2016 International Symposium on Nonlinear Theory and Its Applications,
NOLTA2016, Yugawara, Japan, November 27th-30th, 2016

A Probabilistic Model of Nano-Carbon Materials Based on Probabilistic Current

Shohei Hamada†, Aiko Kawane†, Hisato Fujisaka†, and Takeshi Kamio†

†Faculty of Information Science, Hiroshima City University
Ozuka-higashi, Asa-minami-ku, Hiroshima, 731-3194 Japan
Email: hs199296@sp.info.hiroshima-cu.ac.jp

Abstract—We derived an equation of continuity for the probability density function of electrons on nanocarbon materials. From the derived equation, we built a cellular array model of the materials with hexagonal lattice structure. A virtual electron particle moves on the lattice probabilistically along with probabilistic current in the equation of continuity. From numerical experiments, we found that the cellular array successfully provided numerical samples of electron trajectories on the materials.

1. Introduction

Nanocarbon materials like graphene [1] and carbon nano tubes (CNT) [2] are expected to be used for quantum effect devices because of their high electron mobility and their intrinsic quantum mechanical properties such as Klein tunneling.

Quantum effect devices are often represented by probabilistic models in circuit simulators. If the behavior of electrons in the devices is described by a scalar type of Schrödinger equation, Nelson's stochastic quantization theory is often applied to build the models [3]. However, it is difficult to apply the theory into modeling nanocarbon-based quantum effect devices because electron behavior in the nanocarbon materials is described by a different type of equation, two-dimensional massless Dirac equation [4]. A new method must be established to build the models of nanocarbon-based devices.

In this paper, an equation of continuity for the probability density of an electron in the nanocarbon material is derived. Then, based on the derived equation, a cellular array model of the materials with hexagonal lattice structure is built as a kind of probabilistic cellular automata [5].

2. Nanocarbon Materials

Graphene sheets are composed of carbon atoms bonding to one another as shown in Fig. 1. The carbon atoms A and B, lattice points of a hexagonal lattice, are non-equivalent and adjacent two carbon atoms A and B form a unit cell of graphenes. The behavior of electrons on graphene sheets is described by the following approximate equation:

$$i\hbar\frac{\partial}{\partial t}\boldsymbol{\Psi}(x,y,t) =$$

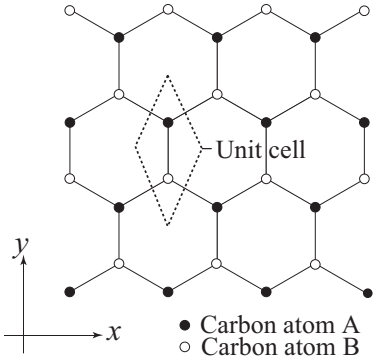

Figure 1: Structure of graphenes.

$$\left[\hbar v_F\left(\boldsymbol{\sigma}_x\hat{k}_x+\boldsymbol{\sigma}_y\hat{k}_y\right)+V(x,y)\right]\boldsymbol{\Psi}(x,y,t) \tag{1}$$

where $\hbar$ is the Plank constant divided by 2π, v_F is the Fermi velocity, and $V(x,y)$ denotes static potential distribution. Wave function$\boldsymbol{\Psi}(x,y,t)$,

$$\boldsymbol{\Psi}(x,y,t)=\begin{pmatrix}\psi_A(x,y,t)\\ \psi_B(x,y,t)\end{pmatrix},\quad \psi_{A,B}:R^3\to C^1 \tag{2}$$

possesses two elements $\psi_{A/B}(x,y,t)$ which are wave functions of the electrons on two sublattices consisting respectively of carbon atoms A and B. The operators in Eq. (1) are defined as $\hat{k}_x\equiv -i\partial/\partial x$, $\hat{k}_y\equiv -i\partial/\partial y$. Pauli spin matrices $\boldsymbol{\sigma}_x$, $\boldsymbol{\sigma}_y$ in the equation are given by

$$\boldsymbol{\sigma}_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \boldsymbol{\sigma}_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix} \tag{3}$$

Equation (1) is the two-dimensional Dirac equation with mass of zero and light speed c replaced by v_F.

A CNT is considered as a cylindrical graphene sheet in structure. We define two linearly independent vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ given by

$$\boldsymbol{e}_{1/2}=\frac{a}{2}(\sqrt{3},\pm 1),\quad a=\sqrt{3}a_{AB} \tag{4}$$

on the graphene sheet, where a_{AB} is the distance between adjacent two A, B carbon atoms. Let a vector oriented in the circumferential direction of the CNT and a vector parallel to the cylinder axis of the CNT or perpendicular to $\boldsymbol{C}_h$

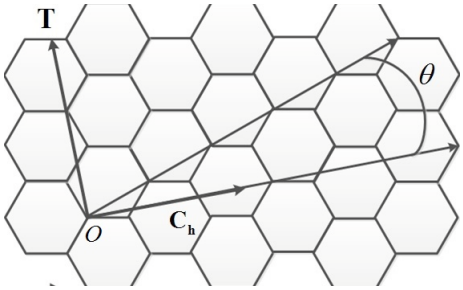

Figure 2: Circumferential and axial vectors $\boldsymbol{C}_h$, $\boldsymbol{T}$ on CNT.

be denoted respectively by $\boldsymbol{C}_h$ and $\boldsymbol{T}$. They are shown in Fig. 2. We express $\boldsymbol{C}_h$ with $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ as

$$\boldsymbol{C}_h = (C_{h,x}, C_{h,y}) = C_1\boldsymbol{e}_1 + C_2\boldsymbol{e}_2 \tag{5}$$

Length of $\boldsymbol{C}_h$ is given by

$$|\boldsymbol{C}_h| = a\sqrt{C_1^2 + C_2^2 + C_1C_2} \tag{6}$$

We set the length as the circumferential length of the CNT. Then, the diameter of the CNT is

$$d_r = \frac{|\boldsymbol{C}_h|}{\pi} \tag{7}$$

In this paper, we assume that $|\boldsymbol{C}_h| \gg a_{AB}$. We set vector $\boldsymbol{T}$ as

$$\begin{aligned} &\boldsymbol{T} = t_1\boldsymbol{e}_1 + t_2\boldsymbol{e}_2 \\ &t_1 = \frac{2C_1 + C_2}{d_r}, \quad t_2 = \frac{C_1 + 2C_2}{d_r} \end{aligned} \tag{8}$$

Then, the length of $\boldsymbol{T}$ is

$$|\boldsymbol{T}| = \frac{\sqrt{3}|\boldsymbol{C}_h|}{d_r} \tag{9}$$

If the vectors $\boldsymbol{C}_h$ and $\boldsymbol{T}$ take particular directions, the wave function of electrons on the CNT can be a solution of Eq. (1) with the periodic condition

$$\boldsymbol{\Psi}(x, y, t) = \boldsymbol{\Psi}(x + mC_{h,x}, y + nC_{h,y}, t), \quad m, n\text{: integers} \tag{10}$$

being satisfied.

3. Equation of Continuity

Let the probability density function and the pseudospin density of an electron on a graphene or a CNT be denoted by $\rho(x, y, t)$ and $s_x(x, y, t)$. In addition, we introduce another function $s_y(x, y, t)$. They are given by

$$\rho(x, y, t) = \psi_A(x, y, t)\psi_A^*(x, y, t) + \psi_B(x, y, t)\psi_B^*(x, y, t) \tag{11}$$

$$s_x(x, y, t) = 2\mathrm{Re}(\psi_A^*(x, y, t)\psi_B(x, y, t)) \tag{12}$$

$$s_y(x, y, t) = 2\mathrm{Im}(\psi_A^*(x, y, t)\psi_B(x, y, t)) \tag{13}$$

and have the following relations:

$$|\psi_A(x, y, t) \pm \psi_B(x, y, t)|^2 = \rho(x, y, t) \pm s_x(x, y, t) \tag{14}$$

$$|\psi_A(x, y, t) \pm i\psi_B(x, y, t)|^2 = \rho(x, y, t) \mp s_y(x, y, t) \tag{15}$$

Let the complex conjugates of $\boldsymbol{\Psi}$, $\sigma_{x/y}$, and $\hat{k}_{x,y}$ be denoted by $\boldsymbol{\Psi}^*$, $\sigma_{x/y}^*$, and $\hat{k}_{x,y}^*$, respectively. Then, the complex conjugate equation of Eq. (1) is given by

$$\begin{aligned} -i\hbar\frac{\partial}{\partial t}\boldsymbol{\Psi}^*(x, y, t) = \\ \left[\hbar v_F\left(\sigma_x^*\hat{k}_x^* + \sigma_y^*\hat{k}_y^*\right) + V(x, y)\right]\boldsymbol{\Psi}^*(x, y, t) \end{aligned} \tag{16}$$

Adding the innor products between Eq. (1) and $\boldsymbol{\Psi}^*$ and between Eq. (16) and $\boldsymbol{\Psi}$, we obtain

$$\begin{aligned} &\frac{\partial}{\partial t}(\psi_A(x, y, t)\psi_A^*(x, y, t) + \psi_B(x, y, t)\psi_B^*(x, y, t)) \\ &\quad = -v_F(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}) \cdot \\ &\quad ((\psi_A^*(x, y, t)\psi_B(x, y, t) + \psi_A(x, y, t)\psi_B^*(x, y, t)), \\ &\quad -i(\psi_A^*(x, y, t)\psi_B(x, y, t) - \psi_A(x, y, t)\psi_B^*(x, y, t)))^T \end{aligned} \tag{17}$$

Equation (17) can be expressed as

$$\frac{\partial}{\partial t}\rho(x, y, t) + \mathrm{div}\boldsymbol{J} = 0 \tag{18}$$

$$\boldsymbol{J} = v_F(s_x, s_y)^T \tag{19}$$

Since Eq. (18) is so called an equation of continuity, $\boldsymbol{J}$ is considered as probabilistic current. When the wave function of Eq. (1) is a plane wave give by

$$\boldsymbol{\Phi}(x, y, t) = \begin{pmatrix} 1 \\ \exp(i\theta) \end{pmatrix}\exp(i(k_x x + k_y y))\exp\left(-i\frac{E(k_x, k_y)}{\hbar}t\right) \tag{20}$$

$$E(k_x, k_y) = \sqrt{k_x^2 + k_y^2}, \quad \theta = \arctan\left(\frac{k_y}{k_x}\right) \tag{21}$$

the directions of $\boldsymbol{J}$ is given by θ, which coincides with the direction of the propagation of $\boldsymbol{\Phi}$. Then, it is inevitable that Eq. (18) has been derived.

4. Probabilistic Model

A model to be proposed is a hexagonal lattice whose sites A and B are distinguished, as shown in Fig. 1. A virtual electron particle moves from a cite to one of three adjacent sites randomly in a unit time Δt. We explain the random motion in detail. We denote three vectors from a site A to its three adjacent sites B by $\boldsymbol{a}_i$, $i = 1, 2, 3$, as shown in Fig 3, and probabilities that a particle on the site A moves to the three sites B are denoted by p_i. The three vectors are give by

$$\boldsymbol{a}_1 = \boldsymbol{e}_1 - \frac{1}{3}(\boldsymbol{e}_1 + \boldsymbol{e}_2) \tag{22}$$

$$\boldsymbol{a}_2 = \boldsymbol{e}_2 - \frac{1}{3}(\boldsymbol{e}_1 + \boldsymbol{e}_2) \tag{23}$$

$$\boldsymbol{a}_3 = -(\boldsymbol{a}_1 + \boldsymbol{a}_2) \tag{24}$$

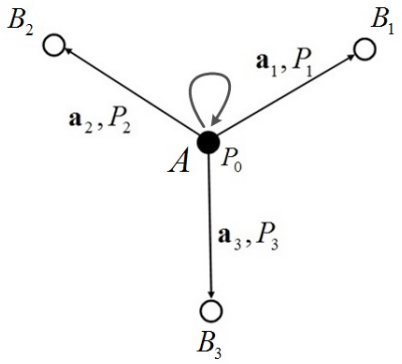

Figure 3: Three vectors from site A to its three adjacent sites B.

When the particle does not stay in an identical site for more than one unit time, we have

$$\sum_{i=1}^{3} p_i = 1 \tag{25}$$

From the discussion at the end of Section 3, a wave packet with momentum distributed around (k_x, k_y) also propagates in the direction of θ approximately. Then, the expectation of the velocity of the particle should be proportional to the probabilistic current, which is represented by

$$\sum_{i=1}^{3} p_i \boldsymbol{a}_i = b\boldsymbol{J}, \quad \text{Proportional constant: } b \in R \tag{26}$$

Equations (25) and (26) are combined as

$$\begin{pmatrix} 1 \\ bv_F s_x \\ bv_F s_y \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ a_{1,x} & a_{2,x} & a_{3,x} \\ a_{1,y} & a_{2,y} & a_{3,y} \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \tag{27}$$

where $(a_{i,x}, a_{i,y})^T = \boldsymbol{a}_i$, i = 1,2,3. From Eq. (27), probabilities p_i are obtained as

$$\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \frac{1}{3\Delta} \begin{pmatrix} 1 + 2\boldsymbol{a}_1 \cdot b\boldsymbol{J} \\ 1 + 2\boldsymbol{a}_2 \cdot b\boldsymbol{J} \\ 1 + 2\boldsymbol{a}_3 \cdot b\boldsymbol{J} \end{pmatrix} \tag{28}$$

$$\Delta = \boldsymbol{a}_1 \times \boldsymbol{a}_2 + \boldsymbol{a}_2 \times \boldsymbol{a}_3 + \boldsymbol{a}_3 \times \boldsymbol{a}_1 \tag{29}$$

where $\cdot$ and $\times$ are inner and outer product operators. Coefficient b should be chosen so that $p_i \geq 0$.

By solving Eq. (1), computing Eq. (19) with the solution $\boldsymbol{\Psi}(x, y, t)$, and using Eq. (28), we determine p_i. Probabilities that the particle moves from a site B to the three adjacent sites A are determined similarly. Then, sample trajectories of the random motion of the particle can be obtained.

5. Numerical Experiments

Let (x', y') be a two dimensional orthogonal coordinate system with axes parallel to $\boldsymbol{C}_h$ and $\boldsymbol{T}$. Suppose that the new coordinate system is obtained by rotating (x, y) coordinate system by φ. The wave function $\boldsymbol{\Psi}'(x', y', t)$ of Eq. (1) with coordinate (x, y) replaced by (x', y') has the following relation with $\boldsymbol{\Psi}(x, y, t)$:

$$\boldsymbol{\Psi}'(x', y', t) = \begin{pmatrix} \exp(i\frac{\varphi}{2})\Psi_A \\ \exp(-i\frac{\varphi}{2})\Psi_B \end{pmatrix} \tag{30}$$

From Eqs. (11), (12), and (30), we see that the probability density function and the pseudospin density are conserved on (x', y') plane. Then, we may denote both coordinate systems on graphene and CNT by the same denotation (x, y).

We will deterimne a wave function in the form of wave packet. The initial conditions of the wave packet are set as follows: Center position: (x_0, y_0), Kinetic momenta: $\hbar(k_{x0}, k_{y0})$, Variances of the momenta: $\sigma_{kx} = \sigma_{ky} = \sigma_k$. The initial form of the packet can then be expressed as

$$\phi_0(k_x, k_y) = \frac{1}{\sqrt{2\pi\sigma_k}} \exp\left(-\frac{1}{4}\left(\frac{k_x - k_{x0}}{\sigma_k}\right)^2 - \frac{1}{4}\left(\frac{k_y - k_{y0}}{\sigma_k}\right)^2 - ik_x x_0 - ik_y y_0 \right) \tag{31}$$

The evolving wave packet is expanded in a series of plane wave solutions (20). Its continuation form is given by

$$\boldsymbol{\Psi}(x, y, t) = \int\int \boldsymbol{\Phi}(x, y, t)\phi_0 dk_x dk_y \tag{32}$$

If the integration on k_y is discretized with step size of Δk_y given by

$$\Delta k_y = \frac{2\pi}{|\boldsymbol{C}_h|} \tag{33}$$

that is, Eq. (32) is in the form of the Riemann sum, the wave packet satisfies periodic condition (10). Then, a packet propagating on a CNT is obtained.

Using wave function (32), we compute probabilistic current $\boldsymbol{J}$ from Eqs. (12), (13), and (19) and then probabilities (28) are determined. Figure 4 shows a wave packet contour-plotted at t = 0 and 30 and a sample trajectory of a virtual electron particle between time interval [0, 30]. They are computed on the following conditions: a_{AB} = 0.5, $\hbar k_{x0}$ = $10 \cdot \cos(\pi/4)$, $\hbar k_{y0} = 10 \cdot \sin(\pi/4)$, σ_k = 0.2, and Δt = 0.4. Figure 5 shows another pair of a wave packet and a sample trajectory computed on the other conditions that a_{AB} = 1.0, $\hbar k_{x0} = 10 \cdot \cos(\pi/3)$, $\hbar k_{y0} = 10 \cdot \sin(\pi/3)$, σ_k = 0.2, and Δt = 0.6. We see that both the wave packet and the virtual electron particle move almost the same distances in almost the same directions on each condition set.

6. Conclusions

We have presented a method to compute sample trajectories of electrons on nanocarbon materials. Our future subjects include developing the method so that the trajectories distribute in accordance with the probability density function.

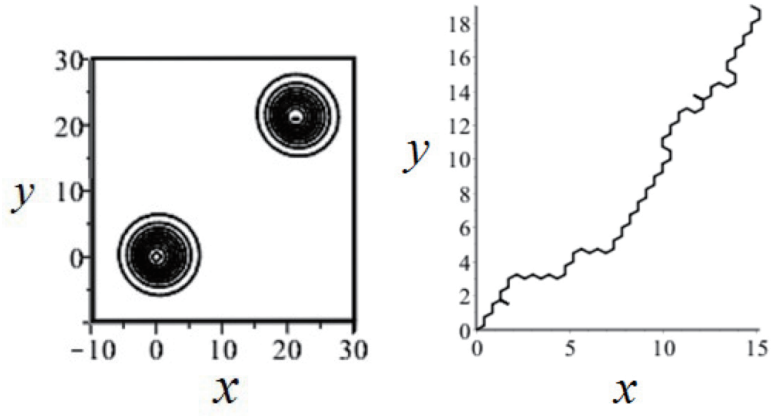

Figure 4: A wave packet at $t = 0$ and 30 and a sample trajectory for time interval [0, 30] when $\theta = \pi/4$.

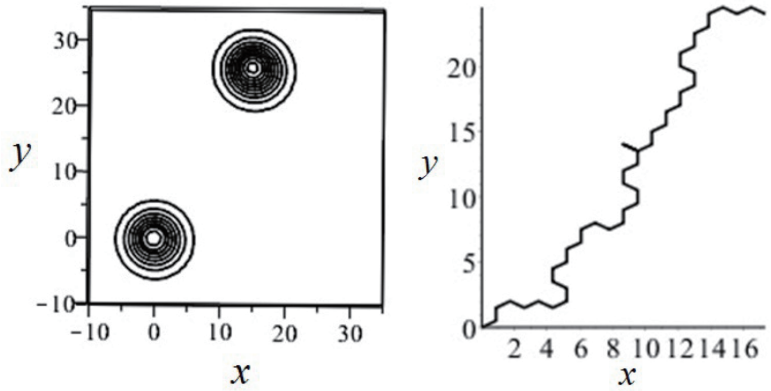

Figure 5: A wave packet at $t = 0$ and 30 and a sample trajectory for time interval [0, 30] when $\theta = \pi/3$.

Acknowledgment

This work was supported by JSPS KAKENHI Grant No. 15K06075.

References

[1] M. I. Katsnelson, *Graphene – Carbon in Two Dimensions*, Cambridge University Press, 2012.

[2] K. Varga and J. A. Driscoll, *Computational Nanoscience*, Cambridge University Press, 2011.

[3] E. Nelson, "Derivation of the Schrödinger Equation from Newtonian Mechanics," *Physical Review*, Vol. 150, No. 4, pp.1079-1085, 1966.

[4] B. Thaller, *The Dirac Equation*, Springer-Verlag, 1992.

[5] A. Ilachinski, *Cellular Automata – A Discrete Universe*, World Scientific, 2001.