



Electron in triangular graphene dots

J. Hrivnák, L. Motlochová

Czech Technical University in Prague, Faculty of Nuclear Sciences and
Physical Engineering, Břehová 7, 115 19 Praha 1

September 6, 2022

AAMP XIX, Prague, Czech Republic

Motivation

General aim

(non-relativistic) electron propagation in triangular graphene quantum dots

Mathematical part

- honeycomb lattice via the root and weight lattices of the crystallographic root system A_2
- armchair and zigzag honeycomb Fourier–Weyl transforms

Physical part

- Hamiltonian description of discrete quantum billiard-type systems on honeycomb lattice
- incorporation of boundary conditions

References

- J. Hrivnák, L. Motlochová, *On electron propagation in triangular graphene quantum dots*, J. Phys. A: Math. Theor. **55** (2022) 125201
- J. Hrivnák, L. Motlochová, *Discrete cosine and sine transforms generalized to honeycomb lattice*, J. Math. Phys. **59** (2018) 063503
- J. Hrivnák, L. Motlochová, *Discrete cosine and sine transforms generalized to honeycomb lattice II. Zigzag boundaries*, J. Math. Phys. **62** (2021) 093504
- T. Czyżycki, J. Hrivnák, L. Motlochová, *Generalized Dual-Root Lattice Transforms of Affine Weyl Groups*, Symmetry **12** (2020) 1018
- A. Brus, J. Hrivnák, L. Motlochová, *Quantum particle on dual root lattice in Weyl alcove*, J. Phys. A: Math. Theor. **54** (2021) 095202
- A. U. Klimyk, J. Patera, *Orbit functions*, SIGMA **2** (2006) 006
- R. V. Moody, J. Patera, *Orthogonality within the families of C -, S -, and E -functions of any compact semisimple Lie group*, SIGMA **2** (2006) 076

Outline

1 Honeycomb Fourier–Weyl Transforms

- Root and weight lattices
- Triangular honeycomb dots
- Honeycomb Weyl orbit functions

2 Electron propagation in TGQDs

- Hamiltonians
- Time-independent Schrödinger equations
- Electronic probability densities

Root system A_2

- the **irreducible crystallographic root system** $\Pi(A_2)$ of rank 2
- the set of **simple roots** $\Delta = \{\alpha_1, \alpha_2\} \subset \Pi$, $\text{span}_{\mathbb{R}} \Delta = \mathbb{R}^2$, scalar product $\langle \cdot, \cdot \rangle$
- roots of the same length with relative angle $2\pi/3$

$$\langle \alpha_1, \alpha_1 \rangle = \langle \alpha_2, \alpha_2 \rangle = 2, \quad \langle \alpha_1, \alpha_2 \rangle = -1$$

- \mathbb{Z} -dual ω -basis $\{\omega_1, \omega_2\}$

$$\langle \omega_i, \alpha_j \rangle = \delta_{ij}, \quad i, j \in \{1, 2\}$$

- reflections** r_i , $i \in \{1, 2\}$ for $x \in \mathbb{R}^2$

$$r_i x = x - \langle x, \alpha_i \rangle \alpha_i$$

- Weyl group** W generated by r_1, r_2
- group of the **sign homomorphisms** $\Sigma = \{1, \sigma^e\} \simeq \mathbb{Z}_2$

$$1(w) = 1, \quad \sigma^e(w) = \det(w)$$

Root and weight lattices

- **even Weyl group** W^e

$$W^e = \{w \in W \mid \sigma^e(w) = 1\}$$

- **root lattice** Q and **weight lattice** P

$$Q = \mathbb{Z}\alpha_1 + \mathbb{Z}\alpha_2$$

$$P = \mathbb{Z}\omega_1 + \mathbb{Z}\omega_2$$

- disjoint **decompositions of the lattices** P and $\frac{1}{3}Q$

$$P = Q \cup \{\omega_1 + Q\} \cup \{-\omega_1 + Q\}$$

$$\frac{1}{3}Q = P \cup \left\{\frac{1}{3}\alpha_1 + P\right\} \cup \left\{-\frac{1}{3}\alpha_1 + P\right\}$$

- **extended affine Weyl group** W_P^{aff} and **affine Weyl group** $W^{\text{aff}} \subset W_P^{\text{aff}}$

$$W_P^{\text{aff}} = P \rtimes W$$

$$W^{\text{aff}} = Q \rtimes W$$

- **fundamental domains** $F_P \subset F \subset \mathbb{R}^2$
- coordinate x_0 of $x = x_1\omega_1 + x_2\omega_2 \in MF$, $x_0 = M - x_1 - x_2$

$$x \equiv [x_0, x_1, x_2]_M$$

Counting functions

- magnifying factor $M \in \mathbb{N}$, **counting functions** $h_M : MF \rightarrow \mathbb{N}$ and $\varepsilon : F \rightarrow \mathbb{N}$

$$h_M(x) = |\text{Stab}_{W^{\text{aff}}} \left(\frac{x}{M} \right)|, \quad \varepsilon(x) = \frac{|W|}{h_1(x)}$$

- **retraction homomorphism** $\psi : W^{\text{aff}} \rightarrow W$ for $z = T(q)w \in W^{\text{aff}}$

$$\psi(z) = w$$

- for any $a \in \mathbb{R}^2$ there exists $a' \in F$ and $z[a] \in W^{\text{aff}}$ such that

$$a = z[a]a'$$

Function $\chi^\sigma : \mathbb{R}^2 \rightarrow \{-1, 0, 1\}$

$$\chi^\sigma(a) = \begin{cases} \sigma \circ \psi(z[a]), & \sigma \circ \psi(\text{Stab}_{W^{\text{aff}}}(a)) = 1 \\ 0, & \sigma \circ \psi(\text{Stab}_{W^{\text{aff}}}(a)) = \{1, -1\} \end{cases}$$

- **signed fundamental domain** $F^\sigma \subset F$

$$F^\sigma = \{x \in F \mid \chi^\sigma(x) = 1\}$$

Outline

1 Honeycomb Fourier–Weyl Transforms

- Root and weight lattices
- **Triangular honeycomb dots**
- Honeycomb Weyl orbit functions

2 Electron propagation in TGQDs

- Hamiltonians
- Time-independent Schrödinger equations
- Electronic probability densities

Armchair honeycomb dots

- W^{aff} -invariant **honeycomb lattice** A_M subtractively

$$A_M = \frac{1}{M}(P \setminus Q) = A_M^+ \cup A_M^-$$

- sublattices** of the honeycomb lattice A_M

$$A_M^+ = \frac{1}{M}(\omega_1 + Q)$$

$$A_M^- = \frac{1}{M}(-\omega_1 + Q)$$

- armchair sign function** $\text{sga} : A_M \rightarrow \{1, -1\}$, $\text{sga}(wa) = \text{sga}(a)$, $w \in W$

$$\text{sga}(a) = \begin{cases} 1, & a \in A_M^+, \\ -1, & a \in A_M^- \end{cases}$$

- armchair neighbourhood sets** $B_{A,M}^{(k)}(a) \subset A_M$, $k \in \{0, 1, 2\}$

$$B_{A,M}^{(0)}(a) = a$$

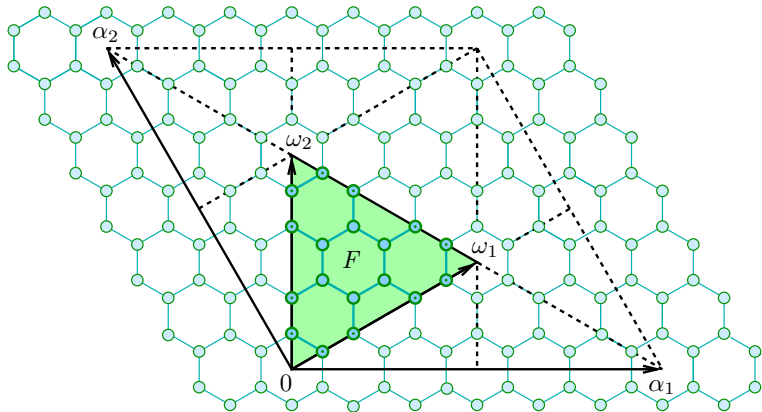
$$B_{A,M}^{(1)}(a) = a + \text{sga}(a) W^e \left(\frac{\omega_1}{M} \right)$$

$$B_{A,M}^{(2)}(a) = a + W \left(\frac{\alpha_1}{M} \right)$$

- armchair honeycomb dots** $H_{A,M}^\sigma$, $\sigma \in \Sigma$

$$H_{A,M}^\sigma = A_M \cap F^\sigma$$

Armchair honeycomb dots $H_{A,6}^\sigma$



Armchair weight sets

- weight sets $L_M^\sigma \subset P, \sigma \in \Sigma$

$$L_M^\sigma = P \cap MF^\sigma$$

- weight sets in Kac coordinates

$$L_M^1 = \left\{ [\lambda_0, \lambda_1, \lambda_2]_M \mid \lambda_0, \lambda_1, \lambda_2 \in \mathbb{Z}^{\geq 0} \right\}$$

$$L_M^{\sigma^e} = \{ [\lambda_0, \lambda_1, \lambda_2]_M \mid \lambda_0, \lambda_1, \lambda_2 \in \mathbb{N} \}$$

- armchair weight sets** $L_{A,M}^{\sigma,\pm}$

$$L_{A,M}^{\sigma,\pm} = \{ \lambda \in L_M^\sigma \mid (\lambda_0 > \lambda_1, \lambda_0 > \lambda_2) \vee (\lambda_0 = \lambda_1 > \lambda_2) \}$$

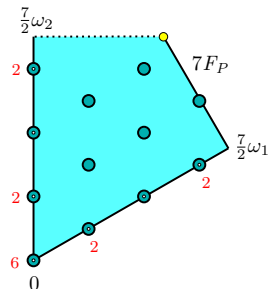
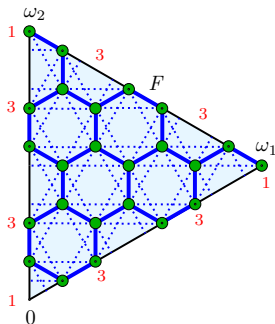
- sums of numbers of weights in $L_{A,M}^{\sigma,+}$ and $L_{A,M}^{\sigma,-}$

$$\left| L_{A,M}^{\sigma,+} \right| + \left| L_{A,M}^{\sigma,-} \right| = \left| H_{A,M}^\sigma \right|$$

- armchair weight transformation** $\gamma_2 : L_M^1 \rightarrow P$ for $\lambda \in L_M^1$

$$\gamma_2 \lambda = (r_1 r_2)^2 \lambda + M \omega_2$$

Armchair honeycomb dots $H_{A,7}^\sigma$ and weight sets $L_{A,7}^{\sigma,\pm}$



Zigzag honeycomb dots

- W^{aff} -invariant **honeycomb lattice** Z_M subtractively

$$Z_M = \frac{1}{M}(\frac{1}{3}Q \setminus P) = Z_M^+ \cup Z_M^-$$

- **sublattices** of the honeycomb lattice Z_M

$$Z_M^+ = \frac{1}{M}(\frac{1}{3}\alpha_1 + P)$$

$$Z_M^- = \frac{1}{M}(-\frac{1}{3}\alpha_1 + P)$$

- **zigzag sign function** $\text{sgz} : Z_M \rightarrow \{1, -1\}$, $\text{sgz}(wa) = \sigma^e(w) \text{sgz}(a)$,
 $w \in W$

$$\text{sgz}(a) = \begin{cases} 1, & a \in Z_M^+, \\ -1, & a \in Z_M^- \end{cases}$$

- **zigzag neighbourhood sets** $B_{Z,M}^{(k)}(a) \subset Z_M$, $k \in \{0, 1, 2\}$

$$B_{Z,M}^{(0)}(a) = a$$

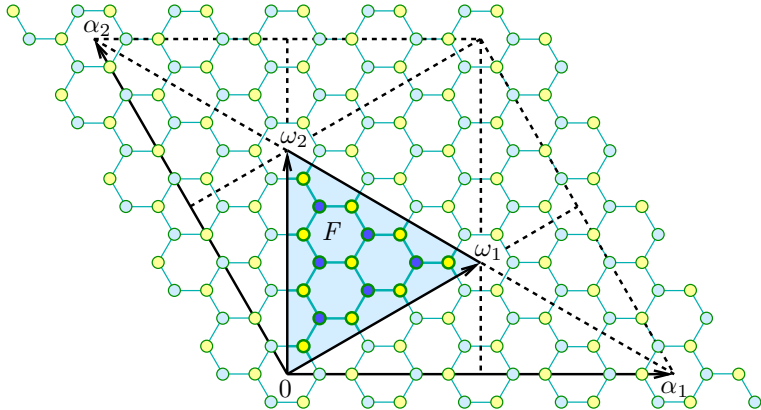
$$B_{Z,M}^{(1)}(a) = a + \text{sgz}(a) W^e \left(\frac{\alpha_1}{3M} \right)$$

$$B_{Z,M}^{(2)}(a) = a + [W^e \left(\frac{\omega_1}{M} \right) \cup W^e \left(-\frac{\omega_1}{M} \right)]$$

- **zigzag honeycomb dots** $H_{Z,M}^\sigma$, $\sigma \in \Sigma$

$$H_{Z,M}^\sigma = Z_M \cap F^\sigma$$

Zigzag honeycomb dots $H_{Z,4}^\sigma$



Zigzag weight sets

- zigzag boundary weight subsets of L_M^1

$$L_M^{Z,a} = \left\{ [0, \lambda_1, \lambda_2]_M \mid \lambda_1, \lambda_2 \in \mathbb{N} \right\}$$

$$L_M^{Z,c} = \left\{ [\lambda_0, 0, \lambda_2]_M \mid \lambda_0, \lambda_2 \in \mathbb{N} \right\} \cup \left\{ [\lambda_0, \lambda_1, 0]_M \mid \lambda_0, \lambda_1 \in \mathbb{N} \right\}$$

$$O_M^Z = \{[M, 0, 0]_M\}$$

- **zigzag weight sets** $L_{Z,M}^{\sigma,\pm}$

$$L_{Z,M}^{1,+} = L_{Z,M}^{\sigma^e,-} = L_M^{\sigma^e} \cup L_M^{Z,a}$$

$$L_{Z,M}^{1,-} = L_{Z,M}^{\sigma^e,+} = L_M^{\sigma^e} \cup O_M^Z \cup L_M^{Z,c}$$

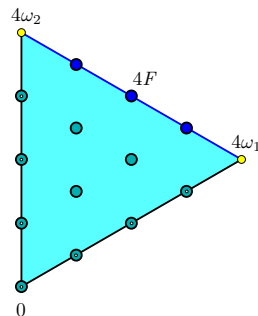
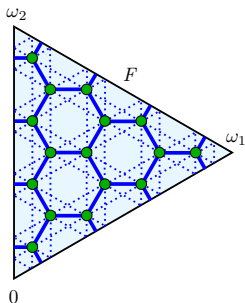
- sums of numbers of weights in $L_{Z,M}^{\sigma,+}$ and $L_{Z,M}^{\sigma,-}$

$$|L_{Z,M}^{\sigma,+}| + |L_{Z,M}^{\sigma,-}| = |H_{Z,M}^{\sigma}|$$

- **zigzag weight transformation** $\beta_1 : L_M^1 \rightarrow P$ for $\lambda \in L_M^1$

$$\beta_1 \lambda = r_1 r_2 r_1 \lambda + M(\omega_1 + \omega_2)$$

Zigzag honeycomb dots $H_{Z,4}^\sigma$ and weight sets $L_{Z,4}^{\sigma,\pm}$



Outline

1 Honeycomb Fourier–Weyl Transforms

- Root and weight lattices
- Triangular honeycomb dots
- Honeycomb Weyl orbit functions

2 Electron propagation in TGQDs

- Hamiltonians
- Time-independent Schrödinger equations
- Electronic probability densities

Weyl orbit functions

- **Weyl orbit functions** (C - and S -functions) $\varphi_b^\sigma : \mathbb{R}^2 \rightarrow \mathbb{C}, \sigma \in \Sigma, b \in \mathbb{R}^2, x \in \mathbb{R}^2$

$$\varphi_b^\sigma(x) = \sum_{w \in W} \sigma(w) e^{2\pi i \langle wb, x \rangle}$$

- **even Weyl orbit functions** (E -functions) $\Xi_b : \mathbb{R}^2 \rightarrow \mathbb{C}, b \in \mathbb{R}^2, x \in \mathbb{R}^2$

$$\Xi_b(x) = \sum_{w \in W^e} e^{2\pi i \langle wb, x \rangle}$$

- product-to-sum formulas of φ_b^σ and $\varphi_b^{\sigma'}, \sigma, \sigma' \in \Sigma, x, y \in \mathbb{R}^2$

$$\varphi_b^\sigma(x) \varphi_b^{\sigma'}(y) = \sum_{w \in W} \sigma'(w) \varphi_b^{\sigma \cdot \sigma'}(x + wy)$$

- (anti)symmetries for $x' \in F$ and $x \in W^{\text{aff}} x'$

$$\varphi_\lambda^\sigma(x) = \chi^\sigma(x) \varphi_\lambda^\sigma(x')$$

Armchair orbit functions

- extension coefficients $\mu_{0,\lambda}^{A,\sigma,\pm}$ and $\mu_{2,\lambda}^{A,\sigma,\pm}$, $\sigma \in \Sigma$, $\lambda \in L_{A,M}^{\sigma,\pm}$

$$\mu_{0,\lambda}^{A,\sigma,\pm} = \operatorname{Re} \left\{ \left(1 + \frac{i}{\sqrt{3}} \right) \Xi_{\lambda} \left(\frac{\omega_1}{M} \right) \right\}$$

$$\mu_{2,\lambda}^{A,\sigma,\pm} = \operatorname{Re} \left\{ \left(1 - \frac{i}{\sqrt{3}} \right) \Xi_{\lambda} \left(\frac{\omega_1}{M} \right) \right\} \pm \left| \Xi_{\lambda} \left(\frac{\omega_1}{M} \right) \right|$$

- armchair orbit functions** $h_{\lambda}^{A,\sigma,\pm} : \mathbb{R}^2 \rightarrow \mathbb{C}$, $\lambda \in L_{A,M}^{\sigma,\pm}$, $\sigma \in \Sigma$, $x \in \mathbb{R}^2$

$$h_{\lambda}^{A,\sigma,\pm}(x) = \mu_{0,\lambda}^{A,\sigma,\pm} \varphi_{\lambda}^{\sigma}(x) + \mu_{2,\lambda}^{A,\sigma,\pm} \varphi_{\gamma_2 \lambda}^{\sigma}(x)$$

- normalization functions $\mu^{A,\sigma,\pm} : L_{A,M}^{\sigma,\pm} \rightarrow \mathbb{R}^{>0}$ for $\lambda \in L_{A,M}^{\sigma,\pm}$

$$\mu^{A,\sigma,\pm}(\lambda) = \left| \Xi_{\lambda} \left(\frac{\omega_1}{M} \right) \right| \left(2 \left| \Xi_{\lambda} \left(\frac{\omega_1}{M} \right) \right| \pm \operatorname{Re} \left\{ (1 - \sqrt{3}i) \Xi_{\lambda} \left(\frac{\omega_1}{M} \right) \right\} \right)$$

- discrete orthogonality relations**

$$\sum_{a \in H_{A,M}^{\sigma}} \varepsilon(a) \left[h_{\lambda}^{A,\sigma,\pm}(a) \right]^* h_{\lambda'}^{A,\sigma,\pm}(a) = 12M^2 h_M(\lambda) \mu^{A,\sigma,\pm}(\lambda) \delta_{\lambda\lambda'}, \quad \lambda, \lambda' \in L_{A,M}^{\sigma,\pm}$$

$$\sum_{a \in H_{A,M}^{\sigma}} \varepsilon(a) \left[h_{\lambda}^{A,\sigma,+}(a) \right]^* h_{\lambda'}^{A,\sigma,-}(a) = 0, \quad \lambda \in L_{A,M}^{\sigma,+}, \quad \lambda' \in L_{A,M}^{\sigma,-}$$

Zigzag orbit functions

- extension coefficients $\mu_{0,\lambda}^{Z,\sigma,\pm}$ and $\mu_{1,\lambda}^{Z,\sigma,\pm}$, $\sigma \in \Sigma$, $\lambda \in L_{Z,M}^{\sigma,\pm}$

$$\mu_{0,\lambda}^{Z,\sigma,\pm} = \sigma(r_1) \operatorname{Re} \left\{ \left(1 - \frac{i}{\sqrt{3}} \right) \Xi_\lambda \left(\frac{\alpha_1}{3M} \right) \right\}$$

$$\mu_{1,\lambda}^{Z,\sigma,\pm} = \operatorname{Re} \left\{ \left(1 + \frac{i}{\sqrt{3}} \right) \Xi_\lambda \left(\frac{\alpha_1}{3M} \right) \right\} \pm \left| \Xi_\lambda \left(\frac{\alpha_1}{3M} \right) \right|$$

- zigzag orbit functions** $h_\lambda^{Z,\sigma,\pm} : \mathbb{R}^2 \rightarrow \mathbb{C}$, $\lambda \in L_{Z,M}^{\sigma,\pm}$, $\sigma \in \Sigma$, $x \in \mathbb{R}^2$

$$h_\lambda^{Z,\sigma,\pm}(x) = \mu_{0,\lambda}^{Z,\sigma,\pm} \varphi_\lambda^\sigma(x) + \mu_{1,\lambda}^{Z,\sigma,\pm} \varphi_{\beta_1 \lambda}^\sigma(x).$$

- normalization functions $\mu^{Z,\sigma,\pm} : L_{Z,M}^{\sigma,\pm} \rightarrow \mathbb{R}^{>0}$ for $\lambda \in L_{Z,M}^{\sigma,\pm}$

$$\mu^{Z,\sigma,\pm}(\lambda) = 2 \left| \Xi_\lambda \left(\frac{\alpha_1}{3M} \right) \right| \left(2 \left| \Xi_\lambda \left(\frac{\alpha_1}{3M} \right) \right| \pm \operatorname{Re} \left\{ \left(1 + \sqrt{3}i \right) \Xi_\lambda \left(\frac{\alpha_1}{3M} \right) \right\} \right)$$

- discrete orthogonality relations**

$$\sum_{a \in H_{Z,M}^\sigma} \left[h_\lambda^{Z,\sigma,\pm}(a) \right]^* h_{\lambda'}^{Z,\sigma,\pm}(a) = 3M^2 \mu^{Z,\sigma,\pm}(\lambda) \delta_{\lambda\lambda'}, \quad \lambda, \lambda' \in L_{Z,M}^{\sigma,\pm},$$

$$\sum_{a \in H_{Z,M}^\sigma} \left[h_\lambda^{Z,\sigma,+}(a) \right]^* h_{\lambda'}^{Z,\sigma,-}(a) = 0, \quad \lambda \in L_{Z,M}^{\sigma,+}, \lambda' \in L_{Z,M}^{\sigma,-}$$

Outline

- 1 Honeycomb Fourier–Weyl Transforms
 - Root and weight lattices
 - Triangular honeycomb dots
 - Honeycomb Weyl orbit functions

- 2 Electron propagation in TGQDs
 - **Hamiltonians**
 - Time-independent Schrödinger equations
 - Electronic probability densities

Armchair Hamiltonians

- **energy parameters** $I_k \in \mathbb{R}$, with $k \in \{0, 1, 2\}$ and I_1 positive, an electron with the on-site energy $E_0 = -I_0$ propagating with amplitudes iI_1/\hbar and iI_2/\hbar per unit time to the nearest and next-to-nearest lattice positions
- orthonormal **armchair position bases** $|a; A, \sigma\rangle$, $\sigma \in \Sigma$, $a \in H_{A,M}^\sigma$ span the complex Hilbert spaces $\mathcal{H}_{A,M}^\sigma$

- coupling sets

$$N_{A,M}^{(k)}(a, a') = W^{\text{aff}} a' \cap B_{A,M}^{(k)}(a)$$

- **hopping operators** for $a, a' \in H_{A,M}^\sigma$

$$\left\langle a; A, \sigma \left| \widehat{I}_{A,M}^{\sigma, (k)} \right| a'; A, \sigma \right\rangle = -I_k \varepsilon^{\frac{1}{2}}(a) \varepsilon^{-\frac{1}{2}}(a') \sum_{d \in N_{A,M}^{(k)}(a, a')} \chi^\sigma(d)$$

- **tight-binding Hamiltonians** $\widehat{H}_{A,M}^\sigma : \mathcal{H}_{A,M}^\sigma \rightarrow \mathcal{H}_{A,M}^\sigma$

$$\widehat{H}_{A,M}^\sigma = \widehat{I}_{A,M}^{\sigma, (0)} + \widehat{I}_{A,M}^{\sigma, (1)} + \widehat{I}_{A,M}^{\sigma, (2)}$$

Zigzag Hamiltonians

- orthonormal **zigzag position bases** $|a; Z, \sigma\rangle, \sigma \in \Sigma, a \in H_{Z,M}^\sigma$ span the complex Hilbert spaces $\mathcal{H}_{Z,M}^\sigma$

- coupling sets

$$N_{Z,M}^{(k)}(a, a') = W^{\text{aff}} a' \cap B_{Z,M}^{(k)}(a)$$

- **hopping operators** for $a, a' \in H_{Z,M}^\sigma$

$$\left\langle a; Z, \sigma \left| \hat{I}_{Z,M}^{\sigma, (k)} \right| a'; Z, \sigma \right\rangle = -I_k \sum_{d \in N_{Z,M}^{(k)}(a, a')} \chi^\sigma(d)$$

- **tight-binding Hamiltonians** $\hat{H}_{Z,M}^\sigma : \mathcal{H}_{Z,M}^\sigma \rightarrow \mathcal{H}_{Z,M}^\sigma$

$$\hat{H}_{Z,M}^\sigma = \hat{I}_{Z,M}^{\sigma, (0)} + \hat{I}_{Z,M}^{\sigma, (1)} + \hat{I}_{Z,M}^{\sigma, (2)}$$

Armchair momentum bases

- armchair orthonormal **momentum bases** $|\lambda; A, \sigma, \pm\rangle \in \mathcal{H}_{A,M}^\sigma$,
 $\lambda \in L_{A,M}^{\sigma,\pm}$

$$|\lambda; A, \sigma, \pm\rangle = \sum_{a \in H_{A,M}^\sigma} |a; A, \sigma\rangle \langle a; A, \sigma | \lambda; A, \sigma, \pm\rangle$$

where

$$\langle a; A, \sigma | \lambda; A, \sigma, \pm\rangle = \sqrt{\frac{\varepsilon(a)}{12M^2 h_M(\lambda) \mu^{A,\sigma,\pm}(\lambda)}} h_\lambda^{A,\sigma,\pm}(a)$$

- energy functions** $E_A^{(1),\pm}, E_A^{(2)} : F_P \rightarrow \mathbb{R}$ for $x \in F_P$

$$E_A^{(1),\pm}(x) = \pm I_1 |\Xi_{\omega_1}(x)|$$

$$E_A^{(2)}(x) = -2I_2 \operatorname{Re} \{ \Xi_{\alpha_1}(x) \}$$

Zigzag momentum bases

- zigzag orthonormal **momentum bases** $|\lambda; Z, \sigma, \pm\rangle \in \mathcal{H}_{Z,M}^\sigma$, $\lambda \in L_{Z,M}^{\sigma,\pm}$

$$|\lambda; Z, \sigma, \pm\rangle = \sum_{a \in H_{Z,M}^\sigma} |a; Z, \sigma\rangle \langle a; Z, \sigma | \lambda; Z, \sigma, \pm\rangle,$$

where

$$\langle a; Z, \sigma | \lambda; Z, \sigma, \pm\rangle = \sqrt{\frac{1}{3M^2\mu^{Z,\sigma,\pm}(\lambda)}} h_\lambda^{Z,\sigma,\pm}(a)$$

- energy functions** $E_Z^{(1),\pm}, E_Z^{(2)} : F \rightarrow \mathbb{R}$ for $x \in F$

$$E_Z^{(1),\pm}(x) = \pm I_1 \left| \Xi_{\frac{\alpha_1}{3}}(x) \right|$$

$$E_Z^{(2)}(x) = -2I_2 \operatorname{Re} \{ \Xi_{\omega_1}(x) \}$$

Outline

- 1 Honeycomb Fourier–Weyl Transforms
 - Root and weight lattices
 - Triangular honeycomb dots
 - Honeycomb Weyl orbit functions

- 2 Electron propagation in TGQDs
 - Hamiltonians
 - Time-independent Schrödinger equations
 - Electronic probability densities

Time-independent armchair Schrödinger equations

Theorem

Let $L_{A,M}^{\sigma,\pm}$ be the armchair weight sets which correspond to the magnifying factor $M \in \mathbb{N}$ and sign homomorphism $\sigma \in \Sigma$ and let $|\lambda; A, \sigma, \pm\rangle \in \mathcal{H}_{A,M}^{\sigma}$, $\lambda \in L_{A,M}^{\sigma,\pm}$ be the vectors of the armchair momentum basis. Then **each vector** $|\lambda; A, \sigma, \pm\rangle \in \mathcal{H}_{A,M}^{\sigma}$ **satisfies** for the armchair Hamiltonian $\hat{H}_{A,M}^{\sigma}$ the **time-independent armchair Schrödinger equation**,

$$\hat{H}_{A,M}^{\sigma} |\lambda; A, \sigma, \pm\rangle = E_{A,\lambda,M}^{\sigma,\pm} |\lambda; A, \sigma, \pm\rangle,$$

with the **eigenenergy** $E_{A,\lambda,M}^{\sigma,\pm} \in \mathbb{R}$ determined by the armchair energy functions as

$$E_{A,\lambda,M}^{\sigma,\pm} = E_0 + E_A^{(1),\pm} \left(\frac{\lambda}{M} \right) + E_A^{(2)} \left(\frac{\lambda}{M} \right).$$

Time-independent zigzag Schrödinger equations

Theorem

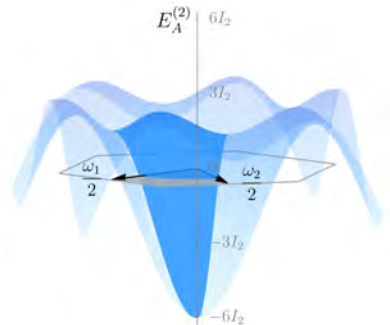
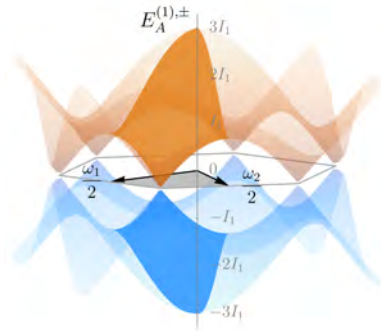
Let $L_{Z,M}^{\sigma,\pm}$ be the zigzag weight sets which correspond to the magnifying factor $M \in \mathbb{N}$ and sign homomorphism $\sigma \in \Sigma$ and let $|\lambda; Z, \sigma, \pm\rangle \in \mathcal{H}_{Z,M}^{\sigma}$, $\lambda \in L_{Z,M}^{\sigma,\pm}$ be the vectors of the zigzag momentum basis. Then **each vector** $|\lambda; Z, \sigma, \pm\rangle \in \mathcal{H}_{Z,M}^{\sigma}$ **satisfies** for the zigzag Hamiltonian $\hat{H}_{Z,M}^{\sigma}$ the **time-independent zigzag Schrödinger equation**,

$$\hat{H}_{Z,M}^{\sigma} |\lambda; Z, \sigma, \pm\rangle = E_{Z,\lambda,M}^{\sigma,\pm} |\lambda; Z, \sigma, \pm\rangle,$$

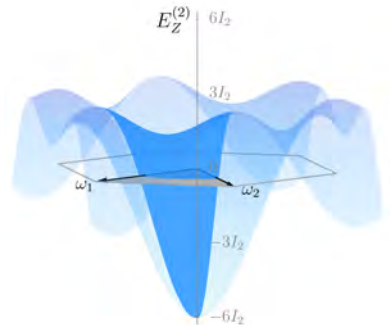
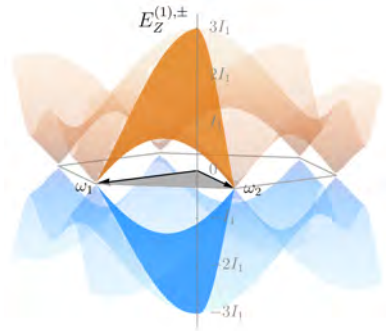
with the **eigenenergy** $E_{Z,\lambda,M}^{\sigma,\pm} \in \mathbb{R}$ determined by the zigzag energy functions as

$$E_{Z,\lambda,M}^{\sigma,\pm} = E_0 + E_Z^{(1),\pm} \left(\frac{\lambda}{M} \right) + E_Z^{(2)} \left(\frac{\lambda}{M} \right).$$

Electronic band structure of the triangular armchair graphene dots



Electronic band structure of the triangular zigzag graphene dots



Outline

- 1 Honeycomb Fourier–Weyl Transforms
 - Root and weight lattices
 - Triangular honeycomb dots
 - Honeycomb Weyl orbit functions

- 2 Electron propagation in TGQDs
 - Hamiltonians
 - Time-independent Schrödinger equations
 - Electronic probability densities

Armchair electronic probability densities

Theorem

Let $L_{A,M}^{\sigma,\pm}$ be the armchair weight sets which correspond to the magnifying factor $M \in \mathbb{N}$ and sign homomorphism $\sigma \in \Sigma$ and let $P_M[\lambda; A, \sigma, \pm]$, $\lambda \in L_{A,M}^{\sigma,\pm}$ be the armchair electronic probability densities. Then the **armchair probability densities** $P_M[\lambda; A, \sigma, +]$ and $P_M[\lambda; A, \sigma, -]$ **coincide** for each $\lambda \in L_{A,M}^{\sigma,+}$ and evaluate for $a \in H_{A,M}^\sigma$ as

$$P_M[\lambda; A, \sigma, \pm](a) = |\langle a; A, \sigma \mid \lambda; A, \sigma, \pm \rangle|^2 = \frac{\varepsilon(a)}{12M^2 h_M(\lambda)} |\varphi_\lambda^\sigma(a)|^2.$$

Zigzag electronic probability densities

Theorem

Let $L_{Z,M}^{\sigma,\pm}$ be the zigzag weight sets which correspond to the magnifying factor $M \in \mathbb{N}$ and sign homomorphism $\sigma \in \Sigma$ and let $P_M[\lambda; Z, \sigma, \pm]$, $\lambda \in L_{Z,M}^{\sigma,\pm}$ be the zigzag electronic probability densities given for $a \in H_{Z,M}^\sigma$ as

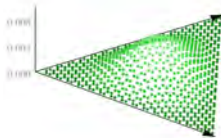
$$P_M[\lambda; Z, \sigma, \pm](a) = |\langle a; Z, \sigma \mid \lambda; Z, \sigma, \pm \rangle|^2 = \frac{1}{3M^2 \mu^{Z,\sigma,\pm}(\lambda)} \left| h_\lambda^{Z,\sigma,\pm}(a) \right|^2.$$

Then the **zigzag probability densities** $P_M[\lambda; Z, \sigma^e, \pm]$ and $P_M[\lambda; Z, 1, \mp]$ **coincide** for any $\lambda \in L_{Z,M}^{\sigma^e,\pm}$,

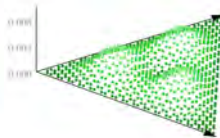
$$P_M[\lambda; Z, \sigma^e, \pm] = P_M[\lambda; Z, 1, \mp].$$

Electronic probability densities of the triangular armchair dots

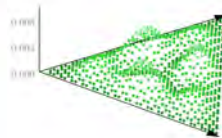
$P_{50}[(1, 1); A, \sigma^e, \pm]$



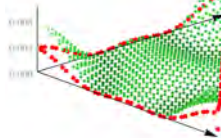
$P_{50}[(2, 1); A, \sigma^e, \pm]$



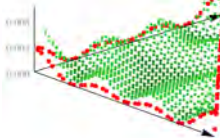
$P_{50}[(3, 1); A, \sigma^e, \pm]$



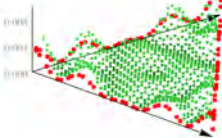
$P_{50}[(1, 1); A, 1, \pm]$



$P_{50}[(2, 1); A, 1, \pm]$

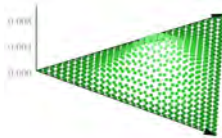


$P_{50}[(3, 1); A, 1, \pm]$

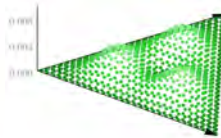


Electronic probability densities of the triangular zigzag dots

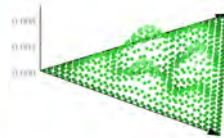
$P_{29}[(1, 1); Z, \sigma^e, -]$



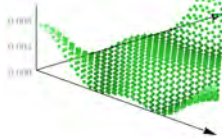
$P_{29}[(2, 1); Z, \sigma^e, -]$



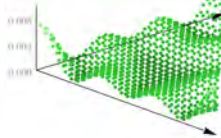
$P_{29}[(3, 1); Z, \sigma^e, -]$



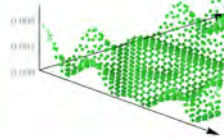
$P_{29}[(1, 1); Z, \sigma^e, +]$



$P_{29}[(2, 1); Z, \sigma^e, +]$



$P_{29}[(3, 1); Z, \sigma^e, +]$



Summary

- **electron propagations** in the triangular armchair and zigzag graphene quantum dots surrounded by the Neumann and Dirichlet walls determined by the **four Hamiltonians**
- **honeycomb Weyl orbit functions** and the corresponding **discrete Fourier–Weyl transforms**
- **energy spectra** corresponding to the electron armchair and zigzag stationary states exactly calculated
- armchair **Neumann boundary effect**, armchair energy relations transform exactly to the standard graphene tight-binding next-to-nearest neighbour coupling **energy bands**
- zigzag probability **density role switching** between the Dirichlet/Neumann boundary behaviour and the valence/conduction states
- (ideal) zigzag **edge states, repulsive** behaviour of **Neumann walls** predicted for zigzag conduction states
- effects of the three corner positions, zero energy states, higher-degree couplings, energy degeneracy, magnetic field, representations of $SU(3)$

References

- A. V. Rozhkov, F. Nori, *Exact wave functions for an electron on a graphene triangular quantum dot*, Phys. Rev. B **81** (2010) 155401
- J. Akola, H. P. Heiskanen, M. Manninen, *Edge-dependent selection rules in magic triangular graphene flakes*, Phys. Rev. B **77** (2008) 193410
- A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, *The electronic properties of graphene*, Rev. Mod. Phys. **81** (2009) 109–162
- S. Phark et al., *Direct Observation of Electron Confinement in Epitaxial Graphene Nanoislands*, ACS Nano **5** (2011) 8162–8166
- M. Zarenia, A. Chaves, G. A. Farias, F. M. Peeters, *Energy levels of triangular and hexagonal graphene quantum dots: A comparative study between the tight-binding and Dirac equation approach*, Phys. Rev. B **84** (2011) 245403
- Q. Zhang et al., *Investigation of edge states in artificial graphene nano-flakes*, J. Phys.: Condens. Matter **33** (2021) 225003