Abstract: This paper proposes a probabilistic particle model of single-electrons on graphene. The behavior of a single-electron on graphene is described approximately by the massless Dirac equation. The electron is non-relativistic and given pseudo-spin. The Dirac equation originally describes the motion of a relativistic quantum particle with actual spin. Then, it has seemed difficult that the Nelson’s stochastic quantization theory could build a particle model of the electron on graphene since the theory can deal with only non-relativistic quantum particles with spin not being taken into account. In this paper, Nelson’s theory is interpreted by using probability density function and probability density current so that it can build a particle model of a single-electron on graphene. Single-electrons on a graphene nano-ribbon and on a graphene sheet in constant magnetic field were modeled as probabilistic particles. The models were described by nonlinear stochastic ordinary differential equations. It has been numerically confirmed that probability distributions of the electron models coincide with distributions derived from the wave functions.

Key Words: nonlinear stochastic ordinary differential equation, graphene, particle model, quantum wave

1. Introduction

Nano-carbon materials like graphene [1–3] and carbon nanotubes [4] are expected to be applied to electronic devices because of their high electron mobility. A graphene sheet is composed of carbon atoms bonding to one another to form honeycomb structure. Because of the structure, the behavior of an electron on graphene is described approximately by the massless Dirac equation or the Weyl equation [5]. The Dirac equation originally describes the motion of relativistic fermions. The wave function of the equation, referred to as spinor, is a vector of two complex-valued functions implying not only the location but also the spin orientation of the fermion.

Electrons possess both particle and wave natures. Electrons are represented by probabilistic particles in circuit simulator models of active quantum effect devices like semiconductor-based single-electron transistors [6, 7], while electrons have been depicted by quantum waves in the research of
passive electron waveguides and filters on semiconductor substrates [8–10]. The authors have asserted unification of the representation of electrons for integrated simulation of circuits built of both passive and active quantum devices. Since the circuit simulator models of the active quantum devices are available today, electrons in the passive quantum devices should be modeled as probabilistic particles [11–13]. In this paper, the authors insist again on transforming expression of electrons in graphene-based passive devices [14–18] from wave representation to particle representation.

Theories on wave-to-particle transformation without high computational complexity were established by D. Bohm [19] and E. Nelson [12, 20]. However, the theories seem applicable only to the transformations for quantum particles which are non-relativistic and whose spin does not need to be taken into account, that is, particles whose motion is described by the Schrödinger equation to be given in subsections 2.1 and 3.1. Although a single-electron on graphene is expressed by a spinor as a solution of the Dirac-type wave equation, the electron is inherently non-relativistic and the implication of its spinor is pseudo-spin. This means that the motion of the single-electron can be described by the Schrödinger equation. Therefore, the theories are considered to be applicable to the wave-to-particle transformation for the single-electron on graphene.

In this paper, Nelson’s theory for the wave-to-particle transformation is interpreted by using probability density function and probability density current so that it can be applicable to particle-modeling of a single-electron on graphene. Single-electrons on a graphene nano-ribbon and on a graphene sheet in constant magnetic field are modeled as probabilistic particles. The models are described by nonlinear stochastic ordinary differential equations.

2. Wave equation, probability density function, and probability density current

2.1 Fundamental Dirac-type wave equation

Graphene [1–4] is composed of carbon atoms bonding to one another to form honeycomb structure as shown in Fig. 1. 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 graphene. In this subsection, we assume that electromagnetic field is not applied to the graphene.

When a single-electron on the graphene is expressed microscopically (in subnanometer scale) as a quantum wave, its behavior is governed by the following Schrödinger equation:

$$i\hbar \frac{\partial \psi(x, y, t)}{\partial t} = H\psi(x, y, t), \quad H = -\frac{\hbar^2}{2m_e} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + V(x, y)$$

(1)

where $\hbar$ is the Plank constant divided by $2\pi$, $m_e$ is the mass of an electron, and $V(x, y)$ denotes static potential energy expressing, for example, effect of ripples and wrinkles of a graphene sheet on the electron behavior [2, 21]. Microscopic energy of interaction between carbon atoms and the electron is also contained in $V(x, y)$.

In Reference [4], wave function, $\psi(x, y, t) : \mathbb{R}^3 \to \mathbb{C}$, is described by the following form:

$$\psi(x, y, t) = \sum_{\mathbf{r}_A} w_A(\mathbf{r}_A, t) \phi((x, y) - \mathbf{r}_A, t) + \sum_{\mathbf{r}_B} w_B(\mathbf{r}_B, t) \phi((x, y) - \mathbf{r}_B, t)$$

(2)
where \( \phi(x,y,t) \) is the wave function of the \( p_z \) orbital of a carbon atom located at the origin, \( r_A \) and \( r_B \) denote respectively the coordinate points of carbon atoms A and B. In the tight-binding approximation [3], the squares of the absolute values of \( w_A(r_A,t) \) and \( w_B(r_B,t) \) are the probabilities that the electron is in carbon atoms A and B at \( r_A \) and \( r_B \). In Reference [1,3], the wave function is divided into two parts, the first and the second summations of Eq. (2), and the Schrödinger Eq. (1) is expressed as the following system of two partial differential equations:

\[
\begin{align*}
\frac{\hbar}{i} \frac{\partial}{\partial t} \Phi(x,y,t) &= \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \Phi(x,y,t), \\
\Phi(x,y,t) &= \begin{bmatrix} \sum w_A(r_A,t) \phi((x,y) - r_A,t) \\ \sum w_B(r_B,t) \phi((x,y) - r_B,t) \end{bmatrix}
\end{align*}
\]

(3)

(4)

where \( h_{ij}, i,j = 1,2 \), are partial differential operator elements of the Hamiltonian in \( 2 \times 2 \) matrix form.

In mesoscopic scale, description of the electron behavior on graphene can be a system of partial differential equations of continuum approximation \( \Psi(x,y,t) \) of \( [w_A(r_A,t), w_B(r_B,t)]^T \). This new mesoscopic system of equations possesses a new Hamiltonian \( H \) in the form of \( 2 \times 2 \) matrix. If the electron takes a state of low energy near the Fermi level, the second and the higher-order spatial differential operators of the elements \( H_{ij}, i,j = 1,2 \), of \( H \) can be neglected.

By the expression of the Hamiltonian in \( 2 \times 2 \) matrix form, the continuum approximation as \( \Psi(x,y,t) \), and the neglect of higher-order spatial differentials of \( H_{ij} \), the non-relativistic electron governed by the Schrödinger Eq. (1) is represented by a relativistic particle described by the following massless Dirac-type equation:

\[
\frac{\hbar}{i} \frac{\partial}{\partial t} \Psi(x,y,t) = \left\{ hv_F \left( \sigma_x \dot{k}_x + \sigma_y \dot{k}_y \right) + V(x,y) \right\} \Psi(x,y,t)
\]

(5)

where \( v_F \) is the Fermi velocity. Microscopic interaction between carbon atoms and the electron is no more contained in potential term \( V(x,y) \) explicitly since the wave function \( \Psi(x,y,t) \) represents mesoscopic electron behavior.

The operators \( \dot{k}_x, \dot{k}_y \) in Eq. (5) are defined as

\[
\dot{k}_x = -i \frac{\partial}{\partial x}, \quad \dot{k}_y = -i \frac{\partial}{\partial y}
\]

(6)

The Pauli spin matrices \( \sigma_x, \sigma_y \) in Eq. (5) are given by

\[
\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}
\]

(7)

Wave function \( \Psi(x,y,t) \),

\[
\Psi(x,y,t) = \begin{bmatrix} \psi_A(x,y,t) \\ \psi_B(x,y,t) \end{bmatrix}, \quad \psi_A/B(x,y,t) : R^3 \rightarrow C^1
\]

(8)

is a vector of two complex-valued elements \( \psi_A/B(x,y,t) \) which are wave functions of an electron on two sub-lattices each of which consists of only carbon atoms A or B like the elements of \( \Phi \) given by Eq. (4). Therefore, probability density function \( \rho(x,y,t) \) of the electron should be

\[
\rho(x,y,t) = \psi_A(x,y,t) \psi_A^*(x,y,t) + \psi_B(x,y,t) \psi_B^*(x,y,t)
\]

(9)

The Dirac equation originally describes the motion of relativistic fermions [5]. Its wave function in the same form as Eq. (8) is called spinor whose first and second elements respectively imply the probabilities that spin of the fermion takes orientations Up and Down. On the other hand, \( \psi_A(x,y,t) \) and \( \psi_B(x,y,t) \) of \( \Psi(x,y,t) \) of the single-electron on graphene respectively show the probabilities that the electron is on sub-lattices A and B. Therefore, we say that spinor \( \Psi(x,y,t) \) has pseudo-spin.
We let \( \hat{k}_{x/y}^* = -\hat{k}_{x/y} \) and the conjugate transposes of \( \sigma_{x/y} \) and \( \Psi(x, y, t) \) be denoted by \( \sigma_{x/y}^* \) and \( \Psi^*(x, y, t) \), respectively. Then, the conjugate transpose of Eq. (5) is given by

\[
-i\hbar \frac{\partial}{\partial t} \Psi^*(x, y, t) = \hbar v_F \left[ \hat{k}_x^*, \hat{k}_y^* \right] \Psi^*(x, y, t). \left[ \sigma_{x}^*, \sigma_{y}^* \right] + \Psi^*(x, y, t)V(x, y)
\]

(10)

Adding the products of \( \Psi^*(x, y, t) \) and Eq. (5) and of Eq. (10) and \( \Psi(x, y, t) \), we obtain

\[
\frac{\partial}{\partial t} \rho(x, y, t) + \nabla \cdot \mathbf{J} = 0
\]

(12)

\[
\mathbf{J} = 2v_F (\mathbf{R}(\psi_A^*(x, y, t)\psi_B(x, y, t)), \mathbf{I}(\psi_A^*(x, y, t)\psi_B(x, y, t)))
\]

(13)

where \( \nabla = [\partial/\partial x, \partial/\partial y] \) and \( \mathbf{R}(\chi) \) and \( \mathbf{I}(\chi) \) indicate the real and imaginary parts of \( \chi \), respectively. Since Eq. (12) is so-called an equation of continuity, \( \mathbf{J} \) is considered as probability density current. Assume that wave function \( \Psi(x, y, t) \) is a plane wave given by

\[
\Psi(x, y, t) = \left[ \begin{array}{c} 1 \\ \exp(i\theta) \end{array} \right] \exp(i(k_xx + k_yy)) \exp \left( -i\frac{E(k_x, k_y)}{\hbar}t \right)
\]

(14)

The eigenenergy \( E(k_x, k_y) \) and the directions \( \theta \) of the wave are

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

(15)

From Eq. (13), we find that direction \( \theta \) of the plane wave propagation coincides with the direction of \( \mathbf{J} \). Then, it is inevitable that Eq. (12) has been derived.

### 2.2 Wave equation with vector potential term

In this subsection, we assume that a graphene sheet is in electromagnetic field. We set \( z \)-axis perpendicular to \( x \) and \( y \)-axes which are on the graphene sheet. Let scalar and vector potentials be denoted by \( A_0 \) and \( \mathbf{A} \) or

\[
\mathbf{A} = [A_x, A_y, A_z]
\]

(16)

Relations between electric field \( \mathbf{E} \) and \( A_0 \) and between magnetic field \( \mathbf{B} \) and \( \mathbf{A} \) are respectively given by

\[
\mathbf{E} = -\nabla A_0, \quad \mathbf{B} = \nabla \times \mathbf{A}
\]

(17)

where \( \nabla = [\partial/\partial x, \partial/\partial y, \partial/\partial z] \). Under the vector potential, canonical momentum operator \( \mathbf{\pi} \) is given by [22]

\[
\mathbf{\pi} = [\hat{\pi}_x, \hat{\pi}_y, \hat{\pi}_z] = \mathbf{p} - e\mathbf{A}, \quad \mathbf{p} = -i\hbar \nabla
\]

(18)

where \( e \) denotes elementary charge. Here, we impose conditions that \( A_z = 0 \) and then \( \hat{\pi}_z = 0 \). Equation (5) is then transformed into

\[
i\hbar \frac{\partial}{\partial t} \Psi(x, y, t) = \{-v_F [\sigma_x, \sigma_y] \cdot [\hat{\pi}_x, \hat{\pi}_y] + eA_0 + V(x, y)\} \Psi(x, y, t)
\]

(19)

Equation (19) describes the behavior of a single-electron on the graphene under potentials \( A_0 \) and \( [A_x, A_y, 0] \). We see in this equation that the scalar and vector potentials respectively generate terms \( eA_0 \) and \( v_F e(\mathbf{A}_x, \sigma_x + A_y\sigma_y) \) which are regarded as new potential terms. Similarly to Eq. (10), the complex conjugate equation of Eq. (19) can be described as
\(-i\hbar \frac{\partial}{\partial t} \Psi^*(x, y, t) = -v_F [\hat{\pi}^*_x, \hat{\pi}^*_y] \Psi^*(x, y, t), \begin{bmatrix} \sigma^*_x, \sigma^*_y \end{bmatrix} + \Psi^*(x, y, t) \{eA_0 + V(x, y)\}\) \hspace{1cm} (20)

where \(\hat{\pi}^*_x, \hat{\pi}^*_y\) are the complex conjugates of \(\hat{\pi}_x, \hat{\pi}_y\). Adding the products of \(\Psi^*(x, y, t)\) and Eq. (19) and of Eq. (20) and \(\Psi(x, y, t)\), we obtain

\[\frac{\partial}{\partial t} \rho(x, y, t) + \nabla \cdot J = 0 \] \hspace{1cm} (21)

\[J = 2v_F (R(\psi^*_A(x, y, t)\psi_B(x, y, t)), I(\psi^*_A(x, y, t)\psi_B(x, y, t))) \] \hspace{1cm} (22)

Equations (21) and (22) are the same equations as equation of continuity (12) and probability density current (13), respectively. This means that the effect of electric and magnetic fields \(E, B\) on the motion of an electron does not appear explicitly in probability density current \(J\).

### 3. Stochastic quantization

#### 3.1 Stochastic quantization for the Schrödinger equation

**3.1.1 Bohm’s quantum potential theory**

Behavior of a single non-relativistic quantum particle represented as a quantum wave is described by the Schrödinger Eq. (1). We show it again here.

\[i\hbar \frac{\partial \psi}{\partial t} = H\psi(x, y, t), \quad H = -\frac{\hbar^2}{2m_e} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x, y) \] \hspace{1cm} (23)

This equation does not deal with spin motion of the particle. We express the complex-valued wave function of the equation with amplitude \(R(x, y, t)\) and phase \(S(x, y, t)\) as

\[\psi(x, y, t) = R(x, y, t) \exp(i\frac{S(x, y, t)}{\hbar}) \] \hspace{1cm} (24)

Substituting Eq. (24) in Eq. (23), we obtain the real and imaginary parts of the equation given by

\[\frac{\partial S(x, y, t)}{\partial t} + H = 0, \] \hspace{1cm} (25)

\[H = \frac{1}{2m_e} \left\{ \left(\frac{\partial S(x, y, t)}{\partial x}\right)^2 + \left(\frac{\partial S(x, y, t)}{\partial y}\right)^2 \right\} + V(x, y) + Q(x, y, t), \] \hspace{1cm} (26)

\[Q = -\frac{\hbar^2}{2m_e} R(x, y, t) \left(\frac{\partial^2 R(x, y, t)}{\partial x^2} + \frac{\partial^2 R(x, y, t)}{\partial y^2}\right) \] \hspace{1cm} (27)

Equation (25) is regarded as the Hamilton-Jacobi equation representing a classical energy-conservative system with a potential given by the sum of classical potential \(V(x, y)\) and a quantum potential term \(Q(x, y, t)\). Equation (26) is regarded as an equation of continuity in terms of probability density and Eq. (27) expresses probability density current. In the quantum potential theory, a quantum particle is modeled as a classical particle which is governed by Eq. (25) and moves along the current of probability density given by Eq. (27) \[12, 19\].

**3.1.2 Nelson’s stochastic quantization theory**

A probabilistic particle fluctuating by receiving white Gaussian random force is described by the forward generalized Langevin equation,
\[ [dx, dy] \equiv [x(t + dt), y(t + dt)] - [x(t), y(t)] \]
\[ = b(x, y, t) dt + \sqrt{\nu} [d\Gamma_x(t), d\Gamma_y(t)], \]  
\[ [d\Gamma_x(t), d\Gamma_y(t)] \equiv [\Gamma_x(t + dt), \Gamma_y(t + dt)] - [\Gamma_x(t), \Gamma_y(t)] \]

or the backward equation,
\[ [dx, dy] \equiv [x(t), y(t)] - [x(t - dt), y(t - dt)] \]
\[ = b_*(x, y, t) dt + \sqrt{\nu} [d\Gamma_x(t), d\Gamma_y(t)], \]
\[ [d\Gamma_x(t), d\Gamma_y(t)] \equiv [\Gamma_x(t), \Gamma_y(t)] - [\Gamma_x(t - dt), \Gamma_y(t - dt)] \]

Terms \( b(x, y, t) \) and \( b_*(x, y, t) \) in Eqs. (28) and (29) are drift terms which are defined by the following ensemble-average velocities:
\[ b(x, y, t) = D \left[ x(t), y(t) \right] = \lim_{\Delta t \to 0} \left\langle \frac{[x(t + \Delta t), y(t + \Delta t)] - [x(t), y(t)]}{\Delta t} \right\rangle \]
\[ b_*(x, y, t) = D_* \left[ x(t), y(t) \right] = \lim_{\Delta t \to 0} \left\langle \frac{[x(t), y(t)] - [x(t - \Delta t), y(t - \Delta t)]}{\Delta t} \right\rangle \]

The elements of variation \([d\Gamma_x(t), d\Gamma_y(t)]\) of random term \([\Gamma_x(t), \Gamma_y(t)]\) in Eqs. (28) and (29) are white Gaussian fluctuations. They possess the following correlation properties:
\[ < d\Gamma_{x/y}(t) d\Gamma_{x/y}(t + \tau) > = 2\delta(\tau), \quad < d\Gamma_x(t) d\Gamma_y(t + \tau) > = 0, \]

Consider that the probabilistic particle moves in a potential field \( U(x, y, t) \). The equation of average motion for the particle is described by
\[ m_e \alpha(x, y, t) = - \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] U(x, y, t) \]

In this equation, \( \alpha(x, y, t) \) is average acceleration given by
\[ \alpha(x, y, t) = \frac{1}{2} (DD_* + D_* D) [x(t), y(t)] = \frac{1}{2} (Db_*(x, y, t) + D_* b(x, y, t)) \]
\[ \frac{\partial}{\partial t} \rho(x, y, t) = - \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] b(x, y, t) \rho(x, y, t) + \frac{\nu}{2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \rho(x, y, t) \]
\[ - \frac{\partial}{\partial t} \rho(x, y, t) = \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] b_*(x, y, t) \rho(x, y, t) + \frac{\nu}{2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \rho(x, y, t) \]

By subtracting Eq. (36) from Eq. (35), we obtain the following equation of continuity in terms of probability density distribution \( \rho(x, y, t) \):
\[ \frac{\partial}{\partial t} \rho(x, y, t) = - \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] \frac{1}{2} (b(x, y, t) + b_*(x, y, t)) \rho(x, y, t) \]

We equate two equations of motion (25) and (33) and two equations of continuity (26) and (37) and we let diffusion coefficient \( \nu \) in Eqs. (28), (29), (35), and (36) be given by
\[ \nu = \frac{h}{m_e} \]
These equations show that a probabilistic particle model described by the generalized Langevin Eq. (28) and the Fokker-Planck Eq. (35) is constructed from the wave function (24) of the Schrödinger Eq. (23) [12, 20]. Note that the former equation, Eq. (28), is a nonlinear stochastic ordinary differential equation.

3.2 Stochastic quantization for graphene

As Eqs. (41) and (42) show, components $u(x, y, t)$ and $v(x, y, t)$ of drift term $b(x, y, t)$ are expressed respectively with amplitude $R(x, y, t)$ and phase $S(x, y, t)$ of the wave function. Probability density function $\rho(x, y, t)$ of the quantum particle whose motion is governed by the Schrödinger equation is $R(x, y, t)^2$, i.e.,

$$\psi(x, y, t)\psi^*(x, y, t) = R(x, y, t)^2 = \rho(x, y, t)$$

(43)

From Eqs. (27), (42), and (43), we obtain

$$\frac{1}{m_e} \left[ \frac{\partial S(x, y, t)}{\partial x}, \frac{\partial S(x, y, t)}{\partial y} \right] \frac{1}{2} \log \rho(x, y, t) = \frac{J(x, y, t)}{\rho(x, y, t)}$$

(44)

Then, we attain

$$u(x, y, t) = \frac{\hbar}{m_e} \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] \frac{1}{2} \log \rho(x, y, t)$$

(45)

$$v(x, y, t) = \frac{J(x, y, t)}{\rho(x, y, t)}$$

(46)

Equations (45) and (46) show that a probabilistic particle model can be built if probability density function and probability density current are obtained. The probability density function and the probability density current for a non-relativistic single-electron with pseudo-spin on graphene are expressed with the two elements $\psi_{A/B}(x, y, t)$ of spinor-type wave function $\Psi(x, y, t)$ of the Dirac-type wave equation, as given in Eq. (9) and Eq. (13) or (22). Therefore, the single-electron on graphene can be represented by a probabilistic particle which is described by the Langevin and Fokker-Planck equations.

4. Numerical experiments

4.1 Nano-ribbon graphene

Figure 2 shows two kinds of graphene ribbons [2, 23–25]. Both sides of nano-ribbons are called zigzag edges if only carbon atoms A locate on one side of the ribbon and only carbon atoms B locate inevitably on other side (see Figs. 2(a) and 1) while the sides on which both atoms A and B locate
Fig. 3. Time-evolving probability density function on armchair nano-ribbon.

alternately are called armchair edges (see Figs. 2(b) and 1). In this subsection, we construct and
evaluate a probabilistic particle model of a single-electron on an armchair graphene nano-ribbon.

The potential term of the Dirac-type wave equation is set simply as \( V(x, y) = 0 \). If the potential
term is constant, \( V(x, y) = V_0 \), or constant scalar potential \( A_0 \) is applied, eigenenergy \( E \) given by
Eq. (15) shifts by \( V_0 \) or \( eA_0 \). Therefore, the change of the single-electron behavior is trivial. If \( V(x, y) \)
is a function of \( x \) and \( y \), the spinor of the electron on a nano-ribbon can be computed as presented,
for example, in [26]. As mentioned in section 3, the Langevin equation as a mathematical particle
model of the single-electron can be established as long as a spinor-type wave function is obtained
analytically or numerically for a given potential term.

Let an armchair nano-ribbon with length \( L \) between the two edges (nano-ribbon of width \( L \)) be set
on \( x - y \) plane as shown in Fig. 2(b). Boundary conditions on two elements \( \psi_{A/B}(x, y, t) \) of spinor
\( \Psi(x, y, t) \) are

\[
\psi_A(0, y, t) = \psi_B(0, y, t) = 0, \quad \psi_A(L, y, t) = \psi_B(L, y, t) = 0
\]

(47)
on the edges of the armchair nano-ribbon. The spinor-type wave function given the boundary con-
ditions is described by Eq. (A-1) in Appendix A. If the probability density function (9) distributing
initially in the Gaussian form along \( y \)-axis is given by Eq. (A-5), coefficients \( c_k \) of the \( y \)-directional
components of the wave function (A-1) are computed according to Eq. (A-10). We constructed the
wave function with 200 components each of which is multiplied by \( c_k \).

The constants of Dirac-type wave Eq. (5) are normalized as \( \hbar = 1.0 \) and \( v_F = 1.0 \). The width
of the ribbon is set to \( L = 1.0 \). The propagation mode in \( x \)-direction is set simply to fundamental mode,
i.e., \( n = 1 \) in Eq. (A-3). Wave number \( k_0 \) in Eq. (A-10) is determined so that initial velocity given
by Eq. (A-8) is \( v_0 = 0.5 \).

Figure 3 shows time-evolving probability density function \( \rho(x, y, t) \) given by Eq. (9).

We computed probability density current \( J(x, y, t) \) given by Eq. (13). From the computed function
\( \rho(x, y, t) \) and current \( J(x, y, t) \), a probabilistic particle model is built as mentioned in subsection 3.2.
Five sample trajectories of the particle model starting at \( (x, y) = (0.5, 0) \) are shown for \( 0 \leq t \leq 50 \)
in Fig. 4. Locations of the particles at time \( t = 10, 20, 30, 40, \) and 50 are marked on the trajectories

508
Fig. 4. Sample trajectories of the particle model on armchair nano-ribbon.

Fig. 5. Marginal probability density of particle locations $x$ and $y$ on armchair nano-ribbon at $t = 30$.

with circles. Figure 5 shows the marginal distributions of coordinates $x$ and $y$ of $10^4$ particle locations at time $t = 30$. Their initial locations distributed as given by Eq. (A-5). Marginal distributions of $x$ and $y$ obtained from probability density function $\rho(x, y, t = 30)$ are also shown in Fig. 5 with red curves.

We compared the marginal distributions obtained from the particle model and from the probability density function as follows: We express the marginal distributions of $x$-coordinate of the particles by the following equation:

$$\rho_p(x, t) = \frac{N_i(x, t)}{N_p}, \quad (48)$$

$N_i(x, t)$: The number of particles whose $x$-coordinate is $x \in \Delta I_i$ at time $t$,

$$\Delta I_i : \left[ \frac{L_{x,i}}{l_x}, \frac{L_{x,i}}{l_x} (i + 1) \right], 0 \leq i (\text{integer}) < l_x,$$

$L_x = L$, $l_x$: the number of intervals $\Delta I_i$,

$N_p$: The number of the particles ($= 10^4$)

The marginal distributions of $y$-coordinate is similarly expressed by

$$\rho_p(y, t) = \frac{N_j(y, t)}{N_p}, \quad (49)$$
$N_j(y,t)$: The number of particles whose $y$-coordinate is $y \in \Delta I_j$ at time $t$,

$\Delta I_j : \left[ \frac{L_y}{l_y} j, \frac{L_y}{l_y} (j + 1) \right], j_{\text{min}} \leq j (\text{integer}) < j_{\text{max}}$,

$L_y = y_{\text{max}} - y_{\text{min}}, \quad L_y$: the number of intervals $\Delta I_j$,

$j_{\text{min}} = \frac{y_{\text{min}}}{L_y/l_y}, \quad j_{\text{max}} = \frac{y_{\text{max}}}{L_y/l_y}$,

$N_p$: The number of the particles ($=10^4$)

We set $l_x = l_y = 30$. Marginal distributions of $x$ and $y$ can be defined also from the probability density function as

$$\rho_w(x,t) = \int_{y_{\text{min}}}^{y_{\text{max}}} \rho(x,y,t) \, dy$$  \hspace{1cm} (50)

and

$$\rho_w(y,t) = \int_0^L \rho(x,y,t) \, dx$$  \hspace{1cm} (51)

respectively. The differences between $\rho_p(x,t)$ and $\rho_w(x,t)$ and between $\rho_p(y,t)$ and $\rho_w(y,t)$ are evaluated respectively by computing

$$\Delta \rho_x = \int_0^L |\rho_p(x,t) - \rho_w(x,t)| \, dx$$  \hspace{1cm} (52)

and

$$\Delta \rho_y = \int_{y_{\text{min}}}^{y_{\text{max}}} |\rho_p(y,t) - \rho_w(y,t)| \, dy$$  \hspace{1cm} (53)

at time $t_1 = 30$. The evaluation results are $\Delta \rho_x = 0.079$ and $\Delta \rho_y = 0.072$. As a result, we can say that the proposed particle model possesses almost the same statistical properties as the spinor-type wave function.

### 4.2 Graphene in constant magnetic field

We compute the behavior of a single-electron on a graphene sheet in $x-y$ plane where vector potential called the symmetric gauge given by

$$A = \frac{B_0}{2} [-y, x, 0]$$  \hspace{1cm} (54)

and zero scalar potential, $A_0 = 0$, are applied. From Eqs. (17) and (54), magnetic field is given by

$$B = [0, 0, B_0]$$  \hspace{1cm} (55)

That is, magnetic field $B$ is perpendicular to the graphene sheet. The potential term in Eq. (19) is $V(x,y) = 0$.

In Appendix B, the spinor-type eigenfunctions $\Psi_{m,n}(\xi, \theta,t)$ with non-negative integer quantum numbers $(n,m)$ are given in polar coordinate system $(\xi, \theta)$ which is related to orthogonal coordinate system $(x, y)$ as follows:

$$\sqrt{\omega_0/2} x = \xi \cos \theta, \quad \sqrt{\omega_0/2} y = \xi \sin \theta, \quad \hbar \omega_0 = 2eB_0$$  \hspace{1cm} (56)

Figure 6 shows probability density function $\rho(\xi, \theta)$ obtained from the eigenfunctions $\Psi_{m,n}(\xi, \theta,t)$. It is found in Appendix C and Fig. 6 that $\rho(\xi, \theta)$ is independent of $\theta$. Figure 7 shows the probability density as a function of $\xi$. It is mentioned in Appendix C that azimuth-directional component $u_\theta(\xi, \theta,t)$ of $u(\xi, \theta,t)$ and radial-directional component $v_\xi(\xi, \theta,t)$ of $v(\xi, \theta,t)$ are zero. Figure 8 shows non-zero drift components $u_\xi(\xi)$ and $v_\theta(\xi)$. From Fig. 8, it is expected that behavior of the particle model of the electron is cyclotron motion on $n+1$ circles. Figure 9 shows the behavior when $(n,m) = (0,2), (1,3)$, and $(2,4)$. If quantum fluctuation is supposed to be zero or $\nu = 0$, the particle model behaves as shown in Fig. 10, circular as expected. Figure 11 shows the probability distribution of the
location, radial $r$, of $10^4$ particles. Normalized distributions in Fig. 7 are also plotted with respect to $r$ in Fig. 11 with red curves.

We compared these two distributions shown in Fig. 11 by computing marginal probability densities given by

$$\rho_p(r) = \frac{N_i(r)}{N_p},$$  \hspace{1cm} (57)

$N_i(r)$: The number of particles whose $r$-coordinate is $r \in \Delta r_i$,

$$\Delta r_i = \left[ \frac{r_{\max}}{l_r}, \frac{r_{\max}}{l_r} (i + 1) \right), \hspace{0.5cm} 0 \leq i (: \text{integer}) < l_r,$$

$N_p$: The number of the particles ($= 10^4$)
Fig. 9. Cyclotron motion of the particle model with quantum noise.

Fig. 10. Cyclotron motion of the particle model without quantum noise.

Fig. 11. Distribution of particle locations on graphene in the vector potential.

\[ \rho_{w}(r) = \int_{t_0}^{t_1} \int_{0}^{2\pi} \rho(r, \theta, t) d\theta dt, \quad t_0 = 0, \quad t_1 = 30 \] (58)

and evaluating

\[ \Delta \rho_r = \int_{0}^{r_{\max}} |\rho_p(r) - \rho_w(r)| dr \] (59)

for \( r = 30 \). The evaluation results in \( \Delta \rho_r = 0.18, 0.11, \) and 0.13 when \((n, m) = (0, 2), (1, 3), \) and \((2, 4)\), respectively. These results validate that the constructed particle model and the spinor-type wave function possess almost the same statistical properties.
5. Conclusions
A probabilistic particle model of single-electrons on graphene has been constructed. Nelson’s stochastic quantization theory could be applied to build the particle model by the interpretation of the theory with probability density function and probability density current. In the second numerical example presented in subsection 4.2, this interpretation has lead to the consequence that the azimuth-directional component $u_\theta$ and the radial-directional component $v_r$ of drift term $b$ of the particle model are zero, which reduced the computational cost of the electron trajectories. It was verified by the numerical experiments that the behaviors of the constructed particle models were stochastically almost equivalent to those of the wave functions. One of the future subjects related to this work is to incorporate probabilistic variable in terms of actual spin into the proposed probabilistic model.

Acknowledgments
A part of this work was supported by JSPS KAKENHI Grant No. 19K04394.

Appendix
A. The spinor-type wave functions for armchair nano-ribbon
From References [23–25], spinor-type wave functions propagating on an armchair nano-ribbon can be described in continuous form by

$$\Psi(x, y, t) = \left[ \psi_A(x, y, t) \psi_B(x, y, t) \right] = \left( \sum_{k=k_{\min}}^{k=k_{\max}} c_k \begin{bmatrix} \phi_{A,k}(x, y, t) \\ \phi_{B,k}(x, y, t) \end{bmatrix} \right) \sin(px),$$ (A-1)

$$\begin{bmatrix} \phi_{A,k}(x, y, t) \\ \phi_{B,k}(x, y, t) \end{bmatrix} = \left[ -S \sqrt{\epsilon_p + \exp \left(-\frac{i k^2}{2}\right)} \right] \left[ \epsilon_p + \exp \left(\frac{i k^2}{2}\right) \right] \exp(i k y) \exp \left(-i \frac{E(p, k)}{\hbar} t \right), \quad S = \pm 1$$ (A-2)

with continuous independent spatial variables $x$ and $y$. Equation (A-1) satisfies boundary conditions (47) if $x$-directional wave number $p$ is

$$p = \frac{\pi}{L} n, \quad n: \text{mode number}$$ (A-3)

Energy $E(p, k)$ in Eq. (A-2) is determined for $y$-directional wave number $k$ as

$$E(p, k) = \sqrt{\left(\epsilon_p + \exp \left(-\frac{i k^2}{2}\right)\right) \left(\epsilon_p + \exp \left(\frac{i k^2}{2}\right)\right)}, \quad \epsilon_p = 2 \cos p$$ (A-4)

The probability density function distributing initially in the Gaussian form on $y$-axis is expressed as

$$\rho(x, y, 0) = f_0(x) g_0(y),$$ (A-5)

$$f_0(x) = \sin^2 \left(\frac{n \pi x}{L}\right),$$ (A-6)

$$g_0(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{y^2}{2\sigma^2}\right)$$ (A-7)

If the initial velocity of a wave packet with initial distribution (A-5) is $v_0$ in $y$-direction, there exists a wave number $k_0$ satisfying

$$v_0 = \frac{1}{\hbar} \frac{\partial E(p, k)}{\partial k} \bigg|_{k=k_0} = -\frac{1}{2\hbar} \epsilon_p \sin \left(\frac{\pi p}{L}\right), \quad k_{\min} < k_0 < k_{\max}$$ (A-8)

From Eqs. (A-1) and (A-5), we have

$$\psi_A(x, y, 0) \psi_A^*(x, y, 0) = \psi_B(x, y, 0) \psi_B^*(x, y, 0) = \frac{1}{2} f_0(x) g_0(y)$$ (A-9)

From Eq. (A-9), coefficients $c_k$ of the $y$-directional components in Eq. (A-1) are determined by the following equation:

$$c_{k'} + k_0 c_{k'+k_0} E(k' + k_0, p) = \sqrt{a_{k'} a_{k'_L}}, \quad a_{k'_L}: \text{Fourier coefficients of} \frac{1}{2} g_0(y)$$ (A-10)
B. The spinor-type eigenfunctions in symmetric gauge

By referring to [27–31], the eigenfunctions of Eq. (19) can be derived as follows: Let creation operators in terms of integer quantum numbers $m$ and $n$ be denoted by $C_M$ and $C_N$. They are given by

$$C_M = \frac{\exp(-i\theta)}{2} \left( -\frac{\partial}{\partial \xi} + \frac{i}{\xi} \frac{\partial}{\partial \theta} + \xi \right)$$  \hspace{1cm} (B-1)

$$C_N = \frac{\exp(i\theta)}{2} \left( -\frac{\partial}{\partial \xi} - \frac{i}{\xi} \frac{\partial}{\partial \theta} + \xi \right)$$  \hspace{1cm} (B-2)

Eigenfunctions $\Psi_{m,n}(\xi,\theta,t)$ has the following form:

$$\Psi_{m,n}(\xi,\theta,t) = \Psi_{m,n}(\xi,\theta)e^{-(iE_\mu/t)}, \quad E_n = \hbar v_F \sqrt{n}\omega_0$$  \hspace{1cm} (B-3)

$$\Psi_{m,n}(\xi,\theta) = \frac{1}{\sqrt{2}} \begin{bmatrix} \psi_{m,n-1}(\xi,\theta) \\ i\psi_{m,n}(\xi,\theta) \end{bmatrix}$$

$$\Psi_{m,0}(\xi,\theta) = \begin{bmatrix} 0 \\ i\psi_{m,0}(\xi,\theta) \end{bmatrix}$$

$$\psi_{0,0}(\xi,\theta) = K_0 \exp \left( -\frac{1}{2}\xi^2 \right), \quad K_0 : \text{Normalization constant}$$

By applying operators $C_M$ and $C_N$ to $\psi_{0,0}(\xi,\theta)$, elements $\psi_{m,n}(\xi,\theta)$ are obtained as

$$\psi_{m,n}(\xi,\theta) = \frac{(C_M)^m(C_N)^n}{\sqrt{m!n!}} \psi_{0,0}(\xi,\theta)$$

$$= (-1)^{m(n,m,n)} \frac{\omega_0 \min(m,n)!}{4\pi \max(m,n)!} \xi^{n-m} \exp \left( -\frac{\xi^2}{2} + i(n-m)\theta \right) L_{\min(m,n)}(\xi^2)$$  \hspace{1cm} (B-4)

where $L_a(\xi)$ is the associated Laguerre polynomial given by

$$L_a(\xi) = \sum_{\gamma=0}^{\alpha} (-1)^{\beta+\gamma} \frac{(\alpha!)^2}{(\alpha+\gamma)!(\alpha-\beta-\gamma)\gamma!} x^\gamma$$  \hspace{1cm} (B-5)

C. Polar coordinate drift term of the particle model in vector potential

Let a generalized Langevin equation in polar coordinate ($\xi, \theta$) be expressed as

$$[d\xi, \xi d\theta] = [u_\xi(\xi,\theta,t), u_\phi(\xi,\theta,t)] dt + [v_\xi(\xi,\theta,t), v_\phi(\xi,\theta,t)] dt + \sqrt{\nu} \left[ d\Gamma(\xi(t),d\Gamma(\theta(t)) \right]$$  \hspace{1cm} (C-1)

where the drift components $[u_\xi(\xi,\theta,t), u_\phi(\xi,\theta,t)]$ and $[v_\xi(\xi,\theta,t), v_\phi(\xi,\theta,t)]$ are coordinate transformation of $u(x,y,t)$ and $v(x,y,t)$ given by Eqs. (45) and (46). Relation between variations $[dx,dy]$ and $[d\xi, d\theta]$ determined by the generalized Langevin equations in orthogonal and polar coordinate systems are given by

$$[d\xi, d\theta] = \frac{\sqrt{\omega_0}}{2} [dx, dy] M(-\theta), \quad M(-\theta) = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}$$  \hspace{1cm} (C-2)

From Eqs. (45), (46), (C-2), and

$$\frac{\sqrt{\omega_0}}{2} \left[ \frac{\partial}{\partial x} \frac{\partial}{\partial y} \right] = \left[ \frac{\partial}{\partial \xi} \frac{1}{\xi} \frac{\partial}{\partial \theta} \right] M(\theta)$$  \hspace{1cm} (C-3)

we obtain

$$[u_\xi(\xi,\theta,t), u_\phi(\xi,\theta,t)] = \frac{\hbar}{m_e} \left[ \frac{\partial}{\partial \xi} \frac{1}{\xi} \frac{\partial}{\partial \theta} \right] \frac{1}{2} \log \rho(\xi,\theta,t)$$  \hspace{1cm} (C-4)
\[ v_\xi(\xi, \theta, t), v_\theta(\xi, \theta, t) = \frac{\sqrt{\omega_0}}{m_e \rho(\xi, \theta, t)} [R(\psi_A^*(\xi, \theta, t)\psi_B(\xi, \theta, t)), I(\psi_A^*(\xi, \theta, t)\psi_B(\xi, \theta, t))] M(-\theta) \quad (C-5) \]

When spinor \([\psi_A(\xi, \theta, t), \psi_B(\xi, \theta, t)]^T\) is an eigenfunction (B-3) whose elements are given by Eq. (B-4), it is easily found that the probability density function \(\rho(\xi, \theta, t)\) is independent of azimuth \(\theta\) and, triably, of time \(t\). Then,

\[ u\rho(\xi, \theta, t) = 0 \quad (C-6) \]

From the first equality of Eq. (B-4), we find

\[ \psi_{m,n}(\xi, \theta) = \frac{1}{\sqrt{n}} C_N \psi_{m,n-1}(\xi, \theta) \quad (C-7) \]

Substituting Eq. (B-3) into \([\psi_A(\xi, \theta, t), \psi_B(\xi, \theta, t)]\) in Eq. (C-5) and using Eq. (C-7), we attain

\[ v_\xi(\xi, \theta, t) = 0 \quad (C-8) \]

References

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

[2] A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, and A.K. Geim, “The Electron properties of graphene,” *Reviews of Modern Physics*, vol. 81, no. 1, pp. 109–162, 2009.

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

[4] T. Ando, “Theory of electronic states and transport in carbon nanotubes,” *Journal of the Physical Society of Japan*, vol. 74, no. 3, pp. 777–817, 2005.

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

[6] C. Wasshuber, *Computational Single-Electronics*, Springer, 2001.

[7] J. Gubernatis, N. Kawashima, and P. Werner, *Quantum Monte Carlo Methods: Algorithms for Lattice Models*, Cambridge University Press, 2016.

[8] J. Xia, D. Liu, and W. Sheng, *Quantum Waveguide in Microcircuits*, Pan Stanford Publishing, 2018.

[9] J.B. Wang and S. Midgley, “Electron transport in quantum waveguides,” *Journal of Computational and Theoretical Nanoscience*, vol. 4, no. 3, pp. 408–432, 2007.

[10] J.A. Alamo, C.C. Eugster, Q. Hu, M.R. Melloch, and M.J. Rooks, “Electron waveguide devices,” *Superlattices and Microstructures*, vol. 23, no. 1, pp. 121–137, 1998.

[11] N. Hirami, H. Fujisaka, and T. Kamio, “Probabilistic particle modeling of quantum wave propagation with reflection, transmission, and coupling,” *Proc. IEEE ISCAS’14*, pp. 478–481, 2014.

[12] I. Nakamura, N. Hirami, and H. Fujisaka, “Representation of electrons on multi-stage coupled electron waveguides by waves and particles,” *NOLTA*, vol. E10-N, no. 2, pp. 206–220, 2019.

[13] S. Hayakawa, N. Hirami, and H. Fujisaka, “Representation of electrons on symmetric electron-wave stub-filters by waves and particles,” *NOLTA*, vol. E10-N, no. 4, pp. 414–430, 2019.

[14] J. Nakabayashi, D. Yamamoto, and S. Kurihara, “Band-Selective Filter in a Zigzag Graphene Nanoribbon,” *Physical Review Letters*, vol. 102, 066803 (4pp), 2009.

[15] W. Huang, S.-J. Liang, E. Kyoseva, and L.K. Ang, “A new coupling mechanism between two graphene electron waveguides for ultrafast switching,” *Semiconductor Science and Technology*, vol. 33, 035014 (8pp), 2018.

[16] R.R. Hartmann, N.J. Robinson, and M.E. Portnoi, “Smooth electron waveguides in graphene,” *Physical Review B*, vol. 81, 245431 (8pp), 2010.

[17] J. Lan, E. Ye, W. Sui, and X. Zhao, “Admittance of T-stub graphene nanoribbon structure,” *Physical Chemistry Chemical Physics*, vol. 15, no. 2, pp. 671–679, 2013.

[18] D. Mencarelli, T. Rozzi, and L. Pierantoni, “Scattering matrix approach to multichannel transport in many lead graphene nanoribbons,” *Nanotechnology*, vol. 21, 155701 (10pp), 2010.

[19] D. Bohm, “A suggested interpretation of the quantum theory in terms of hidden variables I, II,” *Physical Review*, vol. 85, no. 2, pp. 166–193, 1952.

[20] E. Nelson, “Derivation of the Schrödinger equation from Newtonian mechanics,” *Physical Review*, vol. 150, no. 4, pp. 1079–1085, 1966.
[21] E. Kim and A.H. Castro Neto, “Graphene as an electronic membrane,” Europhysics Letters, vol. 84, 57007 (5pp), 2008.
[22] C. Cohen-Tannoudji, B. Diu, and F. Laloë, Quantum mechanics, vol. 1, Wiley, 1991.
[23] K. Wakabayashi, K. Sasaki, T. Nakanishi, and T. Enoki, “Electronic states of graphene nanoribbons and analytical solutions,” Science and Technology of Advanced Materials, vol. 11, 054504 (18pp), 2010.
[24] K. Sasaki and K. Wakabayashi, “Chiral gauge theory for the graphene edge,” Physical Review B, vol. 82, 035421 (15pp), 2010.
[25] K. Sasaki, K. Wakabayashi, and T. Enoki, “Electron wave function in armchair graphene nanoribbons,” Journal of the Physical Society of Japan, vol. 80, no. 4, 044710 (7pp), 2011.
[26] L.S. Cavalcante, A. Chaves, D.R. da Costa, G.A. Farias, and F.M. Peeters, “All-strain based valley filter in graphene nanoribbons using snake states,” Physical Review B, vol. 94, 075432 (8pp), 2016.
[27] M.O. Goerbig, “The quantum Hall effect in graphene – A theoretical perspective,” Comptes Rendus Physique, vol. 12, no. 4, pp. 369–378, 2011.
[28] Y. Zheng and T. Ando, “Hall conductivity of a two-dimensional graphite system,” Physical Review B, vol. 65, 245420 (11pp), 2002.
[29] S. Kuru, J. Negro, and L.M. Nieto, “Exact analytic solutions for a Dirac electron moving in graphene under magnetic fields,” Journal of Physics: Condensed Matter, 455305 (11pp), 2009.
[30] L. Sourrouille, “Spin-1/2 Landau levels in the symmetric gauge from the zero energy modes,” Journal of Physics Communications, vol. 2, 045030 (13pp), 2018.
[31] E. Diaz-Bautista, J. Negro, and L.M. Nieto, “Partial coherent states in graphene,” Journal of Physics: Conference Series, vol. 1194, 012025 (13p), 2019.