ON POINTWISE PRODUCTS OF ELLIPTIC EIGENFUNCTIONS

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ABSTRACT. We consider eigenfunctions of Schrödinger operators on a $d-$dimensional bounded domain Ω (or a $d-$dimensional compact manifold Ω) with Dirichlet conditions. These operators give rise to a sequence of eigenfunctions $(\phi_n)_{n\in\mathbb{N}}$. We study the subspace of all pointwise products

$$A_n = \operatorname{span}\{\phi_i(x)\phi_j(x) : 1 \le i, j \le n\} \subseteq L^2(\Omega).$$

Clearly, that vector space has dimension $\dim(A_n) = n(n+1)/2$. We prove that products $\phi_i\phi_j$ of eigenfunctions are simple in a certain sense: for any $\varepsilon > 0$, there exists a low-dimensional vector space B_n that almost contains all products. More precisely, denoting the orthogonal projection $\Pi_{B_n} : L^2(\Omega) \to B_n$, we have

$$\forall\ 1 \le i, j \le n \qquad \|\phi_i\phi_j - \Pi_{B_n}(\phi_i\phi_j)\|_{L^2} \le \varepsilon$$

and the size of the space $\dim(B_n)$ is relatively small

$$\dim(B_n) \lesssim \left(\frac{1}{\varepsilon} \max_{1 \le i \le n} \|\phi_i\|_{L^\infty}\right)^d n.$$

In the generic delocalized setting, this bound grows linearly up to logarithmic factors: pointwise products of eigenfunctions are low-rank. This has implications, among other things, for the validity of fast algorithms in electronic structure computations.

1. INTRODUCTION

Throughout this paper, we let L be a uniformly elliptic second-order partial differential operator of Schrödinger type

$$Lu = -\operatorname{div}(a(x) \cdot \nabla u) + V(x)u$$

on a $d-$dimensional bounded domain Ω (or a smooth $d-$dimensional compact manifold Ω) with Dirichlet conditions and smooth coefficients $a, V \in C^\infty$. This operator L gives rise to a sequence of eigenfunctions $L\phi_k = \lambda_k\phi_k$ which we assume to be L^2-normalized and which span $L^2(\Omega)$. We ask a very simple question.

Question. What can be said about the function $\phi_i(x)\phi_j(x)$?

Clearly, by L^2-orthogonality, the function $\phi_i(x)\phi_j(x)$ has mean value 0 if $i \ne j$ but what else can be said about its spectral resolution, for example, the size of $\langle\phi_i\phi_j, \phi_k\rangle$? There are very few results overall; some results have been obtained in the presence of additional structure

assumptions on Ω connected to number theory (see Bernstein & Reznikoff [1], Krötz & Stanton [9] and Sarnak [12]). Already the simpler question of understanding L^2-size of the product is highly nontrivial: a seminal result of Burq-Gérard-Tzetkov [4] states

$$\|\phi_\mu \phi_\lambda\|_{L^2} \lesssim \min(\sqrt{\lambda}, \sqrt{\mu})\|\phi_\lambda\|_{L^2}\|\phi_\mu\|_{L^2}$$

on compact two-dimensional manifolds without boundary (this has been extended to higher dimensions [3,5]). A recent result of the second author [14] (see also [6]) shows that one would generically (i.e., on typical manifolds in the presence of quantum chaos) expect $\phi_i(x)\phi_j(x)$ to be mainly supported at eigenfunctions having their eigenvalue close to $\max\{\lambda_i, \lambda_j\}$ and that deviation from this phenomenon, as in the case of Fourier series on $\mathbb{T}$ for example, requires eigenfunctions to be strongly correlated at the wavelength in a precise sense.

In this paper, we ask the question on the numerical rank of the space spanned by the pointwise products of eigenfunctions

$$A_n = \mathrm{span}\left\{\phi_i(x)\phi_j(x) : 1 \leq i, j \leq n\right\}.$$

This is a natural quantity for measuring the complexity of the products but also motivated by the density fitting approximation to the electron repulsion integral in the quantum chemistry literature. Given a set of eigenfunctions, the four-center two-electron repulsion integral

$$(ij|kl) = \int_{\Omega \times \Omega} \frac{\phi_i(x)\phi_j(x)\phi_k(y)\phi_l(y)}{|x-y|} dx dy$$

is a central quantity in electronic structure theories. If we are working with the first n eigenfunctions $(\phi_i)_{1 \leq i \leq n}$, then one has to evaluate $\mathcal{O}(n^4)$ integrals.

It has been empirically observed in the literature (see e.g., [10] by the first author and Lexing Ying) that the space A_n can in practice be very well approximated by another vector space B_n with $\dim(B_n) \sim c \cdot n$, often referred as density fitting. This then drastically reduces the number of integrals in need of evaluation to $\mathcal{O}(n^2)$. Our result is inspired by the empirical success of density fitting and gives a mathematical justification.

2. The results

We state our main result: pointwise products of delocalized eigenfunctions are low-rank.

Theorem 1 (Main Theorem). *For any $\varepsilon > 0, n \in \mathbb{N}$, there exists a space B_n such that*

$$\forall\ i, j \leq n \qquad \|\phi_i\phi_j - \Pi_{B_n}(\phi_i\phi_j)\|_{L^2} \leq \varepsilon$$

and such that $\dim(B_n)$ is relatively small

$$\dim(B_n) \lesssim_{\Omega, a, V} \left(\frac{1}{\varepsilon} \max_{1 \leq i \leq n} \|\phi_i\|_{L^\infty}\right)^d n.$$

We emphasize that for generic differential operators on generic domains, we expect the eigenfunctions to be delocalized and their $L^\infty-$norm to be governed by the random wave heuristic: in particular, we expect the maximum to grow logarithmically. Theorem 1 is thus optimal in the quantum chaotic setting (up to at most logarithmic factors). It is an

interesting question whether the logarithm can be removed. As a corollary of Theorem 1, we obtain unconditional nontrivial results in low dimensions $d = 1, 2$.

Corollary 2. *We have*

$$\dim(B_n) \lesssim_{\Omega,a,V} \begin{cases} \varepsilon^{-1} \cdot n & \text{if } d = 1 \\ \varepsilon^{-2} \cdot n^{3/2} & \text{if } d = 2. \end{cases}$$

The case $d = 1$ is clearly optimal and well in line with classical intuition (the WKB asymptotic suggests that things behave asymptotically like trigonometric functions which one would expect to behave like Fourier series whose products are low-rank).

In light of the four-center two-electron repulsion integral, which is a somewhat better behaved quantity due to the smoothing effects of the potential, it is natural to look for a similar result in a function spaces that captures the smoothing of the potential: since $|x - y|^{-1}$ is the fundamental solution of the Laplacian in $\mathbb{R}^3$, the appropriate space for physically relevant problems in $\Omega \subset \mathbb{R}^3$ is the homogeneous Sobolev space H^{-1} norm (also known as the Coulomb norm or the Beppo-Levi norm) equipped with

$$\|f\|_{\dot{H}^{-1}}^2 = \langle f - \bar{f}, \Delta^{-1}(f - \bar{f}) \rangle,$$

where $\bar{f}$ is the average of f, so that the above definition makes sense also for closed manifold.

Theorem 3 (Variant in $\dot{H}^{-1}$). *For any $\varepsilon > 0, n \in \mathbb{N}$, there exists a space B_n such that*

$$\forall \, i, j \leq n \qquad \|\phi_i \phi_j - \Pi_{B_n}(\phi_i \phi_j)\|_{\dot{H}^{-1}} \leq \varepsilon$$

such that $\dim(B_n)$ *is relatively small*

$$\dim(B_n) \lesssim_{\Omega,a,V} \left(\frac{1}{\varepsilon} \max_{1 \leq i \leq n} \|\phi_i\|_{L^\infty} \right)^{\frac{d}{2}} \sqrt{n}.$$

Note that this improves the bound in the L^2 case by essentially a square root. Here, we can obtain an unconditional result that improves on the trivial bound for all dimensions $d \leq 6$. We also note that it matches the linear scaling for $d = 3$.

Corollary 4 (Variant in $\dot{H}^{-1}$). *We have*

$$\dim(B_n) \lesssim_{\Omega,a,V} \varepsilon^{-\frac{d}{2}} n^{\frac{d+1}{4}}.$$

It is clear that the underlying low-rankness phenomenon is of great relevance in a variety of settings (e.g., fast algorithms for electronic structure theories [10, 11], etc.); it is also clear that similar arguments to the ones contained in this paper can be used to obtain low-rankness results of a similar flavor in a variety of function spaces. One of the most interesting questions is whether it is possible to have $\dim(B_n) \sim n$. Corollary 2 shows that this is the case for ordinary differential equations in L^2; it would be interesting to have concrete examples and counterexamples in higher dimensions – unfortunately many of the cases that can be made explicit (the torus $\mathbb{T}^d$, the sphere $\mathbb{S}^d$) seem exceedingly non-generic.

3. Proofs

Proof of Theorem 1. We first prove an elementary inequality: let $1 \leq i, j \leq n$ and

$$-\text{div}(a(x)\nabla\phi_i) + V\phi_i = \lambda_i\phi_i \qquad \text{and} \qquad -\text{div}(a(x)\nabla\phi_j) + V\phi_j = \lambda_j\phi_j$$

with the normalization $\|\phi_i\|_{L^2} = \|\phi_j\|_{L^2} = 1$, then we have

$$(1) \qquad \langle (-\text{div}(a(x)\nabla(\phi_i\phi_j))) + V\phi_i\phi_j, \phi_i\phi_j \rangle \lesssim_{a,V} (\lambda_n + 1) \max_{1 \leq i \leq n} \|\phi_i\|_{L^\infty}^2.$$

We separate the relevant quantity into two terms. The first one is fairly simple, we observe that $V \in C^\infty(\Omega)$ and thus, by L^2-normalization of the eigenfunctions,

$$\begin{aligned}
\langle V\phi_i\phi_j, \phi_i\phi_j \rangle &= \int_\Omega V\phi_i^2\phi_j^2 dx \\
&\leq \|V\|_{L^\infty} \max_{1 \leq i \leq n} \|\phi_i\|_{L^\infty}^2 \lesssim_V \max_{1 \leq i \leq n} \|\phi_i\|_{L^\infty}^2
\end{aligned}$$

The second term can be rewritten using integration by parts as

$$\begin{aligned}
\langle (-\text{div}(a(x)\nabla(\phi_i\phi_j))), \phi_i\phi_j \rangle &= \int_\Omega a(x)(\nabla(\phi_i\phi_j) \cdot \nabla(\phi_i\phi_j)) dx \\
&\leq \left(\max_{x \in \Omega} a(x) \right) \|\nabla(\phi_i\phi_j)\|_{L^2}^2.
\end{aligned}$$

The product rule and the triangle inequality yield

$$\begin{aligned}
\|\nabla(\phi_i\phi_j)\|_{L^2} &= \|\phi_i\nabla\phi_j + \phi_j\nabla\phi_i\|_{L^2} \\
&\leq \|\nabla\phi_j\|_{L^2}\|\phi_i\|_{L^\infty} + \|\nabla\phi_i\|_{L^2}\|\phi_j\|_{L^\infty}.
\end{aligned}$$

However, we also have, with integration by parts,

$$\begin{aligned}
\|\nabla\phi_i\|_{L^2}^2 &= \int_\Omega \nabla\phi_i \cdot \nabla\phi_i dx \\
&\leq \left(\min_{x \in \Omega} a(x) \right)^{-1} \int_\Omega a(x)\nabla\phi_i \cdot \nabla\phi_i dx \\
&= \left(\min_{x \in \Omega} a(x) \right)^{-1} \int_\Omega -\text{div}(a(x)\nabla\phi_i)\phi_i dx \\
&= \left(\min_{x \in \Omega} a(x) \right)^{-1} \int_\Omega (\lambda_i\phi_i - V\phi_i)\phi_i dx \\
&\lesssim_a \lambda_n + \|V\|_{L^\infty}.
\end{aligned}$$

This concludes the proof of (1).

Expanding the product

$$\phi_i\phi_j = \sum_{k=1}^{\infty} \langle \phi_i\phi_j, \phi_k \rangle \phi_k,$$

we obtain, since ϕ_k are the eigenfunctions,

$$\langle(-\mathrm{div}(a(x)\nabla(\phi_i\phi_j)) + V\phi_i\phi_j, \phi_i\phi_j\rangle = \left\langle \sum_{k=1}^{\infty} \lambda_k\langle\phi_i\phi_j, \phi_k\rangle\phi_k, \sum_{k=1}^{\infty}\langle\phi_i\phi_j, \phi_k\rangle\phi_k \right\rangle$$
$$= \sum_{k=1}^{\infty} \lambda_k|\langle\phi_i\phi_j, \phi_k\rangle|^2.$$

This shows, for any $r \in \mathbb{N}$,

$$\langle(-\mathrm{div}(a(x)\nabla(\phi_i\phi_j)) + V\phi_i\phi_j, \phi_i\phi_j\rangle \geq \lambda_r \left\|\Pi_{>r}(\phi_i\phi_j)\right\|_{L^2}^2,$$

where we have introduced the short hand notation $\Pi_{>r} = \Pi_{\mathrm{span}\{\phi_k|k>r\}}$. Combined this with (1) we get for any $r \in \mathbb{N}$ that

$$\lambda_r \left\|\Pi_{>r}(\phi_i\phi_j)\right\|_{L^2}^2 \lesssim (\lambda_n + 1) \max_{1\leq i\leq n} \|\phi_i\|_{L^\infty}^2.$$

Using Weyl's law, we have (independently of the domain or manifold Ω and with an implicit constant converging to 1 as $\min(r, n) \to \infty$)

$$\lambda_r \sim \lambda_n \left(\frac{r}{n}\right)^{2/d}.$$

and therefore

$$\left\|\Pi_{>r}(\phi_i\phi_j)\right\|_{L^2} \lesssim \left(\frac{n}{r}\right)^{1/d} \max_{1\leq i\leq n} \|\phi_i\|_{L^\infty}.$$

Setting

$$r \sim \left(\frac{1}{\varepsilon} \max_{1\leq i\leq n} \|\phi_i\|_{L^\infty}\right)^d n$$

makes the projection smaller than $\lesssim \varepsilon$. $\qquad\square$

Proof of Corollary 2. To pass from Theorem 1 to Corollary 2 is straightforward: we make use of the $L^\infty - L^2$ estimate of elliptic eigenfunctions due to Hörmander [8] (see Sogge [13] for the extension to general elliptic operators): let ϕ be an L^2-normalized eigenfunction of L on a compact smooth manifold associated with eigenvalue λ, we have

$$\|\phi\|_{L^\infty} \leq C\lambda^{\frac{d-1}{4}}.$$

Combined with the Weyl's law, we thus obtain

(2) $$\max_{1\leq i\leq n} \|\phi_i\|_{L^\infty} \lesssim_{\Omega,a,V} \lambda_n^{\frac{d-1}{4}} \sim_{\Omega,a} \left(n^{2/d}\right)^{\frac{d-1}{4}} \sim n^{\frac{d-1}{2d}}.$$

Corollary 2 immediately follows. $\qquad\square$

Proof of Theorem 3. We introduce the eigenfunctions of $-\Delta$ as $(\psi_k)_{k\in\mathbb{N}}$ having eigenvalues μ_k. These eigenvalues are fairly closely related to λ_k which follows immediately from the min-max characterization

$$\lambda_k = \inf_{V_k\subset C_c^\infty(\Omega)} \max_{f\in V_k} \frac{\int_\Omega |\nabla f|^2}{\int_\Omega f^2} \qquad \text{and} \qquad \mu_k = \inf_{V_k\subset C_c^\infty(\Omega)} \max_{f\in V_k} \frac{\int_\Omega a(x)|\nabla f|^2 + Vf^2}{\int_\Omega f^2},$$

where the infimum runs over all $k-$dimensional subspaces of functions in $C_c^\infty(\Omega)$. This implies

$$\left(\min_{x\in\Omega} a(x)\right)\lambda_k - \|V\|_{L^\infty} \le \mu_k \le \left(\max_{x\in\Omega} a(x)\right)\lambda_k + \|V\|_{L^\infty}.$$

This shows that in the spectral definition of the $\dot{H}^{-1}-$norm

$$\|f\|_{\dot{H}^{-1}}^2 = \sum_{k=1}^\infty \frac{|\langle f, \psi_k\rangle|^2}{\mu_k}$$

it is possible to obtain an equivalent norm by replacing the eigenvalues of the Laplacian μ_k with the eigenvalues of the Schrödinger operator λ_k. We will now study the size of the projection onto the orthogonal space of the first r eigenfunctions of the Laplacian

$$\begin{aligned}
\|\Pi_{>r}(\phi_i\phi_j)\|_{\dot{H}^{-1}}^2 &= \sum_{k=r+1}^\infty \frac{|\langle\phi_i\phi_j,\psi_k\rangle|^2}{\mu_k} \\
&\lesssim_{\Omega,a,V} \sum_{k=r+1}^\infty \frac{|\langle\phi_i\phi_j,\psi_k\rangle|^2}{\lambda_k} \\
&\lesssim \frac{1}{\lambda_r}\sum_{k=r+1}^\infty |\langle\phi_i\phi_j,\psi_k\rangle|^2 = \frac{1}{\lambda_r}\|\Pi_{>r}(\phi_i\phi_j)\|_{L^2}^2,
\end{aligned}$$

where the projection $\Pi_{>r}$ is now onto the orthogonal complement of the first r Laplacian eigenfunctions. We again use

$$\|\nabla(\phi_i\phi_j)\|_{L^2} \le \|\nabla\phi_i\|_{L^2}\|\phi_j\|_{L^\infty} + \|\nabla\phi_j\|_{L^2}\|\phi_i\|_{L^\infty}$$

and

$$\|\nabla\phi_i\|_{L^2}^2 \lesssim_a \int_\Omega -\mathrm{div}(a(x)\nabla\phi_i)\phi_i \lesssim_a \lambda_n + \|V\|_{L^\infty}.$$

Then, however, the equivalence of the eigenvalues implies

$$\lambda_r\|\Pi_{>r}(\phi_i\phi_j)\|_{L^2}^2 \le \sum_{k=1}^\infty \lambda_k|\langle\phi_i\phi_j,\psi_k\rangle|^2 \lesssim_{\Omega,a,V} \sum_{k=1}^\infty \mu_k|\langle\phi_i\phi_j,\psi_k\rangle|^2$$

and integration by part shows

$$\begin{aligned}
\sum_{k=1}^\infty \mu_k|\langle\phi_i\phi_j,\psi_k\rangle|^2 &= \left\langle \sum_{k=1}^\infty \mu_k\langle\phi_i\phi_j,\psi_k\rangle\psi_k, \sum_{k=1}^\infty \langle\phi_i\phi_j,\psi_k\rangle\psi_k \right\rangle \\
&= \int_{-\Omega} -\Delta(\phi_i\phi_j)\phi_i\phi_j dx \\
&= \|\nabla(\phi_i\phi_j)\|_{L^2}^2 \lesssim_{a,V} \lambda_n \max_{1\le i\le n}\|\phi_i\|_{L^\infty}^2.
\end{aligned}$$

Using Weyl's law, the above inequalities yield

$$\begin{aligned}
\|\Pi_{>r}(\phi_i\phi_j)\|_{\dot{H}^{-1}} &\lesssim \frac{\sqrt{\lambda_n}}{\lambda_r}\max_{1\le i\le n}\|\phi_i\|_{L^\infty} \\
&\lesssim n^{1/d}r^{-2/d}\max_{1\le i\le n}\|\phi_i\|_{L^\infty}.
\end{aligned}$$

This is smaller than ε for

$$r \gtrsim \left(\frac{1}{\varepsilon} \max_{1 \leq i \leq n} \|\phi_i\|_{L^\infty} \right)^{\frac{d}{2}} \sqrt{n}.$$

The unconditional result Corollary 4 follows from another application of

$$\max_{1 \leq i \leq n} \|\phi_i\|_{L^\infty} \lesssim n^{\frac{d-1}{2d}}.$$

$\square$

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