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Schrödinger Operators on a Zigzag Supergraphene-Based Carbon Nanotube

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Abstract. Throughout this paper, we study the spectrum of a periodic Schrödinger operator on a zigzag super carbon nanotube, which is a generalization of the zigzag carbon nanotube. We prove that its absolutely continuous spectrum has the band structure. Moreover, we show that its eigenvalues with infinite multiplicities consisting of the Dirichlet eigenvalues and points embedded in the spectral band for some corresponding Hill operator. We also give the asymptotics for the spectral band edges.

AMS subject classifications: 34L05, 34L15, 34B45

Key words: Carbon nanotube, zigzag nanotube, supergraphene, quantum graph, spectral gap, band structure, Floquet–Bloch theory, Hill operator.

1 Introduction

The Royal Swedish Academy of Sciences has awarded the Nobel Prize in Physics for 2010 to A. Geim and K. Novoselov for groundbreaking experiments regarding the two-dimensional material graphene (Fig. 1). Graphene is a thin monolayer of pure carbons located in the vertexes of the hexagonal lattice. Although its thickness is a single atom size, graphene is also known as the strongest materials. Moreover, graphene has outstanding properties on the thermal and electrical conduction and tribology. Thus, graphene nowadays plays important roles in the field of mechanical engineering. These days, mathematicians are also interested in the spectral theory for differential and difference Schrödinger operators on the metric and discrete graph corresponding to materials with nanostructures. As stated in the opening paragraph of [3], researchers recently are suggesting new models of two-dimensional carbon allotropes and studying its properties as materials before they are synthesized. Graphene-like models are called *graphynes*. Do

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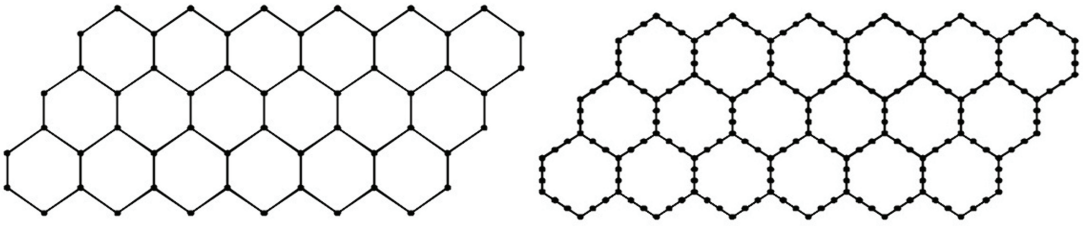

Fig. 1: Graphene (left) and supergraphene (right).

and Kuchment [3] studied the dispersion relations and spectra of Schrödinger operators on one of graphynes, namely, the 2-dimensional lattice consisting of hexagons and rhombuses. In the dispersion relation, they found spectral gaps and conical Dirac points, which are important in the theory of the solid state physics, especially in that of topological insulators. The motivation of [3] originated from the paper [4] by chemists. Enyashin and Ivanovski suggested 14 types of graphynes in their paper [4]. Their paper includes the results of dispersion relation. From the view point of quantum graphs, there are spectral results for graphyne and its nanotubes consisting of hexagons and rhombuses [2, 3]. In the graphynes appearing in [4], we also find *supergraphene* (see also [20]). According to the paper [20], it reads that supergraphene is formed when the carbon-carbon bonds in graphene are completely replaced by carbine-like chains (Fig. 1).

Throughout this paper, we construct the spectral theory of Schrödinger operators on a supergraphene-based carbon nanotube. Standard carbon nanotubes are graphene sheets with a cylindrical structure (Fig. 2). Single-wall carbon nanotubes are classified into three classes: zigzag, armchair and chiral. The spectral theory for Schrödinger operators on the graphene and the carbon nanotubes are constructed in [10, 12]. In this paper, we suggest a new supergraphene-based zigzag carbon nanotube, which can be called a zigzag super carbon nanotube, and study its spectral properties by a quantum graph approach [1].

Let us define a metric graph Γ^N corresponding to zigzag super carbon nanotube (Fig. 2) for a fixed $N\in\mathbb{N}$. We put $\mathbb{J}=\{1,2,3,4,5,6,7,8,9\}$, $\mathbf{e}_0=(0,0,1)$, $\mathbb{Z}_N=\mathbb{Z}/(N\mathbb{Z})=\{0,1,2,\cdots,N-1\}$ and $R_N=\frac{\sqrt{3}}{4\sin\frac{\pi}{2N}}$. For $k\in\mathbb{Z}_N$, let $c_k=\cos\frac{\pi k}{N}$, $s_k=\sin\frac{\pi k}{N}$ and $\kappa_k=R_N(c_k,s_k,0)$. For $\omega=(n,j,k)\in\mathcal{Z}:=\mathbb{Z}\times\mathbb{J}\times\mathbb{Z}_N$, we define the edge $\Gamma_\omega=\{\mathbf{x}=3\mathbf{r}_\omega+t\mathbf{e}_\omega\mid t\in[0,1]\}$, where

$$
\begin{aligned}
&\mathbf{e}_{n,1,k}=\mathbf{e}_{n,2,k}=\mathbf{e}_{n,3,k}=\mathbf{e}_0,\quad \mathbf{e}_{n,4,k}=\mathbf{e}_{n,5,k}=\mathbf{e}_{n,6,k}=\kappa_{n+2k+1}-\kappa_{n+2k}+\frac{\mathbf{e}_0}{2},\\
&\mathbf{e}_{n,7,k}=\mathbf{e}_{n,8,k}=\mathbf{e}_{n,9,k}=-\left(\kappa_{n+2k+2}-\kappa_{n+2k+1}-\frac{\mathbf{e}_0}{2}\right),\\
&\mathbf{r}_{n,1,k}=\kappa_{n+2k}+\frac{3n}{2}\mathbf{e}_0,\quad \mathbf{r}_{n,2,k}=\mathbf{r}_{n,1,k}+\frac{1}{3}\mathbf{e}_{n,1,k},\quad \mathbf{r}_{n,3,k}=\mathbf{r}_{n,2,k}+\frac{1}{3}\mathbf{e}_{n,2,k},\\
&\mathbf{r}_{n,4,k}=\mathbf{r}_{n,1,k}+\mathbf{e}_0,\quad \mathbf{r}_{n,5,k}=\mathbf{r}_{n,4,k}+\frac{1}{3}\mathbf{e}_{n,4,k},\quad \mathbf{r}_{n,6,k}=\mathbf{r}_{n,6,k}+\frac{1}{3}\mathbf{e}_{n,5,k},\\
&\mathbf{r}_{n,7,k}=\mathbf{r}_{n+1,0,k}-\mathbf{e}_{n,7,k},\quad \mathbf{r}_{n,8,k}=\mathbf{r}_{n+1,0,k}-\frac{2}{3}\mathbf{e}_{n,7,k},\quad \mathbf{r}_{n,9,k}=\mathbf{r}_{n+1,0,k}-\frac{1}{3}\mathbf{e}_{n,7,k}.
\end{aligned}
$$