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Quantum Chaos Analysis of a Nanocrystal's Electronic Transport Properties

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Abstract: The electronic transport through a nano-scale device is an interesting topic for both experimental and theoretical physicists, addressing development of new nano-devices. Among the synthesized carbon nanostructures as the materia prima for development of nano-devices, graphene sheets has attracted a lot of attention among researchers. Exceptional properties including carriers with extremely large mobilities and truly two dimensional geometry have made graphene as a promising candidate for replacing semiconductors in the future of nanotechnology. It seems that for a more comprehensive insight of electronic transport properties of the graphene, we could use new frames. The electronic properties of carbon based nanostructures can be well described using a 2-D tight-binding model. Since the motion of an electron is a quantum phenomenon and the tight-binding model describes such motions within an atomic lattice, so graphene and other synthesized carbon nanostructure dynamics can be well studied through the quantum chaos theory. Present study discusses different regimes of conductivity in a 2-D tight-binding model. For this purpose, we apply quantum chaos theory. Spectral statistics of energy levels are used to get consecutive level spacing distribution as an identifier of electronic properties of the device. In order to find best configuration of the crystal for metallic regime, different arrays of onsite energies and hopping constants are analyzed. Our results can report different regimes of conductivity and transition between metallic and insulator phases.

Keywords: Nano-device; Graphene, Electronic transport; Tight-binding model; Quantum chaos; Consecutive level spacing distribution

PACS classifications: 05.45.Mt, 73.63.-b

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1. Introduction

The electron transport through a nano-scale device is an interesting topic for both experimental and theoretical physicists. Among the synthesized carbon nano-structures as the materia prima for development of nano-technologies, carbon nanotubes and graphene sheets possess remarkable electronic features and are considered promising for novel technologies and applications [1–3]. The structure of graphene, composed of tightly packed carbon atoms, is similar to a honeycomb lattice. Based on exceptional properties of the graphene, a great interest has recently been raised on its electronic properties. All of these features indicate that understanding the conductivity properties of graphene is of substantial value. The tight-binding can well describe the conductivity properties of graphene. The tight-binding is a quantum model to describe electron transport within an atomic lattice, so its dynamics can be well studied through quantum chaos theory. This field is a rapidly rising star on the horizon of science. In recent years, some efforts have been conducted to generalize the theory of classical chaos to quantum systems. Much of these efforts are focused on finding chaos indicators in the quantized systems whose classical equivalent has a chaotic behavior. The random matrix theory (RMT), as a cornerstone of quantum chaos theory, gives a fairly simple description of statistical properties of energy level fluctuations. Especially in quantum chaos, RMT provides an statistical frame to analysis of the quantum systems whose classical counterpart are chaotic. Bohigas-Giannoni-Schmit conjecture states that quantum Hamiltonians with chaotic classical dynamics must follow the statistical properties of classical Gaussian ensembles. While according to Berry-Tabor conjecture, quantum Hamiltonians whose classical counterparts are integrable Poisson law holds [4].
Based on this controversy here we try to study electronic properties of a 2-D tigh-binding model. The aim of this study is to find different conditions for which the system is subjected to a transition between insulator and metal regimes. The transition to conductivity under the effects of external perturbations will be studied through consecutive level spacing distribution P(r).

2. Model and Method

The tight-binding Hamiltonian for describing electronic properties of a 2-D system considering that electrons can hope to both nearest- and next-nearest-neighbor atoms using second-quantization has the form (we use units such that $\hbar = 1$)

$$H = \sum_i \varepsilon_i a_i^\dagger a_i - t \sum_{<i,j>} (a_i^\dagger a_j + H.c.) - t' \sum_{<<i,k>>} (a_i^\dagger a_k + H.c.). \quad (1)$$

where $a_i^\dagger$ (a_i) is the electron creation (annihilation) operator on site i. $t(\approx 2.8)$ stands for the nearest-neighbor hopping energy, and $t'(\approx 0.1)$ is the next-nearest-neighbor hopping energy.
RMT is based on the spectral fluctuations of the quantum systems. As is known, different quantum systems may have very different spectral fluctuations. To rule out the unpleasant effects of this difference, Oganesyan and Huse [5] suggested a creative idea defined as follows.

Let consider a typical quantum system characterized by its energy levels $\{E_1, E_2, ..., E_N\}$, with $(E_i < E_{i+1})$ and the nearest-neighbor spacings $s_n = E_{n+1} - E_n$. The new quantity can be defined as the ratio

$\gamma = \frac{min(r_n, r_{n-1})}{max(r_n, r_{n-1})}$, where $r_n = \frac{s_n}{s_n - 1}$. Let $P(r)dr$ be the probability distribution of consecutive level spacings r, so it is possible to write

$$P_I(r) = \frac{1}{(1+r)^2}. \tag{2}$$

$$P_M(r) = \frac{27}{8}\frac{r + r^2}{(1 + r + r^2)^{5/2}}. \tag{3}$$

where $P_I(r)$ ($P_M(r)$) stands for insulator (metallic) regimes. For the metallic regime, the hopping term causes level repulsion and so Wigner distribution holds for consecutive level spacings. While, an insulator has a different energy spectrum. In this limit, the energy spectrum consists of randomly distributed energies. It is well known that the consecutive ratios of random uncorrelated spacings follows the Poisson distribution. We therefore expect that the spectral fluctuations in the localized regime (insulator phase) to be dominated by the Poisson distribution [6,7].

3. Results

We have tried to analyze the electronic properties of a 2-D system modelled by tight-binding model. Hereafter we use the 2-D model described in (1). The site energy ε_i can depend on the external factors which can affect configuration of the lattice. Our purpose is to find different alignments which can cause the studied system to transit between insulator and metallic regimes. Assuming these considerations we study two different configurations of onsite energies.

Case 1. First we assume that not any external factor affect onsite energies and so $\varepsilon_i = 0$ for all sites. In this case, the electrons are not able to transport across the lattice and so the system is in the semi-insulator regime. The wave-functions are nearly localized and this reduces the electron transport property of the system. The results are shown in Figs. 1 and 2. Our analyses show also that shifting onsite energies by a fixed amount does not affect the conductivity properties and the system continues to remain in insulator regime.

Figure 1. Probability of finding electron on different sites of the lattice. This figure shows that the wave-function is nearly localized and the system is in the semi-insulator phase.

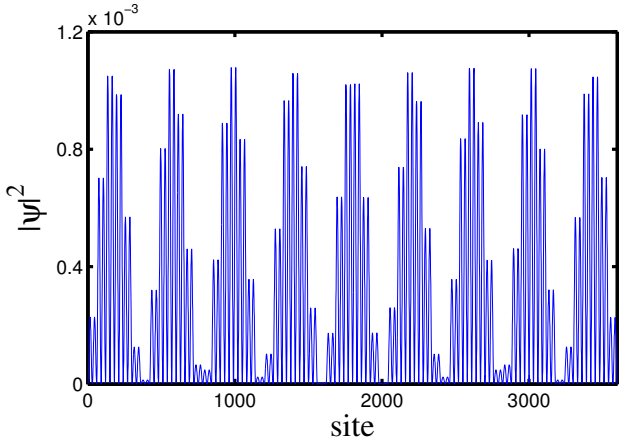
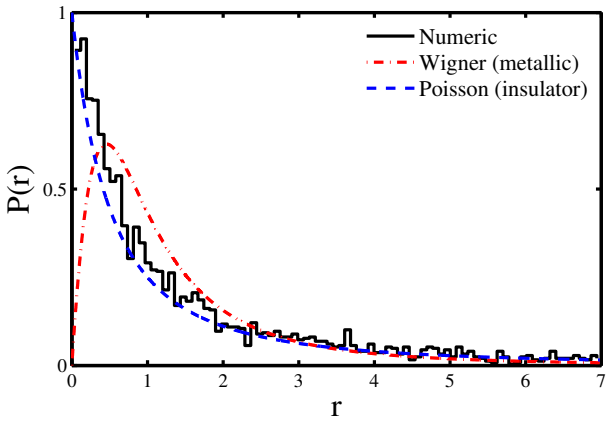


Figure 2. Consecutive level spacing distribution $P(r)$. Numerical results show that the $P(r)$ distribution for the system in case 1 is close to Poisson distribution and so its electronic property is similar to insulator ones.



Case 2. Finally we assume that the energy vary disorderly between 0 and -2.8 values. This case can arise as a result of random thermal baths such as Langevin thermostat. In this case due to the level repulsion between energy levels, the electronic property of the studied system is dramatically changed. The results are shown in Figs. 3 and 4. Evidently, in this case the consecutive level spacing distribution of the system follows the Wigner distribution and the probability of finding electron on different sites is delocalized. So, it can be stated that randomly distribution of onsite energies can shift the conductivity properties of the system from insulator to metallic regime.

Figure 3. Probability of finding electron on different sites of the lattice. This figure shows that the wave-function is fully delocalized.

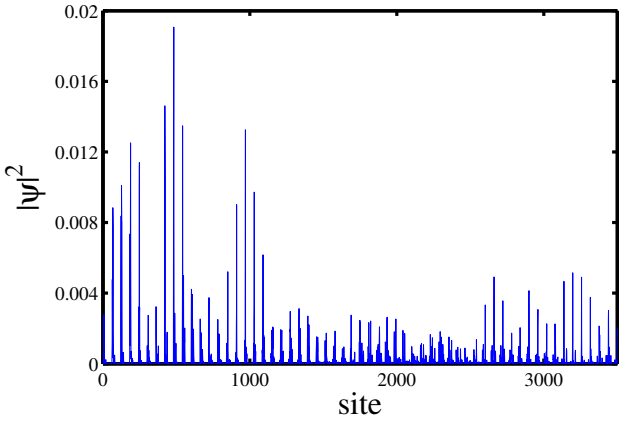
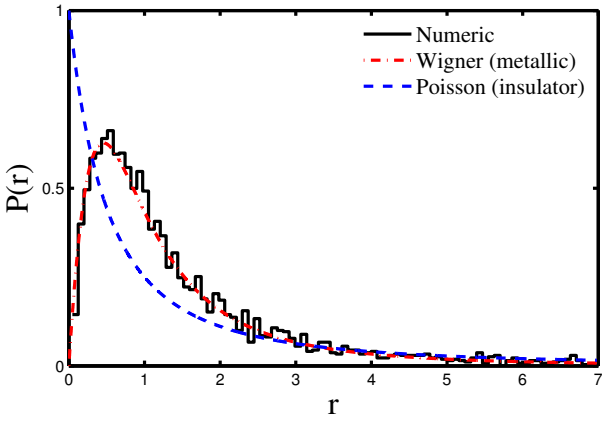


Figure 4. Consecutive level spacing distribution $P(r)$. Numerical results show that the $P(r)$ distribution for the system in case 2 follows the Wigner distribution and so its electronic property is similar to metal ones.



4. Conclusions

In present study we tried to analyze conductivity properties of a 2-D system under the impact of external factors. For this purpose we used 2-D tight-binding model with nearest and next-nearest neighbor hoppings to describe electron transport within the lattice. We followed our goal through two different configurations. Our results showed that when the system is isolated from the environment or its onsite energies are shifted by a fixed amount, insulator behavior is dominant for the electronic properties of the studied system. Finally, it was seen that changing onsite energies according to a disorder pattern can change the conductivity property of the studied system and it can act as a metal.

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