Quantum Mechanical Diffusion of a Magnetized Particle in the Presence of a Field Particle in the Extended Gyration Cycle

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Abstract. We have developed a code to solve the two-dimensional time-dependent Schrödinger equation, for a magnetized proton in the presence of a fixed field particle and of a uniform magnetic field. In the relatively high-speed case, the fast-speed proton has the similar behaviors to those of classical theories. In the low-speed case the magnitudes both in mechanical momentum $mv = |m\boldsymbol{v}|$, where m is the mass and $\boldsymbol{v}$ is the velocity of the particle, and position $r = |\boldsymbol{r}|$ are appreciably decreasing with time. However, the kinetic energy $K = m\langle \boldsymbol{v}^2 \rangle / 2$ and the potential energy $U = \langle qV \rangle$, where q is the electric charge of the particle and V is the scalar potential, do not show appreciable changes. This is because of the increasing variances, i.e. uncertainty, both in momentum and position. The increment in variance of momentum corresponds to the decrement in the magnitude of momentum: Part of energy is transferred from the directional (the kinetic) energy to the uncertainty (the zero-point) energy.

1 Introduction

We have shown in Ref. [1], 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 ~10^{20} m^{-3} and a temperature of T~10keV. After this time the wavefunctions of neighbouring particles would overlap, as a result the conventional classical analysis may lose its validity: Plasmas may behave like extremely-low-density liquids, not gases, since the *size* of each particle is of the same order of the interparticle separation.

In Refs. [2–4], we have also shown that for distant encounters in typical fusion plasmas of a temperature $T = 10\,\mathrm{keV}$ and $n = 10^{20}\,\mathrm{m}^{-3}$, the average potential energy $\langle U \rangle \sim 30\,\mathrm{meV}$ is as small as the uncertainty in energy $\Delta E \sim 40\,\mathrm{meV}$, and for a magnetic field $B \sim 3\,\mathrm{T}$, the spatial size of the wavefunction in the plane perpendicular to the magnetic field is as large as the magnetic length $\ell_B \sim 10^{-8}$ m which is much larger than the typical electron wavelength $\lambda_e \sim 10^{-11}$ m, and is around one-tenth of the average interparticle separation $\Delta\ell$.

2 Schrödinger Equation

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

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

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

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

where the magnetic length ℓ_B is the initial standard deviation, and $\boldsymbol{k}_0=m\boldsymbol{v}_0/\hbar$ is the initial wavenumber vector. Here m is the mass of the particle under consideration, $\boldsymbol{v}_0$ 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

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

where I is a unit matrix, H the numerical Hamiltonian matrix, and $\{\psi^{\mathrm{n}}\}$ 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: 512cores/3GB @1.54GHz) [1-6].

2.1 Electrostatic potential due to a field particle

Here we have assumed that the field particle is a quantum-mechanical particle centred at the origin with the wavefunction ψ_f similar to that given in Eq. (3), but is fixed in space and time, as

$$\psi_f(r)=\frac{\exp\left(-\dfrac{x^2+y^2}{2\ell_B^2}\right)}{\sqrt{\pi\ell_B^2}}\times\frac{\exp\left(-\dfrac{z^2}{2\sigma_z^2}\right)}{\sqrt{\sqrt{\pi}\sigma_z}}$$

where σ_z^2 is the variance in position in z-direction. In magnetically confined fusion plasmas, $\sigma_z\sim h/mv_0\ll\ell_B$ holds, so that the square of the second factor can be approximately the same as a Dirac delta function $\delta(z)$ centred at $z=0$. Thus the electrostatic potential φ_{f} in the x-y plane, due to the distributed charge is given by

$$\varphi_{\mathrm{f}}(R)\simeq\frac{q_f}{4\pi\varepsilon_0\ell_B^2}\frac{4}{\pi}\int_0^\infty\frac{R'e^{-(R'/\ell_B)^2}}{R+R'}K(M)\,dR',$$

where $R=\sqrt{x^2+y^2}$, q_{f} is an electric charge of the field particle, ε_0 is the vacuum permittivity, and $K(M)$ is the complete elliptic integral of the first kind with the parameter M being defined as $M\equiv4RR'/(R+R')^2$ [8].

3 Numerical Results

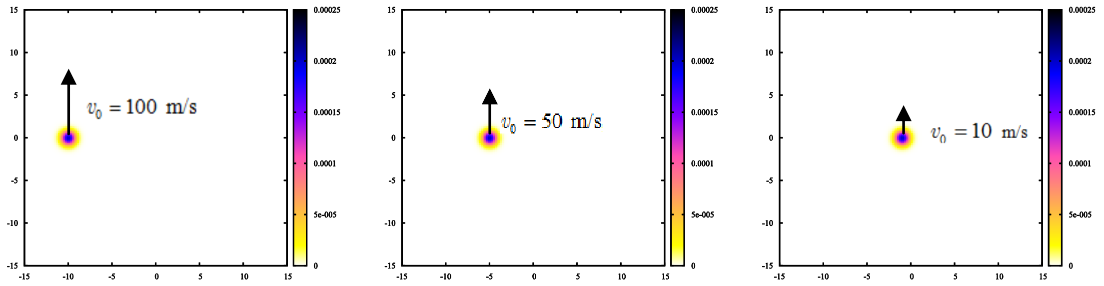
In our numerical calculation, we normalized the following parameters for analysis, as listed in Table 1. Lengths are normalized by cyclotron radius of a proton with a speed of 10 m/s in a magnetic field of 10 T. The cyclotron frequency in such a case is used for normalization of the time.

The magnetic length for a proton in $B=10\,\mathrm{T}$, $\ell_B\equiv\sqrt{\hbar/eB}\sim10^{-8}\,\mathrm{m}$ is a measure for the spread of a wave function in the plane perpendicular to the magnetic field. With these normalization, Planck constant $\hbar\sim0.60$, initial uncertainty in position $\ell_B^2\equiv\hbar/eB\sim0.78^2$ and initial uncertainty in kinetic momentum $(3/2)\hbar eB\sim0.91$ are order of unity. Note that the kinetic energy of a classical proton speed $v_0\sim27$ m/s in $B=10\,\mathrm{T}$ corresponds to the uncertainty of the momentum. In the numerical results to be presented in the following subsections, the Schrödinger Equation is solved for the time duration of fifty cyclotron rotations by a proton.

For low-speed case, $v_0 = 50$ m/s and $v_0 = 10$ m/s, initially the Probability Distribution Function (PDF) is a circular shape and changes to elongated shape at second gyration. This phenomenon extended further for each gyration. Eventually at the 40th gyration, the PDF of the particle tends to have almost uniformly distributes along the classical cyclotron orbit, as shown in Fig. 1, in which the width of the distribution is nearly the magnetic length of $\ell_B = \sqrt{\hbar/qB}$ as shown in Fig. 2.

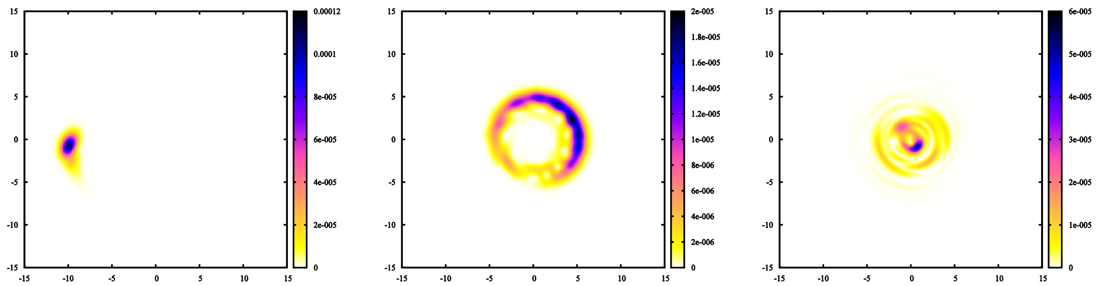
Table 1 Normalized parameter for mass of the particle, charge, magnetic flux density, velocity, length and time.

Parameters	Normalization
Mass of the particle	$m = 1.6722\times10^{-27}$ kg
Charge	$q = 1.602\times10^{-19}$ C
Magnetic flux density	$B = 10$ T
Velocity	$\bar{v} = 10$ m/s
Length	$\bar{\rho} = 1.04382\times10^{-8}$ m
Time	$\bar{t} = 1.04382\times10^{-9}$ s



Initial speed $v_0 = 100$ m/s Initial speed $v_0 = 50$ m/s Initial speed $v_0 = 10$ m/s

Fig. 1. Initial condition ($t = 0$) of Probability Density Function (PDF) of a single charged particle, in the presence of a fixed field particle at the origin.



Initial speed $v_0 = 100$ m/s Initial speed $v_0 = 50$ m/s Initial speed $v_0 = 10$ m/s

Fig. 2. The PDF of a single charged particle, in the presence of a fixed field particle at the origin, after 40 gyrations.

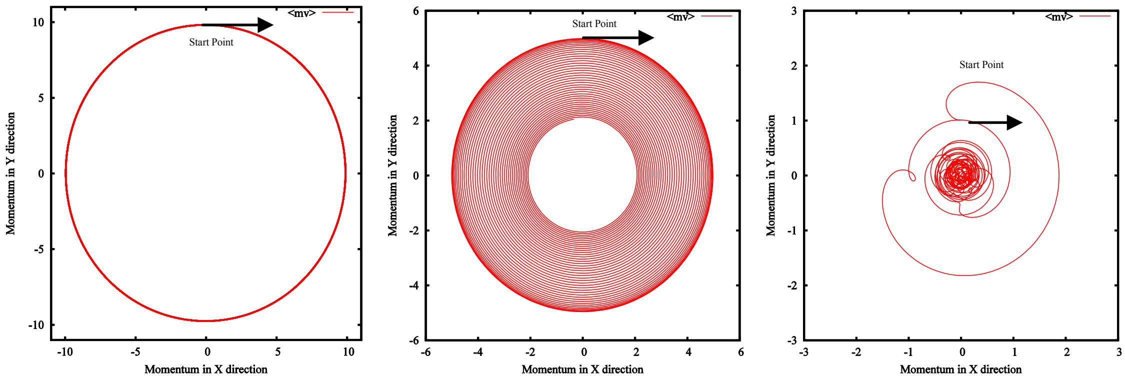
4 Summary

We have solved the two-dimensional time-dependent Schrödinger Equation for a magnetized proton in the presence of a fixed field particle with an electric charge of $2\times10^{-5}e$ and of a uniform magnetic field of $B = 10\text{T}$. In the relatively high-speed case of $v_0 = 100$ m/s, the behaviours are similar to those of classical ones. However, in the low-speed case of $v_0 = 50$ m/s and $v_0 = 10$ m/s, the magnitudes both in momentum $mv = |m\mathbf{v}|$ and position r = |r| are appreciably decreasing with time as shown in Fig 3 and Fig 4. The kinetic energy $K = m\langle \mathbf{v}^2 \rangle / 2$

and the potential energy $U = \langle qV \rangle$ do not show appreciable changes except for a small amplitude oscillation, because of the increasing variances, i.e. uncertainty, both in momentum and position.

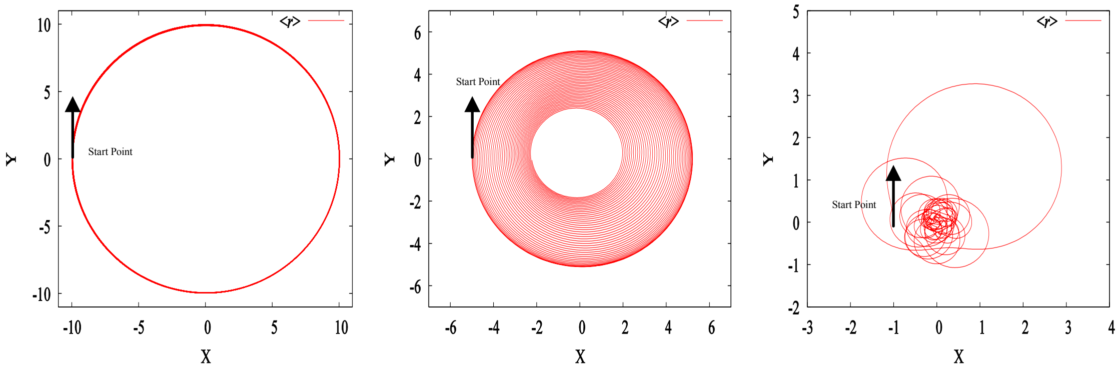
The increment in variance of momentum corresponds to the decrement in the magnitude of momentum: Part of energy is transferred from the directional (the kinetic) energy to the uncertainty (the zero-point) energy.

In summary, quantum-mechanical analyses are necessary for slow particles with mass m and charge q in the presence of magnetic field B, whose kinetic energy K is of the order of $\hbar qB/2m$.



Initial speed $v_0 = 100$ m/s Initial speed $v_0 = 50$ m/s Initial speed $v_0 = 10$ m/s

Fig. 3. Normalized expectation values of momentum $\boldsymbol{p} = \langle m\boldsymbol{v} \rangle$ after 40 gyrations.



Initial speed $v_0 = 100$ m/s Initial speed $v_0 = 50$ m/s Initial speed $v_0 = 10$ m/s

Fig. 4. Normalized expectation position $\langle \boldsymbol{r} \rangle$ after 40 gyrations.

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