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Product rule for gauge invariant Weyl symbols and its application to the semiclassical description of guiding centre motion

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Abstract. We derive a product rule for gauge invariant Weyl symbols which provides a generalization of the well known Moyal formula to the case of non-vanishing electromagnetic fields. Applying our result to the guiding centre problem we expand the guiding centre Hamiltonian into an asymptotic power series with respect to both Planck's constant \hbar and an adiabaticity parameter already present in the classical theory. This expansion is used to determine the influence of quantum-mechanical effects on guiding centre motion.

1. Introduction

In many physical applications charged particles are exposed to strong time-independent magnetic fields $B(x)$ and additional electrostatic potentials $\phi(x)$. Important examples are the magnetic confinement of plasmas, trapping of ions in accelerator facilities [1] as well as the quantum Hall effect [2]. Classically, the motion in such field configurations may be visualized as a fast rotation in the plane perpendicular to the magnetic field ('gyration'), with the centre of the circular orbit moving slowly parallel to the magnetic field lines and drifting very slowly across both electric and magnetic field lines ('guiding centre motion'). The underlying assumption that clearly distinguishable timescales of motion exist is known as 'guiding centre approximation' or, more generally by, 'adiabatic approximation.'

To separate gyration and guiding centre motion, different kinds of perturbative calculations have been applied in classical mechanics [3–7]. Adiabatic invariants and equations of motion for the guiding centre may be derived in a systematic way from Hamiltonian theory [8–13]. For a semiclassical description of guiding centre motion the method invented by Littlejohn [10, 11] using non-canonical, but gauge invariant phase space coordinates turns out to be the best starting point. There, like in all classical investigations of the guiding centre problem, a dimensionless expansion parameter ϵ is introduced by replacing the electric charge q with q/ϵ [4, 14]. Physically, ϵ represents the ratio of the gyroradius to the scale lengths of the external fields and is interpreted as an adiabatic parameter. Employing symplectic geometrical techniques, relations between the guiding centre (phase space) coordinates and the particle's position and velocity are obtained which take the form of asymptotic power series in ϵ . After writing down the Hamiltonian in terms of the guiding centre coordinates, its dependence on

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the rapidly oscillating gyration angle is removed by means of averaging Lie transforms. The equations of motion resulting from the guiding centre Hamiltonian confirm that the magnetic moment caused by the gyration is an adiabatic invariant.

In low-temperature experiments the total energies of the particles are of order of the lowest Landau levels in the magnetic field $\mathbf{B}(\mathbf{x})$. Therefore, quantum-mechanical effects have to be taken into account when deriving equations of motion for the guiding centre. So far this has been done only in the special case of a charged particle in the magnetic field outside of a rectilinear current filament [15, 16]. To explicitly determine the quantum corrections to guiding centre motion in arbitrary field configurations a method is needed which results in an expansion of the quantized guiding centre Hamiltonian into a formal power series in both the (classical) parameter ϵ and Planck's constant \hbar . The quantum guiding centre theory developed by Maraner in two inspiring papers [17, 18] uses only the magnetic length $l_B = \sqrt{\hbar c / (q|\mathbf{B}|)}$ as expansion parameter. The power series expansion of the guiding centre Hamiltonian operator with respect to l_B does not distinguish between terms of adiabatic origin already present in classical mechanics and quantum corrections caused by the non-commutativity of the operator algebra. For experimental purposes, however, it is very important to know whether the classical picture is valid even at low temperatures or whether quantum effects dominate guiding centre motion.

A first step to answer this question lies in the observation that there is great formal resemblance between guiding centre motion and adiabatic motion of neutral spinning particles in an inhomogeneous magnetic field [19]. The latter has recently been studied in more detail because it represents a standard example for the occurrence of 'geometrical' forces in dynamical systems [20–23]. A semiclassical investigation of this motion [24] involves a multicomponent version of the Weyl calculus [25–27]. It has the appealing feature that two different expansion parameters are used: one, ϵ_a , connected with adiabaticity (i.e. the assumption that the magnetic field does not change appreciably during a precession period) and another, ϵ_s , proportional to \hbar , controlling the validity of the semiclassical approximation. In the diagonalized Hamiltonian, which describes orbital motion, the potential terms are expanded with respect to both ϵ_a and ϵ_s . To achieve the same goal for the guiding centre Hamiltonian, the Wigner–Weyl formalism [28, 29] therefore seems to provide the appropriate tools.

In general, the Weyl transform of a quantum-mechanical operator is a uniquely determined phase space function which may be defined as follows [30–32]: starting from the fundamental operators \hat{x} and \hat{p} , a particular, continuously indexed basis $\hat{\Delta}(\mathbf{x}, \mathbf{p})$ of the operator space is constructed. (Here, as in the following, the hat denotes an operator.) The representation of an arbitrary operator \hat{A} as a linear combination of the operators $\hat{\Delta}(\mathbf{x}, \mathbf{p})$ involves c -number coefficients which are labelled by the continuous variables \mathbf{x} and \mathbf{p} . They constitute a function $A_W(\mathbf{x}, \mathbf{p})$ on phase space which is denoted as the Weyl symbol of the operator \hat{A} . The relation between the symbol $C_W(\mathbf{x}, \mathbf{p})$ associated with an operator product $\hat{C} = \hat{A}\hat{B}$ and the symbols $A_W(\mathbf{x}, \mathbf{p})$ and $B_W(\mathbf{x}, \mathbf{p})$ of its factors is given by a nontrivial composition rule known as the Moyal formula [33].

If a magnetic field $\mathbf{B}(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x})$ is present, however, the Weyl correspondence should be re-defined, because the gauge dependence of the canonical momentum \hat{p} causes the basic operators $\hat{\Delta}(\mathbf{x}, \mathbf{p})$ to be gauge dependent as well. As shown in [34] this leads to the undesirable consequence that the Weyl symbol of a gauge invariant operator becomes gauge dependent and that, vice versa, the operator corresponding to a gauge invariant phase space function is itself in general not gauge independent. The most natural way to include the principle of gauge invariance into the Weyl formalism is to replace the (gauge dependent) canonical momentum \hat{p} appearing in the definition of $\hat{\Delta}(\mathbf{x}, \mathbf{p})$ by the (gauge invariant) kinetic momentum $\hat{k} = m\hat{v} = \hat{p} - (q/c)\hat{A}(\hat{x})$ [34–36]. The coefficient function of an operator \hat{A}

(not to be confused with the vector potential) with respect to the new set of basic operators $\hat{\Delta}(\mathbf{x}, \mathbf{k})$ will be denoted in the following as the gauge invariant Weyl symbol $A_W(\mathbf{x}, \mathbf{k})$ of \hat{A} . One can show that $A_W(\mathbf{x}, \mathbf{k})$ is a gauge invariant phase space function if and only if \hat{A} is gauge invariant (for more details cf [36] and section 2). Obviously, the product rule for gauge invariant Weyl symbols will be different from the usual Moyal formula.

After comparing ordinary and gauge invariant Weyl calculus in a little more detail, we will explicitly derive the gauge invariant generalization of Moyal's formula in the next section and discuss its most important properties. In section 3, the gauge invariant Weyl formalism will be applied to separate the different timescales occurring in the motion of charged particles in external electromagnetic fields within a semiclassical framework. As a result we will expand both guiding centre coordinates and the guiding centre Hamiltonian into asymptotic power series with respect to the adiabatic parameter ϵ and Planck's constant \hbar . Section 4 contains a summary of our results and conclusions concerning the influence of quantum effects on guiding centre motion which can be derived from our expansion of the guiding centre Hamiltonian. Finally, we compare our results to the quantum-mechanical calculations of Maraner. In the appendix, the classical guiding centre theory for the motion of a charged particle in a magnetic field of constant direction and an additional electrostatic field is summarized.

2. Product rule for gauge invariant Weyl symbols

In order to set the stage for our computations, let us briefly review some basic features of the ordinary Weyl transform valid in a six-dimensional flat phase space in the absence of magnetic fields [30–32, 37, 38]. Starting with the set of generating Heisenberg operators

$$\hat{T}(\mathbf{u}, \mathbf{v}) \equiv \exp[i(\mathbf{u} \cdot \hat{\mathbf{p}} + \mathbf{v} \cdot \hat{\mathbf{x}})] \quad (1)$$

we introduce a basis

$$\hat{\Delta}(\mathbf{x}, \mathbf{p}) \equiv \left(\frac{\hbar}{2\pi}\right)^3 \int d^3\mathbf{u} d^3\mathbf{v} \exp[i(\mathbf{u} \cdot \mathbf{p} + \mathbf{v} \cdot \mathbf{x})] \hat{T}(-\mathbf{u}, -\mathbf{v}) \quad (2)$$

of the operator space which is labeled by the continuous classical variables \mathbf{x} and \mathbf{p} . If an operator \hat{A} is written as a linear combination of the $\hat{\Delta}(\mathbf{x}, \mathbf{p})$,

$$\hat{A} = \int \frac{d^3\mathbf{x} d^3\mathbf{p}}{h^3} \hat{\Delta}(\mathbf{x}, \mathbf{p}) A_W(\mathbf{x}, \mathbf{p}) \quad (3)$$

the uniquely determined coefficient function

$$A_W(\mathbf{x}, \mathbf{p}) = \int d^3\mathbf{x}' \langle \mathbf{x}' | \hat{A} \hat{\Delta}(\mathbf{x}, \mathbf{p}) | \mathbf{x}' \rangle \equiv \text{Tr}[\hat{A} \hat{\Delta}(\mathbf{x}, \mathbf{p})] \quad (4)$$

is called the Weyl symbol associated with \hat{A} . Here, as in the following, we leave aside questions of convergence and the mathematical problem of characterizing the class of operators for which expansions like (3) exist.

From equations (1)–(4) and the duplication formula

$$\hat{T}(\mathbf{u}, \mathbf{v}) \hat{T}(\mathbf{u}', \mathbf{v}') = \exp\left[i\frac{\hbar}{2}(\mathbf{u} \cdot \mathbf{v}' - \mathbf{u}' \cdot \mathbf{v})\right] \hat{T}(\mathbf{u} + \mathbf{u}', \mathbf{v} + \mathbf{v}') \quad (5)$$

one can immediately determine the relation between the Weyl symbol $C_W(\mathbf{x}, \mathbf{p})$ of a product operator $\hat{C} = \hat{A}\hat{B}$ and the symbols of its factors. The result is the well known Moyal formula

$$C_W(\mathbf{x}, \mathbf{p}) = \exp\left[\frac{i\hbar}{2} \sum_{i=1}^3 \left(\frac{\partial}{\partial b_i} \frac{\partial}{\partial z_i} - \frac{\partial}{\partial a_i} \frac{\partial}{\partial y_i} \right)\right] A_W(\mathbf{z}, \mathbf{a}) B_W(\mathbf{y}, \mathbf{b}) \Big|_{\substack{y=z=x \\ a=b=p}} \quad (6)$$

where the subscript ‘ i ’ characterizes the Cartesian coordinates of a vector, i.e. 1, 2, 3 stands for x, y, z respectively, and the auxiliary vectors $\mathbf{a}, \mathbf{b}, \mathbf{y}, \mathbf{z}$ specify which of the factors $A_W(\mathbf{x}, \mathbf{p}), B_W(\mathbf{x}, \mathbf{p})$ has to be differentiated with respect to \mathbf{x} and \mathbf{p} . Note that the operator in the exponential is just the ordinary (\mathbf{x}, \mathbf{p}) Poisson bracket operator, so that expanding the right-hand side of (6) with respect to \hbar yields

$$C_W(\mathbf{x}, \mathbf{p}) = A_W(\mathbf{x}, \mathbf{p})B_W(\mathbf{x}, \mathbf{p}) + \frac{i\hbar}{2}\{A_W, B_W\} + \mathcal{O}(\hbar^2). \quad (7)$$

Equation (6) may also be interpreted as defining a bilinear, associative and non-commutative product on the space of symbols,

$$C_W(\mathbf{x}, \mathbf{p}) \equiv A_W(\mathbf{x}, \mathbf{p}) * B_W(\mathbf{x}, \mathbf{p}) \quad (8)$$

denoted as the star product or Weyl product.

Suppose we are given a phase space function of the form

$$f(\mathbf{x}, \mathbf{p}) = x_i^m p_j^n \quad (9)$$

with $m, n \in \mathbb{N}_0$ (= non-negative integers). Evaluating equation (3) we obtain the corresponding operator [39]

$$\hat{f}(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = \frac{1}{2^m} \sum_{l=0}^m \binom{m}{l} \hat{x}_i^l \hat{p}_j^n \hat{x}_i^{m-l}. \quad (10)$$

It can be constructed in the following way. Take \hat{x}_i m times, \hat{p}_j n times, put them in all possible permutations with equal weights and divide by the number of terms. The result is called the totally symmetrized or Weyl ordered product, written as $\text{Symm}(\hat{x}_i^m \hat{p}_j^n)$. Applying the commutation relation $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$ one can bring the \hat{p}_j 's together at various positions of the product with no terms proportional to \hbar remaining. Due to the linearity of the Weyl transform, equations (9) and (10) generalize to any analytic function on phase space.

So far we have used position \mathbf{x} and canonical momentum \mathbf{p} as basic variables. If a magnetic field $\mathbf{B}(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x})$ is switched on, the canonical momentum is no longer completely physical because of its gauge dependence. However, the operator of the kinetic momentum,

$$\hat{\mathbf{k}} \equiv \hat{\mathbf{p}} - \frac{q}{c} \hat{\mathbf{A}}(\hat{\mathbf{x}}) = m\hat{\mathbf{v}} \quad (11)$$

is gauge invariant because its expectation value is not effected by a gauge transformation [40].

If we replace the canonical momentum $\hat{\mathbf{p}}$ in (1) with the kinetic momentum $\hat{\mathbf{k}}$, the operators

$$\hat{T}(\mathbf{u}, \mathbf{v}) \equiv \exp[i(\mathbf{u} \cdot \hat{\mathbf{k}} + \mathbf{v} \cdot \hat{\mathbf{x}})] \quad (12)$$

become gauge invariant and hence the basic operators

$$\hat{\Delta}(\mathbf{x}, \mathbf{k}) \equiv \left(\frac{\hbar}{2\pi}\right)^3 \int d^3\mathbf{u} d^3\mathbf{v} \exp[i(\mathbf{u} \cdot \mathbf{k} + \mathbf{v} \cdot \mathbf{x})] \hat{T}(-\mathbf{u}, -\mathbf{v}) \quad (13)$$

are gauge invariant as well. The Weyl symbol $A_W(\mathbf{x}, \mathbf{k})$ of an operator \hat{A} is now defined with respect to the new basis in the same way as in the field-free case,

$$A_W(\mathbf{x}, \mathbf{k}) = \text{Tr}[\hat{A} \hat{\Delta}(\mathbf{x}, \mathbf{k})] \quad (14)$$

or, equivalently,

$$\hat{A} = \int \frac{d^3\mathbf{x} d^3\mathbf{k}}{h^3} \hat{\Delta}(\mathbf{x}, \mathbf{k}) A_W(\mathbf{x}, \mathbf{k}). \quad (15)$$

From equation (14) and the properties of gauge invariant operators (cf [40]) it is obvious that the Weyl symbol of a gauge invariant operator does not change its value under gauge

transformations. Thus, viewed as a phase space function, the symbol is also gauge invariant. According to equation (15) the opposite is also true: The operator corresponding to a gauge invariant phase space function is itself gauge invariant, i.e. its mean value does not change under gauge transformations.

Writing $A_W(\mathbf{x}, \mathbf{k})$ as a Fourier integral,

$$A_W(\mathbf{x}, \mathbf{k}) = \int d^3\mathbf{u} d^3\mathbf{v} \exp[i(\mathbf{u} \cdot \mathbf{k} + \mathbf{v} \cdot \mathbf{x})] \tilde{A}(\mathbf{u}, \mathbf{v}) \tag{16}$$

one can show by inserting definition (13) into (14) that the Fourier transform $\tilde{A}(\mathbf{u}, \mathbf{v})$ may also be obtained from

$$\tilde{A}(\mathbf{u}, \mathbf{v}) = \left(\frac{\hbar}{2\pi}\right)^3 \text{Tr}[\hat{A}\hat{T}(-\mathbf{u}, -\mathbf{v})]. \tag{17}$$

According to (13), (15), and (16) the operator \hat{A} can similarly be expressed in terms of $\tilde{A}(\mathbf{u}, \mathbf{v})$ via

$$\hat{A} = \int d^3\mathbf{u} d^3\mathbf{v} \tilde{A}(\mathbf{u}, \mathbf{v}) \hat{T}(\mathbf{u}, \mathbf{v}). \tag{18}$$

Equations (12), (16) and (18) are the gauge invariant generalization of Weyl's original correspondence rule [28] for phase space functions and quantum-mechanical operators.

To derive a product rule for gauge invariant Weyl symbols we will have to evaluate matrix elements of the form $\langle \mathbf{x}' | \hat{A} | \mathbf{x} \rangle$. For this purpose it is advantageous to express the operator $\exp(i\mathbf{u} \cdot \hat{\mathbf{k}})$ occurring in $\hat{T}(\mathbf{u}, \mathbf{v})$ by the translation operator $\exp(i\mathbf{u} \cdot \hat{\mathbf{p}})$. As proven in [36], $\exp(i\mathbf{u} \cdot \hat{\mathbf{k}})$ and $\exp(i\mathbf{u} \cdot \hat{\mathbf{p}})$ are related by

$$\begin{aligned} \exp(i\mathbf{u} \cdot \hat{\mathbf{k}}) &= \exp(i\mathbf{u} \cdot \hat{\mathbf{p}}) \exp\left\{-i\frac{q}{c}\mathbf{u} \cdot \int_0^1 \hat{A}(\hat{\mathbf{x}} - \hbar\tau\mathbf{u})d\tau\right\} \\ &= \exp\left\{-i\frac{q}{c}\mathbf{u} \cdot \int_0^1 \hat{A}(\hat{\mathbf{x}} + \hbar\tau\mathbf{u})d\tau\right\} \exp(i\mathbf{u} \cdot \hat{\mathbf{p}}). \end{aligned} \tag{19}$$

Using this equation the properties of the translation operator, and the Baker–Campbell–Hausdorff-type formula

$$\begin{aligned} \hat{T}(\mathbf{u}, \mathbf{v}) &= \exp(-i\mathbf{u} \cdot \mathbf{v}/2) \exp(i\mathbf{u} \cdot \hat{\mathbf{k}}) \exp(i\mathbf{v} \cdot \hat{\mathbf{x}}) \\ &= \exp(i\mathbf{u} \cdot \mathbf{v}/2) \exp(i\mathbf{v} \cdot \hat{\mathbf{x}}) \exp(i\mathbf{u} \cdot \hat{\mathbf{k}}) \end{aligned} \tag{20}$$

a straightforward calculation shows that the product of two gauge invariant \hat{T} operators may be cast into the form

$$\begin{aligned} \hat{T}(\mathbf{u}, \mathbf{v})\hat{T}(\mathbf{u}', \mathbf{v}') &= \exp\left\{i\frac{q}{c}\mathbf{u} \cdot \int_0^1 [\hat{A}(\hat{\mathbf{x}} + \hbar\tau(\mathbf{u} + \mathbf{u}')) - \hat{A}(\hat{\mathbf{x}} + \hbar\tau\mathbf{u})]d\tau\right\} \\ &\quad \times \exp\left\{i\frac{q}{c}\mathbf{u}' \cdot \int_0^1 [\hat{A}(\hat{\mathbf{x}} + \hbar\tau(\mathbf{u} + \mathbf{u}')) - \hat{A}(\hat{\mathbf{x}} + \hbar\tau\mathbf{u} + \hbar\tau\mathbf{u}')]d\tau\right\} \\ &\quad \times \left[i\frac{\hbar}{2}(\mathbf{u} \cdot \mathbf{v}' - \mathbf{u}' \cdot \mathbf{v})\right] \hat{T}(\mathbf{u} + \mathbf{u}', \mathbf{v} + \mathbf{v}') \end{aligned} \tag{21}$$

which reduces to the ordinary duplication formula (5) if the vector potential $\mathbf{A}(\mathbf{x})$ vanishes.

After these preliminary remarks we are ready to determine the Weyl symbol $C_W(\mathbf{x}, \mathbf{k})$ of the operator product $\hat{C} = \hat{A}\hat{B}$ in terms of $A_W(\mathbf{x}, \mathbf{k})$ and $B_W(\mathbf{x}, \mathbf{k})$. From equations (18) and (21) we find that

$$\begin{aligned} \hat{C} = \hat{A}\hat{B} &= \int d^3\mathbf{u} d^3\mathbf{v} d^3\mathbf{U} d^3\mathbf{V} \tilde{A}(\mathbf{u}, \mathbf{v}) \tilde{B}(\mathbf{U} - \mathbf{u}, \mathbf{V} - \mathbf{v}) \\ &\quad \times \exp\left[i\frac{\hbar}{2}(\mathbf{u} \cdot \mathbf{V} - \mathbf{U} \cdot \mathbf{v})\right] \hat{F}(\mathbf{u}, \mathbf{U}; \hat{\mathbf{x}}) \hat{T}(\mathbf{U}, \mathbf{V}) \end{aligned} \tag{22}$$

where we introduced the function

$$\begin{aligned}
 F(\mathbf{u}_1, \mathbf{u}_2; \mathbf{x}) &\equiv \exp \left\{ i \frac{q}{c} \mathbf{u}_1 \cdot \int_0^1 [\mathbf{A}(\mathbf{x} + \hbar(1-\tau)\mathbf{u}_1 + \hbar\tau\mathbf{u}_2) - \mathbf{A}(\mathbf{x} + \hbar\tau\mathbf{u}_1)] d\tau \right. \\
 &\quad \left. - i \frac{q}{c} \mathbf{u}_2 \cdot \int_0^1 [\mathbf{A}(\mathbf{x} + \hbar(1-\tau)\mathbf{u}_1 + \hbar\tau\mathbf{u}_2) - \mathbf{A}(\mathbf{x} + \hbar\tau\mathbf{u}_2)] d\tau \right\} \\
 &\equiv \exp \left[i \frac{q}{c} f(\mathbf{u}_1, \mathbf{u}_2; \mathbf{x}) \right] \tag{23}
 \end{aligned}$$

which is equal to unity in the field-free case $\mathbf{A}(\mathbf{x}) \equiv 0$. Note that in (22) F depends on the position operator $\hat{\mathbf{x}}$ and hence is itself an operator.

Inserting (22) into (17) and making use of (19), (20) and the completeness of the position eigenstates $|\mathbf{x}\rangle$ yields the Fourier transform of $C_W(\mathbf{x}, \mathbf{k})$,

$$\begin{aligned}
 \tilde{C}(\mathbf{u}, \mathbf{v}) &= \left(\frac{\hbar}{2\pi} \right)^3 \int d^3\mathbf{x} d^3\mathbf{u}' d^3\mathbf{v}' d^3\mathbf{V} \tilde{A}(\mathbf{u}', \mathbf{v}') \tilde{B}(\mathbf{u} - \mathbf{u}', \mathbf{V} - \mathbf{v}') \\
 &\quad \times \exp[i(\mathbf{V} - \mathbf{v}) \cdot \mathbf{x}] \exp \left\{ i \frac{\hbar}{2} [(\mathbf{u} + \mathbf{u}') \cdot \mathbf{V} - \mathbf{u} \cdot (\mathbf{v} + \mathbf{v}')] \right\} F(\mathbf{u}', \mathbf{u}; \mathbf{x}) \tag{24}
 \end{aligned}$$

so that as an intermediate result the Weyl symbol of \hat{C} reads

$$\begin{aligned}
 C_W(\mathbf{x}, \mathbf{k}) &= \int d^3\mathbf{u}' d^3\mathbf{v}' d^3\mathbf{u}'' d^3\mathbf{v}'' \tilde{A}(\mathbf{u}', \mathbf{v}') \tilde{B}(\mathbf{u}'', \mathbf{v}'') \exp \left[i \frac{\hbar}{2} (\mathbf{u}' \cdot \mathbf{v}'' - \mathbf{u}'' \cdot \mathbf{v}') \right] \\
 &\quad \times F \left(\mathbf{u}', \mathbf{u}' + \mathbf{u}''; \mathbf{x} - \frac{\hbar}{2} (\mathbf{u}' + \mathbf{u}'') \right) \exp \{ i [(\mathbf{v}' + \mathbf{v}'') \cdot \mathbf{x} + (\mathbf{u}' + \mathbf{u}'') \cdot \mathbf{k}] \} \tag{25}
 \end{aligned}$$

where $\mathbf{u}'' \equiv \mathbf{u} - \mathbf{u}'$, $\mathbf{v}'' \equiv \mathbf{V} - \mathbf{v}'$. As a next step we want to express the right-hand side of (25) in terms of $A_W(\mathbf{x}, \mathbf{k})$, $B_W(\mathbf{x}, \mathbf{k})$ and their derivatives with respect to \mathbf{x} and \mathbf{k} . A helpful observation is that by setting $\mathbf{A}(\mathbf{x}) \equiv 0$ the above equation reduces to the one appearing in the derivation of the ordinary product rule [30].

To employ a comparable algorithm in the case of a non-zero vector potential we have to extract \mathbf{u}' and \mathbf{u}'' from the integrals in $F(\mathbf{u}', \mathbf{u}' + \mathbf{u}''; \mathbf{x} - \hbar(\mathbf{u}' + \mathbf{u}'')/2)$. For this purpose the vector potentials occurring in the exponent of (23) are expanded into Taylor series around the position \mathbf{x} . After evaluating the integrals and carrying out some additional algebraic manipulations we obtain

$$\begin{aligned}
 f(\mathbf{u}', \mathbf{u}' + \mathbf{u}''; \mathbf{x} - \hbar(\mathbf{u}' + \mathbf{u}'')/2) &= \sum_{n=1}^{\infty} \frac{\hbar^n}{n!} \left(-\frac{1}{2} \right)^{n+1} \frac{1}{(n+1)^2} \sum_{\substack{r,j,l \\ i_1, \dots, i_{n-1}=1}}^3 \epsilon_{jlr} \frac{\partial^{n-1} B_r}{\partial x_{i_1} \dots \partial x_{i_{n-1}}} u'_j u''_l \sum_{k=1}^n \binom{n+1}{k} \\
 &\quad \times [(1 - (-1)^k)(n+1) - (1 - (-1)^{n+1})k] u'_{i_1} \dots u'_{i_{k-1}} u''_{i_k} \dots u''_{i_{n-1}} \tag{26}
 \end{aligned}$$

where ϵ_{jlr} denotes the totally antisymmetric tensor in three dimensions.

The most important result of the preceding calculation is that the expansion of f includes only derivatives of the magnetic field $\mathbf{B}(\mathbf{x})$. Physically this was to be expected because the product of two gauge invariant symbols is itself gauge invariant. Therefore the integrand on the right-hand side of (25) must not depend on the chosen gauge. As all other factors satisfy this condition, the function $F(\mathbf{u}', \mathbf{u}' + \mathbf{u}''; \mathbf{x} - \hbar(\mathbf{u}' + \mathbf{u}'')/2)$ has to be gauge invariant as well. This is certainly true if it is a functional of the magnetic field.

Now we continue just like in the field-free case. Writing

$$\exp \{ i [(\mathbf{v}' + \mathbf{v}'') \cdot \mathbf{x} + (\mathbf{u}' + \mathbf{u}'') \cdot \mathbf{k}] \} = \exp \{ i (\mathbf{v}' \cdot \mathbf{z} + \mathbf{u}' \cdot \mathbf{a}) \} \exp \{ i (\mathbf{v}'' \cdot \mathbf{y} + \mathbf{u}'' \cdot \mathbf{b}) \} \Big|_{\substack{\mathbf{y}=\mathbf{z}=\mathbf{x} \\ \mathbf{a}=\mathbf{b}=\mathbf{k}}} \tag{27}$$

we may generate the variables u'_i, u''_i, v'_i, v''_i occurring in an analytic function which is multiplied to the right by this exponential by differentiating the latter with respect to the auxiliary variables a_i, b_i, y_i, z_i . This is formally equivalent to substituting

$$u'_i \rightarrow -i \frac{\partial}{\partial a_i} \quad u''_i \rightarrow -i \frac{\partial}{\partial b_i} \quad v'_i \rightarrow -i \frac{\partial}{\partial z_i} \quad v''_i \rightarrow -i \frac{\partial}{\partial y_i} \quad (28)$$

in the analytic function. Hence, if we introduce gauge invariant operators

$$\mathcal{L} \equiv \frac{1}{2} \sum_{i=1}^3 \frac{\partial}{\partial a_i} \frac{\partial}{\partial y_i} - \frac{\partial}{\partial b_i} \frac{\partial}{\partial z_i} \quad (29)$$

$$\begin{aligned} \mathcal{L}_n \equiv & \left(\frac{i}{2}\right)^{n+1} \frac{1}{(n+1)^2 n!} \sum_{\substack{r,j,l \\ i_1, \dots, i_{n-1}=1}}^3 \epsilon_{jlr} \frac{\partial^{n-1} B_r}{\partial x_{i_1} \dots \partial x_{i_{n-1}}} \frac{\partial}{\partial a_j} \frac{\partial}{\partial b_l} \sum_{k=1}^n \binom{n+1}{k} \\ & \times [(1 - (-1)^k)(n+1) - (1 - (-1)^{n+1})k] \frac{\partial}{\partial a_{i_1}} \dots \frac{\partial}{\partial a_{i_{k-1}}} \frac{\partial}{\partial b_{i_k}} \dots \frac{\partial}{\partial b_{i_{n-1}}} \quad (30) \end{aligned}$$

$n \in \mathbb{N}$, and leave aside questions of convergence, we may write

$$\begin{aligned} & \exp[i\hbar(\mathbf{u}' \cdot \mathbf{v}'' - \mathbf{u}'' \cdot \mathbf{v}')/2] \exp\{i[(\mathbf{v}' + \mathbf{v}'') \cdot \mathbf{x} + (\mathbf{u}' + \mathbf{u}'') \cdot \mathbf{k}]\} \\ & = \exp[-i\hbar\mathcal{L}] \exp[i(\mathbf{v}' \cdot \mathbf{z} + \mathbf{u}' \cdot \mathbf{a})] \exp[i(\mathbf{v}'' \cdot \mathbf{y} + \mathbf{u}'' \cdot \mathbf{b})] \Big|_{\substack{y=z=x \\ a=b=k}} \quad (31) \end{aligned}$$

and

$$\begin{aligned} & F(\mathbf{u}', \mathbf{u}' + \mathbf{u}''; \mathbf{x} - \hbar(\mathbf{u}' + \mathbf{u}'')/2) \exp\{i[(\mathbf{v}' + \mathbf{v}'') \cdot \mathbf{x} + (\mathbf{u}' + \mathbf{u}'') \cdot \mathbf{k}]\} \\ & = \exp\left[-i\frac{q}{c} \sum_{n=1}^{\infty} \hbar^n \mathcal{L}_n\right] \exp[i(\mathbf{v}' \cdot \mathbf{z} + \mathbf{u}' \cdot \mathbf{a})] \exp[i(\mathbf{v}'' \cdot \mathbf{y} + \mathbf{u}'' \cdot \mathbf{b})] \Big|_{\substack{y=z=x \\ a=b=k}}. \quad (32) \end{aligned}$$

All operators \mathcal{L} and \mathcal{L}_n , $n \in \mathbb{N}$, commute with one another because they contain a_i, b_i, y_i, z_i only as differentiating variables (the magnetic field $B(\mathbf{x})$ and its derivatives occurring in \mathcal{L}_n depend on the position \mathbf{x} and are hence not effected by a differentiation with respect to these variables). Therefore, the integrand in (25) can be generated by the action of the operator

$$\mathcal{P} \equiv \exp\left[-i\hbar\mathcal{L} - i(q/c) \sum_{n=1}^{\infty} \hbar^n \mathcal{L}_n\right] \quad (33)$$

on $\exp[i(\mathbf{v}' \cdot \mathbf{z} + \mathbf{u}' \cdot \mathbf{a})] \exp[i(\mathbf{v}'' \cdot \mathbf{y} + \mathbf{u}'' \cdot \mathbf{b})] \Big|_{\substack{y=z=x \\ a=b=k}}$. Taking the total differential operator outside of the integral (25) we finally obtain

$$C_W(\mathbf{x}, \mathbf{k}) = \exp\left[-i\hbar\mathcal{L} - i\frac{q}{c} \sum_{n=1}^{\infty} \hbar^n \mathcal{L}_n\right] A_W(\mathbf{z}, \mathbf{a}) B_W(\mathbf{y}, \mathbf{b}) \Big|_{\substack{y=z=x \\ a=b=k}} \equiv [A_W * B_W](\mathbf{x}, \mathbf{k}) \quad (34)$$

which is the generalization of Moyal's formula to gauge invariant Weyl symbols. As in the case of the ordinary Weyl transform one can show that the star product defined (34) is bilinear and associative.

Before turning to the semiclassical analysis of guiding centre motion, let us investigate equation (34) in more detail. Expanding the exponential operator \mathcal{P} into a power series with respect to \hbar yields

$$\begin{aligned} \mathcal{P} = & 1 - i\hbar \left(\mathcal{L} + \frac{q}{c} \mathcal{L}_1\right) - \hbar^2 \left[\frac{1}{2} \left(\mathcal{L} + \frac{q}{c} \mathcal{L}_1\right)^2 + i\frac{q}{c} \mathcal{L}_2\right] \\ & + i\hbar^3 \left[\frac{1}{6} \left(\mathcal{L} + \frac{q}{c} \mathcal{L}_1\right)^3 + i\frac{q}{c} \left(\mathcal{L} + \frac{q}{c} \mathcal{L}_1\right) \mathcal{L}_2 - \frac{q}{c} \mathcal{L}_3\right] + \mathcal{O}(\hbar^4). \quad (35) \end{aligned}$$

The second term on the right-hand side of (35) is equal to $i\hbar/2$ times the (\mathbf{x}, \mathbf{p}) Poisson bracket operator. This is seen most easily by expressing the Poisson bracket of two arbitrary phase space functions in terms of \mathbf{x} - and \mathbf{k} -derivatives,

$$\{f, g\} = \sum_{i=1}^3 \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial k_i} - \frac{\partial f}{\partial k_i} \frac{\partial g}{\partial x_i} + \frac{q}{c} \sum_{j,l,r=1}^3 \epsilon_{jlr} \frac{\partial f}{\partial k_j} \frac{\partial g}{\partial k_l} B_r. \quad (36)$$

A comparison of (7) and (35) shows that the first-order terms of both expansions coincide. However, the higher order terms in (7) turn out to be gauge dependent and hence differ from those in (35).

Using their definitions (29), (30), one can derive the following symmetry properties of the operators $\mathcal{L}, \mathcal{L}_n$,

$$\mathcal{L}^m(B_W, A_W) = (-1)^m \mathcal{L}^m(A_W, B_W) \quad (37)$$

$$\mathcal{L}_n^m(B_W, A_W) = (-1)^{nm} \mathcal{L}_n^m(A_W, B_W) \quad m \in \mathbb{N} \quad (38)$$

which cause the star product to be non-commutative. The difference

$$A_W * B_W - B_W * A_W \equiv [A_W, B_W]_M \quad (39)$$

is called the Moyal bracket of A_W and B_W . According to (35) it may be expanded into

$$[A_W, B_W]_M \equiv \mathcal{M}(A_W B_W) = \left\{ -2i\hbar \left(\mathcal{L} + \frac{q}{c} \mathcal{L}_1 \right) + 2i\hbar^3 \left[\frac{1}{6} \left(\mathcal{L} + \frac{q}{c} \mathcal{L}_1 \right)^3 + i \frac{q}{c} \left(\mathcal{L} + \frac{q}{c} \mathcal{L}_1 \right) \mathcal{L}_2 - \frac{q}{c} \mathcal{L}_3 \right] + \mathcal{O}(\hbar^5) \right\} A_W B_W \quad (40)$$

where the leading order term is just $i\hbar\{A_W, B_W\}$. In contrast to the ordinary Weyl calculus the gauge invariant Moyal bracket operator \mathcal{M} cannot be written in closed form.

Finally one can prove from (34) by induction that the Weyl symbol of the operator

$$\hat{A} = \text{Symm}(\hat{k}_{i_1} \hat{k}_{i_2} \dots \hat{k}_{i_n}) \quad i_j \in \{1, 2, 3\}, \quad 1 \leq j \leq n \quad (41)$$

is given by

$$A_W = k_1^{n_1} k_2^{n_2} k_3^{n_3} \quad n_1 + n_2 + n_3 = n \quad (42)$$

if \hat{k}_i , $1 \leq i \leq 3$, appears n_i times in the operator product $\hat{k}_{i_1} \hat{k}_{i_2} \dots \hat{k}_{i_n}$. The relation above is a direct consequence of the non-commutativity of the Cartesian components of $\hat{\mathbf{k}}$. In general, if $f(\mathbf{x})$ is an analytic function of \mathbf{x} , the operator related to

$$A_W = f(\mathbf{x}) k_1^{n_1} k_2^{n_2} k_3^{n_3} \quad (43)$$

reads

$$\hat{A} \equiv \text{Symm}_{\{\hat{k}_{i_j}\}} \left(\frac{1}{2} \sum_{l=0}^n \binom{n}{l} \hat{k}_{i_1} \hat{k}_{i_2} \dots \hat{k}_{i_{n-l}} \hat{f}(\hat{\mathbf{x}}) \hat{k}_{i_{n-l+1}} \dots \hat{k}_{i_n} \right) \quad (44)$$

where $n = n_1 + n_2 + n_3$ and $\text{Symm}_{\{\hat{k}_{i_j}\}}$ denotes symmetrization with respect to the operators \hat{k}_{i_j} .

3. Semiclassical description of guiding centre motion

We will now apply the gauge invariant Weyl formalism to describe the motion of a charged particle of mass m in a strong time-independent magnetic field $\mathbf{B}(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x})$ and an additional electrostatic field $\mathbf{E}(\mathbf{x}) = -\nabla\phi(\mathbf{x})$ semiclassically. The influence of the latter has not been taken into account in quantum-mechanical calculations [17, 18] so far. Assuming that

the guiding centre approximation is valid, we are in particular interested in the lowest-order quantum-mechanical correction to the guiding centre Hamiltonian.

To incorporate the guiding centre approximation into our theory, we follow the classical calculations and introduce an adiabatic parameter ϵ by replacing the electric charge q of the particle by q/ϵ [10, 11],

$$q \rightarrow \frac{q}{\epsilon}. \tag{45}$$

Physical results are recovered at the end of our calculation by setting $\epsilon = 1$. In the guiding centre approximation we are speaking of the order of an expression in terms of its behaviour as $\epsilon \rightarrow 0$. The physical meaning and mathematical details of this limit are discussed in greater detail in [4, 14]. We adopt the convention that the particle variables x and v as well as the fields A and B are held constant in this limiting process, i.e. are independent of ϵ . Since the guiding centre approximation breaks down when the component E_{\parallel} of the electric field parallel to B is of the same magnitude as $|B|$, we take $E_{\parallel} = \mathcal{O}(\epsilon)$ [11].

For reasons of notational convenience we will further on suppress the constants q, m, c , which is equivalent to the following scaling of physical quantities,

$$\begin{aligned} x &\rightarrow \frac{1}{\sqrt{m}}x & p &\rightarrow \sqrt{m}p & v &\rightarrow \frac{1}{\sqrt{m}}v \\ \Phi &\rightarrow \frac{1}{q}\Phi & A &\rightarrow \frac{\sqrt{m}c}{q}A & B &\rightarrow \frac{mc}{q}B & E &\rightarrow \frac{\sqrt{m}}{q}E. \end{aligned} \tag{46}$$

The corresponding backward transformations restore the correct physical units in our results. Note that with respect to this scaling particle velocity and kinetic momentum are equal.

Due to the foregoing conventions, the operator \mathcal{P} introduced in (34) takes the form

$$\tilde{\mathcal{P}} \equiv \exp \left[-i\hbar\tilde{\mathcal{L}} - \frac{i}{\epsilon} \sum_{n=1}^{\infty} \hbar^n \tilde{\mathcal{L}}_n \right] \tag{47}$$

where $\tilde{\mathcal{L}}, \tilde{\mathcal{L}}_n$ denote the scaled versions of $\mathcal{L}, \mathcal{L}_n$. Since each of the operators $\tilde{\mathcal{L}}_n$ has ϵ^{-1} attached to it, a simple reasoning shows that the term proportional to \hbar^n in the corresponding expansion of $\tilde{\mathcal{P}}$ includes terms of all orders in ϵ^{-1} from 0 to n . Therefore, we may formally write

$$\tilde{\mathcal{P}} \equiv \sum_{n=0}^{\infty} \hbar^n \mathcal{P}_n \equiv \sum_{n=0}^{\infty} \sum_{m=-n}^0 \hbar^n \epsilon^m \mathcal{P}_{n,m}. \tag{48}$$

The operators $\mathcal{P}_{n,m}$ contain derivatives of order $n - |m|$ with respect to the position variables y, z and derivatives of order $n + |m|$ with respect to the kinetic momentum (= velocity) variables a, b . As a consequence of the symmetry properties of $\tilde{\mathcal{L}}, \tilde{\mathcal{L}}_n$ no terms of even power in \hbar occur in the expansion of the (scaled) Moyal bracket operator $\tilde{\mathcal{M}}$,

$$\tilde{\mathcal{M}} = 2 \sum_{n=0}^{\infty} \hbar^{2n+1} \mathcal{P}_{2n+1} = 2 \sum_{n=0}^{\infty} \sum_{m=-(2n+1)}^0 \hbar^{2n+1} \epsilon^m \mathcal{P}_{2n+1,m}. \tag{49}$$

Suppose now we are given symbols of the form

$$A_W = \sum_{n=0}^{\infty} \hbar^n A_n = \sum_{m,n=0}^{\infty} \hbar^n \epsilon^m A_{n,m} \quad B_W = \sum_{n=0}^{\infty} \hbar^n B_n = \sum_{m,n=0}^{\infty} \hbar^n \epsilon^m B_{n,m} \tag{50}$$

with the coefficients being analytical functions of x and k . From (48) and (50) we obtain the following expansion for the star product of A_W and B_W ,

$$A_W * B_W = \sum_{n=0}^{\infty} \sum_{i=0}^n \sum_{m=-i}^{\infty} \sum_{l=m}^{m+i} \hbar^n \epsilon^m \mathcal{P}_{i,m-l} \sum_{r=0}^{n-i} \sum_{s=0}^l A_{r,s} B_{n-i-r,l-s}. \tag{51}$$

A similar calculation yields for the Moyal bracket of A_W and B_W

$$\begin{aligned} [A_W, B_W]_M &= \sum_{n=0}^{\infty} \hbar^n \left[\sum_{m=0}^n [1 - (-1)^m] \mathcal{P}_m \left(\sum_{l=0}^{n-m} A_l B_{n-m-l} \right) \right] \\ &= \sum_{n=0}^{\infty} \sum_{i=0}^n \sum_{m=-i}^{\infty} \sum_{l=m}^{m+i} \hbar^n \epsilon^m [1 - (-1)^i] \mathcal{P}_{i,m-l} \sum_{r=0}^{n-i} \sum_{s=0}^l A_{r,s} B_{n-i-r,l-s}. \end{aligned} \quad (52)$$

Let us now determine the symbols of both guiding centre coordinates and the guiding centre Hamiltonian. The basic features of our method become most transparent if the direction of the magnetic field is held constant with the electric field being perpendicular to it. In addition, this case is notationally easier to handle than the more general one in which the directions of both fields are varying arbitrarily. Therefore, we will consider in the following a charged particle in a magnetic field $\mathbf{B} = B(x, y)\mathbf{e}_z$ and electrostatic potential $\phi(x, y)$ neglecting its motion parallel to \mathbf{B} . This kind of planar motion in a strong two-dimensional magnetic field (i.e. of constant direction) is intensively studied in the context of the quantum Hall effect [2]. There, the electric field is weak compared with \mathbf{B} , which in our scaling is equivalent to assuming that \mathbf{E} is of order ϵ , $\mathbf{E} = \mathcal{O}(\epsilon)$. Classically, this means that the $\mathbf{E} \times \mathbf{B}$ drift is of the same order of magnitude as the ∇B drift [7]. Using scaled velocity operators $\hat{v}_i = \hat{p}_i - \epsilon^{-1} A_i = \hat{k}_i$, $i = 1, 2$, the Hamiltonian in such a field configuration reads

$$\hat{H} = \frac{1}{2} (\hat{v}_x^2 + \hat{v}_y^2) + \hat{\phi}(\hat{x}, \hat{y}). \quad (53)$$

Its Weyl symbol is obtained by replacing operators with their corresponding phase space functions, taking into account that the symbol of $\hat{v}_i^2 = \hat{v}_i \hat{v}_i$ is equal to $v_i * v_i$,

$$H_W = \frac{1}{2} (v_x * v_x + v_y * v_y) + \phi(x, y). \quad (54)$$

In the special case of a homogeneous magnetic field $\mathbf{B} = B\mathbf{e}_z$, it is well known that the operators

$$\hat{V}_x = B^{-1/2} \hat{v}_x \quad \hat{V}_y = B^{-1/2} \hat{v}_y \quad (55)$$

are canonically conjugate and the Hamiltonian has the form of a one-dimensional harmonic oscillator. Physically, \hat{V}_x and \hat{V}_y describe the gyration around the magnetic field lines. To get a complete set of conjugate operators including \hat{V}_x and \hat{V}_y , one has to replace the particle coordinates with the operators

$$\hat{X} = \hat{x} + \epsilon B^{-1} \hat{v}_y \quad \hat{Y} = \hat{y} - \epsilon B^{-1} \hat{v}_x \quad (56)$$

of the guiding centre position. In equations (55) and (56) questions of ordering need not be taken into consideration because B is a real valued constant. The non-vanishing commutators of $\hat{X}, \hat{Y}, \hat{V}_x, \hat{V}_y$ are

$$[\hat{V}_x, \hat{V}_y] = i \frac{\hbar}{\epsilon} \quad [\hat{X}, \hat{Y}] = i \frac{\hbar \epsilon}{B}. \quad (57)$$

The Weyl symbols of these operators are obtained by replacing $\hat{x}, \hat{y}, \hat{v}_x, \hat{v}_y$ in (55) and (56) with the corresponding phase space functions. We denote them as guiding centre symbols and—leaving away the subscript ‘W’—write X, Y, V_x, V_y or \mathbf{X}, \mathbf{V} for them. Their Moyal brackets resemble the commutators (57) of the related operators.

Generalizing the results for the homogeneous field to the case of an arbitrary two-dimensional magnetic field we are looking for a set of symbols (X, Y, V_x, V_y) whose non-vanishing Moyal brackets are given by

$$[V_x, V_y]_M = i \frac{\hbar}{\epsilon} \quad [X, Y]_M = i \frac{\hbar \epsilon}{B(X, Y)}. \quad (58)$$

Their different orders with respect to ϵ indicate the different timescales of motion. They are separated because the symbols X, Y of the guiding centre position commute with those of the gyration velocity V_x, V_y . The latter are again conjugate to one another.

Concerning the Moyal bracket of the guiding centre position components X and Y two remarks are necessary. First, the symbol $B(X, Y)$ specifies the strength of the magnetic field at the position of the guiding centre. The corresponding operator is uniquely determined if X and Y are expressed in terms of the particle coordinates x, y, v_x, v_y and the correspondence rule (43), (44) for arbitrary Weyl symbols and their operators is applied. Second, one could think of replacing X, Y with Euler potentials $x^1(X, Y), x^2(X, Y)$ [41], thus obtaining a set of conjugate variables to describe guiding centre motion. However, Euler potentials are non-physical in the same sense as the vector potential \mathbf{A} is. Moreover, in a three-dimensional magnetic field we get four non-canonical guiding centre coordinates instead of X and Y [11]. To transform them into two pairs of canonically conjugate variables one has to find functions which are less familiar than Euler potentials and much more difficult to construct. Therefore we will keep using non-canonical coordinates X, Y to specify the position of the guiding centre.

From classical guiding centre theory [10] it is well known that (X, Y, V_x, V_y) can be chosen in such a way that $J \equiv V_x^2 + V_y^2$ is a constant of motion which may be interpreted as the generalized magnetic moment of gyration. As a direct consequence of the relations (58) the guiding centre Hamiltonian must therefore depend on V_x, V_y only by means of J and its powers. Accordingly, to find an appropriate set of guiding centre symbols we have to proceed as follows. First we determine symbols X, Y, V_x, V_y satisfying (58). Next we express the particle phase space coordinates (x, y, v_x, v_y) in terms of them and insert our result into the Hamiltonian (54). If the latter contains V_x, V_y in other combinations than J we have to transform to a new set of averaged guiding centre symbols (\bar{X}, \bar{V}) satisfying the same Moyal bracket relations, but H_W depending on the gyration velocities only via $\bar{V}_x * \bar{V}_x + \bar{V}_y * \bar{V}_y$. This symbol transformation is an analogue of the near-identity Lie transform carried out in the classical calculation [10, 11].

To begin with, let us analyse the Moyal bracket relations (58) in more detail. Assuming that the guiding centre symbols can be expanded into power series with respect to \hbar and ϵ as specified in (50), the Moyal brackets take the form (52) with almost all coefficients vanishing. Only those of $\hbar\epsilon^{-1}$ and $\hbar\epsilon$ are different from zero if $A = V_x, B = V_y$ and $A = X, B = Y$, respectively. As stated earlier, the \hbar -term of the Moyal bracket $[A_W, B_W]_M$ is proportional to the Poisson bracket of A_0 and B_0 . Therefore, the zero-order terms (with respect to \hbar) of the guiding centre symbols satisfy the Poisson bracket relations of classical guiding centre theory. Hence we identify them with the classical guiding centre coordinates, in agreement with the fact that in the limit $\hbar \rightarrow 0$ Weyl symbols become classical functions [37]. As we will refer to them frequently in the remainder of this section, the results of the classical guiding centre theory in a two-dimensional magnetic field (using Cartesian coordinates) are briefly summarized in the appendix.

Concerning higher-order terms of the \hbar -expansion of the guiding centre symbols one can show that

$$A_{2n+1} = 0 \quad B_{2n+1} = 0 \quad n \in \mathbb{N}_0 \quad (59)$$

which means that only even powers in \hbar occur. In addition, one can prove that the coefficients $A_{2n,i}$ are zero for $0 \leq i \leq 2n - 1$. For $i \geq 2n$ they turn out to be homogeneous polynomials of degree $i - 2n + 1$ (with respect to the particle velocity components) for the components of \mathbf{V} and of degree $i - 2n$ for the components of \mathbf{X} . Hence, the expansions of the guiding centre

symbols with respect to \hbar and ϵ take the form

$$V_i = \sum_{m,n=0}^{\infty} \hbar^{2n} \epsilon^{2n+m} \sum_{\substack{k_1+k_2 \\ =m+1}} v_x^{k_1} v_y^{k_2} V_i^{(k_1,k_2)}(x, y) \quad (60)$$

$$X_i = \sum_{m,n=0}^{\infty} \hbar^{2n} \epsilon^{2n+m} \sum_{\substack{k_1+k_2 \\ =m}} v_x^{k_1} v_y^{k_2} X_i^{(k_1,k_2)}(x, y) \quad (61)$$

where $i = 1, 2$ denotes the Cartesian components of \mathbf{V} and \mathbf{X} . The coefficient functions $V_i^{(k_1,k_2)}(x, y)$, $X_i^{(k_1,k_2)}(x, y)$ in (60), (61) are functionals of the electric and magnetic fields and thus gauge invariant.

To express the Hamiltonian (54) in terms of the guiding centre symbols we have to find the corresponding backward transformations. Formally they are given by

$$v_i = \sum_{m,n=0}^{\infty} \hbar^{2n} \epsilon^{2n+m} \sum_{\substack{k_1+k_2 \\ =m+1}} V_x^{k_1} V_y^{k_2} v_i^{(k_1,k_2)}(X, Y) \quad (62)$$

$$x_i = \sum_{m,n=0}^{\infty} \hbar^{2n} \epsilon^{2n+m} \sum_{\substack{k_1+k_2 \\ =m}} V_x^{k_1} V_y^{k_2} x_i^{(k_1,k_2)}(X, Y). \quad (63)$$

Again, the coefficient functions $v_i^{(k_1,k_2)}(X, Y)$, $x_i^{(k_1,k_2)}(X, Y)$ are gauge independent.

The products of symbols in (60)–(63) are defined point-wise. To derive corresponding relations between the particle operators \hat{x} , \hat{v} and the guiding centre operators \hat{X} , \hat{V} from (60)–(63), we have to introduce the star product on the right-hand side of these equations. In (60) and (61) this is simply done by making use of the correspondence rule (43),(44). In the case of the backward transformations (62), (63) we have to ‘translate’ the classical result (A7)–(A10) given in the appendix into operator ‘language’ to obtain the lowest-order term with respect to \hbar . It will turn out that this is enough to determine the lowest-order quantum-mechanical correction to the guiding centre Hamiltonian.

To this end we first conclude from equation (48) that for any two symbols A_W , B_W their point-wise product and star product differ by $\sum_{n=1}^{\infty} \hbar^n \mathcal{P}_n(A_W, B_W)$. Since the Moyal brackets of the components (X, Y) of the guiding centre position and the gyration velocity (V_x, V_y) vanish, we have for two arbitrary functions $f(X, Y)$ and $g(V_x, V_y)$

$$f(X, Y) * g(V_x, V_y) = g(V_x, V_y) * f(X, Y). \quad (64)$$

As an example,

$$B^{1/2}(X, Y) * V_x = V_x * B^{1/2}(X, Y) = B^{1/2}(X, Y) V_x + \hbar^2 \mathcal{P}_2(B^{1/2}, V_x) + \mathcal{O}(\hbar^4) \quad (65)$$

with $\mathcal{P}_2(B^{1/2}, V_x)$ being of order ϵ , so that the difference between $B^{1/2} V_x$ and $B^{1/2} * V_x$ is of order $\hbar^2 \epsilon$.

The fact that the symbols x , y , v_x , v_y represent self-adjoint operators leads directly to the substitutions

$$V_x V_y \rightarrow \frac{1}{2}(V_x * V_y + V_y * V_x) \quad V_x^2 V_y \rightarrow V_x * V_y * V_x \quad V_y^2 V_x \rightarrow V_y * V_x * V_y \quad (66)$$

in equations (A7)–(A10), because the symbols on the right-hand side of (66) correspond to self-adjoint operators. Further computations show that the replacement of the point-wise product with the star product in equations (A7)–(A10) leads to corrections which are at least of order $\hbar^2 \epsilon$ or $\hbar \epsilon^2$. Therefore, up to terms of order ϵ^2 the relations between the particle operators (symbols) and the guiding centre operators (symbols) formally coincide with the classical result (A7)–(A10), if the point-wise product is replaced by the star product and the

substitution rules (66) for products of gyration velocities are taken into account. For this reason we refrain from writing them down explicitly and refer the interested reader to the appendix.

Next, we insert the results for v_x, v_y into the Hamiltonian (54) and expand the potential $\phi(x, y)$ into a Taylor series around the guiding centre position (X, Y) replacing again point-wise products with star products. Naively one would expect from our previous results that the symbol Hamiltonian is of the form

$$H_W = H_{cl} + \mathcal{O}(\epsilon^2 \hbar, \epsilon \hbar^2) \quad (67)$$

with H_{cl} being formally equal (in the sense described above) to the classical Hamiltonian function (A11). However, as pointed out earlier, H_W should depend on the gyration velocity components V_x, V_y only by means of the magnetic moment of gyration, $J = V_x * V_x + V_y * V_y$, and its powers. When evaluating the products $v_x * v_x$ and $v_y * v_y$ we have to change the ordering of the symbols V_x, V_y accordingly. Since their Moyal bracket is of order $\hbar \epsilon^{-1}$, additional terms compared to the classical Hamiltonian occur. A straightforward calculation shows that the lowest order correction originates from the ϵ^2 -term in the classical Hamiltonian function. It is of order \hbar^2 . Leaving away from now on the multiplication symbol '*' for reasons of notational simplicity, the Weyl symbol of the guiding centre Hamiltonian finally turns out to be

$$\begin{aligned} H_W = & \frac{1}{2} B (V_x^2 + V_y^2) + \phi(X, Y) + \frac{\epsilon^2}{16B^2} [(-3B_{,x}^2 + BB_{,xx} - 3B_{,y}^2 + BB_{,yy})(V_x^2 + V_y^2)^2 \\ & + 4(3E_x B_{,x} - BE_{x,x} + 3E_y B_{,y} - BE_{y,y})(V_x^2 + V_y^2) - 8(E_x^2 + E_y^2)] \\ & + \frac{\hbar^2}{16B^2} (-B_{,x}^2 + BB_{,xx} - B_{,y}^2 + BB_{,yy}) + \mathcal{O}(\epsilon \hbar^2, \epsilon^2 \hbar, \epsilon^3). \end{aligned} \quad (68)$$

Here, squares of symbols are star products of equal factors, electric and magnetic fields have to be evaluated at the guiding centre position and the comma in a subscript denotes differentiation with respect to the following coordinate(s). Using two-dimensional vector notation equation (68) may be written in a more compact form,

$$\begin{aligned} H_W = & \frac{1}{2} BJ + \phi(X, Y) + \frac{\epsilon^2}{16B^2} [(B \Delta B - 3|\nabla B|^2)J^2 + 4(3E \cdot \nabla B - B \nabla \cdot E)J - 8|E|^2] \\ & + \frac{\hbar^2}{16B^2} (B \Delta B - |\nabla B|^2) + \mathcal{O}(\epsilon \hbar^2, \epsilon^2 \hbar, \epsilon^3) \end{aligned} \quad (69)$$

where scalar products denote summation over Weyl products of vector components. Due to the use of the gauge invariant Weyl calculus, the expansion of H_W involves only gauge invariant quantities. Thus, the higher-order terms of the guiding centre Hamiltonian will be gauge independent as well.

Up to second order in \hbar and ϵ the Hamiltonian H_W in (68) depends on the gyration velocities already via $V_x * V_x + V_y * V_y$, even though we have not carried out the averaging transform mentioned before. The reason for this is that we used averaged classical guiding centre coordinates (as given in the appendix) as zero-order terms (with respect to \hbar) in the general expansion (60) of the guiding centre symbols.

The term proportional to \hbar^2 in (68) specifies the lowest-order quantum-mechanical correction to the classical guiding centre Hamiltonian. It does not depend on the electrostatic field $E = -\nabla \phi$. We will comment on its magnitude in the next section.

Employing the same procedure to the more general case of a three-dimensional magnetic field and arbitrarily oriented electric field, the leading quantum correction to the classical Hamiltonian function turns out to be of second order in \hbar as well. However, the results for the guiding centre symbols and the guiding centre Hamiltonian are notationally cumbersome and

do not shed new light on our method. Therefore, we refrain from writing them down explicitly in this paper.

4. Summary and conclusion

There are two major results of our investigations: first, the product rule for gauge invariant Weyl symbols, as specified in equations (29), (30) and (34). They are a generalization of the well known Moyal formula valid in the usual Weyl formalism. The leading-order term in the \hbar -expansion (40) of the Moyal bracket is proportional to the Poisson bracket, which is expressed in terms of derivatives with respect to position \boldsymbol{x} and kinetic momentum \boldsymbol{k} . The higher-order terms in (40) are of a more complex structure and cannot be written as powers of the Poisson bracket operator. The question about their interpretation in terms of the modified phase space geometry in the presence of electromagnetic fields [42–44] may serve as an interesting starting point for further, more mathematical studies.

The Weyl symbol H_W of the guiding centre Hamiltonian, equation (68), represents the second major result of this paper. The method used to derive it makes extensive use of the product rule for gauge invariant Weyl symbols. The great advantage of this approach lies in the fact that the adiabatic parameter ϵ can be incorporated into the gauge invariant Weyl calculus in a straightforward manner. Consequently, all expansions are carried out with respect to both ϵ and Planck's constant \hbar .

Let us now investigate the importance of quantum-mechanical effects on guiding centre motion by comparing the magnitudes of the ϵ^2 - and \hbar^2 -term in the guiding centre Hamiltonian (68) at low particle energies. Taking into account the quantization of energy levels we replace the gyration energies $\frac{1}{2}B(V_x^2 + V_y^2)$ with the corresponding harmonic oscillator eigenvalues $(n + \frac{1}{2})\hbar\omega_B$, where $\omega_B \equiv |qB|/(mc)$ is the cyclotron frequency at the position of the guiding centre. In the absence of an electric field the guiding centre Hamiltonian for a spinless particle takes the form (using vector notation)

$$H_W = \left(n + \frac{1}{2}\right)\hbar\omega_B + \frac{\hbar^2(n + \frac{1}{2})^2}{4mB^2}(B\Delta B - 3|\nabla B|^2) + \frac{\hbar^2}{16mB^2}(B\Delta B - |\nabla B|^2) \quad (70)$$

with correct physical units restored in the way explained at the beginning of section 3. The second term in (70) is the adiabatic correction (with ϵ set to unity) which now contains \hbar due to energy quantization. Only for small oscillator (= gyration) quantum numbers n the lowest order classical and quantum-mechanical corrections are of the same magnitude, otherwise the classical term dominates. From classical guiding centre theory, however, it is known that at low particle energies the influence of adiabatic corrections on guiding centre motion is negligibly small. Since the magnitude of the leading quantum-mechanical correction in (70) does not depend on the particle energy, we conclude that quantum effects on guiding centre motion may be neglected at all energy scales. Thus, when carrying out experiments with charged particles in inhomogeneous magnetic fields even at very low temperatures, the motion of the guiding centre is described excellently by the lowest-order classical equations. This is also true if an additional electrostatic field \boldsymbol{E} is switched on, because according to (68) the magnitude of the lowest-order quantum-mechanical correction does not depend on \boldsymbol{E} . As a general result of our investigations we may therefore say that guiding centre motion is not effected by quantum mechanics.

Note that if the quantum number n becomes too large in equation (70), the adiabatic correction dominates over the first (gyrative) term in the Hamiltonian. This parallels the breakdown of classical guiding centre theory at large particle energies.

Let us finally compare our result (68) for the guiding centre Hamiltonian with the quantum-mechanical calculation [17] of Maraner, who investigated the motion of a charged spinning particle in a two-dimensional magnetic field. The interaction between the magnetic moment $\boldsymbol{\mu}$ of the particle and the external magnetic field is included into the Hamiltonian by the potential $-\boldsymbol{\mu} \cdot \mathbf{B}$. Since the component μ_z of the magnetic moment parallel to $\mathbf{B} = B(x, y)\mathbf{e}_z$ is a constant of motion we may replace $-\boldsymbol{\mu} \cdot \mathbf{B}$ by the scalar term $-\mu_z B(x, y)$. Thus, the classical Hamiltonian function reads

$$H = \frac{1}{2}(v_x^2 + v_y^2) - \mu_z B(x, y). \quad (71)$$

The term $-\mu_z B(x, y)$ may be interpreted as a special case of a time-independent scalar potential $\phi(x, y)$. A straightforward calculation shows that the corresponding guiding centre symbol Hamiltonian is given by

$$H'_W = \frac{1}{2}BJ - \mu_z B + \frac{\epsilon^2}{16B^2}[(B\Delta B - 3|\nabla B|^2)J(J - 4\mu_z) - 8\mu_z^2 B^{-2}|\nabla B|^2] \\ + \frac{\hbar^2}{16B^2}(B\Delta B - |\nabla B|^2) + \mathcal{O}(\epsilon\hbar^2, \epsilon^2\hbar, \epsilon^3) \quad (72)$$

where the magnetic field and its derivatives have to be taken at the guiding centre position. Substituting $\mu_z = -g\hbar\sigma_3$ (g = gyromagnetic factor of the particle, $\sigma_3 = \pm 1$ for spin- $\frac{1}{2}$ particles), H'_W takes the same form as the Hamiltonian operator derived by Maraner. However, in (72) there are two expansion parameters ϵ and \hbar distinguishing between adiabatic and quantum mechanical corrections to the guiding centre Hamiltonian whereas in [17] the only expansion parameter is the magnetic length $l_B = \sqrt{\hbar c/(q|B|)}$.

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Appendix

In this appendix we will briefly summarize the classical guiding centre theory for the motion of a charged particle in a two-dimensional magnetic field $\mathbf{B} = B(x, y)\mathbf{e}_z$ and an electrostatic field $\mathbf{E} = -\nabla\phi(x, y)$. We closely follow the Hamiltonian method developed by Littlejohn which employs non-canonical, but gauge invariant coordinates in phase space. For further details the interested reader is referred to [10, 11].

To incorporate the classical result into the symbol calculus we have to determine the Cartesian components V_x, V_y of the gyration velocity instead of the generalized gyrophase θ and magnetic momentum J . The reason lies in the difficulty of defining a quantum-mechanical operator corresponding to the classical angle variable θ . This choice of guiding centre phase space coordinates has the disadvantage that in order to compute (X, Y, V_x, V_y) we cannot apply the elegant geometric method of [10, 11].

Introducing the adiabatic parameter ϵ in the standard way, i.e. by replacing the charge q by q/ϵ , and scaling physical quantities according to equation (46) we are looking for phase space functions (X, Y, V_x, V_y) whose non-vanishing Poisson brackets are given by

$$\{V_x, V_y\} = \frac{1}{\epsilon} \quad \{X, Y\} = \frac{\epsilon}{B(X, Y)}. \quad (A1)$$

Again, their different order with respect to ϵ indicates the different timescales of motion.

The resulting guiding centre coordinates are not uniquely determined by the Poisson bracket relations. In order to facilitate the following computations it is of advantage to choose them in the simplest form possible. To lowest order they are proportional to the related particle coordinates. Therefore, V_x, V_y are rapidly oscillating functions of time because the particle velocity components v_x, v_y depend on the gyration angle θ .

Next, we have to find the corresponding backward transformations, i.e. to write the particle coordinates (x, y, v_x, v_y) as functions of (X, Y, V_x, V_y) . Inserting the result into the Hamiltonian function

$$H = \frac{1}{2}(v_x^2 + v_y^2) + \phi(x, y) \quad (\text{A2})$$

the latter takes the form of an asymptotic series with respect to ϵ with the coefficients being gauge invariant functions of the guiding centre coordinates. To exclude rapidly oscillating terms in this expansion, the Hamiltonian should depend on the gyration velocity components only by means of $J = V_x^2 + V_y^2$ and its powers, because to lowest order in ϵ J does not depend on the gyration angle θ . This can be achieved by carrying out a near-identity coordinate transformation $(X, Y, V_x, V_y) \rightarrow (\bar{X}, \bar{Y}, \bar{V}_x, \bar{V}_y)$ to a new set of (averaged) guiding centre coordinates. They have to satisfy the same Poisson bracket relations (A1) so that the related magnetic moment $\bar{J} = \bar{V}_x^2 + \bar{V}_y^2$ becomes a constant of motion and at the same time the dynamics of the guiding centre position decouples from that of the gyration. Such a kind of symplectic transformation may be expressed in terms of Lie generators (cf [10, 11]).

As a result, up to second order in ϵ the averaged guiding centre coordinates read (leaving out the bar over them and using commas in the subscripts to denote differentiation with respect to the following coordinate(s))

$$X = x + \epsilon B^{-1} v_y + \frac{\epsilon^2}{2B^3} (B_{,y} v_x - B_{,x} v_y) v_y + \mathcal{O}(\epsilon^3) \quad (\text{A3})$$

$$Y = y - \epsilon B^{-1} v_x - \frac{\epsilon^2}{2B^3} (B_{,y} v_x - B_{,x} v_y) v_x + \mathcal{O}(\epsilon^3) \quad (\text{A4})$$

$$\begin{aligned} V_x = & B^{-1/2} v_x + \frac{\epsilon}{2B^{5/2}} (B_{,y} v_x^2 + B_{,x} v_x v_y + 2B_{,y} v_y^2 + BB_{,y}) \\ & + \frac{\epsilon^2}{16B^{9/2}} [(-5B_{,x}^2 - BB_{,xx} + 13B_{,y}^2 - 5BB_{,yy})v_x^3 \\ & - 2(4B_{,x}B_{,y} + 2BB_{,xy} - c_1)v_x^2 v_y \\ & + (-15B_{,x}^2 + 7BB_{,xx} + 23B_{,y}^2 - 13BB_{,yy})v_x v_y^2 \\ & + 2(-14B_{,x}B_{,y} + 6BB_{,xy} + c_1)v_y^3 \\ & + 4B(B_{,x}E_x + BE_{x,x} - 7B_{,y}E_y - 3BE_{y,y})v_x \\ & + 2B(c_2 + 9B_{,x}E_y + 9B_{,y}E_x - 8BE_{x,y})v_y] + \mathcal{O}(\epsilon^3) \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} V_y = & B^{-1/2} v_y - \frac{\epsilon}{2B^{5/2}} (2B_{,x} v_x^2 + B_{,y} v_x v_y + B_{,x} v_y^2 + BB_{,x}) \\ & + \frac{\epsilon^2}{16B^{9/2}} [2(-14B_{,x}B_{,y} + 6BB_{,xy} - c_1)v_x^3 \\ & + (23B_{,x}^2 - 13BB_{,xx} - 15B_{,y}^2 + 7BB_{,yy})v_x^2 v_y \\ & - 2(4B_{,x}B_{,y} + 2BB_{,xy} + c_1)v_x v_y^2 \\ & + (13B_{,x}^2 - 5BB_{,xx} - 5B_{,y}^2 - BB_{,yy})v_y^3 \\ & - 2B(c_2 - 7B_{,x}E_y - 7B_{,y}E_x)v_x \\ & + 4B(-7B_{,x}E_x + 3BE_{x,x} + B_{,y}E_y + BE_{y,y})v_y] + \mathcal{O}(\epsilon^3) \end{aligned} \quad (\text{A6})$$

with the corresponding backward transformation

$$x = X - \epsilon B^{-1/2} V_y - \frac{\epsilon^2}{2B^2} (2B_{,x} V_x^2 + B_{,y} V_x V_y + B_{,x} V_y^2 - 2B_x) + \mathcal{O}(\epsilon^3) \quad (\text{A7})$$

$$y = Y + \epsilon B^{-1/2} V_x - \frac{\epsilon^2}{2B^2} (B_{,y} V_x^2 + B_{,x} V_x V_y + 2B_{,y} V_y^2 - 2E_y) + \mathcal{O}(\epsilon^3) \quad (\text{A8})$$

$$\begin{aligned} v_x = & B^{1/2} V_x - \frac{\epsilon}{B} [(B_{,x} V_x + B_{,y} V_y) V_y - E_y] \\ & + \frac{\epsilon^2}{16B^{5/2}} [(-11B_{,x}^2 + BB_{,xx} - 3B_{,y}^2 + BB_{,yy}) V_x^3 \\ & - 4(5B_{,x} B_{,y} + BB_{,xy} + c_1/2) V_x^2 V_y \\ & + (B_{,x}^2 + 5BB_{,xx} - 15B_{,y}^2 - 3BB_{,yy}) V_x V_y^2 \\ & + 4(B_{,x} B_{,y} + BB_{,xy} - c_1/2) V_y^3 \\ & + 4(3B_{,x} E_x - BE_{x,x} + B_{,y} E_y + BE_{y,y}) V_x \\ & - 2(c_2 - B_{,x} E_y - B_{,y} E_x) V_y] + \mathcal{O}(\epsilon^3) \end{aligned} \quad (\text{A9})$$

$$\begin{aligned} v_y = & B^{1/2} V_y + \frac{\epsilon}{B} [(B_{,x} V_x + B_{,y} V_y) V_x - E_x] + \frac{\epsilon^2}{16B^{5/2}} [4(B_{,x} B_{,y} + BB_{,xy} + c_1/2) V_x^3 \\ & + (-15B_{,x}^2 - 3BB_{,xx} + B_{,y}^2 + 5BB_{,yy}) V_x^2 V_y \\ & + 4(5B_{,x} B_{,y} + BB_{,xy} - c_1/2) V_x V_y^2 \\ & + (-3B_{,x}^2 + BB_{,xx} - 11B_{,y}^2 + BB_{,yy}) V_y^3 \\ & + 2(c_2 + 3B_{,x} E_y + 3B_{,y} E_x - 8BE_{x,y}) V_x \\ & + 4(B_{,x} E_x + BE_{x,x} + 3B_{,y} E_y - BE_{y,y}) V_y] + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{A10})$$

In (A5), (A6), (A9), (A10), c_1 and c_2 are arbitrary constants which remain unaffected by the requirement that the Hamiltonian has to be independent of the gyration angle up to second order in ϵ (for more details concerning the ambiguity of guiding centre coordinates cf [45]). In (A7)–(A10) the fields and their derivatives have to be evaluated at the guiding centre position (X, Y) .

In terms of the guiding centre coordinates, the Hamiltonian reads

$$\begin{aligned} H = & \frac{1}{2} B(V_x^2 + V_y^2) + \phi(X, Y) + \frac{\epsilon^2}{16B^2} [(-3B_{,x}^2 + BB_{,xx} - 3B_{,y}^2 + BB_{,yy})(V_x^2 + V_y^2)^2 \\ & + 4(3E_x B_{,x} - BE_{x,x} + 3E_y B_{,y} - BE_{y,y})(V_x^2 + V_y^2) - 8(E_x^2 + E_y^2)] \\ & + \mathcal{O}(\epsilon^3) \end{aligned} \quad (\text{A11})$$

which may be written in a more compact form by employing two-dimensional vector notation,

$$\begin{aligned} H = & \frac{1}{2} B J + \phi(X, Y) + \frac{\epsilon^2}{16B^2} [(B \Delta B - 3|\nabla B|^2) J^2 + 4(3\mathbf{E} \cdot \nabla B - B \nabla \cdot \mathbf{E}) J - 8|\mathbf{E}|^2] \\ & + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{A12})$$

In (A11) and (A12) the fields and potentials have to be evaluated at the guiding centre position (X, Y) . For obvious reasons the last two expressions are denoted as the classical guiding centre Hamiltonian.

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