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# Numerical Analysis of Quantum Mechanical $\nabla B$ Drift III<sup>\*)</sup>

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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 8 - 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  $2.610 \times 10^{-5}$  - 5.219 m. Previously, we found out that the variance, or the uncertainty, in position can be expressed as  $d\sigma_r^2/dt = 4.3\hbar v_0/qB_0L_B$ , 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 research, it was numerically found that the variance, or the uncertainty, in total momentum can be expressed as  $d\sigma_p^2/dt = 0.57\hbar qB_0v_0/L_B$ . In this expression, we found out that mass,  $m$  does not affect both our newly developed expression for uncertainty in position and total momentum.

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**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

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  $n \sim 10^{20} \text{ m}^{-3}$  and a temperature of  $T \sim 10 \text{ keV}$ . After this time the wavefunctions of neighbouring particles would overlap, as a result the conventional classical analysis may lose its validity.

Further on, in previous papers [2], we have investigated the dependence of the variance  $\sigma_r^2$  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. We have shown that the variance, or the uncertainty, in position can be expressed as  $d\sigma_r^2/dt = 4.1\hbar v_0/qB_0L_B$ .

In this paper, as an extension of the paper [1] and [2], we investigated the dependence of the variance in total momentum  $\sigma_p^2$  on parameters such as  $m$ ,  $q$ ,  $v_0$ ,  $B_0$ , and  $L_B$ . Uncertainty in total momentum has the same important role as uncertainty in position, in quantum mechanics studies of plasma fusion.

In section 2, we solve two dimensional Schrödinger equation for a wavefunction  $\psi$  at position  $\mathbf{r}$  and time  $t$ . In

section 3, we show final results of the uncertainty, in position and total momentum after subtracting its numerical error.

## 2. Schrödinger Equation

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

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

where  $\varphi$  and  $\mathbf{A}$  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  $\mathbf{r} = \mathbf{r}_0$  with  $\mathbf{r}_0$  being the initial center of  $\psi$ , is given by

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

where  $\sigma_0$  is the initial standard deviation, and  $\mathbf{k}_0 = m\mathbf{v}_0/\hbar$  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. (1) and (2) above become as

$$\left( \mathbf{I} - \frac{\Delta t}{2i\hbar} \mathbf{H} \right) \{\psi^{n+1}\} = \left( \mathbf{I} + \frac{\Delta t}{2i\hbar} \mathbf{H} \right) \{\psi^n\}, \quad (3)$$

where  $\mathbf{I}$  is a unit matrix,  $\mathbf{H}$  the numerical Hamiltonian matrix, and  $\{\psi^n\}$  stands for the discretized set of the two di-

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mensional 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: 512cores/3GB @1.54 GHz) [1–4].

## 2.1 Exact wavefunction in a uniform magnetic field

The exact solution  $\psi(\mathbf{r}, t)$  for the two-dimensional Schrödinger Eq. (2) with a uniform magnetic field with a Landau gauge [5], of  $A_x = -By$ ,  $A_y = 0$ ,  $A_z = 0$ , is shown below,

$$\psi(\mathbf{r}, t) = \frac{e^{ikx}}{\sqrt{\sqrt{\pi}\ell_B}} \exp\left(-\frac{1}{2\ell_B^2}\left(y - \frac{u(t)}{\omega}\right)^2\right) \times \exp\left[i\left(\frac{y_0^2 \sin 2\omega t}{4\ell_B^2} - \frac{yy_0 \sin \omega t}{\ell_B^2} - \frac{\omega t}{2}\right)\right], \quad (4)$$

where  $\ell_B \equiv \sqrt{\hbar/qB}$  is the magnetic length [5], 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 the case of uniform magnetic field,  $L_B = \infty$ ,  $\sigma_r^2(t) = \ell_B^2 = \text{const.}$

## 3. Numerical Results

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 this paper, we use normalization unit as shown in Ref. [2].

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].

Figure 1 shows the time evolution of the variance in position and total momentum for  $v_0 = 10$  m/s in a uniform magnetic field. The variance of position oscillates with cyclotron period which half of the cyclotron period in total momentum.

Figure 2 shows the time evolution of the variance in total momentum for both uniform magnetic field and non-uniform magnetic field, which are defined as

$$\sigma_P^2 = \int_{\Sigma} \psi^* (-i\hbar \nabla - \langle P \rangle)^2 \psi d^2 \mathbf{r}, \quad (5)$$

where  $\langle P \rangle$  is the total momentum:

$$\langle P \rangle = \int_{\Sigma} \psi^* (-i\hbar \nabla) \psi d^2 \mathbf{r}. \quad (6)$$

### 3.1 Numerical error

As for the numerical error in variance, our code is capable of accurately reproducing the time dependent vari-

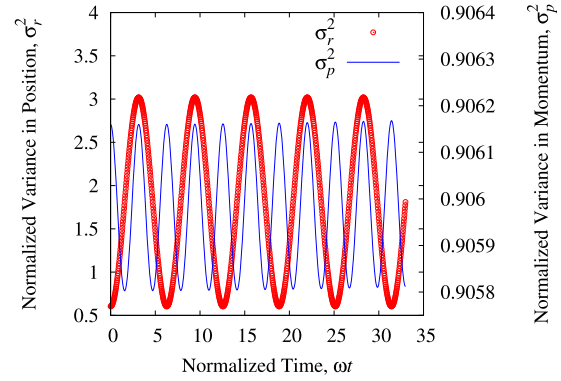


Fig. 1 Normalized variance  $\sigma_r^2$  in position, red plot, and  $\sigma_p^2$ , in total momentum, blue line, for uniform magnetic field  $L_B = \infty$ .

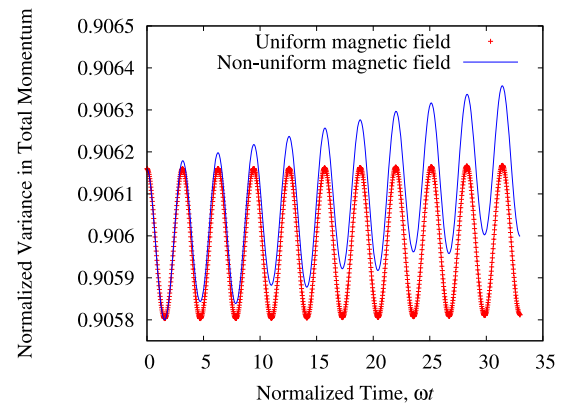


Fig. 2 Comparison of  $\sigma_p^2$ , between uniform magnetic field  $L_B = \infty$ , in red plot, and non-uniform magnetic field  $L_B = 5.219 \times 10^{-4}$  m, in blue line. With magnetic flux density  $B = 10$  T.

ance in position  $\sigma_r^2(t)$  and total momentum  $\sigma_p^2(t)$  in uniform magnetic field which an exact solution is available [1]. 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) [2]. Heisenberg uncertainty principle states that  $\sigma_r(t)\sigma_p(t) \geq \hbar/2$ , therefore, the variance in total momentum also remains constant for uniform magnetic field. However, there is slight increment in variance as shown in Fig. 2. The difference between numerical calculation and theoretical value in this research is attributed to numerical errors [2]. Both variance in position and variance in total momentum are assumed to consist of numerical error, therefore, we perform numerical subtraction as in Ref. [2]. For non-uniform magnetic field, the peak variance grows with time as results of diffusion. The variance grows faster in higher magnetic flux density region as shown in Fig. 3.

In our numerical calculation, both non-uniform magnetic field variance and uniform magnetic field variances behave non-linearly, as shown in Fig. 4. This is due to numerical error accumulated throughout the calculation. In this case, both non-uniform magnetic field and uniform magnetic fields' increments in variance are consisting of

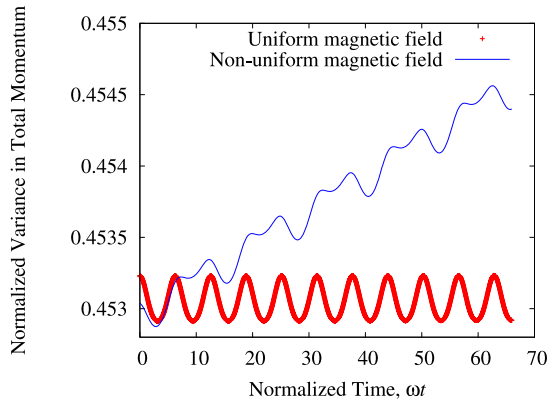


Fig. 3 Comparison of  $\sigma_p^2$ , between uniform magnetic field  $L_B = \infty$ , in red plot, and non-uniform magnetic field  $L_B = 5.219 \times 10^{-5}$  m, in blue line. With magnetic flux density  $B = 50$  T.

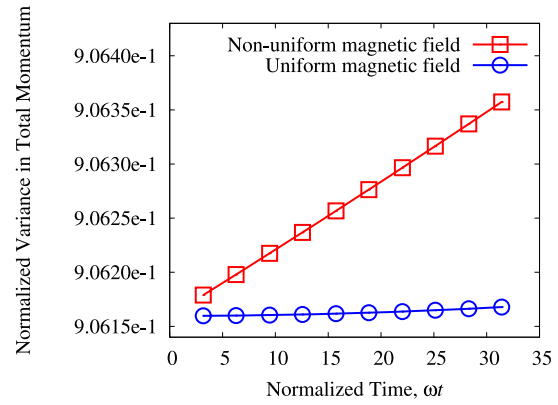


Fig. 5 Comparison of normalized increment of peak variance in total momentum,  $\sigma_p^2$ , between uniform magnetic field  $L_B = \infty$ , in blue circle, compared with  $L_B = 5.219 \times 10^{-4}$  m, in red square.

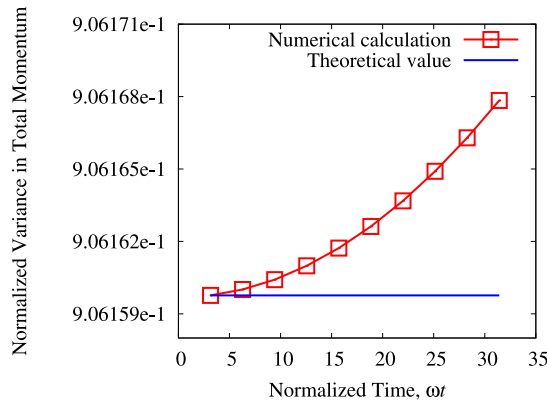


Fig. 4 Comparison of  $\sigma_p^2$ , normalized peak variance in total momentum of uniform magnetic field  $L_B = \infty$ , between numerical calculation, in red and theoretical  $\sigma_p^2$ , in blue line.

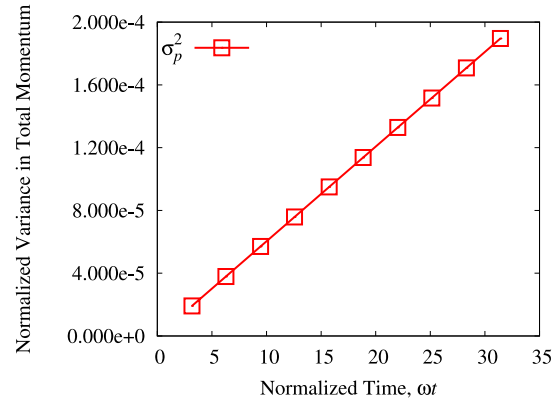


Fig. 6 Linear normalized increment of peak variance in total momentum  $\sigma_p^2$ , for non-uniform magnetic field  $L_B = 5.219 \times 10^{-4}$  m after subtraction of its numerical error.

the same numerical errors. 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 as shown in Fig. 5.

After subtraction of non-uniform magnetic field's peak variance with uniform magnetic field's peak variance, we obtain a linear relationship for the increment in variance of total momentum with time as shown in Fig. 6. By considering particle gyration base time, we equalize each result to the same cyclotron frequency. From Fig. 6, we obtain a single data for our final expression, which after we perform multiple sets of calculation, we reach to the final results shown in Fig. 7.

### 3.2 Expansion rate of variance in position and total momentum

In this paper, we use multiple set of parameters; initial speed of 8 - 100 m/s, mass of the particle at  $1.6722 \times 10^{-27}$  -  $1.6722 \times 10^{26}$  kg, magnetic field at the origin of 5 - 10 T, gradient scale length of  $2.610 \times 10^{-5}$  -  $5.219$  m and charge of  $1.602 \times 10^{-19}$  -  $6.408 \times 10^{-19}$  C. Total 38 sets of

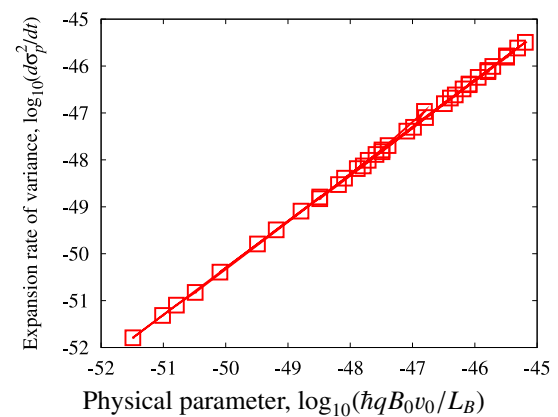


Fig. 7 Expansion rate of variance in total momentum with different sets of parameters of  $m$ ,  $q$ ,  $v_0$ ,  $B_0$  and  $L_B$ .

data were used.

We perform calculation for uncertainty in total momentum using numerical results for these parameter sets, we found a new relation between expansion rate of variance and the physical parameters. The final results are

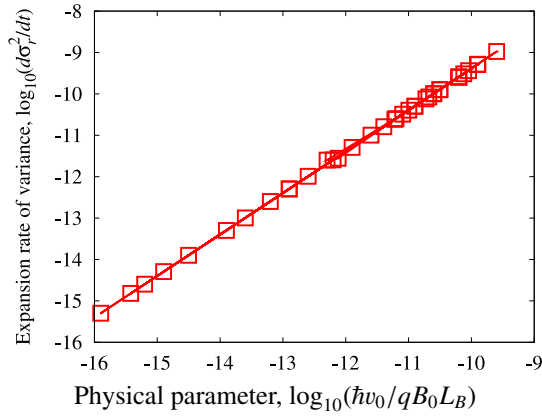


Fig. 8 Expansion rate of variance in position with different sets of parameters of  $m$ ,  $q$ ,  $v_0$ ,  $B_0$  and  $L_B$ .

shown in Fig. 7 with logarithm of base 10 scale. Figure 7 is graph of physical parameter,  $\log_{10}(\hbar q B_0 v_0 / L_B)$  against expansion rate of variance,  $\log_{10}(d\sigma_r^2/dt)$ .

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 in total momentum as a function of  $m$ ,  $q$ ,  $v_0$ ,  $B_0$  and  $L_B$ ,

$$\log_{10}\left(\frac{d\sigma_r^2}{dt}\right) = \log_{10}\left(\hbar q B_0 \frac{v_0}{L_B}\right) - \log 0.2432, \quad (7)$$

which leads to

$$\frac{d\sigma_r^2}{dt} = 0.57 \hbar q B_0 \frac{v_0}{L_B} \quad [\text{kg}^2 \text{m}^2 / \text{s}^3]. \quad (8)$$

We further improve our results in our previous paper [2] for expansion rate of variance in position with as shown in Fig. 8. Figure 8 is graph of physical parameter,  $\log_{10}(\hbar v_0 / q B_0 L_B)$  against expansion rate of variance,  $\log_{10}(d\sigma_r^2/dt)$ . Including additional new calculation data, there are slight changes in our nondimensional numerical factor, which our new result become;

$$\frac{d\sigma_r^2}{dt} = 4.3 \frac{\hbar}{q B_0} \frac{v_0}{L_B} \quad [\text{m}^2 / \text{s}]. \quad (9)$$

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

## 4. Summary

Previously we had shown that conventional classical analysis may lose its validity as the wavefunctions of neighbouring particles would overlap to each another [1]. As the extension of the paper [1], we have solved the two-dimensional time-dependent Schrödinger equation for a single particle in the presence of a non-uniform magnetic field for different set of parameters such as  $m$ ,  $q$ ,  $v_0$ ,  $B_0$  and  $L_B$ . It is shown that the expansion rate for position increases linearly as  $d\sigma_r^2/dt = 4.3 \hbar v_0 / q B_0 L_B$  and the correspond expansion rate for total momentum increases linearly as  $d\sigma_p^2/dt = 0.57 \hbar q B_0 v_0 / L_B$ . Both of these expressions are derived using numerical calculation. We are also interested in developing theoretical expansion rate of variance for both position and momentum. For these studies, we left it for future work.

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