Numerical Analysis of Quantum-Mechanical Non-Uniform $E \times B$ Drift[*)]

Shun-ichi OIKAWA, Wataru KOSAKA[1)] and Poh Kam CHAN[1)]

Faculty of Engineering, Hokkaido University, N-13, W-8, Sapporo 060-8628, Japan
[1)]*Graduate School of Engineering, Hokkaido University, N-13, W-8, Sapporo 060-8628, Japan*

(Received 18 November 2013 / Accepted 28 February 2014)

We have numerically solved the two-dimensional time-dependent Schödinger equation for a magnetized proton in the presence of a uniform electric field and a nonuniform magnetic field with a gradient scale length of L_B. It is shown that the particle mass and the electric field do not affect the time rate of variance change at which variance increases with time, and their characteristic times are of the order of L_B/v_0 sec with v_0 being the initial particle speed.

Keywords: Schrödinger equation, E × B drift, uncertainty, uniform magnetic field, magnetic length, quantum mechanical effect

DOI: 10.1585/pfr.9.3401033

1. Introduction

We have shown in the previous papers [1–4] for the cases of ∇B drift that the variance, or the uncertainty, in position σ_r^2 grows with time. For typical fusion plasmas with a temperature $T \sim 10$ keV and a number density of $n = 10^{20}\,\mathrm{m}^{-3}$, 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: Plasmas may behave more-or-less like extremely-low-density liquids, not gases, since the *size* of each particle is of the same order of the interparticle separation.

We have also pointed out in Refs. [5–7] that (i) 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 (ii) 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 $\ell_B \sim 10^{-8}\,\mathrm{m}$ [8] which is much larger than the typical electron wavelength $\lambda_e \sim 10^{-11}\,\mathrm{m}$, and is around one-tenth of the average interparticle separation $\Delta\ell \sim 10^{-7}\,\mathrm{m}$.

In this paper, quantum mechanical effects of a uniform electric field and a nonuniform magnetic field will be studied.

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

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

where $V = V(\boldsymbol{r})$ and $\boldsymbol{A} = \boldsymbol{A}(\boldsymbol{r})$ stand for the scalar and vector potentials, m and q the mass and electric charge of the particle under consideration, and $\mathrm{i} \equiv \sqrt{-1}$ the imaginary unit. When the corresponding classical particle has a momentum $\boldsymbol{p}_0 = m\boldsymbol{v}_0$, where $\boldsymbol{v}_0$ is the initial velocity, at a position $\boldsymbol{r} = \boldsymbol{r}_0$ at a time $t = 0$, the initial condition for the wavefunction $\psi(\boldsymbol{r}, 0)$ can be given [9, 10] 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 $\boldsymbol{k}_0 = m\boldsymbol{v}_0/\hbar$ is the initial wavenumber vector. We will solve Eqs. (1) and (2) using the finite difference method (FDM) in space with the Crank-Nicolson scheme [2, 4, 9]. The numerical errors for the Crank-Nicolson scheme with the central difference in space

$$\{\psi\}^{n+1} \equiv \mathsf{U}\{\psi\}^n, \tag{3}$$

where

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

are quadratic over both the time step Δt and the space step $\Delta x = \Delta y$. Here the superscript n represents time-label, I and H are unit matrix and numerical Hamiltonian matrix [6, 9]. This time integrator is not only unconditionally stable but also norm-conserving scheme for discretized wavefunction $\{\psi\}$, the latter of which leads to the strict particle conservation, irrespective of Δt, Δx and Δy, since the matrix H in Eq. (4) is Hermitian so that the matrix U is unitary; the norm $\|\{\psi\}\|$ = const with time.

We will also adopt the successive over relaxation (SOR) scheme for time integration in Eq. (3). The size

---

author's e-mail: oikawa@qe.eng.hokudai.ac.jp

*) This article is based on the presentation at the 23rd International Toki Conference (ITC23).

of spatial discretization for the *two-dimensional* FDM in (x, y) plane should be sufficiently small to satisfy

$$\Delta x \sim \Delta y \ll \frac{1}{k_0} = \frac{\lambda_0}{2\pi}, \tag{5}$$

where λ_0 is the de Broglie wavelength. This restriction Eq. (5) on Δx and Δy demands a lot of computer memory for fast particles.

2.1 Exact solution for uniform electric and magnetic fields

In the case of uniform electric and magnetic fields with $\boldsymbol{E} = -\nabla V(y) = E\boldsymbol{e}_y$ and $\boldsymbol{B} = \nabla \times \boldsymbol{A}(y) = B\boldsymbol{e}_z$, the Hamiltonian operator $\hat{H}$ does not depend on x. Thus, the momentum operator in x direction $\hat{P}_x = -\mathrm{i}\hbar\partial/\partial x$ is commutable with $\hat{H}$, and can be replaced with its eigenvalue $\hbar k_x$, where the wavefunction $\psi(x, y, t)$ has the form of $\mathrm{e}^{\mathrm{i}(k_x x - \mathcal{E}t/\hbar)}\varphi(y)$ with $\mathcal{E} \equiv \langle \hat{H} \rangle$ being the energy eigenvalue. In this case, Schrödinger equation (1) becomes

$$\left(\eta^2 - \frac{\partial^2}{\partial \eta^2}\right)\varphi = \frac{2}{\hbar\omega}\left[\mathcal{E} - \left(\hbar k_x - \frac{mE}{2B}\right)\frac{E}{B}\right]\varphi, \tag{6}$$

where $\omega \equiv qB/m$ is the cyclotron angular frequency, and

$$\eta \equiv \frac{qBy + \hbar k_x - mE/B}{\sqrt{\hbar qB}}. \tag{7}$$

A function $H(\eta)$ with $\varphi(\eta) \equiv H(\eta)\exp\left(-\eta^2/2\right)$ satisfies Hermite differential equation [11] so that $\varphi(\eta)$ is given by

$$\varphi_N(\eta) = \frac{H_N(\eta)}{\sqrt{2^N N!\sqrt{\pi}}}\exp\left(-\frac{\eta^2}{2}\right), N = 0, 1, \ldots, \tag{8}$$

where $H_N(\eta)$ is the Hermite polynomials. Since the eigenvalue in Eq. (6) for φ_N is $2N + 1$, the energy eigenvalue for the corresponding wavefunction ψ_N is

$$\mathcal{E}_N = \hbar\omega\left(N + \frac{1}{2}\right) + \left(\hbar k_x - \frac{mE}{2B}\right)\frac{E}{B}. \tag{9}$$

The first term in Eq. (9) is the same as that of a harmonic oscillator [10] with the frequency ω, and the second term is due apparently to the $\boldsymbol{E} \times \boldsymbol{B}$ drift.

For the initial condition given in Eq. (2) with $\boldsymbol{v}_0 = (u_0, 0)$, we have

$$\psi(\eta, t) = \frac{\mathrm{e}^{-\mathrm{i}(\Omega t + \Theta(\eta, t))}}{\pi^{1/4}}\exp\left[-\frac{(\eta - \langle\eta\rangle)^2}{2}\right], \tag{10}$$

$$\Omega = \frac{1}{2}\left[\omega + \frac{m}{\hbar}\left(u_0 - \frac{E}{2B}\right)\frac{E}{B}\right], \tag{11}$$

$$\Theta(\eta, t) = \eta_0\left(\eta\sin\omega t - \frac{\eta_0}{4}\sin 2\omega t\right), \tag{12}$$

where $\langle\eta\rangle$ is the expectation value of particle position. Using the definition of η in the Eq. (7)

$$\langle y \rangle \equiv y_0 - \left(u_0 - \frac{E}{B}\right)\frac{1 - \cos\omega t}{\omega}, \tag{13}$$

which comes from the fact that the total momentum in x direction $P_x = mu - qBy$ is kept constant, i.e. the Poisson bracket of $[\hat{P}_x, \hat{H}] = 0$. Although the exact solution Eq. (10) does not include x, its expectation value $\langle x \rangle$ is found as

$$\langle x \rangle \equiv x_0 + \left(u_0 - \frac{E}{B}\right)\frac{\sin\omega t}{\omega} + \frac{E}{B}t, \tag{14}$$

since $[\hat{P}_y + qBx - qEt, \hat{H}] = 0$, i.e. $\langle \hat{P}_y \rangle + qB\langle x \rangle - qEt =$ const [8], which leads to the $\boldsymbol{E} \times \boldsymbol{B}$ drift. The expectation value of position $\langle \boldsymbol{r} \rangle = (\langle x \rangle, \langle y \rangle)$ is exactly the same as the classical one $\boldsymbol{r}(t)$, so are other expectation values except for uncertainty, such as energy of $\mathcal{E} = \langle \mathrm{i}\hbar\partial/\partial t \rangle = \langle \hat{H} \rangle = mu_0^2/2 - qEy_0 + \hbar\omega/2$.

Thus, Eq. (10) has all the information on the particle under consideration. It should be noted that the variance in position $\sigma_r^2 = \hbar/qB$ does not change with time in the presence of a uniform electric and a magnetic field.

3. Numerical Results

In what follows, velocity and time are normalized by 10 m/s and the cyclotron frequency for a proton in $B =$ 10 T with a speed of 10 m/s, thus position is normalized by the cyclotron radius of the proton. The magnetic length [8] for a proton in $B = 10$ T, $\ell_B \equiv \sqrt{\hbar/eB} \sim 10^{-8}$ m is a measure for the spread of a wave function in the plane perpendicular to the magnetic field. With these normalization, Planck constant $\hbar \sim 0.6038$, initial uncertainty in position $\ell_B^2 = \hbar/eB \sim 0.7771^2$ and initial uncertainty in kinetic momentum $3/2(\hbar eB) \sim 0.9058$ are of order of unity. It should be noted that the kinetic energy of a classical proton speed ~ 27 m/s in $B = 10$ 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 a time duration of five cyclotron rotations by a proton in the presence of an electrostatic potential of $V = V(y) = -Ey$ and a vector potential of $\boldsymbol{A} = \boldsymbol{A}(y) = -By(1 - y/2L_B)\boldsymbol{e}_x$ with L_B being the gradient scale length of the magnetic field.

3.1 Numerical errors

The relative numerical errors in energy $\mathcal{E}$, total momentum P_x, and particle conservation are quite small, as shown in Fig. 1 for initial mechanical momentum of $m\boldsymbol{v}_0 = (mu_0 = 0, mv_0 = 5)$ at $\boldsymbol{r}_0 = (x_0 = -5, y_0 = 0)$, an electric field $E = 0$, and a magnetic field $B = 1$ with $L_B = \infty$. Initial values of the conserved quantities in such a case are energy $\mathcal{E} = 12.92$, momentum $\langle P_x \rangle = \langle -\mathrm{i}\hbar\partial_x \rangle = mu_0 - qBy_0 = 0$ with $|\boldsymbol{P}| \sim mv_0 = 5$, and the particle conservation of

$$\int_\Sigma \rho(\boldsymbol{r}, t)\,\mathrm{d}^2\boldsymbol{r} = 1. \tag{15}$$

The relative error in energy is almost identical with that in particle conservation because of the unitarity of the numer-

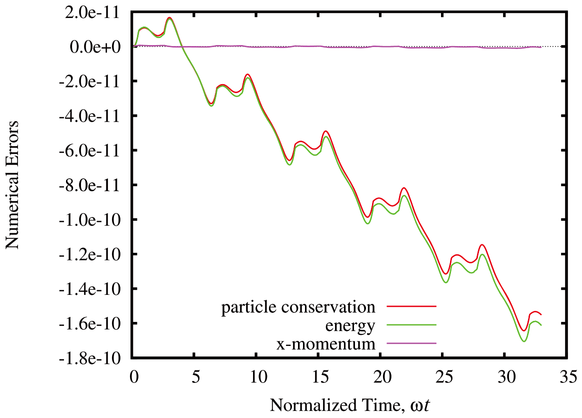

Fig. 1 Time evolution of relative errors in energy, momentum and particle conservation for $E = 0$, $B = 1$ and initial mechanical momentum $(mu_0, mv_0) = (0, 5)$.

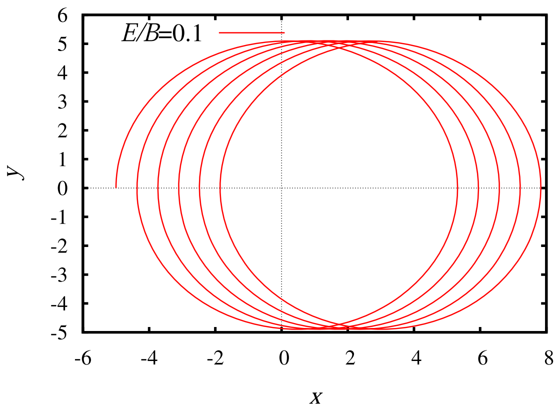

Fig. 2 Time evolution of the expectation of position $\langle \boldsymbol{r} \rangle$ for $\boldsymbol{r}_0 = (-5, 0)$, $m\boldsymbol{v}_0 = (0, 5)$, $B = 1$ and $E = 0.1$. Since normalized period of gyration is 2π, the drift speed $(\langle x(2\pi)\rangle - \langle x(0)\rangle)/2\pi$ is close to $E/B = 0.1$.

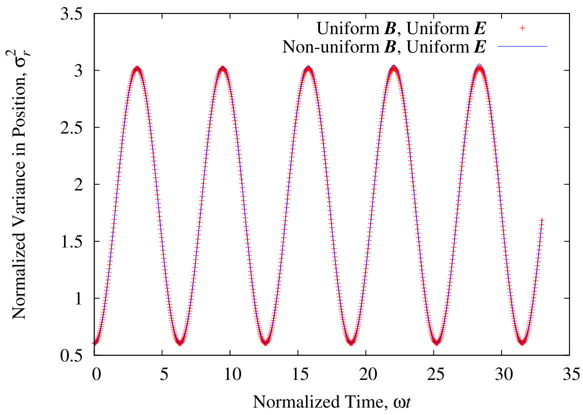

Fig. 3 Time evolution of variance in position $\sigma_r^2 = \left\langle \boldsymbol{r}^2 \right\rangle - \langle \boldsymbol{r} \rangle^2$ for initial speed of $v_0 = 5$, $E = 10^{-4}$, and $B = 1$ with $L_B = \infty$ or $L_B = 10^4$.

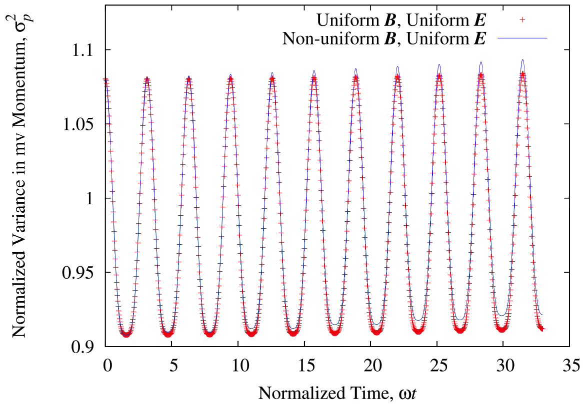

Fig. 4 Time evolution of variance $\sigma_p^2 = \left\langle \boldsymbol{p}^2 \right\rangle - \langle \boldsymbol{p} \rangle^2$ in mechanical momentum $\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla - q\boldsymbol{A}$ for initial speed of $v_0 = 5$, $E = 10^{-4}$, and $B = 1$ with $L_B = \infty$ or $L_B = 10^4$.

ical time-shift operator U, and of the Hermitian nature of numerical Hamiltonian operator H given in Eq. (3).

Note that the normalized initial speed of $v_0 = 5$, i.e. 50 m/s, which is much slower than the thermal speed of fusion plasmas, is assumed here due to a numerical reason: required numerical grid sizes Δx and Δy in Eq. (5) need to be much smaller than the de Broglie wavelength that is inversely proportional to the particle speed.

3.2 $\boldsymbol{E} \times \boldsymbol{B}$ drift

Figure 2 shows the time evolution of the expectation of position $\langle \boldsymbol{r} \rangle$ for $\boldsymbol{r}_0 = (-5, 0)$, $\boldsymbol{v}_0 = (0, 5)$, uniform magnetic field of $\boldsymbol{B} = 1\boldsymbol{e}_z$ with $L_B = \infty$, and $\boldsymbol{E} = 0.1\boldsymbol{e}_y$. The classical $\boldsymbol{E} \times \boldsymbol{B}$ drift velocity in this case is $0.1\boldsymbol{e}_x$. on the other hand, the numerical drift speeds in x-direction of

$$\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} \equiv \frac{\langle x(2\pi)\rangle - \langle x(0)\rangle}{2\pi}, \tag{16}$$

are in the range of 0.10001–0.10008, and are close to classical $\boldsymbol{E} \times \boldsymbol{B}$ drift speed of $E/B = 0.1$, in which the normalized period of gyration is 2π.

3.3 Time evolution of variances

Figures 3 and 4 show the time evolution of variances in position $\sigma_r^2 = \left\langle \boldsymbol{r}^2 \right\rangle - \langle \boldsymbol{r} \rangle^2$ and mechanical momentum $\sigma_p^2 = \left\langle \boldsymbol{p}^2 \right\rangle - \langle \boldsymbol{p} \rangle^2$ in mechanical momentum $\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla - q\boldsymbol{A}$, respectively for $B = 1$ and initial speed is $v_0 = 5$. Red points in both figures show the variance for the case of uniform magnetic field, and blue lines for nonuniform magnetic field with the gradient scale length of $L_B = 10^4$. It is seen that the peaks of variances grow with time.

Although the variances for uniform magnetic field case should not change with time from Eq. (10), they slightly grows with time due to numerical errors, especially due to finite difference approximation. Let us define the difference of $\sigma_{\text{peak}}^2(t)$ between the nonuniform, i.e. finite L_B, and uniform, $L_B = \infty$, magnetic field cases,

$$\Delta\sigma_{\text{peak}}^2 \equiv \sigma_{\text{peak,nonuniform}}^2 - \sigma_{\text{peak,uniform}}^2, \tag{17}$$

which would gives us the physical time rate of variance

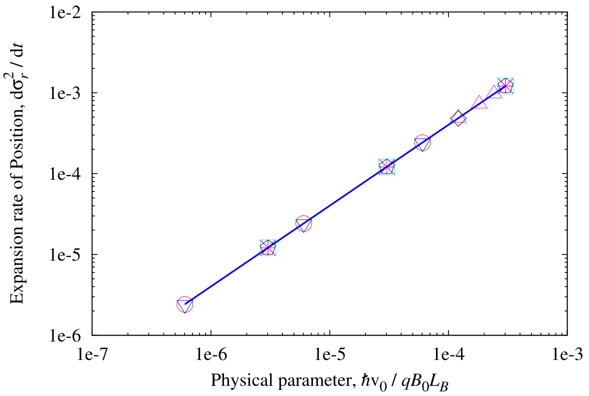

Fig. 5 Expansion rate of variance in position vs. $\hbar v_0/qBL_B$. Each point shape, such as ◇ and □, corresponds to the same electric field E.

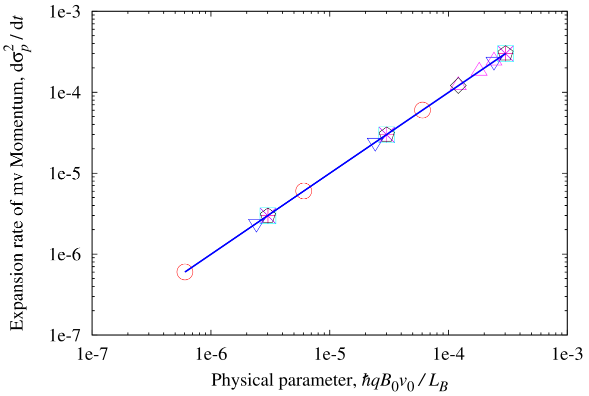

Fig. 6 Expansion rate of variance in mechanical momentum vs. $\hbar v_0/qBL_B$. Each point shape, such as ◇ and □, corresponds to the same electric field E.

change [1, 2] as

$$\frac{d\sigma^2}{dt} \equiv \frac{\Delta\sigma^2_{\text{peak}}(2\pi) - \Delta\sigma^2_{\text{peak}}(0)}{2\pi}, \tag{18}$$

where 2π is the normalized period of the cyclotron motion.

3.4 Rate of changes in variances

For various combinations of physical parameters, such as m, q, v_0, E, B, and L_B, similar analyses as in the preceding section give us the relationship between the expansion rate of variances in position σ_r^2 as a function of $\hbar v_0/qBL_B$, as shown in Fig. 5, and in mechanical momentum σ_p^2 as a function of $\hbar v_0 qB/L_B$ in Fig. 6. Also depicted are the fitting lines in blue. Note that the variances clearly on the respective fitting lines. The expansion rates both for position and mechanical momentum have the following expressions

$$\frac{d\sigma_r^2}{dt} = 4.014 \times \frac{\hbar v_0}{qBL_B}, \tag{19}$$

$$\frac{d\sigma_p^2}{dt} = 0.995 \times \frac{\hbar qBv_0}{L_B}, \tag{20}$$

both of which do not depend on the particle mass m nor the electric field $\boldsymbol{E}$. It should be noted that the initial variance in position is $\sigma_r^2(0) = \hbar/qB$ which is the magnetic length squared, and that in momentum is $\sigma_p^2(0) = \hbar qB$, thus the characteristic times τ are $\tau_r \sim L_B/4v_0$ for position and $\tau_p \sim L_B/v_0$ sec for momentum, respectively.

4. Summary

We have solved the two-dimensional time-dependent Schödinger equation for a magnetized proton in the presence of a uniform electric field and a nonuniform magnetic field with a gradient scale length of L_B. It is shown that the particle mass and the electric field do not affect the time rate of variance expansion at which variances increase with time, and their characteristic times are of the order of L_B/v_0 sec.

Acknowledgment

The authors would like to thank Prof. Y. Matsumoto, Prof. M. Itagaki for their fruitful discussions on the subject. Part of the SOR coding for a GPU was done by Mr. R. Ueda. This research was partially supported by a Grant-in-Aid for Scientific Research (C), 21560061.

[1] S. Oikawa and P.K. Chan, Plasma Fusion Res. **8**, 2401142 (2013).
[2] P.K. Chan, S. Oikawa and E. Okubo, Plasma Fusion Res. **7**, 2401106 (2012).
[3] S. Oikawa, E. Okubo and P.K. Chan, Plasma Fusion Res. **7**, 2401034 (2012).
[4] S. Oikawa, T. Shimazaki and E. Okubo, Plasma Fusion Res. **6**, 2401058 (2011).
[5] S. Oikawa, T. Oiwa and T. Shimazaki, Plasma Fusion Res. **5**, S2024 (2010).
[6] S. Oikawa, T. Shimazaki and T. Oiwa, Plasma Fusion Res. **5**, S2025 (2010).
[7] S. Oikawa, T. Oiwa and T. Shimazaki, Plasma Fusion Res. **5**, S1050 (2010).
[8] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*: *Non-relativistic Theory*, 3rd ed., translated from the Russian by J. B. Sykes and J. S. Bell (Pergamon Press, Oxford, 1977).
[9] H. Natori and T. Munehisa, J. Phys. Soc. Jpn. **66**, 351 (1997).
[10] J.J. Sakurai, *Modern Quantum Mechanics*, Rev. ed., (Addison-Wesley, Reading, 1994).
[11] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, 1965).