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Author(s)	Kosaka, Wataru; Oikawa, Shun-ichi; Chan, Poh Kam
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Numerical Analysis of Quantum-Mechanical Non-uniform $\mathbf{E} \times \mathbf{B}$ Drift: Non-uniform electric field

Wataru Kosaka ^{a,*}, Shun-ichi Oikawa ^b and Poh Kam Chan ^a

^a Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan

^b Faculty of Engineering, Hokkaido University, Sapporo 060-8628, Japan

Abstract. We have numerically solved the two-dimensional time-dependent Schrödinger equation for a charged particle in the presence of a non-uniform electric field $\mathbf{E} = E(1 - y/L_E)\mathbf{e}_y$ as well as a non-uniform magnetic field $\mathbf{B} = B(1 - y/L_B)\mathbf{e}_z$. It is shown that such a non-uniformity of the electric field does not affect the time rate of the variance, or uncertainty, changes in position and momentum, while that of the magnetic field does.

Keywords: Schrödinger equation, uncertainty, non-uniform magnetic field, non-uniform electric field, quantum mechanical effect, expansion rate, GPU parallel computing

1. Introduction

The charged particles drift in the presence of a magnetic field $\mathbf{B}$, the drifts include ∇B drift, curvature drift and $\mathbf{E} \times \mathbf{B}$ drift if there exist an electric field $\mathbf{E}$. The two-dimensional time-dependent Schrödinger equation have been already solved for a charged particle in the presence of a non-uniform magnetic field and a uniform electric field, in which it was shown that the variance, or the uncertainty, in position $\sigma_r^2(t)$ grows with time [1–5]. For the typical fusion plasma with a temperature $T \sim 10$ keV and a number density of $n \sim 10^{20} \text{ m}^{-3}$, the standard deviation $\sigma_r(t)$ would reach the interparticle separation $n^{-1/3}$ in a time interval of the order of 10^{-4} sec. After this time the wavefunctions of neighboring particles would overlap, as a result the conventional classical analysis may lose its validity [1]. In Ref. [1] mentioned above, the uniform electric field have been assumed. In this paper, quantum mechanical effects of a non-uniform electric field and a non-uniform magnetic field will be studied. In section 2, methods of numerical analysis of time-dependent Schrödinger equation is briefly described. In section 3, time evolution of the variances and their dependence on physical parameters, e.g. m, q, v_0, B, L_B, E , and L_E are shown. Section 4 summarizes the study.

2. Schrödinger equation

The unsteady Schrödinger equation for wavefunction $\psi(\mathbf{r}, t)$, at a position $\mathbf{r}$ and a time t , is given by

*Corresponding author: Wataru Kosaka, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan, E-mail: wataru_k@fusion.qe.eng.hokudai.ac.jp

$$i\hbar \frac{\partial \psi}{\partial t} = \left[\frac{1}{2m} \left(-i\hbar \nabla - q\mathbf{A} \right)^2 + qV \right] \psi, \quad (1)$$

where $V = V(\mathbf{r})$ and $\mathbf{A} = \mathbf{A}(\mathbf{r})$ stand for the scalar and vector potentials, m and q the mass and electric charge of the particle, and $i \equiv \sqrt{-1}$ the imaginary unit, $\hbar$ the reduced Planck constant.

2.1. Numerical analysis

In the Cartesian coordinate system (x, y, z) , we assume the magnetic field $\mathbf{B} \parallel \mathbf{e}_z$ and the electric field $\mathbf{E} \perp \mathbf{e}_z$, where $\mathbf{e}_z$ is z -direction unit vector. In this case, the wavefunction $\psi(x, y, z, t)$ is decomposed into $\psi(x, y, t)$ which corresponds to cyclotron motion in x - y plane and $\psi(z, t)$ which corresponds to free particle motion in z -direction.

We will solve Eq. (1) with an appropriate initial condition in x - y plane, using the finite difference method (FDM) in space with the Crank-Nicolson scheme [1–5].

For the Crank-Nicolson scheme with the central difference method in space, partial differential equation Eq. (1) is reduced to the following matrix equation,

$$\left(\mathbf{I} - \frac{\Delta t}{2i\hbar} \mathbf{H} \right) \{\psi^{n+1}\} = \left(\mathbf{I} + \frac{\Delta t}{2i\hbar} \mathbf{H} \right) \{\psi^n\}. \quad (2)$$

Here, $\{\psi^n\}$ stands for the discretized wavefunction, the superscript n represents the time-label, $\mathbf{I}$ and $\mathbf{H}$ are the unit matrix and the numerical Hamiltonian matrix [1–5]. Assuming the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, the numerical Hamiltonian matrix $\mathbf{H} \equiv \{H_{i,j}\}$ is written as follows,

$$H_{i,j} = \frac{1}{2m} \left[\nabla_{i,j}^2 + 2i\hbar q \mathbf{A}_{i,j} \cdot \nabla_{i,j} + (q\mathbf{A}_{i,j})^2 \right] + qV_{i,j}, \quad (3)$$

where $\mathbf{A}_{i,j}$ and $\nabla_{i,j}$ represent the discretized operators, as

$$\nabla_{i,j}^2 \psi = \frac{\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}}{\Delta x^2} + \frac{\psi_{i,j-1} - 2\psi_{i,j} + \psi_{i,j+1}}{\Delta y^2}, \quad (4)$$

and the subscripts i and j represent x - and y - node numbers. Equations (2) and (3) are quadratic in accuracy over both the time step Δt and the grid size Δx and Δy .

The time integrator $\mathbf{U}$ is derived from Eq. (2) as,

$$\mathbf{U} \equiv \left(\mathbf{I} - \frac{\Delta t}{2i\hbar} \mathbf{H} \right)^{-1} \left(\mathbf{I} + \frac{\Delta t}{2i\hbar} \mathbf{H} \right). \quad (5)$$

It should be noted that the time integrator is not only unconditionally stable but also norm-conserving for discretized wavefunction $\{\psi\}$. The latter leads to the strict particle conservation, irrespective of Δt , Δx and Δy , since the matrix $\mathbf{H}$ is Hermitian, so that the matrix $\mathbf{U}$ is unitary; the Euclidean norm $\|\{\psi\}\|_2 = \text{const}$ with time [1].

We will also adopt the successive over relaxation (SOR) scheme for time integration in Eq. (2).

$$\{\psi^{n+1}\}^{(k+1)} = \{\psi^{n+1}\}^{(k)} + \omega_{\text{SOR}} \{R\}^{(k)}, \quad (6)$$

where

$$\{R\} = \frac{1}{\alpha} \left[\{\phi^n\} - \left(1 - \frac{\Delta t}{2i\hbar} \mathbf{H} \right) \{\psi^{n+1}\} \right], \quad (7)$$

$$\{\phi^n\} = \left(1 + \frac{\Delta t}{2i\hbar} \mathbf{H} \right) \{\psi^n\}, \quad (8)$$

$\{R\}$ is the residual in Eq. (2), α stands for the diagonal element in LHS of Eq. (2), superscript (k) represents the number of iterations, ω_{SOR} is the relaxation factor and $\omega_{\text{SOR}} = 1.01$ is adopted in this study. For the convergence criterion, we have used the following,

$$\frac{1}{N_x N_y} \sum_{i,j=1}^{N_x, N_y} |R_{i,j}|^2 \leq \epsilon_{\text{SOR}}, \quad (9)$$

where N_x and N_y represent the number of nodes in x - and y -direction, and $\epsilon_{\text{SOR}} = 5 \times 10^{-31}$ in this study.

Since Eq. (6) can be executed in parallel, we have used a graphics processing unit (GPU) [9] for this purpose.

3. Numerical results

In the numerical results to be presented in the following, physical parameters are normalized as; mass of the particle $m = m_p = 1.6722 \times 10^{-27}$ kg, charge $q = e = 1.602 \times 10^{-19}$ C, velocity $v = 10 \text{ ms}^{-1}$ and magnetic field $B = 10 \text{ T}$ [1]. Thus, normalization constants of length ρ , time t and electric field E are $\rho = m_p v / eB = 1.0438 \times 10^{-8} \text{ m}$, $t = m_p / eB = 1.0438 \times 10^{-9} \text{ s}$ and $E = vB = 100 \text{ Vm}^{-1}$. The Schrödinger equation is solved in the presence of a scalar potential of $qV = -qEy(1 - y/2L_E)$ and a vector potential of $q\mathbf{A} = -qBy(1 - y/2L_B)\mathbf{e}_y$, where L_E and L_B stand for a gradient scale length of a electric field and magnetic field.

When the corresponding classical particle has a canonical momentum $\mathbf{p}_0 = m\mathbf{v}_0 + q\mathbf{A}(\mathbf{r}_0)$, where $\mathbf{v}_0$ is the initial velocity at a position $\mathbf{r} = \mathbf{r}_0$, initially at a time $t = 0$, the initial condition for the wavefunction $\psi(\mathbf{r}, 0)$ can be given [6, 7] by

$$\psi(\mathbf{r}, 0) = \frac{1}{\sqrt{\pi}\sigma_B} \exp \left[-\frac{(\mathbf{r} - \mathbf{r}_0)^2}{2\sigma_B^2} + i\mathbf{k}_0 \cdot \mathbf{r} \right], \quad (10)$$

where $\mathbf{k}_0 = \mathbf{p}_0/\hbar$ is the initial wavenumber vector, and $\sigma_B \equiv \sqrt{\hbar/qB}$ is known as the magnetic length in quantum mechanics [8].

3.1. Numerical errors

There are three invariants of motion, the energy $\mathcal{E} = \langle \hat{H} \rangle$, the canonical momentum in x -direction $P_x = \langle -i\hbar\partial/\partial x \rangle = \langle m\hat{v}_x - q\hat{A}_x \rangle$, since the potentials V and $\mathbf{A}$ do not depend on x , as well as particle conservation $\int_{\Sigma} |\psi|^2 dS = 1$. Here, $\langle \hat{f} \rangle$ stands for the expectation value of an operator $\hat{f}$, i.e. $\langle \hat{f} \rangle = \int_{\Sigma} \psi^* \hat{f} \psi dS$. The absolute numerical errors in these invariants are quite small as shown Fig. 1.

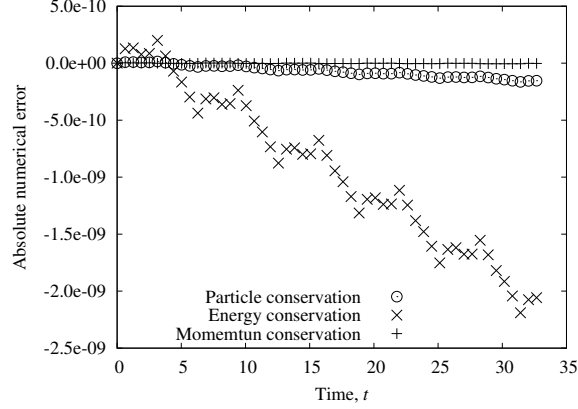


Fig. 1. Absolute errors for the invariants of a particle, energy and x-component of the canonical momentum for $q = m = B = 1$, $v_0 = 5$, $E = 10^{-3}$ and $L_E = L_B = 10^{-4}$. Their initial values are 1 (exact), ~ 5 and ~ 13 .

3.2. Time evolution of variances

The time dependent variances in position $\sigma_r^2(t)$ and mechanical momentum $\sigma_{mv}^2(t)$ oscillate with each gyration period, such as $2\pi/\omega_c$ and π/ω_c , where ω_c is the cyclotron frequency, as shown Fig. 2. In both uniform and non-uniform conditions, the variances slightly grow with time. Since the exact variances should not grow with time in the presence of a uniform electromagnetic field, these time evolution $\sigma_{\text{non-uniform}}^2(t)$ are due purely to numerical errors. On the other hand, the time evolution $\sigma_{\text{uniform}}^2(t)$ in the presence of the non-uniform electromagnetic field consists of physical increment and about the same numerical errors as the case of the uniform field. Thus, let us define the increment of variances, $\Delta\sigma^2(t)$, between $\sigma_{\text{non-uniform}}^2(t)$ and $\sigma_{\text{uniform}}^2(t)$, as [1, 2]

$$\Delta\sigma^2(t) = \sigma_{\text{non-uniform}}^2(t) - \sigma_{\text{uniform}}^2(t). \quad (11)$$

The increment $\Delta\sigma^2(t)$ shows the physical time evolution of variances, as shown in Fig. 3. Also depicted in the figure is a fitting line, which represents the time averaged evolution of variance. Let us also define the expansion rate in position $d\sigma_r^2/dt$ and mechanical momentum $d\sigma_{mv}^2/dt$, using the fitting lines' gradient.

3.3. Rate of changes in variances

For various combinations of physical parameters, such as m , q , v_0 , E , B , L_B and L_E , similar analyses to that in the preceding section give us the relationship between the expansion rate of variances in position $d\sigma_r^2(t)/dt$ as a function of $\hbar v_0/qBL_B$, as shown in the left panel of Fig. 4, and in mechanical momentum $d\sigma_{mv}^2(t)/dt$ as a function of $\hbar qBv_0/L_B$ in the right panel of Fig. 4. Also depicted are the fitting lines. It is noted that the variances clearly on the respective fitting lines of

$$\frac{d\sigma_r^2}{dt} = (2.00 \pm 0.03) \frac{\hbar}{qB} \frac{v_0}{L_B}, \quad (12)$$

$$\frac{d\sigma_{mv}^2}{dt} = (1.030 \pm 0.005) \hbar qB \frac{v_0}{L_B}, \quad (13)$$

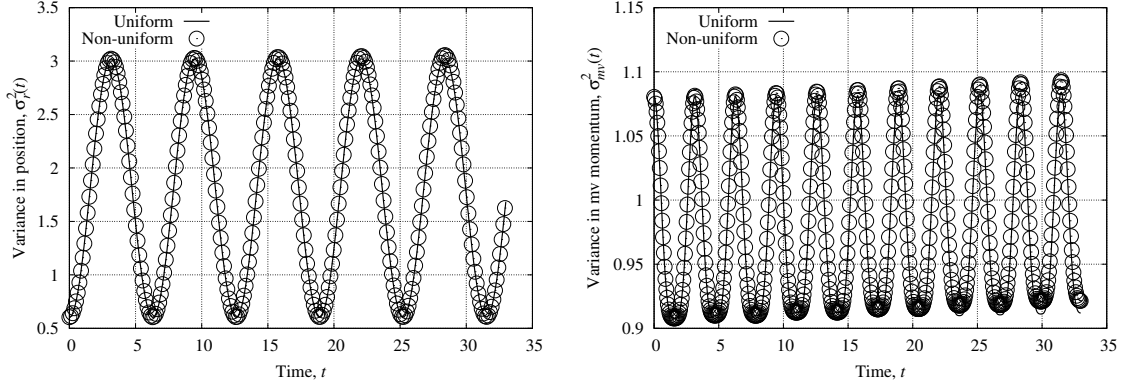


Fig. 2. Time evolution of variance in position $\sigma_r^2(t) = \langle r^2 \rangle - \langle r \rangle^2$ (left) and in mechanical momentum $\sigma_{mv}^2(t) = \langle (mv)^2 \rangle - \langle mv \rangle^2$ (right), for initial velocity $v_0 = 5$, charge $q = 1$, mass $m = 1$, electric field $E = 10^{-3}$ with $L_E = 10^{-4}$, magnetic field $B = 1$, thus $\omega_c = 1$, with $L_B = 10^{-4}$ or ∞ .

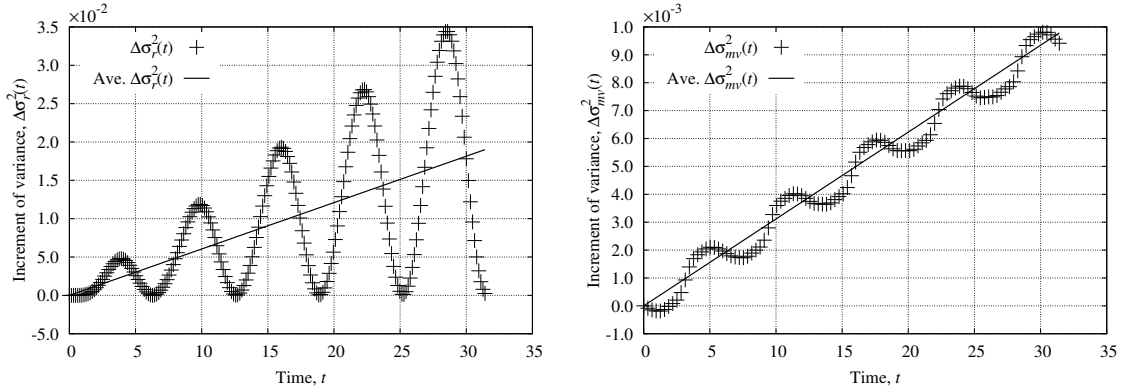


Fig. 3. Time evolution of increment of variance in position $\Delta\sigma_r^2(t)$ (left), and mechanical momentum $\Delta\sigma_{mv}^2(t)$ (right). Ave. $\Delta\sigma_r^2(t)$ and Ave. $\Delta\sigma_{mv}^2(t)$ stand for the time average over the cyclotron period, for the case presented in Fig. 2.

both of which do not depend on the particle mass m , the magnitude of electric field E nor the gradient scale length of electric field L_E . Therefore, it is shown that the non-uniform electric field $\mathbf{E} = E(1 - y/L_E)\mathbf{e}_y$ does not affect the expansion rates while the non-uniform magnetic field $\mathbf{B} = B(1 - y/L_B)\mathbf{e}_z$ does.

Let us apply the expansion rate to the typical fusion plasma with a temperature $T = 10$ keV, number density $n = 10^{20} \text{ m}^{-3}$, a magnetic field $B = 5$ T and a gradient scale length of magnetic field $L_B = 3$ m, which is the major axis of a torus. When we take a proton for the charged particle and the thermal velocity $v_{\text{th}} \sim 1.352 \times 10^6 \text{ m/s}$ for v_0 in Eq. (13), the standard deviation $\sigma_r^2(t)$ of the proton reaches the interparticle separation $n^{-1/3}$ in a time interval 0.38 msec. In contrast, the ion-ion collision time is about 20 msec [10]. Thus, overlapping of wavefunctions of neighboring protons would occur before the conventional collision time.

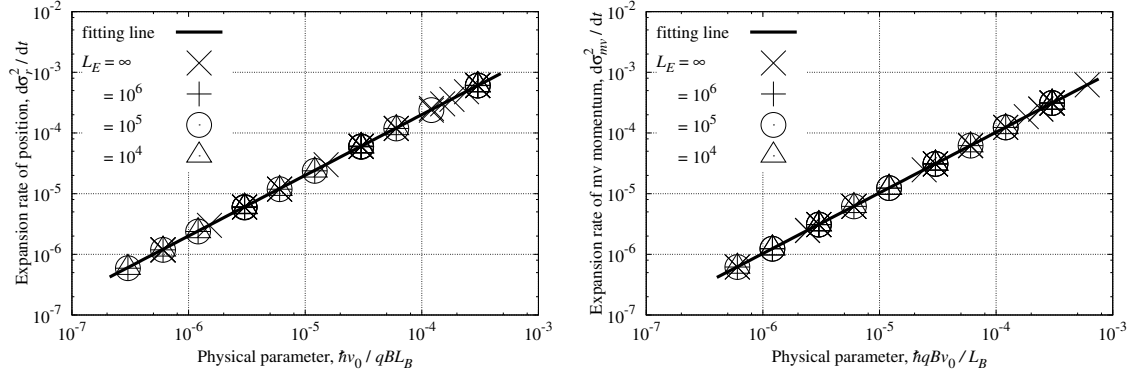


Fig. 4. Expansion rate of variance in position vs. $\hbar v_0/qBL_B$ (left) and in mechanical momentum vs. $\hbar qBv_0/L_B$ (right). Each point shape, such as $\diamond$ and $\square$, corresponds to the same gradient scale length of electric field L_E .

4. Summary

We have solved the two-dimensional time-dependent Schrödinger equation for a charged particle in the presence of a non-uniform electric field $\mathbf{B} = B(1 - y/L_B) \mathbf{e}_z$ and magnetic field $\mathbf{E} = E(1 - y/L_E) \mathbf{e}_y$. It is shown that the particle mass and the electric field do not affect the expansion rate as long as the electric field has the uniform gradient.

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