Use of Quantum Mechanical Methods to Obtain a Bohm-Type Coefficient of Diffusion. Part II

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The research reported in an article previously published in this journal is pursued here further on. A staircase profile of the graphical representation of the absolute value of the expression for Bohm-type diffusion in two dimensions is analyzed allowing the suggestion that its shape could be related to the well-known structure of levels of the quantized square of the guiding center radius vector and that this structure could be responsible for the appearance of the successive steps in such a profile. When these considerations are taken into account, the expression for Bohm-type diffusion in two dimensions is normalized according to the formula for the quantized square of the guiding center radius vector and a diffusion coefficient whose value is $\frac{4}{\pi}$ times the Bohm diffusion coefficient is obtained for large values of the independent variable.

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1. Introduction

The diffusive motion of particles in different media is an interesting phenomenon in several fields and its nature has been an important subject of study. For example, charged particles in magnetized plasmas diffuse in various modes, among which the Bohm diffusion [1] still eludes an explanation based on first principles.

In Ref. [2] a simple quantum mechanical model to treat an electron with thermal energy kT in a dilute magnetized plasma in the presence of an electric potential is considered; there, an expression for Bohm-type diffusion that describes the behaviour of the mean square value of the x component of the displacement of the guiding center of the electron's orbit is obtained. From this expression two coefficients of diffusion were deduced, viz.: one of magnitude $\frac{\hbar}{\sqrt{2}m}$, characterized by a step size comparable to the linear dimensions of the area of uncertainty of the guiding center, the other being a Bohm-type coefficient of diffusion of magnitude $\frac{ckT}{\sqrt{2}eB}$ with a step size comparable to the Larmor radius.

In the present paper, it is found that the graphical representation of the absolute value of the expression for Bohm-type diffusion in two dimensions presents a staircase profile with a mean slope equal to one. The separation between successive steps of this profile turns out to be of the same order of magnitude as the separation between successive levels of the well-known quantized square of the guiding center radius vector. Then an analysis is carried out from the expression for Bohm-type diffusion in two dimensions; from this analysis it is suggested that the structure of levels of the quantized square of the guiding center radius vector could give rise to the series of steps present in that profile. Taking into account these considerations, the expression for Bohm-type diffusion in two dimensions is normalized according to the formula for the quantized square of the guiding center radius vector, to make the separation between successive steps in the graph of the normalized expression be the same as the separation between successive levels of the quantized square of the guiding center radius vector. The Bohm-type coefficient of diffusion that produces this normalized expression for large values of the independent variable results in a quantity which is $\frac{4}{\pi}$ times the Bohm diffusion coefficient.

2. Bohm-type diffusion

Let us first transcribe as Eq. (1), Eq. (39) of Ref. [2] which is the expression for Bohm-type diffusion

$$\langle x_0^2\rangle = \langle N_\mathrm{d}\rangle\langle \dot{x}_0^2\rangle t^2 f(\theta)\,. \tag{1}$$

The origin of this expression is traced back to the solution of a quantum mechanical equation of motion in the quasi-classical approximation for the x component of the displacement of the orbit's guiding center of a single electron with thermal energy kT in a dilute magnetized plasma in the presence of an electrical potential that simulates an electrical fluctuation which drives the guiding center drift. In Eq. (1) x_0 is the x component of the displacement of the guiding center of the electron's, orbit, t is the time, the symbol $\langle\cdot\rangle$ represents the mean value

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taken in terms of quasi-classical states of the harmonic oscillator, the dot indicates the derivative with respect to time, $\langle N_\mathrm{d}\rangle = \frac{kT}{\hbar\omega_\mathrm{c}}$ and $\langle \dot{x}_0^2\rangle = \frac{kT}{\sqrt{2}m}$ (see Eq. (32) of Ref. [2]). The function $f(\theta)$ in Eq. (1) is given by the expression (see Eq. (24), Ref. [2]):

$$f(\theta) = \frac{\sin^2\theta}{\theta^2} + \mathrm{i}\left(\frac{1}{\theta} - \frac{\sin 2\theta}{2\theta^2}\right), \tag{2}$$

where $\theta = \frac{\Omega t}{2}$, $\Omega = \omega_\mathrm{c}\langle N_\mathrm{d}\rangle$, $\omega_\mathrm{c} = \frac{eB}{mc}$ is the cyclotron frequency. Using the definitions given above, the variable θ is written as $\frac{kT}{2\hbar}t$.

The real and imaginary parts of Eq. (2) are the Hilbert transform of each other [3] and fulfill the requisites for a dispersion relation in the time domain (see text below Eq. (24) of Ref. [2]).

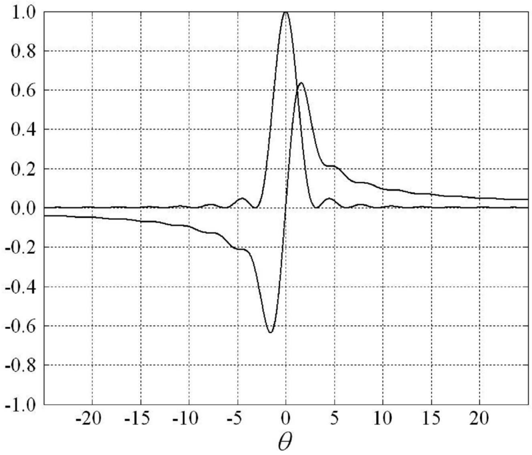

Fig. 1. Real (symmetrical) and imaginary (antisymmetrical) parts of the function $f(\theta)$ given by Eq. (2).

Figure 1 represents the real (symmetrical) and imaginary (antisymmetrical) parts of Eq. (2). Using the definitions of θ, $\langle \dot{x}_0^2\rangle$ and $\langle N_\mathrm{d}\rangle$ given above, Eq. (1) may be rewritten as follows:

$$\langle x_0^2\rangle = 2\sqrt{2}\frac{\hbar c}{eB}\theta^2 f(\theta). \tag{3}$$

In order to take into account simultaneously the information contained in the real and imaginary parts of Eq. (2), its absolute value will be used for the purposes of the present paper; it is expressed as

$$|f(\theta)| = \left[\frac{\sin^4\theta}{\theta^4} + \left(\frac{1}{\theta} - \frac{\sin 2\theta}{2\theta^2}\right)^2\right]^{1/2}. \tag{4}$$

Then the absolute value of Eq. (3) is written as

$$\left|\langle x_0^2\rangle\right| = 2\sqrt{2}\frac{\hbar c}{eB}\theta^2\,|f(\theta)|\,, \tag{5}$$

where the expression $\theta^2|f(\theta)|$ is represented by the staircase curve 2 of Fig. (2).

3. Analysis of the staircase structure of curve 2 in Fig. 2

The following features of curve 2 in Fig. 2 are noticeable:

1. The staircase structure shown there is an infinite set of steps of a ladder whose successive projections on both axes are equidistant. The mean slope of the curve is unity.
2. It is noticed from the figure that the value of $\theta^2|f(\theta)|$ changes very slowly at the steps, causing the contribution of $\theta^2|f(\theta)|$ to the diffusion of the guiding center to be very small there.
3. Calculations show that in each step there exists a point at which the derivative of $\theta^2|f(\theta)|$ takes the value of zero.
4. Calculations show that successive zeroes of the derivative of $\theta^2|f(\theta)|$ are equidistant along the directions of the abscissa and the ordinate.

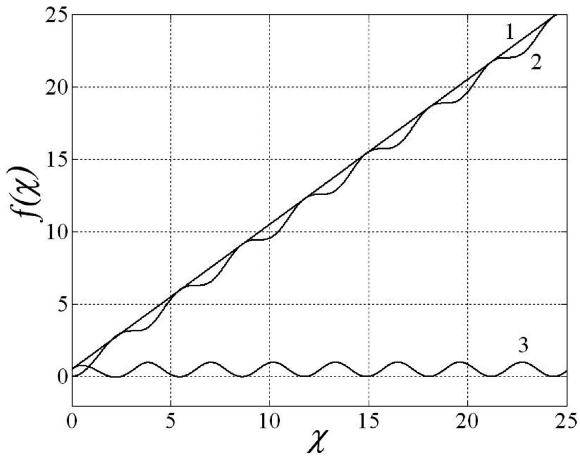

Fig. 2. Curve 3 represents the difference between curves 1 and 2 which are described in the text.

A possible explanation for the presence of the staircase structure of curve 2 in Fig. 2 could rest on the fact that the square of the radius vector of the guiding center with respect to a given origin is quantized in a similar fashion as is the energy of the harmonic oscillator (see Ref. [4], page 758). Therefore, as the guiding center diffuses, it passes through the equidistant successive levels of its quantized squared radius vector in such a way that its structure of levels modulates the motion, producing the phenomenon described by the expression $\theta^2|f(\theta)|$ of Eq. (5). Thus, Eq. (5) and curve 2 of Fig. 2 keep evidences of a discrete behaviour revealing the existence of a structure of levels in the diffusion of the guiding center; in the next section it will be seen that this structure of levels is compatible with Eq. (6) below for the eigenvalues of the squared radius vector of the guiding center.

4. The eigenvalues of Γ_n^2

The expression for the eigenvalues of the square of the radius vector of the guiding center is reproduced here; see Ref. [4], p. 758

$$\Gamma_n^2 = 2\frac{\hbar c}{eB}\left(n + \frac{1}{2}\right), \tag{6}$$

where $\frac{\hbar c}{eB}$ is comparable to the uncertainty area of the guiding center (see Eqs. (6), (7) of Ref. [2]) and $n = 0$, 1, 2, ... is the corresponding quantum number. This quantum number and the one for the oscillator energy take on the same set of values $(0, 1, 2, \ldots)$ but correspond to different operators (see Ref. [4], pp. 754, 758). Equation (6) expresses the concept that the square of the guiding center radius vector is quantized and can assume any of an infinite set of discrete stationary states. Since in the absence of an external electrical perturbation the guiding center does not move, the quantum number n assumes the value $n = 0$. However, in the presence of a perturbing electric field that classically drives the guiding center drift, the number n can take on higher values. In this circumstance the thermal average of Eq. (6) is taken in terms of the Boltzmann factor $\exp\left(-\frac{E_n}{kT}\right)$, where E_n is the harmonic oscillator energy, i.e.:

$$\Gamma_{n_{\rm av}}^2 = 2\frac{\hbar c}{eB}\left(n_{\rm av} + \frac{1}{2}\right), \tag{7}$$

where $n_{\rm av}$ turns out to be

$$n_{\rm av} = \frac{1}{\exp\left(\frac{\hbar\omega_{\rm c}}{kT}\right) - 1}\,.$$

For $\frac{kT}{\hbar\omega_{\rm c}} \gg 1$, as is usual in many experiments, the last expression is reduced to $n_{\rm av} \approx \frac{kT}{\hbar\omega_{\rm c}}$ so that, neglecting the term $\frac{1}{2}$ in Eq. (7), the thermal average of Γ_n^2 is now written as

$$\Gamma_{n_{\rm av}}^2 \approx \frac{\hbar c}{eB}\frac{kT}{\hbar\omega_{\rm c}} = \frac{v_{\rm th}^2}{\omega_{\rm c}^2} = \rho_{\rm L}^2, \tag{8}$$

where $\rho_{\rm L}$ is the Larmor radius, which is the step size in the Bohm and Bohm-type diffusion (see for example Ref. [5] and Eq. (43), Ref. [2]). Notice that expression (8) was achieved independently of any consideration of the behaviour of Eq. (5) which means that in the presence of an external perturbation, the thermal average of the "excited" squared radius vector of the guiding center inherently assumes a value comparable to $\rho_{\rm L}^2$. On the other hand, notice that the numerical coefficients of Eqs. (5), (6) are of the same order of magnitude, which could imply that the separation between the successive "plateaus" of curve 2 depicted in Fig. 2 is related to the separation between levels in Eq. (6). This implication may support what was said before in the sense that the staircase profile of curve 2 shown in Fig. 2 is generated by the passage of the guiding center through the structure of levels of Eq. (6); this item will be given further attention in the following section. Now, it can be seen from curve 2 in Fig. 2 that the width of the steps is $\Delta\theta \approx 1$; also, if one consider that (see text below Eq. (2)) then the associated time interval Δt is consistent with the uncertainty principle for time and energy since $\Delta\theta = \frac{kT}{2\hbar}\Delta t \approx 1$ or $(kT)\Delta t \geq \hbar$, where Δt is the time it takes the mean square of the guiding center radius vector to "traverse" each plateau (level) of curve 2 in Fig. 2.

5. Analysis of Eq. (5)

The aim of this section is to obtain additional information about the nature of Bohm-type diffusion through the handling of Eq. (5). The symmetry of the problem of the motion of the guiding center on the x–y plane with the magnetic field pointing along the positive z-direction permits the writing of a similar equation for the y coordinate of the guiding center location

$$\left|\langle y_0^2\rangle\right| = 2\sqrt{2}\frac{hc}{eB}\theta^2\left|f(\theta)\right|. \tag{9}$$

Therefore, considering Eqs. (5), (9), the expression for the corresponding mean square radius vector of the guiding center position is

$$\left|\langle x_0^2\rangle\right| + \left|\langle y_0^2\rangle\right| = \left|\langle r_0^2\rangle\right| = 4\sqrt{2}\frac{\hbar c}{eB}\theta^2\left|f(\theta)\right|. \tag{10}$$

In the following, the parenthesis part of Eq. (6) and the function $\theta^2|f(\theta)|$ which appears in Eq. (10) will be graphically compared in terms of the generic variable χ, considering that the eigenvalues n may be localized on certain points of the straight line 1 of Fig. 2; on this straight line the value $n = 0$ corresponds to the ordinate $\frac{1}{2}$.

The curves depicted in Fig. 2 are: $f_1(\chi) = \chi + \frac{1}{2}$, $f_2(\chi) = \chi^2|f(\chi)|$, $f_3(\chi) = f_1(\chi) - f_2(\chi)$. Somewhere on the straight line $f_1(\chi)$ there are located the eigenvalues $n = 1, 2, \ldots$; the eigenvalue $n = 0$ corresponds to $\chi = 0$ and represents the "zero-point squared radius vector" of Γ_n^2. However, curve 2 lacks a "zero-point squared radius vector" different from zero because of the quasi--classical origin of Eq. (10), see Ref. [2], Eq. (16). It is observed from Fig. 2 that the general trend of graphs $f_1(\chi)$ and $f_2(\chi)$ is the same and that the curve $f_1(\chi)$ is slightly secant to the knees of the curve $f_2(\chi)$ for small values of χ, whence the curve $f_3(\chi)$ should show small negative values not seen under the scale chosen to draw Fig. 2. For intermediate and high values of χ, $f_1(\chi)$ is tangent to the knees of $f_2(\chi)$.

Continuing the graphical analysis, Fig. 3 shows the following curves drawn in terms of the generic variable χ: $f_1(\chi) = \chi$, $f_2(\chi) = \chi^2|f(\chi)|$, $f_3(\chi) = f_1(\chi) - f_2(\chi)$, $f_4(\chi) = \frac{\rm d}{{\rm d}\chi}[\chi^2|f(\chi)|]$. The straight line $f_1(\chi)$ with slope unity is introduced in Fig. 3 to pinpoint interesting features of curve $f_2(\chi)$. To analyze the curves of Fig. 3, it is convenient to write down the derivative of the function $\theta^2|f(\theta)|$ which appears in Eq. (10):

$$\frac{\rm d}{{\rm d}\theta}\theta^2\left|f(\theta)\right| = \frac{4\theta\sin^2\theta}{\sqrt{2 + 4\theta^2 - 2\cos 2\theta - 4\theta\sin 2\theta}}\,. \tag{11}$$

For $\theta \geq 0$ the zeroes of Eq. (11) are located at $\theta = \lambda\pi$, where $\lambda = 0, 1, 2, \ldots$

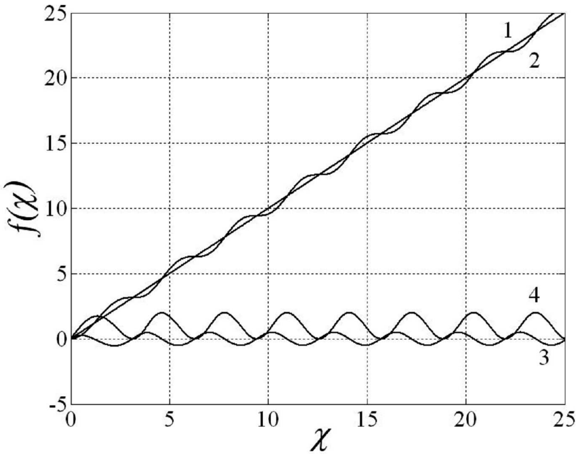

Fig. 3. Curve 3 represents the difference between curves 1 and 2, which are described in the text. Curve 4 represents the derivative of curve 2. Curve 4 never assumes negative values for $\chi \geq 0$. The intersections of curves 1 and 2 at the plateaus occur at the zeroes of curve 4 which are $\chi = \lambda\pi$, where $\lambda = 0, 1, 2, \ldots$.

Several features are noticeable in Fig. 3:

1. The intersections of curves $f_1(\chi)$ and $f_2(\chi)$ at the plateaus occur at the zeroes of curve $f_4(\chi)$ and the zeroes of even order of curve $f_3(\chi)$.

2. In particular the zeroes of $f_4(\chi)$ for $\chi \geq 0$ occur at $\chi = \lambda\pi$, where $\lambda = 0, 1, 2, \ldots$

3. The intersections of curves $f_1(\chi)$ and $f_2(\chi)$ at the successive plateaus are therefore separated by π on the abcissa axis. In fact, considering that straight line 1 has a unity slope, the successive intersections at the plateaus are separated by π in the horizontal and vertical directions.

4. The horizontal and vertical distances from the origin to the intersection on the first plateau are equal to π.

Considering the analysis of Figs. 2, 3 and the above features, the following statements are proposed:

1. The curves $f_2(\chi)$ in Figs. 2, 3, which represent the variable part of Eq. (10) with their structure of equidistant steps, describe the diffusion of the guiding center and its passing through the structure of discrete levels of Eq. (6).

2. These levels are located on the intersection points of curves 1, 2 at the plateaus of curve 2 in Fig. 3. The intersection points at the plateaus are also zeroes of $f_4(\chi)$ and correspond to the values $\chi = \lambda\pi$, where $\lambda = 0, 1, 2, \ldots$

3. Each step is associated with the diffusion of the guiding center through each level of Eq. (6).

4. The points on $f_2(\chi)$ at which $f_4(\chi) = 0$ in Fig. 3 may be enumerated with the eigenvalues $n = 1, 2, \ldots$; the eigenvalue $n = 0$ corresponds to the origin.

5. As a consequence of the above items, the separation between steps of $f_2(\chi)$ should be equal to the separation between levels in Eq. (6).

These statements will be used in the next section.

6. Final form of the expression for Bohm-type diffusion

From the information obtained so far, related to the structure of levels of the expression $\theta^2|f(\theta)|$ and its similarity to the structure of levels of Eq. (6), it is possible to propose a final form for the Bohm-type diffusion expression given by Eq. (10). This proposal is based upon the periodicity of $\theta^2|f(\theta)|$ and its structure of levels, which is similar to that in Eq. (6), in which the separation between successive levels is $2\frac{\hbar c}{eB}$; accordingly, let Eq. (10) be normalized in such a way that the separation between its successive steps be this same quantity. This is achieved by considering the statements of Sect. 5, from which it is deduced that a change of $\Delta\theta = \pi$ corresponds to a change of the same amount in the function $\theta^2|f(\theta)|$, i.e. $\Delta(\theta^2|f(\theta)|) = \pi$, in particular at the points $\lambda\pi$. Therefore, to obtain the corresponding change between successive steps of $2\frac{\hbar c}{eB}$ from Eq. (10) it is necessary to rewrite this as

$$\left|\langle r_0^2\rangle\right| = \frac{2}{\pi}\frac{\hbar c}{eB}\theta^2\left|f(\theta)\right|. \tag{12}$$

This expression represents the trajectory followed by $|\langle r_0^2\rangle|$ as a structure of steps (levels) continuously connected with a separation between them by an amount equal to $2\frac{\hbar c}{eB}$ just as Eq. (6) represents a discrete structure of levels with this same separation between them. Then Eq. (12) serves to describe the diffusion of the guiding center through the levels of $\mathit{\Gamma}_n^2$. Expression (12) for Bohm-type diffusion describes the diffusion of the guiding center on the plane of the Larmor orbit. Notice that electrical perturbations outside the plane of the Larmor orbit will induce, apart from the Bohm-type diffusion on the plane of the Larmor orbit, motions of the guiding center along the z axis (along the magnetic field). These motions, however are not important for diffusion across the magnetic field lines. In this sense, Bohm-type diffusion of the guiding center is a purely two-dimensional phenomenon occurring on the plane of the Larmor orbit. Finally, a Bohm-type diffusion coefficient can be obtained from Eq. (12) for large values of θ (large values of t); indeed, for these values of θ, $|f(\theta)|$ behaves as $\frac{1}{\theta}$ and for $\theta = \frac{kT}{2\hbar}t$ Eq. (12) reduces to

$$\left|\langle r_0^2\rangle\right| = \frac{1}{\pi}\frac{ckT}{eB}t. \tag{13}$$

If the displacement of the guiding center is considered as a two-dimensional random walk on the plane of the Larmor orbit, then the mean square displacement is $\langle r_0^2\rangle = 4Dt$ [6]; therefore Eq. (13) can be written as:

$$4Dt = \frac{1}{\pi}\frac{ckT}{eB}t, \tag{14}$$

or

$$D = \frac{1}{4\pi}\frac{ckT}{eB} = \frac{4}{\pi}D_{\mathrm{B}}, \tag{15}$$

where D_{B} is the Bohm diffusion coefficient $\frac{1}{16}\frac{ckT}{eB}$. On the other hand, for $t \approx \omega_{\mathrm{c}}^{-1}$ Eq. (13) produces $|\langle r_0^2\rangle| \cong \rho_{\mathrm{L}}^2$

which is the step size in the Bohm and Bohm-type diffusion.

7. Concluding remarks

The presence of the staircase profile in the graph of the expression for Bohm-type diffusion in two dimensions was explained in terms of the following idea. As the guiding center diffuses, it passes over the quantized structure of the square of its radius vector in such a way that this structure of equidistant levels manifests itself through the presence of the successive equidistant steps in the staircase profile. A normalized form of the expression that describes two-dimensional Bohm-type diffusion was deduced by taking as a model the expression for the quantized square of the guiding center radius vector.

The separation between successive steps in the graph of the expression for Bohm-type diffusion in two dimensions is the same as the separation between the levels of the quantized square of the guiding center radius vector. The Bohm-type coefficient of diffusion that produces this expression for large values of θ turns out to be $\frac{4}{\pi}$ times the Bohm diffusion coefficient. The results obtained from the work undertaken in this paper support the hypothesis proposed in Ref. [2] that a Bohm-type coefficient of diffusion could be deduced by means of a quantum mechanical approach. Moreover, it should be emphasized that by using the simple model proposed in Ref. [2], the numerical factor in the Bohm-type coefficient of diffusion achieved in the present paper is in close agreement with that in the Bohm coefficient of diffusion.

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References

[1] D. Bohm, E.H.S. Burhop, H.S.W. Massey, R.W. Williams, in: *A Study of the Arc Plasma in the Characteristics of Electrical Discharges in Magnetic Fields*, Eds. A. Guthrie, R.W. Wakerling, 1st ed., McGraw Hill, New York 1949, p. 173.

[2] H. Jiménez-Domínguez, *Acta Phys. Pol. A* **116**, 197 (2009).

[3] F.W. King, University of Wisconsin — Eau Claire `fking@uwec.edu`, private communication.

[4] C. Cohen-Tannoudji, B. Diu, F. Laloë, *Quantum Mechanics*, Vol. 1, Wiley, New York 1977.

[5] N. Rostoker, M.W. Binderbauer, H.J. Monkhorst, *Science* **278**, 1419 (1997).

[6] S. Chandrasekhar, *Rev. Mod. Phys.* **15**, 1 (1943), Eq. (174).