Quantum graph model of a graphyne and graphyne nanotubes

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Graphene - 2D hexagonal carbon allotrope
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2010 Nobel prize in physics.
Wonderful properties: stronger than steel, transparent, better electric conductivity than copper.
Band functions and spectral bands. Might cross/overlap.
Dirac points

Why remarkable electric properties?
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Stable Dirac points!
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- Quantum graph model - P. Kuchment and O. Post
- 2D Schrödinger - C. Fefferman, M. Weinstein, G. Berkolaiko, A. Comech
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High promise.
Nanotubes

Carbon nanotubes: layers of graphene/graphyne rolled onto a cylinder
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Spectrum depends on the type of nanotubes.
Graphyne and Schrödinger operators

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Quantum graph = graph + metric + differential operator
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\[ H = -\frac{d^2}{dx^2} + q(x) \]
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\[ H = - \frac{d^2}{dx^2} + q(x) \]

\[ q_0(x) \] - even real potential on \([-0.5,0.5]\] transferred to invariant potential \( q(x) \)
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Neumann vertex condition
Graphyne nanotubes and Schrödinger operators

Graphyne nanotube $T_p, p = (3, 1)$
Graphyne nanotubes and Schrödinger operators

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$u(x)$ is a function on $G$ s.t. $u(x + p_1e_1 + p_2e_2) = u(x)$.
Graphyne nanotubes and Schrödinger operators

Graphyne nanotube $T_p, p = (3, 1)$

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$u(x)$ is a function on $G$ s.t. $u(x + p_1e_1 + p_2e_2) = u(x)$. Neumann vertex condition
Graphyne spectrum

\[ \sigma_{sc}(H) = \emptyset \]

\[ \sigma_{ac}(H) = \sigma(H_{\text{per}}) \]

\[ H_{\text{per}} = -\frac{d^2}{dx^2} + q(x) \text{ on } \mathbb{R} \]

\[ \sigma_{pp}(H) = \sum D \] and is located at band edges

\[ \sum D \text{ of } -\frac{d^2}{dx^2} + q_0(x) \text{ on } [-0.5,0.5] \]

Eigenvalues \( \lambda \in \sigma_{pp}(H) \) - infinite multiplicity

Description of all compactly bounded eigenfunctions - generators

Each band of \( \sigma(H_{\text{per}}) \) consists of three touching bands of \( \sigma(H) \)

Stable Dirac cones at touching points of spectral bands

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- $\sigma_{pp}(H) = \Sigma_D$ and is located at band edges
  - $\Sigma_D$ - Dirichlet spectrum of $-d^2/dx^2 + q_0(x)$ on $[-0.5,0.5]$
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- **Stable Dirac cones** at touching points of spectral bands
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Compactely supported eigenfunctions generating eigenspaces are provided (simple/tube loop eigenfunctions)
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Eigenvalues - infinite multiplicity
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'y' versus 'e'

Why could graphyne be better than graphene?
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Stable Dirac points
Directionality

Directional conductance

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Quantum graph model of a graphyne and graphyne nanotubes
Reduction from quantum graph to discrete graph model
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   • Reduce study from infinite graph to fundamental domain using Floquet-Bloch theory.
Proof outline

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2. Analyze explicitly (construct the eigenfunctions-generators)
References


Thank you!