, \end{cases} \qquad i \in \{x, y, z\}$$

Lattice and dual lattice

$N = 8$

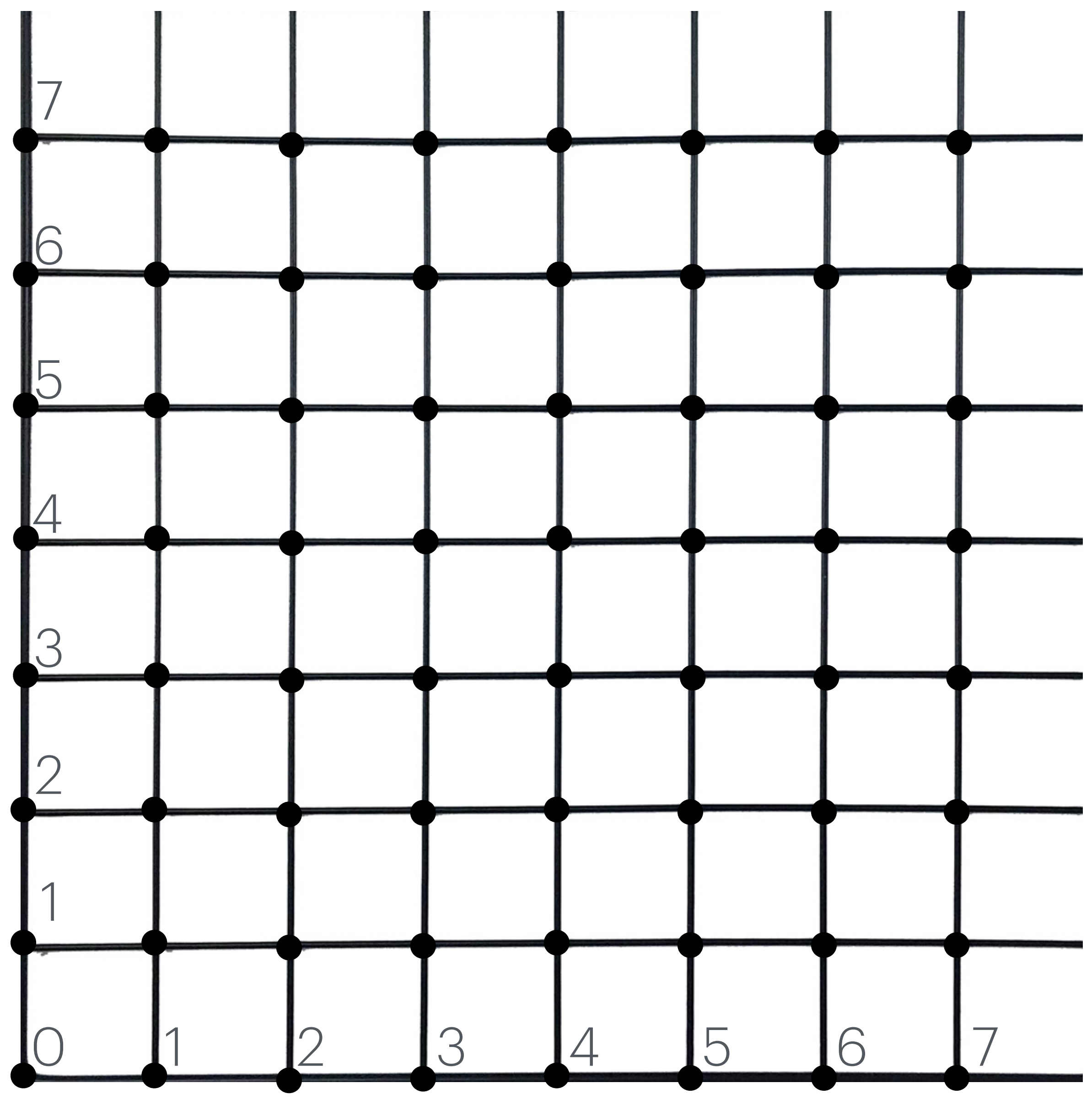
Lattice

$\mathbf{m}$



Dual lattice

$\mathbf{n}$



k-mapping in 2D

$$k_i(\mathbf{n}) = \frac{2\pi}{L} \times \begin{cases} n_i, & 0 \le n_i \le \lfloor \frac{N}{2} \rfloor, \\ n_i - N, & \lfloor \frac{N}{2} \rfloor < n_i \le N-1 \end{cases}$$

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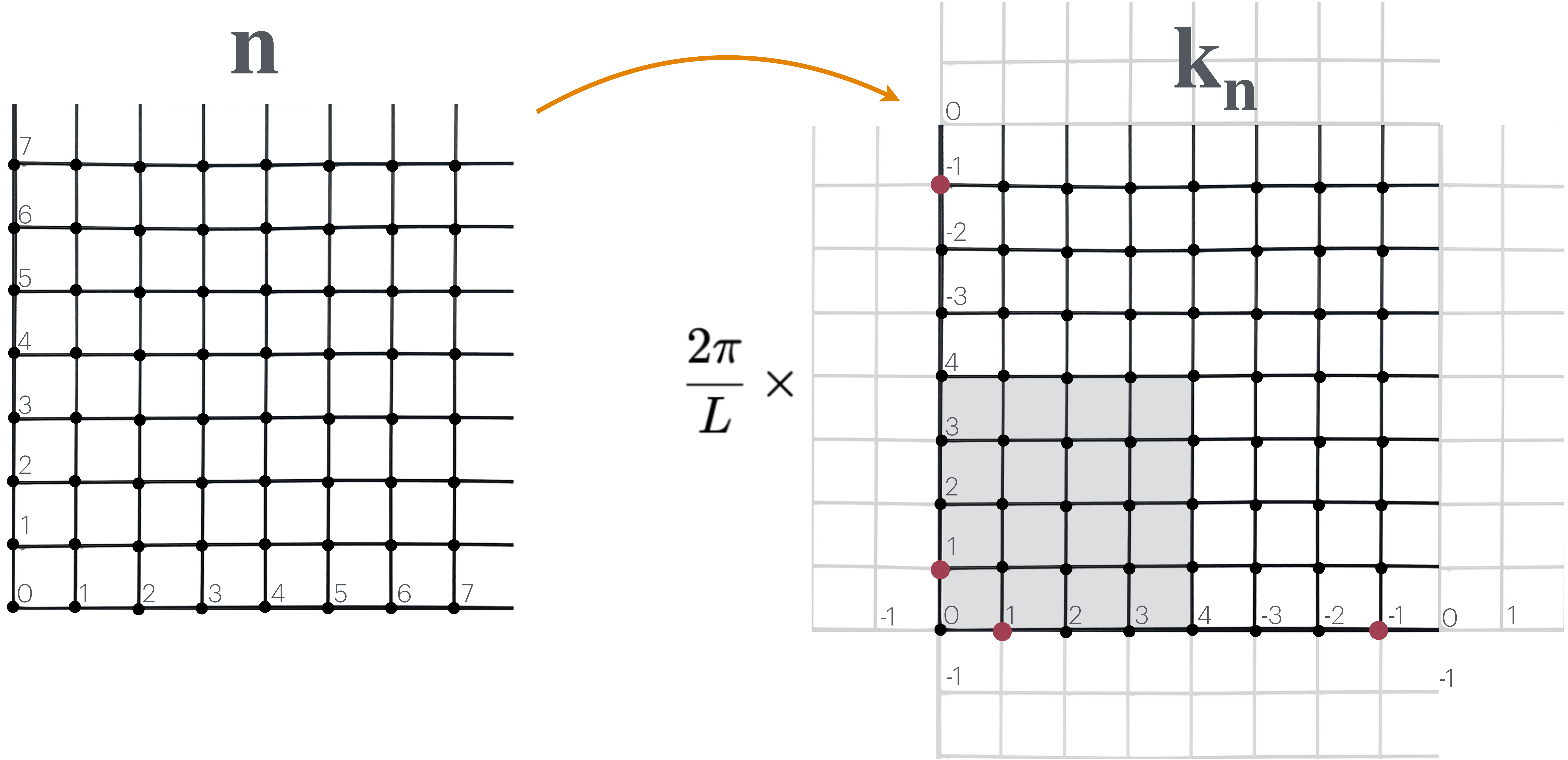

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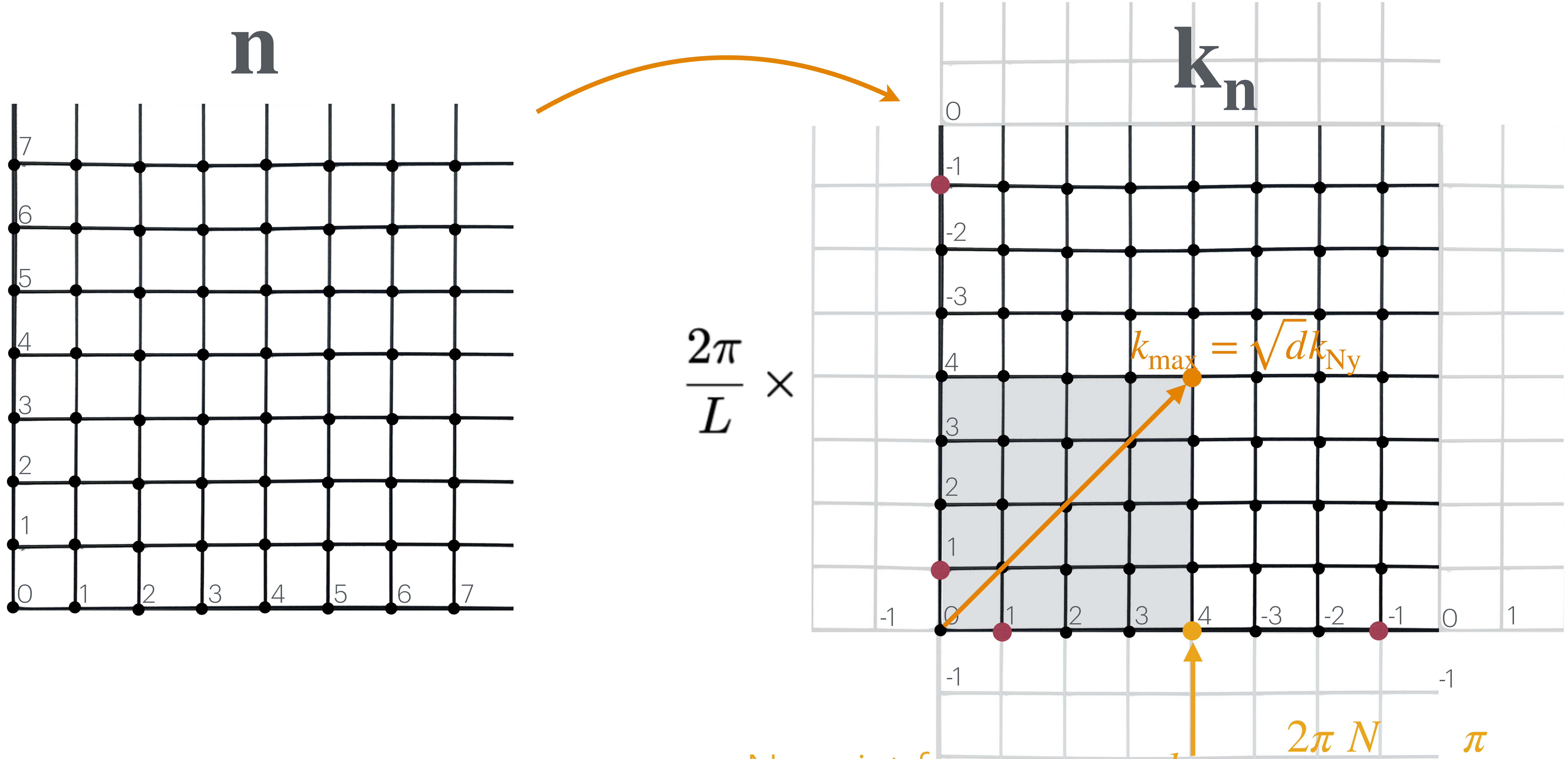

Nyquist frequency: $k_{Ny} = \frac{2\pi}{L}\frac{N}{2} = \frac{\pi}{\Delta x}$

the highest frequency that can be accurately captured in a N-sampled signal

Discrete Fourier Transform

- For some field sampled on discrete lattice sites $f_{\mathbf{m}} \equiv f(\mathbf{x}_{\mathbf{m}})$ with $\mathbf{x}_{\mathbf{m}} = \Delta x\, \mathbf{m}$ the **Discrete Fourier Transform (DFT)** is defined as:

Discrete Fourier transform

$$\tilde{f}_{\mathbf{n}} = \frac{V}{N^3} \sum_{\mathbf{m}\in\mathcal{N}} f_{\mathbf{m}}\, e^{-i\frac{2\pi}{N}\,\mathbf{n}\cdot\mathbf{m}}$$

Inverse transform

$$f_{\mathbf{m}} = \frac{1}{V} \sum_{\mathbf{n}\in\mathcal{N}} \tilde{f}_{\mathbf{n}}\, e^{i\frac{2\pi}{N}\,\mathbf{n}\cdot\mathbf{m}}$$

dual lattice $\mathbf{n}$

Map from lattice

$$\mathbf{m}\,,\ \mathbf{x}_{\mathbf{m}} = \frac{L}{N}\,\mathbf{m}$$

$$k_i(\mathbf{n}) = \frac{2\pi}{L} \times \begin{cases} n_i, & 0 \le n_i \le \left\lfloor \frac{N}{2} \right\rfloor, \\ n_i - N, & \left\lfloor \frac{N}{2} \right\rfloor < n_i \le N-1 \end{cases}$$

From Continuum to Lattice

Continuum

$$\tilde{f}(\mathbf{k}) = \int_{\mathbb{R}^3} d^3x\, f(\mathbf{x})\, e^{-i\mathbf{k}\cdot\mathbf{x}}$$

$$\left\langle \tilde{f}(\mathbf{k})\tilde{f}^*(\mathbf{k}')\right\rangle = (2\pi)^3\delta^{(3)}(\mathbf{k}-\mathbf{k}')\, P(\mathbf{k})$$

$$P(\mathbf{k}) \sim \frac{1}{V_{\mathbb{R}}}\left\langle |\tilde{f}(\mathbf{k})|^2\right\rangle$$

$$P(k) \approx \frac{1}{4\pi}\int d\Omega_{\hat{\mathbf{k}}} \frac{|\tilde{f}(\mathbf{k})|^2}{V_{\mathbb{R}}}\Bigg|_{|\mathbf{k}|=k}.$$

Lattice

$$\tilde{f}_{\mathbf{n}} = \frac{V}{N^3}\sum_{\mathbf{m}\in\mathcal{N}} f_{\mathbf{m}}\, e^{-i\frac{2\pi}{N}\,\mathbf{n}\cdot\mathbf{m}}$$

$$\langle \tilde{f}_{\mathbf{n}}\tilde{f}^*_{\mathbf{n}'}\rangle = V\, P_{\mathbf{n}}\,\delta_{\mathbf{n}\mathbf{n}'}$$

$$P_{\mathbf{n}} = \frac{1}{V}\langle|\tilde{f}_{\mathbf{n}}|^2\rangle$$

$$P(k) \approx \widehat{P}(k) \equiv \frac{1}{N_k}\sum_{k_{\mathbf{n}}\in\text{shell}(k)} \frac{|\tilde{f}_{\mathbf{n}}|^2}{V},$$

k-shell binning in 2D

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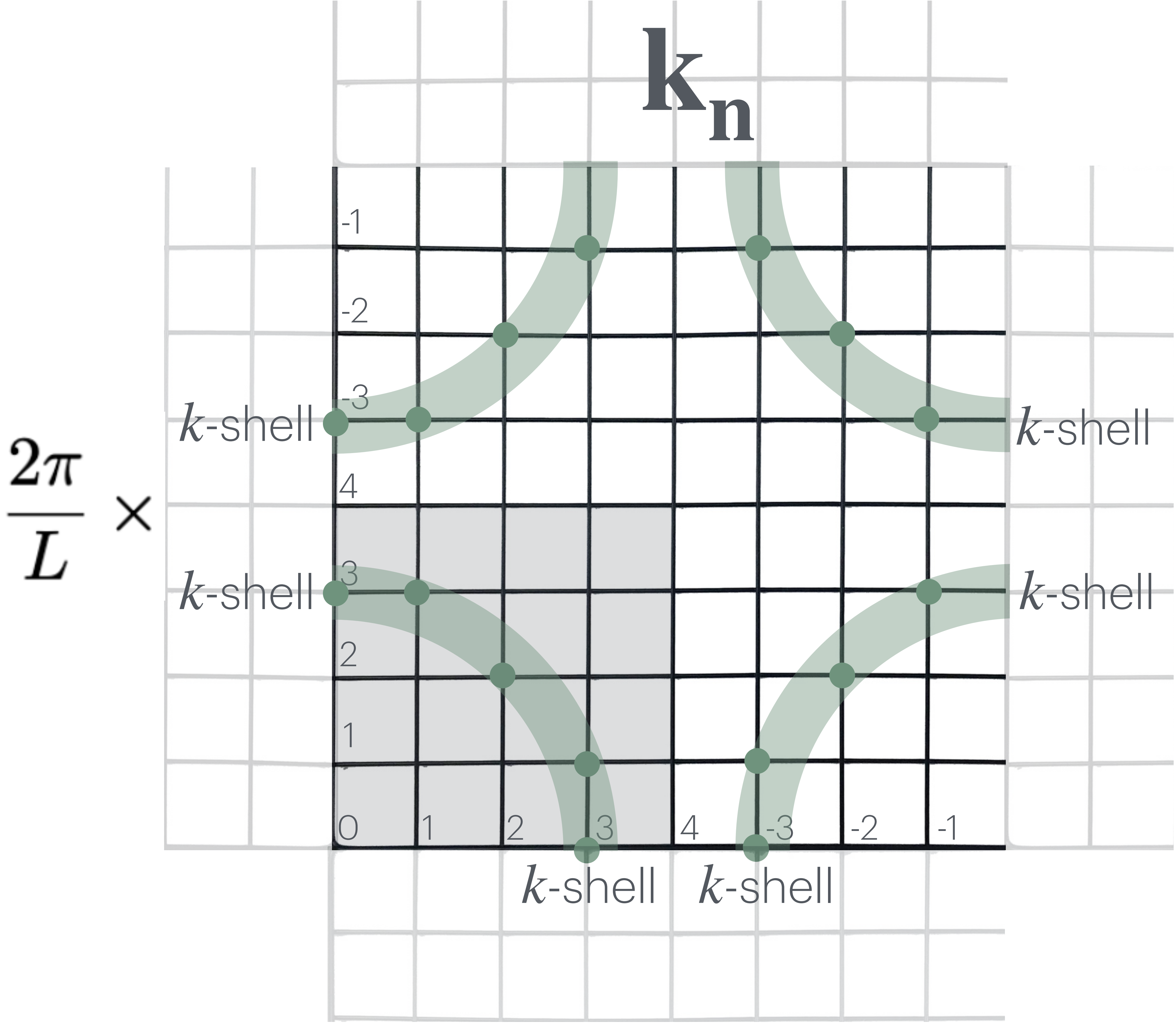

$N_k = 16$

Take-away message

- Pick your favorite DFT library to compute $\tilde{f}_{\mathbf{n}}$ from $f_{\mathbf{m}} \equiv f(\mathbf{x}_{\mathbf{m}})$ (Check normalization!)

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- Bin $\mathbf{k_n}$ into shells k and compute the average of all $\frac{|\tilde{f}_{\mathbf{n}}|^2}{V}$ falling into that shell: $\frac{1}{N_k} \sum_{k_{\mathbf{n}} \in \mathrm{shell}(k)} \frac{|\tilde{f}_{\mathbf{n}}|^2}{V}$

Take-away message

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- Bin $\mathbf{k}_{\mathbf{n}}$ into shells k and compute the average of all $\frac{|\tilde{f}_{\mathbf{n}}|^2}{V}$ falling into that shell: $\frac{1}{N_k} \sum_{k_{\mathbf{n}} \in \text{shell}(k)} \frac{|\tilde{f}_{\mathbf{n}}|^2}{V}$
- **Identify this average as an estimator of the Power spectrum:**

$$\boxed{P(k) \approx \widehat{P}(k) \equiv \frac{1}{N_k} \sum_{k_{\mathbf{n}} \in \text{shell}(k)} \frac{|\tilde{f}_{\mathbf{n}}|^2}{V},}$$

- **Hence:** *Very simple and quick to compute Power Spectra on the Lattice!*

Case study: the velocity spectrum

The velocity spectrum

- We consider a velocity field $\mathbf{u}(\mathbf{x})$ with Fourier transform: $\tilde{u}_i(\mathbf{k}) = \int d^3x \, u_i(\mathbf{x}) \, e^{-i\mathbf{k}\cdot\mathbf{x}}$
- Define the *Power Spectrum Tensor* $P_{ij}(\mathbf{k})$: $\langle \tilde{u}_i(\mathbf{k}) \, \tilde{u}_j^*(\mathbf{k}') \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{k} - \mathbf{k}') \, P_{ij}(\mathbf{k})$.
- The kinetic energy density (per unit mass) is the variance of the velocity field:

$$\boxed{K = \frac{1}{2} \langle u^2 \rangle = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} P_{ii}(\mathbf{k}),} \qquad \text{with } P_{ii}(\mathbf{k}) = \textstyle\sum_{i=1}^{3} P_{ii}(\mathbf{k})$$

- Assume isotropy:

$$K = \frac{1}{2} \int_0^\infty \frac{4\pi k^2}{(2\pi)^3} P_{ii}(k) \, dk = \int_0^\infty \underbrace{\left[\frac{k^2}{4\pi^2} P_{ii}(k) \right]}_{E_u(k)} dk$$

and define **the kinetic energy spectrum**

$$\boxed{E_u(k) = \frac{k^2}{4\pi^2} P_{ii}(k), \qquad K = \int_0^\infty E_u(k) \, dk,}$$

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The velocity spectrum

Longitudinal and transverse decomposition

- Any vector field can be decomposed into a longitudinal (curl-free) part and a transverse (divergence-free) part.
- In Fourier space:

  Longitudinal: project onto $\hat{\mathbf{k}}$

  $$\tilde{u}_{L,i}(\mathbf{k}) = \hat{k}_i\big(\hat{k}_j\tilde{u}_j(\mathbf{k})\big)$$

  Transverse: subtract longitudinal from total

  $$\tilde{u}_{T,i}(\mathbf{k}) = \tilde{u}_i(\mathbf{k}) - \tilde{u}_{L,i}(\mathbf{k}) = \big(\delta_{ij} - \hat{k}_i\hat{k}_j\big)\tilde{u}_j(\mathbf{k})$$

- The Power Spectrum tensor splits into L and T parts:

  $$P_{mn}(\mathbf{k}) = P_L(k)\,\hat{k}_m\hat{k}_n + P_T(k)\,\big(\delta_{mn} - \hat{k}_m\hat{k}_n\big)$$
  $$P_{ii}(k) = P_L(k) + 2P_T(k)$$

- The total kinetic energy can now be computed as:

  $$K = \int_0^\infty \left[E_L(k) + E_T(k)\right] dk$$

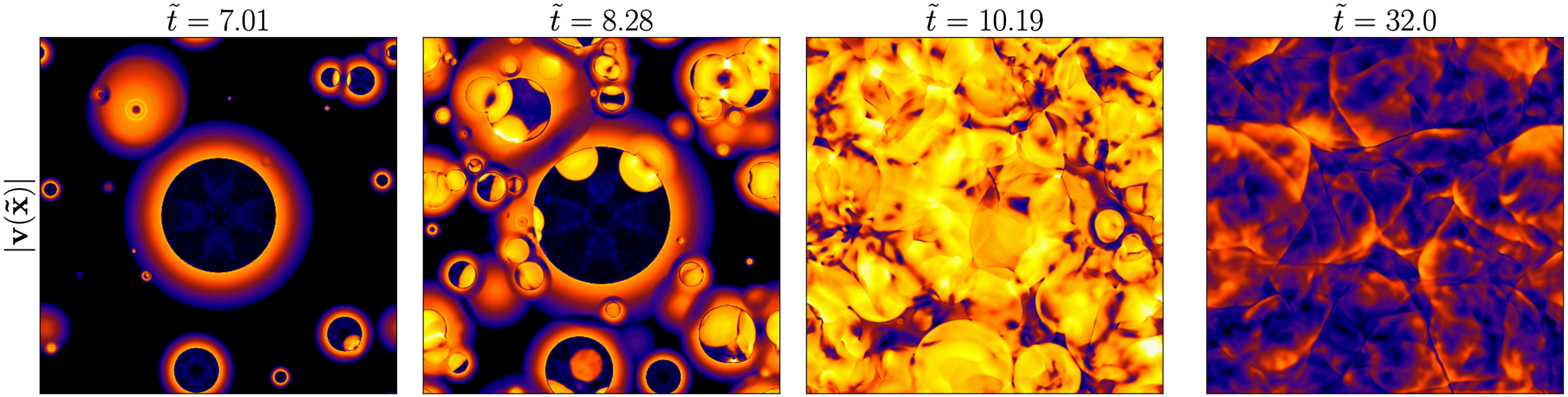
  May include factor of 2 here

with

$$E_L(k) = \frac{k^2}{4\pi^2} P_L(k), \qquad E_T(k) = \frac{k^2}{2\pi^2} P_T(k).$$

The velocity spectrum

Eg: Growth of vorticity



Uncollided sound-shells

$\Downarrow$

Only compressional modes

$\Downarrow$

$E_T(k) = E_u(k) - E_L(k) = 0$

Plane-wave expansion

Linear evolution:
non interacting Sound-waves

$\Downarrow$

$E_T(k) = 0$

Non-linear evolution:
interacting acoustic modes

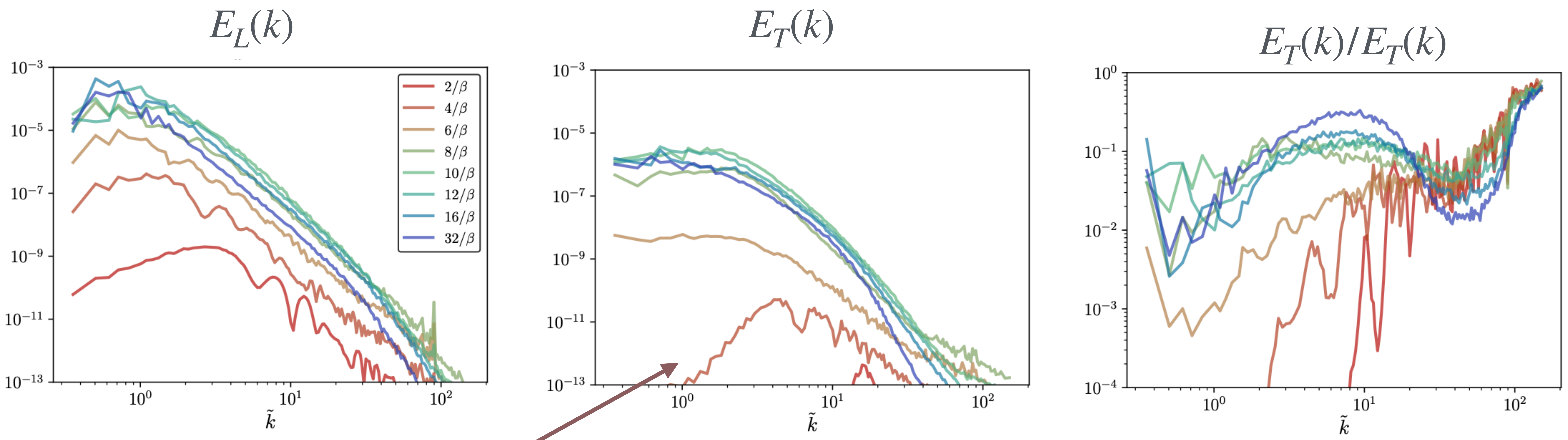
$\Downarrow$

$E_T(k) \neq 0$

$E_T(k) \neq 0$ is a tracer of non-linear evolution and turbulence.

The velocity spectrum

Eg: Growth of vorticity



- $E_T(k)$ **initially vanishing, much smaller** than the **compressional component** $E_L(k)$
- **Transfer** of **energy** from **longitudinal** to **transverse** modes
- **Transverse** velocity spectrum **grows with time (**Generation of vorticity, evolution is non-linear**)**

Hence: ***Velocity spectra (Longitudinal and Transverse) are tools to understand the dynamics, energy transport, non-linear evolution, vorticity/turbulence, etc.***