Parseval frames of exponentially decaying Wannier functions

Peter Kuchment

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Definition

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There exists a larger Hilbert space H_1 and its ortho-normal basis $\{e_j\}$

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There exists a larger Hilbert space H_1 and its ortho-normal basis $\{e_j\}$ s.t.

$$\psi_j = P_H^\perp e_j$$

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$$||f||^2 = \sum_j |(f, \psi_j)|^2$$

Theorem (D. Larson)

There exists a larger Hilbert space H_1 and its ortho-normal basis $\{e_j\}$ s.t.

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 $P_{H}^{\perp}: H_{1} \mapsto H$ - orthogonal projector. (Converse statement clearly also holds.)

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The uses of frames are numerous

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If \mathcal{E} is non-trivial, i.e. not isomorphic to $K \times \mathbb{C}^m$, then there is no continuous basis $e_1(k), \ldots, e_m(k)$ in the fiber.

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There always exists a continuous Parseval frame $\psi_j(k)$ in the fibers of \mathcal{E} .

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There always exists a continuous Parseval frame $\psi_j(k)$ in the fibers of \mathcal{E} .

Indeed, embed \mathcal{E} into a trivial finite-dimensional Hilbert bundle $k \times H$ (always possible)

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Continuous frame

There always exists a continuous Parseval frame $\psi_j(k)$ in the fibers of \mathcal{E} .

Indeed, embed \mathcal{E} into a trivial finite-dimensional Hilbert bundle $k \times H$ (always possible) and project an o.-n. basis into \mathcal{E}_{\bullet}

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Two common functional "bases" in \mathbb{R}^n :

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Two common functional "bases" in \mathbb{R}^n : **Plane waves**

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Two common functional "bases" in \mathbb{R}^n : **Plane waves** $e^{ix \cdot \xi}$, $\xi \in \mathbb{R}^n$.

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$$f\mapsto \int_{\mathbb{R}^n}f(x)e^{ix\cdot\xi}dx$$

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 δ -functions

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 δ -functions $\delta(x - x_0)$, $x_0 \in \mathbb{R}^n$.

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$$f\mapsto \int_{\mathbb{R}^n}f(x)e^{ix\cdot\xi}dx$$

 δ -functions $\delta(x - x_0)$, $x_0 \in \mathbb{R}^n$. Expansion: function values

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$$f \mapsto f(x_0)$$

Plane waves $\Leftrightarrow \quad \delta$ -functions relation: $e^{ix \cdot \xi_0} \stackrel{FT}{\Leftrightarrow} \delta(\xi - \xi_0)$

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Periodic PDEs and Floquet-Bloch expansion - a crash course of solid state physics

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Periodic Schrödinger operator $L(x, D) := -\Delta + V(x)$

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Periodic Schrödinger operator $L(x, D) := -\Delta + V(x)$, V - potential periodic w.r.t. \mathbb{Z}^n -shifts. (More general operators L and lattices Γ are possible). Fundamental domain $W := [0,1]^n$ and torus $\mathbb{T} := \mathbb{R}^n / \mathbb{Z}^n$. Dual lattice $\Gamma^* := 2\pi \mathbb{Z}^n$. Its fundamental domain: Brillouin zone $B = [-\pi, \pi]^n$. Dual torus $\mathbb{T}^* := \mathbb{R}^n / 2\pi \mathbb{Z}^n \approx \{e^{ik} = z = (z_1, \dots, z_n) \mid |z_j| = 1\} \subset \mathbb{C}^n$. Floquet-Bloch direct integral decomposition:

$$L^{2}(\mathbb{R}^{n}) = \int_{B}^{\bigoplus} L^{2}(W) dk = \int_{\mathbb{T}^{*}}^{\bigoplus} L^{2}(W) dz.$$

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Over $z \in \mathbb{T}^*$

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Over $z \in \mathbb{T}^*$ – *z*-automorphic functions $f(x + p) = z^p f(x), p \in \mathbb{Z}^n$

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Floquet-Bloch-Gelfand transform

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$$f(x)\mapsto \widehat{f}(k,x)=\sum_{\gamma\in\Gamma}f(x+\gamma)e^{-ik\cdot\gamma}$$

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Floquet-Bloch-Gelfand transform

$$f(x)\mapsto \widehat{f}(k,x)=\sum_{\gamma\in\Gamma}f(x+\gamma)e^{-ik\cdot\gamma}$$

Its inversion:

$$f(x) = \int_{\mathbb{T}^*} \widehat{f}(k, x) dk.$$

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Operator L(z) = L(k) in the fiber – the restriction of L.

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Operator L(z) = L(k) in the fiber – the restriction of L. Dispersion relation: graph of $\sigma(L(z)), z \in \mathbb{T}$.

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Spectrum:

Operator L(z) = L(k) in the fiber – the restriction of L. Dispersion relation: graph of $\sigma(L(z)), z \in \mathbb{T}$.



Spectrum:

$$\sigma(L) = \bigcup_{\mathbb{T}} \sigma(L(z))$$

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 $I_j = \bigcup \lambda_j(k)$ - single band

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$$I_j = \bigcup \lambda_j(k)$$
 - single band or $S = \bigcup_{i=j}^{j+m-1} I_i$ - composite band

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 $I_j = \bigcup \lambda_j(k)$ - single band or $S = \bigcup_{i=j}^{j+m-1} I_i$ - composite band separated by gaps from the rest of the spectrum.

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 $I_j = \bigcup \lambda_j(k)$ - single band or $S = \bigcup_{i=j}^{j+m-1} I_i$ - composite band separated by gaps from the rest of the spectrum. Spectral subspace H_S for L in $L^2(\mathbb{R}^n)$:

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Spectral projector onto $H_S(z)$ in $L^2(W)$ is analytic in z.

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$$\Lambda_S := \bigcup_{\mathbb{T}^*} H_S(z)$$

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Bloch eigenfunction $-u_z(x) = z^x u(x)$ with periodic u.

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analytically) dependent on $z \in \mathbb{T}^*$ Bloch functions $u_{i,z}$.

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Equivalent to the **triviality of the spectral bundle** Λ_S .

Triviality generically does not hold (e.g., in the presence of magnetic fields, Thouless '84).

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Triviality holds if n = 1 (W. Kohn '59) or if there is **time reversal** symmetry $z \mapsto z^{-1} \Leftrightarrow k \mapsto -k$ and either m = 1 (Nenciu '85)

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Triviality holds if n = 1 (W. Kohn '59) or if there is **time reversal** symmetry $z \mapsto z^{-1} \Leftrightarrow k \mapsto -k$ and either m = 1 (Nenciu '85), or $n \leq 3$ (Panati '07).

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Time reversal symmetry occurs if the coefficients of the operator are real (e.g., magnetic fields are excluded).

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 $u_z(x)$ – Bloch eigenfunction corresponding to a band S.

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Wannier functions

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$$u_z(x)$$
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Wannier functions

• Wannier function
$$w(x) = \int_{m_*} u_z(x) dz$$

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Wannier functions

- Wannier function $w(x) = \int_{\mathbb{T}^*} u_z(x) dz$
- Smoothness w.r.t. z of $u_z \Leftrightarrow \text{decay of } w(x)$.

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- Wannier function $w(x) = \int_{\mathbb{T}^*} u_z(x) dz$
- Smoothness w.r.t. z of $u_z \Leftrightarrow \text{decay of } w(x)$.
- Analyticity of u_z w.r.t. $z \Leftrightarrow$ exponential decay of w.

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Wannier functions

- Wannier function $w(x) = \int_{\mathbb{T}^*} u_z(x) dz$
- Smoothness w.r.t. z of $u_z \Leftrightarrow \text{decay of } w(x)$.
- Analyticity of u_z w.r.t. $z \Leftrightarrow$ exponential decay of w.
- Shifts w(x − γ), γ ∈ Γ pairwise orthogonal ⇔ ||u_z(x)|| is z-independent.

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Wannier functions

- Wannier function $w(x) = \int_{\mathbb{T}^*} u_z(x) dz$
- Smoothness w.r.t. z of $u_z \Leftrightarrow \text{decay of } w(x)$.
- Analyticity of u_z w.r.t. $z \Leftrightarrow$ exponential decay of w.
- Shifts w(x − γ), γ ∈ Γ pairwise orthogonal ⇔ ||u_z(x)|| is z-independent.
- Orthonormal analytic basis $u_{j,z}$ in $\Lambda_S \Leftrightarrow$ orthonormal basis $w_j(x \gamma)$ of exp. decaying Wannier functions in H_S .

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An example of WF in Barium Titanate

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So, what can one do?

Parseval frames of Wannier functions

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Theorem (P.K.)

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- The number *l* is the smallest dimension of the fiber of a trivial vector bundle over T^{*} that contains an isomorphic copy of Λ_S. In particular, *l* ≤ 2ⁿm.
- l = m iff Λ_S is trivial, in which case there exists an o.-n. basis of exponentially decaying Wannier functions in H_S .

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Scheme of the proof

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• Find an *I*-dimensional trivial bundle Λ such that $\Lambda \approx \Lambda_S \bigoplus \Lambda'$.

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- Apply to {e_j} an analytic projector P(z) onto Λ_S orthogonal over T^{*} to get the Wannier functions {w_j}.

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A counterexample to Kadison-Singer (KSC) conjecture?

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Kadison-Singer Problem: Does every pure state on the (abelian) von Neumann algebra D of bounded diagonal operators on l_2 have a unique extension to a (pure) state on the von Neumann algebra $B(l_2)$ of all bounded linear operators on the Hilbert space l_2 ?

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Q.: Do frames of this kind in the spaces of L^2 -sections of non-trivial vector bundles over tori provide counterexamples to Kadison-Singer conjecture?

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THANK YOU

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