## Parseval frames of exponentially decaying Wannier functions

Peter Kuchment

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H-Hilbert space

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

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Plane waves $\Leftrightarrow \quad \delta$-functions relation: $e^{i x \cdot \xi_{0}} \stackrel{F T}{\Leftrightarrow} \delta\left(\xi-\xi_{0}\right)$

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$\mathbb{T}^{*}:=\mathbb{R}^{n} / 2 \pi \mathbb{Z}^{n} \approx\left\{e^{i k}=z=\left(z_{1}, \ldots, z_{n}\right)| | z_{j} \mid=1\right\} \subset \mathbb{C}^{n}$.

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Floquet-Bloch direct integral decomposition:

$$
L^{2}\left(\mathbb{R}^{n}\right)=\int_{B}^{\oplus} L^{2}(W) d k=\int_{\mathbb{T}^{*}}^{\oplus} L^{2}(W) d z
$$

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Bloch eigenfunction $-u_{z}(x)=z^{x} u(x)$ with periodic $u$. An analog of a plane wave (periodically modulated plane wave).
Let $S=I_{j}=\bigcup \lambda_{j}(k)$ - single band or composite band
$S=\bigcup_{i=j}^{j+m-1} I_{i}$.
We look for $m$ linearly independent nicely (continuously, analytically) dependent on $z \in \mathbb{T}^{*}$ Bloch functions $u_{j, z}$. Equivalent to the triviality of the spectral bundle $\Lambda_{S}$. Triviality generically does not hold (e.g., in the presence of magnetic fields, Thouless '84).

## Sufficient triviality conditions

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).

Time reversal symmetry occurs if the coefficients of the operator are real (e.o. maonetic fields are_excluded).

Peter Kuchment

## Wannier functions

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An example of WF in Barium Titanate

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So, what can one do?

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- The number $/$ is the smallest dimension of the fiber of a trivial vector bundle over $\mathbb{T}^{*}$ that contains an isomorphic copy of $\Lambda_{S}$. In particular, $I \leq 2^{n} m$.
- $I=m$ iff $\Lambda_{S}$ is trivial, in which case there exists an o.-n. basis of exponentially decaying Wannier functions in $H_{S}$.


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- Apply to $\left\{e_{j}\right\}$ an analytic projector $P(z)$ onto $\Lambda_{S}$ orthogonal over $\mathbb{T}^{*}$ to get the Wannier functions $\left\{w_{j}\right\}$.


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THANK YOU

