Quantum Mechanical Plasma Scattering

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We have solved the two-dimensional time-dependent Schödinger equation for a particle with and without the interparticle potential in a fusion plasma. It was shown that spatial extent of a free particle grows monotonically in time. Such expansion leads to a spatial extent or size of a proton of the order of the average interparticle separation $\Delta\ell \equiv n^{-1/3} \sim 2\times10^{-7}$ m in a time interval of $10^6 \times \Delta\ell/v_{\rm th} \sim 10^{-7}$ sec for a plasma with a density $n \sim 10^{20}\,{\rm m}^{-3}$ and a temperature $T = mv_{\rm th}^2/2 \sim 10\,{\rm keV}$. It was also shown that, under a Coulomb potential, the wavefunction of a charged particle first shrink and expand in time. In the expansion phase, at times $t \geq 10^{-10}$ sec, the size of particle in the presence of a Coulomb potential is much larger than that in the absence of it.

Keywords: Ehrenfest's theorem, quantum mechanical scattering, plasma, diffusion

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1. Introduction

In considering the diffusion of plasmas correctly, it was pointed out more than half a century ago [1, 2] that one must consider the wave character of charged particles when the temperature T is high, i.e. the relative speeds of interacting particles are fast. The criterion on the classical theory to be valid in terms of relative speed g in a hydrogen plasma is given in Ref. [2], as

$$g \ll \frac{2e^2}{4\pi\epsilon_0\hbar} = 4.4\times10^6\ {\rm m/s}, \tag{1}$$

where $e = 1.60\times10^{-19}$ C and $\hbar \equiv h/2\pi = 1.05\times10^{-34}$ J·s stand for the elementary electric charge and the reduced Planck constant. As discussed in Ref. [2], an electron passing through a circular aperture of radius a will be spread out by diffraction through angles of about $\lambda/2\pi a$, where λ is the material wavelength h/mg. If this angle exceeds the classical deflection angle, $\chi = 2\arctan(Z_ie^2/4\pi\epsilon_0 mg^2a)$, for an electron passing by at a distance a from an ion of charge Z_ie, the deflections produced by the most distant encounters will be materially increased. The ratio of the quantum mechanical to the classical deflection is $2Z_i\alpha c/g$, where $\alpha \equiv e^2/4\pi\epsilon_0\hbar c \approx 1/137$ is the fine structure constant. If Z_i is unity, this ratio equals one for a velocity of 4.4×10^6 m/s, as shown on the right hand side of Eq. (1).

In contemporary fusion plasmas with $T \sim 10\,{\rm keV}$ or higher, ions as well as electrons should be treated quantum mechanically. In current plasma physics, however, the quantum mechanical effects enters as a minor correction to the Coulomb logarithm, $\ln\Lambda$, in the case of close encounters [3]. Nonetheless, the neoclassical theory [4] is capable of predicting a lot of phenomena such as those related to the current conduction. Such phenomena linearly depend on the change in velocity $\Delta\boldsymbol{v}$ or in position $\Delta\boldsymbol{r}$. The average or expectation value of $\Delta\boldsymbol{v} \equiv \boldsymbol{v}(t+\Delta t) - \boldsymbol{v}(t)$ conforms to the classical prediction ${}^{\rm CL}\Delta\boldsymbol{v}$ due to the Ehrenfest's theorem: for operators $\hat{\boldsymbol{\xi}} = \boldsymbol{v} = -({\rm i}\hbar/m)\nabla$, and $\boldsymbol{r}$

$$\langle\Delta\hat{\boldsymbol{\xi}}\rangle = \left\langle {}^{\rm CL}\Delta\boldsymbol{\xi} + {}^{\rm QM}\Delta\hat{\boldsymbol{\xi}}\right\rangle = {}^{\rm CL}\Delta\boldsymbol{\xi}, \tag{2}$$

since the quantum-mechanical changes, ${}^{\rm QM}\Delta\hat{\boldsymbol{\xi}}$ due to *quantum-mechanical force*, are averged out. However, diffusion is quadratic in $\Delta\boldsymbol{g}$ or $\Delta\boldsymbol{r}$:

$$\left\langle\left(\Delta\hat{\boldsymbol{\xi}}\right)^2\right\rangle = \left({}^{\rm CL}\Delta\boldsymbol{\xi}\right)^2 + \left\langle\left({}^{\rm QM}\Delta\hat{\boldsymbol{\xi}}\right)^2\right\rangle > \left({}^{\rm CL}\Delta\boldsymbol{\xi}\right)^2. \tag{3}$$

Thus, $\left\langle(\Delta\boldsymbol{r})^2\right\rangle$ and $\left\langle(\Delta\boldsymbol{g})^2\right\rangle$ are always larger than the classical predictions. It shold be noted that the latter quantity is closely related to the scattering cross section, and accordingly to diffusion. This might be the reason why we cannot understand the so-called anomalous diffusion using classical theories that only give correct $\langle\Delta\hat{\boldsymbol{\xi}}\rangle$.

In this connection, we have shown in Ref. [5, 6] that (i) for distant encounters in typical fusion plasmas of $T = 10\,{\rm keV}$ and $n = 10^{20}\,{\rm m}^{-3}$, the average potential energy $\langle U\rangle \sim 30\,{\rm meV}$ is as small as the uncertainty in energy $\Delta E \sim 40\,{\rm meV}$, and (ii) for a magnetic field $B = 2\,{\rm T}$, the spatial size of the wavefunction in the plane perpendicular to the magnetic field is as large as $\ell_{\rm B} \sim 2\times10^{-8}$ m which is much larger than the typical electron wavelength $\lambda_{\rm e} \sim 10^{-11}$ m. So we will numerically solve the time-dependent Schrödinger equation to find $\left\langle\left(\Delta\hat{\boldsymbol{\xi}}\right)^2\right\rangle$.

2. Schrödinger Equation

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

$${\rm i}\hbar\frac{\partial\psi}{\partial t} = \left\{\frac{1}{2\,m}\left(-{\rm i}\hbar\nabla\right)^2 + U\right\}\psi, \tag{4}$$

where $U = U(\boldsymbol{r})$ stands for the potential energy, m the mass of the particle under consideration, ${\rm i} \equiv \sqrt{-1}$ the imaginary

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unit, and $\hbar \equiv h/2\pi$ the reduced Planck constant. When the corresponding classical particle has a momentum $\boldsymbol{p}_0 = m\boldsymbol{v}_0$ at a position $\boldsymbol{r} = \boldsymbol{r}_0$ at a time $t = 0$, the initial condition for the wavefunction is given by

$$\psi(\boldsymbol{r}, 0) = \frac{1}{\sqrt{\pi}\sigma_0} \exp\left(-\frac{(\boldsymbol{r} - \boldsymbol{r}_0)^2}{2\sigma_0^2} + \mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{r}\right), \qquad (5)$$

where $\boldsymbol{r}_0$ is the initial center of ψ, σ_0 is the initial standard deviation and $\boldsymbol{k}_0$ is the initial wave vector, $\boldsymbol{k}_0 = m\boldsymbol{v}_0/\hbar$.

We will solve Eqs. (4) and (5) using the finite difference method (FDM) in space with the Crank-Nicholson scheme

$$\left(\mathsf{I} - \frac{\Delta t}{2\mathrm{i}\hbar}\mathsf{H}\right)\left\{\psi^{n+1}\right\} = \left(\mathsf{I} + \frac{\Delta t}{2\mathrm{i}\hbar}\mathsf{H}\right)\{\psi^n\}, \qquad (6)$$

where I is a unit matrix, and

$$\{\psi^n\} \equiv \{\psi\left(x_i = i\Delta x, j\Delta y, t_n = n\Delta t\right)\}, \qquad (7)$$

stands for the discretized set of the two-dimensional time-dependent wavefunction $\psi\left(x, y, t\right)$ at a discrete time $t_n = n\Delta t$ to be solved numerically. The numerical Hamiltonian operator H on $\{\psi\}$ is defined as

$$\left\{\frac{1}{2\,m}\left(-\mathrm{i}\hbar\nabla\right)^2 + U\right\}\psi \to \mathsf{H}\left\{\psi\right\}. \qquad (8)$$

We will adopt the successive over relaxation (SOR) scheme for time integration in Eq. (6). The corresponding classical equation of motion will also be solved in order to check the validity of the numerical results.

In the nemerical analysis of one-dimensional Schrödinger equation for a free particle ($U = 0$), the initial momentum is given, using a *one-dimensional* version of Eq. (5), as

$$\langle p_0\rangle = \hbar k_0 \sum_{i=-\infty}^{\infty} \frac{\sin k_0\Delta x}{k_0\Delta x}\left|\psi_i\right|^2 \Delta x, \qquad (9)$$

which becomes $\hbar k_0$ in the limit of $\Delta x \to 0$, i.e., $\sin k_0\Delta x \to k_0\Delta x$. Therefore, the size of spatial discretization for the *two-dimensional* FDM in (x, y) plane should be sufficiently small to satisfy

$$\Delta x \sim \Delta y \ll \frac{1}{k_0} = \frac{\lambda_0}{2\pi}, \qquad (10)$$

where λ_0 is the de Broglie wavelength. This restriction Eq. (10) on Δx and Δy demands a lot of computer memory for fast particles. When Eq. (10) does not hold, the initial momentum vector $\langle \boldsymbol{p}\left(t = 0\right)\rangle$ numerically points to untiparallel direction to $\hbar\boldsymbol{k}_0$.

3. Numerical Results

We will consider a hydrogen ion in a fusion plasma which has the density of $n = 10^{20}\,\mathrm{m}^{-3}$ and a temperature of $T = 10\,\mathrm{keV}$ in the presence of a magnetic flux density $B = 2\,\mathrm{T}$. In what follows lengths and velocities are normalized by the average interpaticle separation $\Delta\ell \equiv n^{-1/3} \sim 2 \times 10^{-7}$ and the thermal speed $v_{\mathrm{th}} \equiv \sqrt{2T/m} \sim 10^6\,\mathrm{m/s}$, respectively.

The magnetic length [7] for a proton in $B = 2\,\mathrm{T}$,

$$\ell_{\mathrm{B}} \equiv \sqrt{\frac{\hbar}{eB}} \sim 2 \times 10^{-8}\,\mathrm{m} \qquad (11)$$

is a measure for the spread of a wave function in a direction perpendicular to magnetic field, and is around one-tenth of the average interparticle separation $\Delta\ell$.

3.1 Free particle

First let us assume $U = 0$ in Eq. (4), i.e. a free particle. The exact solution for a two-dimensional case is known as

$$\left|\psi\left(\boldsymbol{r}, t\right)\right|^2 = \frac{\exp\left[-\dfrac{\left(\boldsymbol{r} - \boldsymbol{r}_0 - \boldsymbol{v}_0 t\right)^2}{\sigma^2\left(t\right)}\right]}{\pi\sigma^2\left(t\right)}, \qquad (12)$$

where

$$\sigma\left(t\right) = \sqrt{1 + \left(\frac{\hbar t}{m\sigma_0^2}\right)^2}\,\sigma_0. \qquad (13)$$

Even in this simple case, a great deal of the computer memory and CPU time will be required in order to solve the Schrödinger equation for a plasma particle, because the de Broglie wavelength decreases inversely in proportion to $v_0 = |\boldsymbol{v}_0|$. Therefore, v_0 is assumed to be $10\,\mathrm{m/s}$.

Figure 1 shows the time-dependent standard deviation $\sigma = \sigma\left(t\right)$ for the an impact parameter of $b = \Delta\ell/2$, which increases by a factor of 3.4 during a time interval of $\Delta t = \Delta\ell/v_0 = n^{-1/3}/v_0$ with $n = 10^{20}\,\mathrm{m}^{-3}$. In other words, the wavefunction of a particle with arbitrary speed spreads spatially 3.4 times the initial *size* when particle interactions are so weak that free particle approximation holds. The calculated $\sigma(t)$ is in good agreement with the theoretical value given by Eq. (13).

It should be noted that the numerical results on $\sigma\left(t\right)$ for different initial speed v_0 are the same as Fig. 1 with $v_0 = 10\,\mathrm{m/s}$, as suggested in Eq. (13) that does not depend on v_0.

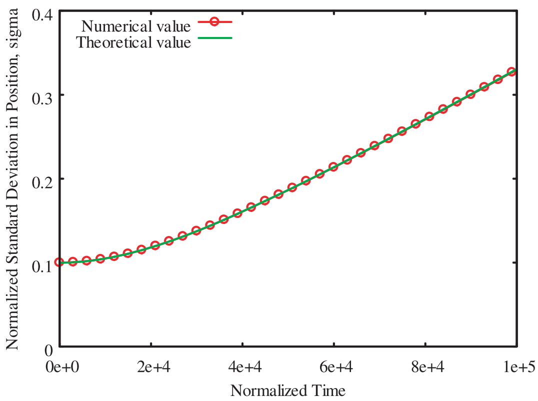

Fig. 1 Normalized standard deviation, σ, in position vs time t with $v_0 = 10\,\mathrm{m/s}$. The impact parameter is $b = \Delta\ell/2$.

Such expansion leads to a spatial extent or size of a proton of the order of the average interparticle separation $\Delta\ell \equiv n^{-1/3} \sim 2 \times 10^{-7}$ meter in a time interval of $10 \times \Delta\ell / v_{\rm th} \sim 10^{-12}$ sec for a plasma with a density $n \sim 10^{20}\,{\rm m}^{-3}$ and a temperature $T = mv_{\rm th}^2/2 \sim 10\,{\rm keV}$.

3.2 Effects of interparticle potential

Here we have assumed that the scatterer is also a quantum-mechanical particle centered at the origin with the wavefunction $\psi_{\rm s}$ similar to that given in Eq. (5), but is fixed in space and time, as

$$\psi_{\rm s}(\boldsymbol{r}) = \frac{1}{\sqrt{\pi}\ell_{\rm B}} \exp\left(-\frac{\boldsymbol{r}^2}{2\ell_{\rm B}^2}\right). \tag{14}$$

In a non-dimensional form, the Coulomb potential $U(\boldsymbol{r})$ due to distributed particle is given as

$$U(\boldsymbol{r}) = \frac{b_0}{r} \,\mathrm{erf}\left(\frac{r}{\ell_{\rm B}}\right), \tag{15}$$

where $b_0 = e^2/4\pi\epsilon_0 \Delta\ell m v_{\rm th}^2$ stands for the impact parameter for $\pi/2$ scattering normalized by $\Delta\ell$. When the scatterer is a point charge, the error function $\mathrm{erf}(\cdot)$ in Eq. (15) should be replaced by unity.

3.2.1 Momenta of particles

Figures 2 and 3 show the time-dependent momentum $\boldsymbol{p} = \left(p_x, p_y\right)$ for $v_0 = 1$ m/s with the impact parameters of $b = \Delta\ell/2$ and $b = 0$, respectively. Here, $\boldsymbol{v}_0$ is the initial velocity directed to $+y$. Obtained time evolutions of particle's momenta agree with the classical ones until the normalized time of approximately $t \sim 500$ with the velocity $v(t = 500) \sim 100 \times v_0$ due to acceleration by the Coulomb force. After this time, however, the numerical momenta deviate from classical ones. The reason for this deviation is that, at around $t \sim 500$, the wavenumber becomes large, $k \sim 100 \times k_0$, as a result the restriction, Eq. (10), on the spatial grid size breaks. The relative error in momentum p_x can be expressed as

$$\frac{\sin k_y \Delta y}{k_y \Delta y} - 1 = -\frac{1}{3!}\left(k_y \Delta y\right)^2 + \frac{1}{5!}\left(k_y \Delta y\right)^4 + \cdots, \tag{16}$$

which, at $t \sim 500$ and later times, is 10^4 times or more as large as that at $t = 0$. Therefore, even though the grid size satisfies the restriction, Eq. (10), at $t = 0$, the acceleration makes it at stake in time.

3.2.2 Spatial extent of particles

Figure 4 depicts the evolution of the spatial extent of a particle $\sigma = \sigma(t)$:

$$\sigma^2(t) = \int \psi^*(\boldsymbol{r}, t)\left(\boldsymbol{r} - \langle \boldsymbol{r} \rangle\right)^2 \psi(\boldsymbol{r}, t)\, \mathrm{d}^2\boldsymbol{r}, \tag{17}$$

for the initial speed v_0 of 1, 10 and 100 m/s with that for the free particle. It is seen in Fig. 4 that, at first, all wavefunctions contract, or shrink, in time, i.e. $\sigma(t) < \sigma(0)$,

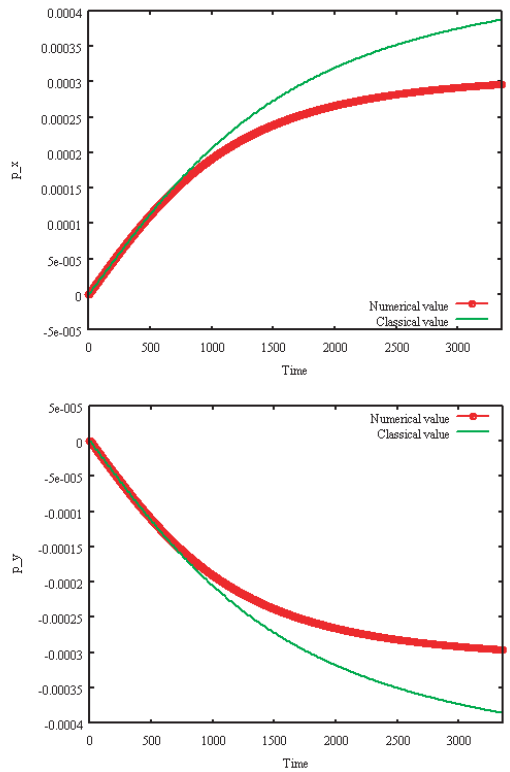

Fig. 2 Time evolution of normalized momenta p_x (top) and p_y (bottom) for $v_0 = 1$ m/s and $b = \Delta\ell/2$.

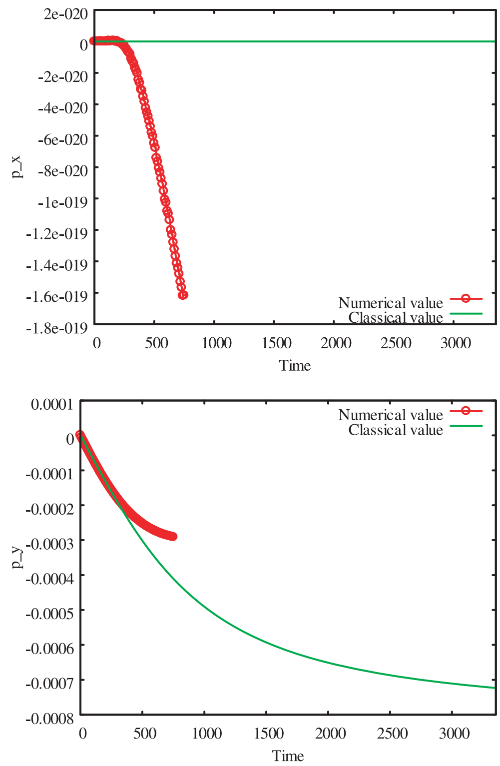

Fig. 3 Time evolution of normalized momenta p_x (top) and p_y (bottom) for $v_0 = 1$ m/s and $b = 0$, i.e. head-on collision.

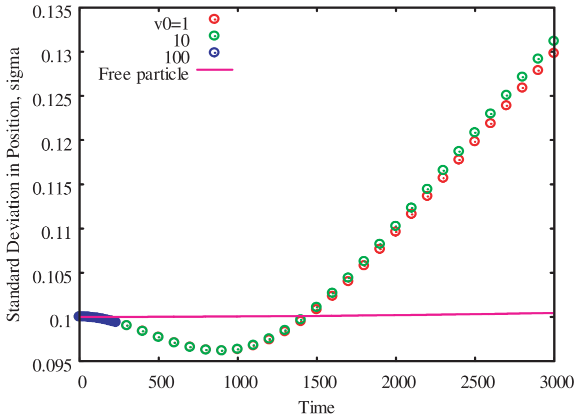

Fig. 4 Normalized standard deviation, σ, in position vs normalized time t with initial speeds of $v_0 = 1$, 10 and 100 m/s. Impact parameter is $b = \Delta\ell/2$.

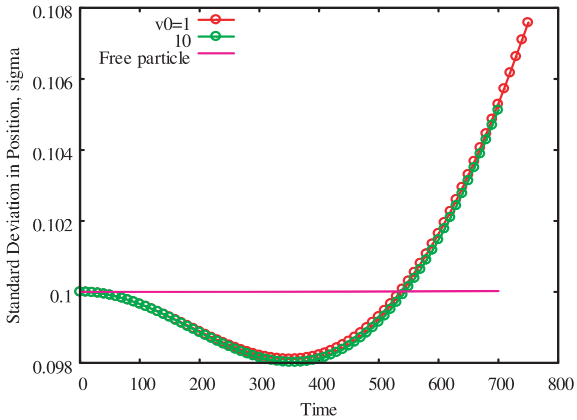

Fig. 5 Normalized standard deviation, σ, in position vs normalized time t with initial speeds of $v_0 = 1$, and 10 m/s. Impact parameter is $b = 0$.

then they gradually expand. Such contraction and expansion correspond to phases of approaching- and going-away-from the scatterer of the classical particle. The spatial size of particles under the Coulomb potential is larger than that of free particles at normalized times of $t > 1500$, i.e., 1.5×10^{-10} sec for ions in fusion plasmas, as shown in Fig. 4.

As was shown in Figs. 2 and 3 with Eq. (16), the numerical errors in momenta at $t > 500$ due to acceleration become larger than those at $t \sim 0$, and so do those in $\sigma(t)$. In spite of this, the time evolution of $\sigma(t)$ for different initial speeds seems the same, as shown in Fig. 4. If the difference of $\sigma(t)$, especially between $v_0 = 1$ m/s and $v_0 = 10$ m/s, is solely due to the numerical origin, i.e., insufficient grid divisions, it would not be required to solve the Schrödinger equation for faster particles with speeds of $v > 4.4 \times 10^6$ m/s, as stated in Eq. (1).

4. Summary

We have solved the two-dimensional time-dependent Schödinger equation for a particle with and without the interparticle potential in a fusion plasma. It was shown that spatial extent of a free particle grows monotonically in time. Such expansion leads to a spatial extent or size of a proton of the order of the average interparticle separation $\Delta\ell \equiv n^{-1/3} \sim 2 \times 10^{-7}$ m in a time interval of $10^6 \times \Delta\ell/v_{\rm th} \sim 10^{-7}$ sec for a plasma with a density $n \sim 10^{20}\,{\rm m}^{-3}$ and a temperature $T = mv_{\rm th}^2/2 \sim 10$ keV. Unfortunately, the calculation presented here is valid for a time t much less than the cycrotron period of the order of 10^{-8} sec for ions, because the initial wavefunction adopted includes the magnetic length, $\ell_{\rm B} = \sqrt{\hbar/qB}$.

It was also shown that, under a Coulomb potential due to a distributed particle, the wavefunction of a charged particle first shrink and expand in time, and that the expansion is much faster than that for free ions at times of $t > 1500 \times \Delta t \sim 3 \times 10^{-10}$ sec for $b = \Delta\ell/2$ and $t > 530 \times \Delta t \sim 10^{-10}$ sec for $b = 0$, respectively.

In summary, quantum-mechanical analyses are necessary for magnetized plasmas, since the wavefunction of their constituents overlaps with one another in a short time compared to the classical collision times.

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