Maximally Localized Wannier Functions

Andreas Klöckner

Valentine's Day 2007

Outline

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What are Photonic Crystals?

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- Typical PCs have a *Band gap*

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Roughly: *A perfect, nanoscale, omnidirectional mirror.*
(Don't take the "mirror" part too literally.)

Mother Nature: "Been there, done that."

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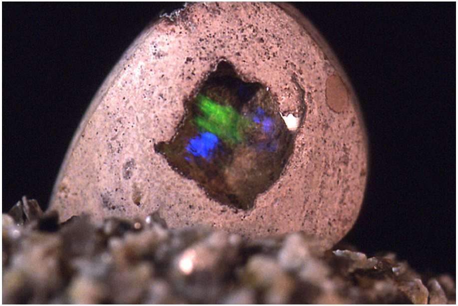

(from `http://geomuseum.tu-clausthal.de/`)

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- 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?

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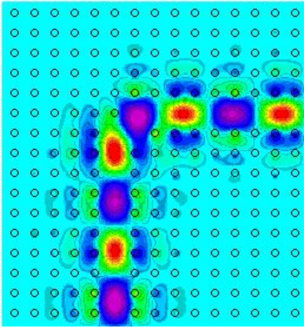

(from http://ab-initio.mit.edu/photons/bends/)

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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.

A few ways of making PCs

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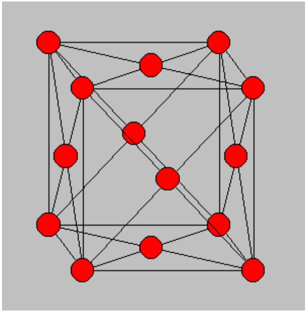


(from http://ece-www.colorado.edu/~bart/book/bravais.htm)

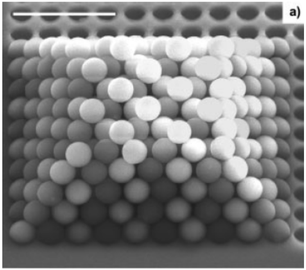
A few ways of making PCs

Maybe like this:

A few ways of making PCs

Maybe like this:

Stack some latex and silica spheres. . .



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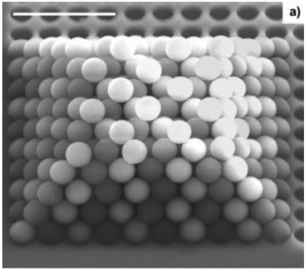
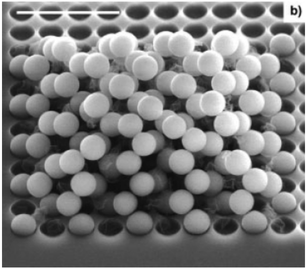


. . . dissolve half of them. . .



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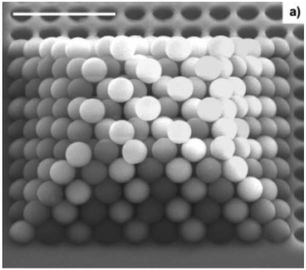

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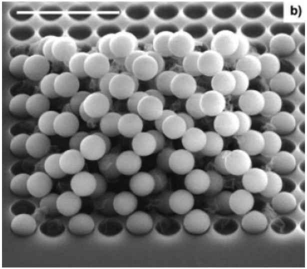

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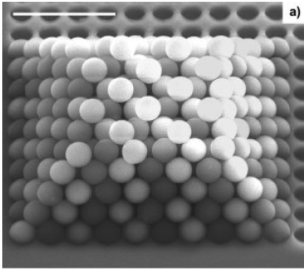

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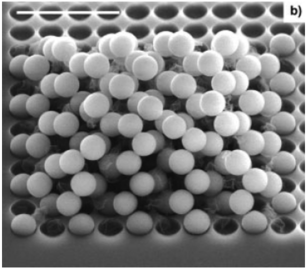

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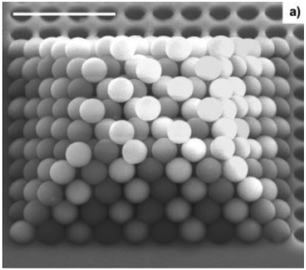

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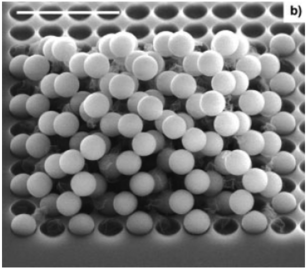

. . . bake that. . . make a Silicon inverse of it. . . Ta-daa!

(from `http://ab-initio.mit.edu/photons/tutorial/`, as are the next few examples)

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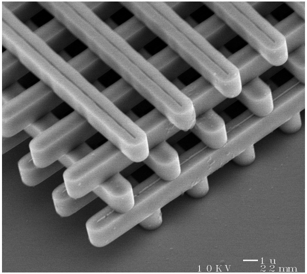

. . . called the "woodpile structure".

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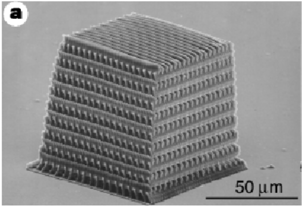

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Obviously, there's a lot to do for the experimentalists. . .
Let's not disturb them and get on with *our* work.

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But periodic BCs forbid them. Not good.

Which BCs are right?

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To admit a plane wave with wave vector $\mathbf{k}$,

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

would be suitable.

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Existence, uniqueness? $\to$ d^2 equations, d^2 unknowns, $\mathbf{R}_j$ are a basis.

Meaning of the Reciprocal Lattice

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The Brillouin Zone

Our proposed BCs

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are invariant under addition of a reciprocal lattice vector $\mathbf{K}$ to the wave vector $\mathbf{k}$.

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So $\mathbf{k}$ can remain restricted to a primitive unit cell of the reciprocal lattice.
Give this unit cell a special name: The *Brillouin Zone B*.

Right Track?

But are these BCs right?

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There is an answer in the fourth volume of Reed and Simon, but it's a bit intimidating at first.

The Floquet Transform

Theorem (Plancherel's Theorem for the Floquet Transform)

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

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

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

$$\langle \varphi, \psi \rangle_{L^2(B\times L^2_\varepsilon(P))} = \frac{1}{\lambda(B)} \int_B \langle \varphi_{\mathbf{k}}, \psi_{\mathbf{k}} \rangle_P \, d\mathbf{k}.$$

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Our BCs follow from the Floquet Transform:

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$$(\text{let } \mathbf{R}'' := \mathbf{R}-\mathbf{R}') \quad = \sum_{\mathbf{R}''\in L} e^{i\mathbf{k}\cdot(\mathbf{R}''+\mathbf{R}')} f(\mathbf{r}-\mathbf{R}'')$$

Floquet and the BCs

Our BCs follow from the Floquet Transform:

$$
\begin{aligned}
(\mathcal{U}f)_{\mathbf{k}}(\mathbf{r}+\mathbf{R}') &= \sum_{\mathbf{R}\in L} e^{i\mathbf{k}\cdot\mathbf{R}} f(\mathbf{r}+\mathbf{R}'-\mathbf{R}) \\
(\text{let } \mathbf{R}'' := \mathbf{R}-\mathbf{R}') \quad &= \sum_{\mathbf{R}''\in L} e^{i\mathbf{k}\cdot(\mathbf{R}''+\mathbf{R}')} f(\mathbf{r}-\mathbf{R}'') \\
&= e^{i\mathbf{k}\cdot\mathbf{R}'} (\mathcal{U}f)_{k}(\mathbf{r})
\end{aligned}
$$

Inverse of the Floquet Transform

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

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

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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)

$$\mathcal{U}\left(-\frac{\nabla^2}{\varepsilon}\right)\mathcal{U}^{-1} = \frac{1}{\lambda(B)}\int_B^{\oplus} H(\mathbf{k})d\mathbf{k},$$

with $H(\mathbf{k}) := -\nabla^2/\varepsilon$ *on* $L^2_\varepsilon(P)$ *under the boundary conditions*

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

$$\boldsymbol{\nabla}\varphi(\mathbf{r}+\mathbf{R})\cdot\mathbf{n} = e^{i\mathbf{k}\cdot\mathbf{R}}\boldsymbol{\nabla}\varphi(\mathbf{r})\cdot\mathbf{n}$$

Consequences

- The BCs allow an intuitive "tiling" of all space with the solution on a unit cell.

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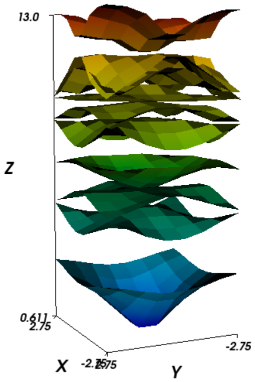
- One can prove that–away from degeneracies–the eigenvalues and eigenmodes have a C^1 dependency on $\mathbf{k}$, so the eigenvalues form "sheets" called *bands*.
- Plotting the eigenvalues ω over the Brillouin Zone gives the *Dispersion Relation*.

An Example Dispersion Relation



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More Consequences

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

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

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

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- The construction is really analogous to the Fourier transform.

Computing the Bloch Modes

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- Obtain the N Bloch modes with the smallest eigenvalues, where $N \approx 10 \dots 20$. (The spectrum of $H(\mathbf{k})$ is discrete and unbounded above.)

Outline

A Harmless Question

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Well, we get *Wannier functions*.

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Definition (Wannier Function)

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More generally, the nth Wannier function $w_{n,\mathbf{R}}$ centered at $\mathbf{R}$ is defined as

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i.e.

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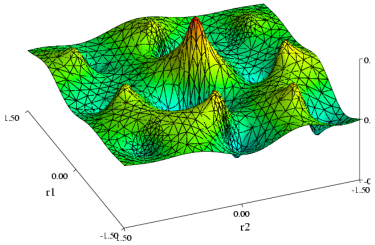

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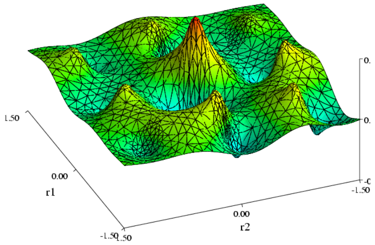

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Unfortunately, the choice of that constant matters when computing Wannier Functions.
To resolve the ambiguity, we demand that our Wannier functions be *maximally localized*, i.e. have minimal second moment

$$\Omega_n := \left\langle r^2 w_{n,\mathbf{0}}, w_{n,\mathbf{0}} \right\rangle_{\mathbb{R}^d} - \left| \left\langle \mathbf{r} w_{n,\mathbf{0}}, w_{n,\mathbf{0}} \right\rangle_{\mathbb{R}^d} \right|^2.$$

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So the problem gets more difficult as we refine the Brillouin Zone Discretization.

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Unfortunately, this does not work for entangled bands.

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$\rightarrow$ mixtures of existing Bloch modes with "mixing matrix" U.

To maintain orthogonality, we demand that $U^{(\mathbf{k})}$ be unitary.

Summary

So, our problem becomes to find a set of $U^{(\mathbf{k})}$ such that

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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 $\mathbf{k}$-space

Theorem

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

$$\langle \mathbf{r} w_{n,\mathbf{0}}, w_{m,\mathbf{R}} \rangle_{\mathbb{R}^d} = \frac{1}{\lambda(B)} \int_B e^{i\mathbf{k}\cdot\mathbf{R}} \langle i\boldsymbol{\nabla}_{\mathbf{k}} u_{n,\mathbf{k}}, u_{m,\mathbf{k}} \rangle_P \, d\mathbf{k}$$

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So if we approximate the $\mathbf{k}$-gradients (say by FD), we can obtain a computable expression for the spread.

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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. . .

So, does it work?

So...

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Yes.

So. . .

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So, does it work?
Yes. But. . . There are cases where it does not work as beautifully.

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- 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.

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- (Conjecture) MLWFs are real-valued.
- (Experimental evidence) Expansions of propagation modes in MLWFs converge very fast.

References

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Busch et al. re-used M-V's method for photonic crystals.

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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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- Dipl.-Phys. Matthias Schillinger (Karlsruhe/UCF)

Questions?

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