Numerical Analysis of Quantum Mechanical ∇B Drift II*)

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We have solved the two-dimensional time-dependent Schrödinger equation for a single particle in the presence of a non-uniform magnetic field for initial speed of 10–100 m/s, mass of the particle at 1–10 m_p, where m_p is the mass of a proton. Magnetic field at the origin of 5–10 T, charge of 1–4 e, where e is the charge of the particle and gradient scale length of 2.610×10^{-5}–5.219 m. It was numerically found that the variance, or the uncertainty, in position can be expressed as $\mathrm{d}\sigma_r^2/\mathrm{d}t = 4.1\hbar v_0/qB_0L_B$, where m is the mass of the particle, q is the charge, v_0 is the initial speed of the corresponding classical particle, B_0 is the magnetic field at the origin and L_B is the gradient scale length of the magnetic field. In this expression, we found out that mass, m does not affect our newly developed expression.

Keywords: grad-B drift, magnetic length, Landau state, quantum mechanical scattering, plasma, diffusion, expansion time, expansion rate of variance

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1. Introduction

It is well known that a charged particle in the presence of a non-uniform magnetic field $\boldsymbol{B}$ tend to move to regions of weak magnetic field via collisions/interaction with other particles. In quantum mechanics the probability density function (PDF) for a charged particle in the presence of a uniform magnetic field $\boldsymbol{B} = B_0\boldsymbol{e}_z$ along the z-axis in the x-y plane perpendicular to the field is given by

$$\rho(\boldsymbol{r}, t) = \frac{qB_0}{\pi\hbar} \exp\left[-\frac{qB_0}{\hbar} \left(\boldsymbol{r} - \langle \boldsymbol{r}(t) \rangle\right)^2\right], \tag{1}$$

where $\langle \boldsymbol{r}(t) \rangle$ stands for the expectation value of the position that is the same as the time-dependent position of the corresponding classical particle. The tendency towards weak $B = |\boldsymbol{B}|$ field region stated above makes the probability density function (PDF) of the particle broader than that for a uniform field case. This makes the PDF of the particle broad compared with that for a uniform magnetic field.

In the case of a non-uniform field, we have developed a code to solve the time-dependent Schrödinger equation in the presence of a non-uniform magnetic field. In the previous paper [1], we have shown that the quantum mechanical variance in position may reach the square of the interparticle separation in a time interval of the order of 10^{-4} sec for typical magnetically confined fusion plasmas with a number density of $n \sim 10^{20}\,\mathrm{m}^{-3}$ and a temperature of $T \sim 10\,\mathrm{keV}$.

In this paper, as an extension of the paper [1], we investigated the dependence of the variance σ_r^2 in position on parameters such as m, q, v_0, B_0, and L_B, where m is the mass of the particle, q is the charge, v_0 is the initial speed of the corresponding classical particle, B_0 is the magnetic field at the origin and L_B is the gradient scale length of the magnetic field.

In section 2, we use two dimensional Schrödinger equation for a wavefunction ψ at position $\boldsymbol{r}$ and time t. In section 3, we show methodology we use for numerical subtraction and the final results of our finding after subtracting its numerical error.

2. Schrödinger Equation

In this research we have solved the two-dimensional Schrödinger equation for a wavefunction ψ at position $\boldsymbol{r}$ and time t,

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \left[\frac{1}{2\,m}\left(-\mathrm{i}\hbar\nabla - q\boldsymbol{A}\right)^2 + q\varphi\right]\psi, \tag{2}$$

where φ and $\boldsymbol{A}$ stand for the scalar and vector potentials, m and q the mass and electric charge of the particle under consideration, $i \equiv \sqrt{-1}$ the imaginary unit, and $\hbar = h/2\pi$ the reduced Planck constant.

The initial condition for wavefunction at $\boldsymbol{r} = \boldsymbol{r}_0$ with $\boldsymbol{r}_0$ being the initial centre of ψ, is given by

$$\psi(\boldsymbol{r}, 0) = \frac{1}{\sqrt{\pi}\sigma_0} \exp\left[-\frac{(\boldsymbol{r} - \boldsymbol{r}_0)^2}{2\sigma_0^2} + \mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{r}\right], \tag{3}$$

where σ_0 is the initial standard deviation, and $\boldsymbol{k}_0 = mv_0/\hbar$ is the initial wavenumber vector. Where m is the mass of the particle under consideration, v_0 is the initial velocity of the corresponding classical particle.

By using the finite difference method in space with Crank-Nicolson scheme for the time integration, Eqs. (2) and (3) above become as

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$$\left(\mathrm{I} - \frac{\Delta t}{2i\hbar}\mathrm{H}\right)\left\{\psi^{n+1}\right\} = \left(\mathrm{I} + \frac{\Delta t}{2i\hbar}\mathrm{H}\right)\left\{\psi^{n}\right\}, \tag{4}$$

where I is a unit matrix, H the numerical Hamiltonian matrix, and $\{\psi^n\}$ stands for the discretized set of the two dimensional time-dependent wavefunction $\psi(x, y, t)$ at a discrete time $t_n = n\Delta t$ to be solved numerically.

We use successive over relaxation (SOR) scheme for time integration in our numerical calculation. Calculation is done on a GPU (Nvidia GTX-580: 512 cores/3 GB @1.54 GHz) [1, 2].

2.1 Exact wavefunction in a uniform magnetic field

The exact solution $\psi(\boldsymbol{r}, t)$ for the two-dimensional Schrödinger Eq. (2) with a uniform magnetic field with a Landau gauge [3], of $A_x = -By$, $A_y = 0$, $A_z = 0$, is shown below,

$$\psi(\boldsymbol{r}, t) = \frac{e^{ikx}}{\sqrt{\sqrt{\pi}\ell_B}} \exp\left(-\frac{1}{2\ell_B^2}\left(y - \frac{u(t)}{\omega}\right)^2\right) \times \exp\left[i\left(\frac{y_0^2 \sin 2\omega t}{4\ell_B^2} - \frac{y y_0 \sin \omega t}{\ell_B^2} - \frac{\omega t}{2}\right)\right], \tag{5}$$

where $\ell_B \equiv \sqrt{\hbar/qB}$ is the magnetic length [3], the $\omega \equiv qB/m$ is the cyclotron frequency, $y_0 = k\ell_B^2$, and $u(t)$ is classical velocity of the particle in x-direction. By referring to Eq. (4) above, we can conclude that the standard deviation, variance, or uncertainty, in position remain constant throughout the time. In case of uniform magnetic field, $L_B = \infty$, $\sigma_r^2(t) = \ell_B^2 = \text{const.}$

3. Numerical Results

In our numerical calculation, we normalized the following parameters for analysis, as listed in Table 1. Lengths are normalized by cyclotron radius of a proton with a speed of 10 m/s in a magnetic field of 10 T. The cyclotron frequency in such a case is used for normalization of the time.

Throughout the calculation, we use normalized grid size of $\Delta x = \Delta y = 0.02$ and normalized time step of $\Delta t = 2\pi \times 10^{-5}$. This normalized grid size is sufficiently small to use as noted in Ref. [1].

Table 1 Normalized parameter for mass of the particle, charge, magnetic flux density, velocity, length and time.

Parameters	Normalization
Mass of the particle	$m = 1.6722 \times 10^{-27}$ kg
Charge	$q = 1.602 \times 10^{-19}$ C
Magnetic flux density	$B = 10$ T
Velocity	$\bar{v} = 10$ m/s
Length	$\bar{\rho} = 1.04382 \times 10^{-8}$ m
Time	$\bar{t} = 1.04382 \times 10^{-9}$ s

3.1 Numerical conservation of momentum and energy

The canonical momentum in x-direction, $P_x = mv_x + qA_x$, is conserved as much as 10–11 digits. In this case, we used a normalized initial momentum of $mv = (0, 1)$. Results shown in Fig. 1, errors of momentum in x-direction, are sufficiently small enough for validity.

We obtain energy error in the particle at a certain time by comparing our numerical results with initial value. The results are proven small enough for validity as shown in Fig. 2. Energy in our calculation is conserved as much as 10–11 digits. In this research, our normalized initial energy, $E \simeq 95.3 \sim 10^2$, is used to compare with our numerical calculation. Note that initial energy is of order of $E = 10^2$, thus the relative error in energy is around 10^{-11}.

Figure 3 compares the trajectory of the particle $\boldsymbol{r}$ in non-uniform magnetic field in the normalized x-y plane between the quantum-mechanical expectation $\langle \boldsymbol{r} \rangle$ and the classical orbit $\boldsymbol{r}(t)$ with a normalized initial position of $\boldsymbol{r}(0) = (-10, 0)$. Comparison of guiding-centre position $\boldsymbol{r}_{\mathrm{G}}$ is shown in the Ref. [1].

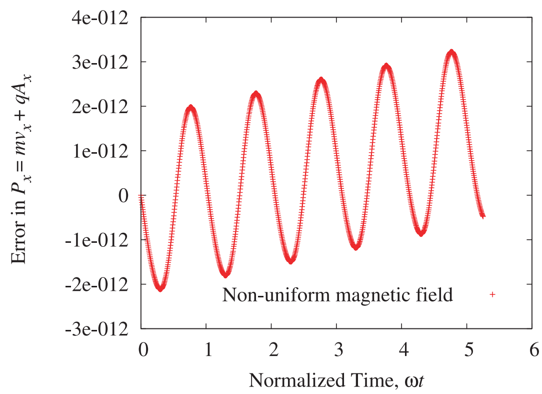

Fig. 1 Numerical Error in momentum in x-direction for non-uniform magnetic field $L_B = 5.219 \times 10^{-4}$ m.

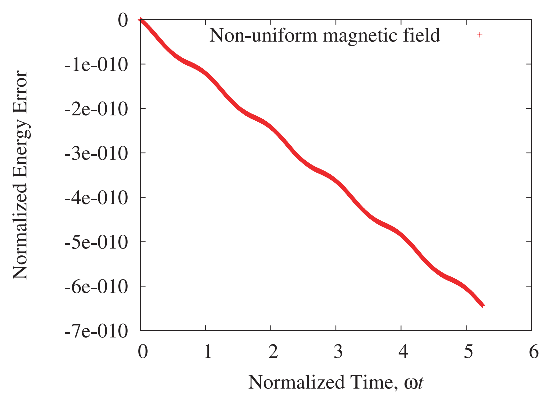

Fig. 2 Numerical error in energy of non-uniform magnetic field with $L_B = 5.219 \times 10^{-4}$ m.

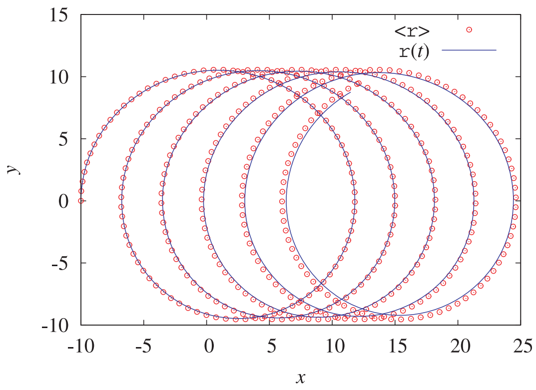

Fig. 3 Comparison of the trajectory of the particle $\boldsymbol{r}$ in non-uniform magnetic field, $L_B = 5.219 \times 10^{-11}$ m between quantum-mechanical expectation $\langle \boldsymbol{r} \rangle$ in red, classical orbit $\boldsymbol{r}(t)$ in blue.

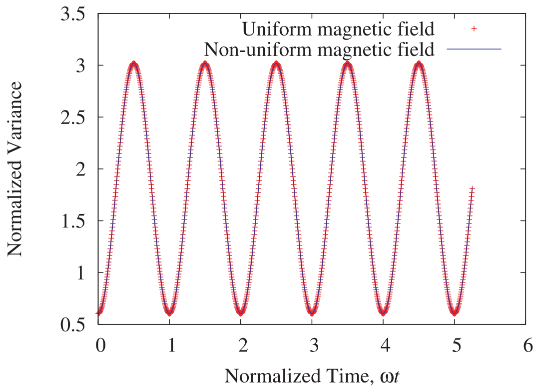

Fig. 4 Comparison of σ_r^2 between uniform magnetic field $L_B = \infty$, red plot, and non-uniform magnetic field $L_B = 5.219 \times 10^{-4}$ m, in blue.

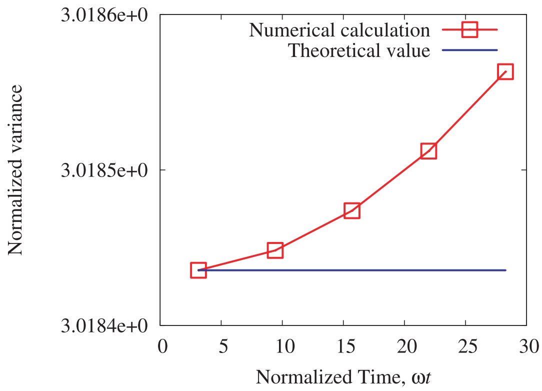

Fig. 5 Comparison of σ_r^2, normalized peak variance in position of uniform magnetic field $L_B = \infty$, between numerical calculation, in red and theoretical σ_r^2, in blue dotted line.

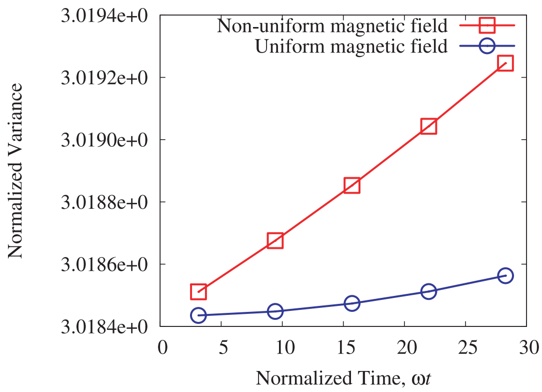

Fig. 6 Comparison of σ_r^2, normalized increment of peak variance in position σ_r^2 between uniform magnetic field $L_B = \infty$, in blue circle, compare with $L_B = 5.219 \times 10^{-4}$ m, in red square.

3.2 Variance in position

The variance, or the uncertainty, in position of a particle is shown in Fig. 4. In our numerical calculation, we numerically calculate the particle until 5 gyrations. Both uniform magnetic field $L_B = \infty$, and non-uniform magnetic field $L_B = 5.219 \times 10^{-4}$ m variance in position, σ_r^2, have small difference in value.

We recorded each maximum or top peak of the normalized variance for both uniform magnetic field $L_B = \infty$, and non-uniform magnetic field $L_B = 5.219 \times 10^{-4}$ m Thus, we have 5 maximum or top peak values as shown in Fig. 5.

3.3 Numerical error subtraction

For uniform magnetic field, $L_B = \infty$, the variance in position should remain constant: $\sigma_r^2(t) = \ell_B^2$ as given by Eq. (4). However, there is slight increment in variance as shown in Fig. 5. The difference between numerical calculation and theoretical value in this research is attributed to numerical errors due to inevitable non-zero grid size and time step as well as the finite bit calculation.

In our numerical calculation, both non-uniform magnetic field and uniform magnetic fields' increments in variance are assumed to consist the same numerical errors. In this case, both non-uniform magnetic field variance and uniform magnetic field variances behave non-linearly, as shown in Fig. 6. Since this numerical error is undesirable in our calculation, we subtract the increment in variance for the non-uniform magnetic field from that for the non-uniform magnetic field.

After subtraction of non-uniform magnetic field's peak variance with uniform magnetic field's peak variance, we get a linear relationship for the increment in variance with time as shown in Fig. 7.

3.4 Expansion rate of variance

In this paper, we use multiple set of parameters; initial speed of 10–100 m/s, mass of the particle at 1.6722×10^{-27}–1.6722×10^{-26} kg, magnetic field at the origin of 5–10 T, gradient scale length of 2.610×10^{-5}–5.219 m and charge of 1.602×10^{-19}–6.408×10^{-19} C. Total 29 sets of data were used.

Using numerical results for these parameter sets, we

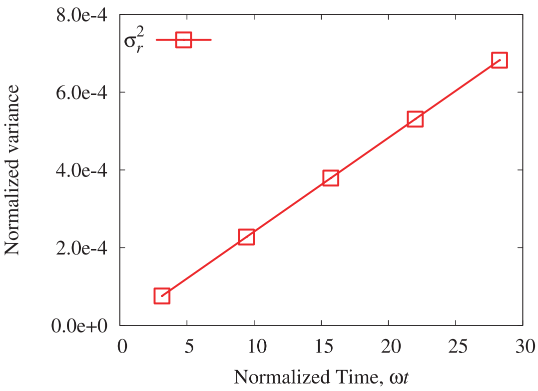

Fig. 7 Normalized increment of peak variance in position σ_r^2 for non-uniform magnetic field $L_B = 5.219 \times 10^{-4}$ m after subtraction with uniform magnetic field $L_B = \infty$ peak variance in position σ_r^2.

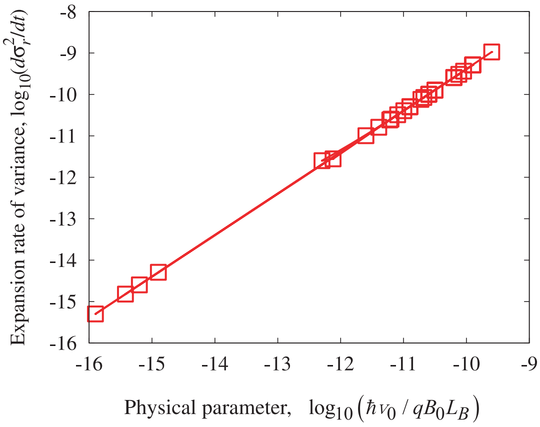

Fig. 8 Expansion rate of variance with different sets of parameters of m, q, v_0, B_0 and L_B.

found a new relation between expansion rate of variance and the physical parameters. The final results are shown in Fig. 8 with logarithm of base 10 scale. Figure 8 is graph of physical parameter, $\log_{10}(\hbar v_0/qB_0L_B)$ against expansion rate of variance, $\log_{10}\left(\mathrm{d}\sigma_r^2/\mathrm{d}t\right)$.

Expansion rate increases linearly with different set of parameters such as m, q, v_0, B_0 and L_B. We found that changes of mass, m, do not affect on our newly developed expression for the expansion rate of variance.

Using numerical analysis method, we developed new expression for expansion rate as a function of m, q, v_0, B_0 and L_B,

$$\log_{10}\left(\frac{\mathrm{d}\sigma_r^2}{\mathrm{d}t}\right) = \log_{10}\left(\frac{\hbar}{qL_B}\frac{v_0}{B_0}\right) + \log 0.6097, \qquad (6)$$

which leads to

$$\frac{\mathrm{d}\sigma_r^2}{\mathrm{d}t} = 4.1\frac{\hbar}{qB_0}\frac{v_0}{L_B} \quad [\mathrm{m}^2/\mathrm{s}]. \qquad (7)$$

It is interesting to note that there is no mass, m, dependence for the expression above. In plasmas, however, the mass dependence, or the isotope effect, may appear through the replacement of $v_0 \sim v_{\mathrm{th}} = \sqrt{2k_{\mathrm{B}}T/m}$, where v_{th} is the thermal speed, k_{B} is the Boltzmann constant and T is the temperature.

4. Summary

We have solved the two-dimensional time-dependent Schrödinger equation for a single particle in the presence of a non-uniform magnetic field for difference set of parameters such as m, q, v_0, B_0 and L_B. It is shown that the expansion rate increases linearly as $\mathrm{d}\sigma_r^2/\mathrm{d}t = 4.1\hbar v_0/qB_0L_B$. This expression has been derived using numerical calculation. We are also interested in developing theoretical expansion rate of variance. For these studies, we left it for future work.

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