A Priori Generalization Analysis of the Deep Ritz Method for Solving High Dimensional Elliptic Partial Differential Equations

Jianfeng Lu JIANFENG@MATH.DUKE.EDU
Departments of Mathematics, Physics, and Chemistry, Duke University, Box 90320, Durham, NC 27708.
Yulong Lu LU@MATH.UMASS.EDU
Department of Mathematics and Statistics, Lederle Graduate Research Tower, University of Massachusetts, 710 N. Pleasant Street, Amherst, MA 01003.
Min Wang WANGMIN@MATH.DUKE.EDU
Mathematics Department, Duke University, Box 90320, Durham, NC 27708.

Editors: Mikhail Belkin and Samory Kpotufe

Abstract

This paper concerns the a priori generalization analysis of the Deep Ritz Method (DRM) [W. E and B. Yu, 2017], a popular neural-network-based method for solving high dimensional partial differential equations. We derive the generalization error bounds of two-layer neural networks in the framework of the DRM for solving two prototype elliptic PDEs: Poisson equation and static Schrödinger equation on the d-dimensional unit hypercube. Specifically, we prove that the convergence rates of generalization errors are independent of the dimension d, under the a priori assumption that the exact solutions of the PDEs lie in a suitable low-complexity space called spectral Barron space. Moreover, we give sufficient conditions on the forcing term and the potential function which guarantee that the solutions are spectral Barron functions. We achieve this by developing a new solution theory for the PDEs on the spectral Barron space, which can be viewed as an analog of the classical Sobolev regularity theory for PDEs.

Keywords: Neural Networks, Partial Differential Equations, Generalization, Regularity, Barron Space.

1. Introduction

Numerical solutions to high dimensional partial differential equations (PDEs) have been a longstanding challenge in scientific computing. The impressive advance of deep learning has offered exciting possibilities for algorithmic innovations. In particular, it is a natural idea to represent solutions of PDEs by (deep) neural networks to exploit the rich expressiveness of neural networks representation. The parameters of neural networks are then trained by optimizing some loss functions associated with the PDE. Natural loss functions can be designed using the variational structure, similar to the Ritz-Galerkin method in classical numerical analysis of PDEs. Such method is known as the Deep Ritz Method (DRM) (E and Yu, 2018; Khoo et al., 2019). Methods in a similar spirit has been also developed in the computational physics literature (Carleo and Troyer, 2017) for solving eigenvalue problems arising from many-body quantum mechanics, under the framework of variational Monte Carlo method (McMillan, 1965). Despite wide popularity and many successful applications of the DRM and other approaches of using neural networks to solve high-dimensional PDEs, the analysis of such methods is scarce and still not well understood. This paper aims to provide an a priori generalization error analysis of the DRM with dimension-explicit estimates.

Generally speaking, the error of using neural networks to solve high dimensional PDEs can be decomposed into the following parts:

- Approximation error: the error of approximating the solution of a PDE using neural networks;
- Generalization error: this refers to the error of the neural network-based approximate solution on predicting unseen data. The variational problem involves integrals in high dimension, which can be expensive to compute. In practice Monte Carlo methods are usually used to approximate those high dimensional integrals and thus the miminizer of the surrogate model (known as empirical risk minimization) would be different from the minimizer of the original variational problem;
- Training (or optimization) error: this is the error incurred by the optimization algorithm used in the training of neural networks for PDEs. Since the parameters of the neural networks are obtained through an optimization process, it might not be able to find the best approximation to the unknown solution within the function class.

Note that from a numerical analysis point of view, these errors already appear for conventional Galerkin methods. Indeed, taking finite element methods for example, the approximation error is the error of approximating the true solution in the finite element space; the generalization error can be seen as the discretization error caused by numerical quadrature of the variational formulation; the optimization error corresponds to the computational error in the conventional numerical PDEs due to the inaccurate resolution of linear or nonlinear finite dimensional discrete system. Although classical numerical analysis for PDEs in low dimensions has formed a relatively complete theory in the last several decades, the error analysis of neural network methods is much more challenging for high dimensional PDEs and requires new ideas and tools. In fact, the three components of error analysis highlighted above all face new difficulties.

For approximation, as is well known, high dimensional problems suffer from the curse of dimensionality, if we proceed with standard regularity-based function spaces such as Sobolev spaces or Hölder spaces as in conventional numerical analysis. In fact, even using deep neural networks, the approximation rate for functions in such spaces deteriorate as the dimension becomes higher; see (Yarotsky, 2017, 2018). Therefore, to obtain better approximation rates that scale mildly in the large dimensionality, it is natural to assume that the function of interest lies in a suitable smaller function space which has low complexity compared to Sobolev or Hölder spaces so that the function can be efficiently approximated by neural networks in high dimensions. The first function class of this kind is the so-called *Barron space* defined in the seminal work Barron (1993); see also (Bach, 2017; Klusowski and Barron, 2018; E et al., 2019; Siegel and Xu, 2020a,b) for more variants of Barron spaces and their neural-network approximation properties. In the present paper we will introduce a discrete version of Barron's definition of such space using the idea of spectral decomposition and because of this we adopt the terminology of *spectral Barron space* following (Siegel and Xu, 2020b; E et al., 2020) to distinguish it from the other versions. As the Barron spaces are very different from the usual Sobolev spaces, for PDE problems, one has to develop novel *a priori* estimates and correspondingly approximation error analysis. In particular, a new solution theory for high dimensional PDEs in those low-complexity function spaces needs to be developed. This paper makes an initial attempt in establishing a solution theory in the spectral Barron space for a class of elliptic PDEs.

The analysis of the generalization error is also intimately related to the function class (e.g. neural networks) we use, in particular its complexity. This makes the generalization analysis quite different from the analysis of numerical quadrature error in an usual finite element method. We face a trade-off between the approximation and generalization: To reduce the approximation error, one would like to use an approximation ansatz which involves large number of degrees of freedom, however, such choice will incur large generalization error.

The training of the neural networks also remains to be a very challenging problem since the associated optimization problem is highly non-convex. In fact, even under a standard supervised learning setting, we still largely lack understanding of the optimization error, except in simplified setting where the optimization dynamics is essentially linear, see e.g., (Jacot et al., 2018; Chizat et al., 2019; Ghorbani et al., 2019). The analysis for PDE problems would face similar, if not severer, difficulties, and it is beyond the scope of our current work.

In this work, we provide a rigorous analysis to the approximation and generalization errors of the DRM for high dimensional elliptic PDEs. We will focus on relative simple PDEs (Poisson equation and static Schrödinger equation) to better convey the idea and illustrate the framework, without bogging the readers down with technical details. Our analysis, as already suggested by the discussions above, which is based on identifying a correct functional analysis setup and developing the corresponding *a priori* analysis and complexity estimates, will provide dimension-independent generalization error estimates.

1.1. Related Works

Several previous works on analysis of neural-network based methods for high-dimensional PDEs focus on the aspect of representation, i.e., whether a solution to the PDE can be approximated by a neural network with quantitative error control; see e.g., (Grohs et al., 2018; Hutzenthaler et al., 2020). Fixing an approximation space, the generalization error can be controlled by analyzing complexity such as covering numbers, see e.g., (Berner et al., 2020) for a specific PDE problem.

More recently, several papers (Shin et al., 2020a; Mishra and Molinaro, 2020; Shin et al., 2020b; Luo and Yang, 2020) considered the generalization error analysis of the physics informed neural network (PINNs) approach based on residual minimization for solving PDEs (Lagaris et al., 1998; Raissi et al., 2019). In particular, the work (Shin et al., 2020a) established the consistency of the loss function such that the approximation converges to the true solution as the training sample increases under the assumption of vanishing training error. For the generalization error, Mishra and Molinaro (Mishra and Molinaro, 2020) carried out an a-posteriori-type generalization error analysis for PINNs, and proved that the generalization error is bounded by the training error and quadrature error under some stability assumptions of the PDEs. To avoid the issue of curse of dimensionality in quadrature error, the authors also considered the cumulative generalization error which involves a validation set. The paper (Shin et al., 2020b) proved both a priori and a posterior estimates for residual minimization methods in Sobolev spaces. The paper (Luo and Yang, 2020) obtained a priori generalization estimates for a class of second order linear PDEs by assuming (but without verifying) that the exact solutions of PDEs belong to a Barron-type space.

Different from the previous generalization error analysis, we derive a priori and dimension-explicit generalization error estimates under the assumption that the solutions of the PDEs lie in the spectral Barron space that is more aligned with (Barron, 1993). More importantly, we justify such assumption by developing a novel solution theory in the spectral Barron space for the PDEs of consideration. This regularity theory is one of the main contributions of our work, which separates our results with the above mentioned ones. A similar regularity theory has been established in Lu and Lu (2021) for the ground state of the Schrödinger operator.

It is worth mentioning that in the very recent preprints E and Wojtowytsch (2020) and Chen et al. (2021), the authors considered the regularity theory of high dimensional PDEs defined on the whole space in the Barron space introduced by (E et al., 2019). Their results shared a similar spirit as our analysis of PDE regularity theory in the spectral Barron space (see Theorem 5), while we focus on PDEs on finite domain, and as a result, we have to develop different Barron function spaces from those used for the whole space. The authors of (E and Wojtowytsch, 2020) also provided some counterexamples to regularity theory for PDE problems defined on non-convex domains, while we would only focus on simple domain (in fact hypercubes) in this work.

While we focus on the variational principle based approach for solving high dimensional PDEs using neural networks, we note that many other approaches have been developed, such as the deep BSDE method based on the control formulation of parabolic PDEs (Han et al., 2018), the deep Galerkin method based on the weak formulation (Sirignano and Spiliopoulos, 2018), methods based on the strong formulation (residual minimization) such as the PINNs (Lagaris et al., 1998; Raissi et al., 2019), the diffusion Monte Carlo type approach for high-dimensional eigenvalue problems (Han et al., 2020), just to name a few. It would be interesting future directions to extend our analysis to these methods.

1.2. Our Contributions

We analyze the generalization error of two-layer neural networks for solving two prototype elliptic PDEs in the framework of DRM. Specifically we make the following contributions:

- We define a spectral Barron space $\mathcal{B}^s(\Omega)$ on a d-dimensional unit hypercube $\Omega = [0,1]^d$ that extend the Barron's original function space (Barron, 1993) from the whole space to bounded domain; see the definition in (10). In the generalization theory we develop, we assume that the solutions lie in the spectral Barron space.
- We show that the spectral Barron functions in $\mathcal{B}^2(\Omega)$ can be well approximated in H^1-norm by two-layer neural networks with either ReLU or Softplus activation functions without curse of dimensionality. Moreover, the parameters (weights and biases) of the two-layer neural networks are controlled explicitly in terms of the spectral Barron norm. The bounds on the neural-network parameters play an essential role in controlling the generalization error of the neural nets. See Theorem 2 (and also Theorem 17 in Appendix B.3) for the approximation results.
- We derive generalization error bounds of the neural-network solutions for solving Poisson equation and the static Schrödinger equation under the assumption that the solutions belong to the Barron space $\mathcal{B}^2(\Omega)$. We emphasize that the convergence rates in our generalization error bounds are dimension-independent and that the prefactors in the error estimates depend at most polynomially on the dimension and the Barron norms of the solutions, indicating that the DRM overcomes the curse of dimensionality when the solutions of the PDEs are spectral Barron functions. See Theorem 3 for the generalization results.
- Last but not the least, we develop new well-posedness theory for the solutions of Poisson and static Schrödinger equations in the spectral Barron space, providing sufficient conditions to verify the earlier assumption on the solutions made in the generalization analysis. The new solution theory can be viewed as an analog of the classical PDE theory in Sobolev or Hölder spaces. See Theorem 5 for the new solution theory in spectral Barron space.

1.3. Notation

We use $|x|_p$ to denote the p-norm of a vector $x \in \mathbb{R}^d$. When $p = 2$ we write $|x| = |x|_2$.

2. Set-Up and Main Results

2.1. Set-Up of PDEs

Let $\Omega = [0, 1]^d$ be the unit hypercube on $\mathbb{R}^d$. Let $\partial\Omega$ be the boundary of Ω. We consider the following two prototype elliptic PDEs on Ω equipped with the Neumann boundary condition: Poisson equation

$$-\Delta u = f \text{ on } \Omega, \qquad \frac{\partial u}{\partial \nu} = 0 \text{ on } \partial\Omega \tag{1}$$

and the static Schrödinger equation

$$-\Delta u + Vu = f \text{ on } \Omega, \qquad \frac{\partial u}{\partial \nu} = 0 \text{ on } \partial\Omega. \tag{2}$$

Throughout the paper, we make the minimal assumption that $f \in L^2(\Omega)$ and $V \in L^\infty(\Omega)$ with $V(x) \geq V_{\min} > 0$, although later we will impose stronger regularity assumptions on f and V. In particular, in our high dimensional setting, we would certainly need to restrict the class of f and V, otherwise just prescribing such general functions numerically would already incur curse of dimensionality. The well-posedness of the solutions to the Poisson equation and static Schrödinger equation in the Sobolev space $H^1(\Omega)$ as well as the variational characterizations of the solutions are standard and are summarized in the proposition below, whose proof is provided in Appendix E.

Proposition 1 *(i) Assume that $f \in L^2(\Omega)$ with $\int_\Omega f dx = 0$. Then there exists a unique weak solution $u_P^* \in H^1_\diamond(\Omega) := \{u \in H^1(\Omega) \mid \int_\Omega u dx = 0\}$ to the Poisson equation (1). Moreover, we have that*

$$u_P^* = \underset{u \in H^1(\Omega)}{\arg\min}\, \mathcal{E}_P(u) := \underset{u \in H^1(\Omega)}{\arg\min} \Big\{ \frac{1}{2} \int_\Omega |\nabla u|^2 dx + \frac{1}{2}\Big(\int_\Omega u dx \Big)^2 - \int_\Omega f u dx \Big\}, \tag{3}$$

and that for any $u \in H^1(\Omega)$,

$$2(\mathcal{E}(u) - \mathcal{E}(u_P^*)) \leq \|u - u_P^*\|^2_{H^1(\Omega)} \leq 2 \max\{2C_P + 1, 2\}(\mathcal{E}(u) - \mathcal{E}(u_P^*)), \tag{4}$$

where C_P is the Poincaré constant on the domain Ω, i.e., for any $v \in H^1(\Omega)$,

$$\Big\| v - \int_\Omega v dx \Big\|^2_{L^2(\Omega)} \leq C_P \|\nabla v\|^2_{L^2(\Omega)}.$$

(ii) Assume that $f, V \in L^\infty(\Omega)$ and that $0 < V_{\min} \leq V(x) \leq V_{\max} < \infty$ for all $x \in \Omega$ and some constants $V_{\min}$ and $V_{\max}$. Then there exists a unique weak solution $u_S^* \in H^1(\Omega)$ to the static Schrödinger equation (2). Moreover, we have that

$$u_S^* = \underset{u \in H^1(\Omega)}{\arg\min}\, \mathcal{E}_S(u) := \underset{u \in H^1(\Omega)}{\arg\min} \Big\{ \frac{1}{2} \int_\Omega |\nabla u|^2 + V|u|^2 \, dx - \int_\Omega f u dx \Big\}, \tag{5}$$

and that for any $u \in H^1(\Omega)$

$$\frac{2}{\max(1, V_{\max})}(\mathcal{E}(u) - \mathcal{E}(u_S^*)) \leq \|u - u^*\|^2_{H^1(\Omega)} \leq \frac{2}{\min(1, V_{\min})}(\mathcal{E}(u) - \mathcal{E}(u_S^*)). \tag{6}$$

The variational formulations (3) and (5) are the basis of the DRM (E and Yu, 2018) for solving those PDEs. The main idea is to train neural networks to minimize the (population) loss defined by the Ritz energy functional $\mathcal{E}$. More specifically, let $\mathcal{F} \subset H^1(\Omega)$ be a hypothesis function class parameterized by neural networks. The DRM seeks the optimal solution to the population loss $\mathcal{E}$ within the hypothesis space $\mathcal{F}$. However, the population loss requires evaluations of d-dimensional integrals, which can be prohibitively expensive when $d \gg 1$ if traditional quadrature methods were used. To circumvent the curse of dimensionality, it is natural to employ the Monte Carlo method for computing the high dimensional integrals, which leads to the so-called *empirical loss (or risk) minimization.*

2.2. Empirical Loss Minimization

Let us denote by $\mathcal{P}_\Omega$ the uniform probability distributions on the domain Ω. Then the loss functional $\mathcal{E}_P$ and $\mathcal{E}_S$ can be rewritten in terms of expectations under $\mathcal{P}_\Omega$ as

$$\mathcal{E}_P(u) = |\Omega| \cdot \mathbf{E}_{X\sim\mathcal{P}_\Omega}\Big[\frac{1}{2}|\nabla u(X)|^2 - f(X)u(X)\Big] + \frac{1}{2}\Big(|\Omega| \cdot \mathbf{E}_{X\sim\mathcal{P}_\Omega} u(X)\Big)^2,$$
$$\mathcal{E}_S(u) = |\Omega| \cdot \mathbf{E}_{X\sim\mathcal{P}_\Omega}\Big[\frac{1}{2}|\nabla u(X)|^2 + \frac{1}{2}V(X)|u(X)|^2 - f(X)u(X)\Big].$$

To define the empirical loss, let $\{X_j\}_{j=1}^n$ be an i.i.d. sequence of random variables distributed according to $\mathcal{P}_\Omega$. Define the empirical losses $\mathcal{E}_{n,P}$ and $\mathcal{E}_{n,S}$ by setting

$$\begin{aligned}\mathcal{E}_{n,P}(u) &= \frac{1}{n}\sum_{j=1}^n \Big[|\Omega| \cdot \Big(\frac{1}{2}|\nabla u(X_j)|^2 - f(X_j)u(X_j)\Big)\Big] + \frac{1}{2}\Big(\frac{|\Omega|}{n}\sum_{j=1}^n u(X_j)\Big)^2,\\ \mathcal{E}_{n,S}(u) &= \frac{1}{n}\sum_{j=1}^n \Big[|\Omega| \cdot \Big(\frac{1}{2}|\nabla u(X_j)|^2 + \frac{1}{2}V(X_j)|u(X_j)|^2 - f(X_j)u(X_j)\Big)\Big].\end{aligned} \tag{7}$$

Given an empirical loss $\mathcal{E}_n$, the empirical loss minimization algorithm seeks u_n which minimizes $\mathcal{E}_n$, i.e.

$$u_n = \arg\min_{u\in\mathcal{F}} \mathcal{E}_n(u). \tag{8}$$

Here we have suppressed the dependence of u_n on $\mathcal{F}$. We denote by $u_{n,P}$ and $u_{n,S}$ the minimal solutions to the empirical loss $\mathcal{E}_{n,P}$ and $\mathcal{E}_{n,S}$, respectively.

2.3. Main Results

The goal of the present paper is to obtain quantitative estimates for the generalization error between the minimal solution $u_{n,S}$ and $u_{n,P}$ computed from the finite data points $\{X_j\}_{j=1}^n$ and the exact solutions when the spacial dimension d is large. Our primary interest is to derive such estimates which scales mildly with respect to the increasing dimension d. To this end, it is necessary to assume that the true solutions lie in a smaller space which has a lower complexity than Sobolev spaces. Specifically we will consider the spectral Barron space defined below via the cosine transformation.

Let $\mathcal{C}$ be a set of cosine functions defined by

$$\mathcal{C} := \Big\{\Phi_k\Big\}_{k\in\mathbb{N}_0^d} := \Big\{\prod_{i=1}^d \cos(\pi k_i x_i) \mid k_i \in \mathbb{N}_0\Big\}. \tag{9}$$

Given $u \in L^1(\Omega)$, let $\{\hat{u}(k)\}_{k\in\mathbb{N}_0^d}$ be the expansion coefficients of u under the basis $\{\Phi_k\}_{k\in\mathbb{N}_0^d}$. Let us define for $s \geq 0$ the spectral Barron space $\mathcal{B}^s(\Omega)$ on Ω by

$$\mathcal{B}^s(\Omega) := \Big\{u \in L^1(\Omega) : \sum_{k\in\mathbb{N}_0^d} (1 + \pi^s |k|_1^s)|\hat{u}(k)| < \infty\Big\}. \tag{10}$$

The spectral Barron norm of a function u on $\mathcal{B}^s(\Omega)$ is given by

$$\|u\|_{\mathcal{B}^s(\Omega)} = \sum_{k\in\mathbb{N}_0^d} (1 + \pi^s |k|_1^s)|\hat{u}(k)|.$$

Observe that a function $f \in \mathcal{B}^s(\Omega)$ if and only if $\{\hat{u}(k)\}_{k\in\mathbb{N}_0^d}$ belongs to the weighted ℓ^1-space $\ell^1_{W_s}(\mathbb{N}_0^d)$ on the lattice $\mathbb{N}_0^d$ with the weights $W_s(k) = (1 + \pi^s|k|_1^s)$. When $s = 2$, we adopt the short-hand notation $\mathcal{B}(\Omega)$ for $\mathcal{B}^2(\Omega)$. Our definition of spectral Barron space is strongly motivated by the seminar work Barron (1993) and other recent works (Bach, 2017; Klusowski and Barron, 2018; E et al., 2019; Siegel and Xu, 2020a). The original Barron function f in (Barron, 1993) is defined on the whole space $\mathbb{R}^d$ whose Fourier transform $\hat{f}(w)$ satisfies that $\int |\hat{f}(\omega)||\omega| d\omega < \infty$. Our spectral Barron space $\mathcal{B}^s(\Omega)$ with $s = 1$ can be viewed as a discrete analog of the original Barron space from (Barron, 1993).

The most important property of the Barron functions is that those functions can be well approximated by two-layer neural networks without the curse of dimensionality. To make this more precise, let us define the class of two-layer neural networks to be used as our hypothesis space for solving PDEs. Given an activation function ϕ, a constant $B > 0$ and the number of hidden neurons m, we define

$$\mathcal{F}_{\phi,m}(B) := \Big\{c + \sum_{i=1}^m \gamma_i \phi(\omega_i \cdot x - t_i), |c| \leq 2B, |w_i|_1 = 1, |t_i| \leq 1, \sum_{i=1}^m |\gamma_i| \leq 4B\Big\}. \tag{11}$$

In the present paper, we mainly consider solving the PDEs within the hypothesis space $\mathcal{F}_{\phi,m}(B)$ with a special Softplus (Dugas et al., 2001; Glorot et al., 2011) activation function. Recall the Softplus function $\mathrm{SP}(z) = \ln(1 + e^z)$ and its rescaled version $\mathrm{SP}_\tau(z)$ defined also for $\tau > 0$,

$$\mathrm{SP}_\tau(z) = \frac{1}{\tau}\mathrm{SP}(\tau z) = \frac{1}{\tau}\ln(1 + e^{\tau z}).$$

In is important to observe that the rescaled Softplus $\mathrm{SP}_\tau(z)$ can be viewed as a smooth approximation of the ReLU function since $\mathrm{SP}_\tau(z) \to \mathrm{ReLU}(z)$ as $\tau \to 0$ for any $z \in \mathbb{R}$ (see Lemma 20 for a quantitative statement). The Softplus activation function is smooth and hence more suitable for PDE applications which involve derivatives, compared with ReLU.

Our first result concerns the approximation of spectral Barron functions in $\mathcal{B}(\Omega)$ by two-layer neural networks with the activation function SP_τ.

Theorem 2 *Define the function class $\mathcal{F}_{\mathrm{SP}_\tau,m}(B)$ by setting $\phi = \mathrm{SP}_\tau$ in (11). Then for any $u \in \mathcal{B}(\Omega)$, there exists a two-layer neural network $u_m \in \mathcal{F}_{\mathrm{SP}_\tau,m}(\|u\|_{\mathcal{B}(\Omega)})$ with activation function SP_τ with $\tau = \sqrt{m}$, such that*

$$\|u - u_m\|_{H^1(\Omega)} \leq \frac{\|u\|_{\mathcal{B}(\Omega)}(6\log m + 30)}{\sqrt{m}}.$$

The proofs of Theorem 2 can be found in Section B. A similar approximation result was first proved in the seminar paper Barron (1993) where the same approximation rate $O(m^{-\frac{1}{2}})$ was also obtained when approximating the Barron function defined on the whole space with two-layer neural nets with the sigmoid activation function in the L^∞-norm.

Now we are ready to state the main generalization results of two-layer neural networks for solving Poisson and the static Schrödinger equations.

Theorem 3 *(i) Let u_P^* solve the Poisson equation (1) with $\|u_P^*\|_{\mathcal{B}(\Omega)} < \infty$. Let $u_{n,S}^m$ be the minimizer of the empirical loss $\mathcal{E}_{n,P}$ in the set $\mathcal{F} = \mathcal{F}_{\mathrm{SP}_\tau,m}(\|u_P^*\|_{\mathcal{B}(\Omega)})$ with $\tau = \sqrt{m}$. Then it holds that*

$$\mathbf{E}\big[\mathcal{E}_P(u_{n,P}^m) - \mathcal{E}_P(u_P^*)\big] \leq \frac{C_1\sqrt{m}(\sqrt{\log m}+1)}{\sqrt{n}} + \frac{C_2(\log m+1)^2}{m}. \tag{12}$$

Here $C_1 > 0$ depends polynomially on $\|u_P^*\|_{\mathcal{B}(\Omega)}, d, \|f\|_{L^\infty(\Omega)}$, and $C_2 > 0$ depends quadratically on $\|u_P^*\|_{\mathcal{B}(\Omega)}$.

(ii) Let u_S^* solve the static Schrödinger equation (2) with $\|u_S^*\|_{\mathcal{B}(\Omega)} < \infty$. Let $u_{n,S}^m$ be the minimizer of the empirical loss $\mathcal{E}_{n,S}$ in the set $\mathcal{F} = \mathcal{F}_{\mathrm{SP}_\tau,m}(\|u_S^*\|_{\mathcal{B}(\Omega)})$ with $\tau = \sqrt{m}$. Then it holds that

$$\mathbf{E}\big[\mathcal{E}_S(u_{n,S}^m) - \mathcal{E}_S(u_S^*)\big] \leq \frac{C_3\sqrt{m}(\sqrt{\log m}+1)}{\sqrt{n}} + \frac{C_4(\log m+1)^2}{m}. \tag{13}$$

Here $C_3 > 0$ depends polynomially on $\|u_S^*\|_{\mathcal{B}(\Omega)}, d, \|f\|_{L^\infty(\Omega)}, \|V\|_{L^\infty(\Omega)}$ and $C_4 >$ depends quadratically on $\|u_S^*\|_{\mathcal{B}(\Omega)}$.

Remark 4 *By setting $m = n^{\frac{1}{3}}$ in Theorem 3 and thanks to the equivalent estimates on H^1-error and the energy excess as shown in Proposition 1, one obtains for some constant $C_5 > 0$ that*

$$\max\Big\{\mathbf{E}\|u_n^m - u^*\|_{H^1(\Omega)}^2, \mathbf{E}\big[\mathcal{E}(u_n^m) - \mathcal{E}(u^*)\big]\Big\} \leq \frac{C_5(\log n)^2}{n^{\frac{1}{3}}}.$$

where u_n^m denotes the neural network solution $u_{n,P}^m$ (or $u_{n,S}^m$), u^* denotes the exact solution u_P^* (or u_S^*) and $\mathcal{E}$ denotes the Ritz loss $\mathcal{E}_P$ (or $\mathcal{E}_S$).

Theorem 3 shows that the convergence rates of the generalization errors of the neural-network solution for Poisson and the static Schrödinger equations do not suffer from the curse of dimensionality under the key assumption that their exact solutions belong to the spectral Barron space $\mathcal{B}(\Omega)$ (which will be justified below). A proof sketch of Theorem 3 can be found in Section 3.1 and the detailed proof is deferred to Appendix C.

We also comment that one can obtain high-probability versions of the generalization bounds in Theorem 3 by utilizing a PAC-type generalization analysis via the Rademacher complexity (see e.g. (Shalev-Shwartz and Ben-David, 2014, Theorem 26.5)). We refer the interested reader to our companion paper Lu and Lu (2021) for a high-probability generalization bound of a neural network method for solving the Schrödinger eigenvalue problem.

Finally we verify the key low-complexity assumption by establishing a new well-posedness theory for Poisson and the static Schrödinger equations in spectral Barron spaces.

Theorem 5 *(i) Assume that $f \in \mathcal{B}^s(\Omega)$ with $s \geq 0$ and $\hat{f}_0 = \int_\Omega f(x)dx = 0$. Then the solution u^*_P of Poisson equation satisfies that $u^*_P \in \mathcal{B}^{s+2}(\Omega)$ and that*

$$\|u^*_P\|_{\mathcal{B}^{s+2}(\Omega)} \leq 2\|f\|_{\mathcal{B}^s(\Omega)}.$$

In particular, when $s = 0$ we have $\|u^*_P\|_{\mathcal{B}(\Omega)} \leq 2\|f\|_{\mathcal{B}^0(\Omega)}$.

(ii) Assume that $f \in \mathcal{B}^s(\Omega)$ with $s \geq 0$ and $V \in \mathcal{B}^s(\Omega)$ with $V(x) \geq V_{\min} > 0$ for every $x \in \mathbb{R}^d$. Then the solution u^*_S of the static Schrödinger problem (2) satisfies that $u \in \mathcal{B}^{s+2}(\Omega)$ and that

$$\|u^*_S\|_{\mathcal{B}^{s+2}(\Omega)} \leq C_6\|f\|_{\mathcal{B}^s(\Omega)}. \tag{14}$$

In particular, when $s = 0$ we have $\|u^*_S\|_{\mathcal{B}(\Omega)} \leq C_6\|f\|_{\mathcal{B}^0(\Omega)}$.

The a priori estimates above can be viewed as analogs of the standard Sobolev regularity estimate $\|u\|_{H^{s+2}(\Omega)} \leq C\|f\|_{H^s(\Omega)}$. In contrast to the standard proof of Sobolev regularity of PDEs, based on bootstrapping the weak derivative estimates of the solution, Theorem 5 is proved by showing that cosine coefficients $\hat{u}$ of the solutions lie in the weighted ℓ^1 space associated to the Barron space. The proof ideas are sketched in Section 3.2 and the full proof can be found in Appendix D.2.

3. Proof Sketch of Main Results

3.1. Proof Sketch of Theorem 3

We start with useful abstract generalization error bounds for the empirical loss minimization.

Abstract Generalization Error Bound. To simply the notation, we suppress the problem-dependent subscript P or S and denote by u_n the minimizer of the empirical loss $\mathcal{E}_n$ over the hypothesis space $\mathcal{F}$. Recall that u^* is the exact solution of the PDE. We aim to bound the energy excess $\Delta\mathcal{E}_n := \mathcal{E}(u_n) - \mathcal{E}(u^*)$. By definition we have that $\Delta\mathcal{E}_n \geq 0$. To bound $\Delta\mathcal{E}_n$ from above, we first decompose $\Delta\mathcal{E}_n$ as

$$\Delta\mathcal{E}_n = \mathcal{E}(u_n) - \mathcal{E}_n(u_n) + \mathcal{E}_n(u_n) - \mathcal{E}_n(u_\mathcal{F}) + \mathcal{E}_n(u_\mathcal{F}) - \mathcal{E}(u_\mathcal{F}) + \mathcal{E}(u_\mathcal{F}) - \mathcal{E}(u^*). \tag{15}$$

Here $u_\mathcal{F} = \arg\min_{u\in\mathcal{F}} \mathcal{E}(u)$. Since u_n is the minimizer of $\mathcal{E}_n$, $\mathcal{E}_n(u_n) - \mathcal{E}_n(u_\mathcal{F}) \leq 0$. Therefore taking expectation on both sides of (15) gives

$$\mathbf{E}\Delta\mathcal{E}_n \leq \underbrace{\mathbf{E}[\mathcal{E}(u_n) - \mathcal{E}_n(u_n)]}_{\Delta\mathcal{E}_{\text{gen}}} + \underbrace{\mathbf{E}[\mathcal{E}_n(u_\mathcal{F})] - \mathcal{E}(u_\mathcal{F})}_{\Delta\mathcal{E}_{\text{bias}}} + \underbrace{\mathcal{E}(u_\mathcal{F}) - \mathcal{E}(u^*)}_{\Delta\mathcal{E}_{\text{approx}}}. \tag{16}$$

Observe that $\Delta\mathcal{E}_{\text{gen}}$ and $\Delta\mathcal{E}_{\text{bias}}$ are the statistical errors: the first term $\Delta\mathcal{E}_{\text{gen}}$ describing the generalization error of the empirical loss minimization over the hypothesis space $\mathcal{F}$ and the second term $\Delta\mathcal{E}_{\text{bias}}$ being the bias coming from the Monte Carlo integration. Whereas the third term $\Delta\mathcal{E}_{\text{approx}}$ is the approximation error incurred by restricting minimizing $\mathcal{E}$ from over the set $H^1(\Omega)$ to $\mathcal{F}$. Thanks to Proposition 1, the third term $\Delta\mathcal{E}_{\text{approx}}$ is equivalent (up to a constant) to $\inf_{u\in\mathcal{F}} \|u - u^*\|^2_{H^1(\Omega)}$. To control the statistical errors, it is essential to bound the *Rademacher complexities* of certain PDE-dependent function classes. Recall for a set of random variables $\{Z_j\}_{j=1}^n$ independently distributed according to $\mathcal{P}_\Omega$ and a function class $\mathcal{S}$ the Rademacher complexity

$$R_n(\mathcal{S}) := \mathbf{E}_Z\mathbf{E}_\sigma\Big[\sup_{g\in\mathcal{S}}\Big|\frac{1}{n}\sum_{j=1}^n \sigma_j g(Z_j)\Big| \;\Big|\; Z_1, \cdots, Z_n\Big],$$

where the expectation $\mathbf{E}_\sigma$ is taken with respect to the independent uniform Bernoulli sequence $\{\sigma_j\}_{j=1}^n$ with $\sigma_j \in \{\pm 1\}$. Define the following two function classes that are closely associated to the variational forms of the Poisson and static Schrödinger equations.

$$\begin{aligned}\mathcal{G}_P &:= \Big\{g : \Omega \to \mathbb{R} \mid g = \frac{1}{2}|\nabla u|^2 - fu \text{ where } u \in \mathcal{F}\Big\},\\ \mathcal{G}_S &:= \Big\{g : \Omega \to \mathbb{R} \mid g = \frac{1}{2}|\nabla u|^2 + \frac{1}{2}V|u|^2 - fu \text{ where } u \in \mathcal{F}\Big\}.\end{aligned} \tag{17}$$

Let $u_{n,P}$ (or $u_{n,S}$) be the minimizer of the empirical risk $\mathcal{E}_{n,P}$ (or $\mathcal{E}_{n,S}$) within the hypothesis class $\mathcal{F}$, and for $E = P$ or S, let us denote $\Delta\mathcal{E}_{n,E} = \mathcal{E}_E(u_{n,E}) - \mathcal{E}_E(u_E^*)$. The following lemma summarizes abstract generalization error bound for the energy excess $\Delta\mathcal{E}_n$ for the two equations, whose proof can be found in Appendix A.

Lemma 6 *Assume that* $\sup_{u\in\mathcal{F}} \|u\|_{L^\infty(\Omega)} < \infty$. *Then we have that*

$$\mathbf{E}\Delta\mathcal{E}_{n,P} \leq 2R_n(\mathcal{G}_P) + 4\sup_{u\in\mathcal{F}}\|u\|_{L^\infty(\Omega)} \cdot R_n(\mathcal{F}) + \frac{1}{2}\inf_{u\in\mathcal{F}}\|u - u^*\|^2_{H^1(\Omega)}, \tag{18}$$

$$\mathbf{E}\Delta\mathcal{E}_{n,S} \leq 2R_n(\mathcal{G}_S) + \frac{1}{2}\inf_{u\in\mathcal{F}}\|u - u^*\|^2_{H^1(\Omega)}. \tag{19}$$

Bounding the Rademacher Complexity Recall the set of two-layer nets $\mathcal{F}_{\mathrm{SP}_\tau,m}(B)$ defined by setting $\phi = \mathrm{SP}_\tau$. We also define the corresponding function classes $\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)$ and $\mathcal{G}_{\mathrm{SP}_\tau,m,S}(B)$ by replacing $\mathcal{F}$ by $\mathcal{F}_{\mathrm{SP}_\tau,m}(B)$ in (17). According to Lemma 6, to bound the generalization error bound (in terms of the energy excess), it is essential to bound the Rademacher complexities of $\mathcal{F}_{\mathrm{SP}_\tau,m}(B), \mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)$ and $\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)$. The next lemma states a bound for $R_n(\mathcal{F}_{\mathrm{SP}_\tau,m}(B))$.

Lemma 7 *For any* $\tau > 0, B > 0$, *it holds that* $R_n(\mathcal{F}_{\mathrm{SP}_\tau,m}(B)) \leq \frac{16(1+\sqrt{d}+\frac{\ln 2}{\tau})B}{\sqrt{n}}$.

The proof of Lemma 7 follows from the contraction principle of the Rademacher complexity. In fact, thanks to the fact that SP_τ is 1-Lipschitz, bounding the complexity of $\mathcal{F}_{\mathrm{SP}_\tau,m}(B)$ can be reduced to bounding that of suitable affine functions. See a detailed proof in Appendix C.1.

Theorem 8 *Assume that* $\|f\|_{L^\infty(\Omega)} \leq F$ *and* $\|V\|_{L^\infty(\Omega)} \leq V_{\max}$. *Consider the sets* $\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)$ *and* $\mathcal{G}_{\mathrm{SP}_\tau,m,S}(B)$ *with* $\tau = \sqrt{m}$. *Then there exist positive constants* $C_P(B,d,F)$ *and* $C_S(B,d,F,V_{\max})$ *depending polynomially on* $B,d,F,V_{\max}$ *such that*

$$R_n(\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)) \leq \frac{C_P(B,d,F)\sqrt{m}(\sqrt{\log m}+1)}{\sqrt{n}}, \tag{20}$$

$$R_n(\mathcal{G}_{\mathrm{SP}_\tau,m,S}(B)) \leq \frac{C_S(B,d,F,V_{\max})\sqrt{m}(\sqrt{\log m}+1)}{\sqrt{n}}. \tag{21}$$

Proof [Proof Sketch of Theorem 8] We will only sketch the key steps for proving the bound on $R_n(\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B))$ and refer a detailed proof to Appendix C.2; The same proof strategy carries over to bounding $R_n(\mathcal{G}_{\mathrm{SP}_\tau,m,S}(B))$.

Step 1. Decomposing the set $\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)$. Let us define two sets of functions

$$\begin{aligned}\mathcal{G}^1_{\mathrm{SP}_\tau,m}(B) &:= \{g : \Omega \to \mathbb{R} \mid g = \frac{1}{2}|\nabla u|^2 \text{ where } u \in \mathcal{F}_{\mathrm{SP}_\tau,m}(B)\},\\ \mathcal{G}^2_{\mathrm{SP}_\tau,m}(B) &:= \{g : \Omega \to \mathbb{R} \mid g = fu \text{ where } u \in \mathcal{F}_{\mathrm{SP}_\tau,m}(B)\}.\end{aligned}$$

Then it is clear that $R_n(\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)) \leq R_n(\mathcal{G}^1_{\mathrm{SP}_\tau,m}(B)) + R_n(\mathcal{G}^2_{\mathrm{SP}_\tau,m}(B))$.

Step 2. Bounding $R_n(\mathcal{G}^1_{\mathrm{SP}_\tau,m}(B))$ and $R_n(\mathcal{G}^2_{\mathrm{SP}_\tau,m}(B))$. The idea is to bound the Rademacher complexity in terms of the metric entropy by using the following celebrated Dudley's theorem Dudley (1967). We present below a restatement of the theorem from (Wolf, 2020, Theorem 1.19).

Theorem 9 (Dudley's theorem (Wolf, 2020, Theorem 1.19)) *Let $\mathcal{F}$ be a function class such that $\sup_{f\in\mathcal{F}} \|f\|_\infty \leq M$. Then the Rademacher complexity $R_n(\mathcal{F})$ satisfies that*

$$R_n(\mathcal{F}) \leq \inf_{0\leq\delta\leq M} \left\{4\delta + \frac{12}{\sqrt{n}} \int_\delta^M \sqrt{\log \mathcal{N}(\varepsilon, \mathcal{F}, \|\cdot\|_\infty)}\, d\varepsilon\right\},$$

where $\mathcal{N}(\varepsilon, \mathcal{F}, \|\cdot\|_\infty)$ denotes the ε-covering number of $\mathcal{F}$ w.r.t the L_∞-norm.

Now we apply Dudley's theorem to bound the δ-covering number of the set $\mathcal{G}^1_{\mathrm{SP}_\tau,m}(B)$ and due to page limit we omit the same process applied to the other set $\mathcal{G}^2_{\mathrm{SP}_\tau,m}(B)$. To construct a cover of $\mathcal{G}^1_{\mathrm{SP}_\tau,m}(B)$, we build covers of the parameter space. Specifically, we consider the larger set $\Theta = [-2B, 2B] \times B^m_1(4B) \times \left(B^d_1(1)\right)^m \times [-1,1]^m$ containing the parameter space associated to (11). The set Θ is endowed with the metric ρ defined for $\theta = (c, \gamma, w, t), \theta' = (c', \gamma', w', t') \in \Theta$ by $\rho_\Theta(\theta, \theta') = \max\{|c - c'|, |\gamma - \gamma'|_1, \max_i |w_i - w'_i|_1, |t - t'|_\infty\}$. It can be shown (see the proof of Lemma 28 in Appendix C.2) that for any $u_\theta, u_{\theta'} \in \mathcal{F}_{\mathrm{SP}_\tau,m}(B)$,

$$\frac{1}{2} \sup_{\theta,\theta'\in\Theta} \||\nabla u_\theta|^2 - |\nabla u_{\theta'}|^2\|_{L^\infty(\Omega)} \leq \Lambda_1 \rho_\Theta(\theta, \theta'),$$

where $\Lambda_1 \leq 32B^2\sqrt{m} + 4B$. This particularly implies that $\mathcal{N}(\delta, \mathcal{G}^1_m, \|\cdot\|_\infty) \leq \mathcal{N}(\frac{\delta}{\Lambda_1}, \Theta, \rho_\Theta)$. In addition, thanks to Proposition 27 in Appendix C.2,

$$\mathcal{N}(\frac{\delta}{\Lambda_1}, \Theta, \rho_\Theta) \leq \frac{4B\Lambda_1}{\delta} \cdot \left(\frac{12B\Lambda_1}{\delta}\right)^m \cdot \left(\frac{3\Lambda}{\delta}\right)^{dm} \cdot \left(\frac{3\Lambda}{\delta}\right)^m. \tag{22}$$

Combining the last two estimates with the Dudley's theorem yields that $R_n(\mathcal{G}^1_{\mathrm{SP}_\tau,m}(B)) \leq C_1(B, d)$ $\sqrt{\frac{m\log m}{n}}$. It follows from similar arguments that $R_n(\mathcal{G}^2_{\mathrm{SP}_\tau,m}(B)) \leq C_2(B, d, F)\sqrt{\frac{m}{n}}$. Here the constants $C_1(B, d)$ and $C_2(B, d, F)$ depend at mostly polynomially on the parameters B, d, F. Combining the last two estimates proves the estimate (20). ∎

Proof [Proof of Theorem 3] We only present the proof of Part (i), Theorem 3 since Part (ii) can be done in the same manner. First from the definition of $\mathcal{F}_{\mathrm{SP}_\tau,m}(B)$, one can obtain that $\sup_{u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)} \|u\|_{L^\infty(\Omega)} \leq 14B$. Then it follows from Lemma 6, Theorem 8, Theorem 2 and Lemma 7 that

$$\begin{aligned}
\mathbf{E}\big[\mathcal{E}_P(u^m_{n,P}) - \mathcal{E}_P(u^*_P)\big] &\leq 2R_n(\mathcal{G}_{\mathrm{SP}_\tau,m,P}) + 4 \sup_{u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)} \|u\|_{L^\infty(\Omega)} \cdot R_n(\mathcal{F}_{\mathrm{SP}_\tau,m}) \\
&\quad + \frac{1}{2} \inf_{u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)} \|u - u^*\|^2_{H^1(\Omega)} \\
&\leq \frac{2C_P(B, d, F)\sqrt{m}(\sqrt{\log m} + 1)}{\sqrt{n}} + \frac{4 \cdot 14 \cdot 16 \cdot B^2(\sqrt{d} + 1 + \frac{\ln 2}{\sqrt{m}})}{\sqrt{n}} + \frac{B^2(6\log m + 30)^2}{2m} \\
&\leq \frac{C_1\sqrt{m}(\sqrt{\log m} + 1)}{\sqrt{n}} + \frac{C_2(\log m + 1)^2}{m},
\end{aligned}$$

where C_1 depends polynomially on B, d and F and C_2 depends only quadratically on B. ∎

3.2. Proof Sketch of Theorem 5

The proof of Part (i) is straightforward and can be found in Appendix D.1. The proof of Part (ii) is more tricky. We only sketch the main idea here and provide the complete proof in Appendix D.2. In fact, by multiplying Φ_k on both sides of the static Schrödinger equation and then integrating, one obtains the following equivalent linear system on the cosine coefficients $\hat{u} = \{\hat{u}_k\}_{k\in\mathbb{N}_0^d}$:

$$|\pi|^2|k|^2\hat{u}_k + \widehat{(Vu)}_k = \hat{f}_k, \quad k \in \mathbb{N}_0^d. \tag{23}$$

This system of equations can be further rewritten as an operator equation

$$(\mathbb{M} + \mathbb{V})\hat{u} = \hat{f} \text{ or equivalently } (\mathbb{I} + \mathbb{M}^{-1}\mathbb{V})\hat{u} = \mathbb{M}^{-1}\hat{f}, \tag{24}$$

where $\mathbb{M}$ is an invertible diagonal multiplication operator with $(\mathbb{M}\hat{u})_k = \pi^2|k|^2\hat{u}_k$ for $k \neq \mathbf{0}$ and $\mathbb{V}$ is a "convolution"-type operator defined by the potential V. In order to show that $u \in \mathcal{B}^{s+2}(\Omega)$, it suffices to show that the equation $(\mathbb{M} + \mathbb{V})\hat{u} = \hat{f}$ has a unique solution $\hat{u} \in \ell^1_{W_s}(\mathbb{N}_0^d)$. In fact, thanks to the boundedness of $\mathbb{V}$ on $\ell^1_{W_s}(\mathbb{N}_0^d)$, it is not hard to show that

$$\|u\|_{\mathcal{B}^{s+2}(\Omega)} \lesssim \|\mathbb{M}\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \lesssim \|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} + \|\hat{f}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)}. \tag{25}$$

Finally we claim that equation (24) has a unique solution $\hat{u} \in \ell^1_{W_s}(\mathbb{N}_0^d)$ and that for some $C_2 > 0$

$$\|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \leq C_2\|\hat{f}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)}. \tag{26}$$

To see this, it is important to observe that $\mathbb{M}^{-1}\mathbb{V}$ is compact on $\ell^1_{W_s}(\mathbb{N}_0^d)$ (using Lemma 35 in Appendix D.2), the operator equation $\mathbb{I} + \mathbb{M}^{-1}\mathbb{V}$ is a Fredholm operator on $\ell^1_{W_s}(\mathbb{N}_0^d)$. By the celebrated Fredholm alternative theorem (see e.g., (Fredholm, 1903) and (Conway, 1990, VII 10.7)), the operator $\mathbb{I} + \mathbb{M}^{-1}\mathbb{V}$ has a bounded inverse $(\mathbb{I} + \mathbb{M}^{-1}\mathbb{V})^{-1}$ if and only if $(\mathbb{I} + \mathbb{M}^{-1}\mathbb{V})\hat{u} = 0$ has a trivial solution. Therefore to prove the bound (26), it suffices to show that $(\mathbb{I} + \mathbb{M}^{-1}\mathbb{V})\hat{u} = 0$ implies $\hat{u} = 0$. Such uniqueness follows directly from the uniqueness of the Schrödinger problem (2). The regularity estimate (14) follows by combining (25) and (26).

4. Numerical Experiments

Poisson Equation. Consider the Poisson equation

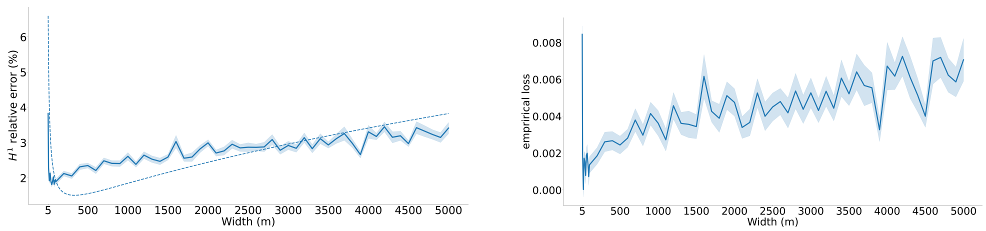
$$-\Delta u = f(x) = \pi^2 \sum_{k=1}^{d} \cos(\pi x_k) \tag{27}$$

in the hupercube Ω subject to a homogeneous Neumann boundary condition. The exact solution is $u_P^*(x) = \sum_{k=1}^d \cos(\pi x_k)$. We further notice that $\int f(x) = 0$. Thus, the unique weak solution u_P^* is also the solution to the argmin problem $\arg\min_{u\in H^1(\Omega)} \mathcal{E}_P(u)$ according to Proposition 1. In practice, the empirical loss $\mathcal{E}_{n,P}(u)$ will be minimized to approximate the PDE solution. u will be parametrized as a neural network. More specifically, a two-layer neural network is used and the activation function is taken to be the rescaled softplus function. While the stochastic gradient descent(SGD) does not guarantee universal optimizer $u^m_{n,P}$, the neural network prediction (denote

Dimension d	2	3	5	10	20	50	100
H^1-relative error(%)	1.04	1.08	1.89	2.09	4.19	5.82	17.59

Table 1: **Poisson equation** (27)**:** H^1-relative error of Ritz prediction $\tilde{u}^m_{n,P}$ ($m = 2,000$ and $n = 100,000$).

by $\tilde{u}^m_{n,P}$) can closely approximate the exact solution u^*_P for various dimensions through sufficient training(Table 1). Moreover, we observe that, with fixed n, as m grows, the H^1-generalization error curve of Ritz prediction exhibits the U-shape, which is consistent to our theoretical upper bound for the error of $u^m_{n,P}$ denoted by $B_P(m) := C_1\frac{\sqrt{m}(\sqrt{\log m}+1)}{\sqrt{n}} + C_2\frac{(\log m+1)^2}{m}$ (see Theorem 3 and Proposition 1). When comparing with the generalization error, the constants in $B_P(m)$ are computed to best fit the error data set (Figure 1).



(a) Solid line: Mean H^1-relative error. Dashed line: $B_P(m)$.

(b) Mean empirical loss $\mathcal{E}_{n,P}(\tilde{u}^m_{n,P})$.

Figure 1: **Poisson equation** (27)**:** H^1-generalization error/empirical loss of Ritz prediction v.s width (m) with $n = 100,000$. Activation function: rescaled Softplus.

Schrödinger Equation. Now let us consider the following Schrödinger equation

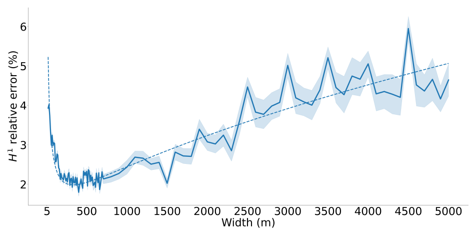
$$-\Delta u + \left(\sum_{k=1}^{\infty} \sin(x_k)\right) u = f(x) = \left(\sum_{k=1}^{d} \sin(\pi x_k) + \pi^2\right)\left(\sum_{k=1}^{d} \cos(\pi x_k)\right) \tag{28}$$

in Ω subject to the zero Neumann boundary condition. The exact solution is again $u^*_S(x) = \sum_{k=1}^d \cos(\pi x_k)$. Similar to last example, we utilize a neural network to solve the minimization problem $\arg\min_{u\in H^1(\Omega)} \mathcal{E}_S(u)$ as defined in Proposition 1 to approximate the solution to the PDE. In this example, different activation functions are tested. We observe that the neural network solution provides a good approximation to the solution of the Schrödinger equation for various dimensions (Table 2). We also observe that the curve of H^1-generalization error and empirical loss for

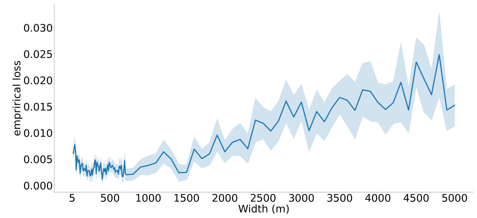
Dimension d	2	3	5	10	20	50	100
H^1-relative error(%)	0.95	1.24	3.54	2.46	5.51	11.70	18.32

Table 2: **Schrödinger equation** (28)**:** H^1-relative error of Ritz prediction $\tilde{u}^m_{n,S}$ ($m = 2,000$ and $n = 300,000$). Activation function : rescaled Softplus.

the approximate solution resulted from a cosine neural network also has a U-shape. Its comparison with the theoretical upper bound $B_S(m) := \frac{C_3\sqrt{m}(\sqrt{\log m}+1)}{\sqrt{n}} + \frac{C_4(\log m+1)^2}{m}$ with fitted constants is presented in Figure 2.



(a) Solid line: Mean H^1-relative error. Dashed line: $B_S(m)$.



(b) Mean empirical loss $\mathcal{E}_{n,S}(\tilde{u}^m_{n,S})$ of Ritz prediction.

Figure 2: **Schrödinger Equation** (28)**:** H^1-relative error/empirical loss $\tilde{u}^m_{n,S}$ v.s width (m) with $n = 300,000$. Activation function: cosine.

5. Conclusion and Discussion

We established dimension-independent rates of convergence for the generalization error of the DRM for solving two simple linear elliptic PDEs under the a priori assumption that the exact solutions lie in the spectral Barron space. Such a priori assumption can be verified using a new solution theory of the PDEs in the Barron space. We would like to discuss some restrictions of the main results and point out some interesting future directions.

First, some preliminary numerical experiments show that the convergence rates in our generalization error estimates may not be sharp. In fact, we expect that the approximation error can be sharpened using two-layer networks with possibly different activation functions and that the statistical error may also be improved with more delicate Rademacher complexity estimates; those questions are to be investigated in future work.

We restricted our attention on two simple elliptic problems to better convey the main ideas. It is natural to consider carrying out similar programs of solving more general PDE problems defined on general bounded domains. The first major difficulty arises when one comes to the definition of Barron functions on a general bounded domain and our spectral Barron functions built on cosine expansions can not be adapted to general domains. Other Barron functions such as the one defined in (E et al., 2019) via integral representation are on bounded domains and may be considered as alternatives, but building a solution theory for PDEs in those spaces seems highly nontrivial; see (E and Wojtowytsch, 2020) for some results and discussions along this direction.

It is also interesting to establish a priori generalization error estimates for other neural network-based methods for PDEs based on alternative loss functions, such as PINNs (Raissi et al., 2019) and the weak adversarial networks (Zang et al., 2020).

Acknowledgments

J.L. and M.W. are supported in part by National Science Foundation via grants DMS-2012286 and CCF-1934964. Y.L. is supported by the start-up fund of the Department of Mathematics and Statistics at UMass Amherst.

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Appendix A. Abstract Generalization Error (Proof of Lemma 6)

Let us start with the proof of the abstract generalization error bound (6) for Poisson equation. To this end, recall the Ritz loss and the empirical loss associated to the Poisson equation

$$\begin{aligned}
\mathcal{E}_P(u) &= |\Omega| \cdot \mathbf{E}_{X\sim\mathcal{P}_\Omega}\Big[\frac{1}{2}|\nabla u(X)|^2 - f(X)u(X)\Big] + \frac{1}{2}\Big(|\Omega|\cdot\mathbf{E}_{X\sim\mathcal{P}_\Omega}u(X)\Big)^2\\
&=: \mathcal{E}^1(u) + \mathcal{E}^2(u),\\
\mathcal{E}_{n,P}(u) &= \frac{1}{n}\sum_{j=1}^n\Big[|\Omega|\cdot\Big(\frac{1}{2}|\nabla u(X_j)|^2 - f(X_j)u(X_j)\Big)\Big] + \frac{1}{2}\Big(\frac{|\Omega|}{n}\sum_{j=1}^n u(X_j)\Big)^2\\
&=: \mathcal{E}_n^1(u) + \mathcal{E}_n^2(u).
\end{aligned}$$

By definition, the bias term $\Delta\mathcal{E}_{\text{bias}}$ in (16) satisfies that

$$\begin{aligned}
\Delta\mathcal{E}_{\text{bias}} &= \mathbf{E}[\mathcal{E}_n^1(u_\mathcal{F})] - \mathcal{E}^1(u_\mathcal{F}) + \mathbf{E}[\mathcal{E}_n^2(u_\mathcal{F})] - \mathcal{E}^2(u_\mathcal{F})\\
&= \frac{1}{2}\mathbf{E}\Big(\frac{|\Omega|}{n}\sum_{j=1}^n u(X_j)\Big)^2 - \frac{1}{2}\Big(|\Omega|\cdot\mathbf{E}_{X\sim\mathcal{P}_\Omega}u(X)\Big)^2\\
&= \frac{1}{2}\mathbf{E}\Big[\Big(\frac{1}{n}\sum_{j=1}^n u_\mathcal{F}(X_j) - \mathbf{E}_{X\sim\mathcal{P}_\Omega}u_\mathcal{F}(X)\Big)\cdot\Big(\frac{1}{n}\sum_{j=1}^n u_\mathcal{F}(X_j) + \mathbf{E}_{X\sim\mathcal{P}_\Omega}u_\mathcal{F}(X)\Big)\Big]\\
&\leq \|u_\mathcal{F}\|_{L^\infty(\Omega)}\cdot\mathbf{E}\sup_{u\in\mathcal{F}}\Big|\frac{1}{n}\sum_{j=1}^n u(X_j) - \mathbf{E}_{X\sim\mathcal{P}_\Omega}u(X)\Big|\\
&\leq 2\sup_{u\in\mathcal{F}}\|u\|_{L^\infty(\Omega)}\cdot R_n(\mathcal{F}),
\end{aligned}$$

where we have used $|\Omega| = 1$ the last inequality follows from Lemma 10.

Lemma 10 *(Wainwright, 2019, Proposition 4.11) Let $\mathcal{F}$ be a set of functions. Then*

$$\mathbf{E}\sup_{u\in\mathcal{F}}\Big|\frac{1}{n}\sum_{j=1}^n u(X_j) - \mathbf{E}_{X\sim\mathcal{P}_\Omega}u(X)\Big| \leq 2R_n(\mathcal{F}).$$

Next we bound the first term $\Delta\mathcal{E}_{\text{gen}}$ in (16). In fact, it follows by Lemma 10 that

$$\begin{aligned}
\Delta\mathcal{E}_{\text{gen}} &\leq \mathbf{E}\sup_{v\in\mathcal{F}}\Big|\mathcal{E}_P(v) - \mathcal{E}_{n,P}(v)\Big|\\
&\leq \mathbf{E}\sup_{v\in\mathcal{F}}\Big|\mathcal{E}^1(v) - \mathcal{E}_n^1(v)\Big| + \mathbf{E}\sup_{v\in\mathcal{F}}\Big|\mathcal{E}^2(v) - \mathcal{E}_n^2(v)\Big|\\
&\leq \mathbf{E}\sup_{g\in\mathcal{G}}\Big|\frac{1}{n}\sum_{j=1}^n g(X_j) - \mathbf{E}_{\mathcal{P}_\Omega}[g]\Big| + \mathbf{E}\sup_{u\in\mathcal{F}}\frac{1}{2}\Big|\Big(\mathbf{E}_{X\sim\mathcal{P}_\Omega}u(X)\Big)^2 - \Big(\frac{1}{n}\sum_{j=1}^n u(X_j)\Big)^2\Big|\\
&\leq 2R_n(\mathcal{G}_P) + \sup_{u\in\mathcal{F}}\|u\|_{L^\infty(\Omega)}\cdot\mathbf{E}\sup_{u\in\mathcal{F}}\Big|\frac{1}{n}\sum_{j=1}^n u(X_j) - \mathbf{E}_{X\sim\mathcal{P}_\Omega}u(X)\Big|\\
&\leq 2R_n(\mathcal{G}_P) + 2\sup_{u\in\mathcal{F}}\|u\|_{L^\infty(\Omega)}R_n(\mathcal{F}).
\end{aligned}$$

Finally owing to the estimate (4) in Proposition 1, the approximation error $\Delta\mathcal{E}_{\text{approx}}$ satisfies that

$$\Delta\mathcal{E}_{\text{approx}} \leq \frac{1}{2}\inf_{u\in\mathcal{F}}\|u-u^*\|^2_{H^1(\Omega)}.$$

Therefore inserting the last three estimates into (16) finishes the proof of (6) on the energy excess $\Delta\mathcal{E}_{n,P}$ in the case of Poisson equation.

Now we proceed to prove an abstract generalization bound for the static Schrödinger equation. First recall the corresponding Ritz loss and the empirical loss as follows

$$\mathcal{E}_S(u) = |\Omega|\cdot\mathbf{E}_{X\sim\mathcal{P}_\Omega}\Big[\frac{1}{2}|\nabla u(X)|^2 + \frac{1}{2}V(X)|u(X)|^2 - f(X)u(X)\Big],$$
$$\mathcal{E}_{n,S}(u) = \frac{1}{n}\sum_{j=1}^n\Big[|\Omega|\cdot\Big(\frac{1}{2}|\nabla u(X_j)|^2 + \frac{1}{2}V(X_j)|u(X_j)|^2 - f(X_j)u(X_j)\Big)\Big].$$

In the Schrödinger case, since the Ritz energy $\mathcal{E}_S$ is linear with respect to the probability measure $\mathcal{P}_\Omega$, the statistical errors $\Delta\mathcal{E}_{\text{gen}}$ and $\Delta\mathcal{E}_{\text{bias}}$ are simpler than those in the Poisson case. In particular, a similar calculation shows that $\Delta\mathcal{E}_{\text{bias}} = 0$ and $\Delta\mathcal{E}_{\text{gen}} \leq 2R_n(\mathcal{G}_S)$. Therefore (19) follows from (16).

Appendix B. Spectral Barron functions on the hypercube and their H^1-approximation (Proof of Theorem 2)

In this section, we discuss the approximation properties two-layer neural networks of spectral Barron functions on the d-dimensional hypercube defined by (10) as well as their neural network approximations. Since our spectral Barron functions are defined via the expansion under the following set of cosine functions:

$$\mathcal{C} = \Big\{\Phi_k\Big\}_{k\in\mathbb{N}_0^d} := \Big\{\prod_{i=1}^d \cos(\pi k_i x_i) \mid k_i\in\mathbb{N}_0\Big\},$$

we start by stating some preliminaries on $\mathcal{C}$ and the product of cosines to be used in the subsequent proofs.

B.1. Preliminary Lemmas

Lemma 11 *The set $\mathcal{C}$ forms an orthogonal basis of $L^2(\Omega)$ and $H^1(\Omega)$.*

Proof First that $\mathcal{C}$ forms an orthogonal basis of $L^2(\Omega)$ follows directly from the Parseval's theorem applied to the Fourier expansion of the even extension of a function u from $L^2(\Omega)$. To see $\mathcal{C}$ is an orthogonal basis of $H^1(\Omega)$, since $\mathcal{C}$ is an orthogonal set of $H^1(\Omega)$, it suffices to show that if $u\in H^1(\Omega)$ satisfying

$$\Big(u,\Phi_k\Big)_{H^1(\Omega)} = 0$$

for all $k \in \mathbb{N}_0^d$, then $u = 0$. In fact, the last display above yields that

$$\begin{aligned} 0 &= \int_\Omega u \cdot \Phi_k dx + \int_\Omega \nabla u \cdot \nabla \Phi_k dx \\ &= \int_\Omega u \cdot (\Phi_k - \Delta \Phi_k) dx \\ &= (1 + \pi^2 |k|^2) \int_\Omega u \cdot \Phi_k dx, \end{aligned}$$

where for the second identity we have used the Green's formula and the fact that the normal derivative of Φ_k vanishes on the boundary of Ω. Therefore we have obtained that $(u, \Phi_k)_{L^2} = 0$ for any $k \in \mathbb{N}_0^d$, which implies that $u = 0$ since $\mathcal{C}$ is an orthogonal basis of $L^2(\Omega)$. ■

Given $u \in L^2(\Omega)$, let $\{\hat{u}(k)\}_{k \in \mathbb{N}_0^d}$ be the expansion coefficients of u under the basis $\{\Phi_k\}_{k \in \mathbb{N}_0^d}$. Then for any $u \in L^2(\Omega)$,

$$u(x) = \sum_{k \in \mathbb{N}_0^d} \hat{u}(k) \Phi_k(x).$$

Moreover, it follows from a straightforward calculation that for $u \in H^1(\Omega)$,

$$\|u\|_{H^1(\Omega)}^2 = \sum_{k \in \mathbb{N}_0^d} \alpha_k (1 + \pi^2 |k|^2) |\hat{u}(k)|^2,$$

where $\alpha_k = \langle \Phi_k, \Phi_k \rangle_{L^2(\Omega)} = 2^{-\sum_{i=1}^d \mathbf{1}_{k_i \neq 0}} \leq 1$. This implies the following characterization of a function from $H^1(\Omega)$ function in terms of its expansion coefficients under $\mathcal{C}$.

Corollary 12 *The space $H^1(\Omega)$ can be characterized as*

$$H^1(\Omega) = \Big\{ u \in L^2(\Omega) \,\Big|\, \sum_{k \in \mathbb{N}_0^d} |\hat{u}(k)|^2 (1 + \pi^2 |k|^2) < \infty \Big\}.$$

The following elementary product formula of cosine functions will also be useful.

Lemma 13 *For any $\{\theta_i\}_{i=1}^d \subset \mathbb{R}$,*

$$\prod_{i=1}^d \cos(\theta_i) = \frac{1}{2^d} \sum_{\xi \in \Xi} \cos(\xi \cdot \theta),$$

where $\theta = (\theta_1, \cdots, \theta_d)^T$ and $\Xi = \{1, -1\}^d$.

Proof The lemma follows directly by iterating the following simple identity

$$\begin{aligned} \cos(\theta_1) \cos(\theta_2) &= \frac{1}{2} \big(\cos(\theta_1 + \theta_2) + \cos(\theta_1 - \theta_2) \big) \\ &= \frac{1}{4} \big(\cos(\theta_1 + \theta_2) + \cos(\theta_1 - \theta_2) + \cos(-\theta_1 - \theta_2) + \cos(-\theta_1 + \theta_2) \big). \end{aligned}$$

■

B.2. Spectral Barron Space and Neural-Network Approximation

Recall for any $s \in \mathbb{N}$ the spectral Barron space $\mathcal{B}^s(\Omega)$ given by

$$\mathcal{B}^s(\Omega) := \Big\{u \in L^1(\Omega) : \sum_{k\in\mathbb{N}_0^d} (1+\pi^s|k|_1^s)|\hat{u}(k)| < \infty\Big\}$$

with associated norm $\|u\|_{\mathcal{B}^s(\Omega)} := \sum_{k\in\mathbb{N}_0^d}(1+\pi^s|k|_1^s)|\hat{u}(k)|$. Recall also the short notation $\mathcal{B}(\Omega)$ for $\mathcal{B}^2(\Omega)$.

Lemma 14 *The following embedding results hold:*
(i) $\mathcal{B}(\Omega) \hookrightarrow H^1(\Omega)$*;*
(ii) $\mathcal{B}^0(\Omega) \hookrightarrow L^\infty(\Omega)$.

Proof (i). If $u \in \mathcal{B}(\Omega)$, then $\|u\|_{\mathcal{B}(\Omega)} = \sum_{k\in\mathbb{N}_0^d}(1+\pi^2|k|_1^2)|\hat{u}(k)| < \infty$. This particularly implies $|\hat{u}(k)| \le \|u\|_{\mathcal{B}(\Omega)}$ for each $k \in \mathbb{N}^d$. Since $\alpha_k \le 1$, we have that

$$\begin{aligned}
\|u\|_{H^1(\Omega)}^2 &= \sum_{k\in\mathbb{N}_0^d} \alpha_k(1+\pi^2|k|_1^2)|\hat{u}(k)|^2 \\
&\le \|u\|_{\mathcal{B}(\Omega)} \sum_{k\in\mathbb{N}_0^d}(1+\pi^2|k|_1^2)|\hat{u}(k)| \\
&= \|u\|_{\mathcal{B}(\Omega)}^2.
\end{aligned}$$

(ii). For $u \in \mathcal{B}^0(\Omega)$, using the fact that $\|\Phi_k\|_{L^\infty(\Omega)} \le 1$ we have that

$$\|u\|_{L^\infty(\Omega)} = \Big\|\sum_{k\in\mathbb{N}_0^d}\hat{u}(k)\Phi_k\Big\|_{L^\infty(\Omega)} \le \sum_{k\in\mathbb{N}_0^d}|\hat{u}(k)| = \|u\|_{\mathcal{B}(\Omega)}.$$

■

Thanks to Lemma 11 and Lemma 13, any function $u \in H^1(\Omega)$ admits the expansion

$$u(x) = \sum_{k\in\mathbb{N}_0^d}\hat{u}(k)\cdot\frac{1}{2^d}\sum_{\xi\in\Xi}\cos(\pi k_\xi\cdot x), \tag{29}$$

where $\hat{u}(k)$ is the expansion coefficient of u under the basis $\mathcal{C}$ and $k_\xi = (k_1\xi_1,\cdots,k_d\xi_d) \in \mathbb{Z}^d$.

Given $u \in \mathcal{B}(\Omega) \subset H^1(\Omega)$, letting $(-1)^{\theta(k)} = \text{sign}(\hat{u}(k))$ with $\theta(k) \in \{0,1\}$, we have from (29) that

$$
\begin{aligned}
u(x) &= \hat{u}(0) + \sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} \hat{u}(k) \cdot \frac{1}{2^d} \sum_{\xi\in\Xi} \cos(\pi k_\xi \cdot x) \\
&= \hat{u}(0) + \sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} |\hat{u}(k)| \,\text{sign}(\hat{u}(k)) \cdot \frac{1}{2^d} \sum_{\xi\in\Xi} \cos(\pi k_\xi \cdot x) \\
&= \hat{u}(0) + \sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} |\hat{u}(k)| \cdot \frac{1}{2^d} \sum_{\xi\in\Xi} \cos(\pi (k_\xi \cdot x + \theta_k)) \\
&= \hat{u}(0) + \sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} \frac{1}{Z_u} |\hat{u}(k)| \,(1+\pi^2|k|_1^2) \cdot \frac{Z_u}{1+\pi^2|k|_1^2} \cdot \frac{1}{2^d} \sum_{\xi\in\Xi} \cos(\pi (k_\xi \cdot x + \theta_k)) \\
&=: \hat{u}(0) + \int g(x,k)\mu(dk),
\end{aligned}
$$

where $\mu(dk)$ is the probability measure on $\mathbb{N}_0^d \setminus \{\mathbf{0}\}$ defined by

$$
\mu(dk) = \sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} \frac{1}{Z_u} \big|\hat{u}(k)\big| (1+\pi^2|k|_1^2)\delta(dk)
$$

with normalizing constant $Z_u = \sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} |\hat{u}(k)|(1+\pi^2|k|_1^2) \leq \|u\|_{\mathcal{B}(\Omega)}$ and

$$
g(x,k) = \frac{Z_u}{1+\pi^2|k|_1^2} \cdot \frac{1}{2^d} \sum_{\xi\in\Xi} \cos(\pi(k_\xi \cdot x + \theta_k)).
$$

Observe that the function $g(x,k) \in C^2(\Omega)$ for every $k \in \mathbb{N}_0^d \setminus \{\mathbf{0}\}$. Moreover, it is straightforward to show that the following bounds hold:

$$
\begin{aligned}
&\|g(\cdot,k)\|_{H^1(\Omega)} = Z_u \sqrt{\frac{\alpha_k}{1+\pi^2|k|_1^2}} \leq \|u\|_{\mathcal{B}(\Omega)}, \\
&\|D^s g(\cdot,k)\|_{L^\infty(\Omega)} \leq Z_u \leq \|u\|_{\mathcal{B}(\Omega)} \text{ for } s = 0,1,2.
\end{aligned}
$$

Let us define for a constant $B > 0$ the function class

$$
\mathcal{F}_{\cos}(B) := \Big\{ \frac{\gamma}{1+\pi^2|k|_1^2} \cos(\pi(k \cdot x + b)), k \in \mathbb{Z}^d \setminus \{\mathbf{0}\}, |\gamma| \leq B, b \in \{0,1\} \Big\}.
$$

It follows from the calculations above that if $u \in \mathcal{B}(\Omega)$, then $\bar{u} := u - \hat{u}(0)$ lies in the H^1-closure of the convex hull of $\mathcal{F}_{\cos}(B)$ with $B = \|u\|_{\mathcal{B}(\Omega)}$. Indeed, if $\{k^i\}_{i=1}^m$ is an i.i.d. sequence of random samples from the probability measure μ, then it follows from Fubini's theorem that

$$\begin{aligned}
&\mathbf{E}\left\|\bar{u}(x)-\frac{1}{m}\sum_{i=1}^{m}g(x,k^i)\right\|_{H^1(\Omega)}^2\\
&=\mathbf{E}\int_{\Omega}\left|\bar{u}(x)-\frac{1}{m}\sum_{i=1}^{m}g(x,k^i)\right|^2dx+\mathbf{E}\int_{\Omega}\left|\nabla\bar{u}(x)-\frac{1}{m}\sum_{i=1}^{m}\nabla g(x,k^i)\right|^2dx\\
&=\frac{1}{m}\int_{\Omega}\mathrm{Var}[g(x,k)]dx+\frac{1}{m}\int_{\Omega}\mathrm{Tr}(\mathrm{Cov}[\nabla g(x,k)])dx\\
&\le\frac{\mathbf{E}\|g(\cdot,k)\|_{H^1(\Omega)}^2}{m}\\
&\le\frac{\|u\|_{\mathcal{B}(\Omega)}^2}{m}.
\end{aligned}$$

Therefore the expected H^1-norm of an average of m elements in $\mathcal{F}_{\cos}(B)$ converges to zero as $m\to\infty$. This in particular implies that there exists a sequence of convex combinations of points in $\mathcal{F}_{\cos}(B)$ converging to $\bar{u}$ in H^1-norm. Since the H^1-norm of any function in $\mathcal{F}_{\cos}(B)$ is bounded by B, an application of Maurey's empirical method (see Lemma 16) yields the following theorem.

Theorem 15 *Let $u\in\mathcal{B}(\Omega)$. Then there exists u_m which is a convex combination of m functions in $\mathcal{F}_{\cos}(B)$ with $B=\|u\|_{\mathcal{B}(\Omega)}$ such that*

$$\|u-\hat{u}(0)-u_m\|_{H^1(\Omega)}^2\le\frac{\|u\|_{\mathcal{B}(\Omega)}^2}{m}.$$

Lemma 16 (Pisier (1981); Barron (1993)) *Let u belongs to the closure of the convex hull of a set $\mathcal{G}$ in a Hilbert space. Let the Hilbert norm of of each element of $\mathcal{G}$ be upper bounded by $B>0$. Then for every $m\in\mathbb{N}$, there exists $\{g_i\}_{i=1}^m\subset\mathcal{G}$ and $\{c_i\}_{i=1}^m\subset[0,1]$ with $\sum_{i=1}^m c_i=1$ such that*

$$\left\|u-\sum_{i=1}^{m}c_ig_i\right\|^2\le\frac{B^2}{m}.$$

B.3. Reduction from Cosine to ReLU Activation

In this section we aim to show that a similar version of Theorem 15 holds when the cosine activation function is replaced by ReLU activation. This is stated precisely in the following theorem.

Theorem 17 *Consider the class of two-layer ReLU neural networks*

$$\mathcal{F}_{\mathrm{ReLU},m}(B):=\Big\{c+\sum_{i=1}^{m}\gamma_i\mathrm{ReLU}(\omega_i\cdot x-t_i),|c|\le 2B,|w_i|_1=1,|t_i|\le 1,\sum_{i=1}^{m}|\gamma_i|\le 4B\Big\}.\quad(30)$$

Then for any $u\in\mathcal{B}(\Omega)$, there exists $u_m\in\mathcal{F}_{\mathrm{ReLU},m}(\|u\|_{\mathcal{B}(\Omega)})$, such that

$$\|u-u_m\|_{H^1(\Omega)}\le\frac{\sqrt{116}\|u\|_{\mathcal{B}(\Omega)}}{\sqrt{m}}.$$

To prove Theorem 17, first notice that every function in $\mathcal{F}_{\cos}(B)$ is the composition of the one dimensional function g defined on $[-1,1]$ by

$$g(z) = \frac{\gamma}{1+\pi^2|k|_1^2}\cos(\pi(|k|_1 z + b)) \tag{31}$$

with $k \in \mathbb{Z}^d \setminus \{\mathbf{0}\}, |\gamma| \leq B$ and $b \in \{0,1\}$, and a linear function $z = w \cdot x$ with $w = k/|k|_1$. It is clear that $g \in C^2([-1,1])$ and g satisfies that

$$\|g^{(s)}\|_{L^\infty([-1,1])} \leq |\gamma| \leq B \text{ for } s = 0,1,2. \tag{32}$$

Since $b \in \{0,1\}$, it also holds that $g'(0) = 0$.

Lemma 18 *Let $g \in C^2([-1,1])$ with $\|g^{(s)}\|_{L^\infty([-1,1])} \leq B$ for $s = 0,1,2$. Assume that $g'(0) = 0$. Let $\{z_j\}_{j=0}^{2m}$ be a partition of $[-1,1]$ with $z_0 = -1, z_m = 0, z_{2m} = 1$ and $z_{j+1} - z_j = h = 1/m$ for each $j = 0,\cdots,2m-1$. Then there exists a two-layer ReLU network g_m of the form*

$$g_m(z) = c + \sum_{i=1}^{2m} a_i \mathrm{ReLU}(\epsilon_i z - b_i), z \in [-1,1] \tag{33}$$

with $c = g(0), b_i \in [-1,1]$ and $\epsilon_i \in \{\pm 1\}, i = 1,\cdots,2m$ such that

$$\|g - g_m\|_{W^{1,\infty}([-1,1])} \leq \frac{2B}{m}. \tag{34}$$

Moreover, we have that $|a_i| \leq \frac{2B}{m}$ and that $|c| \leq B$.

Proof Let g_m be the piecewise linear interpolation of g with respect to the grid $\{z_j\}_{j=0}^{2m}$, i.e.

$$g_m(z) = g(z_{j+1})\frac{z - z_j}{h} + g(z_j)\frac{z_{j+1} - z}{h} \text{ if } z \in [z_j, z_{j+1}].$$

According to (Ascher and Greif, 2011, Chapter 11),

$$\|g - g_m\|_{L^\infty([-1,1])} \leq \frac{h^2}{8}\|g''\|_{L^\infty([-1,1])}.$$

Moreover, $\|g' - g_m'\|_{L^\infty([-1,1])} \leq h\|g''\|_{L^\infty([-1,1])}$. In fact, consider $z \in [z_j, z_{j+1}]$ for some $j \in \{0,\cdots,2m-1\}$. By the mean value theorem, there exist $\xi, \eta \in (z_j, z_{j+1})$ such that $(g(z_{j+1} - g(z_j)))/h = g'(\xi)$ and hence

$$\begin{aligned}\left|g'(z) - \frac{g(z_{j+1}) - g(z_i)}{h}\right| &= \left|g'(z) - g'(\xi)\right| \\ &= |g''(\eta)||z - \xi| \\ &\leq h\|g''\|_{L^\infty([-1,1])}.\end{aligned}$$

This proves the error bound (34).

Next, we show that g_m can be represented by a two-layer ReLU neural network. Indeed, it is easy to verify that g_m can be rewritten as

$$g_m(z) = c + \sum_{i=1}^{m} a_i \mathrm{ReLU}(z_i - z) + \sum_{i=m+1}^{2m} a_i \mathrm{ReLU}(z - z_{i-1}), z \in [-1,1], \tag{35}$$

where $c = g(z_m) = g(0)$ and the parameters a_i defined by

$$a_i = \begin{cases} \frac{g(z_{m+1})-g(z_m)}{h}, & \text{if } i = m+1, \\ \frac{g(z_{m-1})-g(z_m)}{h}, & \text{if } i = m, \\ \frac{g(z_i)-2g(z_{i-1})+g(z_{i-2})}{h}, & \text{if } i > m+1, \\ \frac{g(z_{i-1})-2g(z_i)+g(z_{i+1})}{h}, & \text{if } i < m. \end{cases}$$

Furthermore, by again the mean value theorem, there exists $\xi_1, \xi_2 \in (z_m, z_{m+1})$ such that $|a_{m+1}| = |g'(\xi_1)| = |g'(\xi_1) - g'(0)| = |g''(\xi_2)\xi_1| \leq Bh$. In a similar manner one can obtain that $|a_m| \leq Bh$ and $|a_i| \leq 2Bh$ if $i \notin \{m, m+1\}$.

Finally, by setting $\epsilon_i = -1, b_i = -z_i$ for $i = 1, \cdots, m$ and $\epsilon_i = 1, b_i = z_{i-1}$ for $i = m+1, \cdots, 2m$, one obtains the desired form (33) of g_m. This completes the proof of the lemma. ■

The following proposition is a direct consequence of Lemma 18.

Proposition 19 *Define the function class*

$$\mathcal{F}_{\mathrm{ReLU}}(B) := \Big\{c + \gamma \mathrm{ReLU}(w \cdot x - t), |c| \leq 2B, |w|_1 = 1, |t| \leq 1, |\gamma| \leq 4B\}.$$

Then for any constant $\tilde{c}$ such that $|\tilde{c}| \leq B$, the set $\tilde{c} + \mathcal{F}_{\cos}(B)$ is in the H^1-closure of the convex hull of $\mathcal{F}_{\mathrm{ReLU}}(B)$.

Proof First Lemma 18 states that each C^2-function g with $g'(0) = 0$ and with up to second order derivatives bounded by B can be well approximated in H^1-norm by a linear combination of a constant function and the ReLU functions $\mathrm{ReLU}(\epsilon z - t)$ with the sum of the absolute values of the combination coefficients bounded by $4B$. As a result, the function g defined in (31) lies in the closure of the convex hull of functions $c + \gamma \mathrm{ReLU}(\epsilon z - t)$ with $|c| \leq B, |\gamma| \leq 4B, |t| \leq 1$. Then the proposition follows from absorbing the additive constant $\tilde{c}$ into the constant c in the definition of $\mathcal{F}_{\mathrm{ReLU}}(B)$. ■

With Proposition 19, we are ready to give the proof of Theorem 17.
Proof [Proof of Theorem 17] Observe that if $u \in \mathcal{F}_{\mathrm{ReLU}}(B)$, then

$$\|u\|^2_{H^1(\Omega)} \leq (c + 2\gamma)^2 + \gamma^2 \leq (10^2 + 4^2)B^2 = 116B^2.$$

Therefore Theorem 17 follows directly from Lemma 16, Proposition 19 with $\tilde{c} = \hat{u}(0)$ and the fact that $|\hat{u}(0)| \leq \|u\|_{\mathcal{B}(\Omega)}$. ■

B.4. Reduction from ReLU to Softplus Activation

In this section we aim to prove Theorem 2 by utilizing the approximation Theorem 17. To this end, let us first state a lemma which shows that ReLU can be well approximated by SP_τ for $\tau \gg 1$.

Lemma 20 *The following inequalities hold:*

(i) $$|\mathrm{ReLU}(z) - \mathrm{SP}_\tau(z)| \leq \frac{1}{\tau} e^{-\tau|z|}, \ \forall z \in [-2, 2];$$

(ii) $$|\mathrm{ReLU}'(z) - \mathrm{SP}'_\tau(z)| \leq e^{-\tau|z|}, \ \forall z \in [-2, 0) \cup (0, 2];$$

(iii) $$\|\mathrm{SP}_\tau\|_{W^{1,\infty}([-2,2])} \leq 3 + \frac{1}{\tau}.$$

Proof Notice that $\mathrm{ReLU}(z) - \mathrm{SP}_\tau(z) = -\frac{1}{\tau}\ln(1+e^{-\tau|z|})$. Hence inequality (i) follows from that

$$|\mathrm{ReLU}(z) - \mathrm{SP}_\tau(z)| \leq \frac{1}{\tau}\ln(1+e^{-\tau|z|}) \leq \frac{e^{-\tau|z|}}{\tau},$$

where the second inequality follows from the simple inequality $\ln(1+x) \leq x$ for $x > -1$. In addition, inequality (ii) holds since

$$|\mathrm{ReLU}'(z) - \mathrm{SP}_\tau'(z)| = \Big|\frac{1}{1+e^{\tau|z|}}\Big| \leq e^{-\tau|z|}, \text{ if } z \neq 0.$$

Finally, inequality (iii) follows from that

$$\|\mathrm{SP}_\tau(z)\|_{L^\infty([-2,2])} = \mathrm{SP}_\tau(2) \leq 2 + \frac{1}{\tau}$$

and that

$$|\mathrm{SP}_\tau'(z)| = \Big|\frac{1}{1+e^{\tau z}}\Big| \leq 1.$$

■

Lemma 21 *Let $g \in C^2([-1,1])$ with $\|g^{(s)}\|_{L^\infty([-1,1])} \leq B$ for $s = 0,1,2$. Assume that $g'(0) = 0$. Let $\{z_j\}_{j=-m}^m$ be a partition of $[-1,1]$ with $m \geq 2$ and $z_{-m} = -1, z_0 = 0, z_m = 1$ and $z_{j+1} - z_j = h = 1/m$ for each $j = -m, \cdots, m-1$. Then there exists a two-layer neural network $g_{\tau,m}$ of the form*

$$g_{\tau,m}(z) = c + \sum_{i=1}^{2m} a_i \mathrm{SP}_\tau(\epsilon_i z - b_i), z \in [-1,1] \tag{36}$$

with $c = g(0) \leq B, b_i \in [-1,1], |a_i| \leq 2B/m$ and $\epsilon_i \in \{\pm 1\}, i = 1, \cdots, 2m$ such that

$$\|g - g_{\tau,m}\|_{W^{1,\infty}([-1,1])} \leq 6B\delta_\tau, \tag{37}$$

where

$$\delta_\tau := \frac{1}{\tau}\Big(1+\frac{1}{\tau}\Big)\Big(\log\big(\frac{\tau}{3}\big)+1\Big). \tag{38}$$

Proof Thanks to Lemma 18, there exists g_m of the form

$$g_m(z) = c + \sum_{i=1}^{m} a_i \mathrm{ReLU}(z_i - z) + \sum_{i=m+1}^{2m} a_i \mathrm{ReLU}(z - z_{i-1}), z \in [-1,1] \tag{39}$$

such that $\|g - g_m\|_{W^{1,\infty}([-1,1])} \leq 2B/m$. More importantly, the coefficients a_i satisfies that $|a_i| \leq 2B/m$ so that $\sum_{i=1}^{2m} a_i \leq 4B$. Now let $g_{\tau,m}$ be the function obtained by replacing the activation ReLU in g_m by SP_τ, i.e.

$$g_{\tau,m}(z) = c + \sum_{i=1}^{m} a_i \mathrm{SP}_\tau(z_i - z) + \sum_{i=m+1}^{2m} a_i \mathrm{SP}_\tau(z - z_{i-1}), z \in [-1,1]. \tag{40}$$

Suppose that $z \in (z_j, z_{j+1})$ for some fixed $j < m-1$. Then thanks to Lemma 20 - (i), the bound $|a_i| \leq 2B/m$ and the fact that $|z_i - z| \geq 1/m$ if $i \neq j$ while $z \in (z_j, z_{j+1})$, we have

$$\begin{aligned}|g_m(z) - g_{\tau,m}(z)| &\leq |a_j||\mathrm{ReLU}(z_j - z) - \mathrm{SP}_\tau(z_j - z)| \\ &\quad + \sum_{i=1, i\neq j}^{m} |a_i||\mathrm{ReLU}(z_i - z) - \mathrm{SP}_\tau(z_i - z)| \\ &\quad + \sum_{i=m+1}^{2m} |a_i||\mathrm{ReLU}(z - z_{i-1}) - \mathrm{SP}_\tau(z - z_{i-1})| \\ &\leq \frac{2B}{m\tau} + \frac{2B}{\tau} e^{-\tau|x|} \mathbf{1}_{|x|\geq 1/m}.\end{aligned}$$

Similar bounds hold for the case where $z \in (z_j, z_{j+1})$ for $j > m$. Lastly, if $z \in (z_m, z_{m+1})$, then both the m-th and $m+1$-th term in (39) and (40) depend on z_m, from which we get

$$|g_m(z) - g_{\tau,m}(z)| \leq \frac{4B}{m\tau} + \frac{2B}{\tau} e^{-\tau|x|} \mathbf{1}_{|x|\geq 1/m}.$$

Therefore we have obtained that

$$\|g_m - g_{\tau,m}\|_{L^\infty([-1,1])} \leq \frac{4B}{m\tau} + \frac{2B}{\tau} e^{-\tau|x|} \mathbf{1}_{|x|\geq 1/m}.$$

Thanks to Lemma 20 - (ii), the same argument carries over to the estimate for the difference of the derivatives and leads to

$$\|g'_m - g'_{\tau,m}\|_{L^\infty([-1,1])} \leq \frac{4B}{m} + 2B e^{-\tau|x|} \mathbf{1}_{|x|\geq 1/m}.$$

Combining the estimates above with that $\|g - g_m\|_{W^{1,\infty}([-1,1])} \leq 2B/m$ yields that

$$\begin{aligned}\|g - g_{\tau,m}\|_{W^{1,\infty}([-1,1])} &\leq \|g - g_m\|_{W^{1,\infty}([-1,1])} + \|g_m - g_{\tau,m}\|_{W^{1,\infty}([-1,1])} \\ &\leq \frac{2B}{m} + \frac{4B}{m\tau} + \frac{2B}{\tau} e^{-\tau|x|} \mathbf{1}_{|x|\geq 1/m} \\ &\leq 2B\Big(1 + \frac{1}{\tau}\Big)\Big(\frac{3}{m} + e^{-\frac{\tau}{m}}\Big) \\ &= 6B\delta_\tau.\end{aligned}$$

We have used the fact that $\max_{0<x\leq 1/2} 3x + e^{-\tau x} = \big(\log\big(\frac{\tau}{3}\big) + 1\big)\frac{3}{\tau}$ in the last inequality. The proof of the lemma is finished by combining the estimates above and by rewriting (40) in the form of (36). ■

Now we are ready to present the proof of Theorem 2. To do this, let us define the function class

$$\mathcal{F}_{\mathrm{SP}_\tau}(B) := \Big\{c + \gamma \mathrm{SP}_\tau(w \cdot x - t), |c| \leq 2B, |w|_1 = 1, |t| \leq 1, |\gamma| \leq 4B\Big\}.$$

Note by (iii) of Lemma 20 that

$$\sup_{u \in \mathcal{F}_{\mathrm{SP}_\tau}(B)} \|f\|_{H^1(\Omega)} \leq 2B + 4B\|\mathrm{SP}_\tau\|_{W^{1,\infty}([-2,2])} \leq 14B + \frac{4B}{\tau}. \tag{41}$$

Proof [Proof of Theorem 2] First according to Theorem 15, $u - \hat{u}(0)$ lies in the H^1-closure of the convex hull of $\mathcal{F}_{\cos}(B)$ with $B = \|u\|_{\mathcal{B}(\Omega)}$. Note that each function in $\mathcal{F}_{\cos}(B)$ is a composition of the multivariate linear function $z = w \cdot x$ with $|w| = 1$ and the univariate function $g(z)$ defined in (31) such that $g'(0) = 0$ and $\|g^{(s)}\|_{L^\infty([-1,1])} \leq B$ for $s = 0, 1, 2$. By Lemma 21, such g can be approximated by $g_{\tau,m}$ which lies in the convex hull of the set of functions

$$\Big\{c + \gamma \mathrm{SP}_\tau(\epsilon z - b), |c| \leq B, \epsilon \in \{\pm 1\}, |b| \leq 1, \gamma \leq 4B\Big\}.$$

Moreover, $\|g - g_{\tau,m}\|_{W^{1,\infty}([-1,1])} \leq 6B\delta_\tau$. As a result, we have that

$$\|g(w \cdot x) - g_{\tau,m}(w \cdot x)\|_{H^1(\Omega)} \leq \|g - g_{\tau,m}\|_{W^{1,\infty}([-1,1])} \leq 6B\delta_\tau.$$

This combining with the fact that $|\hat{u}(0)| \leq B$ yields that there exists a function u_τ in the closure of the convex hull of $\mathcal{F}_{\mathrm{SP}_\tau}(B)$ such that

$$\|u - u_\tau\|_{H^1(\Omega)} \leq 6B\delta_\tau.$$

Thanks to Lemma 16 and the bound (41), there exists $u_m \in \mathcal{F}_{\mathrm{SP}_\tau, m}(B)$, which is a convex combination of m functions in $\mathcal{F}_{\mathrm{SP}_\tau}(B)$ such that

$$\|u_\tau - u_m\|_{H^1(\Omega)} \leq \frac{B\Big(\frac{4}{\tau} + 14\Big)}{\sqrt{m}}.$$

Combining the last two inequalities leads to

$$\|u - u_m\|_{H^1(\Omega)} \leq 6B\delta_\tau + \frac{B\Big(\frac{4}{\tau} + 14\Big)}{\sqrt{m}}.$$

Setting $\tau = \sqrt{m} \geq 1$ and using (38), we obtain that

$$\begin{aligned}
\|u - u_m\|_{H^1(\Omega)} &\leq \frac{6B}{\tau}\Big(1 + \frac{1}{\tau}\Big)\Big(\log\Big(\frac{\tau}{3}\Big) + 1\Big) + \frac{B}{\sqrt{m}}\Big(\frac{4}{\tau} + 14\Big) \\
&\leq \frac{6B}{\sqrt{m}} 2\Big(\frac{1}{2}\log(m) + 1\Big) + \frac{18B}{\sqrt{m}} \\
&= \frac{B(6\log(m) + 30)}{\sqrt{m}}.
\end{aligned}$$

This proves the desired estimate. ■

Appendix C. Rademacher complexities of two-layer neural networks (Proof of Theorem 3)

The goal of this section is to derive the Rademacher complexity bounds for some two-layer neural-network function classes that are relevant to the Ritz losses of the Poisson and the static Schrödinger equations, which eventually lead to the proof of Theorem 3.

C.1. Proof of Lemma 7

First let us consider for fixed positive constants C, Γ, W and T the set of two-layer neural networks

$$\begin{aligned}\mathcal{F}_m = \Big\{ u_\theta(x) = c + \sum_{i=1}^m \gamma_i \phi(w_i \cdot x + t_i),\ x \in \Omega, \theta \in \Theta \ \Big|\ |c| \leq C, \sum_{i=1}^m |\gamma_i| \leq \Gamma, \\ |w_i|_1 \leq W, |t_i| \leq T \Big\}.\end{aligned} \tag{42}$$

Here ϕ is the activation function, $\theta = (c, \{\gamma_i\}_{i=1}^m, \{w_i\}_{i=1}^m, \{t_i\}_{i=1}^m)$ denotes collectively the parameters of the two-layer neural network, $\Theta = \Theta_c \times \Theta_\gamma \times \Theta_w \times \Theta_t = [-C, C] \times B_1^m(\Gamma) \times \big(B_1^d(W)\big)^m \times [-T, T]^m$ represents the parameter space. We shall consider the set Θ endowed with the metric ρ defined for $\theta = (c, \gamma, w, t), \theta' = (c', \gamma', w', t') \in \Theta$ by

$$\rho_\Theta(\theta, \theta') = \max\{|c - c'|, |\gamma - \gamma'|_1, \max_i |w_i - w_i'|_1, |t - t'|_\infty\}. \tag{43}$$

Throughout the section we assume that ϕ satisfies the following assumption, which particularly holds for the Softplus activation function.

Assumption 1 *$\phi \in C^2(\mathbb{R})$ and that ϕ (resp. ϕ', the derivative of ϕ) is L-Lipschitz (resp. is L'-Lipschitz) for some $L, L' > 0$. Moreover, there exist positive constants $\phi_{\max}$ and $\phi'_{\max}$ such that*

$$\sup_{w \in \Theta_w, t \in \Theta_t, x \in \Omega} |\phi(w \cdot x + t)| \leq \phi_{\max} \text{ and } \sup_{w \in \Theta_w, t \in \Theta_t, x \in \Omega} |\phi'(w \cdot x + t)| \leq \phi'_{\max}.$$

Recall that the Rademacher complexity of a function class $\mathcal{G}$ is defined by

$$R_n(\mathcal{G}) = \mathbf{E}_Z \mathbf{E}_\sigma \Big[\sup_{g \in \mathcal{G}} \Big| \frac{1}{n} \sum_{j=1}^n \sigma_j g(Z_j) \Big| \ \Big|\ Z_1, \cdots, Z_n \Big].$$

In the subsequent proof, it will be useful to use the following modified Rademacher complexity $\tilde{R}_n(G)$ without the absolute value sign:

$$\tilde{R}_n(\mathcal{G}) = \mathbf{E}_Z \mathbf{E}_\sigma \Big[\sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{j=1}^n \sigma_j g(Z_j) \ \Big|\ Z_1, \cdots, Z_n \Big].$$

The lemma below bounds the Rademacher complexity of $\mathcal{F}_m$.

Lemma 22 *Assume that the activation function ϕ is L-Lipschitz. Then*

$$R_n(\mathcal{F}_m) \leq \frac{4\Gamma L(W\sqrt{d} + T) + 2\Gamma^2 |\phi(0)|}{\sqrt{n}}.$$

Proof Let $\bar{\phi}(x) = \phi(x) - \phi(0)$. First observe that

$$
\begin{aligned}
&\mathbf{E}_\sigma\Big[\sup_{f\in\mathcal{F}_m}\frac{1}{n}\sum_{j=1}^n \sigma_j f(Z_j)\Big|Z_1,\cdots,Z_n\Big]\\
&=\mathbf{E}_\sigma\Big[\sup_{\Theta}\frac{1}{n}\sum_{j=1}^n \sigma_j\big(c+\sum_{i=1}^m \gamma_i\phi(w_i\cdot Z_j+t_i)\big)\Big|Z_1,\cdots,Z_n\Big]\\
&=\mathbf{E}_\sigma\Big[\sup_{\Theta}\frac{1}{n}\sum_{j=1}^n \sigma_j\sum_{i=1}^m \gamma_i\phi(w_i\cdot Z_j+t_i)\Big|Z_1,\cdots,Z_n\Big]\\
&\leq \frac{1}{n}\mathbf{E}_\sigma\Big[\sup_{\Theta}\sum_{i=1}^m\gamma_i\sum_{j=1}^n \sigma_j\bar{\phi}(w_i\cdot Z_j+t_i)\Big|Z_1,\cdots,Z_n\Big]+\frac{1}{n}\mathbf{E}_\sigma\Big[\sup_{\Theta}\sum_{i=1}^m\gamma_i\sum_{j=1}^n\sigma_j\phi(0)\Big]\\
&=: J_1+J_2.
\end{aligned}
$$

Using the fact that $\bar{\phi}(\cdot) = \phi(\cdot) - \phi(0)$ is L-Lipschitz, one has that

$$
\begin{aligned}
J_1 &\leq \frac{1}{n}\sum_{i=1}^m|\gamma_i|\cdot\mathbf{E}_\sigma\Big[\sup_{|w|\leq W,|t|\leq T}\Big|\sum_{j=1}^n\sigma_j\bar{\phi}(w\cdot Z_j+t)\Big|\ \Big|\ Z_1,\cdots,Z_n\Big]\\
&\leq \frac{2\Gamma L}{n}\Big(\mathbf{E}_\sigma\Big[\sup_{|w|\leq W}\Big|\sum_{j=1}^n\sigma_j w\cdot Z_j\Big|\ \Big|\ Z_1,\cdots,Z_n\Big]+\mathbf{E}_\sigma\Big[\sup_{|t|\leq T}\Big|\sum_{j=1}^n\sigma_j t\Big|\Big]\Big)\\
&\leq \frac{2\Gamma L}{n}\Big(W\cdot\mathbf{E}_\sigma\|\sum_{j=1}^n\sigma_j Z_j\|+T\mathbf{E}_\sigma\Big[\Big|\sum_{j=1}^n\sigma_j\Big|\Big]\Big)\\
&\leq \frac{2\Gamma L}{n}\Big(W\cdot\sqrt{\sum_{j=1}^n|Z_j|^2}+T\cdot\sqrt{\mathbf{E}_\sigma\Big[\sum_{j=1}^n\sigma_j^2\Big]}\Big)\\
&\leq \frac{2\Gamma L(W\sqrt{d}+T)}{\sqrt{n}}.
\end{aligned}
$$

Note that in the second inequality we have used the Talagrand's contraction principle (Lemma 23 below). Moreover, since $\sum_{i=1}^m|\gamma_i|\leq\Gamma$, it is easy to see that

$$
\begin{aligned}
J_2 &\leq \frac{\Gamma|\phi(0)|}{n}\mathbf{E}_\sigma\Big[\Big|\sum_{j=1}^n\sigma_j\Big|\Big]\\
&\leq \frac{\Gamma|\phi(0)|}{n}\sqrt{\mathbf{E}_\sigma\Big[\sum_{j=1}^n\sigma_j^2\Big]}\\
&= \frac{\Gamma|\phi(0)|}{\sqrt{n}}.
\end{aligned}
$$

Combining the estimates above and then taking the expectation w.r.t. Z_j yields that $\tilde{R}_n(\mathcal{F}_m) \leq \frac{2\Gamma L(W\sqrt{d}+T)+\Gamma|\phi(0)|}{\sqrt{n}}$. This combined with Lemma 24 below leads to the desired estimate. ■

Lemma 23 (Ledoux-Talagrand contraction (Ledoux and Talagrand, 1991, Theorem 4.12)) *Assume that $\phi : \mathbb{R} \to \mathbb{R}$ is L-Lipschitz with $\phi(0) = 0$. Let $\{\sigma_i\}_{i=1}^n$ be independent Rademacher random variables. Then for any $T \subset \mathbb{R}^n$*

$$\mathbf{E}_\sigma \sup_{(t_1,\cdots,t_n)\in T} \Big| \sum_{i=1}^n \sigma_i \phi(t_i) \Big| \leq 2L \cdot \mathbf{E}_\sigma \sup_{(t_1,\cdots,t_n)\in T} \Big| \sum_{i=1}^n \sigma_i t_i \Big|.$$

Lemma 24 *(Ma, 2018, Lemma 1) Assume that the set of functions $\mathcal{G}$ contains the zero function. Then*

$$R_n(\mathcal{G}) \leq 2\tilde{R}_n(\mathcal{G}).$$

Now we are ready to give the proof of Lemma 7.

Proof [Proof of Lemma 7] Recall the sets of two-layer neural networks

$$\mathcal{F}_{\mathrm{ReLU},m}(B) = \Big\{ c + \sum_{i=1}^m \gamma_i \mathrm{ReLU}(\omega_i \cdot x - t_i), |c| \leq 2B, |w_i|_1 = 1, |t_i| \leq 1, \sum_{i=1}^m |\gamma_i| \leq 4B \Big\},$$
$$\mathcal{F}_{\mathrm{SP}_\tau,m}(B) = \Big\{ c + \sum_{i=1}^m \gamma_i \mathrm{SP}_\tau(\omega_i \cdot x - t_i), |c| \leq 2B, |w_i|_1 = 1, |t_i| \leq 1, \sum_{i=1}^m |\gamma_i| \leq 4B \Big\}.$$

Since both ReLU and SP_τ are 1-Lipschitz and $\mathrm{ReLU}(0) = 0$, $\mathrm{SP}_\tau(0) = \frac{\ln 2}{\tau}$, it follows from Lemma 22 that

$$R_n(\mathcal{F}_{\mathrm{ReLU},m}(B)) \leq \frac{16(\sqrt{d}+1)B}{\sqrt{n}} \quad \text{and} \quad R_n(\mathcal{F}_{\mathrm{SP}_\tau,m}(B)) \leq \frac{16(\sqrt{d}+1+\frac{\ln 2}{\tau})B}{\sqrt{n}}.$$

This proves Lemma 7. ■

C.2. Proof of Theorem 8

Given the source function $f \in L^\infty(\Omega)$ and the potential $V \in L^\infty(\Omega)$, we recall the function classes associated to the Ritz losses of Poisson equation and the static Schrödinger equation

$$\begin{aligned} \mathcal{G}_{m,P} &:= \Big\{ g : \Omega \to \mathbb{R} \;\big|\; g = \frac{1}{2}|\nabla u|^2 - fu \text{ where } u \in \mathcal{F}_m \Big\}, \\ \mathcal{G}_{m,S} &:= \Big\{ g : \Omega \to \mathbb{R} \;\big|\; g = \frac{1}{2}|\nabla u|^2 + \frac{1}{2}V|u|^2 - fu \text{ where } u \in \mathcal{F}_m \Big\}. \end{aligned} \tag{44}$$

In the sequel we aim to bound the Rademacher complexities of $\mathcal{G}_{m,P}$ and $\mathcal{G}_{m,S}$ defined above. This will be achieved by bounding the Rademacher complexities of the following function classes

$$\begin{aligned} \mathcal{G}_m^1 &:= \Big\{ g : \Omega \to \mathbb{R} \;\big|\; g = \frac{1}{2}|\nabla u|^2 \text{ where } u \in \mathcal{F}_m \Big\}, \\ \mathcal{G}_m^2 &:= \Big\{ g : \Omega \to \mathbb{R} \;\big|\; g = fu \text{ where } u \in \mathcal{F}_m \Big\}, \\ \mathcal{G}_m^3 &:= \Big\{ g : \Omega \to \mathbb{R} \;\big|\; g = \frac{1}{2}V|u|^2 \text{ where } u \in \mathcal{F}_m \Big\}. \end{aligned}$$

The celebrated Dudley's theorem will be used to bound the Rademacher complexity in terms of the metric entropy. For this, let us first recall the metric entropy and the Dudley's theorem below.

Let (E, ρ) be a metric space with metric ρ. A δ-*cover* of a set $A \subset E$ with respect to ρ is a collection of points $\{x_1, \cdots, x_n\} \subset A$ such that for every $x \in A$, there exists $i \in \{1, \cdots, n\}$ such that $\rho(x, x_i) \leq \delta$. The δ-covering number $\mathcal{N}(\delta, A, \rho)$ is the cardinality of the smallest δ-cover of the set A with respect to the metric ρ. Equivalently, the δ-covering number $\mathcal{N}(\delta, A, \rho)$ is the minimal number of balls $B_\rho(x, \delta)$ of radius δ needed to cover the set A.

Theorem 25 (Dudley's theorem) *Let $\mathcal{F}$ be a function class such that $\sup_{f\in\mathcal{F}} \|f\|_\infty \leq M$. Then the Rademacher complexity $R_n(\mathcal{F})$ satisfies that*

$$R_n(\mathcal{F}) \leq \inf_{0\leq\delta\leq M} \Big\{4\delta + \frac{12}{\sqrt{n}} \int_\delta^M \sqrt{\log \mathcal{N}(\varepsilon, \mathcal{F}, \|\cdot\|_\infty)}\, d\varepsilon\Big\}.$$

Note that our statement of Dudley's theorem is slightly different from the standard Dudley's theorem Dudley (1967) where the covering number is based on the empirical ℓ^2-metric instead of the L^∞-metric above. However, since L^∞-metric is stronger than the empirical ℓ^2-metric and since the covering number is monotonically increasing with respect to the metric, Theorem 25 follows directly from the classical Dudley's theorem (see e.g. (Wolf, 2020, Theorem 1.19)).

Let us now state an elementary lemma on the covering number of product spaces.

Lemma 26 *Let (E_i, ρ_i) be metric spaces with metrics ρ_i and let $A_i \subset E_i, i = 1, \cdots, n$. Consider the product space $E = \times_{i=1}^n E_i$ equipped with the metric $\rho = \max_i \rho_i$ and the set $A = \times_{i=1}^n A_i$. Then for any $\delta > 0$,*

$$\mathcal{N}(\delta, A, \rho) \leq \prod_{i=1}^n \mathcal{N}(\delta, A_i, \rho_i). \tag{45}$$

Proof It suffices to prove the lemma in the case that $n = 2$, i.e.,

$$\mathcal{N}(\delta, A_1 \times A_2, \rho) \leq \mathcal{N}(\delta, A_1, \rho_1) \cdot \mathcal{N}(\delta, A_2, \rho_2). \tag{46}$$

Indeed, suppose that C_1 and C_2 are δ-covers of A_1 and A_2 respectively. Then it is straightforward that the product set $C_1 \times C_2$ is also a δ-cover of $A_1 \times A_2$ in the space $(E_1 \times E_2, \rho)$ with $\rho = \max(\rho_1, \rho_2)$. Hence $\mathcal{N}(\delta, A_1 \times A_2, \rho) \leq \operatorname{card}(C_1) \cdot \operatorname{card}(C_2)$. Applying this inequality for C_i with $\operatorname{card}(C_i) = \mathcal{N}(\delta, A_i, \rho_i), i = 1, 2$, we obtain (46). The general inequality (45) follows by iterating (46). ■

As a consequence of Lemma 26, the following proposition gives an upper bound for the covering number $\mathcal{N}(\delta, \Theta, \rho_\Theta)$.

Proposition 27 *Consider the metric space (Θ, ρ_Θ) with ρ_Θ defined in (43). Then for any $\delta > 0$, the covering number $\mathcal{N}(\delta, \Theta, \rho_\Theta)$ satisfies that*

$$\mathcal{N}(\delta, \Theta, \rho_\Theta) \leq \frac{2C}{\delta} \cdot \Big(\frac{3\Gamma}{\delta}\Big)^m \cdot \Big(\frac{3W}{\delta}\Big)^{dm} \cdot \Big(\frac{3T}{\delta}\Big)^m.$$

Proof Thanks to Lemma 26,

$$\begin{aligned}\mathcal{N}(\delta,\Theta,\rho) &\leq \mathcal{N}(\delta,\Theta_c,|\cdot|)\cdot\mathcal{N}(\delta,\Theta_\gamma,\|\cdot\|_1)\cdot\Big(\mathcal{N}(\delta,B_2^d(W),\|\cdot\|_2)\Big)^m\cdot\mathcal{N}(\delta,\Theta_t,\|\cdot\|_\infty)\\ &\leq \frac{2C}{\delta}\cdot\Big(\frac{3\Gamma}{\delta}\Big)^m\cdot\Big(\frac{3W}{\delta}\Big)^{dm}\cdot\Big(\frac{3T}{\delta}\Big)^m,\end{aligned}$$

where in the last inequality we have used the fact that the covering number of a d-dimensional ℓ^p-ball of radius r satisfies that

$$\mathcal{N}(\delta,B_p^d(r),\|\cdot\|_p)\leq\Big(\frac{3r}{\delta}\Big)^d.$$

■

Bounding $R_n(\mathcal{G}_m^1)$. We would like to bound $R_n(\mathcal{G}_m^1)$ from above using metric entropy. To this end, let us first bound the covering number $\mathcal{N}(\delta,\mathcal{G}_m^1,\|\cdot\|_\infty)$. Recall the parameters C,Γ,W and T in (42). With those parameters fixed, to simplify expressions, we introduce the following functions to be used in the sequel

$$\mathcal{M}(\delta,\Lambda,m,d) := \frac{2C\Lambda}{\delta}\cdot\Big(\frac{3\Gamma\Lambda}{\delta}\Big)^m\cdot\Big(\frac{3W\Lambda}{\delta}\Big)^{dm}\cdot\Big(\frac{3T\Lambda}{\delta}\Big)^m, \tag{47}$$

$$\begin{aligned}\mathcal{Z}(M,\Lambda,d) := M\big(&\sqrt{(\log(2C\Lambda))_+}+\sqrt{(\log(3\Gamma\Lambda)+d\log(3W\Lambda)+\log(3T\Lambda))_+}\big)\\ &+\sqrt{d+3}\int_0^M\sqrt{(\log(1/\varepsilon))_+}d\varepsilon.\end{aligned} \tag{48}$$

Lemma 28 *Let the activation function ϕ satisfy Assumption 1. Then we have*

$$\mathcal{N}(\delta,\mathcal{G}_m^1,\|\cdot\|_\infty)\leq\mathcal{M}(\delta,\Lambda_1,m,d), \tag{49}$$

where the constant Λ_1 is defined by

$$\Lambda_1=\Big((W+\Gamma)\phi'_{\max}+2\Gamma WL'\Big)\Gamma W\phi'_{\max}. \tag{50}$$

Proof Thanks to Assumption 1, $\sup_{\theta\in\Theta}|\phi'(w\cdot x+t)|\leq\phi'_{\max}$. This implies that

$$\begin{aligned}\max_{\theta\in\Theta}|\nabla u_\theta(x)| &\leq \sum_{i=1}^m|\gamma_i||w_i|_1|\phi'(w_i\cdot x+t_i)|\\ &\leq \Gamma W\phi'_{\max}.\end{aligned}$$

Furthermore, for $\theta,\theta'\in\Theta$, by adding and subtracting terms, we have that

$$\begin{aligned}|\nabla u_\theta(x)-\nabla u_{\theta'}(x)| &\leq \sum_{i=1}^m|\gamma_i-\gamma_i'||w_i||\phi'(w_i\cdot x+t_i)|\\ &+\sum_{i=1}^m|\gamma_i'||w_i-w_i'||\phi'(w_i\cdot x+t_i)|+\sum_{i=1}^m|\gamma_i'||w_i'||\phi'(w_i\cdot x+t_i)-\phi'(w_i'\cdot x+t_i')|\\ &\leq W\phi'_{\max}|\gamma-\gamma'|_1+\Gamma\phi'_{\max}\max_i|w_i-w_i'|_1+\Gamma WL'(\max_i|w_i-w_i'|_1+|t-t'|_\infty)\\ &\leq \Big((W+\Gamma)\phi'_{\max}+2\Gamma WL'\Big)\rho_\Theta(\theta,\theta').\end{aligned}$$

Note that we have also used the fact that $|x| \leq |x|_1$ for any vector $x \in \mathbb{R}^d$. Combining the last two estimates yields that

$$\begin{aligned}\frac{1}{2}\big||\nabla u_\theta(x)|^2 - |\nabla u_{\theta'}(x)|^2\big| &\leq \frac{1}{2}\big|\nabla u_\theta(x) + \nabla u_{\theta'}(x)\big|\big|\nabla u_\theta(x) - \nabla u_{\theta'}(x)\big| \\ &\leq \Lambda_1 \rho_\Theta(\theta,\theta').\end{aligned}$$

This particularly implies that $\mathcal{N}(\delta, \mathcal{G}_m^1, \|\cdot\|_\infty) \leq \mathcal{N}(\frac{\delta}{\Lambda_1}, \Theta, \rho_\Theta)$. Then the estimate (49) follows from Proposition 27 with δ replaced by $\frac{\delta}{\Lambda_1}$. ■

Proposition 29 *Assume that the activation function ϕ satisfies Assumption 1. Then*

$$R_n(\mathcal{G}_m^1) \leq \mathcal{Z}(M_1, \Lambda_1, d) \cdot \sqrt{\frac{m}{n}},$$

where $M_1 = \frac{1}{2}\Gamma^2 W^2 (\phi'_{\max})^2$ and Λ_1 is defined in (50).

Proof Thanks to Assumption 1,

$$\begin{aligned}\sup_{g\in\mathcal{G}_m^2} \|g\|_{L^\infty(\Omega)} &\leq \sup_{u\in\mathcal{F}_m} \frac{1}{2}\|\nabla u\|^2_{L^\infty(\Omega)} \\ &\leq \frac{\Gamma^2 W^2 (\phi'_{\max})^2}{2}.\end{aligned}$$

Then the proposition follows from Lemma 28, Theorem 25 with $\delta = 0$ and $M = M_1 = \frac{\Gamma^2 W^2(\phi'_{\max})^2}{2}$, and the simple fact that $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ for $a, b \geq 0$. ■

Bounding $R_n(\mathcal{G}_m^2)$. The next lemma provides an upper bound for $\mathcal{N}(\delta, \mathcal{G}_m^2, \|\cdot\|_\infty)$.

Lemma 30 *Assume that $\|f\|_{L^\infty(\Omega)} \leq F$ for some $F > 0$. Assume that the activation function ϕ satisfies Assumption 1. Then the covering number $\mathcal{N}(\delta, \mathcal{G}_m^2, \|\cdot\|_\infty)$ satisfies that*

$$\mathcal{N}(\delta, \mathcal{G}_m^2, \|\cdot\|_\infty) \leq \mathcal{M}(\delta, \Lambda_2, m, d).$$

Here the constant Λ_2 is defined by

$$\Lambda_2 = F\big(1 + \phi_{\max} + 2L\Gamma\big). \tag{51}$$

Proof Note that a function $g_\theta \in \mathcal{G}_m^2$ has the form $g_\theta = f u_\theta$. Given $\theta = (c,\gamma,w,t), \theta' = (c',\gamma',w',t') \in \Theta$, we have

$$\begin{aligned}|u_\theta(x) - u_{\theta'}(x)| &\leq |c-c'| + \sum_{i=1}^m |\gamma_i\phi(w_i\cdot x - t_i) - \sum_{i=1}^m \gamma_i'\phi(w_i'\cdot x - t_i')| \\ &\leq |c-c'| + \sum_{i=1}^m |\gamma_i - \gamma_i'|\phi(w_i\cdot x - t_i) + \sum_{i=1}^m |\gamma_i'||\phi(w_i\cdot x - t_i) - \phi(w_i'\cdot x - t_i')|.\end{aligned} \tag{52}$$

Since ϕ satisfies Assumption 1, we have that $|\phi(w_i \cdot x - t_i)| \leq \phi_{\max}$ and that

$$|\phi(w_i \cdot x - t_i) - \phi(w_i' \cdot x - t_i')| \leq L(\sqrt{d}|w_i - w_i'|_1 + |t_i - t_i'|).$$

Therefore, it follows from (52) that

$$\begin{aligned} |u_\theta(x) - u_{\theta'}(x)| &\leq |c - c'| + \phi_{\max}|\gamma - \gamma'|_1 \\ &\quad + L\Gamma(\max_i |w_i - w_i'|_1 + |t - t'|_\infty) \\ &\leq \Big(1 + \phi_{\max} + 2L\Gamma\Big)\rho_\Theta(\theta, \theta'). \end{aligned} \tag{53}$$

This implies that

$$\|g_\theta - g_{\theta'}\|_\infty \leq F\Big(1 + \phi_{\max} + 2L\Gamma\Big)\rho = \Lambda_2 \rho_\Theta(\theta, \theta').$$

As a consequence, $\mathcal{N}(\delta, \mathcal{G}_m^2, \|\cdot\|_\infty) \leq \mathcal{N}(\frac{\delta}{\Lambda_2}, \Theta, \rho_\Theta)$. Then the lemma follows from Proposition 27 with δ replaced by $\frac{\delta}{\Lambda_2}$. ∎

Proposition 31 *Assume that $\|f\|_{L^\infty(\Omega)} \leq F$ for some $F > 0$. Assume that the activation function ϕ is L-Lipschitz. Then*

$$R_n(\mathcal{G}_m^2) \leq \mathcal{Z}(M_2, \Lambda_2, d) \cdot \sqrt{\frac{m}{n}},$$

where $M_2 = F(C + \Gamma\phi_{\max})$ and Λ_2 is defined in (51).

Proof It follows from the definition of $\mathcal{G}_m^2$ and the assumption that $\|f\|_{L^\infty(\Omega)} \leq F$, one has that $\sup_{g \in \mathcal{G}_m^2} \|g\|_{L^\infty(\Omega)} \leq M_2 = F(C + \Gamma\phi_{\max})$. Then the proposition is proved by an application of Theorem 25 with $\delta = 0$, $M = M_2$ and Lemma 30. ∎

Bounding $R_n(\mathcal{G}_m^3)$. The lemma below gives an upper bound for $\mathcal{N}(\delta, \mathcal{G}_m^3, \|\cdot\|_\infty)$.

Lemma 32 *Assume that $\|V\|_{L^\infty(\Omega)} \leq V_{\max}$ for some $V_{\max} < \infty$. Assume that the activation function ϕ satisfies Assumption 1. Then the covering number $\mathcal{N}(\delta, \mathcal{G}_m^3, \|\cdot\|_\infty)$ satisfies that*

$$\mathcal{N}(\delta, \mathcal{G}_m^3, \|\cdot\|_\infty) \leq \mathcal{M}(\delta, \Lambda_3, m, d), \tag{54}$$

where the constant Λ_3 is defined by

$$\Lambda_3 = V_{\max}(C + \Gamma\phi_{\max})\Big(1 + \phi_{\max} + 2L\Gamma\Big). \tag{55}$$

Proof By the definition of $\mathcal{F}_m$ and Assumption 1 on ϕ,

$$\sup_{u \in \mathcal{F}_m} \|u\|_{L^\infty(\Omega)} \leq C + \Gamma\phi_{\max}.$$

Moreover, recall from (53) that for $\theta, \theta' \in \Theta$,

$$|u_\theta(x) - u_{\theta'}(x)| \leq \Big(1 + \phi_{\max} + 2L\Gamma\Big)\rho_\Theta(\theta, \theta').$$

Consequently,

$$\begin{aligned}\Big|\frac{1}{2}V(x)u_\theta^2(x)-\frac{1}{2}V(x)u_{\theta'}^2(x)\Big| &\le \frac{1}{2}|V(x)||u_\theta(x)+u_{\theta'}(x)||u_\theta(x)-u_{\theta'}(x)|\\ &\le \Lambda_3\rho_\Theta(\theta,\theta').\end{aligned}$$

The estimate (54) follows from the same line of arguments used in the proof of Lemma 30. ∎

Proposition 33 *Under the same assumption of Lemma 32, $\mathcal{G}_m^3$ satisfies that*

$$R_n(\mathcal{G}_m^3)\le \mathcal{Z}(M_3,\Lambda_3,d)\cdot\sqrt{\frac{m}{n}},$$

where $M_3=\frac{V_{\max}}{2}(C+\Gamma\phi_{\max})^2$ and Λ_3 is defined in (55).

Proof Note that $\sup_{u\in\mathcal{G}_m^3}\|u\|_{L^\infty(\Omega)}\le M_3=\frac{V_{\max}}{2}(C+\Gamma\phi_{\max})^2$. Then the proposition follows from Theorem 25 with $\delta=0, M=M_3$ and Lemma 32. ∎

The following corollary is a direct consequence of the Propositions 29, 31 and 33.

Corollary 34 *The two sets of functions $\mathcal{G}_{m,P}$ and $\mathcal{G}_{m,S}$ defined in (44) satisfy that*

$$R_n(\mathcal{G}_{m,P})\le(\mathcal{Z}(M_1,\Lambda_1,d)+\mathcal{Z}(M_2,\Lambda_2,d))\cdot\sqrt{\frac{m}{n}}$$

and that

$$R_n(\mathcal{G}_{m,S})\le\sum_{i=1}^{3}\mathcal{Z}(M_i,\Lambda_i,d)\cdot\sqrt{\frac{m}{n}}.$$

Considering the set of two-layer neural networks $\mathcal{F}_{\mathrm{SP}_\tau,m}(B)$ with $\tau=\sqrt{m}$, we define the following associated sets of functions

$$\begin{aligned}\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)&:=\{g:\Omega\to\mathbb{R}\mid g=\frac{1}{2}|\nabla u|^2-fu \text{ where } u\in\mathcal{F}_{\mathrm{SP}_\tau,m,P}(B)\},\\ \mathcal{G}_{\mathrm{SP}_\tau,m,S}(B)&:=\{g:\Omega\to\mathbb{R}\mid g=\frac{1}{2}|\nabla u|^2+\frac{1}{2}V|u|^2-fu \text{ where } u\in\mathcal{F}_{\mathrm{SP}_\tau,m,S}(B)\},\\ \mathcal{G}^1_{\mathrm{SP}_\tau,m}(B)&:=\{g:\Omega\to\mathbb{R}\mid g=\frac{1}{2}|\nabla u|^2 \text{ where } u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)\},\\ \mathcal{G}^2_{\mathrm{SP}_\tau,m}(B)&:=\{g:\Omega\to\mathbb{R}\mid g=fu \text{ where } u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)\}\\ \mathcal{G}^3_{\mathrm{SP}_\tau,m}(B)&:=\Big\{g:\Omega\to\mathbb{R}\;\Big|\; g=\frac{1}{2}V|u|^2 \text{ where } u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)\Big\}.\end{aligned}$$

Now we are ready to prove Theorem 8 by utilizing Corollary 34.

Proof [Proof of Theorem 8] Indeed, from the definition of the activation function SP_τ, we know that $\|\mathrm{SP}'_\tau\|_{L^\infty(\mathbb{R})}\le 1$ and $\|\mathrm{SP}''_\tau\|_{L^\infty(\mathbb{R})}\le\tau=\sqrt{m}$, so SP_τ satisfies Assumption (1) with

$$L=\phi'_{\max}=1, L'=\tau=\sqrt{m},\phi_{\max}\le 3+\frac{1}{\sqrt{m}}\le 4.$$

Note also that $\mathcal{F}_{\mathrm{SP}_\tau,m,P}(B)$ coincides with the set $\mathcal{F}_m$ defined in (42) with the following parameters

$$C = 2B, \Gamma = 4B, W = 1, T = 1. \tag{56}$$

With the parameters above, one has that

$$\begin{aligned} M_1 &= 8B, & \Lambda_1 &\leq 32B^2\sqrt{m} + 4B, \\ M_2 &\leq 18FB, & \Lambda_2 &\leq F(5+8B), \\ M_3 &\leq \frac{V_{\max}}{2}(18B)^2, & \Lambda_3 &\leq 18V_{\max}B(5+8B). \end{aligned}$$

Inserting M_i and $\Lambda_i, i = 1,2,3$ into (48), one can obtain by a straightforward calculation that there exist positive constants $C_1(B,d), C_2(B,d,F)$ and $C_3(B,d,V_{\max})$, depending on the parameters $B, d, F, V_{\max}$ polynomially, such that

$$\begin{aligned} \mathcal{Z}(M_1, \Lambda_1, d) &\leq C_1(B,d)\sqrt{\log m}, \\ \mathcal{Z}(M_2, \Lambda_2, d) &\leq C_2(B,d,F), \\ \mathcal{Z}(M_3, \Lambda_3, d) &\leq C_3(B,d,V_{\max}). \end{aligned}$$

Combining the estimates above with Corollary 5.2 gives directly the Rademacher complexity bounds for $\mathcal{G}_{\mathrm{SP}_\tau,m,P}(B)$ and $\mathcal{G}_{\mathrm{SP}_\tau,m,S}(B)$. ■

C.3. Proof of Theorem 3

We start with the proof of Part (i). Recall that $u^m_{n,P}$ is the minimizer of the empirical loss $\mathcal{E}_{n,P}$ in the set $\mathcal{F} = \mathcal{F}_{\mathrm{SP}_\tau,m}(B)$ with $\tau = \sqrt{m}$, where $B = \|u^*_P\|_{\mathcal{B}(\Omega)}$. From the definition of $\mathcal{F}_{\mathrm{SP}_\tau,m}(B)$, one can obtain that

$$\sup_{u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)} \|u\|_{L^\infty(\Omega)} \leq 14B.$$

Then it follows from Lemma 6, Theorem 8, Theorem 2 and Lemma 7 that

$$\begin{aligned} \mathbf{E}\big[\mathcal{E}_P(u^m_{n,P}) - \mathcal{E}_P(u^*_P)\big] &\leq 2R_n(\mathcal{G}_{\mathrm{SP}_\tau,m,P}) + 4 \sup_{u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)} \|u\|_{L^\infty(\Omega)} \cdot R_n(\mathcal{F}_{\mathrm{SP}_\tau,m}) \\ &\quad + \frac{1}{2}\inf_{u\in\mathcal{F}_{\mathrm{SP}_\tau,m}(B)} \|u-u^*\|^2_{H^1(\Omega)} \\ &\leq \frac{2C_P(B,d,F)\sqrt{m}(\sqrt{\log m}+1)}{\sqrt{n}} + \frac{4\cdot 14\cdot 16\cdot B^2(\sqrt{d}+1+\frac{\ln 2}{\sqrt{m}})}{\sqrt{n}} + \frac{B^2(6\log m + 30)^2}{2m} \\ &\leq \frac{C_1\sqrt{m}(\sqrt{\log m}+1)}{\sqrt{n}} + \frac{C_2(\log m + 1)^2}{m}, \end{aligned}$$

where the constant C_1 depends polynomially on B, d and F and C_2 depends only quadratically on B.

The proof of Part (ii) is almost identical to the proof of Part (i) as shown above and it follows directly from Lemma 6, Theorem 8 and Theorem 2. We omit the details.

Appendix D. Solution Theory of Poisson and Static Schrödinger Equations in Spectral Barron Spaces (Proof of Theorem 5)

This appendix devotes to the proof of Theorem 5, namely to developing a new solution theory for Poisson and the static Schrödinger equations in spectral Barron Spaces. This new theory can be viewed as regularity analysis of high dimensional PDEs in the spectral Barron space.

D.1. Proof of Part(i), Theorem 5

Proof Suppose that $f = \sum_{k\in\mathbb{N}_0^d} \hat{f}_k\Phi_k$ and that f has vanishing mean value on Ω so that $\hat{f}_0 = 0$. Let $\hat{u}_k$ be the cosine coefficients of the solution u_P^* of the Neumann problem for Poisson equation. By testing Φ_k on both sides of the Poisson equation and by taking account of the Neumann boundary condition, one obtains that

$$\begin{aligned}\hat{u}_0 &= 0,\\ \hat{u}_k &= -\frac{1}{\pi^2|k|^2}\hat{f}_k.\end{aligned}$$

As a result,

$$\begin{aligned}\|u_P^*\|_{\mathcal{B}^{s+2}(\Omega)} &= \sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} (1+\pi^{s+2}|k|_1^{s+2})|\hat{u}_k| = \sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} \frac{(1+\pi^{s+2}|k|_1^{s+2})}{\pi^2|k|^2}|\hat{f}_k|\\ &\leq d\sum_{k\in\mathbb{N}_0^d\setminus\{\mathbf{0}\}} (1+\pi^s|k|_1^s)|\hat{f}_k| = d\|f\|_{\mathcal{B}^s(\Omega)}.\end{aligned}$$

This finishes the proof. ∎

D.2. Proof of Part(ii), Theorem 5

First under the assumption of Part(ii) in Theorem 5, there exists a unique solution $u_S \in H^1(\Omega)$ to (2). Moreover,

$$\|\nabla u_S\|_{L^2(\Omega)}^2 + V_{\min}\|u_S\|_{L^2(\Omega)}^2 \leq \|f\|_{L^2(\Omega)}\|u_S\|_{L^2(\Omega)}. \tag{57}$$

Our goal is to show that $u_S \in \mathcal{B}^{s+2}(\Omega)$. To simplify the notation, in what follows we suppress the subscript S when we referring to the solution u_S. Let us first derive an operator equation that is equivalent to the original Schrödinger problem (2). To do this, multiplying Φ_k on both sides of the static Schrödinger equation and then integrating yields the following equivalent linear system on the cosine coefficients $\hat{u} = \{\hat{u}_k\}_{k\in\mathbb{N}_0^d}$:

$$|\pi|^2|k|^2\hat{u}_k + \widehat{(Vu)}_k = \hat{f}_k, \quad k\in\mathbb{N}_0^d. \tag{58}$$

Let us first consider (58) with $k = \mathbf{0}$. Thanks to Corollary 41,

$$\widehat{(Vu)}_0 = \frac{1}{\beta_0}\Big(\sum_{m\in\mathbb{Z}^d}\beta_m^2\hat{u}_{|m|}\hat{V}_{|m|}\Big) = \hat{u}_0\hat{V}_0 + \Big(\sum_{m\in\mathbb{Z}^d\setminus\{\mathbf{0}\}}\beta_m^2\hat{u}_{|m|}\hat{V}_{|m|}\Big),$$

where we have also used the fact that $\beta_0 = 1$. Consequently, equation (58) with $k = \mathbf{0}$ becomes

$$\hat{u}_0 \hat{V}_0 + \sum_{m \in \mathbb{Z}^d \setminus \{\mathbf{0}\}} \beta_m^2 \hat{u}_{|m|} \hat{V}_{|m|} = \hat{f}_0.$$

For $k \neq \mathbf{0}$, using again Corollary 41, equation (58) can be written as

$$|\pi|^2 |k|^2 \hat{u}_k + \frac{1}{\beta_k} \Big(\sum_{m \in \mathbb{Z}^d} \beta_m \hat{u}_{|m|} \beta_{m-k} \hat{V}_{|m-k|} \Big) = \hat{f}_k, \quad k \in \mathbb{N}^d \setminus \{\mathbf{0}\}.$$

Recall that a function $u \in \mathcal{B}^s(\Omega)$ is equivalent to that $\hat{u}_k$ belongs to the weighted ℓ^1-space $\ell^1_{W_s}(\mathbb{N}_0^d)$ with the weight $W_s(k) = 1 + \pi^s |k|_1^s$. We would like to rewrite the above equations as an operator equation on the space $\ell^1_{W_s}(\mathbb{N}_0^d)$. For doing this, let us define some useful operators. Define the operator $\mathbb{M} : \hat{u} \mapsto \mathbb{M}\hat{u}$ by

$$(\mathbb{M}\hat{u})_k = \begin{cases} \hat{V}_0 \hat{u}_0 & \text{if } k = \mathbf{0}, \\ |\pi|^2 |k|^2 \hat{u}_k & \text{otherwise.} \end{cases}$$

Define the operator $\mathbb{V} : \hat{u} \mapsto \mathbb{V}\hat{u}$ by

$$(\mathbb{V}\hat{u})_k = \begin{cases} \sum_{m \in \mathbb{Z}^d \setminus \{\mathbf{0}\}} \beta_m^2 \hat{u}_{|m|} \hat{V}_{|m|} & \text{if } k = \mathbf{0}, \\ \frac{1}{\beta_k} \Big(\sum_{m \in \mathbb{Z}^d} \beta_m \hat{u}_{|m|} \beta_{m-k} \hat{V}_{|m-k|} \Big) & \text{otherwise.} \end{cases}$$

With those operators, the system (58) can be reformulated as the operator equation

$$(\mathbb{M} + \mathbb{V})\hat{u} = \hat{f}. \tag{59}$$

Since $V(x) \geq V_{\min} > 0$ for every x, we have $\hat{V}_0 > 0$. As a direct consequence, the diagonal operator $\mathbb{M}$ is invertible. Therefore the operator equation (59) is equivalent to

$$(\mathbb{I} + \mathbb{M}^{-1}\mathbb{V})\hat{u} = \mathbb{M}^{-1}\hat{f}. \tag{60}$$

In order to show that $u \in \mathcal{B}^{s+2}(\Omega)$, it suffices to show that the equation (59) or (60) has a unique solution $\hat{u} \in \ell^1_{W_s}(\mathbb{N}_0^d)$. Indeed, if $\hat{u} \in \ell^1_{W_s}(\mathbb{N}_0^d)$, then it follows from (59) and the boundedness of $\mathbb{V}$ on $\ell^1_{W_s}(\mathbb{N}_0^d)$ (see (64) in the proof of Lemma 35 below) that

$$\begin{aligned} \|\mathbb{M}\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} &\leq \|\mathbb{V}\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} + \|\hat{f}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \\ &\leq C(d, V)\|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} + \|\hat{f}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)}. \end{aligned} \tag{61}$$

Moreover, this combined with the positivity of $\hat{V}_0$ implies that

$$\begin{aligned} \|u\|_{\mathcal{B}^{s+2}(\Omega)} &= \sum_{k \in \mathbb{N}_0^d} (1 + \pi^{s+2}|k|_1^{s+2})|\hat{u}_k| \\ &= \frac{1}{\hat{V}_0} \cdot \hat{V}_0 |\hat{u}_0| + \sum_{k \in \mathbb{N}^d} \frac{1 + \pi^{s+2}|k|_1^{s+2}}{\pi^2 |k|^2} \cdot \pi^2 |k|^2 |\hat{u}_k| \\ &\leq \max\Big\{\frac{1}{\hat{V}_0}, \Big(\frac{1}{\pi^2} + d\Big)\Big\} \|\mathbb{M}\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \\ &\leq C_1(d, V)(\|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} + \|\hat{f}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)}) \end{aligned} \tag{62}$$

for some $C_1(d, V) > 0$.

Next, we claim that equation (60) has a unique solution $\hat{u} \in \ell^1_{W_s}(\mathbb{N}_0^d)$ and that there exists a constant $C_2 > 0$ such that

$$\|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \leq C_2 \|\hat{f}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)}. \tag{63}$$

To see this, observe that owing to the compactness of $\mathbb{M}^{-1}\mathbb{V}$ as shown in Lemma 35, the operator equation $\mathbb{I} + \mathbb{M}^{-1}\mathbb{V}$ is a Fredholm operator on $\ell^1_{W_s}(\mathbb{N}_0^d)$. By the celebrated Fredholm alternative theorem (see e.g., (Fredholm, 1903) and (Conway, 1990, VII 10.7)), the operator $\mathbb{I} + \mathbb{M}^{-1}\mathbb{V}$ has a bounded inverse $(\mathbb{I} + \mathbb{M}^{-1}\mathbb{V})^{-1}$ if and only if $(\mathbb{I} + \mathbb{M}^{-1}\mathbb{V})\hat{u} = 0$ has a trivial solution. Therefore to obtain the bound (63), it suffices to show that $(\mathbb{I} + \mathbb{M}^{-1}\mathbb{V})\hat{u} = 0$ implies $\hat{u} = 0$. By the equivalence between the Schrödinger problem (2) and (60), we only need to show that the only solution of (2) is zero. Notice that the latter is a direct consequence of (57) and thus this finishes the proof of that the Schrödinger problem (2) has a unique solution in $\mathcal{B}(\Omega)$. Finally, the regularity estimate (14) follows by combining (62) and (63).

Lemma 35 *Assume that $V \in \mathcal{B}^s(\Omega)$ with $V(x) \geq V_{\min} > 0$ for every $x \in \Omega$. Then the operator $\mathbb{M}^{-1}\mathbb{V}$ is compact on $\ell^1_{W_s}(\mathbb{N}_0^d)$.*

Proof Since $\mathbb{M}^{-1}$ is a multiplication operator on $\ell^1_{W_s}(\mathbb{N}_0^d)$ with the diagonal entries converging to zero, it follows from Lemma 36 that $\mathbb{M}^{-1}$ is compact on $\ell^1_{W_s}(\mathbb{N}_0^d)$. Therefore to show the compactness of $\mathbb{M}^{-1}\mathbb{V}$, it is sufficient to show that the operator $\mathbb{V}$ is bounded on $\ell^1_{W_s}(\mathbb{N}_0^d)$. To see this, note that by definition $\beta_k = 2^{\mathbf{1}_k - \sum_{i=1}^d \mathbf{1}_{k_i \neq 0}} \in [2^{1-d}, 2]$. In addition, since $V \in \mathcal{B}^0(\Omega)$, using Corollary 41, one has that

$$\begin{aligned}
\|\mathbb{V}\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} &= \Big| \sum_{m \in \mathbb{Z}^d \setminus \{\mathbf{0}\}} \beta_m^2 \hat{u}_{|m|} \hat{V}_{|m|} \Big| + \sum_{k \in \mathbb{N}^d} \frac{1}{\beta_k} \Big| \sum_{m \in \mathbb{Z}^d} \beta_m \hat{u}_{|m|} \beta_{m-k} \hat{V}_{|m-k|} \Big| (1 + \pi^s |k|_1^s) \\
&\leq 4 \sum_{m \in \mathbb{Z}^d \setminus \{\mathbf{0}\}} |\hat{u}_{|m|}| \sum_{m \in \mathbb{Z}^d \setminus \{\mathbf{0}\}} |\hat{V}_{|m|}| + 2^{d+1} \sum_{m \in \mathbb{Z}^d} \sum_{k \in \mathbb{N}^d} |\hat{u}_{|m|}| |\hat{V}_{|m-k|}| \big(1 + |\pi|^s C_s (|m-k|_1^s + |m|_1^s)\big) \\
&\leq 2^{2d+2} \|\hat{u}\|_{\ell^1(\mathbb{N}_0^d)} \|\hat{V}\|_{\ell^1(\mathbb{N}_0^d)} + 2^{2d+1} \max(1, C_s) \cdot \big(\|\hat{u}\|_{\ell^1(\mathbb{N}_0^d)} \|\hat{V}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} + \|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \|\hat{V}\|_{\ell^1(\mathbb{N}_0^d)} \big) \\
&\leq 2^{2d+3} \max(1, C_s) \cdot \|\hat{V}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \\
&= 2^{2d+3} \max(1, C_s) \cdot \|V\|_{\mathcal{B}^s(\Omega)} \|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)},
\end{aligned} \tag{64}$$

where in the first inequality above we used the elementary inequality $|a+b|^s \leq C_s(|a|^s + |b|^s)$ for some constant $C_s > 0$ and in the second inequality we used the fact that $\sum_{m \in \mathbb{Z}^d} |\hat{u}_{|m|}| \leq 2^d \|\hat{u}\|_{\ell^1(\mathbb{N}_0^d)} \leq 2^d \|\hat{u}\|_{\ell^1_{W_s}(\mathbb{N}_0^d)}$. ■

Lemma 36 *Suppose that $\mathbb{T}$ is a multiplication operator on $\ell^1_{W_s}(\mathbb{N}_0^d)$ defined by for $u = (u_k)_{k \in \mathbb{N}_0^d}$ that $(\mathbb{T}u)_k = \lambda_k u_k$ with $\lambda_k \to 0$ as $\|k\|_2 \to \infty$. Then $\mathbb{T} : \ell^1_{W_s}(\mathbb{N}_0^d) \to \ell^1_{W_s}(\mathbb{N}_0^d)$ is compact.*

Proof It suffices to show that the image of the unit ball in $\ell^1_{W_s}(\mathbb{N}_0^d)$ under the map $\mathbb{T}$ is totally bounded. To this end, given any fixed $\varepsilon > 0$, let $K_0 \in \mathbb{N}$ be such that $|\lambda_k| \leq \varepsilon$ if $\|k\|_2 > K_0$. Denote by $\mathcal{I}_0 : \{k \in \mathbb{N}_0^d : \|k\|_2 \leq K_0\}$ and let d_0 be the cardinality of the index set $\mathcal{I}_0$.

Note that the ball in $\mathbb{R}^{d_0}$ of radius $\max_k\{|\lambda_k| : k \in \mathcal{I}_0\}$ with respect to the weighted 1-norm $\|v\|_{\ell^1_{W_s}} = \sum_{k\in\mathcal{I}_0} |v_k|W_s(k)$ is precompact, so it can be covered by the union of n ε-balls with centers $\{v_1, \cdots, v_n\}$ where $v_i \in \mathbb{R}^{d_0}$. We now claim that the image of the unit ball in $\ell^1_{W_s}(\mathbb{N}_0^d)$ under $\mathbb{T}$ is covered by n 2ε-balls with centers $\{(v_1, \mathbf{0}), \cdots, (v_n, \mathbf{0})\}$. In fact, for $u \in \ell^1_{W_s}(\mathbb{N}_0^d)$ with $\sum_{k\in\mathbb{N}_0^d} |u_k|W_s(k) \leq 1$, one has

$$\mathbb{T}u = \Big((\lambda_k u_k)_{k\in\mathcal{I}_0}, \mathbf{0}\Big) + \Big(\mathbf{0}, (\lambda_k u_k)_{k\notin\mathcal{I}_0}\Big).$$

Suppose that v_{i^*} is the closest center of $\{v_1, \cdots, v_n\}$ to the vector $\big((\lambda_k u_k)_{k\in\mathcal{I}_0}\big)$. Then

$$\begin{aligned}\|Tu - (v_{i^*}, \mathbf{0})\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} &= \sum_{k\in\mathcal{I}_0} |(v_{i^*})_k - (\lambda_k u_k)|W_s(k) + \Big\|\Big(\mathbf{0}, (\lambda_k u_k)_{k\notin\mathcal{I}_0}\Big)\Big\|_{\ell^1_{W_s}(\mathbb{N}_0^d)}\\ &\leq \varepsilon + \varepsilon\Big\|\Big(\mathbf{0}, (u_k)_{k\notin\mathcal{I}_0}\Big)\Big\|_{\ell^1_{W_s}(\mathbb{N}_0^d)} \leq 2\varepsilon.\end{aligned}$$

This finishes the proof. ■

Appendix E. Proof of Proposition 1

E.1. Proof of Part (i), Proposition 1

First, it is well known that the problem (1) has a unique weak solution $u_P^* \in H^1_\diamond(\Omega) = \{u \in H^1(\Omega) : \int_\Omega u dx = 0\}$, i.e.

$$a(u, v) =: \int_\Omega \nabla u \cdot \nabla v = F(v) := \int_\Omega f v dx \text{ for every } v \in H^1_\diamond(\Omega). \tag{65}$$

Moreover, the solution u_P^* satisfies that

$$u_P^* = \underset{u\in H^1_\diamond(\Omega)}{\arg\min}\Big\{\frac{1}{2}\int_\Omega |\nabla u|^2 dx - \int_\Omega f u dx\Big\}.$$

Due to the mean-zero constraint of the space $H^1_\diamond(\Omega)$, the variational formulation above is inconvenient to be adopted as the loss function for training a neural network solution. To tackle this issue, we consider instead the following modified Poisson problem:

$$\begin{aligned} -\Delta u + \lambda \int_\Omega u dx &= f \text{ on } \Omega,\\ \frac{\partial}{\partial \nu} u &= 0 \text{ on } \partial\Omega. \end{aligned} \tag{66}$$

Here $\lambda > 0$ is a fixed constant. By the Lax-Milgram theorem the problem (66) has a unique weak solution $u^*_{\lambda,P}$, which solves

$$a_\lambda(u^*_{\lambda,P}, v) := \int_\Omega \nabla u \cdot \nabla v dx + \lambda \int_\Omega u dx \int_\Omega v dx = F(v) \text{ for every } v \in H^1(\Omega). \tag{67}$$

It is clear that $u^*_{\lambda,P}$ is the solution of the variational problem

$$\arg\min_{u\in H^1(\Omega)}\Big\{\frac{1}{2}\int_\Omega |\nabla u|^2 dx + \frac{\lambda}{2}\Big(\int_\Omega u dx\Big)^2 - \int_\Omega f u dx\Big\}. \tag{68}$$

Furthermore, the lemma below shows that the weak solutions of (66) are independent of λ and they all coincides with u^*_P.

Lemma 37 *Assume that $\lambda > 0$. Let u^*_P and $u^*_{\lambda,P}$ be the weak solution of (1) and (66) respectively with $f \in L^2(\Omega)$ satisfying $\int_\Omega f dx = 0$. Then we have that $u^*_{\lambda,P} = u^*_P$.*

Proof We only need to show that $u^*_{\lambda,P}$ satisfies the weak formulation (65). In fact, since $u^*_{\lambda,P}$ satisfies (67), by setting $v = 1$ we obtain that

$$\lambda \int_\Omega u dx = \int_\Omega f dx = 0.$$

This immediately implies that $a_\lambda(u^*_{\lambda,P}, v) = a(u^*_{\lambda,P}, v)$ and hence $u^*_{\lambda,P}$ satisfies (65). ■

Since the solution to (66) is invariant for all $\lambda > 0$, for simplicity we set $\lambda = 1$ in (68) and this proves (3), i.e.

$$u^*_P = \arg\min_{u\in H^1(\Omega)} \mathcal{E}_P(u) = \arg\min_{u\in H^1(\Omega)}\Big\{\frac{1}{2}\int_\Omega |\nabla u|^2 dx - \int_\Omega f u dx + \frac{1}{2}\Big(\int_\Omega u dx\Big)^2\Big\}. \tag{69}$$

Finally we prove that u^*_P satisfies the estimate (4). To see this, we first state a useful lemma which computes the energy excess $\mathcal{E}(u) - \mathcal{E}(u^*_P)$ with any $u \in H^1(\Omega)$.

Lemma 38 *Let u^*_P be the minimizer of $\mathcal{E}_P$ or equivalently the weak solution of the Poisson problem (66). Then for any $u \in H^1(\Omega)$, it holds that*

$$\mathcal{E}_P(u) - \mathcal{E}_P(u^*_P) = \frac{1}{2}\int_\Omega |\nabla u - \nabla u^*_P|^2 dx + \frac{1}{2}\Big(\int_\Omega u^*_P - u\, dx\Big)^2.$$

Proof It follows from Green's formula and the fact that $u^*_P \in H^1_\diamond(\Omega)$ that

$$\begin{aligned}\mathcal{E}(u^*_P) &= \int_\Omega \frac{1}{2}|\nabla u^*_P|^2 - f u^*_P dx + \underbrace{\frac{1}{2}\Big(\int_\Omega u^*_P dx\Big)^2}_{=0}\\ &= \int_\Omega \frac{1}{2}|\nabla u^*_P|^2 + \Delta u^*_P u^*_P dx\\ &= -\frac{1}{2}\int_\Omega |\nabla u^*_P|^2 dx.\end{aligned}$$

Then for any $u \in H^1(\Omega)$, applying Green's formula again yields

$$\begin{aligned}\mathcal{E}(u) - \mathcal{E}(u^*_P) &= \frac{1}{2}\int_\Omega |\nabla u|^2 dx - \int_\Omega f u dx + \frac{1}{2}\Big(\int_\Omega u dx\Big)^2 + \frac{1}{2}\int_\Omega |\nabla u^*_P|^2 dx\\ &= \frac{1}{2}\int_\Omega |\nabla u|^2 dx + \int_\Omega \Delta u^*_P u dx + \frac{1}{2}\Big(\int_\Omega u dx\Big)^2 + \frac{1}{2}\int_\Omega |\nabla u^*_P|^2 dx\\ &= \frac{1}{2}\int_\Omega |\nabla u - \nabla u^*_P|^2 dx + \frac{1}{2}\Big(\int_\Omega (u^*_P - u)\, dx\Big)^2.\end{aligned}$$

■

Now recall that $C_P > 0$ is the Poincaré constant such that for any $v \in H^1(\Omega)$,

$$\Big\|v - \int_\Omega v dx\Big\|^2_{L^2(\Omega)} \leq C_P \|\nabla v\|^2_{L^2(\Omega)}.$$

As a result,

$$\begin{aligned}\|v\|^2_{H^1(\Omega)} &= \|\nabla v\|^2_{L^2(\Omega)} + \|v\|^2_{L^2(\Omega)}\\ &\leq \|\nabla v\|^2_{L^2(\Omega)} + 2\Big\|v - \int_\Omega v\Big\|^2_{L^2(\Omega)} + 2\Big|\int_\Omega v dx\Big|^2\\ &\leq (2C_P + 1)\|\nabla v\|^2_{L^2(\Omega)} + 2\Big|\int_\Omega v dx\Big|^2.\end{aligned}$$

Therefore, an application of the last inequality with $v = u - u^*_P$ and Lemma 38 yields that

$$\|u - u^*_P\|^2_{H^1(\Omega)} \leq 2\max\{2C_P + 1, 2\}(\mathcal{E}(u) - \mathcal{E}(u^*_P)).$$

On the other hand, it follows from Lemma 38 that

$$\mathcal{E}(u) - \mathcal{E}(u^*_P) \leq \frac{1}{2}\|u - u^*_P\|^2_{H^1(\Omega)}.$$

Combining the last two estimates leads to (4) and hence finishes the proof of Proposition 1-(i).

E.2. Proof of Part (ii), Proposition 1

First the standard Lax-Milgram theorem implies that the static Schrödinger equation has a unique weak solution u^*_S. Moreover, it is not hard to verify that u^*_S solves the equivalent variational problem (5), i.e.

$$u^*_S = \underset{u\in H^1(\Omega)}{\arg\min}\, \mathcal{E}_S(u) = \underset{u\in H^1(\Omega)}{\arg\min} \Big\{\frac{1}{2}\int_\Omega |\nabla u|^2 + V|u|^2\, dx - \int_\Omega f u dx\Big\}.$$

Finally we prove that u^*_S satisfies the estimate (6). For this, we first claim that for any $u \in H^1(\Omega)$,

$$\mathcal{E}_S(u) - \mathcal{E}_S(u^*_S) = \frac{1}{2}\int_\Omega |\nabla u - \nabla u^*_S|^2 dx + \frac{1}{2}\int_\Omega V(u^*_S - u)^2\, dx. \tag{70}$$

In fact, using Green's formula, one has that

$$\begin{aligned}\mathcal{E}_S(u^*_S) &= \int_\Omega \frac{1}{2}|\nabla u^*_S|^2 + \frac{1}{2}V|u^*_S|^2 - f u^* dx\\ &= \int_\Omega \frac{1}{2}|\nabla u^*_S|^2 + \frac{1}{2}V|u^*_S|^2 + (\Delta u^*_S - V u^*_S)u^* dx\\ &= -\frac{1}{2}\int_\Omega |\nabla u^*_S|^2 + V|u^*|^2 dx.\end{aligned}$$

Then for any $u \in H^1(\Omega)$, applying Green's formula again yields

$$\begin{aligned}\mathcal{E}_S(u) - \mathcal{E}_S(u_S^*) &= \frac{1}{2}\int_\Omega |\nabla u|^2 + V|u|^2 dx - \int_\Omega f u dx + \frac{1}{2}\int_\Omega |\nabla u_S^*|^2 + V|u_S^*|^2 dx \\ &= \frac{1}{2}\int_\Omega |\nabla u|^2 + V|u|^2 dx + \int_\Omega (\Delta u_S^* - V u_S^*) u dx + \frac{1}{2}\int_\Omega |\nabla u_S^*|^2 + V|u_S^*|^2 dx \\ &= \frac{1}{2}\int_\Omega |\nabla u - \nabla u_S^*|^2 dx + \frac{1}{2}\int_\Omega V\big(u_S^* - u\big)^2 dx.\end{aligned}$$

The estimate (6) follows directly from the identity (70) and the assumption that $0 < V_{\min} \le V(x) \le V_{\max}$. This completes the proof.

Appendix F. Some Useful Facts on Cosine Series and Convolution

Assume that $u \in L^1(\Omega)$ admits the cosine series expansion

$$u(x) = \sum_{k \in \mathbb{N}_0^d} \hat{u}_k \Phi_k(x),$$

where $\{\hat{u}_k\}_{k \in \mathbb{N}_0^d}$ are the cosine expansion coefficients, i.e.

$$\hat{u}_k = \frac{\int_\Omega u(x)\Phi_k(x)dx}{\int_\Omega \Phi_k^2(x)dx} = \frac{\int_\Omega u(x)\Phi_k(x)dx}{2^{-\sum_{i=1}^d \mathbf{1}_{k_i \neq 0}}}. \tag{71}$$

Let $\Omega_e := [-1, 1]^d$ and define the even extension of u_e of a function u by

$$u_e(x) = u_e(x_1, \cdots, u_d) = u(|x_1|, \cdots, |x_d|), x \in \Omega_e.$$

Let $\tilde{u}_k$ be the Fourier coefficients of u_e. Since u_e is real and even, one has that

$$u_e = \sum_{k \in \mathbb{Z}^d} \tilde{u}_k \cos(\pi k \cdot x),$$

where

$$\tilde{u}_k = \frac{\int_{\Omega_e} u_e(x)\cos(\pi k \cdot x)dx}{\int_{\Omega_e} \cos^2(\pi k \cdot x)dx} = \frac{1}{2^{d - \mathbf{1}_{k \neq \mathbf{0}}}} \int_{\Omega_e} u_e(x)\cos(\pi k \cdot x)dx. \tag{72}$$

By abuse of notation, we use $|k|$ to stand for the vector $(|k_1|, |k_2, |, \cdots, |k_d|)$.

Lemma 39 *For every $k \in \mathbb{Z}^d$, it holds that $\tilde{u}_k = \beta_k \hat{u}_{|k|}$ where $\beta_k = 2^{\mathbf{1}_{k \neq \mathbf{0}} - \sum_{i=1}^d \mathbf{1}_{k_i \neq 0}}$.*

Proof First thanks to Lemma 13 and the evenness of cosine,

$$\begin{aligned}\int_{\Omega_e} u_e(x)\cos(\pi k\cdot x)dx &= \int_{\Omega_e} u_e(x)\cos\Big(\pi\Big(\sum_{i=1}^{d-1}k_ix_i\Big)\Big)\cos(\pi k_dx_d)dx\\ &\quad \underbrace{-\int_{\Omega_e} u_e(x)\sin\Big(\pi\Big(\sum_{i=1}^{d-1}k_ix_i\Big)\Big)\sin(\pi k_dx_d)dx}_{=0}\\ &= \int_{\Omega_e} u_e(x)\cos\Big(\pi\Big(\sum_{i=1}^{d-2}k_ix_i\Big)\Big)\cos(\pi k_{d-1}x_{d-1})\cos(\pi k_dx_d)dx\\ &\quad \underbrace{-\int_{\Omega_e} u_e(x)\sin\Big(\pi\Big(\sum_{i=1}^{d-2}k_ix_i\Big)\Big)\sin(\pi k_{d-1}x_{d-1})\cos(\pi k_dx_d)dx}_{=0}\\ &= \cdots\\ &= \int_{\Omega_e} u_e(x)\prod_{i=1}^{d}\cos(\pi k_ix_i)dx\\ &= 2^d\int_{\Omega} u(x)\Phi_k(x)dx.\end{aligned}$$

In addition, since $\Phi_k = \Phi_{|k|}$ for any $k\in\mathbb{Z}^d$, the lemma follows from the equation above, (71) and (72). ■

The next lemma shows that the Fourier coefficients of the product of two functions u and v are the discrete convolution of their Fourier coefficients. Recall that $\{\tilde{u}_k\}_{k\in\mathbb{Z}^d}$ denote the Fourier coefficients of the even functions u_e.

Lemma 40 *Let $w_e = u_ev_e$. Then $\tilde{w}_k = \sum_{m\in\mathbb{Z}^d}\tilde{u}_m\tilde{v}_{k-m}$.*

Proof By definition, $u_e(x) = \sum_{m\in\mathbb{Z}^d}\tilde{u}_m\cos(\pi m\cdot x)$ and $v_e(x) = \sum_{n\in\mathbb{Z}^d}\tilde{v}_n\cos(\pi n\cdot x)$ Thanks to the fact that

$$\int_{\Omega_e}\cos(\pi\ell\cdot x)\cos(\pi k\cdot x) = 2^{d-\mathbf{1}_{k\neq\mathbf{0}}}\delta_\ell(k),$$

one obtains that

$$\begin{aligned}
\tilde{w}_k &= \frac{1}{2^{d-\mathbf{1}_{k\neq\mathbf{0}}}} \int_{\Omega_e} u_e(x) v_e(x) \cos(\pi k \cdot x) dx \\
&= \frac{1}{2^{d-\mathbf{1}_{k\neq\mathbf{0}}}} \sum_{m\in\mathbb{Z}^d} \sum_{n\in\mathbb{Z}^d} \tilde{u}_m \tilde{v}_n \int_{\Omega_e} \cos(\pi m \cdot x) \cos(\pi n \cdot x) \cos(\pi k \cdot x) dx \\
&= \frac{1}{2^{d-\mathbf{1}_{k\neq\mathbf{0}}}} \sum_{m\in\mathbb{Z}^d} \sum_{n\in\mathbb{Z}^d} \tilde{u}_m \tilde{v}_n \int_{\Omega_e} \frac{1}{2}\Big[\cos(\pi(m+n)\cdot x) + \cos(\pi(m-n)\cdot x)\Big] \cos(\pi k \cdot x) dx \\
&= \frac{1}{2} \sum_{m\in\mathbb{Z}^d} \tilde{u}_m (\tilde{v}_{k-m} + \tilde{v}_{m-k}) \\
&= \sum_{m\in\mathbb{Z}^d} \tilde{u}_m \tilde{v}_{k-m},
\end{aligned}$$

where we have also used that $\tilde{v}_k = \tilde{v}_{-k}$ for any k. ■

Corollary 41 *For any $k \in \mathbb{N}^d$,*

$$\widehat{(uv)}_k = \frac{1}{\beta_k} \sum_{m\in\mathbb{Z}^d} \beta_m \hat{u}_{|m|} \beta_{m-k} \hat{v}_{|m-k|}.$$

Proof Thanks to Lemma 39 and Lemma 40,

$$\widehat{(uv)}_k = \frac{1}{\beta_k} \widetilde{(uv)}_k = \frac{1}{\beta_k} (\tilde{u} * \tilde{v})_k = \frac{1}{\beta_k} \sum_{m\in\mathbb{Z}^d} \beta_m \hat{u}_{|m|} \beta_{m-k} \hat{v}_{|m-k|}.$$

■