

Tight Binding Models for Longitudinally Driven Linear/Nonlinear Lattices

Mark J. Ablowitz

Department of Applied Mathematics
University of Colorado, Boulder
September 2017



Outline

- Introduction
- Study light propagation in longitudinal (z) direction with an optical lattice in transverse ($x-y$) plane
- Systematic method to obtain tight binding approximations for linear/NL lattices with detailed longitudinal structure
- Prototypes: honeycomb (HC) and staggered square (SS) lattices
- Examples of longitudinal structure: helical periodic variation with same rotation/different radii on sublattices, out of phase rotation between sublattices, different frequencies between sublattices,...

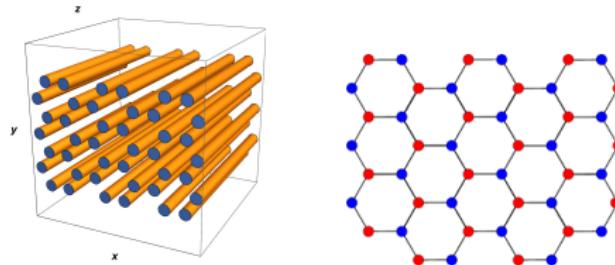
Outline – con't

- Obtain Floquet bands – indicates edge waves; typically two types
 - Unidirectional traveling edge waves: topological: no backscatter, stable w/r defects
 - Non-unidirectional/non-topological waves
- Further asymptotic models can be constructed; yields analytical insight: rapid and slow variation
- In nonlinear problem can find envelope edge solitons satisfying classical 1d-NLS eq; the solitons are stable, they persist over long distances; remain intact around defects, corners
- NL modes–solitons inherit underlying topological properties
- Conclusion

Refs: MJA, C. Curtis, YP Ma (2014-15); MJA, J. Cole (2017)

Introduction

- Investigations of optical lattices extensive
- Paradigm – HC lattice: ‘Photonic Graphene’ (PG)



Left: Uniform HC lattice: z direc'n; Right: x-y plane : HC lattice

- Segev group 2007–conical diffraction; MJA, Y. Zhu, C. Curtis constructed/studied TB models; found conical diffraction & various interesting new NL nonlocal eqn's in certain limits (2009-13)

Introduction–con't

- Topological edge waves were theoretically proposed/observed in magneto-optics, Wang et al 2008-09
- Such waves were found in photonics: HC lattice with longitudinal helical variation, Rechtsman et al 2013
- MJA, YP Ma, C. Curtis (2014), studied TB model, developed asymptotic description linear/NL under assumption of rapid helical variation
- Leykam et al (2016) studied staggered square lattice with helical variation and phase sh'fts between sublattices
- MJA & J. Cole (2017): systematic method to find TB models in lattices with longitudinal structure
- Topological edge/interface/surface waves in physics – very active field of research

Lattice NLS Equation

Maxwell's eq with paraxial approx. \Rightarrow NLS eq with ext pot'l

$$i \frac{\partial \psi}{\partial z} = -\frac{1}{2k_0} \nabla^2 \psi + k_0 \frac{\Delta n(x, y, z)}{n_0} \psi - \gamma |\psi|^2 \psi$$

where: k_0 is input wavenumber

n_0 is the bulk refractive index

$\Delta n/n_0$ is the change of index change relative to n_0

γ is NL index

Non-dimensional NLS Equation

Rescale to non-dimensional form

$$x = \ell x', \quad y = \ell y', \quad z = z_* z', \quad \psi = \sqrt{P_*} \psi'$$

where: ℓ is the lattice scale; P_* : peak input power

Find non-dim NLS eq, ': dimensionless:

$$i \frac{\partial \psi'}{\partial z'} + (\nabla')^2 \psi' - V(x', y', z') \psi' + \sigma |\psi'|^2 \psi' = 0$$

where $z_* = 2k_0 \ell^2$, $V = 2k_0^2 \ell^2 (\Delta n / n_0)$, $\sigma = 2\gamma k_0 \ell^2 P_*$

Drop ' => normalized lattice NLS eq

$$i \frac{\partial \psi}{\partial z} + \nabla^2 \psi - V(x, y, z) \psi + \sigma |\psi|^2 \psi = 0$$

TB Limit

When $|V| \gg 1$, the tight binding (TB) limit, approx the potential by

$$V(\mathbf{r}) \approx \sum_{\mathbf{v}} V_j(\mathbf{r} - \mathbf{v}), \quad j = 1, 2 \quad (\text{nonsimple HC or SS lattice})$$

where $V_j(\mathbf{r})$, denotes the approximating potential with minima at site $S_{\mathbf{v}}$; $V_j(\mathbf{r})$ typically gaussian

Associated localized functions near the potential minima, termed orbitals, are used to approx ψ

TB approx used widely in physics to study lattice systems: uniform linear HC lattices ('Graphene'): Wallace 1947

Longitudinal Variation in Potentials

Typical case nonsimple lattice with two sublattices

$$V_1 = V_1(\mathbf{r} - \mathbf{h}_1(z)), \quad V_2 = V_2(\mathbf{r} - \mathbf{h}_2(z))$$

in nb'hd of sublattices 1, 2 and $\mathbf{h}_j(z)$, $j = 1, 2$ are prescribed (smooth) functions

Simple case, helical variation

$$\mathbf{h}_j(z) = \eta_j \left(\cos \left(\frac{z}{\varepsilon_j} + \chi_j \right), \sin \left(\frac{z}{\varepsilon_j} + \tilde{\chi}_j \right) \right), \quad j = 1, 2$$

Rotating frame

Move to coordinate frame co-moving with the $V_1(\mathbf{r}, z)$ sublattice,

$$\mathbf{r}' = \mathbf{r} - \mathbf{h}_1(z) \quad , \quad z' = z$$

which after the phase transformation

$$\psi = \psi' \exp \left[-i \int_0^z |\mathbf{A}(\xi)|^2 d\xi \right] \text{ with } \mathbf{A}(z) = -\mathbf{h}_1'(z)$$

find lattice NLS with a pseudo-field $\mathbf{A}(z)$ -dropping ':

$$i\partial_z \psi + (\nabla + i\mathbf{A}(z))^2 \psi - V(\mathbf{r}, z)\psi + \sigma |\psi|^2 \psi = 0$$

$V_1(r, z) = V_1(\mathbf{r})$, $V_2(r, z) = V_2(\mathbf{r} - \Delta\mathbf{h}_{21}(z))$, near sites 1, 2 with
 $\Delta\mathbf{h}_{21}(z) = \mathbf{h}_2(z) - \mathbf{h}_1(z)$

NL HC Representation

In non-dim NLS eq using HC lattice with $|V| \gg 1$ substitute

$$\psi(\mathbf{r}, z) \sim \sum_{\nu} [a_{\nu}(z)\phi_{1,\nu}(\mathbf{r}, z) + b_{\nu}(z)\phi_{2,\nu}(\mathbf{r}, z)]$$

where

$$\left(\nabla^2 - \tilde{V}_j(\mathbf{r}, z) \right) \phi_{j,\nu}(\mathbf{r}, z) = -E_j \phi_{j,\nu}(\mathbf{r}, z); \quad j = 1, 2$$

$\phi_{j,\nu}$ are termed orbitals

Substitute ψ into NLS eq. with pseudo-field, multiply
 $\phi_j(\mathbf{r} - \mathbf{p})e^{-i\mathbf{k}\cdot\mathbf{p}}$; $j = 1, 2$ and integrate

Discrete HC System

$$i \frac{da_{mn}}{dz} + e^{i\varphi(z)} (\mathcal{L}_-(z)b)_{mn} + \sigma |a_{mn}|^2 a_{mn} = 0$$

$$i \frac{db_{mn}}{dz} + e^{-i\varphi(z)} (\mathcal{L}_+(z)a)_{mn} + \sigma |b_{mn}|^2 b_{mn} = 0$$

$$(\mathcal{L}_-(z)b)_{mn} = L_0(z)b_{mn} + L_1(z)b_{m-1,n-1}e^{-i\theta_1(z)} + L_2(z)b_{m+1,n-1}e^{-i\theta_2(z)}$$

$$(\mathcal{L}_+(z)a)_{mn} = \tilde{L}_0(z)a_{mn} + \tilde{L}_1(z)a_{m+1,n+1}e^{i\theta_1(z)} + \tilde{L}_2(z)a_{m-1,n+1}e^{i\theta_2(z)},$$

where $\varphi(z), \theta_j(z), L_j(z), \tilde{L}_j(z) \in \mathbb{R}$, $j = 1, 2, 3$ known

Typical Rotation Patterns for Sublattices

- Same rotation, same or different radii:

$$\mathbf{h}_2(z) = R_a \mathbf{h}_1(z) = R_a \eta \left(\cos \left(\frac{z}{\varepsilon} \right), \sin \left(\frac{z}{\varepsilon} \right) \right),$$

- π -Phase offset rotation

$$\mathbf{h}_2(z) = \mathbf{h}_1(z + \varepsilon\pi) = -\eta \left(\cos \left(\frac{z}{\varepsilon} \right), \sin \left(\frac{z}{\varepsilon} \right) \right),$$

- Different frequencies

$$\mathbf{h}_j(z) = \eta \left(\cos \left(\frac{z}{\varepsilon_j} \right), \sin \left(\frac{z}{\varepsilon_j} \right) \right), \quad j = 1, 2,$$

BCs – Linear Floquet Bands

Consider e.g. Zig-Zag; left end BCs

$$a_{mn} = 0 \text{ for } n < 1, \quad b_{mn} = 0 \text{ for } n < 0,$$
$$a_{mn} \rightarrow 0 \text{ as } n \rightarrow \infty, \quad b_{mn} \rightarrow 0 \text{ as } n \rightarrow \infty.$$

Look for solutions of the form

$$a_{mn}(z) = a_n(z; \omega) e^{im\omega}, \quad b_{mn}(z) = b_n(z; \omega) e^{im\omega},$$

Find linear difference eq with periodic coef; use Floquet thy:

$$f(z + L) = e^{-i\alpha(\omega)z} f(z)$$

HC Floquet Bands

HC lattice linear band structure—typical parameters

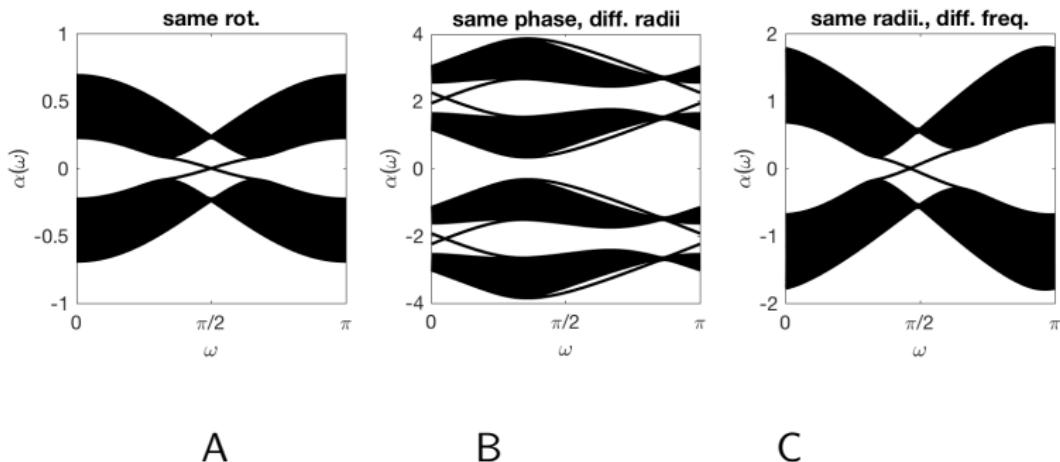


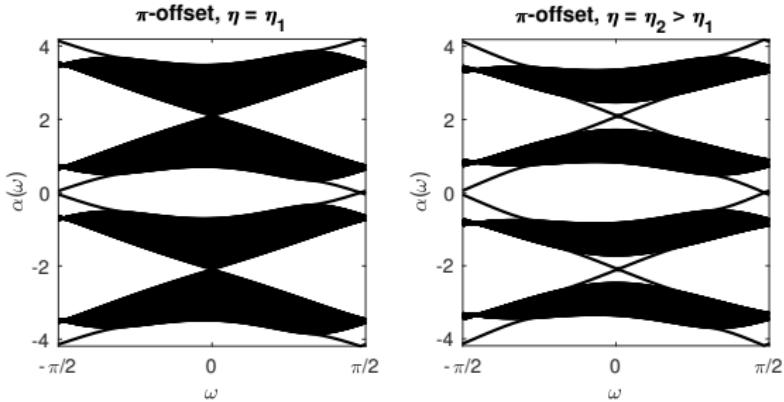
Fig A: same freq, same radii

Fig B: same freq, different radii ($R_2 = R_1/2$)

Fig C: diff freq ($1/\varepsilon_2 = \omega_2 = 2\omega_1 = 1/\varepsilon_1$), same radii

HC Floquet Bands –con't

HC lattice linear band structure—typical parameters



A

B

Figs A & B: π offset, same rotation

Fig B vs Fig A: radius $\eta_2 > \eta_1$

Linear HC Edge Mode Dynamics

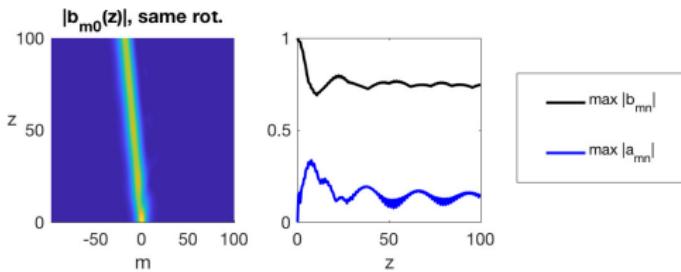


Fig Above: Same rotation, same radii

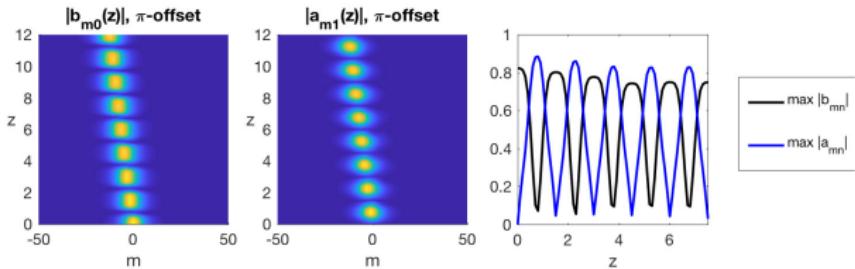
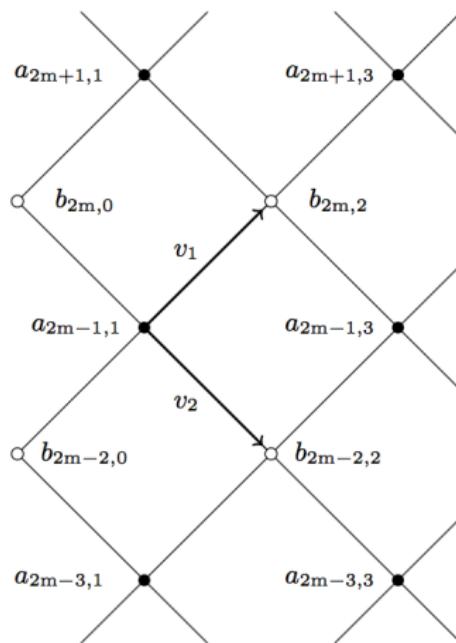


Fig Above: π offset, different radii

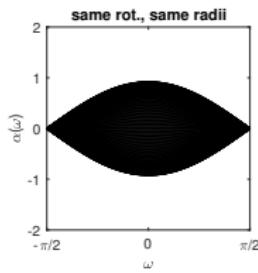
Staggered Square lattice



Analysis to find TB system and Floquet system similar to HC

Staggered Square (SS) Floquet bands

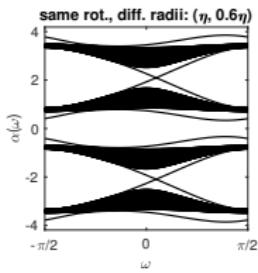
Staggered Square (SS) lattice linear band structure—typical parameters



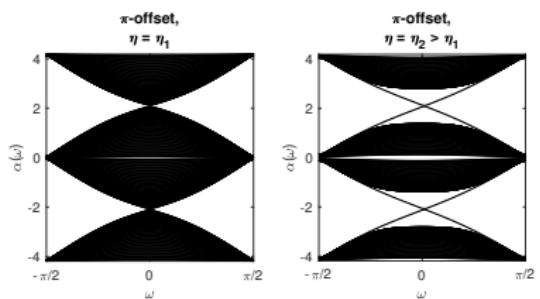
A

A & B: Same rotation

- A: same radii (simple lattice)
- B: different radii ($R_a = 0.6$)

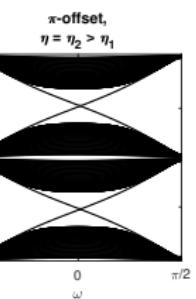


B



C

C & D: π offset, different radii



D

Linear SS Edge Mode Dynamics

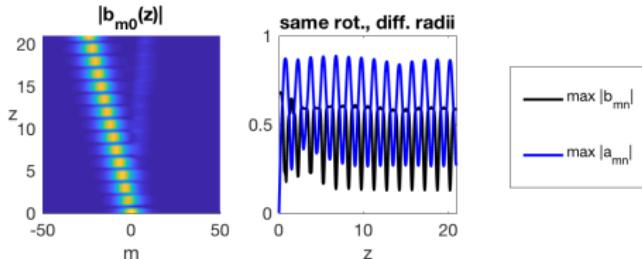


Fig Above: Same rotation, different radii ($R_a = 0.6$)

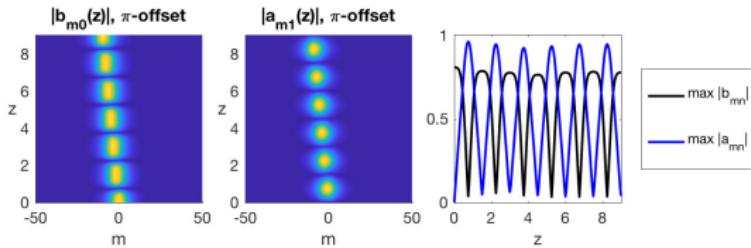


Fig Above: π offset, different radii:

Asymptotics: Rapidly Varying Helical HC Lattice

HC lattice, when each sublattice has same rotation/radius, eqs simplify

Let: $a_{mn} = a_n e^{im\omega}$, $b_{mn} = b_n e^{im\omega}$ find

$$i\partial_z a_n + e^{i\mathbf{d}\cdot\mathbf{A}} (b_n + \rho\gamma^* b_{n-1}) + \sigma|a_n|^2 a_n = 0$$

$$i\partial_z b_n + e^{-i\mathbf{d}\cdot\mathbf{A}} (a_n + \rho\gamma a_{n+1}) + \sigma|b_n|^2 b_n = 0$$

where $\gamma = \gamma(\omega, \mathbf{A}(z))$, ρ : geometric deformation parameter

$\mathbf{A}(z)$ periodic & rapidly varying in z :

$$\mathbf{A} = \mathbf{A}(\zeta), \zeta = \frac{z}{\varepsilon}, |\varepsilon| \ll 1; \text{ expt's: } \varepsilon = 0.24$$

e.g. $\mathbf{A} = \kappa(\sin \zeta, -\cos \zeta)$: 'helical waveguides'

Expt's: Rechtsman et al (2013); Theory: MJA, Curtis, Ma, Cole (2014, 2017)

Edge Modes: Zig-Zag (ZZ)

Multiple scales:

$$a_n = a_n(z, \zeta); \quad b_n = b_n(z, \zeta); \quad \zeta = \frac{z}{\varepsilon}$$

Expand a_n, b_n in powers of ε

Find at leading order: **Edge Modes (ZZ)**, exp decay, left end:

$$a_n \sim 0, \quad b_n \sim C(Z, \omega) r^n, \quad |r| = |r(\omega, \rho; \mathbf{A})| < 1, \quad n \geq 0$$

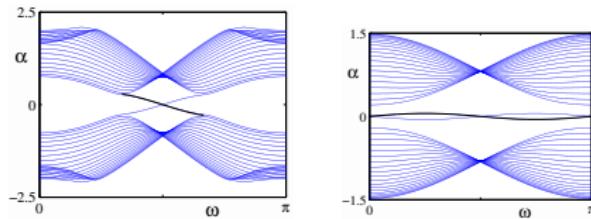
Linear problem (first order):

$$C(Z, \omega) = C_0 \exp(-i\alpha(\omega)Z), \quad Z = \varepsilon z$$

C_0 const. $\alpha(\omega) \equiv \alpha(\omega, \rho; \mathbf{A}) \in \mathbb{R}$: 'edge dispersion relation'
Obtain explicit formulae (Floquet coef)

Linear Problem–Edge Dispersion Relation

Dispersion relations (helical waveguides): $\alpha(\omega)$: thin curves are ‘bulk’ modes; lines in the gap are edge modes ($\rho = 1$):



$$\rho = 1$$

$$\rho = 0.4$$

Left: : ‘Topological Floquet Insulator’ ($\mathcal{I} = 1$)

Right $\rho = 0.4$: Nontopological mode ($\mathcal{I} = 2$)

Nonlinear Edge Wave Envelope Evolution Eq

Discrete Zig-Zag edge mode:

$$a_{mn} \sim 0$$

$$b_{mn} \sim C(Z, y) e^{i\omega_0 m} r^n, \quad |r| < 1$$

where slowly varying ($|\nu| \ll 1$) edge mode envelope C satisfies:

$$i\partial_Z C = \alpha_0 C - i\alpha'_0 \nu C_y - \frac{\alpha''_0}{2} \nu^2 C_{yy} + \frac{i\alpha'''_0}{6} \nu^3 C_{yyy} - \alpha_{nl,0} |C|^2 C + \dots$$

where $\alpha_0 = \alpha(\omega_0)$ etc

If $\mathbf{A} = \mathbf{0}$ then $\alpha = 0$: stationary mode

Linear/NL mode evolution discrete eq agrees with LS/NLS eq

NL topological mode: unidirectional, stable

Typical Linear Edge Wave Evolution–Defects

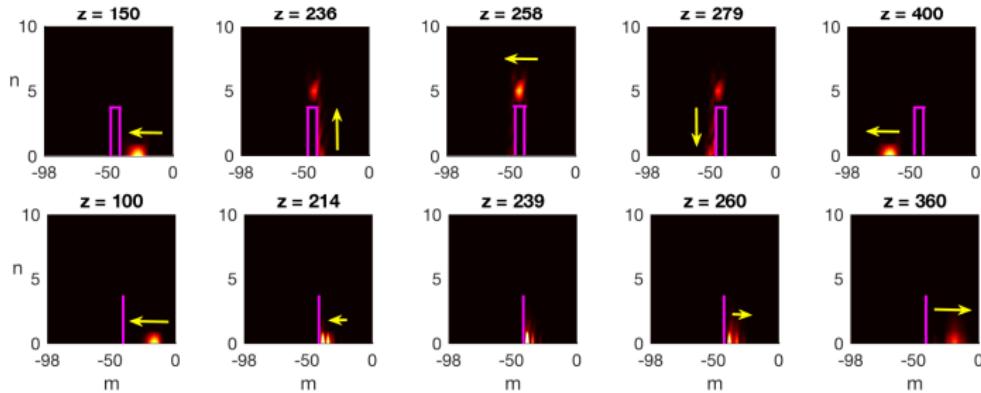


Fig: propagation across defect: left to right

Top fig: Topological mode – wave propagates unidirectionally without losing significant power ($\rho = 1, \omega = \pi/2, \alpha_{nl} = 0$)

Bottom fig: Nontopological mode – wave reflects, broadens/loses significant power ($\rho = 0.4, \omega = \pi/2, \alpha_{nl} = 0$)

NL Edge Wave Propagation Around Defects

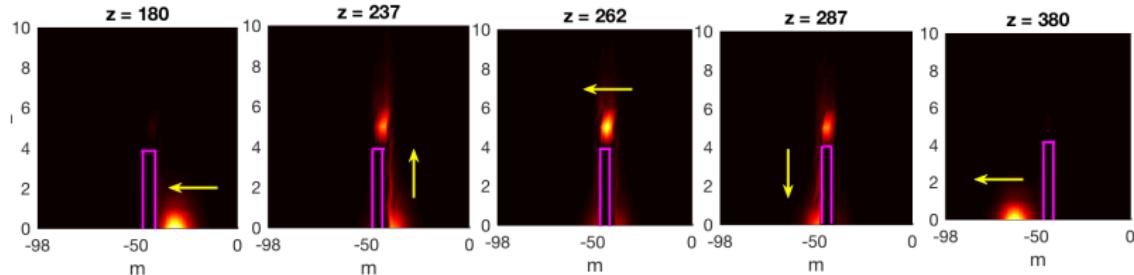
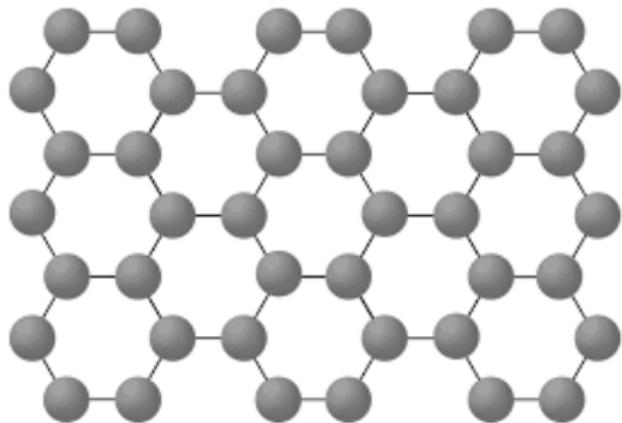


Fig: NL propagation across defect: left to right

NL topological edge wave ($\rho = 1, \alpha_0'' > 0, \alpha_{nl} \neq 0$) propagates without losing significant power

NL edge solitons: unidirectional, propagates across defects

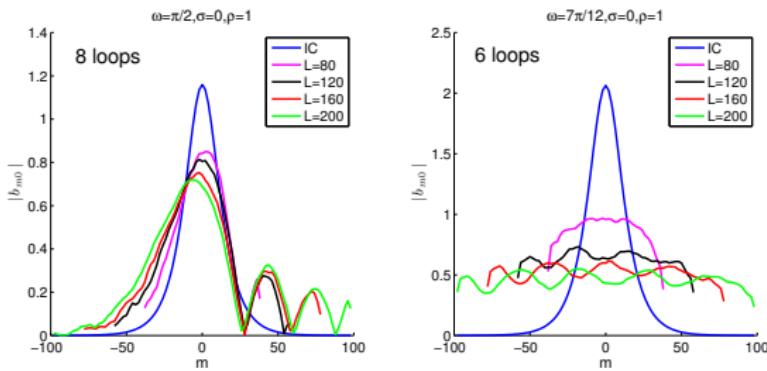
Bounded Graphene: Zig-Zag, Arm Chair Edges



Zig-Zag (ZZ): Left Right; Armchair: Top, Bottom

Mode Propagation–Linear

Linear propagation $\rho = 1$: topological case; different points on the dispersion curve

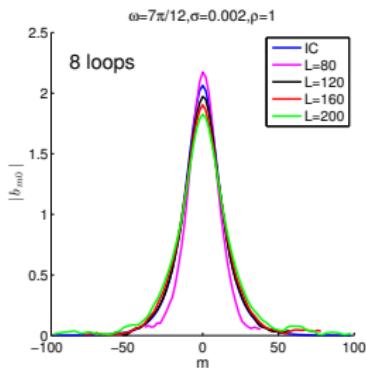
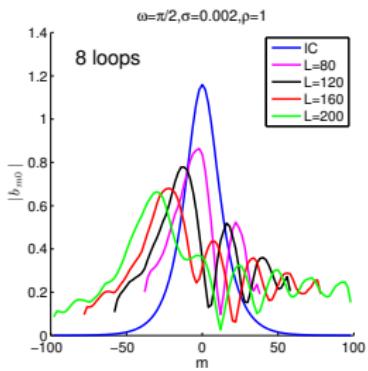


Left: Linear $\omega = \pi/2$
 $\alpha'' = 0, \alpha''' \neq 0$

Right: Linear $\omega = 7\pi/12$
 $\alpha'' \neq 0$

Mode Propagation–NL

NL propagation $\rho = 1$: topological case;; different points on the dispersion curve



Left: NL $\omega = \pi/2$
 $\alpha'' = 0, \alpha''' \neq 0$

Right: NL $\omega = 7\pi/12$: NLS eq
 $\alpha'' \neq 0$

Adiabatic HC Lattice

Take HC lattice, uniform rotation, and $\mathbf{A} = \mathbf{A}(Z)$, where $Z = \varepsilon z$

In lattice system: $a_n = a_n(z, Z)$, $b_n = b_n(z, Z)$

Multiple scales asymptotics:

$$a_n \sim 0; \quad b_n \sim C(Z, \omega) b_n^S(Z)$$

where $b_n^S(Z) = \{r^n(Z); \quad |r| < 1; \quad r = r(\omega, \rho; \mathbf{A}(Z)), \quad n \geq 0\}$

In general edge mode existence ($|r| < 1$) depends on ω, ρ, Z

Modes can ‘disintegrate’ under evolution

Adiabatic HC Lattice-con't

For $b_n \sim C(Z, \omega) b_n^S(Z)$, find at leading order:

$$\partial_Z C + i\alpha_p(Z; \omega)C = 0,$$

where $\alpha_p(Z; \omega)$ may be calculated explicitly

Typical case take: $\mathbf{A}(Z) = \kappa(\sin Z, -\cos Z)$

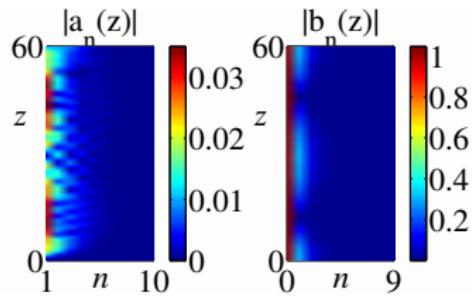
$\alpha_p(Z; \omega)$ is a periodic fcn in Z

$\alpha_p(Z; \omega)$ is termed the 'edge dispersion relation'

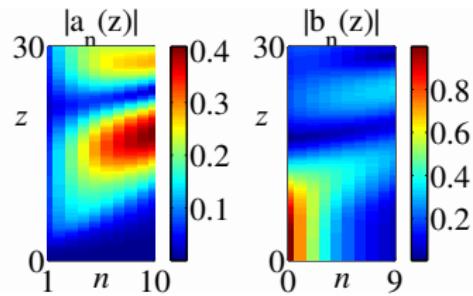
Linear Edge Modes—Under Evolution

Typical linear edge mode evolution—via discrete eq:

$$\varepsilon = 0.1, \kappa = 0.3, \rho = 1$$



(a)



(b)

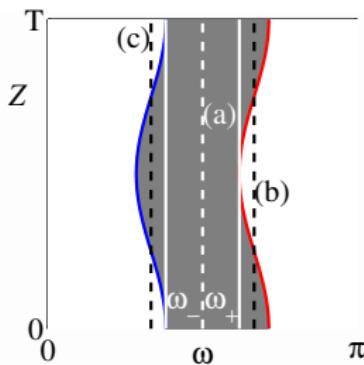
$$\omega_0 = \pi/2$$

$\omega_0 = 2\pi/3$
Mode ‘disintegrates’

Edge Mode Region–Under Evolution

Typical Edge Mode Region Under Evolution:

$$\varepsilon = 0.1, \kappa = 0.3, \rho = 1$$



Mode exists in region in gray; If begin inside ω : $\omega_- < \omega < \omega_+$, then remain. Mode (a) exists for entire period; mode (b) disintegrates at some Z_*

Adiabatic NL Edge Wave Envelope Evolution Eq

Discrete edge mode: $a_{mn} \sim 0$

$$b_{mn} \sim C(Z, y) e^{i\omega_0 m} b_n^S(Z), \quad |r| < 1$$

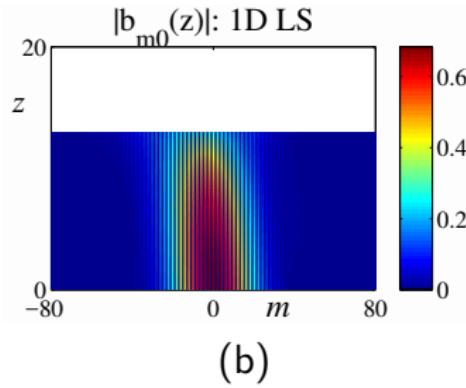
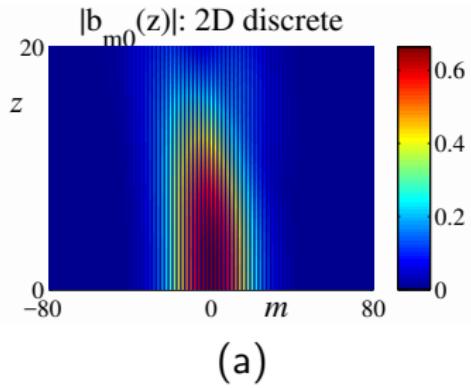
slowly varying ($|\nu| \ll 1$) edge mode envelope C NLS-type eq:

$$\begin{aligned} i\partial_Z C = & \alpha_0(Z)C - i\alpha'_0(Z)\nu C_y - \frac{\alpha''_0(Z)}{2}\nu^2 C_{yy} + \frac{i\alpha'''_0(Z)}{6}\nu^3 C_{yyy} \\ & - \alpha_{nl,0}(Z)|C|^2 C + \dots \end{aligned}$$

$$\alpha_0(Z) = \alpha_p(\omega_0, Z), \quad \alpha'_0(Z) = (\partial_\omega \alpha_p)(\omega_0, Z) \text{ etc.}$$

Adiabatic: Linear Discrete vs. Envelope Eq

Linear discrete system vs. linear envelope eq – at edge: $n = 0$



Left: Discrete eq. evolution;

Right: Envelope evolution:
Stopped at $z \approx 12$ edge state ‘disintegrates’

$$\varepsilon = 0.1, \kappa = 0.3, \rho = 1, \nu = 0.1, \omega_0 = 2\pi/3$$

Conclusion

Photonic lattices with longitudinal variation

- Systematic method to find tight binding equations for complex longitudinally driven lattices
- Special case periodically driven –helical–lattices: Honeycomb and staggered square lattices
- In tight binding (TB) limit find/study discrete linear and NL systems governing wave propagation
- Find Floquet bands; study evolution of edge waves for different sublattice structures: different radii/different frequency/phase offsets...
- Find topological/nontopological edge waves

Conclusion: HC Edge States

Helical Variation I:

Rapid (fast) helical variation:

- Construct asymptotic theory
- Envelope of edge modes satisfy standard NLS eq
- NLS solitons topological case: unidirectional, propagate stably around defects
- Bounded Domain:
 - Linear modes affected by dispersion; integrity of pulses deteriorate
 - NL solitons propagate long distances with little degradation

Conclusion: HC Edge States

Helical Variation II:

Adiabatic helical variation:

- Construct asymptotic theory
- Edge states depend on slow longitudinal coordinate: Z
- Find envelope satisfies NLS-type eq: coefficients depend on Z
- Modes can propagate over entire period or 'disintegrate' over partial period
- Solitons can propagate intact over long distances

Ref.: MJA, C. Curtis, Y-P Ma, J. Cole: 2014 - 2017