Simulating Photonic Crystals

Andreas Klöckner

DAM Pizza Seminar–March 16, 2007

Outline

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What are Photonic Crystals?

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- Periodic Optical Nanomaterials

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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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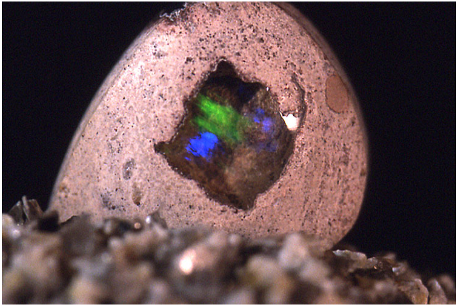

(from `http://geomuseum.tu-clausthal.de/`)

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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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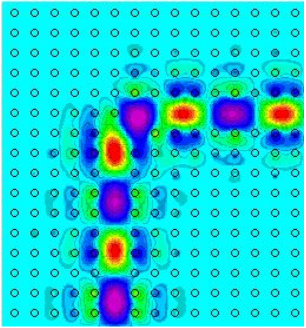

(from `http://ab-initio.mit.edu/photons/bends/`)

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This research seeks to enable *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.

A few ways of making PCs

Materials built from FCC lattices (in 3D) often have band gaps.

A few ways of making PCs

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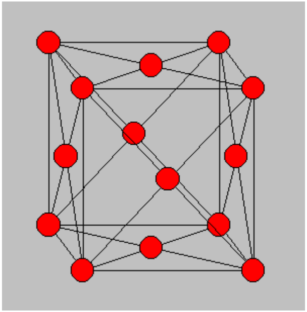


(from `http://ece-www.colorado.edu/~bart/book/bravais.htm`)

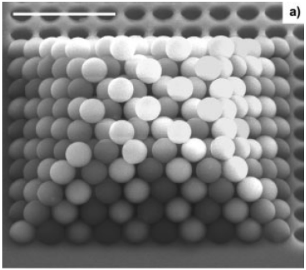
A few ways of making PCs

Maybe like this:

A few ways of making PCs

Maybe like this:

Stack some latex and silica spheres. . .



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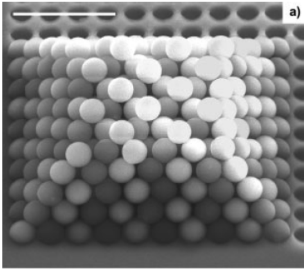
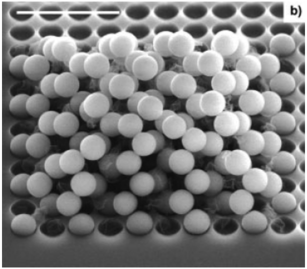


. . . dissolve half of them. . .



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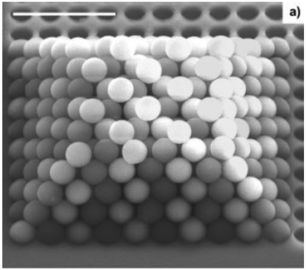

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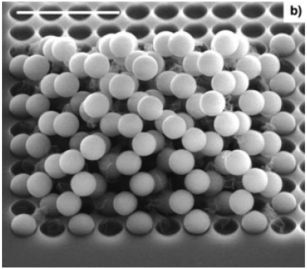

. . . bake that. . .

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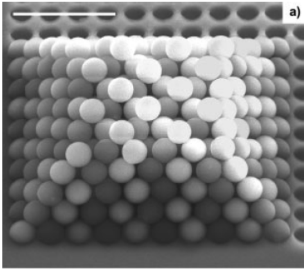

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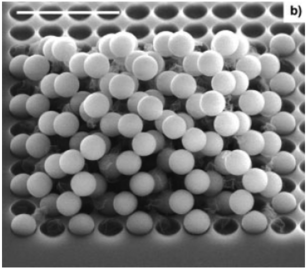

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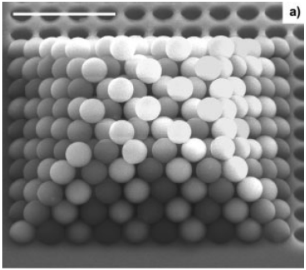

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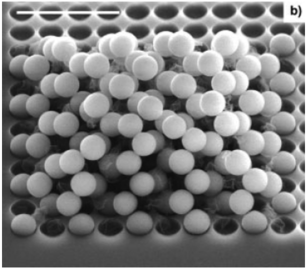

. . . bake that. . . make a Silicon inverse of it. . . Ta-daa!

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

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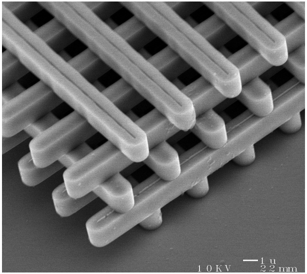

. . . called the "woodpile structure".

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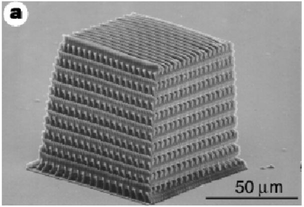

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Oh wait, what about defects?
Obviously, there's a lot to do for the experimentalists. . .
Let's not disturb them and get on with *our* work.

Outline

1. Photonic Crystals
   - Fabrication
2. Eigenproblems with Spatially Periodic Coefficients
   - The Floquet Transform
3. Wannier Functions
   - Minimizing the Spread
4. Concluding Remarks

Maxwell's Equations

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$$\psi(\mathbf{r}+\mathbf{R}) = \psi(\mathbf{r})$$

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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 **k**,

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

would be suitable.

The Reciprocal Lattice

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

Meaning of the Reciprocal Lattice

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

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

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The Brillouin Zone

Our proposed BCs

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

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*

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

Floquet and the BCs

Our BCs follow from the Floquet Transform:

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

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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}'')
\end{aligned}
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Floquet and the BCs

Our BCs follow from the Floquet Transform:

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

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*

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

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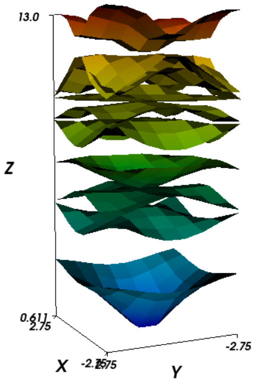
- One can prove that–away from degeneracies–the eigenvalues and eigenmodes have a C^1 dependency on $\mathbf{k}$, so the eigenvalues form “sheets” called *bands*.
- Plotting the eigenvalues ω over the Brillouin Zone gives the *Dispersion Relation*.

An Example Dispersion Relation



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- 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 $N \approx 10 \ldots 20$. (The spectrum of $H(\mathbf{k})$ is discrete and unbounded above.)

Outline

A Harmless Question

So, what happens if we apply the inverse Floquet transform to the Bloch modes?

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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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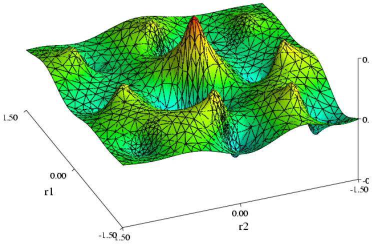

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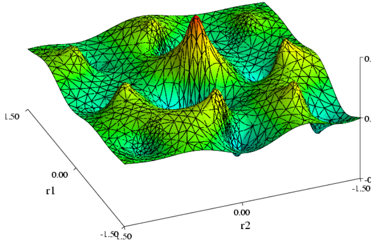

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Unfortunately, the choice of that constant matters when computing Wannier Functions.
To resolve the ambiguity, we demand that our Wannier functions be *maximally localized*, i.e. have minimal second moment

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

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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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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*

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

and

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So if we approximate the **k**-gradients (say by FD), we can obtain a computable expression for the spread.

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- Compute the maximally localized Wannier Functions, using the optimal U.
- Use a grid of MLWFs (centered in each unit cell) as a Galerkin basis to attack large-scale simulation problems, *with defects*.

Finding the Wannier functionns. . .

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Yes.

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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.

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$$-\int \nabla\psi \cdot \nabla\phi + \frac{\omega^2}{c^2}\left[\varepsilon_p + \delta\varepsilon\right]\psi\phi d\mathbf{r} = 0$$

$$-\int \nabla\left(\sum_{n,\mathbf{R}} \alpha_{n,\mathbf{R}} w_{n,\mathbf{R}}\right) \cdot \nabla w_{m,\mathbf{R}'}$$

$$+\frac{\omega^2}{c^2}\left[\varepsilon_p + \delta\varepsilon\right]\left(\sum_{n,\mathbf{R}} \alpha_{n,\mathbf{R}} w_{n,\mathbf{R}}\right) w_{m,\mathbf{R}'} d\mathbf{r} = 0$$

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References

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

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

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- What *exactly* goes on in 3D?
- Can the minimization be made reliable?

Questions?

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