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Optimally localized Wannier functions for quasi one-dimensional nonperiodic insulators

G. Nenciu
Univ. of Bucharest & Inst. of Mathematics "Simion Stoilow" of the Romanian Academy, Romania

Joint work with H. D. Cornean and Alexandrina Nenciu

The problem (W)

$H = (\mathbf{P} - \mathbf{A})^2 + V$, $L^2(\mathbb{R}^d)$,
$\sigma_0 \subset \sigma(H)$-bounded & isolated,
P_0- corresponding spectral projector,
$\mathcal{K} = P_0 L^2(\mathbb{R}^d)$

Find an orth. basis in $\mathcal{K}$, $\{w_{\mathbf{g},j}\}_{\mathbf{g}\in\mathbf{\Gamma},1\leq j\leq m(\mathbf{g})\leq M<\infty}$:

- $\mathbf{\Gamma}$- discrete set in $L^2(\mathbb{R}^d)$, $\alpha > 0$,

- $\int |w_{\mathbf{g},j}(\mathbf{x}-\mathbf{g})|^2 e^{2\alpha|\mathbf{x}-\mathbf{g}|} d\mathbf{x} \leq C < \infty$

Additional requirements

- Symmetries:

time reversal: $[H, K] = 0$, $Kf(\mathbf{x}) = \overline{f(\mathbf{x})}$

$Kw_{\mathbf{g},j} = w_{\mathbf{g},j}$- real Wannier functions.

translations:
$\Gamma = \mathbb{Z}^d$, $V(\mathbf{x}+\mathbf{n}) = V(\mathbf{x})$, $T_{\mathbf{n}} f(\mathbf{x}) = f(\mathbf{x}-\mathbf{n})$,
$[H, T_{\mathbf{n}}] = 0$

$w_{\mathbf{g},j}(\mathbf{x}) = T_{\mathbf{g}} w_{\mathbf{0},j}(\mathbf{x}) = w_{\mathbf{0},j}(\mathbf{x}-\mathbf{g})$

• Optimal localization: which is the largest α i.e. which is the quickest exponential decay.

• The spreading of Wannier functions: maximal localization, very important for computational purposes (Marzari & Vanderbilt 97)

$\|f\| = 1$, $\langle(\Delta A)^2\rangle_f = \langle f, (A - \langle f, Af\rangle)^2 f\rangle$

$\langle(\Delta \mathbf{X})^2\rangle_{w_{\mathbf{g},j}}$ -as small as possible.

Non-triviality

For $\mathbf{A} \neq 0$ the problem **(W)** may not have a solution (Novikov 1981, Thouless 1984).

The main conjecture

For real $V(\mathbf{x})$ and $\mathbf{A} = 0$ the problem **(W)** has always a solution.

• The uniqueness problem.

Construction of Wannier functions: the periodic case (Wannier 1937)

Bloch functions: $H = \int_B^{\oplus} H_{\mathbf{k}} d\mathbf{k}$, $B = \{\mathbf{k} | k_j \in [-\pi, \pi)\}$ (Brillouin zone), $\psi_{n,\mathbf{k}}(\mathbf{x}) = u_{n,\mathbf{k}}(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}}$, $u_{n,\mathbf{k}}(\mathbf{x}) = u_{n,\mathbf{k}}(\mathbf{x}+\mathbf{g})$, $n = 1, 2, ...,$
$H_{\mathbf{k}} \psi_{n,\mathbf{k}} = E_n(\mathbf{k}) \psi_{n,\mathbf{k}}$

Suppose $E_{n_0}(\mathbf{k})$ is nondegenerate for $\mathbf{k} \in B$ (**simple** band):

$$w_{\mathbf{g}}^{n_0}(\mathbf{x}) = (2\pi)^{-d} \int_B \psi_{n_0,\mathbf{k}}(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{g}} d\mathbf{k}$$

The main point (Paley-Wiener theorem):

exponential decay of $w_{\mathbf{g}}^{n_0} \Longleftrightarrow \psi_{n_0,\mathbf{k}}$ analytic and periodic in $\mathbf{k}$

• The Bloch functions are defined by the eigenvalue problem up to a phase factor (non-uniqueness of Wannier functions):

$$\psi_{n_0,\mathbf{k}} = \chi(\mathbf{k})\widetilde{\psi}_{n_0,\mathbf{k}}.$$

• Wannier functions for **composite** band i.e. a group of intersecting bands $E_{n_l}(\mathbf{k})$, $l = 1, 2, ...N, N < \infty$ isolated for all $\mathbf{k}$ from the rest of the spectrum.

$$w_{\mathbf{g},j}(\mathbf{x}) = (2\pi)^{-d} \int_B \sum_l \chi_{j,l}(\mathbf{k})\widetilde{\psi}_{n_l,\mathbf{k}}(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{g}} d\mathbf{k}$$

Questions: i. Can one chose $\chi(\mathbf{k})$ as to make $\psi_{n_0,\mathbf{k}}$ analytic and periodic in $\mathbf{k}$?.

ii. What choice leads to optimally/maximally localized $w_{\mathbf{g}}^{n_0}$?

Answer: Yes for i. Partial answers for ii.

Non-periodic systems: the quasi one-dimensional case

• In (quasi) one dimension **(W)** has a solution with real, optimally and maximally localized (generalized) Wannier functions (i.e. the main conjecture holds true for one quasi dimensional systems).

• **Main open problem.** Prove the main conjecture in higher dimensions.

• How to define Wannier functions (one cannot use the Bloch functions!)

• The way out in the one dimensional case: Kivelson 82, Niu 91; mathematical substantiation: A. Nenciu & N 98.

The main results

$H = \mathbf{P}^2 + V$; $L^2(\mathbb{R}^3)$; $\mathbf{x} = (x_1, \mathbf{x}_\perp)$.

$I_V(R) = \sup_{x_1 \in \mathbb{R}; |\mathbf{x}_\perp| \geq R} \int_{|\mathbf{x}-\mathbf{y}| \leq 1} |V(\mathbf{y})|^2 d\mathbf{y}$
$I_V(R_0) < \infty$; $\lim_{R\to\infty} I_V(R) = 0$
$\sigma_0 \in (-\infty, 0)$, $-E_+ = \sup\{E : E \in \sigma_0\} < 0$
$\mathcal{K} = \mathrm{Ran}(P_0)$; $\quad P_0 = \frac{i}{2\pi} \int_\Gamma (H - z)^{-1} dz$

$g_a(\mathbf{x}) = \sqrt{(x_1 - a)^2 + 1}$; $g_\perp(\mathbf{x}) = \sqrt{|\mathbf{x}_\perp|^2 + 1}$.

Proposition 1. *There exist* $\alpha_\| > 0$, $\alpha_\perp > 0$, $M < \infty$ *such that:*

$$\sup_{a\in\mathbb{R}} \| e^{\alpha_\| g_a(\cdot)} P_0 e^{-\alpha_\| g_a(\cdot)} \| \leq M, \quad \text{and}$$

$$\| e^{\alpha_\perp g_\perp(\cdot)} P_0 e^{\alpha_\perp g_\perp(\cdot)} \| \leq M.$$

Theorem 2. *Let $X_{\|}$ be the operator of multiplication with x_1 in $L^2(\mathbb{R}^3)$ and consider in $\mathcal{K}$ the operator $\hat{X}_{\|} := P_0 X_{\|} P_0$ defined on $\mathcal{D}(\hat{X}_{\|}) = \mathcal{D}(X_{\|}) \cap \mathcal{K}$. Then*

i. *$\hat{X}_{\|}$ is self-adjoint on $\mathcal{D}(\hat{X}_{\|})$;*
ii. *$\hat{X}_{\|}$ has purely discrete spectrum;*
iii. *Let $g \in G := \sigma(\hat{X}_{\|})$ be an eigenvalue, m_g its multiplicity, and $\{W_{g,j}\}_{1 \leq j \leq m_g}$ an orthonormal basis in the eigenspace of $\hat{X}$ corresponding to g. Then for all $\beta \in [0,1]$, there exists $M_1 < \infty$ independent of g, j and β such that:*

$$\int_{\mathbb{R}^3} e^{2(1-\beta)\alpha_{\|}|x_1-g|} e^{2\beta\alpha_{\perp}|\mathbf{x}_{\perp}|} |W_{g,j}(\mathbf{x})|^2 d\mathbf{x} \leq M_1,$$

where $\alpha_{\|}$ and $\alpha_{\perp}$ are the same exponents as for P_0;
iv. *Let $a \in \mathbb{R}$ and $L \geq 1$. Denote by $N(a,L)$ the total multiplicity of the spectrum of $\hat{X}_{\|}$ contained in $[a-L, a+L]$. Then there exists $M_2 < \infty$ such that*

$$N(a,L) \leq M_2 \cdot L.$$

Further properties

- **Optimal exponential decay**

Proposition 3. *Assume that for all* $\alpha < \alpha_0$ *we are given an* a priori *bound*

$$\sup_{a\in\mathbb{R}} \| e^{\alpha g_a(\cdot)} P_0 e^{-\alpha g_a(\cdot)} \| \leq M, \quad \text{and}$$

Then for all $\alpha < \alpha_0$ *there exists* $M_1(\alpha)$*, independent of* g *and* j *such that*

$$\int_{\mathbb{R}^3} e^{2\alpha|x_1-g|} |W_{g,j}(\mathbf{x})|^2 d\mathbf{x} \leq M_1(\alpha).$$

- **Uniqueness**: Up to uninteresting phases.

- **Reality**: One can choose $W_{g,j}(\mathbf{x}) = \overline{W_{g,j}(\mathbf{x})}$

• **Screw symmetry**:

$\mathbf{x}_\perp = (r, \theta), \quad r \geq 0,$

$\theta \in [0, 2\pi)$; $V(x_1, r, \theta) = V(x_1 + 1, r, \theta + \theta_0)$

$(T_n^{\theta_0} f)(x_1, r, \theta) := f(x_1 - n, r, \theta - n\theta_0).$

Proposition 4. *The spectrum of $\hat{X}_\parallel$ consists of a union of p ladders:*

$G = \cup_{j=1}^{p} G_j, \quad G_j = \{g : \ g = g_j + n, \ n \in \mathbb{Z}\}, \quad j \in \{1, 2$

and an orthonormal basis in $\mathcal{K}$ can be chosen as:

$$W_{n,g_j,\alpha_j} := W_{g_j+n,\alpha_j} := T_n^{\theta_0} W_{g_j,\alpha_j},$$
$$n \in \mathbb{Z}, \ j \in \{1, 2, ..., p\}, \ \alpha_j \in \{1, 2, ..., m_{g_j}\}.$$

Main result: the periodic case

Abstract problem (C) (des Cloizeaux 64, N 83,91)

$\mathcal{H}$, $\mathcal{I}_a^d = \{\mathbf{z} \in \mathbb{C}^d || \Im \mathbf{z}| < a\}$, $Q(\mathbf{z})$- projection valued function in $\mathcal{I}_a^d$:

$Q(\mathbf{z}) = Q^*(\overline{\mathbf{z}})$, $Q(\mathbf{z}) = Q(\mathbf{z} + \mathbf{p})$ for $\mathbf{p} \in \mathbb{Z}^d$.

Find $A(z) : \mathcal{H} \to \mathcal{H}$ analytic in $\mathcal{I}_a^d$ satisfying $A(\mathbf{0}) = 1$, $A^{-1}(\mathbf{z}) = A^*(\overline{\mathbf{z}})$, $Q(\mathbf{z}) = A(\mathbf{z})Q(\mathbf{0})A^{-1}(\mathbf{z})$, $A(\mathbf{z})Q(\mathbf{0}) = A(\mathbf{z} + \mathbf{p})Q(\mathbf{0})$

• If problem **(C)** has a solution then for $\{f_m\}_1^{\dim Q_0}$ basis in $Q(\mathbf{0})\mathcal{H}$, $\{A(z)f_m\}_1^{\dim Q_0}$ is an **analytic and periodic** basis in $Q(\mathbf{z})\mathcal{H}$.

• The existence of a solution of **(C)** $\Longleftrightarrow$ triviality of the fiber bundle $Q(\mathbf{z})$ (N 91).

Theorem 5. *(Kohn 58, des Cloizeaux 64; N 83,91; Helffer & Sjostrand 89; Panati 06)*
*i. In the cases below the problem **(C)** has solutions. In addition a solution leading to real, translation invariant, optimally localized Wannier functions has been constructed.*
a. $d = 1$
b. $\sup_{\mathbf{z}\in\mathcal{I}_a^d} \|Q(\mathbf{z}) - Q(\mathbf{0})\| < 1$
c. $\dim Q(\mathbf{0}) = 1$ *and there exists an antiunitary involution* $\theta : \mathcal{H} \to \mathcal{H}$ *such that* $\theta Q(\mathbf{z})\theta = Q(-\mathbf{z})$

ii. For $d = 2, 3$, $\dim Q(\mathbf{0}) < \infty$ *and there exists an antiunitary involution* $\theta : \mathcal{H} \to \mathcal{H}$ *such that* $\theta Q(\mathbf{z})\theta = Q(-\mathbf{z})$ *the problem **(C)** has solutions.*

Open problems in the periodic case

• Generalize Theorem 1ii to arbitrary dimensions (if true!).

• Find a constructive proof of Theorem 1ii.

• Construct maximally localized Wannier functions. Are maximally localized functions among the optimally localized ones. For details and some partial results: Marzari & Vanderbild 97.

• Not discussed: magnetic field case (see Nenciu 1991).

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