

A Probabilistic Cellular Array Model of Dissipative Wave Systems

Shohei Hamada[†], Atsushi Setsuie[†], 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—Electron behavior in nano-carbon materials like graphene sheets and carbon nano tubes is described approximately by the Dirac-type equation. If the quantum electron waves on the materials are planar, the wave equation for the materials is transformed into a one-dimensional classical wave equation. In this paper, we propose a probabilistic cellular array which is a model of one-dimensional classical wave systems with dissipation and can be a stochastic quantization of the nano-carbon quantum systems. We assume particles moving from a cell to an adjacent cell of the cellular array for a unit time step. We then proved analytically that the probability distribution of the particles in terms of their location satisfied the discretized classical wave equation. We also presented numerically that the distribution met the solution of the classical wave equation.

1. Introduction

Nano-carbon devices using graphene sheets and carbon nano tubes (CNT) have been researched. Non-relativistic electrons on graphene [1] are described approximately by the Dirac-type equation that generally describes relativistic quantum mechanical systems [2]. Models of quantum effect devices for conventional circuit simulators like SPICE can be built based on stochastic quantization for non-relativistic quantum mechanical systems [3, 4]. A novel stochastic quantization for relativistic quantum mechanical systems is necessary to build models of graphene-based devices for circuit simulators. Although stochastic quantizations for the relativistic quantum systems have been attempted [5], no quantization suitable to modeling for circuit simulators has yet been invented.

When static scalar potentials on graphene sheets are uniform, the Dirac-type wave equation can be transformed into a classical wave equation describing, for example, distributed parameter electric circuits. In this paper, we consider a stochastic model of classical wave systems which can be a stochastic quantization of the quantum nano-carbon systems. Concretely speaking, we will present a cellular array like probabilistic cellular automata [6] and investigate whether the stochastic behavior of virtual particles on the array meets the classical wave propagation. Preceding cellular automata models of wave systems are not flexible [7]. They can not be dissipative nor their wave propagation speed can not be changed.

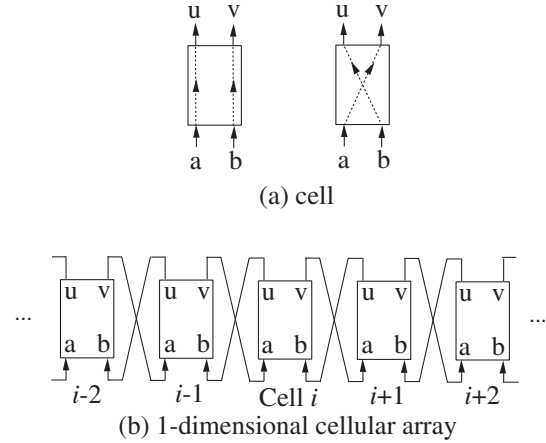


Figure 1: Probabilistic cellular array

2. A Probabilistic Cellular Array Model

Figure 1 shows a probabilistic cellular array and its cell elements [8]. Each cell has two inputs a, b and two outputs u, v . Internal connections between the inputs and outputs are in parallel or crossed as shown in Fig. 1(b). The connections switch randomly. Let probabilities that the cells take parallel and cross connections be denoted by p_{str} and p_{crs} respectively. Then, $p_{str} + p_{crs} = 1$. Let Cell $_i$, a_i , and b_i denote a cell at location i in the cellular array and the two inputs of the cell. Assume that there exists a particle at an input of a cell. The particle passes through the cell and moves to an input of its left and right adjacent cells at probabilities p_{str} and p_{crs} for a unit time interval. If the particle is at a_i at time n , it will locate at b_{i-1} at probability p_{str} or a_{i+1} at probability p_{crs} at time $n + 1$. Then, the input a/b at which the particle locates and the increment/decrement of the particle's location i change every one time step according to a Markovian transition diagram shown in Fig. 2. This cellular array and the change of particle direction by the internal parallel connections correspond respectively to a conductor and electron scattering by thermal vibration of the conductor lattice. That is, dissipation is represented by the change of the direction.

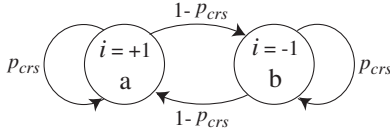


Figure 2: Transition of the direction of particles.

3. Theoretical Analysis

Let probabilities that the particle locates at a_i and b_i at time n be denoted by $a(n, i)$ and $b(n, i)$. Evolutional equations of the probabilities are expressed by

$$a(n+1, i) = p_{crs}a(n, i-1) + p_{str}b(n, i-1) \quad (1)$$

$$b(n+1, i) = p_{str}a(n, i+1) + p_{crs}b(n, i+1) \quad (2)$$

By a z -transformation from discrete time-space domain (n, i) to two-dimensional z -domain (z_t, z_x) , Eqs. (1) and (2) are expressed by

$$\mathbf{M}(z_t, z_x) \begin{bmatrix} \alpha(z_t, z_x) & \beta(z_t, z_x) \end{bmatrix}^T = \mathbf{0} \quad (3)$$

$$\mathbf{M}(z_t, z_x) \equiv \begin{bmatrix} -z_t + p_{crs}z_x^{-1} & (1 - p_{crs})z_x^{-1} \\ (1 - p_{crs})z_x & -z_t + p_{crs}z_x \end{bmatrix} \quad (4)$$

where $\alpha(z_t, z_x)$ and $\beta(z_t, z_x)$ are respectively the z -transforms of $a(n, i)$ and $b(n, i)$. Eliminating $\alpha(z_t, z_x)$ or $\beta(z_t, z_x)$ from Eq. (3), we have

$$\text{Det}(\mathbf{M}(z_t, z_x))\alpha(z_t, z_x) = 0 \quad (5)$$

$$\text{Det}(\mathbf{M}(z_t, z_x))\beta(z_t, z_x) = 0 \quad (6)$$

Inversely z -transforming Eq. (5) from (z_t, z_x) to (n, i) and using the following first-order difference operators,

$$\Delta_t a(n, i) \equiv a(n+1, i) - a(n, i) \quad (7)$$

$$\Delta_x a(n, i) \equiv a(n, i+1) - a(n, i) \quad (8)$$

we obtain

$$\begin{aligned} & \Delta_t a(n+1, i+1) - (2p_{crs} - 1)\Delta_t a(n, i+1) \\ &= p_{crs}(\Delta_x a(n+1, i+1) - \Delta_x a(n+1, i)) \end{aligned} \quad (9)$$

By using the following second-order difference operators

$$\Delta_t^2 a(n, i) \equiv \Delta_t a(n+1, i) - \Delta_t a(n, i) \quad (10)$$

$$\Delta_x^2 a(n, i) \equiv \Delta_x a(n, i+1) - \Delta_x a(n, i) \quad (11)$$

Eq. (9) is expressed as

$$\begin{aligned} & (2p_{crs} - 1)\Delta_t^2 a(n, i+1) + 2(1 - p_{crs})\Delta_t a(n+1, i+1) \\ &= p_{crs}\Delta_x^2 a(n+1, i) \end{aligned} \quad (12)$$

It is obvious from equation set (5, 6) that $b(n, i)$ also satisfies Eq. (12).

Partial difference equation (12) corresponds to the following partial differential equation with continuous independent time and space variables t and x :

$$C_1 \frac{\partial^2 u(t, x)}{\partial t^2} + C_2 \frac{\partial u(t, x)}{\partial t} = C_3 \frac{\partial^2 u(t, x)}{\partial x^2} \quad (13)$$

This equation describes one-dimensional dissipative wave systems. Equation (12) is a discretization of Eq. (13) when spatial and temporal discretization steps are 1.0 and the coefficients are given by $C_1 = 2p_{crs} - 1$, $C_2 = 2(1 - p_{crs})$, $C_3 = p_{crs}$.

When $p_{crs} = 1$, the first-order temporal-difference and differential terms in Eqs. (12) and (13) disappear. Thus, the probabilistic cellular array is a model of lossless wave systems. When $1/2 < p_{crs} < 1$, all the coefficients of the difference terms in Eqs. (12) and (13) are positive. Then, the probabilistic cellular array is a model of dissipative wave systems. When $p_{crs} = 1/2$, the second-order temporal-difference and differential terms in Eqs. (12) and (13) disappear. Thus, the probabilistic cellular array is a model of continuous diffusion systems with no advective term [9].

4. Numerical Experiments

We computed trajectories of 10000 particles starting at Cell_0 from time $n = 1$ to 500 when $p_{crs} = 0.98$. We then obtained probability distributions of the particle location. For comparison, we obtained analytical solutions of wave equation (13) on a condition that initial waveform is a Gaussian wave packet with average of 0 and standard deviation of 0.5. Figures 3 and 4 show the distribution and the solutions.

The initial wave packet divides into forward and backward wave packets. We see diffusion components between the two packets. Because the diffusion phenomenon is slower than the propagation phenomenon, the diffusion components are always between the wave packets. The packet propagation is damped and changed into diffusion components with the time. The propagating packets of the probability distribution and the analytical solution have almost the same damping rate. Macroscopically, the diffusion components of the packet of the probability distribution seem approximately twice as large as those of the analytical solution. Microscopically, there exists no diffusion components at cells with even/odd location indices i when time n is odd/even. Therefore, the distribution density almost agrees with the solution height.

5. Graphene As A Classical Wave System

Stochastic quantizations such as the Nelson's method [10] can represent non-relativistic quantum systems by classical probabilistic processes. On the other hand, as mentioned in Section 2, we have no method of stochastic quantization for relativistic quantum systems described by

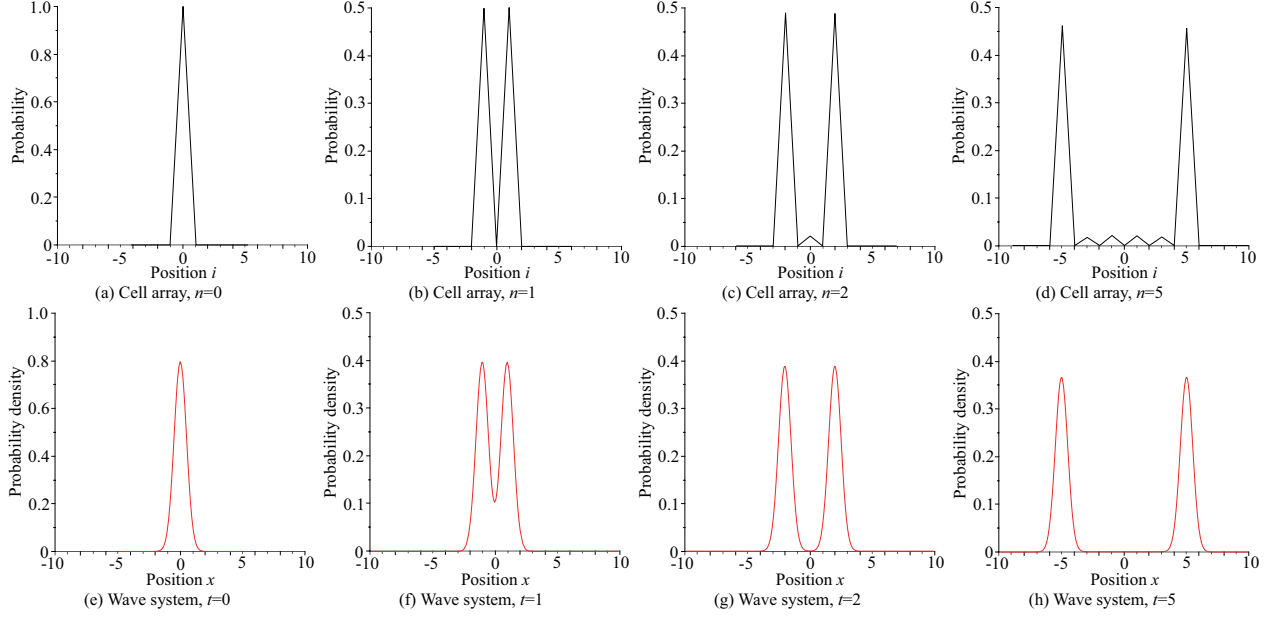


Figure 3: Numerically obtained probability distributions of particle locations and analytical solutions of wave equation ($0 \leq n, t \leq 5$)

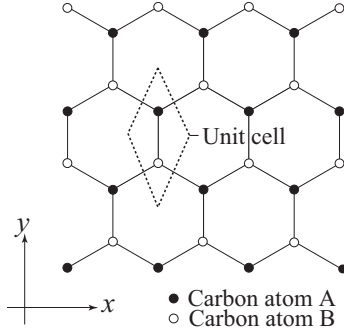


Figure 5: Structure of graphene

the Dirac equations. In this section, we present that a Dirac-type equation describing the behavior of electrons on two-dimensional graphene can be transformed into a classical wave equation and that the cellular array can be a stochastic quantization of graphene on limited conditions.

Graphene sheets are composed of carbons bonding to one another as shown in Fig. 5. For more details on graphene, see [1]. The behavior of electrons on graphene sheets is described by the following approximate equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, y, t) = \left[\hbar v_F (\sigma_x \hat{k}_x + \sigma_y \hat{k}_y) + V(x, y) \right] \Psi(x, y, t) \quad (14)$$

where \hbar is the Plank constant divided by 2π and v_F is the

Fermi velocity. Wave function $\Psi(x, y, t)$

$$\Psi(x, y, t) = \begin{pmatrix} \psi_A(x, y, t) \\ \psi_B(x, y, t) \end{pmatrix}, \quad \psi_{A,B} : R^3 \rightarrow C^1 \quad (15)$$

possesses two elements which are wave functions of the electrons at the two carbon sites A and B. Site A and site B are non-equivalent to form a unit cell of graphenes. The operators in Eq. (14) are defined as $\hat{k}_x \equiv -i\partial/\partial x$, $\hat{k}_y \equiv -i\partial/\partial y$. Pauli spin matrices σ_x , σ_y employed in the equation are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (16)$$

Equation (14) is the two-dimensional Dirac equation with mass of zero and light speed c replaced by v_F .

Let the static scalar potential be spatially uniform, that is $V(x, y) = V$ and the wave function be represented by $\Psi(x, y, t) = \Phi(x, y, t) \exp(iVt/\hbar)$. Then, we obtain the following equation without scalar potential term.

$$i\hbar \frac{\partial}{\partial t} \Phi(x, y, t) = \left[\hbar v_F (\sigma_x \hat{k}_x + \sigma_y \hat{k}_y) \right] \Phi(x, y, t) \quad (17)$$

$$\Phi(x, y, t) = \begin{pmatrix} \phi_A(x, y, t) \\ \phi_B(x, y, t) \end{pmatrix} \quad (18)$$

Eliminating $\phi_A(x, y, t)$ or $\phi_B(x, y, t)$ from Eq. (17), we obtain the following classical wave equation:

$$\frac{\partial^2}{\partial t^2} \phi_{A,B}(x, y, t) = v_F^2 \left(\frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} \right) \phi_{A,B}(x, y, t) \quad (19)$$

When $\phi_A(x, y, t)$ and $\phi_B(x, y, t)$ are planar wave, Eq. (19) becomes a one-dimensional classical equation (13) with no dissipative term.

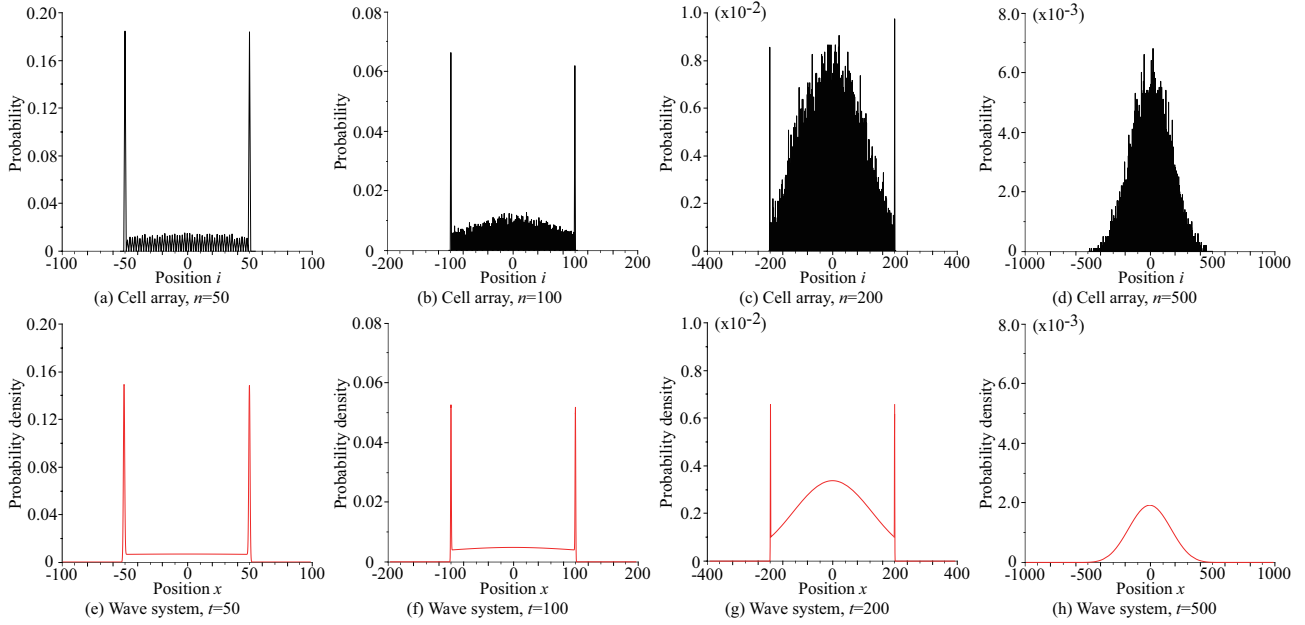


Figure 4: Numerically obtained probability distributions of particle locations and analytical solutions of wave equation ($50 \leq n, t \leq 500$)

6. Conclusions

This paper has presented a probabilistic cellular array model of classical dissipative wave systems and shown analytically and numerically that the model corresponds to the wave systems. It also has been shown that the cellular array can be a stochastic quantization model of graphene sheets on certain conditions. Our future works include extending the cellular array to a two-dimensional model of classical wave systems and to a model of graphene sheets with non-uniform scalar potential.

References

- [1] M. I. Katsnelson, *Graphene – Carbon in Two Dimensions*, Cambridge University Press, 2012.
- [2] B. Thaller, *The Dirac Equation*, Springer, 1992.
- [3] N. Hiram, H. Fujisaka, and T. Kamio, “Probabilistic Particle Modeling of Quantum Wave Propagation with Reflection, Transmission, and Coupling,” *Proc. of International Symposium on Circuits and Systems*, 2014.
- [4] Y. Kawabata, H. Fujisaka, and T. Kamio, “Probabilistic Particle Modeling of Quantum Wave Propagation with Excitation and Refraction,” *Proc. of International Symposium on Circuits and Systems*, 2014.
- [5] D. G. C. McKeon and G. N. Ord, “Time Reversal and a Stochastic Model of the Dirac Equation in an electromagnetic Field,” *Canadian Journal of Physics*, Vol. 82, No. 1, pp.19-27, 2004.
- [6] A. Ilachinski, *Cellular Automata Modeling – A Discrete Universe*, World Scientific Publishing, 2001.
- [7] B. Chopard and M. Droz, *Cellular Automata Modeling of Physical Systems*, Cambridge University Press, 1998.
- [8] H. Fujisaka, T. Kamio, C.-J. Ahn, M. Sakamoto, and K. Haeiwa, “A Sigma-Delta Domain Lowpass Wave Filter,” *IEEE Trans. on Circuits and Systems I*, Vol. 62, No. 1, pp.167-176, 2015.
- [9] K. Nagata, H. Fujisaka, T. Kamio, and K. Haeiwa, “A cellular array model of reaction-diffusion systems for parallel generation of pseudo-random i.i.d. sequences,” *Nonlinear Theory and Its Applications, IEICE*, Vol. 3, No. 4, pp.606-620, 2012.
- [10] E. Nelson, “Derivation of the Schrödinger Equation from Newtonian Mechanics,” *Physical Review*, Vol. 150, No. 4, pp.1079-1085, 1966.