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Spectral properties of multi-layered graphene in a magnetic field

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ABSTRACT

Solvable model of multi-layered graphene in a homogeneous magnetic field is constructed. The spectrum of the Hamiltonian has Hofstadter butterfly type. The comparison of the spectrum for single-layer graphene with that for two-layered and three-layered systems is made.

1. Introduction

Starting from famous Hofstadter paper [1], fractal structure of the spectrum of nanosystems in a magnetic field attracts great attention both theoreticians and experimentalists. It is inspired by the peculiarities of the electron transport in such systems. Experimental observation of this effect in natural systems has remained elusive because the required experimental magnetic field is too high (approximately, 10^5 T) for a typical lattice constant of 0.1 nm. One way to circumvent this difficulty was to construct artificial superlattice to increase the lattice constant [2]. Particularly, one can find this type of the spectrum when dealing with periodic arrays of quantum dots [3–11]. One interesting nanostructure more is graphene. It demonstrates many intriguing properties [12]. We are interested in the spectral properties of electron in graphene in a magnetic field. It is related with the quantum Hall effect [13]. Graphene is two-dimensional (2D) Dirac-like electronic system. Due to this reason, its anomalous quantum Hall effect could be measured [14,15]. To calculate the spectrum for various magnetic field, one uses usually tight-binding approximation (see, e.g., [7]) or zero-range potentials model (see, e.g., [16,17]). The next interesting question is related with a comparison of the spectral results for single-layer graphene and multi-layered graphene structure. In bilayer graphene, the two atomic layers can be stacked together in many different ways, and even be twisted [8,18]. Of course, it has an influence on the spectrum [19,20]. An effect of number of layers is also important. In the present paper we describe the Hofstadter butterfly type structure of the spectrum for one, two and three graphene layers. We deal with layers stacked in the most natural way - the Bernal stacking configuration (see Fig. 1).

2. Model construction

The starting point of the construction is the standard Hamiltonian H_0 of free spinless charged particle (of mass m and charge e) in a homogeneous magnetic field **B** (Landau operator):

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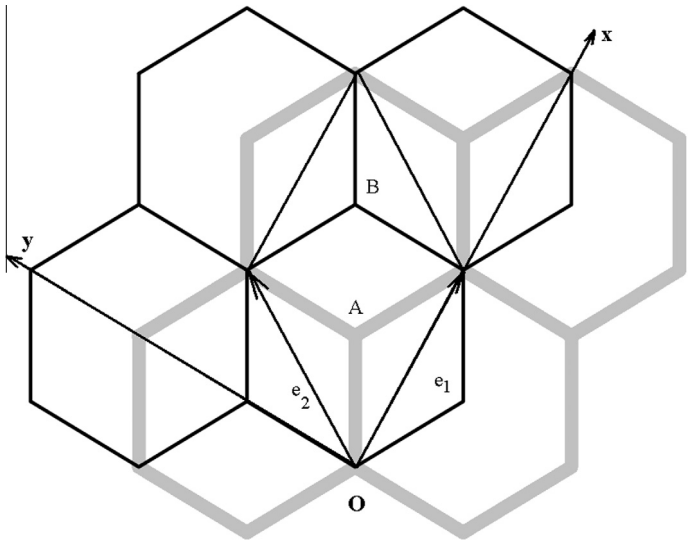

Fig. 1. Geometric structure of bilayer graphene. The Bernal stacking configuration.

$$H_0 = \frac{\hbar}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2. \tag{1}$$

Here $\mathbf{p} = i\hbar\nabla$ is the momentum operator in $\mathbf{R}^3$, $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B}\times\mathbf{r}$ is the vector potential of the magnetic field $\mathbf{B}$ (the symmetric gauge is chosen). It is assumed that the magnetic field is orthogonal to the graphene sheet plane. Below, the following notations are used: $\omega = |e\mathbf{B}|/2c$ is the cyclotron frequency, $\varepsilon_\ell = \hbar\omega(\ell + 1/2)$, $\ell = 0, 1, \ldots$ are the Landau levels of the operator H_0 (1), $\Phi_0 = 2\pi\hbar c/|e|$ is the magnetic flux quantum, $\xi = \mathbf{B}/\Phi_0$ is the density of the magnetic flux. It is well-known that operator H_0 (1) has the continuous spectrum occupying the half-axis $[\varepsilon_0, \infty)$. More precisely, it consists of infinite number of branches:

$$\bigcup_{\ell=0}^{\infty}[\varepsilon_\ell, \infty)$$

Let a be the interatomic distance in single-layer graphene. In real physical system one has $a = 0.142$ nm (see, e.g., [8]). Vectors $\mathbf{a}_1 = (\sqrt{3}a; 0; 0)$ and $\mathbf{a}_2 = \left(\frac{\sqrt{3}}{2}a; \frac{3}{2}a; 0\right)$ are the basic vectors of the Bravais lattice Λ for graphene with the basic cell

$$C_\Lambda = \left\{\mathbf{r}\in\mathbf{R}^3 : 0 \leqslant r_i \leqslant a_i \ (i = 1, 2),\ r_3 \in \mathbf{R}\right\}.$$

The set of nodes (atoms) in the basic cell is marked as $\mathrm{K} \in C_\Lambda$. The set K contains two elements for single-layer graphene, four elements for bilayer graphene, six elements for three-layered graphene, etc. Then, the set

$$\Gamma = \mathrm{K} + \Lambda = \{\boldsymbol{\kappa} + \boldsymbol{\lambda} : \boldsymbol{\kappa} \in \mathrm{K},\ \boldsymbol{\lambda} \in \Lambda\}$$

is the set of all nodes of periodic system with the lattice Λ. As for real graphene samples, the model does not describe correctly the sample edge region.

Fig. 1 shows the lattice structure of bilayer graphene. It corresponds to the most natural physical situation [21]. Let η ($\eta = \xi(\mathbf{a}_1 \times \mathbf{a}_2)$) be the number of the magnetic flux quanta through the basic cell of lattice Λ.

The model Hamiltonian for spinless electron in our system is constructed as a perturbation of the operator (1) by zero-range potentials posed at the nodes of lattice Λ. Formally, the model operator can be written as

$$H = H_0 + \hat{\alpha}\sum_{\boldsymbol{\gamma}\in\Gamma}\delta(\mathbf{r} - \boldsymbol{\gamma}), \tag{2}$$

where $\hat{\alpha}$ is a real constant which characterizes the strength of the point-like potential. Correct mathematical description of the operator (2) is given in the framework of the theory of self-adjoint extensions of symmetric operators [17,22–26]. Let us describe the procedure.

Let $\mathcal{D}$ be the following set

$$\mathcal{D} = \{f \in D(H_0) : f(\boldsymbol{\gamma}) = 0\ \forall\boldsymbol{\gamma} \in \Gamma\}.$$

The operator S is the restriction of the operator H_0 on $\mathcal{D}$. It is a symmetric operator. The model Hamiltonian H is a self-adjoint extension of symmetric operator S. It can be described by the Krein resolvent formula (see, e.g., [27,28]). Let $R(\zeta) = (H - \zeta)^{-1}$