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

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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

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Outline

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Root system A_2

- the **irreducible crystallographic root system** $\Pi(A_2)$ of rank 2
- the set of **simple roots** $\Delta = \{\alpha_1, \alpha_2\} \subset \Pi$, $\mathrm{span}_{\mathbb{R}} \Delta = \mathbb{R}^2$, scalar product $\langle \, , \, \rangle$
- 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** $\Sigma = \{\mathfrak{1}, \sigma^e\} \simeq \mathbb{Z}_2$

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

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Root and weight lattices

- **even Weyl group** W^e

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

- **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 $\frac{1}{3}Q$

$$P = Q \cup \{\omega_1 + Q\} \cup \{-\omega_1 + Q\}$$
$$\tfrac{1}{3}Q = P \cup \left\{\tfrac{1}{3}\alpha_1 + P\right\} \cup \left\{-\tfrac{1}{3}\alpha_1 + P\right\}$$

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

$$W_P^{\mathrm{aff}} = P \rtimes W$$
$$W^{\mathrm{aff}} = Q \rtimes W$$

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

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

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Counting functions

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

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

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

$$\psi(z) = w$$

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

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

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

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

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

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

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Armchair honeycomb dots

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

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

- **sublattices** of the honeycomb lattice A_M

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

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

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

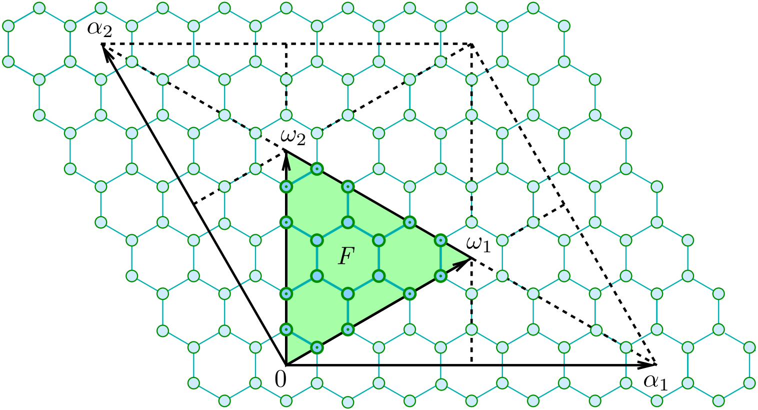
- **armchair neighbourhood sets** $B^{(k)}_{A,M}(a) \subset A_M$, $k \in \{0,1,2\}$

$$B^{(0)}_{A,M}(a) = a$$
$$B^{(1)}_{A,M}(a) = a + \mathrm{sga}(a)\, W^e\left(\tfrac{\omega_1}{M}\right)$$
$$B^{(2)}_{A,M}(a) = a + W\left(\tfrac{\alpha_1}{M}\right)$$

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

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

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



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

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

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

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

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

- 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** $\gamma_2 : L_M^1 \to P$ for $\lambda \in L_M^1$

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

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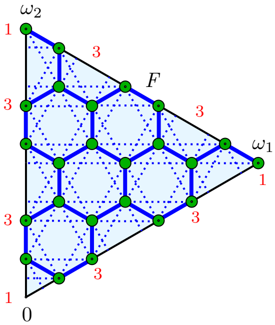
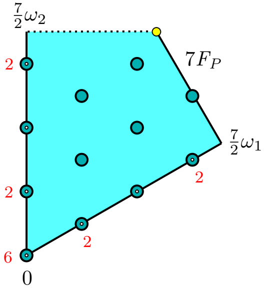
Armchair honeycomb dots $H^{\sigma}_{A,7}$ and weight sets $L^{\sigma,\pm}_{A,7}$





Zigzag honeycomb dots

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

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

- **sublattices** of the honeycomb lattice Z_M

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

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

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

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

$$B^{(0)}_{Z,M}(a) = a$$
$$B^{(1)}_{Z,M}(a) = a + \mathrm{sgz}(a)\, W^e\left(\tfrac{\alpha_1}{3M}\right)$$
$$B^{(2)}_{Z,M}(a) = a + \left[W^e\left(\tfrac{\omega_1}{M}\right) \cup W^e\left(-\tfrac{\omega_1}{M}\right)\right]$$

- **zizgzag honeycomb dots** $H^\sigma_{Z,M}$, $\sigma \in \Sigma$

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

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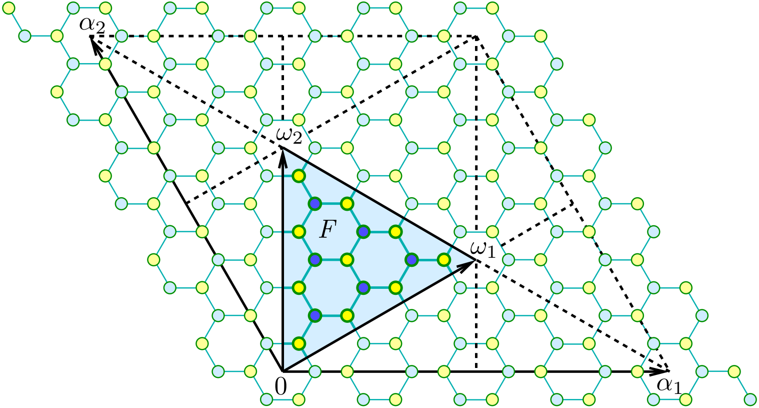
Zigzag honeycomb dots $H^{\sigma}_{Z,4}$



Zigzag weight sets

- zigzag boundary weight subsets of L_M^{1}

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

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

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

- **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 $L_{Z,M}^{\sigma,-}$

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

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

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

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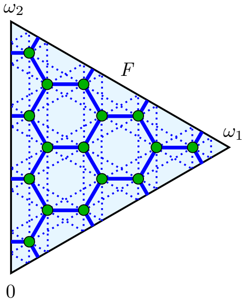
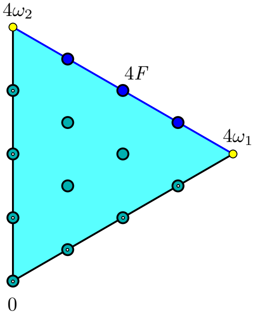
Zigzag honeycomb dots $H^{\sigma}_{Z,4}$ and weight sets $L^{\sigma,\pm}_{Z,4}$





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Weyl orbit functions

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

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

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

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

- 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 $x \in W^{\mathrm{aff}} x'$

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

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Armchair orbit functions

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

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

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

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

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

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

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

- **discrete orthogonality relations**

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

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

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Zigzag orbit functions

- extension coefficients $\mu^{Z,\sigma,\pm}_{0,\lambda}$ and $\mu^{Z,\sigma,\pm}_{1,\lambda}$, $\sigma\in\Sigma$, $\lambda\in L^{\sigma,\pm}_{Z,M}$

$$\begin{aligned}\mu^{Z,\sigma,\pm}_{0,\lambda}&=\sigma(r_1)\,\mathrm{Re}\left\{\left(1-\tfrac{\mathrm{i}}{\sqrt{3}}\right)\Xi_\lambda\left(\tfrac{\alpha_1}{3M}\right)\right\}\\ \mu^{Z,\sigma,\pm}_{1,\lambda}&=\mathrm{Re}\left\{\left(1+\tfrac{\mathrm{i}}{\sqrt{3}}\right)\Xi_\lambda\left(\tfrac{\alpha_1}{3M}\right)\right\}\pm\left|\Xi_\lambda\left(\tfrac{\alpha_1}{3M}\right)\right|\end{aligned}$$

- **zigzag orbit functions** $\mathrm{h}^{Z,\sigma,\pm}_\lambda:\mathbb{R}^2\to\mathbb{C}$, $\lambda\in L^{\sigma,\pm}_{Z,M}$, $\sigma\in\Sigma$, $x\in\mathbb{R}^2$

$$\mathrm{h}^{Z,\sigma,\pm}_\lambda(x)=\mu^{Z,\sigma,\pm}_{0,\lambda}\varphi^\sigma_\lambda(x)+\mu^{Z,\sigma,\pm}_{1,\lambda}\varphi^\sigma_{\beta_1\lambda}(x).$$

- normalization functions $\mu^{Z,\sigma,\pm}:L^{\sigma,\pm}_{Z,M}\to\mathbb{R}^{>0}$ for $\lambda\in L^{\sigma^e}_M$

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

- **discrete orthogonality relations**

$$\sum_{a\in H^\sigma_{Z,M}}\left[\mathrm{h}^{Z,\sigma,\pm}_\lambda(a)\right]^*\mathrm{h}^{Z,\sigma,\pm}_{\lambda'}(a)=3M^2\mu^{Z,\sigma,\pm}(\lambda)\delta_{\lambda\lambda'},\quad\lambda,\lambda'\in L^{\sigma,\pm}_{Z,M},$$

$$\sum_{a\in H^\sigma_{Z,M}}\left[\mathrm{h}^{Z,\sigma,+}_\lambda(a)\right]^\star\mathrm{h}^{Z,\sigma,-}_{\lambda'}(a)=0,\quad\lambda\in L^{\sigma,+}_{Z,M},\ \lambda'\in L^{\sigma,-}_{Z,M}$$

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Outline

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 $\mathrm{i}I_1/\hbar$ and $\mathrm{i}I_2/\hbar$ per unit time to the nearest and next-to-nearest lattice positions
- orthonormal **armchair position bases** $|a; A, \sigma\rangle$, $\sigma \in \Sigma$, $a \in H^\sigma_{A,M}$ span the complex Hilbert spaces $\mathcal{H}^\sigma_{A,M}$
- coupling sets

$$N^{(k)}_{A,M}(a,a') = W^{\mathrm{aff}} a' \cap B^{(k)}_{A,M}(a)$$

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

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

- **tight-binding Hamiltonians** $\widehat{H}^\sigma_{A,M} : \mathcal{H}^\sigma_{A,M} \to \mathcal{H}^\sigma_{A,M}$

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

Zigzag Hamiltonians

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

$$N^{(k)}_{Z,M}(a, a') = W^{\mathrm{aff}} a' \cap B^{(k)}_{Z,M}(a)$$

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

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

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

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

Armchair momentum bases

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

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

where

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

- **energy functions** $E^{(1),\pm}_{A}, E^{(2)}_{A} : F_P \to \mathbb{R}$ for $x \in F_P$

$$E^{(1),\pm}_{A}(x) = \pm I_1 \left|\Xi_{\omega_1}(x)\right|$$
$$E^{(2)}_{A}(x) = -2I_2 \operatorname{Re}\left\{\Xi_{\alpha_1}(x)\right\}$$

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Zigzag momentum bases

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

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

where

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

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

$$E^{(1),\pm}_Z(x) = \pm I_1 \left|\Xi_{\frac{\alpha_1}{3}}(x)\right|$$
$$E^{(2)}_Z(x) = -2I_2 \,\mathrm{Re}\left\{\Xi_{\omega_1}(x)\right\}$$

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Time-independent armchair Schrödinger equations

Theorem

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

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

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

$$E^{\sigma,\pm}_{A,\lambda,M} = E_0 + E^{(1),\pm}_{A}\left(\tfrac{\lambda}{M}\right) + E^{(2)}_{A}\left(\tfrac{\lambda}{M}\right).$$

Time-independent zigzag Schrödinger equations

Theorem

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

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

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

$$E^{\sigma,\pm}_{Z,\lambda,M} = E_0 + E^{(1),\pm}_{Z}\left(\tfrac{\lambda}{M}\right) + E^{(2)}_{Z}\left(\tfrac{\lambda}{M}\right).$$

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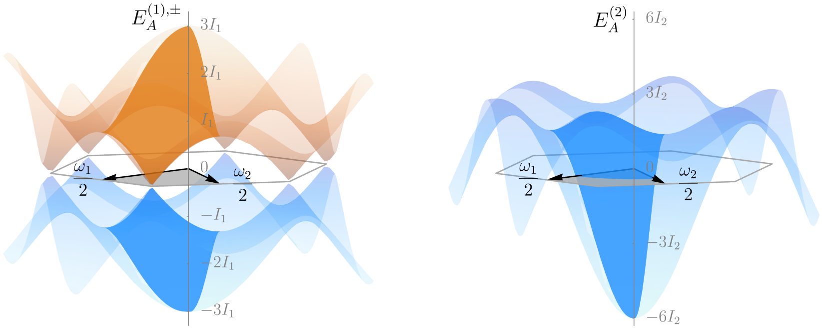
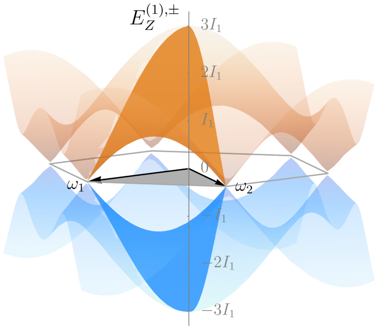
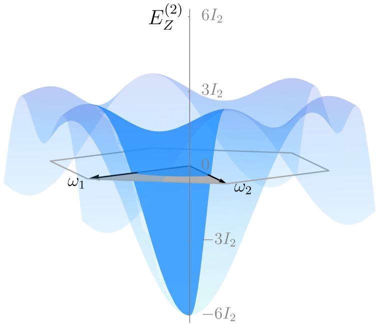
Electronic band structure of the triangular armchair graphene dots



Electronic band structure of the triangular zigzag graphene dots





Outline

Armchair electronic probability densities

Theorem

Let $L^{\sigma,\pm}_{A,M}$ be the armchair weight sets which correspond to the magnifying factor $M \in \mathbb{N}$ and sign homomorphism $\sigma \in \Sigma$ and let $P_M[\lambda; A, \sigma, \pm]$, $\lambda \in L^{\sigma,\pm}_{A,M}$ 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 $\lambda \in L^{\sigma,+}_{A,M}$ and evaluate for $a \in H^{\sigma}_{A,M}$ as

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

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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

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

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

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

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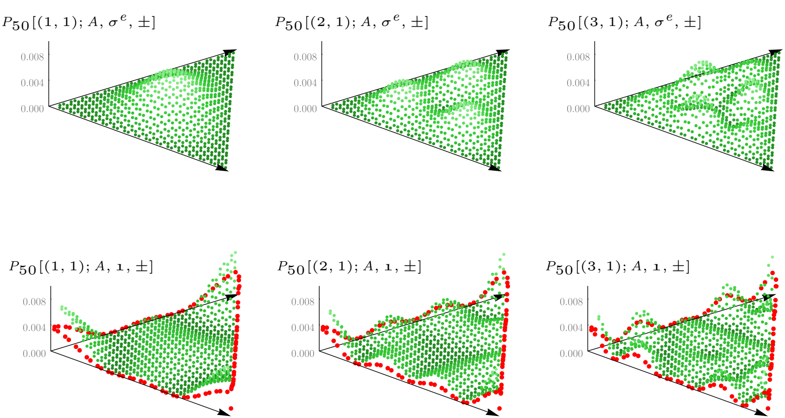
Electronic probability densities of the triangular armchair dots



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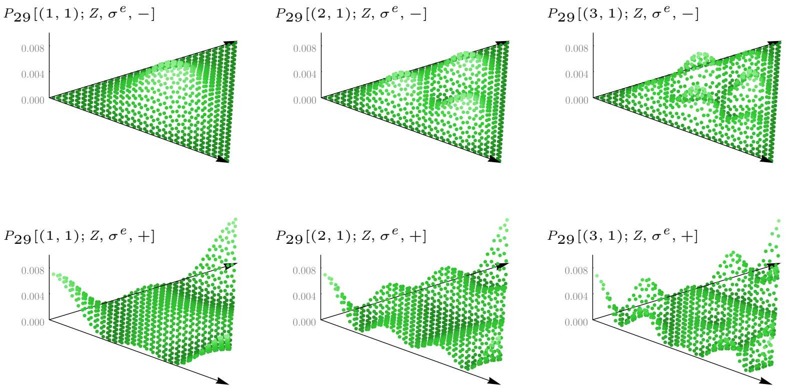
Electronic probability densities of the triangular zigzag dots



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 $SU(3)$

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