

SUPPLEMENTARY MATERIALS: On the Exact Computation of Linear Frequency Principle Dynamics and Its Generalization*

Tao Luo[†], Zheng Ma[‡], Zhi-Qin John Xu[§], and Yaoyu Zhang[¶]

SM1. Fourier transform table. We list the results of one-dimensional Fourier transform in Table SM1 and high-dimensional Fourier transform in Table SM2 used in our proofs.

Table SM1

Fourier transform for 1-dimensional functions used in our proofs.

Function of x	Fourier transform with respect to x
$g(ax)$	$\frac{1}{ a } \mathcal{F}[g]\left(\frac{\xi}{a}\right)$
$g(x - c)$	$\mathcal{F}[g](\xi) e^{-2\pi i c \xi}$
$x^k g(x)$	$\left(\frac{i}{2\pi}\right)^k \frac{d^k}{d\xi^k} \mathcal{F}[g](\xi)$
$g^{(k)}(x)$	$(2\pi i \xi)^k \mathcal{F}[g](\xi)$
1	$\delta(\xi)$
x^k	$\left(\frac{i}{2\pi}\right)^k \delta^{(k)}(\xi)$
$\delta(x - x_0)$	$e^{-2\pi i x_0 \xi}$
$H(x)$ (Heaviside)	$\frac{1}{i2\pi\xi} + \frac{1}{2}\delta(\xi)$
ReLU(x)	$-\frac{1}{4\pi^2\xi^2} + \frac{i}{4\pi}\delta'(\xi)$
tanh(x)	$-i\pi \operatorname{csch}(\pi^2\xi)$
Sigmoid(x)	$-i\pi \operatorname{csch}(2\pi^2\xi) + \frac{1}{2}\delta(\xi)$
$\operatorname{sech}^2(x)$	$2\pi^2\xi \operatorname{csch}(\pi^2\xi)$
$x \operatorname{sech}^2(x)$	$i\pi (1 - \pi^2\xi \operatorname{coth}(\pi^2\xi)) \operatorname{csch}(\pi^2\xi)$

SM2. Proof.

Lemma. (*Lemma 2 in main text*) Given any nonzero vector $\mathbf{w} \in \mathbb{R}^d$ with $\hat{\mathbf{w}} = \frac{\mathbf{w}}{\|\mathbf{w}\|}$, we have

$$(SM2.1) \quad \frac{1}{\|\mathbf{w}\|^d} \delta_{\hat{\mathbf{w}}} \left(\frac{\mathbf{x}}{\|\mathbf{w}\|} \right) = \delta_{\mathbf{w}}(\mathbf{x}).$$

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[†]Corresponding author. School of Mathematical Sciences, CMA-Shanghai, Institute of Natural Sciences, MOE-LSC, and Qing Yuan Research Institute, Shanghai Jiao Tong University, Shanghai, 200240, People's Republic of China (luotao41@sjtu.edu.cn).

[‡]School of Mathematical Sciences, CMA-Shanghai, Institute of Natural Sciences, MOE-LSC, and Qing Yuan Research Institute, Shanghai Jiao Tong University, Shanghai, 200240, People's Republic of China (zhengma@sjtu.edu.cn).

[§]School of Mathematical Sciences, Institute of Natural Sciences, MOE-LSC, and Qing Yuan Research Institute, Shanghai Jiao Tong University, Shanghai, 200240, People's Republic of China (xuzhiqin@sjtu.edu.cn).

[¶]School of Mathematical Sciences, Institute of Natural Sciences, MOE-LSC, and Qing Yuan Research Institute, Shanghai Jiao Tong University, and Shanghai Center for Brain Science and Brain-Inspired Technology, Shanghai, 200240, People's Republic of China (zhyy.sjtu@sjtu.edu.cn).

Table SM2

Fourier transform for d -dimensional functions used in our proofs.

Function of \mathbf{x}	Fourier transform with respect to \mathbf{x}
$g(a\mathbf{x})$	$\frac{1}{ a ^d} \mathcal{F}[g]\left(\frac{\boldsymbol{\xi}}{a}\right)$
$\delta(\mathbf{x} - \mathbf{x}_0)$	$e^{-2\pi i \boldsymbol{\xi}^\top \mathbf{x}_0}$
$g(\boldsymbol{\nu}^\top \mathbf{x})$ (unit vector $\boldsymbol{\nu}$)	$\delta_{\boldsymbol{\nu}}(\boldsymbol{\xi}) \mathcal{F}[g](\boldsymbol{\xi}^\top \boldsymbol{\nu})$
$g(\mathbf{w}^\top \mathbf{x} + b)$	$\delta_{\mathbf{w}}(\boldsymbol{\xi}) \mathcal{F}[g]\left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\ \mathbf{w}\ }\right) e^{2\pi i \frac{b}{\ \mathbf{w}\ } \boldsymbol{\xi}^\top \hat{\mathbf{w}}}$
$g(\mathbf{w}^\top \mathbf{x} + \ \mathbf{w}\ c)$	$\delta_{\mathbf{w}}(\boldsymbol{\xi}) \mathcal{F}[g]\left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\ \mathbf{w}\ }\right) e^{2\pi i c \boldsymbol{\xi}^\top \hat{\mathbf{w}}}$
$\mathbf{x}g(\mathbf{x})$	$\frac{i}{2\pi} \nabla \mathcal{F}[g](\boldsymbol{\xi})$
$\mathbf{x}^\perp g(\mathbf{w}^\top \mathbf{x} + \ \mathbf{w}\ c)$	$\frac{i}{2\pi} \nabla_{\boldsymbol{\xi}^\perp} \left[\delta_{\mathbf{w}}(\boldsymbol{\xi}) \mathcal{F}[g]\left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\ \mathbf{w}\ }\right) e^{2\pi i c \boldsymbol{\xi}^\top \hat{\mathbf{w}}} \right]$
$\mathbf{x}g(\mathbf{w}^\top \mathbf{x} + b)$	$\frac{i}{2\pi} \nabla_{\boldsymbol{\xi}} \left[\delta_{\mathbf{w}}(\boldsymbol{\xi}) \mathcal{F}[g]\left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\ \mathbf{w}\ }\right) e^{2\pi i b \boldsymbol{\xi}^\top \hat{\mathbf{w}} / \ \mathbf{w}\ } \right]$

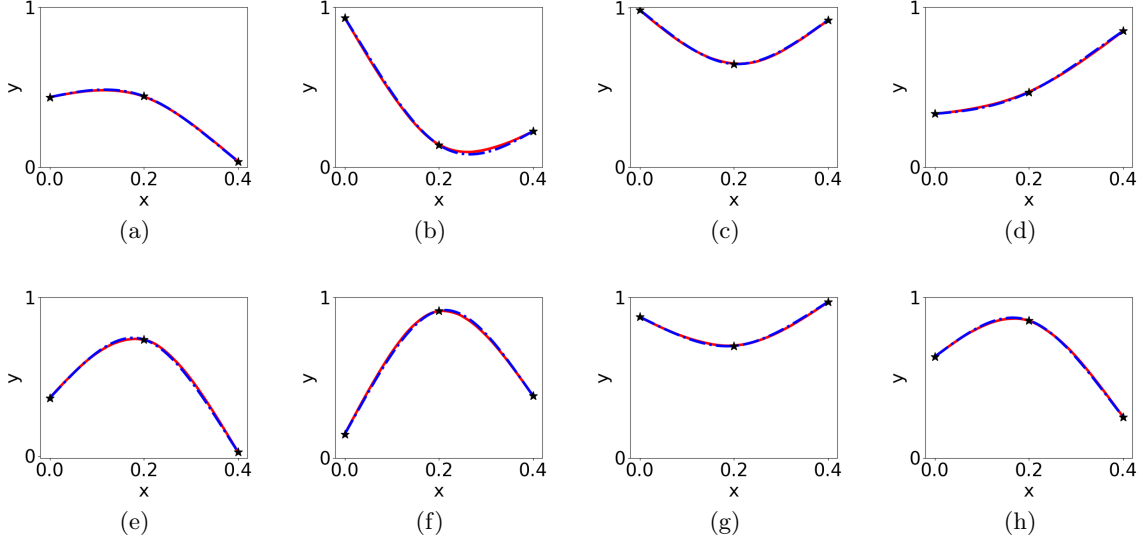


Figure SM1. f_{NN} (red solid) vs. f_{LFP} (blue dashed dot) for a 1-d problem. The setting is the same as the case in Figure 1(a) in main text, except that the label for each data is randomly selected from $[0, 1]$ and the uniform distribution half width U is randomly selected from $[3, 6]$. Each subfigure is one trial.

Proof. This is proved by changing of variables. In fact, for any $\phi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$\begin{aligned}
\left\langle \frac{1}{\|\mathbf{w}\|^d} \delta_{\hat{\mathbf{w}}} \left(\frac{\cdot}{\|\mathbf{w}\|} \right), \phi(\cdot) \right\rangle_{\mathcal{S}'(\mathbb{R}^d), \mathcal{S}(\mathbb{R}^d)} &= \langle \delta_{\hat{\mathbf{w}}}(\cdot), \phi(\|\mathbf{w}\|\cdot) \rangle_{\mathcal{S}'(\mathbb{R}^d), \mathcal{S}(\mathbb{R}^d)} \\
&= \int_{\mathbb{R}} \phi(\|\mathbf{w}\|y\hat{\mathbf{w}}) dy \\
&= \int_{\mathbb{R}} \phi(y\mathbf{w}) dy \\
&= \langle \delta_{\mathbf{w}}(\cdot), \phi(\cdot) \rangle_{\mathcal{S}'(\mathbb{R}^d), \mathcal{S}(\mathbb{R}^d)}. \quad \blacksquare
\end{aligned}$$

Lemma. (Lemma 2 in main text) For any unit vector $\boldsymbol{\nu} \in \mathbb{R}^d$, any nonzero vector $\boldsymbol{w} \in \mathbb{R}^d$ with $\hat{\boldsymbol{w}} = \frac{\boldsymbol{w}}{\|\boldsymbol{w}\|}$, and $g \in \mathcal{S}'(\mathbb{R})$ with $\mathcal{F}[g] \in C(\mathbb{R})$, we have, in the sense of distribution,

$$(SM2.2) \quad (a) \quad \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\boldsymbol{\nu}^\top \boldsymbol{x})](\boldsymbol{\xi}) = \delta_{\boldsymbol{\nu}}(\boldsymbol{\xi}) \mathcal{F}[g](\boldsymbol{\xi}^\top \boldsymbol{\nu}),$$

$$(SM2.3) \quad (b) \quad \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\boldsymbol{w}^\top \boldsymbol{x} + b)](\boldsymbol{\xi}) = \delta_{\boldsymbol{w}}(\boldsymbol{\xi}) \mathcal{F}[g] \left(\frac{\boldsymbol{\xi}^\top \hat{\boldsymbol{w}}}{\|\boldsymbol{w}\|} \right) e^{2\pi i \frac{b}{\|\boldsymbol{w}\|} \boldsymbol{\xi}^\top \hat{\boldsymbol{w}}},$$

$$(SM2.4) \quad (c) \quad \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[\boldsymbol{x}g(\boldsymbol{w}^\top \boldsymbol{x} + b)](\boldsymbol{\xi}) = \frac{i}{2\pi} \nabla_{\boldsymbol{\xi}} \left[\delta_{\boldsymbol{w}}(\boldsymbol{\xi}) \mathcal{F}[g] \left(\frac{\boldsymbol{\xi}^\top \hat{\boldsymbol{w}}}{\|\boldsymbol{w}\|} \right) e^{2\pi i \frac{b}{\|\boldsymbol{w}\|} \boldsymbol{\xi}^\top \hat{\boldsymbol{w}}} \right].$$

Proof. Let $\phi \in \mathcal{S}(\mathbb{R}^d)$ be any test function.

(a) By direct calculation, we have

$$\begin{aligned} \langle \mathcal{F}_{\boldsymbol{x} \rightarrow \cdot} [g(\boldsymbol{\nu}^\top \boldsymbol{x})](\cdot), \phi(\cdot) \rangle_{\mathcal{S}'(\mathbb{R}^d), \mathcal{S}(\mathbb{R}^d)} &= \langle g(\boldsymbol{\nu}^\top \cdot), \mathcal{F}_{\boldsymbol{x} \rightarrow \cdot} [\phi(\boldsymbol{x})](\cdot) \rangle_{\mathcal{S}'(\mathbb{R}^d), \mathcal{S}(\mathbb{R}^d)} \\ &= \langle g(\cdot), \mathcal{F}_{\boldsymbol{y} \rightarrow \cdot} [\phi(\boldsymbol{y}\boldsymbol{\nu})](\cdot) \rangle_{\mathcal{S}'(\mathbb{R}), \mathcal{S}(\mathbb{R})} \\ &= \langle \mathcal{F}_{\boldsymbol{y} \rightarrow \cdot} [g(\boldsymbol{y})](\cdot), \phi(\cdot\boldsymbol{\nu}) \rangle_{\mathcal{S}'(\mathbb{R}), \mathcal{S}(\mathbb{R})} \\ &= \langle \mathcal{F}[g](\cdot\boldsymbol{\nu}^\top \boldsymbol{\nu}), \phi(\cdot\boldsymbol{\nu}) \rangle_{\mathcal{S}'(\mathbb{R}), \mathcal{S}(\mathbb{R})} \\ &= \langle \delta_{\boldsymbol{\nu}}(\cdot) \mathcal{F}[g](\cdot^\top \boldsymbol{\nu}), \phi(\cdot) \rangle_{\mathcal{S}'(\mathbb{R}^d), \mathcal{S}(\mathbb{R}^d)}. \end{aligned}$$

(b) By part (a), we have in the distributional sense

$$\mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\hat{\boldsymbol{w}}^\top \boldsymbol{x})](\boldsymbol{\xi}) = \delta_{\hat{\boldsymbol{w}}}(\boldsymbol{\xi}) \mathcal{F}[g](\boldsymbol{\xi}^\top \hat{\boldsymbol{w}}).$$

Note that

$$\mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\boldsymbol{x} - \boldsymbol{x}_0)](\boldsymbol{\xi}) = \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g](\boldsymbol{\xi}) e^{-2\pi i \boldsymbol{x}_0^\top \boldsymbol{\xi}},$$

then

$$\begin{aligned} \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\hat{\boldsymbol{w}}^\top \boldsymbol{x} + b)](\boldsymbol{\xi}) &= \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\hat{\boldsymbol{w}}^\top (\boldsymbol{x} + b\hat{\boldsymbol{w}}))](\boldsymbol{\xi}) \\ &= \delta_{\hat{\boldsymbol{w}}}(\boldsymbol{\xi}) \mathcal{F}[g](\boldsymbol{\xi}^\top \hat{\boldsymbol{w}}) e^{2\pi i b \hat{\boldsymbol{w}}^\top \boldsymbol{\xi}}. \end{aligned}$$

Therefore

$$\begin{aligned} \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\boldsymbol{w}^\top \boldsymbol{x} + b)](\boldsymbol{\xi}) &= \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\hat{\boldsymbol{w}}^\top \|\boldsymbol{w}\| \boldsymbol{x} + b)](\boldsymbol{\xi}) \\ &= \frac{1}{\|\boldsymbol{w}\|^d} \mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[g(\hat{\boldsymbol{w}}^\top \boldsymbol{x} + b)] \left(\frac{\boldsymbol{\xi}}{\|\boldsymbol{w}\|} \right) \\ &= \frac{1}{\|\boldsymbol{w}\|^d} \delta_{\hat{\boldsymbol{w}}} \left(\frac{\boldsymbol{\xi}}{\|\boldsymbol{w}\|} \right) \mathcal{F}[g] \left(\frac{\boldsymbol{\xi}^\top \hat{\boldsymbol{w}}}{\|\boldsymbol{w}\|} \right) e^{2\pi i \frac{b}{\|\boldsymbol{w}\|} \hat{\boldsymbol{w}}^\top \boldsymbol{\xi}} \\ &= \delta_{\boldsymbol{w}}(\boldsymbol{\xi}) \mathcal{F}[g] \left(\frac{\boldsymbol{\xi}^\top \hat{\boldsymbol{w}}}{\|\boldsymbol{w}\|} \right) e^{2\pi i \frac{b}{\|\boldsymbol{w}\|} \hat{\boldsymbol{w}}^\top \boldsymbol{\xi}}. \end{aligned}$$

(c) This follows from part (b) and the fact that for any function $\tilde{g}(\boldsymbol{x})$

$$\mathcal{F}_{\boldsymbol{x} \rightarrow \boldsymbol{\xi}}[\boldsymbol{x}\tilde{g}(\boldsymbol{x})](\boldsymbol{\xi}) = \frac{i}{2\pi} \nabla_{\boldsymbol{\xi}} [\mathcal{F}[\tilde{g}](\boldsymbol{\xi})].$$

■

Lemma. (Lemma 3 in main text) The dynamics (4.9) has the following expression in the frequency domain for all $\phi \in \mathcal{S}(\mathbb{R}^d)$

$$(SM2.5) \quad \langle \partial_t \mathcal{F}[u], \phi \rangle = -\langle \mathcal{L}[\mathcal{F}[u_\rho]], \phi \rangle,$$

where $\mathcal{L}[\cdot]$ is called Linear F-Principle (LFP) operator is given by

$$\mathcal{L}[\mathcal{F}[u_\rho]] = \int_{\mathbb{R}^d} \hat{K}(\boldsymbol{\xi}, \boldsymbol{\xi}') \mathcal{F}[u_\rho](\boldsymbol{\xi}') d\boldsymbol{\xi}',$$

and

$$(SM2.6) \quad \hat{K}(\boldsymbol{\xi}, \boldsymbol{\xi}') := \mathbb{E}_{\mathbf{q}} \hat{K}_{\mathbf{q}}(\boldsymbol{\xi}, \boldsymbol{\xi}') := \mathbb{E}_{\mathbf{q}} \mathcal{F}_{\mathbf{x} \rightarrow \boldsymbol{\xi}}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}, \mathbf{q})] \cdot \overline{\mathcal{F}_{\mathbf{x}' \rightarrow \boldsymbol{\xi}'}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q})]}.$$

The expectation $\mathbb{E}_{\mathbf{q}}$ is taken w.r.t. initial distribution of parameters.

Proof. For any $\phi \in \mathcal{S}(\mathbb{R}^d)$. since $\partial_t u$ is in $\mathcal{S}'(\mathbb{R}^d)$ and locally integrable, we have

$$\begin{aligned} \langle \partial_t \mathcal{F}[u], \phi \rangle &= \langle \partial_t u, \mathcal{F}[\phi] \rangle \\ &= \int_{\mathbb{R}^d} \partial_t u(\mathbf{x}, t) \int_{\mathbb{R}^d} \phi(\boldsymbol{\xi}) e^{-i2\pi \mathbf{x} \cdot \boldsymbol{\xi}} d\boldsymbol{\xi} d\mathbf{x} \\ &= - \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(\mathbf{x}, \mathbf{x}') u_\rho(\mathbf{x}') d\mathbf{x}' \int_{\mathbb{R}^d} \phi(\boldsymbol{\xi}) e^{-i2\pi \mathbf{x} \cdot \boldsymbol{\xi}} d\boldsymbol{\xi} d\mathbf{x} \\ &= - \int_{\mathbb{R}^{3d}} K(\mathbf{x}, \mathbf{x}') u_\rho(\mathbf{x}') d\mathbf{x}' \phi(\boldsymbol{\xi}) e^{-i2\pi \mathbf{x} \cdot \boldsymbol{\xi}} d\boldsymbol{\xi} d\mathbf{x} \\ &= - \int_{\mathbb{R}^{3d}} \mathbb{E}_{\mathbf{q}} \nabla_{\mathbf{q}} \sigma^*(\mathbf{x}, \mathbf{q}) \cdot \nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q}) u_\rho(\mathbf{x}') d\mathbf{x}' \phi(\boldsymbol{\xi}) e^{-i2\pi \mathbf{x} \cdot \boldsymbol{\xi}} d\boldsymbol{\xi} d\mathbf{x} \\ &= - \mathbb{E}_{\mathbf{q}} \int_{\mathbb{R}^d} \nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q}) u_\rho(\mathbf{x}') d\mathbf{x}' \cdot \int_{\mathbb{R}^{2d}} \nabla_{\mathbf{q}} \sigma^*(\mathbf{x}, \mathbf{q}) e^{-i2\pi \mathbf{x} \cdot \boldsymbol{\xi}} \phi(\boldsymbol{\xi}) d\boldsymbol{\xi} d\mathbf{x} \\ &= - \mathbb{E}_{\mathbf{q}} \int_{\mathbb{R}^d} \nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q}) u_\rho(\mathbf{x}') d\mathbf{x}' \cdot \langle \mathcal{F}_{\mathbf{x} \rightarrow \cdot}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}, \mathbf{q})](\cdot), \phi(\cdot) \rangle. \end{aligned}$$

Since

$$\int_{\mathbb{R}^d} \nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q}) u_\rho(\mathbf{x}') d\mathbf{x}' = \int_{\mathbb{R}^d} \overline{\mathcal{F}_{\mathbf{x}' \rightarrow \boldsymbol{\xi}'}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q})](\boldsymbol{\xi}')} \mathcal{F}_{\mathbf{x}' \rightarrow \boldsymbol{\xi}'}[u_\rho](\boldsymbol{\xi}') d\boldsymbol{\xi}',$$

we have

$$\begin{aligned} \langle \partial_t \mathcal{F}[u], \phi \rangle &= - \mathbb{E}_{\mathbf{q}} \int_{\mathbb{R}^d} \overline{\mathcal{F}_{\mathbf{x}' \rightarrow \boldsymbol{\xi}'}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q})](\boldsymbol{\xi}')} \mathcal{F}_{\mathbf{x}' \rightarrow \boldsymbol{\xi}'}[u_\rho](\boldsymbol{\xi}') d\boldsymbol{\xi}' \cdot \langle \mathcal{F}_{\mathbf{x} \rightarrow \cdot}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}, \mathbf{q})](\cdot), \phi(\cdot) \rangle \\ &= - \mathbb{E}_{\mathbf{q}} \int_{\mathbb{R}^{2d}} \overline{\mathcal{F}_{\mathbf{x}' \rightarrow \boldsymbol{\xi}'}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q})](\boldsymbol{\xi}')} \cdot \mathcal{F}_{\mathbf{x} \rightarrow \boldsymbol{\xi}}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}, \mathbf{q})](\boldsymbol{\xi}) \mathcal{F}_{\mathbf{x}' \rightarrow \boldsymbol{\xi}'}[u_\rho](\boldsymbol{\xi}') d\boldsymbol{\xi}' \phi(\boldsymbol{\xi}) d\boldsymbol{\xi} \\ &= - \int_{\mathbb{R}^{2d}} \hat{K}(\boldsymbol{\xi}, \boldsymbol{\xi}') \mathcal{F}[u_\rho](\boldsymbol{\xi}') d\boldsymbol{\xi}' \phi(\boldsymbol{\xi}) d\boldsymbol{\xi} \\ &= - \langle \mathcal{L}[\mathcal{F}[u_\rho]], \phi \rangle. \end{aligned}$$

■

Theorem. (Theorem 1 in main text) Suppose that Assumption 1 holds. If $\sigma_b \gg 1$, then the dynamics (4.9) has the following expression,

$$(SM2.7) \quad \langle \partial_t \mathcal{F}[u], \phi \rangle = - \langle \mathcal{L}[\mathcal{F}[u_\rho]], \phi \rangle + O(\sigma_b^{-3}),$$

where $\phi \in \mathcal{S}(\mathbb{R}^d)$ is a test function and the LFP operator is given by

$$(SM2.8) \quad \begin{aligned} \mathcal{L}[\mathcal{F}[u_\rho]] &= \frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b\|\boldsymbol{\xi}\|^{d-1}} \mathbb{E}_{a,r} \left[\frac{1}{r} \mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \cdot \mathcal{F}[\mathbf{g}_1] \left(-\frac{\|\boldsymbol{\xi}\|}{r} \right) \right] \mathcal{F}[u_\rho](\boldsymbol{\xi}) \\ &\quad - \frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b} \nabla \cdot \left(\mathbb{E}_{a,r} \left[\frac{1}{r\|\boldsymbol{\xi}\|^{d-1}} \mathcal{F}[\mathbf{g}_2] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \mathcal{F}[\mathbf{g}_2] \left(-\frac{\|\boldsymbol{\xi}\|}{r} \right) \right] \nabla \mathcal{F}[u_\rho](\boldsymbol{\xi}) \right), \end{aligned}$$

where $\Gamma(\cdot)$ is the gamma function. The expectations are taken w.r.t. initial parameter distribution. Here $r = \|\mathbf{w}\|$ with the probability density $\rho_r(r) := \frac{2\pi^{d/2}}{\Gamma(d/2)} \rho_{\mathbf{w}}(r\mathbf{e}_1)r^{d-1}$, $\mathbf{e}_1 = (1, 0, \dots, 0)^\top$.

Proof. For simplicity, we assume that $b \sim \mathcal{N}(0, \sigma_b^2)$, $\sigma_b \gg 1$ in this proof. It is straightforward to extend the proof to general distributions for b as long as it is zero-mean and with variance $\sigma_b \gg 1$.

1. Divide into two parts. Note that

$$(SM2.9) \quad \begin{pmatrix} \mathbf{g}_1(\mathbf{w}^\top \mathbf{x} + b) \\ \mathbf{x} \mathbf{g}_2(\mathbf{w}^\top \mathbf{x} + b) \end{pmatrix} = \begin{pmatrix} \partial_a[a\sigma(\mathbf{w}^\top \mathbf{x} + b)] \\ \partial_b[a\sigma(\mathbf{w}^\top \mathbf{x} + b)] \\ \nabla_{\mathbf{w}}[a\sigma(\mathbf{w}^\top \mathbf{x} + b)] \end{pmatrix} = \nabla_{\mathbf{q}} \sigma^*(\mathbf{x}, \mathbf{q}).$$

One can split the Fourier transformed kernel \hat{K} into two parts, more precisely,

$$\hat{K} = \mathbb{E}_{\mathbf{q}} \hat{K}_{\mathbf{q}}, \quad \hat{K}_{\mathbf{q}} = \hat{K}_{a,b} + \hat{K}_{\mathbf{w}},$$

where

$$\begin{aligned} \hat{K}_{\mathbf{q}}(\boldsymbol{\xi}, \boldsymbol{\xi}') &= \mathbb{E}_{\mathbf{q}} \mathcal{F}_{\mathbf{x} \rightarrow \boldsymbol{\xi}}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}, \mathbf{q})] \cdot \overline{\mathcal{F}_{\mathbf{x}' \rightarrow \boldsymbol{\xi}'}[\nabla_{\mathbf{q}} \sigma^*(\mathbf{x}', \mathbf{q})]}, \\ \hat{K}_{a,b}(\boldsymbol{\xi}, \boldsymbol{\xi}') &= \mathcal{F}[\mathbf{g}_1(\mathbf{w}^\top \mathbf{x} + b)] \cdot \overline{\mathcal{F}[\mathbf{g}_1(\mathbf{w}^\top \mathbf{x}' + b)]}, \\ \hat{K}_{\mathbf{w}}(\boldsymbol{\xi}, \boldsymbol{\xi}') &= \mathcal{F}[\mathbf{x} \mathbf{g}_2(\mathbf{w}^\top \mathbf{x} + b)] \cdot \overline{\mathcal{F}[\mathbf{x} \mathbf{g}_2(\mathbf{w}^\top \mathbf{x}' + b)]}. \end{aligned}$$

For any $\phi, \psi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$(SM2.10) \quad \langle \hat{K}_{\mathbf{q}}, \phi \otimes \psi \rangle := \langle \hat{K}_{\mathbf{q}}, \phi \otimes \psi \rangle_{\mathcal{S}'(\mathbb{R}^{2d}), \mathcal{S}(\mathbb{R}^{2d})} = \int_{\mathbb{R}^{2d}} \hat{K}_{\mathbf{q}}(\boldsymbol{\xi}, \boldsymbol{\xi}') \phi(\boldsymbol{\xi}) \psi(\boldsymbol{\xi}') \, d\boldsymbol{\xi} \, d\boldsymbol{\xi}'.$$

The expressions for $\hat{K}_{a,b}$ and $\hat{K}_{\mathbf{w}}$ are similar.

2. Calculate $\hat{K}_{a,b}(\boldsymbol{\xi}, \boldsymbol{\xi}')$. Since

$$\hat{K}_{a,b}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \delta_{\mathbf{w}}(\boldsymbol{\xi}) \delta_{\mathbf{w}}(\boldsymbol{\xi}') \mathcal{F}[\mathbf{g}_1] \left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right) \cdot \overline{\mathcal{F}[\mathbf{g}_1] \left(\frac{\boldsymbol{\xi}'^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right)} e^{2\pi i b (\boldsymbol{\xi} - \boldsymbol{\xi}')^\top \hat{\mathbf{w}} / \|\mathbf{w}\|},$$

we have

$$\begin{aligned} \langle \hat{K}_{a,b}, \phi \otimes \psi \rangle &= \int_{\mathbb{R}^{2d}} \delta_{\mathbf{w}}(\boldsymbol{\xi}) \delta_{\mathbf{w}}(\boldsymbol{\xi}') \mathcal{F}[\mathbf{g}_1] \left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right) \cdot \overline{\mathcal{F}[\mathbf{g}_1] \left(\frac{\boldsymbol{\xi}'^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right)} e^{2\pi i b (\boldsymbol{\xi} - \boldsymbol{\xi}')^\top \hat{\mathbf{w}} / \|\mathbf{w}\|} \phi(\boldsymbol{\xi}) \psi(\boldsymbol{\xi}') \, d\boldsymbol{\xi} d\boldsymbol{\xi}' \\ &= \int_{\mathbb{R} \times \mathbb{R}} \phi(\eta \mathbf{w}) \psi(\eta' \mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \overline{\mathcal{F}[\mathbf{g}_1](\eta')} e^{2\pi i b (\eta - \eta')} \, d\eta d\eta'. \end{aligned}$$

By assumption $b \sim \mathcal{N}(0, \sigma_b^2)$, i.e., $\rho_b(b) = \frac{1}{\sqrt{2\pi\sigma_b}} e^{-\frac{b^2}{2\sigma_b^2}}$, then $\mathcal{F}[\rho_b](\eta) = e^{-2\pi^2\sigma_b^2\eta^2}$.

$$\begin{aligned} \mathbb{E}_b \left(e^{2\pi i b (\eta - \eta')} \right) &= \int_{\mathbb{R}} \frac{1}{\sqrt{2\pi\sigma_b}} e^{-b^2/2\sigma_b^2} e^{2\pi i b (\eta - \eta')} \, db \\ &= \mathcal{F}[\rho_b](-(\eta - \eta')) \\ &= e^{-2\pi^2\sigma_b^2(\eta - \eta')^2}. \end{aligned}$$

Therefore

$$\begin{aligned} \mathbb{E}_b \left[\langle \hat{K}_{a,b}, \phi \otimes \psi \rangle \right] &= \int_{\mathbb{R} \times \mathbb{R}} \phi(\eta \mathbf{w}) \psi(\eta' \mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \overline{\mathcal{F}[\mathbf{g}_1](\eta')} \mathbb{E}_b \left[e^{2\pi i b (\eta - \eta')} \right] \, d\eta d\eta' \\ &= \int_{\mathbb{R} \times \mathbb{R}} \phi(\eta \mathbf{w}) \psi(\eta' \mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \overline{\mathcal{F}[\mathbf{g}_1](\eta')} e^{-2\pi^2\sigma_b^2(\eta - \eta')^2} \, d\eta d\eta'. \end{aligned}$$

Applying the Laplace method, we have

$$\begin{aligned} \mathbb{E}_b \left[\langle \hat{K}_{a,b}, \phi \otimes \psi \rangle \right] &= \int_{\mathbb{R}} \phi(\eta \mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \left[\int_{\mathbb{R}} \psi(\eta' \mathbf{w}) \overline{\mathcal{F}[\mathbf{g}_1](\eta')} e^{-2\pi^2\sigma_b^2(\eta - \eta')^2} \, d\eta' \right] \, d\eta \\ &= \int_{\mathbb{R}} \phi(\eta \mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \left[\psi(\eta \mathbf{w}) \overline{\mathcal{F}[\mathbf{g}_1](\eta)} \frac{1}{\sqrt{2\pi\sigma_b}} + O(\sigma_b^{-3}) \right] \, d\eta \\ &= \frac{1}{\sqrt{2\pi\sigma_b}} \int_{\mathbb{R}} \phi(\eta \mathbf{w}) \psi(\eta \mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \overline{\mathcal{F}[\mathbf{g}_1](\eta)} \, d\eta + O(\sigma_b^{-3}). \end{aligned}$$

Next we consider the expectation with respect to \mathbf{w} . Up to error of order $O(\sigma_c^{-3})$, we have

$$\begin{aligned} \mathbb{E}_{\mathbf{w}, b} \left[\langle \hat{K}_{a,b}, \phi \otimes \psi \rangle \right] &= \mathbb{E}_{\mathbf{w}} \left[\frac{1}{\sqrt{2\pi\sigma_b}} \int_{\mathbb{R}} \phi(\eta \mathbf{w}) \psi(\eta \mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \overline{\mathcal{F}[\mathbf{g}_1](\eta)} \, d\eta \right] \\ &= \int_{\mathbb{R}^{d+1}} \frac{1}{\sqrt{2\pi\sigma_b}} \phi(\eta \mathbf{w}) \psi(\eta \mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \overline{\mathcal{F}[\mathbf{g}_1](\eta)} \rho_{\mathbf{w}}(\mathbf{w}) \, d\mathbf{w} d\eta. \end{aligned}$$

Here we assume that $\rho_{\mathbf{w}}$ is radially symmetric so $\rho_{\mathbf{w}}(\mathbf{w})$ is a function of $r := \|\mathbf{w}\|$ only. By using spherical coordinate system, we have

$$\begin{aligned} 1 &= \int_{\mathbb{R}^d} \rho_{\mathbf{w}}(\mathbf{w}) \, d\mathbf{w} \\ &= \int_{\mathbb{R}^d} \rho_{\mathbf{w}}(\|\mathbf{w}\| \mathbf{e}_1) \, d\mathbf{w} \\ &= \int_{\mathbb{R}^+} \int_{\mathbb{S}^{d-1}} \rho_{\mathbf{w}}(r \mathbf{e}_1) r^{d-1} \, d\hat{\mathbf{w}} \, dr \\ &= \int_{\mathbb{R}^+} \rho_r(r) \, dr, \end{aligned}$$

where $\hat{\mathbf{w}} \in \mathbb{S}^{d-1}$ and we define

$$(SM2.11) \quad \rho_r(r) := \int_{\mathbb{S}^{d-1}} \rho_{\mathbf{w}}(r\mathbf{e}_1) r^{d-1} d\hat{\mathbf{w}} = \frac{2\pi^{d/2}}{\Gamma(d/2)} \rho_{\mathbf{w}}(r\mathbf{e}_1) r^{d-1},$$

where $\Gamma(\cdot)$ is the gamma function. Then we introduce the following change of variables,

$$\begin{cases} \boldsymbol{\zeta} = \eta \mathbf{w}, \\ r = \|\mathbf{w}\|, \end{cases}$$

whose the Jacobian determinant is

$$\det \left(\frac{\partial(\boldsymbol{\zeta}, r)}{\partial(\mathbf{w}, \eta)} \right) = \det \begin{bmatrix} \eta & 0 & \cdots & 0 & w_1 \\ 0 & \eta & \cdots & 0 & w_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \eta & w_d \\ w_1/r & w_2/r & \cdots & w_d/r & 0 \end{bmatrix} = -r\eta^{d-1} = -r \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right)^{d-1}.$$

Thus

$$(SM2.12) \quad \begin{cases} \mathbf{w} = \frac{r\boldsymbol{\zeta}}{\|\boldsymbol{\zeta}\|} \\ \eta = \frac{\|\boldsymbol{\zeta}\|}{r}, \end{cases}$$

and its Jacobian determinant is

$$\det \left(\frac{\partial(\mathbf{w}, \eta)}{\partial(\boldsymbol{\zeta}, r)} \right) = -\frac{r^{d-1}}{r\|\boldsymbol{\zeta}\|^{d-1}}.$$

So one can obtain,

$$\begin{aligned} \mathbb{E}_{\mathbf{w}, b} \left[\langle \hat{K}_{a,b}, \phi \otimes \psi \rangle \right] &= \int_{\mathbb{R}^{d+1}} \frac{1}{\sqrt{2\pi}\sigma_b} \phi(\eta\mathbf{w}) \psi(\eta\mathbf{w}) \mathcal{F}[\mathbf{g}_1](\eta) \cdot \overline{\mathcal{F}[\mathbf{g}_1](\eta)} \rho_{\mathbf{w}}(r\mathbf{e}_1) d\mathbf{w} d\eta \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^+} \frac{1}{\sqrt{2\pi}\sigma_b} \phi(\boldsymbol{\zeta}) \psi(\boldsymbol{\zeta}) \mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right) \cdot \overline{\mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right)} \frac{r^{d-1}}{r\|\boldsymbol{\zeta}\|^{d-1}} \rho_{\mathbf{w}}(r\mathbf{e}_1) d\boldsymbol{\zeta} dr \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^+} \frac{1}{\sqrt{2\pi}\sigma_b} \phi(\boldsymbol{\zeta}) \psi(\boldsymbol{\zeta}) \mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right) \cdot \overline{\mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right)} \frac{1}{r\|\boldsymbol{\zeta}\|^{d-1}} \left[\frac{\Gamma(d/2)}{2\pi^{d/2}} \rho_r(r) \right] d\boldsymbol{\zeta} dr \\ &= \frac{\Gamma(d/2)}{2\sqrt{2\pi}^{(d+1)/2}\sigma_b} \int_{\mathbb{R}^d} \phi(\boldsymbol{\zeta}) \int_{\mathbb{R}^+} \left[\frac{1}{r\|\boldsymbol{\zeta}\|^{d-1}} \mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right) \cdot \overline{\mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right)} \right] \psi(\boldsymbol{\zeta}) \rho_r(r) dr d\boldsymbol{\zeta}, \end{aligned}$$

Therefore taking $\psi = \mathcal{F}[u_\rho]$, we have

$$(SM2.13) \quad \begin{aligned} \mathcal{L}_{a,b}[\mathcal{F}[u_\rho]] &= \frac{\Gamma(d/2)}{2\sqrt{2\pi}^{(d+1)/2}\sigma_b \|\boldsymbol{\xi}\|^{d-1}} \mathbb{E}_{a,r} \left[\frac{1}{r} \mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \cdot \overline{\mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right)} \right] \mathcal{F}[u_\rho](\boldsymbol{\xi}) \\ &= \frac{\Gamma(d/2)}{2\sqrt{2\pi}^{(d+1)/2}\sigma_b \|\boldsymbol{\xi}\|^{d-1}} \mathbb{E}_{a,r} \left[\frac{1}{r} \mathcal{F}[\mathbf{g}_1] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \cdot \mathcal{F}[\mathbf{g}_1] \left(-\frac{\|\boldsymbol{\xi}\|}{r} \right) \right] \mathcal{F}[u_\rho](\boldsymbol{\xi}). \end{aligned}$$

3. Calculate $\hat{K}_{\mathbf{w}}(\boldsymbol{\xi}, \boldsymbol{\xi}')$. Since

$$\begin{aligned} \hat{K}_{\mathbf{w}}(\boldsymbol{\xi}, \boldsymbol{\xi}') &= \frac{1}{4\pi^2} \nabla_{\boldsymbol{\xi}} \left[\delta_{\mathbf{w}}(\boldsymbol{\xi}) \mathcal{F}[g_2] \left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right) e^{2\pi i b \boldsymbol{\xi}^\top \hat{\mathbf{w}} / \|\mathbf{w}\|} \right] \\ &\quad \cdot \nabla_{\boldsymbol{\xi}'} \left[\overline{\delta_{\mathbf{w}}(\boldsymbol{\xi}') \mathcal{F}[g_2] \left(\frac{\boldsymbol{\xi}'^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right) e^{-2\pi i b \boldsymbol{\xi}'^\top \hat{\mathbf{w}} / \|\mathbf{w}\|}} \right], \end{aligned}$$

we have

$$\begin{aligned} &\langle \hat{K}_{\mathbf{w}}, \phi \otimes \psi \rangle \\ &= \frac{1}{4\pi^2} \int_{\mathbb{R}^d} \phi(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \left[\delta_{\mathbf{w}}(\boldsymbol{\xi}) \mathcal{F}[g_2] \left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right) e^{2\pi i b \boldsymbol{\xi}^\top \hat{\mathbf{w}} / \|\mathbf{w}\|} \right] d\boldsymbol{\xi} \\ &\quad \cdot \int_{\mathbb{R}^d} \psi(\boldsymbol{\xi}') \nabla_{\boldsymbol{\xi}'} \left[\overline{\delta_{\mathbf{w}}(\boldsymbol{\xi}') \mathcal{F}[g_2] \left(\frac{\boldsymbol{\xi}'^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right) e^{-2\pi i b \boldsymbol{\xi}'^\top \hat{\mathbf{w}} / \|\mathbf{w}\|}} \right] d\boldsymbol{\xi}' \\ &= \frac{1}{4\pi^2} \int_{\mathbb{R}^d} \nabla_{\boldsymbol{\xi}} \phi(\boldsymbol{\xi}) \delta_{\mathbf{w}}(\boldsymbol{\xi}) \mathcal{F}[g_2] \left(\frac{\boldsymbol{\xi}^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right) e^{2\pi i b \boldsymbol{\xi}^\top \hat{\mathbf{w}} / \|\mathbf{w}\|} d\boldsymbol{\xi} \\ &\quad \cdot \int_{\mathbb{R}^d} \nabla_{\boldsymbol{\xi}'} \psi(\boldsymbol{\xi}') \overline{\delta_{\mathbf{w}}(\boldsymbol{\xi}') \mathcal{F}[g_2] \left(\frac{\boldsymbol{\xi}'^\top \hat{\mathbf{w}}}{\|\mathbf{w}\|} \right) e^{-2\pi i b \boldsymbol{\xi}'^\top \hat{\mathbf{w}} / \|\mathbf{w}\|}} d\boldsymbol{\xi}' \\ &= \int_{\mathbb{R} \times \mathbb{R}} \nabla \phi(\eta \mathbf{w}) \cdot \nabla \psi(\eta' \mathbf{w}) \mathcal{F}[g_2](\eta) \cdot \overline{\mathcal{F}[g_2](\eta')} e^{2\pi i b(\eta - \eta')} d\eta d\eta'. \end{aligned}$$

By the same computation as for $\hat{K}_{a,b}(\boldsymbol{\xi}, \boldsymbol{\xi}')$, we can get

$$\begin{aligned} &\mathbb{E}_{\mathbf{w},b} \left[\langle \hat{K}_{\mathbf{w}}, \phi \otimes \psi \rangle \right] \\ &= \frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b} \int_{\mathbb{R}^d} \nabla \phi(\boldsymbol{\zeta}) \cdot \int_{\mathbb{R}^+} \left[\frac{1}{r\|\boldsymbol{\zeta}\|^{d-1}} \mathcal{F}[g_2] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right) \cdot \overline{\mathcal{F}[g_2] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right)} \right] \nabla \psi(\boldsymbol{\zeta}) \rho_r(r) dr d\boldsymbol{\zeta} \\ &= \frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b} \int_{\mathbb{R}^d} \nabla \phi(\boldsymbol{\zeta}) \cdot \mathbb{E}_{a,r} \left[\frac{1}{r\|\boldsymbol{\zeta}\|^{d-1}} \mathcal{F}[g_2] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right) \cdot \overline{\mathcal{F}[g_2] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right)} \right] \nabla \psi(\boldsymbol{\zeta}) d\boldsymbol{\zeta} \\ &= -\frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b} \int_{\mathbb{R}^d} \phi(\boldsymbol{\zeta}) \nabla \cdot \left\{ \mathbb{E}_{a,r} \left[\frac{1}{r\|\boldsymbol{\zeta}\|^{d-1}} \mathcal{F}[g_2] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right) \cdot \overline{\mathcal{F}[g_2] \left(\frac{\|\boldsymbol{\zeta}\|}{r} \right)} \right] \nabla \psi(\boldsymbol{\zeta}) \right\} d\boldsymbol{\zeta}. \end{aligned}$$

Thus taking $\psi(\boldsymbol{\xi}) = \mathcal{F}[u_\rho](\boldsymbol{\xi})$, we have

$$(SM2.14) \quad \mathcal{L}_{\mathbf{w}}[\mathcal{F}[u_\rho](\boldsymbol{\xi})] = -\frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b} \nabla \cdot \left(\mathbb{E}_{a,r} \left[\frac{1}{r\|\boldsymbol{\xi}\|^{d-1}} \mathcal{F}[g_2] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \mathcal{F}[g_2] \left(-\frac{\|\boldsymbol{\xi}\|}{r} \right) \right] \nabla \mathcal{F}[u_\rho](\boldsymbol{\xi}) \right).$$

Finally, one can plug (SM2.13) and (SM2.14) into (SM2.5) and obtain the dynamics (SM2.7). ■

Corollary. (Corollary 1 in main text) Suppose that Assumption 1 holds. If $\sigma_b \gg 1$ and $\sigma = \text{ReLU}$, then the dynamics (4.9) has the following expression,

$$(SM2.15) \quad \langle \partial_t \mathcal{F}[u], \phi \rangle = -\langle \mathcal{L}[\mathcal{F}[u_\rho]], \phi \rangle + O(\sigma_b^{-3}),$$

where $\phi \in \mathcal{S}(\mathbb{R}^d)$ is a test function and the LFP operator reads as

$$(SM2.16) \quad \begin{aligned} \mathcal{L}[\mathcal{F}[u_\rho]] &= \frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b} \mathbb{E}_{a,r} \left[\frac{r^3}{16\pi^4 \|\boldsymbol{\xi}\|^{d+3}} + \frac{a^2 r}{4\pi^2 \|\boldsymbol{\xi}\|^{d+1}} \right] \mathcal{F}[u_\rho](\boldsymbol{\xi}) \\ &\quad - \frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b} \nabla \cdot \left(\mathbb{E}_{a,r} \left[\frac{a^2 r}{4\pi^2 \|\boldsymbol{\xi}\|^{d+1}} \right] \nabla \mathcal{F}[u_\rho](\boldsymbol{\xi}) \right). \end{aligned}$$

The expectations are taken w.r.t. initial parameter distribution. Here $r = \|\mathbf{w}\|$ with the probability density $\rho_r(r) := \frac{2\pi^{d/2}}{\Gamma(d/2)} \rho_{\mathbf{w}}(r\mathbf{e}_1) r^{d-1}$, $\mathbf{e}_1 = (1, 0, \dots, 0)^\top$.

Proof. Let

$$(SM2.17) \quad f_a(\mathbf{x}) := \nabla_a [a\text{ReLU}(\mathbf{w} \cdot \mathbf{x} + b)] = \text{ReLU}(\mathbf{w} \cdot \mathbf{x} + b),$$

$$(SM2.18) \quad g_a(z) := \text{ReLU}(z),$$

$$(SM2.19) \quad f_b(\mathbf{x}) := \nabla_b [a\text{ReLU}(\mathbf{w} \cdot \mathbf{x} + b)] = aH(\mathbf{w} \cdot \mathbf{x} + b),$$

$$(SM2.20) \quad g_b(z) := aH(z),$$

so $\mathbf{g}_1(z) = (g_a(z), g_b(z))^\top$ and $g_2(z) = g_b(z)$. Then

$$(SM2.21) \quad \mathcal{F}[g_a](\xi) = -\frac{1}{4\pi^2 \xi^2} + \frac{i}{4\pi} \delta'(\xi),$$

$$(SM2.22) \quad \mathcal{F}[g_b](\xi) = a \left[\frac{1}{i2\pi\xi} + \frac{1}{2} \delta(\xi) \right],$$

By ignoring all $\delta(\xi)$ and $\delta'(\xi)$ related to only the trivial $\mathbf{0}$ -frequency, we obtain

$$(SM2.23) \quad \frac{1}{r} \mathcal{F}[g_a] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \mathcal{F}[g_a] \left(\frac{-\|\boldsymbol{\xi}\|}{r} \right) = \frac{r^3}{16\pi^4 \|\boldsymbol{\xi}\|^4},$$

$$(SM2.24) \quad \frac{1}{r} \mathcal{F}[g_b] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \mathcal{F}[g_b] \left(\frac{-\|\boldsymbol{\xi}\|}{r} \right) = \frac{a^2 r}{4\pi^2 \|\boldsymbol{\xi}\|^2}.$$

We then obtain (SM2.16) by plugging these into (SM2.8). ■

Corollary. (Corollary 2 in main text) Suppose that Assumption 1 holds. If $\sigma_b \gg 1$ and $\sigma = \tanh$, then the dynamics (4.9) has the following expression,

$$(SM2.25) \quad \langle \partial_t \mathcal{F}[u], \phi \rangle = -\langle \mathcal{L}[\mathcal{F}[u_\rho]], \phi \rangle + O(\sigma_b^{-3}),$$

where $\phi \in \mathcal{S}(\mathbb{R}^d)$ is a test function and the LFP operator reads as

$$(SM2.26) \quad \begin{aligned} \mathcal{L}[\mathcal{F}[u_\rho]] &= \frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b \|\boldsymbol{\xi}\|^{d-1}} \mathbb{E}_{a,r} \left[\frac{\pi^2}{r} \text{csch}^2 \left(\frac{\pi^2 \|\boldsymbol{\xi}\|}{r} \right) + \frac{4\pi^4 a^2 \|\boldsymbol{\xi}\|^2}{r^3} \text{csch}^2 \left(\frac{\pi^2 \|\boldsymbol{\xi}\|}{r} \right) \right] \mathcal{F}[u_\rho](\boldsymbol{\xi}) \\ &\quad - \frac{\Gamma(d/2)}{2\sqrt{2}\pi^{(d+1)/2}\sigma_b} \nabla \cdot \left(\mathbb{E}_{a,r} \left[\frac{4\pi^4 a^2}{r^3 \|\boldsymbol{\xi}\|^{d-3}} \text{csch}^2 \left(\frac{\pi^2 \|\boldsymbol{\xi}\|}{r} \right) \right] \nabla \mathcal{F}[u_\rho](\boldsymbol{\xi}) \right). \end{aligned}$$

The expectations are taken w.r.t. initial parameter distribution. Here $r = \|\mathbf{w}\|$ with the probability density $\rho_r(r) := \frac{2\pi^{d/2}}{\Gamma(d/2)} \rho_{\mathbf{w}}(r\mathbf{e}_1) r^{d-1}$, $\mathbf{e}_1 = (1, 0, \dots, 0)^\top$.

Proof. Let

$$(SM2.27) \quad f_a(\mathbf{x}) := \nabla_a [a \tanh(\mathbf{w} \cdot \mathbf{x} + b)] = \tanh(\mathbf{w} \cdot \mathbf{x} + b),$$

$$(SM2.28) \quad g_a(z) := \tanh(z),$$

$$(SM2.29) \quad f_b(\mathbf{x}) := \nabla_b [a \tanh(\mathbf{w} \cdot \mathbf{x} + b)] = a \operatorname{sech}^2(\mathbf{w} \cdot \mathbf{x} + b),$$

$$(SM2.30) \quad g_b(z) := a \operatorname{sech}^2(z),$$

so $\mathbf{g}_1(z) = (g_a(z), g_b(z))^\top$ and $g_2(z) = g_b(z)$. Then

$$(SM2.31) \quad \mathcal{F}[g_a](\xi) = -i\pi \operatorname{csch}(\pi^2 \xi),$$

$$(SM2.32) \quad \mathcal{F}[g_b](\xi) = 2\pi^2 a \xi \operatorname{csch}(\pi^2 \xi).$$

By ignoring all $\delta(\xi)$ and $\delta'(\xi)$ related to only the trivial $\mathbf{0}$ -frequency, we obtain

$$(SM2.33) \quad \frac{1}{r} \mathcal{F}[g_a] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \mathcal{F}[g_a] \left(\frac{-\|\boldsymbol{\xi}\|}{r} \right) = \frac{\pi^2}{r} \operatorname{csch}^2 \left(\frac{\pi^2 \|\boldsymbol{\xi}\|}{r} \right),$$

$$(SM2.34) \quad \frac{1}{r} \mathcal{F}[g_b] \left(\frac{\|\boldsymbol{\xi}\|}{r} \right) \mathcal{F}[g_b] \left(\frac{-\|\boldsymbol{\xi}\|}{r} \right) = \frac{4\pi^4 a^2 \|\boldsymbol{\xi}\|^2}{r^3} \operatorname{csch}^2 \left(\frac{\pi^2 \|\boldsymbol{\xi}\|}{r} \right).$$

We then obtain (SM2.26) by plugging these into (4.17). ■

Lemma. (Lemma 4 in main text) Suppose that H_1 and H_2 are two separable Hilbert spaces and $\mathcal{P} : H_1 \rightarrow H_2$ and $\mathcal{P}^* : H_2 \rightarrow H_1$ is the adjoint of \mathcal{P} . Then all eigenvalues of $\mathcal{P}^*\mathcal{P}$ and $\mathcal{P}\mathcal{P}^*$ are non-negative. Moreover, they have the same positive spectrum. If in particular, we assume that the operator $\mathcal{P}\mathcal{P}^*$ is surjective, then the operator $\mathcal{P}\mathcal{P}^*$ is invertible.

Proof. We consider the eigenvalue problem $\mathcal{P}^*\mathcal{P}\phi_1 = \lambda\phi_1$. Taking inner product with ϕ_1 , we have $\langle \phi_1, \mathcal{P}^*\mathcal{P}\phi_1 \rangle_{H_1} = \lambda \|\phi_1\|_{H_1}^2$. Note that the left hand side is $\|\mathcal{P}\phi_1\|_{H_2}^2$ which is non-negative. Thus $\lambda \geq 0$. Similarly, the eigenvalues of $\mathcal{P}\mathcal{P}^*$ are also non-negative.

Now if $\mathcal{P}^*\mathcal{P}$ has a positive eigenvalue $\lambda > 0$, then $\mathcal{P}^*\mathcal{P}\phi_1 = \lambda\phi_1$ with non-zero vector $\phi_1 \in H_1$. It follows that $\mathcal{P}\mathcal{P}^*(\mathcal{P}\phi_1) = \lambda(\mathcal{P}\phi_1)$. It is sufficient to prove that $\mathcal{P}\phi_1$ is non-zero. Indeed, if $\mathcal{P}\phi_1 = 0$, then $\mathcal{P}^*\mathcal{P}\phi_1 = 0$ and $\lambda = 0$ which contradicts with our assumption. Therefore, any positive eigenvalue of $\mathcal{P}^*\mathcal{P}$ is an eigenvalue of $\mathcal{P}\mathcal{P}^*$. Similarly, any positive eigenvalue of $\mathcal{P}\mathcal{P}^*$ is an eigenvalue of $\mathcal{P}^*\mathcal{P}$.

Next, suppose that $\mathcal{P}\mathcal{P}^*$ is surjective. We show that $\mathcal{P}\mathcal{P}^*\phi_2 = 0$ has only the trivial solution $\phi_2 = 0$. In fact, $\mathcal{P}\mathcal{P}^*\phi_2 = 0$ implies that $\|\mathcal{P}^*\phi_2\|_{H_1}^2 = \langle \phi_2, \mathcal{P}\mathcal{P}^*\phi_2 \rangle_{H_2} = 0$, i.e., $\mathcal{P}^*\phi_2 = 0$. Thanks to the surjectivity of $\mathcal{P}\mathcal{P}^*$, there exists a vector $\phi_3 \in H_2$ such that $\phi_2 = \mathcal{P}\mathcal{P}^*\phi_3$. Let $\phi_1 = \mathcal{P}^*\phi_3 \in H_1$. Hence $\phi_2 = \mathcal{P}\phi_1$ and $\mathcal{P}^*\mathcal{P}\phi_1 = 0$. Taking inner product with ϕ_1 , we have $\|\mathcal{P}\phi_1\|_{H_2}^2 = \langle \phi_1, \mathcal{P}^*\mathcal{P}\phi_1 \rangle_{H_1} = 0$, i.e., $\phi_2 = \mathcal{P}\phi_1 = 0$. Therefore $\mathcal{P}\mathcal{P}^*$ is injective. This with the surjectivity assumption of $\mathcal{P}\mathcal{P}^*$ leads to that $\mathcal{P}\mathcal{P}^*$ is invertible. ■

Theorem. (Theorem 2 in main text) Suppose that $\mathcal{P}\mathcal{P}^*$ is surjective. The above Problems (i) and (ii) are equivalent in the sense that $\phi_\infty = \phi_{\min}$. More precisely, we have

$$(SM2.35) \quad \phi_\infty = h_{\min} = \mathcal{P}^*(\mathcal{P}\mathcal{P}^*)^{-1}(g - \mathcal{P}\phi_{\text{ini}}) + \phi_{\text{ini}}.$$

Proof. Let $\tilde{\phi} = \phi - \phi_{\text{ini}}$ and $\tilde{g} = g - \mathcal{P}\phi_{\text{ini}}$. Then it is sufficient to show the following problems (i') and (ii') are equivalent.

(i') The initial value problem

$$\begin{cases} \frac{d\tilde{\phi}}{dt} = \mathcal{P}^*(\tilde{g} - \mathcal{P}\tilde{\phi}) \\ \tilde{\phi}(0) = 0. \end{cases}$$

(ii') The minimization problem

$$\begin{aligned} & \min_{\tilde{\phi}} \|\tilde{\phi}\|_{H_1}^2, \\ & \text{s.t. } \mathcal{P}\tilde{\phi} = \tilde{g}. \end{aligned}$$

We claim that $\tilde{\phi}_{\text{min}} = \mathcal{P}^*(\mathcal{P}\mathcal{P}^*)^{-1}\tilde{g}$. Thanks to Lemma 4, $\mathcal{P}\mathcal{P}^*$ is invertible, and thus $\tilde{\phi}_{\text{min}}$ is well-defined and satisfies that $\mathcal{P}\tilde{\phi} = \tilde{g}$. It remains to show that this solution is unique. In fact, for any $\tilde{\phi}$ satisfying $\mathcal{P}\tilde{\phi} = \tilde{g}$, we have

$$\begin{aligned} \langle \tilde{\phi} - \tilde{\phi}_{\text{min}}, \tilde{\phi}_{\text{min}} \rangle_{H_1} &= \langle \tilde{\phi} - \tilde{\phi}_{\text{min}}, \mathcal{P}^*(\mathcal{P}\mathcal{P}^*)^{-1}\tilde{g} \rangle_{H_1} \\ &= \langle \mathcal{P}(\tilde{\phi} - \tilde{\phi}_{\text{min}}), (\mathcal{P}\mathcal{P}^*)^{-1}\tilde{g} \rangle_{H_2} \\ &= \langle \mathcal{P}\tilde{\phi}, (\mathcal{P}\mathcal{P}^*)^{-1}\tilde{g} \rangle_{H_2} - \langle \mathcal{P}\tilde{\phi}_{\text{min}}, (\mathcal{P}\mathcal{P}^*)^{-1}\tilde{g} \rangle_{H_2} \\ &= 0. \end{aligned}$$

Therefore,

$$\|\tilde{\phi}\|_{H_1}^2 = \|\tilde{\phi}_{\text{min}}\|_{H_1}^2 + \|\tilde{\phi} - \tilde{\phi}_{\text{min}}\|_{H_1}^2 \geq \|\tilde{\phi}_{\text{min}}\|_{H_1}^2.$$

The equality holds if and only if $\tilde{\phi} = \tilde{\phi}_{\text{min}}$.

For problem (i'), from the theory of ordinary differential equations on Hilbert spaces, we have that its solution can be written as

$$\tilde{\phi}(t) = \mathcal{P}^*(\mathcal{P}\mathcal{P}^*)^{-1}\tilde{g} + \sum_{i \in \mathcal{I}} c_i v_i \exp(-\lambda_i t),$$

where λ_i , $i \in \mathcal{I}$ are positive eigenvalues of $\mathcal{P}\mathcal{P}^*$, \mathcal{I} is an index set with at most countable cardinality, and v_i , $i \in \mathcal{I}$ are eigenvectors in H_1 . Thus $\tilde{\phi}_{\infty} = \tilde{\phi}_{\text{min}} = \mathcal{P}^*(\mathcal{P}\mathcal{P}^*)^{-1}\tilde{g}$.

Finally, by back substitution, we have

$$\phi_{\infty} = \phi_{\text{min}} = \mathcal{P}^*(\mathcal{P}\mathcal{P}^*)^{-1}\tilde{g} + \phi_0 = \mathcal{P}^*(\mathcal{P}\mathcal{P}^*)^{-1}(g - \mathcal{P}\phi_{\text{ini}}) + \phi_{\text{ini}}. \quad \blacksquare$$

Corollary. (Corollary 4 in main text) Let H_1 and H_2 be two separable Hilbert spaces and $\Gamma : H_1 \rightarrow H_1$ be an injective operator. Define the Hilbert space $H_{\Gamma} := \text{Im}(\Gamma)$. Let $g \in H_2$ and $\mathcal{P} : H_{\Gamma} \rightarrow H_2$ be an operator such that $\mathcal{P}\mathcal{P}^* : H_2 \rightarrow H_2$ is surjective. Then $\Gamma^{-1} : H_{\Gamma} \rightarrow H_1$ exists and H_{Γ} is a Hilbert space with norm $\|\phi\|_{H_{\Gamma}} := \|\Gamma^{-1}\phi\|_{H_1}$. Moreover, the following two problems are equivalent in the sense that $\phi_{\infty} = \phi_{\text{min}}$.

(B1) *The initial value problem*

$$\begin{cases} \frac{d\phi}{dt} = \Gamma\Gamma^*\mathcal{P}^*(g - \mathcal{P}\phi) \\ \phi(0) = \phi_{\text{ini}}. \end{cases}$$

(B2) *The minimization problem*

$$\begin{aligned} & \min_{\phi - \phi_0 \in H_\Gamma} \|\phi - \phi_{\text{ini}}\|_{H_\Gamma}, \\ & \text{s.t. } \mathcal{P}\phi = g. \end{aligned}$$

Proof. The operator $\Gamma : H_1 \rightarrow H_\Gamma$ is bijective. Hence $\Gamma^{-1} : H_\Gamma \rightarrow H_1$ is well-defined and H_Γ with norm $\|\cdot\|_{H_\Gamma}$ is a Hilbert space. The equivalence result holds by applying Theorem 2 with proper replacements. More precisely, we replace ϕ by $\Gamma^{-1}\phi$ and \mathcal{P} by $\mathcal{P}\Gamma$. \blacksquare

Corollary. (Corollary 5 in main text) Let $\gamma : \mathbb{R}^d \rightarrow \mathbb{R}^+$ be a positive function, h be a function in $L^2(\mathbb{R}^d)$ and $\phi = \mathcal{F}[h]$. The operator $\Gamma : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ is defined by $[\Gamma\phi](\boldsymbol{\xi}) = \gamma(\boldsymbol{\xi})\phi(\boldsymbol{\xi})$, $\boldsymbol{\xi} \in \mathbb{R}^d$. Define the Hilbert space $H_\Gamma := \text{Im}(\Gamma)$. Let $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\top \in \mathbb{R}^{n \times d}$, $\mathbf{Y} = (y_1, \dots, y_n)^\top \in \mathbb{R}^n$ and $\mathcal{P} : H_\Gamma \rightarrow \mathbb{R}^n$ be a surjective operator

$$(SM2.36) \quad \mathcal{P} : \phi \mapsto \left(\int_{\mathbb{R}^d} \phi(\boldsymbol{\xi}) e^{2\pi i \mathbf{x}_1^\top \boldsymbol{\xi}} d\boldsymbol{\xi}, \dots, \int_{\mathbb{R}^d} \phi(\boldsymbol{\xi}) e^{2\pi i \mathbf{x}_n^\top \boldsymbol{\xi}} d\boldsymbol{\xi} \right)^\top = (h(\mathbf{x}_1), \dots, h(\mathbf{x}_n))^\top.$$

Then the following two problems are equivalent in the sense that $\phi_\infty = \phi_{\text{min}}$.

(C1) *The initial value problem*

$$\begin{cases} \frac{d\phi(\boldsymbol{\xi})}{dt} = (\gamma(\boldsymbol{\xi}))^2 \sum_{i=1}^n \left(y_i e^{-2\pi i \mathbf{x}_i^\top \boldsymbol{\xi}} - [\phi * e^{-2\pi i \mathbf{x}_i^\top (\cdot)}](\boldsymbol{\xi}) \right) \\ \phi(0) = \phi_{\text{ini}}. \end{cases}$$

(C2) *The minimization problem*

$$\begin{aligned} & \min_{\phi - \phi_{\text{ini}} \in H_\Gamma} \int_{\mathbb{R}^d} (\gamma(\boldsymbol{\xi}))^{-2} |\phi(\boldsymbol{\xi}) - \phi_{\text{ini}}(\boldsymbol{\xi})|^2 d\boldsymbol{\xi}, \\ & \text{s.t. } h(\mathbf{x}_i) = y_i, \quad i = 1, \dots, n. \end{aligned}$$

Proof. Let $H_1 = L^2(\mathbb{R}^d)$, $H_2 = \mathbb{R}^n$, $g = \mathbf{Y}$. By definition, Γ is injective. Then by Corollary 4, we have that $\Gamma^{-1} : H_\Gamma \rightarrow L^2(\mathbb{R}^d)$ exists and H_Γ is a Hilbert space with norm $\|\phi\|_{H_\Gamma} := \|\Gamma^{-1}\phi\|_{L^2(\mathbb{R}^d)}$. Moreover, $\|\phi - \phi_{\text{ini}}\|_{H_\Gamma}^2 = \int_{\mathbb{R}^d} (\gamma(\boldsymbol{\xi}))^{-2} |\phi(\boldsymbol{\xi}) - \phi_{\text{ini}}(\boldsymbol{\xi})|^2 d\boldsymbol{\xi}$. We note that $[\mathcal{P}^*\mathbf{Y}](\boldsymbol{\xi}) = \sum_{i=1}^n y_i e^{-2\pi i \mathbf{x}_i^\top \boldsymbol{\xi}}$ for all $\boldsymbol{\xi} \in \mathbb{R}^d$. Thus

$$\begin{aligned} [\mathcal{P}^*\mathcal{P}\phi](\boldsymbol{\xi}) &= \left[\mathcal{P}^* \left(\int_{\mathbb{R}^d} \phi(\boldsymbol{\xi}') e^{2\pi i \mathbf{x}_i^\top \boldsymbol{\xi}'} d\boldsymbol{\xi}' \right)_{i=1}^n \right](\boldsymbol{\xi}) \\ &= \sum_{i=1}^n \int_{\mathbb{R}^d} \phi(\boldsymbol{\xi}') e^{2\pi i \mathbf{x}_i^\top \boldsymbol{\xi}'} d\boldsymbol{\xi}' e^{-2\pi i \mathbf{x}_i^\top \boldsymbol{\xi}} \end{aligned}$$

$$\begin{aligned}
 &= \sum_{i=1}^n \int_{\mathbb{R}^d} \phi(\boldsymbol{\xi}') e^{-2\pi i \mathbf{x}_i^\top (\boldsymbol{\xi} - \boldsymbol{\xi}')} d\boldsymbol{\xi}' \\
 &= \sum_{i=1}^n \left[\phi * e^{-2\pi i \mathbf{x}_i^\top (\cdot)} \right] (\boldsymbol{\xi}).
 \end{aligned}$$

The equivalence result then follows from Corollary 4. ■

Corollary. (Corollary 6 in main text) Let $\gamma : \mathbb{Z}^d \rightarrow \mathbb{R}^+$ be a positive function defined on lattice \mathbb{Z}^d and $\phi = \mathcal{F}[h]$. The operator $\Gamma : \ell^2(\mathbb{Z}^d) \rightarrow \ell^2(\mathbb{Z}^d)$ is defined by $[\Gamma\phi](\mathbf{k}) = \gamma(\mathbf{k})\phi(\mathbf{k})$, $\mathbf{k} \in \mathbb{Z}^d$. Here $\ell^2(\mathbb{Z}^d)$ is set of square summable functions on the lattice \mathbb{Z}^d . Define the Hilbert space $H_\Gamma := \text{Im}(\Gamma)$. Let $X = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\top \in \mathbb{T}^{n \times d}$, $Y = (y_1, \dots, y_n)^\top \in \mathbb{R}^n$ and $\mathcal{P} : H_\Gamma \rightarrow \mathbb{R}^n$ be a surjective operator such as

$$(SM2.37) \quad P : \phi \mapsto \left(\sum_{\mathbf{k} \in \mathbb{Z}^d} \phi(\mathbf{k}) e^{2\pi i \mathbf{x}_1^\top \mathbf{k}}, \dots, \sum_{\mathbf{k} \in \mathbb{Z}^d} \phi(\mathbf{k}) e^{2\pi i \mathbf{x}_n^\top \mathbf{k}} \right)^\top.$$

Then the following two problems are equivalent in the sense that $\phi_\infty = \phi_{\min}$.

(D1) The initial value problem

$$\begin{cases} \frac{d\phi(\mathbf{k})}{dt} = (\gamma(\mathbf{k}))^2 \sum_{i=1}^n \left(y_i e^{-2\pi i \mathbf{x}_i^\top \mathbf{k}} - \left[\phi * e^{-2\pi i \mathbf{x}_i^\top (\cdot)} \right] (\mathbf{k}) \right) \\ \phi(\mathbf{0}) = \phi_{\text{ini}}. \end{cases}$$

(D2) The minimization problem

$$\begin{aligned}
 &\min_{\phi - \phi_{\text{ini}} \in H_\Gamma} \sum_{\mathbf{k} \in \mathbb{Z}^d} (\gamma(\mathbf{k}))^{-2} |\phi(\mathbf{k}) - \phi_{\text{ini}}(\mathbf{k})|^2, \\
 &s.t. \quad h(\mathbf{x}_i) = y_i, \quad i = 1, \dots, n.
 \end{aligned}$$

Proof. Let $H_1 = \ell^2(\mathbb{Z}^d)$, $H_2 = \mathbb{R}^n$, and $g = \mathbf{Y}$. By definition, Γ is injective. Then by Corollary 4, we have that $\Gamma^{-1} : H_\Gamma \rightarrow \ell^2(\mathbb{Z}^d)$ exists and H_Γ is a Hilbert space with norm $\|\phi\|_{H_\Gamma} := \|\Gamma^{-1}\phi\|_{\ell^2(\mathbb{Z}^d)}$. Moreover, $\|\phi - \phi_{\text{ini}}\|_{H_\Gamma}^2 = \sum_{\mathbf{k} \in \mathbb{Z}^d} (\gamma(\mathbf{k}))^{-2} |\phi(\mathbf{k}) - \phi_{\text{ini}}(\mathbf{k})|^2$. We note that $[P^* \mathbf{Y}](\mathbf{k}) = \sum_{i=1}^n y_i e^{-2\pi i \mathbf{x}_i^\top \mathbf{k}}$ for all $\mathbf{k} \in \mathbb{Z}^d$. Thus

$$\begin{aligned}
 [P^* P \phi](\mathbf{k}) &= \left[P^* \left(\sum_{\mathbf{k}' \in \mathbb{Z}^d} \phi(\mathbf{k}') e^{2\pi i \mathbf{x}_i^\top \mathbf{k}'} \right)_{i=1}^n \right] (\mathbf{k}) \\
 &= \sum_{i=1}^n \sum_{\mathbf{k}' \in \mathbb{Z}^d} \phi(\mathbf{k}') e^{2\pi i \mathbf{x}_i^\top \mathbf{k}'} e^{-2\pi i \mathbf{x}_i^\top \mathbf{k}} \\
 &= \sum_{i=1}^n \sum_{\mathbf{k}' \in \mathbb{Z}^d} \phi(\mathbf{k}') e^{-2\pi i \mathbf{x}_i^\top (\mathbf{k} - \mathbf{k}')} \\
 &= \sum_{i=1}^n \left[\phi * e^{-2\pi i \mathbf{x}_i^\top (\cdot)} \right] (\mathbf{k}).
 \end{aligned}$$

The equivalence result then follows from Corollary 4. \blacksquare

Lemma. (Lemma 5 in main text) (i) For $\mathcal{H}_Q = \{h : \|h\|_\gamma \leq Q\}$ with $\gamma : \mathbb{Z}^d \rightarrow \mathbb{R}^+$, we have

$$(SM2.38) \quad \text{Rad}_S(\mathcal{H}_Q) \leq \frac{1}{\sqrt{n}} Q \|\gamma\|_{\ell^2}.$$

(ii) For $\mathcal{H}'_Q = \{h : \|h\|_\gamma \leq Q, |\mathcal{F}[h](\mathbf{0})| \leq c_0\}$ with $\gamma : \mathbb{Z}^{d^*} \rightarrow \mathbb{R}^+$ and $\gamma^{-1}(\mathbf{0}) := 0$, we have

$$(SM2.39) \quad \text{Rad}_S(\mathcal{H}'_Q) \leq \frac{c_0}{\sqrt{n}} + \frac{1}{\sqrt{n}} Q \|\gamma\|_{\ell^2}.$$

Proof. We first prove (ii) since it is more involved. By the definition of the Rademacher complexity

$$(SM2.40) \quad \text{Rad}_S(\mathcal{H}'_Q) = \frac{1}{n} \mathbb{E}_\tau \left[\sup_{h \in \mathcal{H}'_Q} \sum_{i=1}^n \tau_i h(\mathbf{x}_i) \right].$$

Let $\tau(\mathbf{x}) = \sum_{i=1}^n \tau_i \delta(\mathbf{x} - \mathbf{x}_i)$, where τ_i 's are i.i.d. random variables with $\mathbb{P}(\tau_i = 1) = \mathbb{P}(\tau_i = -1) = \frac{1}{2}$. We have $\mathcal{F}[\tau](\mathbf{k}) = \int_\Omega \sum_{i=1}^n \tau_i \delta(\mathbf{x} - \mathbf{x}_i) e^{-2\pi i \mathbf{k}^\top \mathbf{x}} d\mathbf{x} = \sum_{i=1}^n \tau_i e^{-2\pi i \mathbf{k}^\top \mathbf{x}_i}$. Note that

$$(SM2.41) \quad \sup_{h \in \mathcal{H}'_Q} \sum_{i=1}^n \tau_i h(\mathbf{x}_i) = \sup_{h \in \mathcal{H}'_Q} \sum_{i=1}^n \tau_i \bar{h}(\mathbf{x}_i) = \sup_{h \in \mathcal{H}'_Q} \sum_{i=1}^n \tau_i \sum_{\mathbf{k} \in \mathbb{Z}^d} \overline{\mathcal{F}[h](\mathbf{k})} e^{-2\pi i \mathbf{k}^\top \mathbf{x}_i}$$

$$(SM2.42) \quad = \sup_{h \in \mathcal{H}'_Q} \sum_{\mathbf{k} \in \mathbb{Z}^d} \mathcal{F}[\tau](\mathbf{k}) \overline{\mathcal{F}[h](\mathbf{k})}.$$

By the Cauchy–Schwarz inequality,

$$(SM2.43) \quad \sup_{h \in \mathcal{H}'_Q} \sum_{\mathbf{k} \in \mathbb{Z}^d} \mathcal{F}[\tau](\mathbf{k}) \overline{\mathcal{F}[h](\mathbf{k})}$$

$$(SM2.44) \quad \leq \sup_{h \in \mathcal{H}'_Q} \left[\mathcal{F}[\tau](\mathbf{0}) \overline{\mathcal{F}[h](\mathbf{0})} + \left(\sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^2 |\mathcal{F}[\tau](\mathbf{k})|^2 \right)^{1/2} \left(\sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^{-2} |\overline{\mathcal{F}[h](\mathbf{k})}|^2 \right)^{1/2} \right]$$

$$\leq c_0 |\mathcal{F}[\tau](\mathbf{0})| + Q \left(\sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^2 |\mathcal{F}[\tau](\mathbf{k})|^2 \right)^{1/2}.$$

Since $\mathbb{E}_\tau |\mathcal{F}[\tau](\mathbf{0})| \leq (\mathbb{E}_\tau |\mathcal{F}[\tau](\mathbf{0})|^2)^{1/2} = \sqrt{n}$, $\mathbb{E}_\tau |\mathcal{F}[\tau](\mathbf{k})|^2 = \mathbb{E}_\tau \sum_{i,j=1}^n \tau_i \tau_j e^{-2\pi i \mathbf{k}^\top (\mathbf{x}_i - \mathbf{x}_j)} = n$, we obtain

$$(SM2.45) \quad \mathbb{E}_\tau \left[\sup_{h \in \mathcal{H}'_Q} \sum_{i=1}^n \tau_i h(\mathbf{x}_i) \right] \leq c_0 \sqrt{n} + Q \mathbb{E}_\tau \left(\sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^2 |\mathcal{F}[\tau](\mathbf{k})|^2 \right)^{1/2}$$

$$(SM2.46) \quad \leq c_0 \sqrt{n} + Q \left(\mathbb{E}_\tau \sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^2 |\mathcal{F}[\tau](\mathbf{k})|^2 \right)^{1/2}$$

$$(SM2.47) \quad = c_0 \sqrt{n} + Q \sqrt{n} \|\gamma\|_{\ell^2}.$$

This leads to

$$(SM2.48) \quad \text{Rad}_S(\mathcal{H}'_Q) \leq \frac{c_0}{\sqrt{n}} + \frac{1}{\sqrt{n}} Q \|\gamma\|_{\ell^2}.$$

For (ii), the proof is similar to (i). We have

$$(SM2.49) \quad \mathbb{E}_\tau \left[\sup_{h \in \mathcal{H}_Q} \sum_{\mathbf{k} \in \mathbb{Z}^d} \mathcal{F}[\tau](\mathbf{k}) \overline{\mathcal{F}[h](\mathbf{k})} \right] \leq Q \mathbb{E}_\tau \left(\sum_{\mathbf{k} \in \mathbb{Z}^d} (\gamma(\mathbf{k}))^2 |\mathcal{F}[\tau](\mathbf{k})|^2 \right)^{1/2} \leq Q \sqrt{n} \|\gamma\|_{\ell^2}.$$

Therefore

$$(SM2.50) \quad \text{Rad}_S(\mathcal{H}_Q) \leq \frac{1}{\sqrt{n}} Q \|\gamma\|_{\ell^2}. \quad \blacksquare$$

Lemma. (Lemma 6 in main text) Suppose that the real-valued target function $f \in \mathcal{F}_\gamma(\Omega)$ and that the training dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ satisfies $y_i = f(\mathbf{x}_i)$, $i = 1, \dots, n$. If $\gamma : \mathbb{Z}^d \rightarrow \mathbb{R}^+$, then there exists a unique solution h_n to the regularized model

$$(SM2.51) \quad \min_{h \in \mathcal{H}_\gamma(\Omega)} \|h - h_{\text{ini}}\|_\gamma, \quad \text{s.t.} \quad h(\mathbf{x}_i) = y_i, \quad i = 1, \dots, n.$$

Moreover, we have

$$(SM2.52) \quad \|h_n - h_{\text{ini}}\|_\gamma \leq \|f - h_{\text{ini}}\|_\gamma.$$

Proof. By the definition of the FP-norm, we have $\|h_n - h_{\text{ini}}\|_\gamma = \|\mathcal{F}[h_n] - \mathcal{F}[h_{\text{ini}}]\|_{H_\Gamma}$. According to Corollary 6, the minimizer of problem (SM2.51) exists, i.e., h_n exists. Since the target function $f(x)$ satisfies the constraints $f(\mathbf{x}_i) = y_i$, $i = 1, \dots, n$, we have $\|h_n - h_{\text{ini}}\|_\gamma \leq \|f - h_{\text{ini}}\|_\gamma$. \blacksquare

Lemma. (Lemma 7 in main text) Suppose that the real-valued target function $f \in \mathcal{F}_\gamma(\Omega)$ and the training dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ satisfies $y_i = f(\mathbf{x}_i)$, $i = 1, \dots, n$. If $\gamma : \mathbb{Z}^{d^*} \rightarrow \mathbb{R}^+$ with $\gamma^{-1}(\mathbf{0}) := 0$, then there exists a solution h_n to the regularized model

$$(SM2.53) \quad \min_{h \in \mathcal{H}_\gamma(\Omega)} \|h - h_{\text{ini}}\|_\gamma, \quad \text{s.t.} \quad h(\mathbf{x}_i) = y_i, \quad i = 1, \dots, n.$$

Moreover, we have

$$(SM2.54) \quad |\mathcal{F}[h_n - h_{\text{ini}}](\mathbf{0})| \leq \|f - h_{\text{ini}}\|_\infty + \|f - h_{\text{ini}}\|_\gamma \|\gamma\|_{\ell^2}.$$

Proof. Let $f' = f - h_{\text{ini}}$. Since $h_n(\mathbf{x}_i) - f(\mathbf{x}_i) = 0$ for $i = 1, \dots, n$, we have $h_n(\mathbf{x}_i) - f'(\mathbf{x}_i) - h_{\text{ini}}(\mathbf{x}_i) = 0$. Therefore

(SM2.55)

$$\begin{aligned} |\mathcal{F}[h_n - h_{\text{ini}}](\mathbf{0})| &= \left| f'(\mathbf{x}_i) - \sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} \mathcal{F}[h_n - h_{\text{ini}}](\mathbf{k}) e^{2\pi i \mathbf{k}^\top \mathbf{x}_i} \right| \\ (SM2.56) \quad &\leq \|f'\|_\infty + \sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} |\mathcal{F}[h_n - h_{\text{ini}}](\mathbf{k})| \\ (SM2.57) \quad &\leq \|f'\|_\infty + \left(\sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^2 \right)^{\frac{1}{2}} \left(\sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^{-2} |\mathcal{F}[h_n - h_{\text{ini}}](\mathbf{k})|^2 \right)^{\frac{1}{2}} \\ (SM2.58) \quad &\leq \|f'\|_\infty + \|h_n - h_{\text{ini}}\|_\gamma \|\gamma\|_{\ell^2} \\ (SM2.59) \quad &\leq \|f'\|_\infty + \|f'\|_\gamma \|\gamma\|_{\ell^2}. \end{aligned}$$

We remark that the last step is due to the same reason as Lemma 6. ■

Theorem. (Theorem 3 in main text) Suppose that the real-valued target function $f \in \mathcal{F}_\gamma(\Omega)$, the training dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ satisfies $y_i = f(\mathbf{x}_i)$, $i = 1, \dots, n$, and h_n is the solution of the regularized model

$$(SM2.60) \quad \min_{h - h_{\text{ini}} \in \mathcal{F}_\gamma(\Omega)} \|h - h_{\text{ini}}\|_\gamma, \quad \text{s.t.} \quad h(\mathbf{x}_i) = y_i, \quad i = 1, \dots, n.$$

Then we have

(i) given $\gamma : \mathbb{Z}^d \rightarrow \mathbb{R}^+$, for any $\delta \in (0, 1)$, with probability at least $1 - \delta$ over the random training sample, the population risk has the bound

$$(SM2.61) \quad R_{\mathcal{D}}(h_n) \leq \|f - h_{\text{ini}}\|_\gamma \|\gamma\|_{\ell^2} \left(\frac{2}{\sqrt{n}} + 4\sqrt{\frac{2 \log(4/\delta)}{n}} \right).$$

(ii) given $\gamma : \mathbb{Z}^{d^*} \rightarrow \mathbb{R}^+$ with $\gamma(\mathbf{0})^{-1} := 0$, for any $\delta \in (0, 1)$, with probability at least $1 - \delta$ over the random training sample, the population risk has the bound

$$(SM2.62) \quad R_{\mathcal{D}}(h_n) \leq (\|f - h_{\text{ini}}\|_\infty + 2\|f - h_{\text{ini}}\|_\gamma \|\gamma\|_{\ell^2}) \left(\frac{2}{\sqrt{n}} + 4\sqrt{\frac{2 \log(4/\delta)}{n}} \right).$$

Proof. Let $f' = f - h_{\text{ini}}$ and $Q = \|f'\|_\gamma$.

(i) Given $\gamma : \mathbb{Z}^d \rightarrow \mathbb{R}^+$, we set $\mathcal{H}_Q = \{h : \|h - h_{\text{ini}}\|_\gamma \leq Q\}$. According to Lemma 6, the solution of problem (SM2.60) $h_n \in \mathcal{H}_Q$. By the relation between generalization gap and Rademacher complexity [SM1, SM2],

$$(SM2.63) \quad |R_{\mathcal{D}}(h_n) - L_S(h_n)| \leq 2\text{Rad}_S(\mathcal{H}_Q) + 2 \sup_{h, h' \in \mathcal{H}_Q} \|h - h'\|_\infty \sqrt{\frac{2 \log(4/\delta)}{n}}.$$

One of the component can be bounded as follows

$$(SM2.64) \quad \sup_{h, h' \in \mathcal{H}_Q} \|h - h'\|_\infty \leq \sup_{h \in \mathcal{H}_Q} 2\|h - h_{\text{ini}}\|_\infty$$

$$(SM2.65) \quad \leq \sup_{h \in \mathcal{H}_Q} 2 \max_{\mathbf{x}} \left| \sum_{\mathbf{k} \in \mathbb{Z}^d} \mathcal{F}[h - h_{\text{ini}}](\mathbf{k}) e^{2\pi i \mathbf{k}^\top \mathbf{x}} \right|$$

$$(SM2.66) \quad \leq \sup_{h \in \mathcal{H}_Q} 2 \sum_{\mathbf{k} \in \mathbb{Z}^d} |\mathcal{F}[h - h_{\text{ini}}](\mathbf{k})|$$

$$(SM2.67) \quad \leq 2 \sup_{h \in \mathcal{H}_Q} \left(\sum_{\mathbf{k} \in \mathbb{Z}^d} (\gamma(\mathbf{k}))^2 \right)^{\frac{1}{2}} \left(\sum_{\mathbf{k} \in \mathbb{Z}^d} (\gamma(\mathbf{k}))^{-2} |\mathcal{F}[h - h_{\text{ini}}](\mathbf{k})|^2 \right)^{\frac{1}{2}}$$

$$(SM2.68) \quad \leq 2Q \|\gamma\|_{\ell^2}.$$

By Lemma 5,

$$(SM2.69) \quad \text{Rad}_S(\mathcal{H}_Q) \leq \frac{1}{\sqrt{n}} Q \|\gamma\|_{\ell^2}.$$

By optimization problem (SM2.60), $L_S(h_n) \leq L_S(f') = 0$. Therefore we obtain

$$(SM2.70) \quad R_{\mathcal{D}}(h) \leq \frac{2}{\sqrt{n}} \|f'\|_\gamma \|\gamma\|_{\ell^2} + 4 \|f'\|_\gamma \|\gamma\|_{\ell^2} \sqrt{\frac{2 \log(4/\delta)}{n}}.$$

(ii) Given $\gamma : \mathbb{Z}^{d^*} \rightarrow \mathbb{R}^+$ with $\gamma(\mathbf{0})^{-1} := 0$, set $c_0 = \|f'\|_\infty + \|f'\|_\gamma \|\gamma\|_{\ell^2}$. By Lemma 5, 6, and 7, define $\mathcal{H}'_Q = \{h : \|h - h_{\text{ini}}\|_\gamma \leq Q, |\mathcal{F}[h - h_{\text{ini}}](\mathbf{0})| \leq c_0\}$, we obtain

$$(SM2.71) \quad \text{Rad}_S(\mathcal{H}'_Q) \leq \frac{1}{\sqrt{n}} \|f'\|_\infty + \frac{2}{\sqrt{n}} \|f'\|_\gamma \|\gamma\|_{\ell^2}.$$

Also

$$(SM2.72)$$

$$\sup_{h, h' \in \mathcal{H}'_Q} \|h - h'\|_\infty \leq \sup_{h \in \mathcal{H}'_Q} 2 \sum_{\mathbf{k} \in \mathbb{Z}^d} |\mathcal{F}[h - h_{\text{ini}}](\mathbf{k})|$$

$$(SM2.73)$$

$$\leq 2 \sup_{h \in \mathcal{H}'_Q} \left[|\mathcal{F}[h - h_{\text{ini}}](\mathbf{0})| + \left(\sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^2 \right)^{\frac{1}{2}} \left(\sum_{\mathbf{k} \in \mathbb{Z}^{d^*}} (\gamma(\mathbf{k}))^{-2} |\mathcal{F}[h - h_{\text{ini}}](\mathbf{k})|^2 \right)^{\frac{1}{2}} \right]$$

$$(SM2.74)$$

$$\leq 2 \|f'\|_\infty + 4 \|f'\|_\gamma \|\gamma\|_{\ell^2}.$$

Then

$$(SM2.75) \quad R_{\mathcal{D}}(h_n) \leq \frac{2}{\sqrt{n}} \|f'\|_\infty + \frac{4}{\sqrt{n}} \|f'\|_\gamma \|\gamma\|_{\ell^2} + (4 \|f'\|_\infty + 8 \|f'\|_\gamma \|\gamma\|_{\ell^2}) \sqrt{\frac{2 \log(4/\delta)}{n}}. \blacksquare$$

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