From homogenization to linear dispersion relations in periodic structures

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Collaborators and supports

• Collaborators
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  – China: Jun Mei, Yun Lai

• Funding agencies
• Homogenization (Effective medium theory)
  – Introduction to effective medium theories
  – Effective medium theory based on coherent potential approximation for electromagnetic waves
  – Zero-index and energy-balanced coherent perfect absorber and laser

• Linear dispersion relations
  – Introduction to zero-index materials and linear dispersions
  – Perturbation theory and selection rule
  – Classical analogues of topological insulators

• Summary
• Homogenization (Effective medium theory)
  – Introduction to effective medium theories
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• Summary
Effective Medium Theory

Our eyes cannot resolve the fine structures of such a medium! We only see it in an “averaged” sense.

Microstructure | Artificial Material | Effective Medium

$\lambda \gg a$

homogenization

$\varepsilon, \mu$
Conventional effective medium theories are valid in the quasi-static limit:

\[ \lambda_{b} \gg r; \lambda_{s} \gg r; \lambda_{e} \gg r. \]

When resonance occurs: the conditions no longer hold. Our purpose: go beyond the quasi-static limit.
## Our contributions

<table>
<thead>
<tr>
<th>Method</th>
<th>Pros and Cons</th>
<th>Publications</th>
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</table>
| Coherent Potential Approximation | • Analytic solution  
                                   • High frequency  
                                   • Regular shape | PRB 2006, 2007  
Sci Rep 2015 |
| Multiple-scattering Theory     | • Analytic solution  
                                   • Lattice symmetry  
                                   • Complex derivation | PRB 2009, EPL 2011  
PBCM 2011 |
| Field-averaging                | • Arbitrary shape  
                                   • High frequency  
                                   • Prior knowledge | Nat Mater 2011  
OE 2014  
AMSE 2014 |
| Green’s function               | • Exact in 1D  
                                   • High frequency  
                                   • Prior knowledge | PRB 2014 |
Advantage: 1. Go beyond the quasi-static limit (deal with resonance); 2. Analytic

Only requires $\lambda_e \gg a$

$\varepsilon \leftrightarrow 1/\kappa, \mu \leftrightarrow \rho$ for acoustic waves

Extension to anisotropic metamaterials

Wave equation in Elliptic coordinates:

\[
\frac{\partial^2 E_z}{\partial \xi^2} + \frac{\partial^2 E_z}{\partial \eta^2} + c^2 k^2 (\cosh^2 \xi - \cos^2 \eta) E_z = 0, \quad (\xi, \eta) \in (0, \infty) \times (0, 2\pi)
\]

In the limit of \( \frac{1}{2} k_{\text{eff}} (a_0 + b_0) \ll 1 \)

\[
\begin{align*}
\varepsilon_{\text{eff}} + 2\varepsilon_0 \frac{J'_{e0}(q_0; \xi_0)}{k_0^2 a_0 b_0 J_{e0}(q_0; \xi_0)} &= \frac{Y_{e0}(q_0; \xi_0)}{i J_{e0}(q_0; \xi_0)} D_{e0}(0) \frac{D_{e0}(0)}{1 + D_{e0}(0)} \\
\varepsilon_{\text{eff}} + 2\varepsilon_0 \frac{Y'_{e0}(q_0; \xi_0)}{k_0^2 a_0 b_0 Y_{e0}(q_0; \xi_0)} &= \frac{Y'_{e0}(q_0; \xi_0)}{i J'_{e0}(q_0; \xi_0)} D_{e0}(0) \frac{D_{e0}(0)}{1 + D_{e0}(0)} \\
\mu_{\text{eff}, x} - \mu_0 \frac{a_0 J_{o1}(q_0; \xi_0)}{b_0 J'_{o1}(q_0; \xi_0)} &= \frac{Y_{o1}(q_0; \xi_0)}{i J_{o1}(q_0; \xi_0)} D_{o1}(0) \frac{D_{o1}(0)}{1 + D_{o1}(0)} \\
\mu_{\text{eff}, x} - \mu_0 \frac{a_0 Y_{o1}(q_0; \xi_0)}{b_0 Y'_{o1}(q_0; \xi_0)} &= \frac{Y_{o1}(q_0; \xi_0)}{i J'_{o1}(q_0; \xi_0)} D_{o1}(0) \frac{D_{o1}(0)}{1 + D_{o1}(0)} \\
\mu_{\text{eff}, y} - \mu_0 \frac{b_0 J_{e1}(q_0; \xi_0)}{a_0 J'_{e1}(q_0; \xi_0)} &= \frac{Y_{e1}(q_0; \xi_0)}{i J_{e1}(q_0; \xi_0)} D_{e1}(0) \frac{D_{e1}(0)}{1 + D_{e1}(0)} \\
\mu_{\text{eff}, y} - \mu_0 \frac{b_0 Y_{e1}(q_0; \xi_0)}{a_0 Y'_{e1}(q_0; \xi_0)} &= \frac{Y_{e1}(q_0; \xi_0)}{i J'_{e1}(q_0; \xi_0)} D_{e1}(0) \frac{D_{e1}(0)}{1 + D_{e1}(0)}
\end{align*}
\]
Applications

Anisotropic material to perfectly absorb oblique coherent incident waves

On-chip material, in collaboration with Prof. X. Zhang (PSE) and nanofabrication.

X. Zhang and Y. Wu, *Opt. Express.* (Accepted)
About zero-index

- Metamaterials (engineering the real parameter space)

\[ \varepsilon < 0, \mu > 0 \]
\[ \varepsilon > 0, \mu > 0 \]
\[ \varepsilon > 0, \mu < 0 \]
\[ \varepsilon < 0, \mu < 0 \]

\[ \varepsilon \approx 0 \text{ or } \mu \approx 0 \]

\[ \varepsilon \approx 0 \& \mu \approx 0 \]

PRL 100, 033903 (2008)

Nat. Mater. 10 582 (2011)
• Considered detrimental to the performance of metamaterials (metal, resonance...)

Thin layer

\[ t \to 0 \]

\[ A \leq 50\% \]

PRL 100 207402 (2008)


PRL 105 053901 (2010); Physics, 3, 61 (2010)
Manipulate the full complex plane

- Overcoming loss with gain
  - PRL 105, 127401 (2010)
  - Nature 466, 735 (2010)

- and beyond...
  - PT-symmetry: $n(-\vec{r}) = n^*(\vec{r})$
  - PT-symmetric
  - PT-broken
  - Nat. Phys. 6 116 (2010)
  - Science, 346, 972 (2014)
Motivation

• PT symmetry: Loss and gain spatially distributed at different locations

• How about loss and gain carried by different parameters?
  – What if the gain and loss are “balanced”?
Principles

System:
\[
\varepsilon", \mu" > 0 \text{  \&  } \varepsilon'\mu" - \varepsilon"\mu' = 0
\]

\[
n = \sqrt{\varepsilon \mu} \text{ is real}
\]

Real propagation constant

\[
\begin{pmatrix}
  b_2 \\
  b_1
\end{pmatrix} = S
\begin{pmatrix}
  a_1 \\
  a_2
\end{pmatrix} =
\begin{pmatrix}
  t_1 & r_2 \\
  r_1 & t_2
\end{pmatrix}
\begin{pmatrix}
  a_1 \\
  a_2
\end{pmatrix}
\]

Scattering matrix:

Eigenvalues: \( \lambda_{1,2} = t \pm r \)

Eigenvectors \((a_1, a_2) = (1,1)\) and \((1,-1)\)

Scattering coefficients: \( s_m = b_m / a_1 \) \(m = 1,2\)

Coherent incident beams:
\[
a_2 = a_1 e^{i\Delta \varphi}
\]

CPA: \( s = 0 \)

Laser: \( s = \infty \)
More about scattering coefficients

\[ \lambda_{1,2} = t \pm r \]

\[ \varepsilon = 1.2i, \mu = -0.5i \]

CPA or lasing at different \( d \)

\[ \varepsilon = 1.2i, \mu = -1.2i \]

CPA & lasing at the same \( d \)

\[ \varepsilon_r = \mu_r = 0 \]
Energy-balanced ZIM

\[ s_1 = \frac{e^{-ikd} \left[ 2in\mu e^{i\Delta \varphi} - (n^2 - \mu^2) \sin \eta \right]}{2in\mu \cos \eta + (n^2 + \mu^2) \sin \eta} \]

\[ s_2 = \frac{e^{-ikd} \left[ 2in\mu - e^{i\Delta \varphi} (n^2 - \mu^2) \sin \eta \right]}{2in\mu \cos \eta + (n^2 + \mu^2) \sin \eta} \]

\[ \eta = kd \]

<table>
<thead>
<tr>
<th>CPA ( s = 0 )</th>
<th>Laser ( s = \infty )</th>
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<tbody>
<tr>
<td>( \varphi = 0 )</td>
<td>( \varphi = \pi )</td>
</tr>
<tr>
<td>( \varepsilon = n\cot(\eta/2)i )</td>
<td>( \varepsilon = -n\cot(\eta/2)i )</td>
</tr>
<tr>
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</tr>
</tbody>
</table>

\[ \cot(kd/2) = \tan(kd/2) \]

\[ kd = \pi/2 + 2n\pi \]

\[ |\varepsilon| = |\mu| \]

CPA–laser!
Design of ZIM-GL

Goal

\[ \varepsilon = \varepsilon' + i\varepsilon'' \]
\[ \mu = \mu' + i\mu'' \]

Effective medium theory

\[ \varepsilon_{\text{eff}} = 0.0184i, \quad \mu_{\text{eff}} = -0.0184i \]

Photonic crystal

\[ \varepsilon_1 = 1.154 + 0.11i, \quad \varepsilon_2 = 1.07 - 0.054i \]

Loss in core
Gain in shell

\[ \text{Re}(\varepsilon_{\text{eff}}) = \text{Re}(\mu_{\text{eff}}) = 0 \]

\[ \varepsilon_{\text{eff}} = 0.02i, \quad \mu_{\text{eff}} = -0.02i \]
Eigenmodes of the PC

\[ \begin{align*}
\varepsilon_1 &= 1.154 + 0.11i \\
\varepsilon_2 &= 1.07 - 0.054i
\end{align*} \]

Lossy core \( \Rightarrow \epsilon_{\text{eff}} = 0.02i \)

Shell with gain \( \Rightarrow \mu_{\text{eff}} = -0.02i \)

Combination of a monopole and a dipole.
Phase difference of the two coherent incident waves: $\Delta \phi = 0$.

Phase difference of the two coherent incident waves: $\Delta \phi = \pi$.

EMT and Zero-index

- Realization of double-zero-index material (accidental degeneracy)

ZIM at microwave frequencies
Nat. Mater. 10, 582, (2011)

Dirac Cone + flat sheet

All dielectric ZIM at optical frequencies
Nat. Photon. 7, 791 (2013)

&

On-Chip ZIM
Nat. Photon. 9, 738 (2015)

\[ \varepsilon = \varepsilon(\omega_0) + \varepsilon'(\omega_0)(\omega - \omega_0) \]

\[ \mu = \mu(\omega_0) + \mu'(\omega_0)(\omega - \omega_0) \]

\[ \omega = ck \]

\[ \Delta \omega \propto \Delta k, \text{ when } \varepsilon(\omega_0) = \mu(\omega_0) = 0 \]

Elastic ZIM
PRL 115, 175502 (2015)

Linear
Outline

• Homogenization (Effective medium theory)
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• Summary
A honeycomb/triangular lattice of photonic/acoustic crystals, with interesting phenomena such as

- **Conical diffraction** (PRL 98, 103901)
- **Classical analogs of quantum Hall edge states** (PRL 100, 013904; PRA 78, 033834; PRB 80, 155103)
- **Classical analogs of Zitterbewegung** (PRL 100, 113903; PRL 101, 264303; PRL 105, 143902; Opt. Lett. 36, 2513)
- **Pesudo-diffusion at the Dirac point** (PRA 75, 063813; Opt. Commun. 281, 5267; Physica B 405, 2990)
- **Acoustic/elastic analogues of graphene** (PRL 108, 174301; PRB 87, 115143)
Questions

• Is double-zero-index material *necessary* for linear dispersion relations at the Γ point?

• Are linear dispersion relations at the BZ center equivalent to those at the BZ corner?

• Is there a *unified* theory to characterize all of the linear dispersion relations?
A k.p Theory for Classical Waves

Example: Acoustic waves

Acoustic wave equation:

\[
\nabla \cdot \left( \frac{1}{\rho_r(\vec{r})} \nabla p \right) = -\frac{\omega^2}{c_1^2} \cdot \frac{p}{B_r(\vec{r})}
\]

Bloch function near a high symmetry point \( k_0 \)

\[
\psi_{nk}(\vec{r}) = u_{nk}(\vec{r}) e^{i\vec{k} \cdot \vec{r}} = \sum_j A_{nj}(\vec{k}) e^{i(\vec{k} - \vec{k}_0) \cdot \vec{r}} \psi_{j\vec{k}_0}(\vec{r})
\]

\[
\sum_j \left[ \frac{\omega_{j0}^2 - \omega_{nk}^2}{c_1^2} \delta_{lj} - P_{lj}(\vec{k}) \right] A_{nj}(\vec{k}) = 0
\]

\[
\det \left| H - \frac{\omega_{nk}^2 - \omega_{j0}^2}{c_1^2} I \right| = 0
\]

\[
P_{lj}(\vec{k}) = (\vec{k} - \vec{k}_0) \cdot \vec{p}_{lj} - (\vec{k} - \vec{k}_0)^2 q_{lj}
\]

\[
\begin{cases}
\vec{p}_{lj} = i \frac{(2\pi)^2}{\Omega} \int_{\text{unit cell}} \psi_{lk_0}^* (\vec{r}) \left[ \frac{2\nabla \psi_{lk_0}(\vec{r})}{\rho_r(\vec{r})} + \left( \nabla \frac{1}{\rho_r(\vec{r})} \right) \psi_{lk_0}(\vec{r}) \right] d\vec{r}
\end{cases}
\]

\[
q_{lj} = \frac{(2\pi)^2}{\Omega} \int_{\text{unit cell}} \psi_{j\vec{k}_0}^* (\vec{r}) \frac{1}{\rho_r(\vec{r})} \psi_{j\vec{k}_0}(\vec{r}) d\vec{r}
\]
steel rods in water host in a triangular lattice

Example
**BZ Center: Accidental Degeneracy**

Linear dispersions

\[ \frac{\Delta \omega}{\Delta k} = \pm \frac{sc_1^2}{2\omega_0a} \text{ and } 0 \]

\[ s = 10.241 \]

\[ \frac{\omega_0a}{2\pi c_1} = 1.06 \]

Rightarrow

\[ \frac{\Delta \omega}{\Delta k} = \pm 0.769c_1 \text{ and } 0 \]

---

**Single eigenstate**

\[ H = \begin{pmatrix} 0 & i\bar{k} \cdot \bar{L}_{12} & i\bar{k} \cdot \bar{L}_{13} \\ -i\bar{k} \cdot \bar{L}_{12} & 0 & 0 \\ -i\bar{k} \cdot \bar{L}_{13} & 0 & 0 \end{pmatrix} \]

\[ \bar{p}_{lj} = i \langle \psi_{lk_0} | \bar{L} | \psi_{jk_0} \rangle \]

**doubly-degenerate eigenstates**

\[ \bar{L}_{lj} = -i\bar{p}_{lj} \]

\[ |\bar{L}_{12}| = |\bar{L}_{13}| = s/a \]

\[ \bar{L}_{12} \cdot \bar{L}_{13} = 0 \]

**C\textsubscript{6v} Group:**

\[ B_2 \quad E_1 \quad E_2 \]

---

**selection rule**

**contains** \[ A_1 \]

**Linear dispersion.**
**BZ Center: Zero Berry Phase**

**Bloch states**

\[
\Psi_+ (\mathbf{k}) = \left( \frac{1}{\sqrt{2}} \right) \begin{pmatrix} 1 \\ ik \cdot \hat{L}_{12} \\ ik \cdot \hat{L}_{13} \end{pmatrix} e^{ik \cdot \mathbf{r}} \\
\Psi_- (\mathbf{k}) = \left( \frac{1}{\sqrt{2}} \right) \begin{pmatrix} 1 \\ -ik \cdot \hat{L}_{12} \\ -ik \cdot \hat{L}_{13} \end{pmatrix} e^{ik \cdot \mathbf{r}} \\
\Psi_0 (\mathbf{k}) = \left( \frac{1}{\sqrt{2}} \right) \begin{pmatrix} 0 \\ -ik \cdot \hat{L}_{13} \\ ik \cdot \hat{L}_{12} \end{pmatrix} e^{ik \cdot \mathbf{r}}
\]

**Berry phase**

\[
\Gamma_{\pm,0} = i \oint \langle \Psi_{\pm,0} (\mathbf{k}) | \nabla_{\mathbf{k}} | \Psi_{\pm,0} (\mathbf{k}) \rangle \cdot d\mathbf{k} = 0
\]

consistent with the fact that the Hamiltonian cannot be cast into the massless Dirac Hamiltonian

The linear dispersions around BZ center are not really Dirac cones!
**BZ Corner: Deterministic Degeneracy**

**doubly-degenerate eigenstates**

**Selection rule** $C_{3v}$ Group: $E \otimes E \otimes E$ contains $A_1$

**The Dirac Hamiltonian**

$$H = \frac{S}{a} \left[ (\Delta k)_x \sigma_x + (\Delta k)_y \sigma_y \right]$$

**Linear dispersions independent of physical parameters (radii, mass densities, wave velocities)**

$$H = \Delta \vec{k} \cdot \begin{pmatrix} \vec{p}_{11} \\ \text{Re} \vec{p}_{12} + i \text{Im} \vec{p}_{12} \\ \text{Re} \vec{p}_{12} - i \text{Im} \vec{p}_{12} \\ -\vec{p}_{11} \end{pmatrix}$$

**The Dirac Hamiltonian**

$$H = \left( \Delta k \right)_x \left( \tilde{\alpha}_x \cdot \tilde{\sigma} \right) + \left( \Delta k \right)_y \left( \tilde{\alpha}_y \cdot \tilde{\sigma} \right)$$

**unitary transformations**

$$\tilde{\alpha}_x = \left( \left( \text{Re} \vec{p}_{12} \right)_x, -\left( \text{Im} \vec{p}_{12} \right)_x, \left( \vec{p}_{11} \right)_x \right)$$

$$\tilde{\alpha}_y = \left( \left( \text{Re} \vec{p}_{12} \right)_y, -\left( \text{Im} \vec{p}_{12} \right)_y, \left( \vec{p}_{11} \right)_y \right)$$

$$\tilde{\sigma} = \left( \sigma_1, \sigma_2, \sigma_3 \right)$$

$$\begin{align*}
|\tilde{\alpha}_x| &= |\tilde{\alpha}_y| = s/a \\
\tilde{\alpha}_x \cdot \tilde{\alpha}_y &= 0
\end{align*}$$
BZ Corner: Non-Zero Berry Phase

Block states

\[
\Psi_+ (\Delta \vec{k}) = \left( \frac{1}{\sqrt{2}} \right) \left( \begin{array}{c}
\sqrt{1 - \Delta \hat{k} \cdot \vec{M}_{11}} \\
-\Delta \hat{k} \cdot \vec{M}_{12}^* \\
\sqrt{1 - \Delta \hat{k} \cdot \vec{M}_{11}}
\end{array} \right) e^{i \Delta \vec{k} \cdot \vec{r}}
\]

\[
\Psi_- (\Delta \vec{k}) = \left( \frac{1}{\sqrt{2}} \right) \left( \begin{array}{c}
\sqrt{1 + \Delta \hat{k} \cdot \vec{M}_{11}} \\
\Delta \hat{k} \cdot \vec{M}_{12}^* \\
\sqrt{1 + \Delta \hat{k} \cdot \vec{M}_{11}}
\end{array} \right) e^{i \Delta \vec{k} \cdot \vec{r}}
\]

Berry phase

\[
\Gamma_\pm = i \oint \langle \Psi_\pm (\Delta \vec{k}) | \nabla_{\Delta \vec{k}} | \Psi_\pm (\Delta \vec{k}) \rangle \cdot d(\Delta \vec{k})
\]

\[
\Gamma_\pm = -\pi
\]

consistent with that the Hamiltonian can be cast into the Dirac Hamiltonian

The linear dispersions around BZ corners are really Dirac cones!

About Selection Rule

Air Boreholes in Si  $\varepsilon_r = 12.5$
H field out-of-plane
Accidental degeneracy $A_1 \otimes E_1 \otimes E_1$ contains $A_1$

Size of the air boreholes changed.
Accidental degeneracy $A_1 \otimes E_1 \otimes E_2$ does not contain $A_1$

Other Linear Dispersion Relations

**Semi-Dirac Points (anisotropic)**

\[ r_a / a = 0.188, \quad r_b / a = 0.188 \times 1.3 \]

X. Zhang and Y. Wu *Proc. ASME.* 46620 (2014)

**Double-Dirac Points**


Topological Phononic Crystal

Tunable topological transition

Topological Phononic Crystal (QSH)

**Double Dirac cone**

- **k.p model (2\textsuperscript{nd} order perturbation)**
  
  Effective Hamiltonian
  
  $$H^{\text{eff}}(\vec{k}) = \begin{pmatrix}
  M - Bk^2 & Ak_+ & 0 & 0 \\
  A^*k_- & -M + Bk^2 & 0 & 0 \\
  0 & 0 & M - Bk^2 & Ak_-
  \end{pmatrix}$$

  Spin Chern number
  
  $$C_\pm = \pm \frac{1}{2} \left[ \text{sgn}(M) + \text{sgn}(B) \right]$$

  - **Band inversion and mixing**

  **Pseudo Time Reversal**

  **Topological transition**
Topological Photonic Crystal (QSH)

Unit cell (YIG cylinder in air)

\[ R, \hat{\mu}_1 \text{ Can be adjusted} \]

\[
\hat{\mu}_1 = \begin{bmatrix}
\mu & i\kappa & 0 \\
-i\kappa & \mu & 0 \\
0 & 0 & \mu_0
\end{bmatrix}
\]
Edge states (demonstration)

Robust against disorder and TRS broken (magnetic) impurities.

I: $C_\pm = 0$

IV: $C_\pm = (0, -1)$

Magnetic impurities
Spin splitter

$I$ \( C_\pm = 0 \)

$C_\pm = (1,0)$

$II$ \( C_\pm = (0,-1) \)

$III$ \( C_\pm = (1,-1) \)
Summary

• Homogenization (Effective medium theory)
  – Can deal with resonances
  – Predicts double zero-index-materials
  – Enabled the design of EBZIM

• Linear dispersion relations
  – Some are related to double zero-index-materials
  – Can be characterized by a unified theory (k.p)
  – Existence can be determined by a selection rule, solely from symmetry
  – Are starting points for classical analogues of topological insulators
Thank you

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