Maximally Localized Wannier Functions

Andreas Klöckner

Outline

Photonic Crystals
- Fabrication

Eigenproblems with Spatially Periodic Coefficients
- The Floquet Transform

Wannier Functions
- Minimizing the Spread

Outlook and Origins
Outline

1. Photonic Crystals
   - Fabrication

2. Eigenproblems with Spatially Periodic Coefficients
   - The Floquet Transform

3. Wannier Functions
   - Minimizing the Spread

4. Outlook and Origins
Photonic Crystals are

- Periodic Optical Nanomaterials
What are Photonic Crystals?

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- Periodic Optical Nanomaterials
- That can be used to emulate the behavior of electrons in semiconductors—using light
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Photonic Crystals are

- Periodic Optical Nanomaterials
- That can be used to emulate the behavior of electrons in semiconductors—using light
- Typical PCs have a *Band gap*
What is a Band Gap?

A *band gap* is a range of energies for which photons cannot propagate in a material.
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→ an insulator for light
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→ an *insulator* for light

Most materials *absorb*, they don’t insulate.
A band gap is a range of energies for which photons cannot propagate in a material.
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Most materials absorb, they don’t insulate. → energy loss
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Roughly: A *perfect, nanoscale, omnidirectional mirror.*

---

**Notes:**

- Photonic Crystals
  - Fabrication

- Eigenproblems with Spatially Periodic Coefficients
  - The Floquet Transform

- Wannier Functions
  - Minimizing the Spread

- Outlook and Origins

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What is a Band Gap?

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→ an insulator for light

Most materials absorb, they don’t insulate. → energy loss

PBG materials insulate → no energy loss

Roughly: A perfect, nanoscale, omnidirectional mirror. (Don’t take the “mirror” part too literally.)
Mother Nature: “Been there, done that.”

Photonic Crystals occur naturally.
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Photonic Crystals occur naturally. Ever seen an opal?
Mother Nature: “Been there, done that.”

Photonic Crystals occur naturally. Ever seen an opal?

(from http://geomuseum.tu-clausthal.de/)
If PCs are the soup, then defects are the salt

- Semiconductor devices (and thereby all of modern electronics) come from defects in regular crystals.
If PCs are the soup, then defects are the salt

- Semiconductor devices (and thereby all of modern electronics) come from *defects* in regular crystals.
- *Crystals* are only the substrate.
Semiconductor devices (and thereby all of modern electronics) come from *defects* in regular crystals.

*Crystals* are only the substrate.

*Defects* are what we really want.
Example Device: A waveguide

Want to transmit light around a bend with no loss?
Want to transmit light around a bend with no loss?

(from http://ab-initio.mit.edu/photons/bends/)
This research seeks to enable \textit{large-scale} simulation of such structures.
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This means finding the propagating modes.
Bases of Wannier functions promise to be much better suited to this than standard polynomial or plane-wave bases.
Simulation is especially necessary because fabrication is difficult.
Materials built from FCC lattices (in 3D) often have band gaps.
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Materials built from FCC lattices (in 3D) often have band gaps. → Let’s build an FCC lattice!

A few ways of making PCs

Maybe like this:
A few ways of making PCs

Maybe like this:

Stack some latex and silica spheres...
A few ways of making PCs

Maybe like this:

Stack some latex and silica spheres...

...dissolve half of them...

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...bake that... make a Silicon inverse of it...
A few ways of making PCs

Maybe like this:

Stack some latex and silica spheres...  
...dissolve half of them...

...bake that... make a Silicon inverse of it... Ta-daa!

(from http://ab-initio.mit.edu/photons/tutorial/, as are the next few examples)
A few ways of making PCs

That’s too hard.
That’s too hard. Maybe we should think about different structures:
A few ways of making PCs

That’s too hard. Maybe we should think about different structures:

...called the “woodpile structure”.
A few ways of making PCs

But can we mass-produce those?
A few ways of making PCs

But can we mass-produce those? Using Lithography, maybe...
Maximally Localized Wannier Functions

Outlook and Origins

A few ways of making PCs

But can we mass-produce those? Using Lithography, maybe...
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Oh wait, what about defects?
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Obviously, there’s a lot to do for the experimentalists...
A few ways of making PCs

Oh wait, what about defects?
Obviously, there’s a lot to do for the experimentalists. . .
Let’s not disturb them and get on with our work.
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Maximally Localized Wannier Functions
Maxwell’s Equations

The time-harmonic form of Maxwell’s Equations (no charge carriers, $\mu_r \equiv 1$, linear, isotropic materials) reads:

\[
\begin{align*}
-\nabla \times E(r) &= \mu_0 i\omega H(r) \\
\nabla \times H(r) &= \varepsilon_0 \varepsilon(r) i\omega E(r) \\
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(note $\varepsilon_r = \varepsilon$ for simplicity) But actually...
...we will only treat the simpler 2D Transverse Magnetic form:
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But on what domain?
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We approximate our domain as infinite, and given a lattice $L := \{\sum_i n_i \mathbf{R}_i\}$, the permittivity $\varepsilon$ is assumed $L$-periodic. (We’ll deal with defects later.) We would like to compute only on one primitive unit cell. Right BCs on the unit cell $P$?
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Right BCs on the unit cell $P$? Periodic BCs maybe?
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$$\psi(r + R) = \psi(r)$$
Why Periodic BCs are not right

Suppose $\varepsilon \equiv 1$. Then plane waves $e^{ik \cdot r}$ are eigenmodes of the Laplacian.
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But periodic BCs forbid them.
Why Periodic BCs are not right

Suppose $\varepsilon \equiv 1$. Then plane waves $e^{i\mathbf{k}\cdot\mathbf{r}}$ are eigenmodes of the Laplacian.
But periodic BCs forbid them. Not good.
Which BCs are right?

Need to admit at least plane waves.
Which BCs are right?

Need to admit at least plane waves. To admit a plane wave with wave vector $\mathbf{k}$,

$$\psi(r + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi(r)$$

would be suitable.
Here comes a (seemingly) unmotivated definition:
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The reciprocal lattice $\hat{L} := \{ \sum_i n_i K_i \}$, where

$$K_i \cdot R_j = 2\pi \delta_{ij}.$$
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Existence, uniqueness?
The Reciprocal Lattice

Here comes a (seemingly) unmotivated definition:
The reciprocal lattice $\hat{L} := \{\sum_i n_i K_i\}$, where

$$K_i \cdot R_j = 2\pi \delta_{ij}.$$ 

Existence, uniqueness? $\rightarrow$ $d^2$ equations, $d^2$ unknowns, $R_j$ are a basis.
Meaning of the Reciprocal Lattice

Let $\mathbf{K} \in \hat{L}$. Then

$$\psi(\mathbf{r} + \mathbf{R}) = e^{i(\mathbf{k} + \mathbf{K}) \cdot \mathbf{R}} \psi(\mathbf{r})$$
Meaning of the Reciprocal Lattice

Let $K \in \hat{L}$. Then

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= e^{i k \cdot R} e^{i \sum_j n_j K_j \cdot \sum_l m_l R_l} \psi(r)
$$
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Meaning of the Reciprocal Lattice

Let \( \mathbf{K} \in \hat{\mathcal{L}} \). Then

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\psi(\mathbf{r} + \mathbf{R}) = e^{i(k + \mathbf{K} \cdot \mathbf{R})} \psi(\mathbf{r})
\]

\[
= e^{i\mathbf{k} \cdot \mathbf{R}} e^{i\mathbf{K} \cdot \mathbf{R}} \psi(\mathbf{r})
\]

\[
= e^{i\mathbf{k} \cdot \mathbf{R}} e^{i(\sum_j n_j \mathbf{K}_j \cdot (\sum_l m_l \mathbf{R}_l))} \psi(\mathbf{r})
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The Brillouin Zone

Our proposed BCs

$$\psi(r + R) = e^{ik \cdot R} \psi(r),$$

are invariant under addition of a reciprocal lattice vector $K$ to the wave vector $k$. 
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are invariant under addition of a reciprocal lattice vector $K$ to the wave vector $k$. So $k$ can remain restricted to a primitive unit cell of the reciprocal lattice.
Our proposed BCs

\[ \psi(r + R) = e^{i k \cdot R} \psi(r), \]

are invariant under addition of a reciprocal lattice vector \( K \) to the wave vector \( k \).

So \( k \) can remain restricted to a primitive unit cell of the reciprocal lattice.

Give this unit cell a special name: The Brillouin Zone \( B \).
But are these BCs right?
Right Track?

But are these BCs right?
There is an answer in the fourth volume of Reed and Simon, but it’s a bit intimidating at first.
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The Floquet Transform

Theorem (Plancherel’s Theorem for the Floquet Transform)

Define a transform $\mathcal{U}$ on $S(\mathbb{R}^d)$ by

$$(\mathcal{U}f)_k(r) := \sum_{R \in L} e^{i k \cdot R} f(r - R).$$

Then $\mathcal{U}$’s domain may be extended to all of $L^2_\varepsilon(\mathbb{R}^d)$, and it becomes a unitary operator

$$\mathcal{U} : L^2_\varepsilon(\mathbb{R}^d) \to L^2(B \times L^2_\varepsilon(P)),$$

where $L^2(B \times L^2_\varepsilon(P))$ has the inner product

$$\langle \varphi, \psi \rangle_{L^2(B \times L^2_\varepsilon(P))} = \frac{1}{\lambda(B)} \int_B \langle \varphi_k, \psi_k \rangle_P dk.$$
Our BCs follow from the Floquet Transform:

\[(\mathcal{U}f)_k(r + R') = \sum_{R \in L} e^{ik \cdot R} f(r + R' - R)\]
Floquet and the BCs

Our BCs follow from the Floquet Transform:

\[(Uf)_k(r + R') = \sum_{R \in L} e^{i k \cdot R} f(r + R' - R)\]

(let \(R'' := R - R'\))

\[= \sum_{R'' \in L} e^{i k \cdot (R'' + R')} f(r - R'')\]
Our BCs follow from the Floquet Transform:

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\]

\[
= e^{ik \cdot R'} (\mathcal{U}f)_k(r)
\]
Inverse of the Floquet Transform

Theorem (Inverse of $\mathcal{U}$)

$$(\mathcal{U}^{-1}f)(r) = \frac{1}{\lambda(B)} \int_B f_k(r) \, dk.$$
Inverse of the Floquet Transform

Theorem (Inverse of $\mathcal{U}$)

$$(\mathcal{U}^{-1}f)(\mathbf{r}) = \frac{1}{\lambda(B)} \int_B f_k(\mathbf{r}) d\mathbf{k}.$$ 

In plain words: To invert the Floquet transform, just average over all $\mathbf{k}$ in the Brillouin zone.
The transformed Differential Operator

Theorem (Floquet Transform of the Differential Operator)

\[ \mathcal{U} \left( -\frac{\nabla^2}{\varepsilon} \right) \mathcal{U}^{-1} = \frac{1}{\lambda(B)} \int_B^{+} H(k) dk, \]

with \( H(k) := -\nabla^2/\varepsilon \) on \( L_\varepsilon^2(P) \) under the boundary conditions

\[ \varphi(r + R) = e^{ik \cdot R} \varphi(r) \]

\[ \nabla \varphi(r + R) \cdot n = e^{ik \cdot R} \nabla \varphi(r) \cdot n \]
Consequences

- The BCs allow an intuitive “tiling” of all space with the solution on a unit cell.
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- Each $H(k)$ has a complete set of eigenfunctions (“Bloch modes”) $\psi_{m,k}$.
- The Bloch modes are $k$- and $m$-orthogonal:

$$\langle \psi_{n,k}, \psi_{m,k'} \rangle_P = \lambda(B)\delta(k - k')\delta_{n,m}.$$
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- One can prove that—away from degeneracies—the eigenvalues and eigenmodes have a $C^1$ dependency on $k$, so the eigenvalues form “sheets” called bands.
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- One can prove that–away from degeneracies–the eigenvalues and eigenmodes have a $C^1$ dependency on $k$, so the eigenvalues form “sheets” called bands.
- Plotting the eigenvalues $\omega$ over the Brillouin Zone gives the Dispersion Relation.
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An Example Dispersion Relation
More Consequences

- $\mathcal{U}$ unitary $\implies$ a Parseval-like equality
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- $\mathcal{U}$ transforms $-\nabla^2/\varepsilon$ into a direct integral of identical differential operators with varying BCs.
More Consequences

- $\mathcal{U}$ unitary $\Rightarrow$ a Parseval-like equality
- $\mathcal{U}$ transforms $-\nabla^2/\varepsilon$ into a direct integral of \textit{identical} differential operators with \textit{varying} BCs.
- One can also achieve a transform into \textit{varying} operators with \textit{identical} (periodic) BCs by considering

$$u_{n,k}(r) := (\mathcal{P}\psi_{n,k})(r) := e^{-ik \cdot r}\psi_k(r).$$

and $\mathcal{P} H(k) \mathcal{P}^{-1}$. 


More Consequences

- $\mathcal{U}$ unitary $\implies$ a Parseval-like equality
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and $\mathcal{P}H(k)\mathcal{P}^{-1}$.
- The construction is really analogous to the Fourier transform.
Determining the Bloch modes computationally is (relatively) easy now:

- Sample the Brillouin Zone on a regular grid of $k$-points.
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Computing the Bloch Modes

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- For each $k$, solve the eigenvalue problem $H(k)\psi_k = \omega^2/c^2 \psi_k$ using second-order FEM. (BCs require care.)
- Obtain the $N$ Bloch modes with the smallest eigenvalues, where $N \approx 10 \ldots 20$. (The spectrum of $H(k)$ is discrete and unbounded above.)
Maximally Localized Wannier Functions

Andreas Klöckner

Outline

1. Photonic Crystals
   • Fabrication

2. Eigenproblems with Spatially Periodic Coefficients
   • The Floquet Transform

3. Wannier Functions
   • Minimizing the Spread

4. Outlook and Origins
So, what happens if we apply the inverse Floquet transform to the Bloch modes?
So, what happens if we apply the inverse Floquet transform to the Bloch modes? Well, we get *Wannier functions*. 
Wannier Functions

Definition (Wannier Function)

\[ w_{n,0}(r) := U^{-1}(\psi_n) \in L^2_\varepsilon(\mathbb{R}^d). \]

More generally, the \( n \)th Wannier function \( w_{n,R} \) centered at \( R \) is defined as

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i.e.

\[ w_{n,R}(r) = \frac{1}{\lambda(B)} \int_B e^{-i k \cdot R} \psi_{n,k}(r) dk. \]
So, what do they look like?
Maximally Localized Wannier Functions

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Pretty Picture

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Pretty Picture

So, what do they look like?

Yikes!
Pretty Ambiguous

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To resolve the ambiguity, we demand that our Wannier functions be \textit{maximally localized}, i.e. have minimal second moment

\[ \Omega_n := \langle r^2 w_n, 0, w_n, 0 \rangle_{\mathbb{R}^d} - | \langle rw_n, 0, w_n, 0 \rangle_{\mathbb{R}^d} |^2. \]
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- for each sample point $\mathbf{k}$ in the Brillouin zone
- for each band number $n$

So the problem gets more difficult as we refine the Brillouin Zone Discretization.
Minimizing the Spread: Isolated Bands

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To localize the WF for an isolated band,
Minimizing the Spread: Isolated Bands

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Experimentation shows:
To localize the WF for an isolated band, fixing

\[ \arg \psi_{n,k}(\mathbf{r}) = \text{constant over } \mathbf{k}! \]

for a given \( \mathbf{r} \) is enough. (Proof?)

Unfortunately, this does not work for entangled bands.
Minimizing the Spread: Entangled Bands

To deal with degeneracies, we make our problem more complicated:

\[ \psi_{\text{gen}} = \sum_{m=1}^{J} U(k) \psi_m(k) \]

This introduces "generalized" Bloch modes with "mixing matrix" \( U(k) \).

To maintain orthogonality, we demand that \( U(k) \) be unitary.
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So, our problem becomes to find a set of $U^{(k)}$ such that

$$\Omega := \sum_n \Omega_n \rightarrow \min!$$
Summary

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But how do we even compute the spread? We can’t evaluate an integration over all of $\mathbb{R}^d$!
The Spread in $k$-space

Theorem

Let $\psi_{n,k}$ be continuously differentiable in $k$. Then

$$\langle rw_{n,0}, w_{m,R} \rangle_{\mathbb{R}^d} = \frac{1}{\lambda(B)} \int_{B} e^{i k \cdot R} \langle i \nabla_k u_{n,k}, u_{m,k} \rangle_P \, dk$$

and

$$\langle r^2 w_{n,0}, w_{n,0} \rangle_{\mathbb{R}^d} = \frac{1}{\lambda(B)} \int_{B} \langle i \nabla_k u_{n,k}, i \nabla_k u_{n,k} \rangle_P \, dk.$$
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So if we approximate the $k$-gradients (say by FD), we can obtain a computable expression for the spread.
• Compute the spread $\Omega$. 

The Plan

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Outlook and Origins
The Plan

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Maximally Localized Wannier Functions

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The Plan

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- Compute the maximally localized Wannier Functions, using the optimal $U$. 

Compute a grid of MLWFs (centered in each unit cell) as a Galerkin basis to attack large-scale simulation problems, with defects.
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Use a grid of MLWFs (centered in each unit cell) as a Galerkin basis to attack large-scale simulation problems, with defects.
So, does it work?
So, does it work?
Yes.
So, does it work?
Yes. But...
So, does it work?
Yes. But... There are cases where it does not work as beautifully.
Getting stuck in a local minimum
Issues with The Plan

- Getting stuck in a local minimum
- What is a good starting guess?
Issues with The Plan

- Getting stuck in a local minimum
- What is a good starting guess?
- There are several (at least two) valid ways of finding $d\Omega/dU$. More specifically: What inner product do we use on the gradient space of $U$?
The Promise of MLWFs

Several things make WFs ideally suited as a computational basis:

- Wannier functions are $n$- and $R$-orthogonal, i.e.

$$\langle W_{n,R}, W_{m,R'} \rangle_{\mathbb{R}^d} = \delta_{m,n} \delta_{R,R'}.$$
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- They are complete in $L^2_{\varepsilon}$.
- (Conjecture) MLWFs are real-valued.
- (Experimental evidence) Expansions of propagation modes in MLWFs converge very very fast.
This is the method of Marzari and Vanderbilt (1997), which they invented and used for computational chemistry.
This is the method of Marzari and Vanderbilt (1997), which they invented and used for computational chemistry. Busch et al. re-used M-V’s method for photonic crystals.
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Hopes and unanswered questions

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- What exactly goes on in 3D?
- DG could help greatly with the discretization of the Floquet BCs.
How I ended up doing this research

- Prof. Dr. Willy Dörfler (Karlsruhe)
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- Prof. Dr. Willy Dörfler (Karlsruhe)
- Prof. Dr. Kurt Busch (Karlsruhe/UCF)
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- Prof. Dr. Willy Dörfler (Karlsruhe)
- Prof. Dr. Kurt Busch (Karlsruhe/UCF)
- Dipl.-Phys. Matthias Schillinger (Karlsruhe/UCF)
Maximally Localized Wannier Functions

Questions?