Wigner equation for general electromagnetic fields: The Weyl-Stratonovich transform

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Gauge-invariant Wigner theories are formulated in terms of the kinetic momentum, which—being a physical quantity—is conserved after a change of the gauge. These theories rely on a transform of the density matrix, originally introduced by Stratonovich, which generalizes the Weyl transform by involving the vector potential. We thus present an alternative derivation of the Weyl-Stratonovich transform, which bridges the concepts and notions used by the different, available gauge-invariant approaches and thus links physically intuitive with formal mathematical viewpoints. Furthermore, an explicit form of the Wigner equation, suitable for numerical analysis and corresponding to general, inhomogeneous, and time-dependent electromagnetic conditions, is obtained. For a constant magnetic field, the equation reduces to two models: in the case of a constant electric field, this is the ballistic Boltzmann equation, where classical particles are driven by local forces. The second model, derived for general electrostatic conditions, involves novel physics, where the magnetic field acts locally via the Liouville operator, while the electrostatics is determined by the manifestly nonlocal Wigner potential. A significant consequence of our work is the fact that now the constant magnetic field case can be treated with existing numerical approaches developed for the standard, scalar potential Wigner theory. Therefore, in order to demonstrate the feasibility of the approach, a stochastic method is applied to simulate a physically intuitive evolution problem.

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I. INTRODUCTION

The Wigner formulation of quantum mechanics [1] offers certain heuristic and applicational advantages as compared to other formal theories [2] and thus finds increased use in recent years in many different fields [3]. Many classical concepts and notions developed in the phase space are directly adopted or generalized by the Wigner formalism [4]. This establishes a unique correspondence between classical and quantum mechanics, which enables a seamless transition between purely quantum and classical descriptions [5]. In this way the Wigner formalism is very convenient for analyzing physical processes governed by the complicated interplay between quantum-coherent phenomena and effects of decoherence which strive to impose classical behavior [6,7]; in contrast to other quantum mechanical formalisms, which deal with purely mathematical quantities, the Wigner function is a *physical quantity* as it can be directly measured. This aspect has become extremely important in recent times, where one wants to actually visualize the presence of entanglement and nonclassical behavior [8–10]. Entanglement has been called the most important aspect of quantum mechanics [11]. As there is no quantum operator that gives entanglement as an eigenvalue, so its existence has to be provided by visualizing the Wigner function from the experiments. Indeed, the Wigner function, which has real values, but is not necessarily positive definite as its classical counterpart and is thus called a quasiprobability, can be presented as a linear combination of probabilities, which can be measured and used to reconstruct the Wigner function. In particular the latter can be written in terms of expectation values of a displaced and/or rotated parity operator and thus enables to visualize entanglement within a quantum system [9,12].

The formulation of the Wigner theory is historically based on operator quantum mechanics [13,14]. Due to the works of Moyal and Groenewold, the Wigner formalism has been established in the mid-twentieth century as an independent, self-contained formulation of quantum mechanics in terms of the Moyal bracket and the star-product [13–17], introduced already at the level of the fundamental *single particle in potential* problem. It has become common in most quantum mechanical descriptions to introduce the electric field in a scalar potential gauge. This makes it easy to show gauge invariance. The formulation of the Schrödinger's equation in an arbitrary magnetic field is quite well known, beginning already with Darwin and Fock [18–20]. The same holds for the Wigner formalism, having already been reviewed by Carruthers and Zachariasen [21]. In this way, the inclusion of the magnetic field raises the problem of the choice of the gauge.

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We recall the concept of gauge invariance. In classical mechanics, the scalar and the vector potentials provide a mathematically convenient way to describe the particle dynamics governed by the electric and the magnetic fields $\mathbf{E}$ and $\mathbf{B}$. The four potential components determine the six components of $\mathbf{E}$ and $\mathbf{B}$ as follows:

$$\mathbf{B} = \nabla \times \mathbf{A}; \quad \mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}. \tag{1}$$

The values of $\mathbf{B}$ and $\mathbf{E}$ are invariant with respect to a general gauge transform

$$\mathbf{A}' = \mathbf{A} + \nabla\chi; \quad \phi' = \phi - \frac{\partial \chi}{\partial t}, \tag{2}$$

where $\mathbf{A}$ and ϕ and their primed counterparts are the old and new sets of vector and scalar potentials and χ can be freely chosen within a certain class of functions.

In the Newtonian picture, transport is usually discussed in terms of the Boltzmann equation. It is the force due to the applied electric and magnetic fields that is important. Quantum mechanics is different. The Schrödinger equation, and any other quantum description, depends directly upon the potentials themselves. While this may seem like a minor difference, this is just not the case. In fact, Wigner himself [1], actually, described the modifications to thermodynamics due to the much more complicated dependence upon the potentials in quantum mechanics. He was the first to introduce an effective potential as a method to modify classical systems to account for (weak) quantum effects. This is an important approach highly utilized in todays semiconductor modeling and simulation [14,22]. In the simplest case, quadratic potentials do not give rise to modifications in the Wigner equation of motion, as this reduces to the Boltzmann equation, but stronger variations of the potential certainly give rise to much more complicated terms.

The transform (2) provides equivalent formulations of a given quantum mechanical problem, which, however, are characterized by different theoretical and numerical peculiarities. An emblematic example is related to Wannier-Stark localized states [23] and accelerated Bloch states [24], which provide two possible ways of describing electron transport in superlattices governed by a homogeneous electric field. The problem polarized the scientific society into two parts, speculating about the correctness of the former or the latter approach. Finally it has been shown that the two pictures are equivalent and related to the choice of a vector ($\phi = 0$) or a scalar ($\mathbf{A} = 0$) potential gauge [25,26].

In the following, we review related research, which considers the Wigner equation in conjunction with (2). However, most research works focus on the effect of the magnetic field, so that the electromagnetic Wigner model is derived after a choice of a concrete gauge for the potentials.

Levinson [27] observed that in the case of homogeneous electric and magnetic fields the physical system has a translational symmetry. This should hold for the Wigner function f_w and the density matrix ρ. However, for example, $\langle \mathbf{p}|\hat{\rho}|\mathbf{p}'\rangle$ in representation $\mathbf{p}$ of the canonical momentum $\hat{\mathbf{p}} = -i\hbar\nabla$, related to the kinetic momentum $\mathbf{P} = \mathbf{p} - e\mathbf{A}(\mathbf{r})$, has off-diagonal elements. In contrast, the density matrix of the kinetic momentum has diagonal elements only due to the translational invariance, where $\langle \mathbf{P}|\hat{\rho}|\mathbf{P}\rangle$ gives the kinetic momentum distribution function. This imposes a relationship between $\mathbf{p}$ and $\mathbf{p}'$ and thus a conjunction between gauge transform and translation operations. A gauge, where the constant part of the electric field is described by a scalar potential and the alternating, time-dependent part by a vector potential, has been conveniently chosen for the analysis. Levinson claimed the following relationship between the spatial variables of the density matrix:

$$\langle \mathbf{r} + \mathbf{a}|\hat{\rho}|\mathbf{r}' + \mathbf{a}\rangle = e^{\frac{ie}{\hbar}A(\mathbf{a})\cdot(\mathbf{r}-\mathbf{r}')}\langle \mathbf{r}|\hat{\rho}|\mathbf{r}'\rangle. \tag{3}$$

The Wigner transform of this equality gives rise to

$$f_w(\mathbf{p}, \mathbf{r}) = f_w(\mathbf{P}), \tag{4}$$

together with the evolution equation for $f_w(\mathbf{P})$. An important peculiarity is that the differential part of the derived Wigner equation resembles the Liouville operator corresponding to the case of the magnetic field.

Constant magnetic field forms of the Wigner function have been further utilized in many studies. The entire microwave field ($\mathbf{E}$ and $\mathbf{B}$) were used in the Jaynes-Cummings model [28]. The field is also considered in optics, especially with squeezed states [29–31].

One of the first Wigner function simulations considering the magnetic field in electron transport is due to Kluksdahl *et al.* [32]. A Wigner equation is derived under constant magnetic field conditions and in a symmetric gauge to analyze the magnetoconductance of a single barrier tunneling structure. The equation is then solved with a finite difference approach in a two-dimensional simulation domain x, y. The barrier is assumed independent on the y coordinate, which simplifies the numerical task. Notably, this is also one of the first computer simulations of a two-dimensional Wigner function problem: as it will be further discussed, robust multi-dimensional algorithms for phase space quantum electron transport have only been developed recently [14].

Materdey and Seyler [33,34] consider a uniform magnetic field and use a symmetric gauge to develop a Wigner theory and applied it to calculate the quantum dielectric function and to explore De-Haas–van Alphen oscillations and magnetic field localization. Two alternative definitions of the Wigner function are introduced via alternative combinations of the canonical momentum and the vector potential operators: $\hat{\mathbf{P}} = \hat{\mathbf{p}} - e\hat{\mathbf{A}}$ and $\hat{\mathbf{D}} = \hat{\mathbf{p}} + e\hat{\mathbf{A}}$. In the first case, we recognize the kinetic momentum operator $\hat{\mathbf{P}}$, while in the second case, the Wigner function is expressed via the expectation value in a given Schrödinger state $|\psi\rangle$ of the operator $\hat{\mathcal{W}} = e^{-\frac{i}{2\hbar}\mathbf{s}\cdot\hat{\mathbf{D}}^*}e^{\frac{i}{2\hbar}\mathbf{s}\cdot\hat{\mathbf{D}}}$. The authors show that both $\hat{\mathbf{P}}$ and $\hat{\mathcal{W}}$ are invariant under a gauge transform and give a preference to $\hat{\mathbf{D}}$. Nevertheless, the physical derivations are in terms of the kinetic momentum $\mathbf{P}$.

If a quantum phase space theory is developed in terms of the canonical momentum $\mathbf{p}$, then the dynamical functions of the physical quantities are also obtained in terms of $\mathbf{p}$; hence the practical importance of the kinetic momentum. In this way, generic physical quantities of the kinetic momentum, expressed as functions of the canonical momentum, involve the vector potential and hence depend on the chosen gauge. Consequently, a change of the gauge requires to develop a novel theory and in particular to recalculate the set of the dynamical functions. Therein lies the fundamental motivation and need to develop a gauge-independent Wigner theory.

In a very recent work of Iafrate, Sokolov, and Krieger [35], the Wigner theory for Bloch electrons in homogeneous electric and magnetic fields of arbitrary time dependence has been developed. The electric field is treated in a vector potential gauge and the magnetic field is in the symmetric gauge. In this way, the basis is given by accelerated Bloch states. Next, a change to a new set of variables gives rise to a gauge-invariant Wigner function of position, kinetic momentum, and time. The resulting equation for free electrons, which resembles the classical Boltzmann counterpart, consistently depends only on the forces $\mathbf{B}$ and $\mathbf{E}$. The approach is then generalized for arbitrary energy bands. Besides the theoretical value of the paper, it also promotes the practical importance of a gauge-invariant Wigner formalism in solids. We note that Maxwell's equations require an inhomogeneous electric field to give a time varying magnetic field.

Alternative approaches are used to derive the gauge-invariant formalism. A gauge-invariant Wigner approach under general electromagnetic conditions was developed at a high formal level of abstraction by Serimaa *et al.* [36], with a further generalization to include radiation reactions [37]. The derivation is based on the concept of a generating operator

$$\hat{T}(\mathbf{s},\mathbf{q}) = e^{\frac{i}{\hbar}(\mathbf{s}\hat{\mathbf{P}}+\mathbf{q}\hat{\mathbf{r}})} \quad \hat{\mathbf{P}} = \hat{\mathbf{p}} - e\hat{\mathbf{A}}(\mathbf{r}), \tag{5}$$

where the vector potential may contain also quantized degrees of freedom. Then the gauge-independent Wigner operator (GIWO) $\hat{W}(\mathbf{P},\mathbf{r})$, which is a function of the $\mathbf{P}, \mathbf{r}$ variables, is defined as a Fourier transform of (5)

$$\hat{W}(\mathbf{P},\mathbf{r}) = C\int d\mathbf{s}\int d\mathbf{q} e^{-\frac{i}{\hbar}(\mathbf{sP}+\mathbf{qr})}\hat{T}(\mathbf{s},\mathbf{q}), \tag{6}$$

where C is a dimension-dependent normalization constant. The equation of motion for GIWO is derived in terms of operators $\hat{\mathbf{E}}$, $\hat{\mathbf{B}}$, where the functional dependence of electric and magnetic vectors on the position is replaced by the operator $\hat{\mathbf{R}} = \mathbf{r} + i\hbar\tau\nabla_{\mathbf{P}}$ and where τ is a one-dimensional variable. The gauge-independent Wigner function (GIWF) is defined as the trace of the GIWO with the density operator

$$f_w = \mathrm{Tr}(\hat{W}\hat{\rho}). \tag{7}$$

Accordingly, the equation for the GIWF is obtained by the trace of the GIWO equation, multiplied by the density operator. We note that the GIWF equation is formulated with the help of the pseudodifferential operators $\hat{\mathbf{E}}$ and $\hat{\mathbf{B}}$. That is, in the Taylor expansion of the electromagnetic field functions, the position argument is replaced by the operator $\hat{\mathbf{R}}$ which contains $\nabla_{\mathbf{P}}$. This gives rise to consecutive powers of $\mathbf{P}$ derivatives acting on f_w. This means that the derived equation is implicit with respect to its mathematical appearance, in particular, the order of the $\mathbf{P}$ derivatives depends on the functional dependence on the position of the considered electromagnetic field. Equation (7) is an implicit expression for f_w, where functional dependence can be obtained only after the action of differential operators in $\hat{W}$ on the density matrix. Nevertheless, it is possible to find an explicit form of (7), which connects the Wigner function to the position-dependent density matrix [36]. A Baker-Campbell-Hausdorff (BCH) representation of the operator $\hat{T}$ was derived by Serimaa *et al.*, which, after inserting in (7) and applying the trace operation, gives rise to a Fourier type of transform of the density matrix, where the argument of the exponent depends on both the kinetic momentum and the vector potential. It generalizes the Weyl transform of the standard, scalar potential Wigner theory and is reduced to the latter if the vector pontential becomes zero. The resulting expression, first obtained by Stratonovich [38] and thus called Weyl-Stratonovich (WS) transform, will be in the focus of this paper.

Levanda and Fleurov [39] also apply this transform to derive "quantum analogs of Hamilton-Jacobi and the Boltzmann kinetic equations." They, however, associate the transform to another work, which was published ten years after the paper of Stratonovich. We note that the derived equations are again implicitly formulated with the help of two operator functions. The sinc function, denoted by $j_0(x)$, and the function $j_1(x) = \sin(x)/x^2 - \cos(x)/x$, where the argument x is replaced by the operator $\Delta = \hbar\frac{\partial}{\partial\mathbf{r}}\frac{\partial}{\partial\mathbf{P}}$. As discussed, such formulations have their theoretical value but lack practical applicability for numerical implementations due to their implicit formulations.

Definition (6) has been already applied within the pragmatic approach developed by Kubo [40] under the name "quantum analog of a delta function in the phase space" and denoted by $\hat{\Delta}(\hat{\mathbf{p}},\hat{\mathbf{r}})$ (the canonical pair of operators). It establishes an one-to-one correspondence between the operator $\hat{D}(\hat{\mathbf{p}},\hat{\mathbf{r}})$ and the dynamical functions $D_s(\mathbf{p},\mathbf{r})$, corresponding to a generic physical quantity D: $D_s = C\mathrm{Tr}(\hat{D}\hat{\Delta})$. The dynamical functions are used to introduce the differential operators $\hat{D}_s(\mathbf{p} - i\frac{\hbar}{2}\nabla_{\mathbf{r}}, \mathbf{r} + i\frac{\hbar}{2}\nabla_{\mathbf{p}})$, called Wigner operators. They have the property to recover the corresponding dynamical function when acting on the unity function: $\hat{D}_W \cdot 1 = D_s$. Wigner operators are used to prove the relationship

$$\mathrm{Tr}(\hat{D}\hat{F}) = C\int d\mathbf{p}\int d\mathbf{r} D_W F_W \cdot 1 = C\int d\mathbf{p}\int d\mathbf{r} D_s F_s. \tag{8}$$

If $\hat{F}$ is chosen to be the density operator, (8) can be applied to calculate expectation values of physical observables as phase space integrals with the corresponding Wigner function. Furthermore, this result can be used to formulate a gauge-independent expressions for the physical observables. According to Kubo [40]: "Now, a Wigner distribution function, originally defined as a function of $\mathbf{p}$ and $\mathbf{r}$, can be regarded as a function of $\mathbf{P}$ and $\mathbf{r}$ simply by change of the independent variables." The Jacobian of the change of the variables, as defined by the relationship between the canonical and kinetic momentum, equals to 1. In this way, Kubo develops a "Wigner representation of quantum mechanics …characterized by the use of noncanonical variables." The evolution equation for the Wigner function in this representation derived under constant magnetic field conditions is "…exactly the same as that in the absence of a magnetic field" plus a term, which is the same as the Lorentz force term in the classical Liouville equation.

The intuitive and physically founded approach suggested by Stratonovich [38] in the year 1956 is based on the expressions for the spatially local mean values of products of components of the canonical momentum (position representation). The search of a gauge-invariant Wigner function is then equivalent to a search of an invariant formulation of the corresponding values of the kinetic momentum. The analysis of the way the former modifies after a gauge transform (2) $\mathbf{A}' = \mathbf{A} + \nabla\chi,\ \rho'(\mathbf{r}_1, \mathbf{r}_2) = e^{i\chi(\mathbf{r}_1) - i\chi(\mathbf{r}_2)}\rho(\mathbf{r}_1, \mathbf{r}_2)$ suggests a change of the operator variables, which gives rise to expressions for the local mean value of products of components of the kinetic momentum. These expressions are used to define the local characteristic function, which obeys a differential equation and can be explicitly solved. The gauge-invariant Wigner distribution is obtained after a Fourier transform of the solution, thus giving the WS transform. However, the corresponding Wigner evolution equation is not stated explicitly. This fact is fully understandable, having in mind that 60 years ago there were neither powerful computers, nor numerical methods with which to solve the equation.

In this work, we show that the formal [36], the pragmatic [40], and the intuitive [38] approaches can be bridged with the help of a first-order differential equation, associating canonical transformations with a change of the variables. The equation links the density matrix to the characteristic function of the local mean values of products of kinetic momentum components. The solution of the equation, obtained as a product of an exponential function of the vector potential with the density matrix, which is the characteristic function, is then Fourier-transformed to obtain the kinetic momentum-dependent Wigner function from the density matrix: the WS transform. The Wigner equation is then derived from the evolution equation for the position-dependent density matrix formulated by using scalar and vector potentials, corresponding to general, inhomogeneous, and time-dependent electromagnetic conditions. The WS transform is then applied to involve the kinetic momentum. The equation has an explicit mathematical structure in the sense that the differential and integral operations are fixed and independent from the electric and magnetic fields, which appear as regular functions of the position. Two cases corresponding to constant magnetic field are considered; in particular, the usual validation that the equation reduces to the Boltzmann counterpart under homogeneous conditions is presented. The work concludes with discussing numerical aspects based on simulations of the evolution of an initial Wigner function governed by a magnetic field.

II. ELECTROMAGNETIC POTENTIALS IN THE WIGNER PICTURE

We consider the evolution of a charged particle driven by electric and magnetic fields described by a fixed set of vector and scalar potentials $\mathbf{A}(\mathbf{r})$ and $\phi(\mathbf{r}) = V(\mathbf{r})/e$. The time dependence of $\mathbf{A}$ is not written explicitly. From a classical point of view the particle evolution is governed by forces. Electromagnetic potentials are introduced as a mathematical construct, which simplifies the calculations and have no physical significance [41]. Quantum descriptions explicitly depend on the potentials via the Hamiltonian. As previously mentioned, a gauge transform can entirely change the theoretical formulation in terms of physical descriptors. However, consistently, a gauge transform preserves the values of the physical averages and thus the physical picture. This means that theoretical formulations related to different gauges are related by unitary transforms.

We begin with the operator picture, which provides the historical way to introduce the Wigner function, and we recall that an operator $\hat{G}$ can be used to formulate a unitary mapping of the algebra of quantum operators $\hat{b}$ into itself by

$$\hat{b}(\alpha) = e^{-i\alpha\hat{G}}\hat{b}e^{i\alpha\hat{G}}\,, \tag{9}$$

with the corresponding equation of motion:

$$\dot{\hat{b}}(\alpha) = \frac{d\hat{b}(\alpha)}{d\alpha} = i[\hat{b}(\alpha), \hat{G}]_-\,. \tag{10}$$

This is a first-order differential equation with a solution uniquely determined by the initial condition $\hat{b}_i$. Alternative ways to formulate exponential transforms involving the operator $\hat{G}$ in the space of the state functions (which give rise to similar first-order differential equations) are given in Appendix A. The logical steps of our derivations are unified via considerations of such kind of transforms, which will be frequently referred to. In the next section, we consecutively introduce the concepts and notions needed for the derivation of the exponential transform expressed in terms of the chosen gauge.

A. Gauge and transform of pure states

We consider a single particle in the electric potential, $\mathbf{B} = 0$. The Hamiltonian in an arbitrary gauge $\mathbf{A}, \phi$ is

$$H = \frac{1}{2m}(\hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r}))^2 + V(\mathbf{r})\,, \tag{11}$$

where $\hat{\mathbf{p}} = -i\hbar\nabla$ is the canonical momentum operator. H governs the evolution of the state ψ' via the Schrödinger equation:

$$\left(\frac{\hbar^2}{2m}\left(i\nabla + \frac{e}{\hbar}\mathbf{A}(\mathbf{r})\right)^2 + V(\mathbf{r})\right)\psi' = i\hbar\frac{\partial\psi'}{\partial t}\,. \tag{12}$$

We seek a transform that changes the state ψ' to a state ψ in a picture, where the kinetic operator in the inner brackets obtains a simple form. In accordance with (9), the solution ψ' is sought by the mapping $\psi'(\mathbf{r}, t) = e^{i\alpha G(\mathbf{r})}\psi(\mathbf{r}, t)$. This gives rise to the equation

$$\begin{aligned}\left(i\nabla + \frac{e}{\hbar}\mathbf{A}(\mathbf{r})\right)\psi' &= -(\alpha\nabla G(\mathbf{r}))\psi'(\mathbf{r}, t) + ie^{i\alpha G(\mathbf{r})}\nabla\psi(\mathbf{r}, t)\\ &\quad + \frac{e}{\hbar}\mathbf{A}(\mathbf{r})\psi'(\mathbf{r}, t) = ie^{i\alpha G(\mathbf{r})}\nabla\psi(\mathbf{r}, t).\end{aligned} \tag{13}$$

This expression is simplified under the condition

$$\alpha\nabla G(\mathbf{r}) = \frac{e}{\hbar}\mathbf{A}(\mathbf{r})\,, \tag{14}$$

which effectively removes the vector potential from the operator. We see that α can be associated to G or equivalently set to 1. The approach gives rise to a Schrödinger equation with a potential $(V(\mathbf{r}) + \frac{\hbar\partial G(\mathbf{r})}{\partial t})$. Hence, provided that the solution of (14) exists, which is the case for zero magnetic field, the mapping corresponds to a change of the gauge from the initial set of vector and scalar potentials $\mathbf{A}, \phi$ to the set 0, and $\phi + \frac{\hbar\partial G(\mathbf{r})}{e\partial t}$. The major conclusion—after a generalization for $\mathbf{B} \neq 0$—is that quantum physics is invariant under gauge transforms. However, here, we draw two additional conclusions from Eqs. (13) and (14). It follows that the argument $\mathbf{B}$ of the Wigner function obtained by the Fourier transform $e^{i\mathbf{Bs}}$ of $\psi^*(\mathbf{r}+\mathbf{s}/2)\psi(\mathbf{r}-\mathbf{s}/2)$ is the kinetic momentum. Second, the differential equation (13), which has been used to introduce ψ, actually determines the argument of the exponential transform via (14). We also imposed the constrain $\alpha = 1$, as the latter can be associated to G. In what follows, we apply the same scheme to derive the transform which links the density matrix to the Wigner function of the kinetic momentum.

B. Gauge and transform of mixed states

Here, we merely formulate the problem for the general case of mixed states. The evolution equation for the density operator $\rho i\hbar\frac{\partial}{\partial t}\rho = [H,\rho]_-$ in a coordinate representation, is written for the chosen set of potentials $\mathbf{A}$, V in the center of mass coordinates $\mathbf{x} = \frac{\mathbf{r}'+\mathbf{r}''}{2}$, $\quad \mathbf{s} = \mathbf{r}' - \mathbf{r}''$ as follows:

$$\frac{1}{2mi\hbar}\left\{\sum_l 2\left[i\hbar\frac{\partial}{\partial x_l} + eA_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - eA_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]\right.$$
$$\times\left[i\hbar\frac{\partial}{\partial s_l} + \frac{e}{2}A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right) + \frac{e}{2}A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)\right]$$
$$\left.+2m\left[V\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - V\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]\right\}\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)$$
$$= \frac{\partial\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)}{\partial t}. \tag{15}$$

The equation is now ready for a Fourier transform with respect to the $\mathbf{s}$ variable, in order to introduce the Wigner phase space representation.

The magnetic field involves novel terms via the dependence of the vector potential on $\mathbf{s}$. From a formal point of view, an equation for f_W can be readily obtained. Indeed, after multiplying (15) by $e^{i\mathbf{sp}/\hbar}$ and integrating over $\mathbf{s}$, we can expand the functions A_l and V on $\mathbf{s}$ around $\mathbf{x}$. After that, in the obtained Taylor expansions, we can replace $\mathbf{s}$ by $i\hbar\frac{\partial}{\partial\mathbf{p}}$ and associate the integration to the product of the exponent and the density matrix. In this way, we obtain an equation for the Wigner function in terms of gauge-dependent pseudodifferential operators determined by the chosen vector and scalar potentials. However, as already discussed, this way has definite drawbacks. First of all, any novel choice of the gauge gives rise to a novel mathematical appearance, which affects the differential operations and their order. Second, dynamical functions of the kinetic momentum, corresponding to generic quantities, such as velocity and energy, obtain a novel form with the novel gauge. Thus we have a gauge-specific Wigner function, Wigner equation, and physical quantities. Nevertheless, the operator form of the equation can be convenient for physical analysis, presented in Appendix B.

We, therefore, continue according to Sec. II A by formally seeking a transformation, to simplify the differential part of (15). It will appear that these entirely mathematical considerations have a deep physical meaning which links the characteristic function of the kinetic momentum with the Wigner equation.

C. Derivation of the transform

We are looking for an *Ansatz* for ρ, which simplifies (15). The basic obstacle to follow the standard way by directly applying a Fourier transform with respect to $\mathbf{s}$ are the brackets with the vector potential components, which also depend on $\mathbf{s}$. In the spirit of Sec. II A, we seek to replace these operators with the derivatives of another quantity $\vec{\alpha}$. We follow Sec. II A and seek a transform of the density matrix:

$$\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2},\vec{\alpha}\right)$$
$$= e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\left[i\hbar\nabla_{\mathbf{s}} + \frac{e}{2}\mathbf{A}\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right) + \frac{e}{2}\mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)\right]}$$
$$\times\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right). \tag{16}$$

We maintain the dependence of both $\mathbf{s}$ and $\vec{\alpha}$ and will impose a relevant constrain after gaining experience about the properties of (16). In the best case, we expect that this approach will give a set of three derivatives $\frac{\partial\rho}{\partial\alpha_l}$, which to replace the operators $[i\hbar\frac{\partial}{\partial s_l} + \frac{e}{2}A_l(\mathbf{x}-\frac{\mathbf{s}}{2}) + \frac{e}{2}A_l(\mathbf{x}+\frac{\mathbf{s}}{2})]$ in (15) as in the considered example with the gauge transform. This will give a convenient form for applying the Fourier transform and introducing the Wigner picture. We also need to explore the meaning of the momentum variable introduced by the Fourier transform. Is it related to the kinetic or to the canonical momentum?

In the following, we explore the properties of (16), which is an implicit relation, since the corresponding function of $x, s, \vec{\alpha}$ can be obtained only after expanding the exponent and applying the consecutive powers of the operators on ρ. To introduce an approach for evaluating implicit (or operator) functions of the type of (16), we first examine the one-dimensional version of the task.

1. One-dimensional problem

The operator function

$$\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha\right) = e^{-\frac{i}{\hbar}\alpha[i\hbar\frac{\partial}{\partial s}+\frac{e}{2}A(x-\frac{s}{2})+\frac{e}{2}A(x+\frac{s}{2})]}$$
$$\times\rho\left(x+\frac{s}{2},x-\frac{s}{2}\right) \tag{17}$$

obeys the differential equation

$$i\hbar\frac{\partial}{\partial\alpha}\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha\right)$$
$$= \left[i\hbar\frac{\partial}{\partial s} + \frac{e}{2}A\left(x-\frac{s}{2}\right) + \frac{e}{2}A\left(x+\frac{s}{2}\right)\right]$$
$$\times\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha\right). \tag{18}$$

As shown in Appendix C, equation (18) has an explicit solution with respect to the involved variables:

$$\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha\right) = e^{-\frac{i}{\hbar}\int_0^1\alpha d\tau[\frac{e}{2}A(x-\frac{s+\alpha\tau}{2})+\frac{e}{2}A(x+\frac{s+\alpha\tau}{2})]}$$
$$\times\rho\left(x+\frac{s+\alpha}{2},x-\frac{s+\alpha}{2}\right). \tag{19}$$

This solution obeys the same initial condition suggested by (17) $\rho(x+\frac{s}{2}, x-\frac{s}{2}, \alpha=0) = \rho(x+\frac{s}{2}, x-\frac{s}{2})$ and hence (17) and (19) coincide.

These considerations suggest a way to explicitly evaluate the functional dependence of such operator-defined functions. From a given operator function we first obtain the corresponding differential equation and then find a solution which obeys the same initial condition. We summarize the used approach which will be further needed for our analysis. Both, (17) and (19) satisfy the differential equation (18). Here the argument is α, all other variables are treated as parameters, in particular the right-hand side contains ρ and the first derivative of ρ with respect to s where all arguments, except α, are fixed as parameters. Thus this equation can be formally regarded as an ordinary first-order differential equation where the initial condition determines the solution. The same logic will be pursued for the general three-dimensional case.

2. Multidimensional problem

It is very tempting to interpret the exponent of (16) as three consecutive transformations of type (17) for the components of $\vec{\alpha}$. Unfortunately, this fails since the operators in the arguments do not commute: the BCH formula for the product of two exponential operators

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}+[\hat{A},\hat{B}]_-+\cdots}, \tag{20}$$

where $\cdots$ denotes nested commutators of $\hat{A}$ and $\hat{B}$, indicates that the product of the exponents results in an exponent of the sum of the operators only if the commutator is zero. Furthermore, as suggested by (20), in the general case, the partial derivatives of the operator $\hat{C} = e^{\alpha_1\hat{A}+\alpha_2\hat{B}}$, which is of the form of the exponential operator in (16), differ from the derivatives of $\hat{D} = e^{\alpha_1\hat{A}}e^{\alpha_2\hat{B}}$. Their calculation is straightforward and gives rise to equations of the desired type $\partial\hat{D}/\partial\alpha_1 = \hat{A}\hat{D}$, as suggested by (19). $\hat{C} = \hat{D}$ only when the operators $\hat{A}$ and $\hat{B}$ commute. Hence (16) introduces an equation of the type of (C3) only if the increment $\delta\vec{\alpha}$ is along a fixed direction $\vec{\alpha}^0$. In this case, $\vec{\alpha} = \beta\vec{\alpha}^0$ and the increment is determined by $\delta\beta$, which actually reduces the gradient into the one-dimensional β derivative. This makes the two operators $\hat{A} = \beta\vec{\alpha}_0\cdot(i\hbar\nabla_{\mathbf{s}} + \frac{e}{2}\mathbf{A}(\cdot - \cdot) + \frac{e}{2}\mathbf{A}(\cdot + \cdot))$ and $\hat{B} = \frac{\beta+\delta\beta}{\beta}\hat{A}$ proportional and thus commutative. Then, according to the BCH formula, the β derivative can be easily computed, giving rise to the equation:

$$\begin{aligned} i\hbar\sum_l \alpha_l \frac{\partial\rho}{\partial\alpha_l}(\mathbf{x},\mathbf{s},\vec{\alpha}) &= \left\{\sum_l \alpha_l\left[A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right) + A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) + i\hbar\frac{\partial}{\partial s_l}\right]\right\} \\ &\quad\times\rho(\mathbf{x},\mathbf{s},\vec{\alpha}). \end{aligned} \tag{21}$$

As it will be shown in the next section, (21) is the actual relationship or the *demanded* transform: it appears as a basic entity in the transition from canonical to kinetic momentum representation, necessary for evaluating the physical averages.

3. Characteristic function

The expectation value of the canonical momentum operator $\hat{\mathbf{p}}$ is given by

$$\overline{\mathbf{p}} = \mathrm{Tr}(\hat{\mathbf{p}}\hat{\rho}) = \int d\mathbf{r}'d\mathbf{r}''\langle\mathbf{r}''\hat{\mathbf{p}}|\mathbf{r}'\rangle\langle\mathbf{r}'|\hat{\rho}|\mathbf{r}''\rangle\,, \tag{22}$$

where $\hat{\rho}$ is the density operator corresponding to Eq. (15). This equation can be rewritten with the help of the operator equality

$$\langle\mathbf{r}''|\hat{\mathbf{p}}|\mathbf{r}'\rangle = \delta(\mathbf{r}'-\mathbf{r}'')(-i\hbar)\nabla_{\mathbf{r}'} = \delta(\mathbf{r}'-\mathbf{r}'')(+i\hbar)\nabla_{\mathbf{r}''}\,, \tag{23}$$

which is obtained from the definition of an adjoint operator $\hat{A}^*$: $\langle\mathbf{r}'|\hat{A}^*|\mathbf{r}''\rangle = (\langle\mathbf{r}''|\hat{A}|\mathbf{r}'\rangle)^*$. The mean value (22) of the canonical momentum is then

$$\begin{aligned} \overline{\mathbf{p}} &= \int d\mathbf{r}'d\mathbf{r}''\frac{1}{2}\delta(\mathbf{r}'-\mathbf{r}'')(-i\hbar)(\nabla_{\mathbf{r}'}-\nabla_{\mathbf{r}''})\langle\mathbf{r}'|\hat{\rho}|\mathbf{r}''\rangle \\ &= \int d\mathbf{x}d\mathbf{s}\delta(\mathbf{s})(-i\hbar)\nabla_{\mathbf{s}}\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right). \end{aligned} \tag{24}$$

With the help of this result we can evaluate also the expectation value of the kinetic momentum, whose operator in position representation is given by

$$\hat{\mathbf{P}}(\mathbf{r})|\mathbf{r}\rangle = (\hat{\mathbf{p}} - e\mathbf{A})|\mathbf{r}\rangle = -(i\hbar\nabla_{\mathbf{r}} + e\mathbf{A}(\mathbf{r}))|\mathbf{r}\rangle\,.$$

The expectation value is expressed in phase space coordinates as follows:

$$\begin{aligned} \overline{\mathbf{P}} &= \int d\mathbf{r}'d\mathbf{r}''\frac{1}{2}\delta(\mathbf{r}'-\mathbf{r}'')(-i\hbar(\nabla_{\mathbf{r}'}-\nabla_{\mathbf{r}''}) - e\mathbf{A}(\mathbf{r}') \\ &\quad - e\mathbf{A}(\mathbf{r}''))\langle\mathbf{r}'|\hat{\rho}|\mathbf{r}''\rangle \\ &= -\int d\mathbf{x}d\mathbf{s}\delta(\mathbf{s})\left[i\hbar\nabla_{\mathbf{s}} + \frac{e}{2}\mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) + \frac{e}{2}\mathbf{A}\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right] \\ &\quad\times\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right) = \int d\mathbf{x}\overline{\mathbf{P}}(\mathbf{x})\,. \end{aligned} \tag{25}$$

The definition of the density $\overline{\mathbf{P}}(\mathbf{x})$ stems from the last two lines of (25). This result is easily generalized for $\overline{\mathbf{P}}(\mathbf{x})^n$. Thus, after a multiplication by $\vec{\alpha}$, it holds

$$\begin{aligned} \left(\frac{i}{\hbar}\vec{\alpha}\cdot\overline{\mathbf{P}}(\mathbf{x})\right)^n &= \left\{-\frac{i}{\hbar}\vec{\alpha}\cdot\left[i\hbar\nabla_{\mathbf{s}} + \frac{e}{2}\mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)\right.\right. \\ &\quad\left.\left.+\frac{e}{2}\mathbf{A}\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]\right\}^n\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)\Big|_{\mathbf{s}=0}\,. \end{aligned} \tag{26}$$

The notation $|_{\mathbf{s}=0}$ means that the exponential operator first acts on the density matrix and then $\mathbf{s}$ is set to zero in the resulting expression. This result invokes the concept of the characteristic function from the probability theory: if the value of the quantity $\overline{Q}^n$ is given by the first integral

$$\overline{Q}^n = \int dQ\,Q^n f(Q) \quad \text{it follows} \quad \overline{Q}^n = \frac{d^n}{i^n d\alpha^n}\kappa(\alpha)|_{\alpha=0}\,. \tag{27}$$

Here, $f(Q)$ plays the role of a distribution function and $\kappa(\alpha)$ is the characteristic function defined by

$$\kappa(\alpha) = \int dQ e^{i\alpha Q} f(Q) = \sum_n \frac{1}{n!}(i\alpha)^n \overline{Q}^n = e^{i\alpha\overline{Q}},$$
$$f(Q) = \frac{1}{2\pi}\int dQ e^{-i\alpha Q}\kappa(\alpha). \tag{28}$$

This notion is generalized for the multivariate case

$$\kappa(\alpha, x) = \int dQ e^{i\alpha Q} f(Q, x) = \sum_n \frac{(i\alpha)^n}{n!}\overline{Q}^n(x) = e^{i\alpha\overline{Q}(x)},$$
$$f(Q, x) = \frac{1}{2\pi}\int dQ e^{-i\alpha Q}\kappa(\alpha, x) \tag{29}$$

and then applied in conjunction with (26) to give

$$\kappa(\vec{\alpha}, \mathbf{x}) = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\overline{\mathbf{P}}(\mathbf{x})} = e^{-\frac{i}{\hbar}\vec{\alpha}\cdot[i\hbar\nabla_{\mathbf{s}} + \frac{e}{2}\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}}{2}) + \frac{e}{2}\mathbf{A}(\mathbf{x}-\frac{\mathbf{s}}{2})]}$$
$$\times \rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right)\bigg|_{\mathbf{s}=0}. \tag{30}$$

We conclude that Eq. (16) provides the characteristic function κ and thus is of physical importance for the computation of the averaged quantities in the limit $\mathbf{s} = 0$. The latter discriminates $\mathbf{s}$ from $\vec{\alpha}$ in the result and thus is the constrain needed to consider the transform as a change of variables. Moreover, as previously discussed, methods are available to evaluate such operator functions.

In what follows, we first utilize our experience in obtaining (19) to calculate the explicit form of the characteristic function from (16). Then, we obtain the differential equation corresponding to this equation. Finally, we obtain a gauge-independent formulation of the Wigner function.

D. The Weyl-Stratonovich transform

In complete analogy with the transition from (17) to (19), we associate to (16) the following expression:

$$\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}, \vec{\alpha}\right) = e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\int_0^1 d\tau[\frac{e}{2}\mathbf{A}(\mathbf{x}-\frac{\mathbf{s}+\vec{\alpha}\tau}{2}) + \frac{e}{2}\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}+\vec{\alpha}\tau}{2})]}$$
$$\times \rho\left(\mathbf{x}+\frac{\mathbf{s}+\vec{\alpha}}{2}, \mathbf{x}-\frac{\mathbf{s}+\vec{\alpha}}{2}\right). \tag{31}$$

Now, we need to show that this expression is equivalent to (16), that is, that both quantities satisfy a common differential equation under the same initial condition. Besides, also the condition for relevance of the derivatives of (16) must be satisfied, namely,

$$\alpha_1 = \beta\alpha_1^0; \quad \alpha_2 = \beta\alpha_2^0; \quad \alpha_3 = \beta\alpha_3^0. \tag{32}$$

In this way, the components of the unit vector are not variables, but play the role of parameters. The arguments of ρ then become $\mathbf{x}, \mathbf{s}, \vec{\alpha} = \beta\vec{\alpha}^0$. Accordingly, we consider the following expression:

$$\rho(\mathbf{x}, \mathbf{s}, \beta, \vec{\alpha}^0) = e^{-\frac{i}{\hbar}\frac{e}{2}\sum_l \int_0^\beta d\tau\alpha_l^0\{A_l(x_1-\frac{s_1+\alpha_1^0\tau}{2}, x_2-\frac{s_2+\alpha_2^0\tau}{2}, x_3-\frac{s_3+\alpha_3^0\tau}{2}) + A_l(x_1+\frac{s_1+\alpha_1^0\tau}{2}, x_2+\frac{s_2+\alpha_2^0\tau}{2}, x_3+\frac{s_3+\alpha_3^0\tau}{2})\}}\rho\left(\mathbf{x}+\frac{\mathbf{s}+\beta\vec{\alpha}^0}{2}, \mathbf{x}-\frac{\mathbf{s}+\beta\vec{\alpha}^0}{2}\right). \tag{33}$$

As shown in Appendix D, this expression obeys the differential equation (21) under the same initial condition as the expression (16). Then the characteristic function $\kappa(\vec{\alpha}, \mathbf{x}) = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\overline{\mathbf{P}}(\mathbf{x})} = \rho(\mathbf{x}, 0, \vec{\alpha})$ can be written as

$$\kappa(\vec{\alpha}, \mathbf{x}) = e^{-\frac{i}{\hbar}\frac{e}{2}\vec{\alpha}\cdot\int_{-1}^1 d\tau\mathbf{A}(\mathbf{x}+\frac{\vec{\alpha}\tau}{2})}\rho\left(\mathbf{x}+\frac{\vec{\alpha}}{2}, \mathbf{x}-\frac{\vec{\alpha}}{2}\right). \tag{34}$$

According to (29), the inverse Fourier transform of κ corresponds to the distribution function f. Consequently, the definition of the Wigner function in terms of the kinetic momentum is the inverse Fourier transform of (34). By replacing $\vec{\alpha}$ by the standard notation $\mathbf{s}$, it is obtained:

$$f_w(\mathbf{P}, \mathbf{x}) = \int \frac{d\mathbf{s}}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}\mathbf{s}\cdot\mathbf{P}} e^{-\frac{i}{\hbar}\frac{e}{2}\mathbf{s}\cdot\int_{-1}^1 d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})}$$
$$\times \rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right). \tag{35}$$

E. Section summary

We conclude the first part of the paper by giving an overview of the logical structure of the presented approach. The exponential operator relation (16) has been introduced merely to simplify the mathematical aspects of the Fourier transformation of (15) in analogy with the gauge transform of the wave function of Sec. II A. From the perspective of canonical transforms, which in Hamilton mechanics give rise to a change of variables, the relation introduces a novel variable $\vec{\alpha}$. The constrain needed for the replacement of $\mathbf{s}$ by $\vec{\alpha}$ is to be further specified within the effort to separate the vector potential from the terms containing derivatives on the new variable. However, since the components of the momentum operator are noncommutative, the BCH formula does not allow independent separation of these components and they can be unified only via Eq. (21) instead. It appears that this equation is entirely sufficient for the desired change of variables. First, it is shown that the characteristic function of the kinetic momentum (30) has the form of (16) under the constrain $\mathbf{s} = 0$. It follows that (30) satisfies the differential equation (21). Then, following Stratonovich, an explicit solution of the equation is found under the same initial condition, namely function (34), which after a Fourier transform gives rise to the WS transform (35). Serimaa *etal.* elaborated basically the same logical structure working entirely with the involved exponential operators: the generating operator (5) is a counterpart of the characteristic function. The Fourier transform is the GIWO (6), giving the Wigner function via (7). Finally, the BCH representations of the generating operator $\hat{T} = e^{i(\mathbf{s}\hat{\mathbf{P}}+\mathbf{q}\hat{\mathbf{r}})/\hbar}$ are derived with the help of the explicit solution of a first-order differential equation, obtained from the β derivative of the operator $\hat{T}(\beta) = e^{i\beta(\mathbf{s}\hat{\mathbf{P}}+\mathbf{q}\hat{\mathbf{r}})/\hbar}$.

In our approach, we follow the idea to reduce the mathematical complexity rather than to formulate an alternative gauge-invariant theory. By following this line, it appears that many concepts utilized before, such as a change of variables, the characteristic function and BCH relations may be combined to present the derivation of the transformation (35) from another perspective. This transformation gives rise to a gauge-invariant equation, which is derived in the next section entirely in terms of regular functions and without any involvement of pseudodifferential operators.

III. THE WIGNER EQUATION

The equation of motion of the function (35) is obtained from (15) by firstly multiplying by the exponent factor $e^{-\frac{i}{\hbar}\mathbf{s}\cdot(\cdot\quad\cdot)}$ in (35) and then integrating over $\mathbf{s}$. The idea is to associate the exponential factor to ρ in order to recover the definition (35). This involves lengthy calculations, so that the consecutive terms are considered separately. Details about their evaluation is given in Appendix E.

We first consider the term with the differential operators in the first two rows of (15):

$$\mathcal{D} = \frac{1}{2mi\hbar}\frac{1}{(2\pi\hbar)^3}\int d\mathbf{s} e^{-\frac{i}{\hbar}\mathbf{s}\cdot(\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2}))}\Bigg\{\sum_l 2\left[i\hbar\frac{\partial}{\partial x_l} + eA_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - eA_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]$$
$$\times\left[i\hbar\frac{\partial}{\partial s_l} + \frac{e}{2}A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right) + \frac{e}{2}A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)\right]\Bigg\}\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right). \tag{36}$$

We shift the exponent to the right after the first parentheses in the square bracket by using the equality

$$e^{-\frac{i}{\hbar}\mathbf{s}\cdot(\cdot\quad\cdot)}\left[i\hbar\frac{\partial}{\partial x_l} + eA_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - eA_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right] = \left\{i\hbar\frac{\partial}{\partial x_l} - \frac{e}{2}\int_{-1}^{1}d\tau\left[\mathbf{s}\times\mathbf{B}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right]_l\right\}e^{-\frac{i}{\hbar}\mathbf{s}\cdot(\cdot\quad\cdot)} \tag{37}$$

derived in Appendix E 1.

Next, we move the exponent to the right of the second bracket of (36) with the help of expression

$$e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\left[i\hbar\frac{\partial}{\partial s_l} + \frac{e}{2}A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) + \frac{e}{2}A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right] = \left\{i\hbar\frac{\partial}{\partial s_l} - P_l - \frac{e}{2}\int_{-1}^{1}d\tau\frac{\tau}{2}\left[\mathbf{s}\times\mathbf{B}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right]_l\right\}$$
$$\times e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]} \tag{38}$$

derived in Appendix E 2. In this way, term D (36) becomes

$$\mathcal{D} = \frac{1}{2mi\hbar}\frac{1}{(2\pi\hbar)^3}\int d\mathbf{s}\left(\sum_l 2\left\{i\hbar\frac{\partial}{\partial x_l} - \frac{e}{2}\int_{-1}^{1}d\tau\left[\mathbf{s}\times\mathbf{B}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right]_l\right\}\left\{-P_l - \frac{e}{2}\int_{-1}^{1}d\tau\frac{\tau}{2}\left[\mathbf{s}\times\mathbf{B}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right]_l\right\}\right)$$
$$\times e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right). \tag{39}$$

Note that the operator $i\hbar\frac{\partial}{\partial s_l}$ in the second bracket of (38) has been canceled by the integration over $\mathbf{s}$ since ρ vanishes if the arguments approach infinity. Thus $\mathcal{D}$ becomes

$$\mathcal{D} = \int\frac{d\mathbf{s}}{(2\pi\hbar)^3}\left(-\frac{\mathbf{P}}{m}\cdot\frac{\partial}{\partial\mathbf{x}} + \left\{-\frac{\partial}{\partial\mathbf{x}}\cdot\frac{e}{2m}\int_{-1}^{1}d\tau\frac{\tau}{2}\left[\mathbf{s}\times\mathbf{B}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right] + \frac{e}{2i\hbar}\int_{-1}^{1}d\tau\frac{\mathbf{P}}{m}\cdot\left[\mathbf{s}\times\mathbf{B}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right]\right.\right.$$
$$\left.\left. - \frac{e}{2i\hbar}\frac{e}{2}\int_{-1}^{1}\int_{-1}^{1}d\tau d\eta\left[\mathbf{s}\times\mathbf{B}\left(\mathbf{x}+\frac{\mathbf{s}\eta}{2}\right)\right]\cdot\left[\mathbf{s}\times\mathbf{B}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right]\frac{\tau}{2}\right\}\right)e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right). \tag{40}$$

We denote by $(\mathbf{sB})_F(\mathbf{P}, \mathbf{x}, \tau)$ the Fourier transform of $[\mathbf{s}\times\mathbf{B}(\mathbf{x}+\frac{\mathbf{s}\eta}{2})]$. With the help of Appendix E 3 this gives

$$\mathcal{D} = \left\{-\frac{\mathbf{P}}{m}\cdot\frac{\partial}{\partial\mathbf{x}} + \int d\mathbf{P}'\left[-\frac{\partial}{\partial\mathbf{x}}\cdot\frac{e}{2m}\int_{-1}^{1}d\tau\frac{\tau}{2}(\mathbf{sB})_F(\mathbf{P}', \mathbf{x}, \tau) + \frac{e}{2i\hbar}\int_{-1}^{1}d\tau\frac{\mathbf{P}}{m}\cdot(\mathbf{sB})_F(\mathbf{P}', \mathbf{x}, \tau)\right.\right.$$
$$\left.\left. - \frac{e}{2i\hbar}\frac{e}{2}\int_{-1}^{1}\int_{-1}^{1}d\tau d\eta\int d\mathbf{P}''(\mathbf{sB})_F(\mathbf{P}', \mathbf{x}, \eta)\cdot(\mathbf{sB})_F(\mathbf{P}'-\mathbf{P}'', \mathbf{x}, \tau)\frac{\tau}{2}\right]\right\}f_W(\mathbf{P}-\mathbf{P}', \mathbf{x}). \tag{41}$$

We note that the gradient in the first term in the square brackets acts on the product of the rest of this term with f_W.

Next in turn is the term with the scalar potential in the third row of (15):

$$\mathcal{P} = \frac{1}{(2\pi\hbar)^3}\int \frac{d\mathbf{s}}{i\hbar} e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\left[V\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - V\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right) = \int d\mathbf{P}' V_w(\mathbf{P}', \mathbf{x}) f_w(\mathbf{P}-\mathbf{P}', \mathbf{x}), \tag{42}$$

where we immediately recognize the Wigner potential.

The last term $\mathcal{T}$ is the $\mathbf{s}$ integral of the product of the right-hand side of (15) and the exponent factor. $\mathcal{T}$ can be expressed in terms of $\partial f_w(\mathbf{P},\mathbf{x})/\partial t$ by taking the time derivative of (35):

$$\mathcal{T} = \frac{1}{(2\pi\hbar)^3}\int d\mathbf{s} e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\frac{\partial\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right)}{\partial t} = \frac{\partial}{\partial t} f_w(\mathbf{P},\mathbf{x}) - \frac{e}{2(2\pi\hbar)^3 i\hbar}\int_{-1}^{1} d\tau \int d\mathbf{s}\,\mathbf{s}\cdot\frac{\partial \mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)}{\partial t}$$
$$\times e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right). \tag{43}$$

Observing that the vector potential does not appear as an explicit variable in the expressions for $\mathcal{D}$ and $\mathcal{P}$, we follow the idea to eliminate it from the equation under derivation: the second equation in (1) can be used to express the time derivative of the vector potential via the electric field and the gradient of the scalar potential:

$$-\frac{\partial \mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)}{\partial t} = \mathbf{E}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right) + \frac{\partial}{\partial \mathbf{x}}\phi\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right). \tag{44}$$

Furthermore, the τ integral in the term with the scalar potential can be evaluated as follows:

$$\begin{aligned}&\frac{e}{2(2\pi\hbar)^3 i\hbar}\int_{-1}^{1} d\tau\mathbf{s}\cdot\frac{\partial}{\partial\mathbf{x}}\phi\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\\ &= \frac{1}{(2\pi\hbar)^3 i\hbar}\int_{-1}^{1} d\tau\frac{\partial}{\partial\tau}V\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\\ &= \frac{1}{(2\pi\hbar)^3 i\hbar}\left[V\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - V\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right].\end{aligned} \tag{45}$$

Thus the contribution of the gradient of the scalar potential to (43) is equal to the Wigner potential term $\mathcal{P}$. The two terms cancel each other on both sides of Eq. (15). The contribution of the electric field $\mathbf{E}$ to $\mathcal{T}$ can be evaluated according to Appendix E 3 to

$$\mathcal{T} = \frac{\partial}{\partial t} f_w(\mathbf{P},\mathbf{x}) + \frac{e}{2i\hbar}\int d\mathbf{P}'\int_{-1}^{1} d\tau(\mathbf{s}\cdot\mathbf{E})_F(\mathbf{P}',\mathbf{x},\tau)$$
$$\times f_w(\mathbf{P}-\mathbf{P}',\mathbf{x}),$$

where $(\mathbf{s}\cdot\mathbf{E})_F(\mathbf{P}',\mathbf{x},\tau)$ is the Fourier transform of the function $\mathbf{s}\cdot\mathbf{E}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})$. In this way, we can obtain a closed differential equation for f_w, namely,

$$\mathcal{D} = \mathcal{T}. \tag{46}$$

This equation has the important property to be independent from the choice of the set of the electromagnetic potentials. Indeed, all operators now depend on the kinetic momentum $\mathbf{P}$, the position $\mathbf{x}$, and the time via the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$.

In the next section, we consider two cases of constant magnetic field and discuss related physical aspects.

A. Constant magnetic field

1. Homogeneous electromagnetic conditions

The derived equation is first verified against the emblematic test involving homogeneous electromagnetic conditions. The expression for $\mathcal{D}$ considerably simplifies in the case of a homogeneous magnetic field. For convenience, we consider (41). The first term in the square brackets completely disappears since $\mathbf{B}$ is a constant and the integration over τ can be performed directly. The same holds for the last term where the integrand is an odd function of τ. The equality $\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = \mathbf{b}\cdot(\mathbf{c}\times\mathbf{a})$ can be applied to the only surviving term in the square brackets to obtain

$$\int d\mathbf{s}\frac{ie}{\hbar(2\pi\hbar)^3}\frac{\mathbf{P}}{m}\times\mathbf{B}\cdot\mathbf{s}e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}$$
$$\times\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2}, \mathbf{x}-\frac{\mathbf{s}}{2}\right) = e\frac{\mathbf{P}}{m}\times\mathbf{B}\cdot\frac{\partial}{\partial\mathbf{P}} f_W(\mathbf{P},\mathbf{x}). \tag{47}$$

The term on the right-hand side of equation (46) can be easily evaluated in the case of constant field $\mathbf{E}$. Finally, we obtain

$$\left[\frac{\partial}{\partial t} + \frac{\mathbf{P}}{m}\cdot\frac{\partial}{\partial\mathbf{x}} + e\left(\mathbf{E}+\frac{\mathbf{P}}{m}\times\mathbf{B}\right)\cdot\frac{\partial}{\partial\mathbf{P}}\right] f_w(\mathbf{P},\mathbf{x}) = 0. \tag{48}$$

Equation (48) recovers equation (30) from the paper of Iafrate *et al.* [35] and is identical to the classical evolution equation for a ballistic particle driven by electromagnetic forces.

Now, (48) is easily recognized as the equivalent of the Boltzmann equation. However, the quadratic terms in the vector potential have disappeared, as have the higher-order terms of the Wigner potential. The quadratic terms in the vector potential are well known to lead to Landau quantization by introducing harmonic oscillator effects and it is well known that the Wigner equation of motion does not incorporate these quadratic quantization terms. In that sense, any such quantization has to be put in via the adjoint equation, and the Wigner function then becomes a sum over the various occupied eigenfunctions, each individually transformed on its own. Thus each eigenstate of the quantized system satisfies (48), and the result for the final Wigner function is then a sum over these individual results.

2. General electric conditions

We assume that the electric field has a general spatial dependence. As the magnetic field remains homogeneous, all considerations of the previous section remain valid; in particular Eq. (47). Furthermore, under an arbitrary gauge the vector potential is time-independent as the magnetic field is, and we can conveniently refer to Eq. (43) where only the time derivative of the Wigner function remains. As the second term on the right of this equation becomes zero, the considerations after the equation show that the Wigner potential term $\mathcal{P}$, Eq. (42), survives so that the following equation is readily obtained:

$$\left[\frac{\partial}{\partial t} + \frac{\mathbf{P}}{m}\cdot\frac{\partial}{\partial \mathbf{x}} + e\frac{\mathbf{P}}{m}\times\mathbf{B}\cdot\frac{\partial}{\partial \mathbf{P}}\right] f_w(\mathbf{P},\mathbf{x}) = \int d\mathbf{P}' V_w(\mathbf{P}-\mathbf{P}',\mathbf{x}) f_w(\mathbf{P}',\mathbf{x}), \tag{49}$$

where the Wigner potential

$$V_w(\mathbf{P},\mathbf{x}) = \frac{1}{(2\pi\hbar)^3}\int \frac{d\mathbf{s}}{i\hbar} e^{-\frac{i}{\hbar}\mathbf{s}\cdot\mathbf{P}}\left[V\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - V\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]$$

is linked to the electric force via Eqs. (44) and (45). The left-hand side is the Liouville operator, which describes the acceleration of a particle over Newtonian trajectory. The force is now given by the magnetic field, which manifests its local character. If **B** is set to zero, we recognize the standard scalar potential Wigner equation. The latter provides a full quantum description of the processes governed by the electric potential like tunneling and interference [42]. In particular, while the physical picture related to (48) is governed by the local electromagnetic forces, here the effects of the potential are widely nonlocal. It affects the physical behavior at places where the electric force is practically zero [43]. Now, the interplay of the magnetic field with these effects can be conveniently studied in the phase space. On the left-hand side of Eq. (49), **B** is still local in space and this gives the opportunity to study the interplay by comparison with the solutions of the classical equation (48) and the zero magnetic field version of (49). As we discuss in the next section, the case of a constant magnetic field is fully approachable by the existing numerical models developed in terms of phase space particles.

The remaining terms of (40) are enabled in the case of a general spatial dependence of **B**. We expect that they will introduce nonlocality in the action of the magnetic field as suggested by the spatial derivative in the first term and the spatial convolution structure of the integrals in the last term in the square brackets of $\mathcal{D}$. The effects carried by these terms are not yet explored; their explicit formulation in phase space terms (40) is the first step in this direction, which paves the way for development of numerical approaches which can handle general electromagnetic conditions.

IV. COMPUTATIONAL ASPECTS

The basic similarities between the concepts and notions of classical mechanics and quantum mechanics in phase space motivated the development of particle methods for solving the Wigner equation almost three decades ago [44]. Different particle approaches have been developed since then [2,4,5], which focus mainly on the electrostatic problem in a scalar potential gauge. In particular, the concept of signed particles, which has matured for already 15 years [45], is based on the application of stochastic approaches for solving integral equations to different integral forms of the Wigner equation. The concept is not a single, unique particle model, but comprises a set of particle attributes which can be combined and modified to develop suitable algorithms, specific for the physical aspects of the analyzed problem. Some of these attributes are, however, fundamental and give rise to a heuristic picture of quantum mechanics in terms of particles: first derived from the Wigner theory, the signed particle concept can be postulated to derive back the Wigner formalism [46]. Basic attributes are particle sign, particle generation, and particle annihilation. In a signed particle approach pointlike particles are enabled with classical features, such as drift over Newtonian (field-less) trajectories but carry the quantum information by their positive or negative sign. The mean value of a generic physical quantity A, represented by a phase space function, is evaluated by the sum $\sum_n \mathrm{sign}(n) A_n$ for all particles n in a desired region, where $\mathrm{sign}(n)$ is the sign of the nth particle and A_n the corresponding value of the physical quantity. During the evolution each particle generates couples of one positive and one negative particle, according to rules dictated by the Wigner potential, and propagate in space by distinct but fixed momentum (no acceleration). Particles with opposite sign which meet in the phase space annihilate each-other since they have a common probabilistic future but opposite contribution to the physical averages. These concepts, developed to solve the electrostatic version (**B** =0) of Eq. (49), have been successfully applied recently to many problems. In particular in a proof of concept simulation, showing that the Newton second law can be reproduced by generation/annihilation of unaccelerated signed particles [47] and for two- and three-dimensional problems [43,48]. This shows that a signed particle approach is a promising platform for numerical models for solving the Wigner equation for general electromagnetic conditions. Indeed, it is a method enabling simulations of multi-dimensional problems as posed by the inclusion of the magnetic field. The mathematical structure of the terms in the square brackets in (40) are similar to the Wigner potential term on the right-hand side of (49). This suggests that nonlocal effects due to the magnetic field are introduced if the latter is inhomogeneous, as it is in the case of the electric counterpart. This also indicates that a numerical incorporation of these terms should be in conjunction with their convolution structure as in the case of a gauge transform of the scalar potential Wigner equation [41]. Furthermore, such transform can be used to modify the Wigner potential in a way which is more convenient with respect to computational efficiency [41]. However, the numerical aspects of such a generalization are beyond the scope of this work: most importantly, the available signed particle approach is fully capable to simulate the interplay between constant magnetic and general spatially dependent electric fields posed by Eq. (49). One of the advantages of the phase space description is that it allows to conveniently compare classical and quantum behavior. The former is provided by the solution of Eq. (48), where local forces govern the particle evolution. The latter is introduced by the Wigner potential in

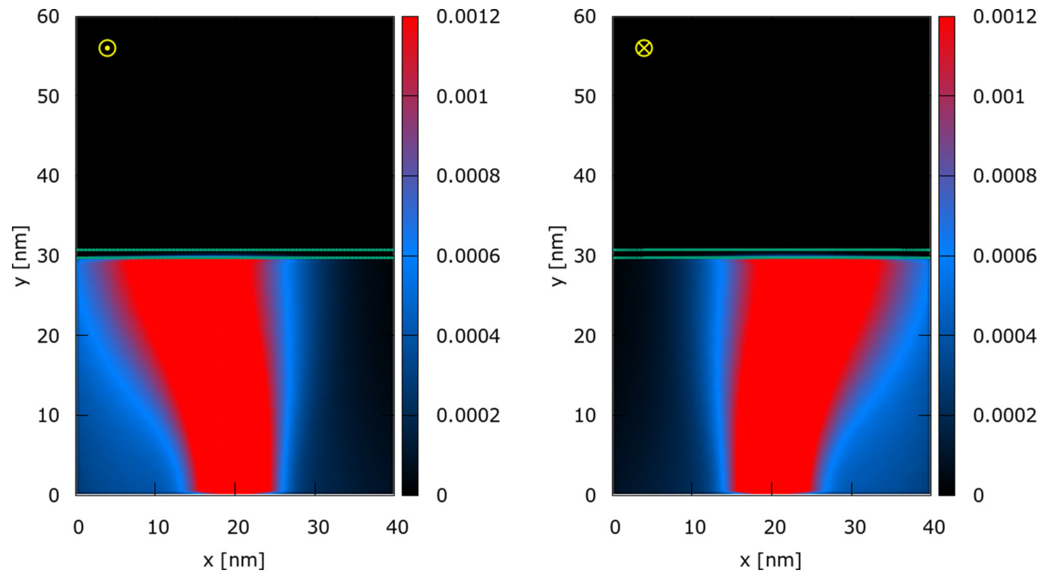

FIG. 1. Classical density corresponding to 6 T (left) and −6 T (right) magnetic field.

(49). We solve the two equations for an initial condition given by a Wigner state corresponding to a minimum uncertainty Gaussian wave packet [4], admissible for both problems. It is non-negative so that it can be interpreted as a probability distribution and it obeys the uncertainty relations. We adopt the physical problem considered in Ref. [32], describing processes of tunneling through a barrier under the action of a constant magnetic field normal to the xy plane of the evolution. The 0.3 eV high, 1-nm-thick barrier is homogeneous along the x direction of the simulation domain with a length of 40 nm. The corresponding length along the y direction is 60 nm, with a coherence length of $L_c = 60$ nm in both directions. The mean kinetic energy of the initial state is 0.1 eV with a standard deviation $\sigma_x = \sigma_y = 3$ nm, corresponding to an equilibrium distribution at 300 K. The effective mass is assumed to be $m_{\rm eff} = 0.19\, m_e$ with m_e being the mass of a free electron. The same state is injected periodically from the boundary until a stationary distribution of the electron density is obtained. This corresponds to a time integration of the density $n(x, y, t)$, corresponding to the evolution of a single state.

Figure 1 shows the classical density described by Eq. (48) for a magnetic field of ±6 T. The local Lorentz force is changed either by switching the direction of the magnetic field, which causes a switch in the beam bending, or by the reflection from the potential barrier which causes 99% of the particles to return on the same path. Only 1% of the particles from the high energetic tail of the initial condition surmount the barrier, so that the upper half of the simulation domain is practically empty. The expected specular symmetry of the ±6 T results is confirmed by the numerical results.

Figure 2, left, shows the quantum density under zero magnetic field conditions. The quantum solution reflects the symmetry of the physical task, which indicates the stability of

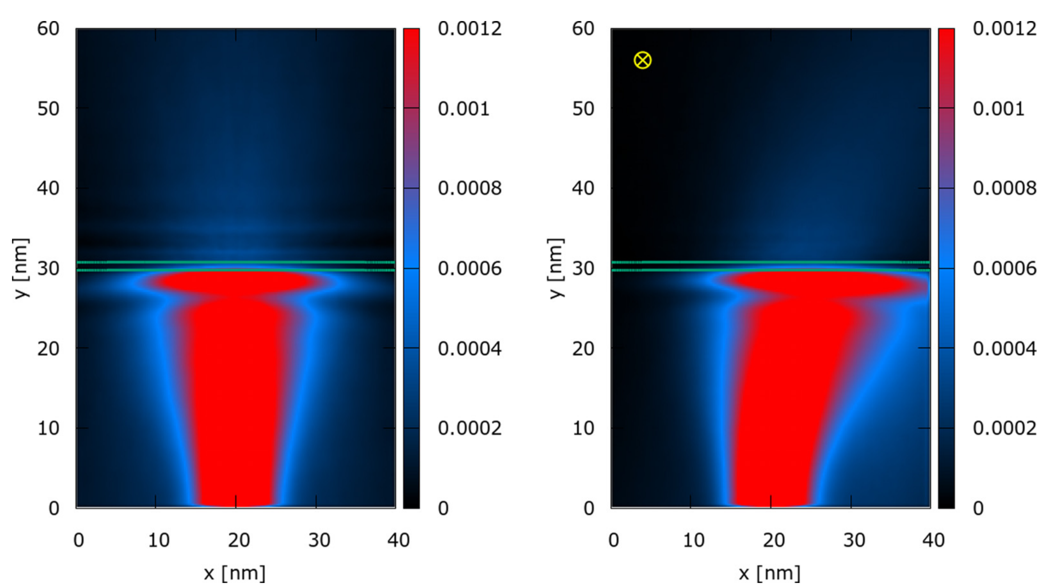

FIG. 2. Quantum density corresponding to 0 T (left) and −6 T magnetic field (right).

the simulation approach. The tunneling is well demonstrated by the pronounced density in the upper half of the domain. We note the nonlocal action of the Wigner potential which affects the density before the barrier. Furthermore, the wave character of the density is a manifestation of the coherent evolution. The application of a 6-T magnetic field lifts the symmetry of the task. The action of the Wigner potential is still nonlocal. However, now the coherence is affected by the magnetic field: the density in the upper half is bent according to the influence of the magnetic field.

V. CONCLUSIONS

The derivation of (35), which aimed at mathematical simplification, underlines the internal relationship between the concepts used by other approaches used to formulate a gauge-invariant Wigner theory. The approach highlights the interplay between physical and mathematical aspects of the latter. The main outcome is not only the WS transform (known since six decades) but also that when the latter is applied to (15), the differential part will be simplified and that the variable $\mathbf{P}$ in the solution of the equation corresponds to the kinetic momentum, which is a gauge-independent quantity. Indeed, the derived equation (46) does not involve electromagnetic potentials, but depends only on the electric and the magnetic fields, which is a manifestation of gauge invariance. Furthermore, the equation has an explicit mathematical structure in the sense that the differential and integral operations are fixed and independent on the electric and magnetic fields: the latter appear as regular functions of the position and time for very general electromagnetic conditions. This is very important for future applications of the equation, which will rely on numerical approaches for finding the solution. The derived equation passed the usual test under homogeneous conditions, when it reduces to the classical ballistic Boltzmann equation for particles governed by the local electromagnetic forces. Equation (49) is also newly derived: the action of the constant magnetic field is local, however, the Wigner potential description is fully quantum and accounts for phenomena such as nonlocality, tunneling, and interference. The interplay of these phenomena with the magnetic force can be readily analyzed with the help of the existing numerical approaches, as illustrated by the presented simulations and discussions. It is important to note that the electric potential is decoupled from the gauge related to the constant magnetic field and thus plays a role of a gauge-invariant quantity determined by the electric potential. Very interesting are the terms in $\mathcal{D}$, which have zero contribution to (49). Their structure resembles the structure of the Wigner potential term and hence they accomplish the full quantum description of the effects caused by the magnetic field. These terms require inhomogeneous magnetic conditions. Thus the study of the involved quantum effects deeply relies on the future development of the numerical approaches for the general electromagnetic conditions.

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APPENDIX A

Alternative relations involving exponent of operators $\hat{G}$ acting in the functional space $\{c\}$ can be formulated:

$$c(\alpha) = e^{i\hat{G}\alpha}c; \quad \dot{c}(\alpha) = i\hat{G}c(\alpha);$$
$$c(\alpha) = e^{i\int_0^\alpha G(\tau)d\tau}c; \quad \dot{c}(\alpha) = i\hat{G}(\alpha)c(\alpha)$$
$$c(\alpha) = e^{i\int_{-\alpha}^\alpha G(\tau)d\tau}c; \quad \dot{c}(\alpha) = i(\hat{G}(\alpha) + \hat{G}(-\alpha))c(\alpha). \tag{A1}$$

These alternative definitions of $c(\alpha)$, give rise to first-order differential equations having solutions, uniquely determined by the initial condition.

APPENDIX B

The following equalities can be proved with the help of the properties of the translation operator $e^{i\hat{\mathbf{p}}\cdot\mathbf{s}/2\hbar}$ where $\hat{\mathbf{p}} = -i\hbar\partial/\partial\mathbf{x}$ so that

$$\frac{1}{2}\frac{\partial}{\partial\mathbf{x}}\cdot\left[\mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)+\mathbf{A}\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right] = \frac{\partial}{\partial\mathbf{x}}\cdot\left[\cos\left(\frac{\hat{\mathbf{p}}\cdot\mathbf{s}}{2\hbar}\right)\mathbf{A}(\mathbf{x})\right],$$
$$\frac{1}{i}\left[\mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-\mathbf{A}\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]\cdot\frac{\partial}{\partial\mathbf{s}} = 2\left[\sin\left(\frac{\hat{\mathbf{p}}\cdot\mathbf{s}}{2\hbar}\right)\mathbf{A}(\mathbf{x})\right]\cdot\frac{\partial}{\partial\mathbf{s}},$$
$$\frac{1}{4}[\mathbf{A}^2\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-\mathbf{A}^2\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)] = \left[\sin\left(\frac{\hat{\mathbf{p}}\cdot\mathbf{s}}{2\hbar}\right)\mathbf{A}(\mathbf{x})\right]\cdot\left[\cos\left(\frac{\hat{\mathbf{p}}\cdot\mathbf{s}}{2\hbar}\right)\mathbf{A}(\mathbf{x})\right].$$

Note that the sine and cosine operators act only inside the square brackets. It is finally obtained

$$\frac{1}{m}\left[i\hbar\frac{\partial}{\partial\mathbf{x}}+e\mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-e\mathbf{A}\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]\cdot\left[i\hbar\frac{\partial}{\partial\mathbf{s}}+\frac{e}{2}\mathbf{A}\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)+\frac{e}{2}\mathbf{A}\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)\right]$$
$$= \frac{e}{\hbar m}\left\{\frac{\partial}{\partial\mathbf{x}}\cdot\frac{\partial}{\partial\mathbf{s}}+\frac{1}{i}\frac{\partial}{\partial\mathbf{x}}\cdot[\cos(\hat{\mathbf{p}}\cdot\mathbf{s}/2\hbar)\mathbf{A}(\mathbf{x})]+2[\sin(\hat{\mathbf{p}}\cdot\mathbf{s}/2\hbar)\mathbf{A}(\mathbf{x})]\cdot\frac{\partial}{\partial\mathbf{s}}\right.$$
$$\left.-\frac{2ie}{\hbar}[\sin(\hat{\mathbf{p}}\cdot\mathbf{s}/2\hbar)\mathbf{A}(\mathbf{x})]\cdot[\cos(\hat{\mathbf{p}}\cdot\mathbf{s}/2\hbar)\mathbf{A}(\mathbf{x})]\right\}. \tag{B1}$$

Here, $\hat{\mathbf{p}}$ is the canonical momentum operator, so that we recognize in the sine and cosine terms operations of translation.

The first two terms with the curly brackets correspond to the term in the Schrödinger equation, which gives a gauge rotation of the electric field relative to the current direction. The last term is what is left from the $\mathbf{A}^2$ contribution to the Schrödinger equation, which can be added to V and thus is responsible for, e.g., Landau quantization. Quantization is lost in (15), which can be seen already in the zero magnetic field case. In particular, if we consider a quadratic scalar potential and zero vector potential gauge, and then transform to the gauge where the scalar potential is zero, from (1) it follows that the last term in (B1) is zero. Thus the evolution equation for the density matrix cannot contain all relevant physics. In this sense, one cannot expect that the latter will reappear in the unitary equivalent Wigner equation: this physics has to arise from the corresponding adjoint equation and must be incorporated in the initial condition. To conclude, Eq. (15) and the corresponding Wigner counterpart are evolution equations where the initial condition determines the solution. Physical solutions correspond to physically relevant initial conditions which introduce the relevant physics in the evolution problem.

APPENDIX C

Equation (18) can be rewritten as

$$\left(\frac{\partial}{\partial\alpha}-\frac{\partial}{\partial s}\right)\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha\right)=-\frac{i}{\hbar}\left[\frac{e}{2}A\left(x-\frac{s}{2}\right)+\frac{e}{2}A\left(x+\frac{s}{2}\right)\right]\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha\right). \tag{C1}$$

We first note that if the right-hand side tends to zero with $A\to 0$, the two partial derivatives compensate each other according to the relation

$$\left(\frac{\partial}{\partial\alpha}-\frac{\partial}{\partial s}\right)f(s+\alpha)=0, \tag{C2}$$

which suggest the particular appearance of s and α as the sum $s+\alpha$ in the argument of the function f. Furthermore, the structure of this equation resembles the equations in the second row in (A1). Thus we seek a solution of the form:

$$\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha\right)=e^{-\frac{i}{\hbar}\int_0^\alpha\hat{G}(x,s,\tau)d\tau}\rho\left(x+\frac{s+\alpha}{2},x-\frac{s+\alpha}{2}\right), \tag{C3}$$

where $\hat{G}$ as suggested by (C1) gives rise to the expression

$$\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha\right)=e^{-\frac{i}{\hbar}\int_0^\alpha d\tau[\frac{e}{2}A(x-\frac{s+\tau}{2})+\frac{e}{2}A(x+\frac{s+\tau}{2})]}\rho\left(x+\frac{s+\alpha}{2},x-\frac{s+\alpha}{2}\right). \tag{C4}$$

To prove that this is the solution of (C1), we first take the α derivative, then the s derivative and subtract.

The equality $\int_0^\alpha d\tau\frac{\partial}{\partial s}F(s+\tau)=F(s+\alpha)-F(s)$ can be used to assist the calculations of the proof. Finally, (C4) obeys the initial condition:

$$\rho\left(x+\frac{s}{2},x-\frac{s}{2},\alpha=0\right)=\rho\left(x+\frac{s}{2},x-\frac{s}{2}\right).$$

APPENDIX D

The β derivative of Eq. (33) can be shortly written as

$$\begin{aligned}i\hbar\frac{\partial\rho}{\partial\beta}(\mathbf{x},\mathbf{s},\beta,\vec{\alpha}^0)=e^{-\frac{i}{\hbar}\frac{e}{2}\sum_l\int_0^\beta d\tau\alpha_l^0(\cdot\quad\cdot)}&\left\{\sum_l\alpha_l^0\left[A_l\left(\mathbf{x}-\frac{\mathbf{s}+\beta\vec{\alpha}^0}{2}\right)+A_l\left(\mathbf{x}+\frac{\mathbf{s}+\beta\vec{\alpha}^0}{2}\right)\right]\right.\\&\left.+i\hbar\frac{\partial}{\partial\beta}\right\}\rho\left(\mathbf{x}+\frac{\mathbf{s}+\beta\vec{\alpha}^0}{2},\mathbf{x}-\frac{\mathbf{s}+\beta\vec{\alpha}^0}{2}\right),\end{aligned} \tag{D1}$$

where two dots correspond to the term in the brackets of the exponential factor in (33). Here, we first replace $i\hbar\frac{\partial}{\partial\beta}$ by $i\hbar\sum_l\alpha_l^0\frac{\partial}{\partial s_l}$ and then move the exponent to the right of the operator in the brackets in order to recover $\rho(\mathbf{x},\mathbf{s},\beta,\vec{\alpha}^0)$, which gives rise to (21).

APPENDIX E

1.

We use the identity

$$\begin{aligned}&e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\left[i\hbar\frac{\partial}{\partial x_l}+eA_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-eA_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]\\&=\left[i\hbar\frac{\partial}{\partial x_l}-\frac{e}{2}\int_{-1}^{1}d\tau\sum_j s_j\frac{\partial A_j}{\partial x_l}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)+e\int_{-1}^{1}d\tau\frac{\partial A_l}{\partial\tau}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right]e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}.\end{aligned}$$

The last integral in the brackets can be rewritten as

$$e\int_{-1}^{1} d\tau \frac{\partial A_l}{\partial \tau}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right) = \int_{-1}^{1} d\tau \frac{e}{2}\sum_j s_j \frac{\partial A_l}{x_j}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)$$

and unified with the previous term to give

$$\int_{-1}^{1} d\tau \frac{e}{2}\sum_j s_j \left(\frac{\partial A_l}{x_j} - \frac{\partial A_j}{x_l}\right)\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right).$$

The term in the brackets gives the components of the magnetic field

$$B_k = \sum_{ij} \epsilon_{ijk}\frac{\partial}{\partial x_i} A_j$$

written with the help of the Levi-Civita tensor ϵ_{ijk}. Due to the importance of this term, we write explicitly the components of $I_m = \sum_j s_j(\frac{\partial A_l}{x_j} - \frac{\partial A_j}{x_l})$.

l	j	sB	I_m
1	2	$s_2(-B_3)$	
1	3	$s_3 B_2$	$s_3B_2 - s_2B_3 = -(\mathbf{s}\times\mathbf{B})_1 = I_1$
2	1	$s_1 B_3$	
2	3	$s_3(-B_1)$	$s_1B_3 - s_3B_1 = -(\mathbf{s}\times\mathbf{B})_2 = I_2$
3	1	$s_1(-B_2)$	
3	2	$s_2 B_1$	$s_2B_1 - s_1B_2 = -(\mathbf{s}\times\mathbf{B})_3 = I_3$

In particular, we conclude that $m = l$.

2.

We use

$$e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1} d\tau \mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\left[i\hbar\frac{\partial}{\partial s_l} + \frac{e}{2}A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) + \frac{e}{2}A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]$$
$$= \left[i\hbar\frac{\partial}{\partial s_l} - P_l - \frac{e}{2}\int_{-1}^{1} d\tau A_l\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right) - \frac{e}{2}\int_{-1}^{1} d\tau\frac{\tau}{2}\sum_j s_j \frac{\partial A_j}{\partial x_l}\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right) + \frac{e}{2}A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) + \frac{e}{2}A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]$$
$$\times e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1} d\tau \mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}. \tag{E1}$$

The third term on the right may be rewritten by using integration by parts:

$$\frac{e}{2}\int_{-1}^{1} d\tau\left[\frac{\partial}{\partial\tau}\tau\right]A_l\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right) = \frac{e}{2}\int_{-1}^{1} d\tau\frac{\partial}{\partial\tau}\left[\tau A_l\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right] - \frac{e}{2}\int_{-1}^{1} d\tau\frac{\tau}{2}\sum_j s_j\frac{\partial A_l\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)}{\partial x_j}. \tag{E2}$$

Inserted back in (E1), the first integral on the right cancels the last two quantities in the curly brackets. Furthermore, the term containing the magnetic field can be easily identified in the expression

$$e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1} d\tau \mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}\left[i\hbar\frac{\partial}{\partial s_l} + \frac{e}{2}A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) + \frac{e}{2}A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]$$
$$= \left[i\hbar\frac{\partial}{\partial s_l} - P_l + \frac{e}{2}\int_{-1}^{1} d\tau\frac{\tau}{2}\sum_j s_j\left(\frac{\partial A_l}{\partial x_j} - \frac{\partial A_j}{\partial x_l}\right)\left(\mathbf{x}+\frac{\mathbf{s}\tau}{2}\right)\right]e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1} d\tau \mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}. \tag{E3}$$

Indeed, we already know that the sum over j gives $I_l = -(\mathbf{s}\times\mathbf{B})_l$.

3.

We consider integrals of the type

$$\mathcal{F}(H) = \int d\mathbf{s}\mathcal{H}(\mathbf{P},\mathbf{x},\mathbf{s})\frac{e^{-\frac{i}{\hbar}\mathbf{s}\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})]}}{(2\pi\hbar)^3}\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right), \tag{E4}$$

$$\begin{aligned}\mathcal{F}(H) &= \int d\mathbf{s}'\left[\int d\mathbf{s}\int d\mathbf{P}'\frac{1}{(2\pi\hbar)^3}e^{-\frac{i}{\hbar}(\mathbf{s}-\mathbf{s}')\cdot\mathbf{P}'}\right]H(\mathbf{P},\mathbf{x},\mathbf{s})\frac{e^{-\frac{i}{\hbar}\mathbf{s}'\cdot[\mathbf{P}+\frac{e}{2}\int_{-1}^{1}d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}'\tau}{2})]}}{(2\pi\hbar)^3}\rho'\left(\mathbf{x}+\frac{\mathbf{s}'}{2},\mathbf{x}-\frac{\mathbf{s}'}{2}\right)\\ &= \int d\mathbf{P}'\left[\int d\mathbf{s}\frac{1}{(2\pi\hbar)^3}e^{-\frac{i}{\hbar}\mathbf{s}\cdot\mathbf{P}'}H(\mathbf{P},\mathbf{x},\mathbf{s})\right]f_w(\mathbf{P}-\mathbf{P}',\mathbf{x}) = \int d\mathbf{P}'H_F(\mathbf{P},\mathbf{x},\mathbf{P}')f_w(\mathbf{P}-\mathbf{P}',\mathbf{x}),\end{aligned}$$

where due to the δ function in the curly brackets, the integral is now separated into integrals on $\mathbf{s}$ and $\mathbf{s}'$. According to the expression in the square brackets, H_F is the Fourier transform of H. We note that the function H can depend implicitly on other variables.

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