Chaos, Solitons and Fractals 99 (2017) 101–108

Contents lists available at ScienceDirect

Chaos, Solitons and Fractals

Nonlinear Science, and Nonequilibrium and Complex Phenomena

journal homepage: www.elsevier.com/locate/chaos

Metal-insulator transition in a disordered nanotube

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ARTICLE INFO

Article history:
Received 27 January 2016
Revised 1 November 2016
Accepted 29 March 2017

Keywords:
Nanotube
Anderson localization transition
Tight-binding
Consecutive level spacing distribution
Multifractal
Electrical current

ABSTRACT

According to the Anderson localization theory, the wavefunctions of a sufficiently strong disordered system are localized. We show that shifting hopping energy between nearest neighbors would induce an anomalous localization-delocalization transition in a disordered square lattice nanotube modelled by tight-binding. For this purpose, the consecutive level spacing statistics and the singularity spectrum analyses were performed. The quantum analysis of singularity spectrum reveals distinctive multifractality structures of the wavefunctions associated with localized and delocalized phases. We find that while in finite-size limit the system has a sudden metal-insulator transition, in large-scale limit the system experiences a rapid but continuous crossover. Interestingly, we report a critical value of hopping energy for which the system behavior is fairly close to metallic phase and especially independent of the system size. Passing this critical value, a great difference in the electronic transport properties of the system occurs. It follows that in the large-scale size, the system tends to follow semi-metallic behavior, while in finite size behaves more like to an insulator. The localization-delocalization transition is also reflected in the electrical current. In accordance with the indicators studied, we find that in delocalized regime there is a spreading electrical current throughout the whole system with an azimuthal symmetric characteristic.

1. Introduction

Motivated by experimental observations of Anderson localization theory [1–4], there has also been a resurgence of interest in exploring the fundamental aspects of electronic transports in quantum models [5,6], in nanoscale devices [7,8], and in DNA molecules [9]. Electronic localization (delocalization) phenomena in quantum systems have long been a central problem in condensed matter physics. A variety of remarkable phenomena such as superconductors with high critical temperatures [10] and interaction driven metal-insulator transitions [11] is well known to arise from electron correlations. However, metal-insulator transition (MIT) which could be defined as the quantum interference among multiple scatterings of an electron with random impurities and defects of material is used for new types of optoelectronic switches [12]. The MIT describing the properties of a critical quantum state at the transition phase has been represented first in the Anderson model [13,14]. The emergence of this phenomenon has been reported experimentally in a wide variety of examples, including light [15], microwaves [16], and matter waves [17]. According to this theory, eigenstates of low-dimensional systems without disorder-correlation are localized and so spread only over a finite and small region, while for long-range correlation it is possible to find extended states [23]. Many conductance studies have addressed the interaction effects using the method of non-equilibrium Keldysh Green functions [18]. In this approach, one assumes non-interacting leads and the non-equilibrium current are obtained as a function of the exact propagators of the interacting cluster (including the contribution of the leads). The requirements and simplification made for employing the Green function method can be considered of the restrictions on the use of this method.

But, similar phenomena occur in few-body quantum systems, which frequently show the emergence of the so-called quantum chaos [19]. As quantum mechanics lack a notion of phase space, we identify transport properties with quantum chaos, now a standard prescription [20,21], and we use the corresponding diagnostic tools. There, upon changing parameters/numbers of degrees of freedom, the classical system can go from regular to chaotic behavior. On a quantum level this results in changes of level statistics, which has been proven to be a powerful probe of the system properties in the context of quantum chaos [22]. As will be seen, this perspective provides sufficient information to capture localization aspects of the studied system.

The absence of delocalized behavior in a two-dimensional disordered system has been well-predicted with the scaling theory [23,24]. Earlier it was suggested that the Anderson model of localization with purely off-diagonal disorder might violate the general statement of scaling theory [25,26]. In addition, accord-

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http://dx.doi.org/10.1016/j.chaos.2017.03.062
0960-0779/

ing to the dimensionality of the space and the universality class [27,28] some exceptions have been reported in the literature. These include electrons having strong spin-orbit coupling [29], integer quantum Hall systems [30,31], tight-binding models with random magnetic fields [32], systems having symplectic symmetry in the presence of strong magnetic field [33]. Furthermore, after the discovery of graphene some experimental and numerical evidences [34] of the existence of mobility edge [35–37] and delocalized states [38,39] have been found. Considering these controversy, we study the metal-insulator transition in a special case of 2D systems. In this picture, it is considered that the hopping energy between nearest neighbors is changed as a result of magnetic field, strain, and so on. Accordingly, we consider a typical 2D crystal with periodic boundary conditions.

In this work, we study the transport properties and transition behavior of a nanotube via the standard tight-binding (TB) model in the presence of an uniform disorder. Due to the quantum nature of the system and metal-insulator mechanism, we have tried to use quantum chaos tools. We find that in localized phase the electronic transport behavior of the system is almost independent of system size, while in delocalized phase there are different patterns. The proximity index reveals a critical value of hopping energy for which the system behavior is close to metallic phase and more importantly, independent of the system size. It follows that in the large-scale size, the system tends to follow semi-metallic conductivity, while in finite size the system behaves more like an insulator. Also, we study electrical current in the delocalized (ergodic) and localized phases. In accordance with the indicators studied, we find that in delocalized regime there is a spreading electrical current in both azimuthal and altitudinal directions with an azimuthal symmetric characteristic.

2. Model

Recent years have witnessed increasing attention on low-dimensional systems. In particular, various two-dimensional (2D) materials are found in recent years [40,41]. The novel and exceptional properties of newfound materials have made them substantial in both fundamental research and applications. Therefore, we have focused on a nanotube by considering a square lattice with periodic boundary conditions shown in Fig. 1. The tight-binding Hamiltonian with nearest-neighbor hopping characterizing the properties of such a system could be written as

$$H = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{<i,j>} t_{i,j}(c_i^\dagger c_j + H.c.). \quad (1)$$

where $t_{i,j}$ is the hopping term between the nearest-neighbor sites. We suppose that on-site energies ε_is are uniformly distributed over [1/2, 1/2]. Considering modification of atomic orbitals due to applied magnetic fields, leads to a modified hopping integral with a variable nature dependent on the strength of the applied field [42]. So, the aim is to understand the interplay of the possibly interactions between neighbors on the transport properties. According to the random matrix theory, statistics of eigenenergies is not only known to be a powerful probe of crossovers between chaotic and integrable systems in quantum chaos, but also the delocalized and localized states can be characterized by energy level statistics [43,44]. Based on this controversy we discuss the results.

3. Results

We try to analyze comprehensively the electronic transport properties of a nanotube modelled by tight-binding Hamiltonian (1). The geometry is determined by a square lattice of N^2 atoms with periodic boundary conditions. We study this system using exact diagonalization with $N = 10, 12, 14$ (10^3 disorder realizations),

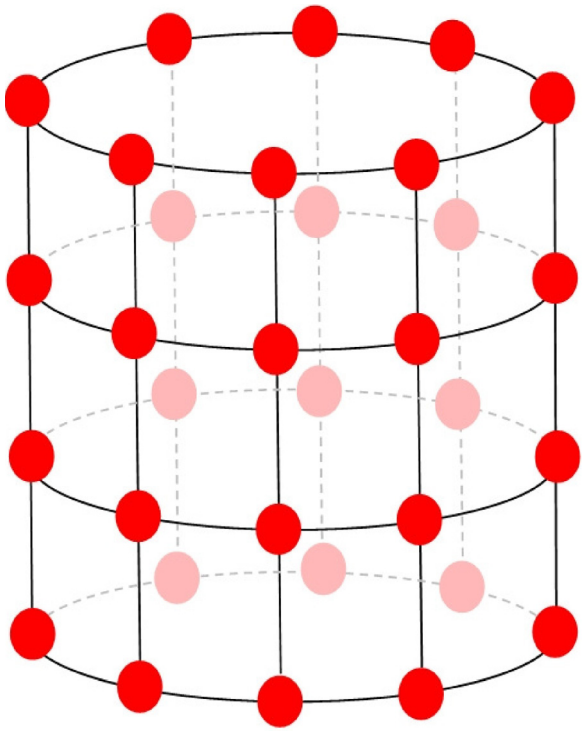

Fig. 1. Schematic view of a nanotube with 8*4 atoms distributed over a cylinder with azimuthal symmetry.

and $N = 40, 50, 60, 70$ (500 realizations) atoms in each direction shown in Fig. 1. This configuration is studied under the change of hopping constant between nearest neighbors by considering $t_{i,j} = t$ for all nearest-neighbor couples.

Characterization of the transition : A rather simple description of energy level statistics [45,46] is provided by the random matrix theory. According to Bohigas–Giannoni–Schmit (Berry–Tabor) conjecture [47] for ensembles of quantum systems with non-integrable (integrable) classical counterparts, different statistics hold for their energy level fluctuations. In order to compare the usual spectral correlations between different fluctuations one may use proximity index η [48].

Let consider a typical quantum system with an ordered set of energy levels $\{E_1, E_2, \ldots E_N\}$ and the nearest-neighbor spacings $s_n = E_{n+1} - E_n$. One can define the following ratio [49,50] $\tilde{r}_n = \frac{\min(s_{n+1}, s_n)}{\max(s_{n+1}, s_n)}$. The mean value $<\tilde{r}>$ provides a more way of proximity to either a Poisson distribution ($\eta = 0$) or a Wigner distribution ($\eta = 1$) via proximity index defined as [48]

$$\eta = \frac{<\tilde{r}> - <\tilde{r}>_P}{<\tilde{r}>_W - <\tilde{r}>_P}. \quad (2)$$

considering $<\tilde{r}>_P \approx 0.3863$ and $<\tilde{r}>_W \approx 0.5359$ [50].

It follows that, the proximity index organizes itself from being close to zero (one) in the insulator (metal) phase to being in between these extremal values in the transition regime, corresponding to a mixing of localized and delocalized states, reflecting a measure of localization-delocalization transition. So, according to deviation from 1 (0), one could determine approaching to each of the extended (localized) states.

In Fig. 2 we show the disorder-averaged proximity index for different values of hopping constant and for $N = 10, 12, 60, 70$. As is evident with increasing hopping parameter, a transition occurs from the localized to delocalized phase. It is clear that for low values of hopping parameter, the system follows Poisson statistics corresponding to a localized state of system. It follows that for fully-