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The Wigner equation in the presence of electromagnetic potentials

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Abstract An analysis of the possible formulations of the Wigner equation under a general gauge for the electric field is presented with an emphasis on the computational aspects of the problem. The numerical peculiarities of those formulations enable alternative computational strategies based on existing numerical methods applied in the Wigner formalism, such as finite difference or stochastic particle methods. The phase space formulation of the problem along with certain relations to classical mechanics offers an insight about the role of the gauge transforms in quantum mechanics.

Keywords Wigner function · Electromagnetic potentials · Gauge transform

1 Introduction

The motion of classical particles is governed by forces, which at any instant act locally causing acceleration over Newtonian trajectories. A charged particle, moving in an electromagnetic medium experiences the Lorentz force, comprised by the joint action of the electric and magnetic fields. Locally means that the value of the force is determined by the phase space position of the particle, i.e., the force and the particle share the same phase space location. Electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ are described by Maxwell's equations, which under certain initial/boundary conditions provide the six unknown components of the two three-dimensional vector-fields. The description of electromagnetic phenomena can be simplified by the introduction of electromagnetic scalar and vector potentials, $\mathbf{A}$ and ϕ, respectively, which reduce the number of the unknown components to four.

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

In his seminal work [1] Lorenz begins with the equations for the scalar and vector potentials and derives Maxwell's equations from these equations. Alternatively the derivation begins from the Maxwell equations written in a general form and yields electromagnetic potentials, which obey certain relations, called gauges, which may be imposed additionally, and in particular the Lorenz and Coulomb gauges. The existence of such a freedom in determining the electromagnetic potential reveals an important property of the Maxwell equations: They are invariant under a gauge transform with a given function χ:

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

From a classical point of view these potentials are a mathematical construct, aiming to simplify calculations, that is, they contain no physical significance.

With the development of quantum mechanics this viewpoint had to be changed. The Schrödinger equation, usually formulated in terms of the potential energy $V(\mathbf{r}) = e\phi(\mathbf{r})$ (e refers to the elementary charge) prompts that not only the first derivative, but all terms in the Taylor expansion of the potential take part in the quantum evolution. The Schrödinger

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equation is based on the Hamilton function, which explicitly depends on the vector potential via the kinetic momentum $\mathbf{p} - e\mathbf{A}$, where $\mathbf{p}$ is the conjugate variable to the position, that is the conjugate momentum. The transition to quantum mechanics is established by replacing $\mathbf{p}$ with $-i\hbar\nabla$. With the help of a gauge transform (2), the Schrödinger equation can be formulated explicitly in terms of the vector potential $\mathbf{A}$, even in the case of a zero magnetic field. We limit our considerations to this case: $\mathbf{B} = 0$ is assumed in the sequel.

An emblematic example about the importance of the general gauge picture is related to the theoretical models for analysis of Bloch electrons moving in solids under the influence of a homogeneous electric field $\mathbf{F}$ [2]. Those models are relevant for the electron dynamics in superlattices and comprise effects related to the periodic potential and the electron acceleration. The two possible ways of description, using Wannier-Stark localized states [3] and accelerated Bloch states (Houston states) [4] polarized the scientific society into two parts, speculating about the correctness of the former or the latter approach. These are indeed very different: The former is characterized by a discrete energy spectrum accounting for the translational crystal symmetry (Wannier-Stark ladder), while the latter by the continuous acceleration of the wave vector in the crystal band structure, gives rise to a periodic electron motion (Bloch oscillations). Finally it has been shown that the Wannier-Stark picture (completed by interband Zener tunneling) is linked by an unitary transform (and thus completely equivalent) to the Bloch representation. An excellent analysis based on a Schrödinger equation/density matrix approach is presented in [5]. In particular, the two pictures are related to a vector or a scalar potential gauge respectively:

$$\mathbf{A} = -\mathbf{E}t;\ \phi = 0; \qquad \mathbf{A} = 0, \phi = -\mathbf{E}\cdot\mathbf{r} \tag{3}$$

It is thus important to maintain quantum mechanical descriptions in the presence of scalar and vector potentials. From a theoretical point of view the problem is particularly solved for pure states: The solution of the Schrödinger equation with a vector potential can be related to the solution of the equation without a vector potential by an exponential phase function which is expressed as a line integral of $\mathbf{A}$. Such a function can be defined as it does not depend on the path of integration if the magnetic field is zero.

The inclusion of the vector potential in more general, mixed state approaches, as is the Wigner representation of quantum mechanics, has a long tradition [6,7]; in particular a gauge-invariant Wigner function based on a unitary transform was suggested decades ago [8]. The transform, which can be viewed as a modification of the definition of the Wigner function [9], actually eliminates the vector potential term from the Wigner equation. The conjugate momentum $\mathbf{p}$ used for the Wigner-Weyl transform now coincides with the kinetic momentum, thus recovering the standard scalar potential gauge Wigner picture [10]. Since also operators must be modified accordingly, the approach gives an advantage, if gauge-invariant operators are considered.

In this paper we analyze the choice of the gauge in the Wigner picture from a different perspective: We focus on the computational aspects of the problem. From our point of view two gauge representations are equivalent, provided that they involve comparable computational efforts. In this sense an equation, where the action of the Wigner potential is presented as a series expansion (cf. [10]), does not favor numerical solution approaches and is thus primarily of academic interest.

An approach is suggested, which maintains the Wigner-Weyl transform. We follow the standard way of derivation of the Wigner formalism from the von-Neumann equation for the density matrix [11]. The vector potential equation for the density matrix in Sect. 2 is reformulated to derive a unitary transform based on a general function $\tilde{G}$, which is discussed in Sect. 2.1. The unitary transform provides an *educated guess* for the density matrix suggested in Sect. 2.2. The calculations in this section give rise to an equation which is numerically solvable, i.e., the developed numerical approaches to the standard Wigner equation can be formally applied to this equation. Until this point, the approach is very general, since it does not depend on the particular properties of $\tilde{G}$. A line integral particularization of $\tilde{G}$, presented in Sect. 3, resembles some expressions known from the literature.

2 Vector potential evolution equations

We consider the evolution of a charged particle driven by electric and magnetic fields described by the vector and scalar potentials $\mathbf{A}(\mathbf{r})$ and $\phi(\mathbf{r}) = V(\mathbf{r})/e$. The Hamiltonian is

$$H = \frac{1}{2m}\left(\hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r})\right)^2 + V(\mathbf{r}) \tag{4}$$

with $\hat{\mathbf{p}} = -i\hbar\nabla_{\mathbf{r}}$ is the adjoined (to the position operator $\hat{\mathbf{r}}$) momentum operator and m is the mass.

We pursue a phase space equation of motion in terms of a Wigner function. The starting equation is the evolution equation for the density operator ρ, which is obtained by the commutator with the Hamiltonian, and has the operator form:

$$i\hbar\frac{\partial}{\partial t}\rho = [H, \rho]_{-} = H\rho - \rho H \tag{5}$$

In a coordinate representation, the equation is expressed in terms of the density matrix $\langle\mathbf{r}'|\rho|\mathbf{r}''\rangle$ by applying $\langle\mathbf{r}'|$ to the left and $|\mathbf{r}''\rangle$ to the right of (5):

$$\frac{1}{2m}\left[\sum_l\left(i\hbar\frac{\partial}{\partial r'_l}+eA_l\left(\mathbf{r}'\right)\right)^2 -\sum_l\left(i\hbar\frac{\partial}{\partial r''_l}-eA_l\left(\mathbf{r}''\right)\right)^2\right]\rho\left(\mathbf{r}',\mathbf{r}''\right) +\left(V\left(\mathbf{r}'\right)-V\left(\mathbf{r}''\right)\right)\rho\left(\mathbf{r}',\mathbf{r}''\right)=i\hbar\frac{\partial\rho\left(\mathbf{r}',\mathbf{r}''\right)}{\partial t}, \qquad (6)$$

where for convenience the index t has been skipped.

Equation (6) describes the evolution of a charged particle subject to interaction with scalar and vector potentials. The equation holds for both pure and mixed states and thus may include other operators acting on the density matrix, accounting for alternative processes of interaction with the environment, e.g., with phonons. We change the variables $\mathbf{r}$ and $\mathbf{r}'$ to the center of mass variables $\mathbf{x}=x_1,x_2,x_3$ and $\mathbf{s}=s_1,s_2,s_3$, needed for the Wigner-Weyl transform:

$$\mathbf{x}=\frac{\mathbf{r}'+\mathbf{r}''}{2},\quad \mathbf{s}=\mathbf{r}'-\mathbf{r}'' \quad\leftrightarrow\quad \mathbf{r}'=\mathbf{x}+\frac{\mathbf{s}}{2},\quad \mathbf{r}''=\mathbf{x}-\frac{\mathbf{s}}{2} \qquad (7)$$

Based on this new set of variables, Eq. (6) is formulated as follows:

$$\begin{aligned}\frac{\partial\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)}{\partial t} &=\frac{1}{2mi\hbar}\left[\sum_l\left\{-2\hbar^2\frac{\partial}{\partial s_l}\frac{\partial}{\partial x_l}\right.\right.\\ &+ie\hbar\left(\frac{\partial}{2\partial x_l}A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)+\frac{\partial}{\partial s_l}A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)\right.\\ &\left.+A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)\frac{\partial}{\partial 2x_l}+A_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)\frac{\partial}{\partial s_l}\right)\\ &+ie\hbar\left(\frac{\partial}{2\partial x_l}A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)-\frac{\partial}{\partial s_l}A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right.\\ &\left.+A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\frac{\partial}{\partial 2x_l}-A_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\frac{\partial}{\partial s_l}\right)\\ &\left.+\ e^2A_l^2\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-e^2A_l^2\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right\}\\ &\left.+2m\left(V\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-V\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right)\right]\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)\end{aligned} \qquad (8)$$

We further assume the existence of the functions G_l such that

$$\frac{\partial G_l(\mathbf{y})}{\partial y_l}=\frac{e}{\hbar}A_l(\mathbf{y})\,. \qquad (9)$$

It is important to note that G_l are in general three independent functions, namely they may be bound into a relation only via the gauge obeyed by A_l. In this way the definition of the functions G_l introduces additional - to any gauge transform - degrees of freedom. In the particular case of $G_l=G$ $\forall l$ we obtain the electromagnetic vector potential expressed as a gradient of the function G. This corresponds to the considered case of a zero magnetic filed, so that it is consistent to continue with such a definition of G. However, it is important to keep the general definition which may give a deeper insight in the properties of the derived equations.

With the help of (9) it is shown that the second and the third term on the right of (8) give rise to the equalities:

$$i2\hbar^2\left(\frac{\partial^2}{\partial s_l\partial x_l}G_l\left(\mathbf{x}\pm\frac{\mathbf{s}}{2}\right)-G_l\left(\mathbf{x}\pm\frac{\mathbf{s}}{2}\right)\frac{\partial^2}{\partial s_l\partial x_l}\right) =\pm i2\hbar^2\left[\frac{\partial^2}{\partial s_l\partial x_l},G_l\left(\mathbf{x}\pm\frac{\mathbf{s}}{2}\right)\right]_-$$

By denoting

$$\tilde{G}_l\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)=G_l\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-G_l\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right), \qquad (10)$$

we can rewrite Eq. (8) as follows:

$$\begin{aligned}\frac{\partial\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)}{\partial t} &=\frac{1}{2mi\hbar}\left[\sum_l\left\{-\frac{2\hbar^2\partial^2}{\partial s_l\partial x_l}\right.\right.\\ &+\left[\frac{i2\hbar^2\partial^2}{\partial s_l\partial x_l},\tilde{G}_l\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right]_-\\ &\left.+\ e^2\left(A_l^2\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-A_l^2\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right)\right\}\\ &\left.+2m\left(V\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)-V\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right)\right]\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)\end{aligned} \qquad (11)$$

An application of the Wigner–Weyl transform to this equation provides the corresponding vector-potential Wigner equation. The first and the last terms to the right give rise to the diffusion component in the Liouville operator and the Wigner potential operator. Interestingly, the third term has the same structure as the subsequent potential term. Thus, the the two terms can be associated and processed together. More details about this procedure are discussed in the next section.

Novel from a computational point of view is the commutator term, based on the second mixed derivatives $\partial^2/\partial x_l\partial s_l$ and the three components of the vector function G_l. This formulation already allows to apply the Wigner–Weyl transform and thus enables to solve the obtained equation via numerical solution schemes, such as the finite difference method. However, this commutator term triggers further reformulations of the task as discussed in the next section.

2.1 Unitary transform

The commutator corresponds to a mapping of the differential operator $\partial^2/\partial x_l \partial s_l$ subject to a canonical transform provided by the element $\tilde{G}$ of the dynamical algebra of quantum operators. The transform $U(\alpha)$ is introduced by the unitary operator $e^{i\alpha\tilde{G}}$, where α is a real parameter. We recall that the mapping of any given operator $\hat{b}$ is

$$\hat{b}(\alpha) = U(\alpha)\hat{b} = e^{-i\alpha\tilde{G}}\hat{b}e^{i\alpha\tilde{G}}\,, \tag{12}$$

which is defined as the series:

$$\hat{b}(\alpha) = \hat{b} + (i\alpha)\left[\hat{b},\tilde{G}\right]_- + \frac{(i\alpha)^2}{2!}\left[\left[\hat{b},\tilde{G}\right]_-,\tilde{G}\right]_- + \frac{(i\alpha)^3}{3!}\left[\left[\left[\hat{b},\tilde{G}\right]_-,\tilde{G}\right]_-,\tilde{G}\right]_- + \cdots \tag{13}$$

By taking the derivative of this series with respect to α one obtains:

$$\dot{\hat{b}}(\alpha) = i\left[\hat{b},\tilde{G}\right]_-\,,$$

which is in accordance with (12). We recall that such a commutator defines an automorphism of the algebra $\mathcal{D}$ of the quantum operators - a mapping of $\mathcal{D}$ into itself, which preserves the algebraic structure, namely if $\hat{b} = f(\hat{q},\hat{p})$, $\hat{q}(\alpha) = U(\alpha)\hat{q}$ and $\hat{p}(\alpha) = U(\alpha)\hat{p}$ then

$$\hat{b}(\alpha) = U(\alpha)\hat{b} = U(\alpha)f\left(\hat{q},\hat{p}\right) = f\left(\hat{q}(\alpha),\hat{p}(\alpha)\right)\,.$$

This prompts that the appearances of the commutator elements in the differential part of (11) is a result of such a transform, which gives rise to the following approach.

2.2 Approach for the density matrix

We assume that

$$\alpha = 1; \qquad \tilde{G}\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right) = \sum_m \tilde{G}_m\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)$$

so that the density matrix contains the factor:

$$\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right) = e^{i\tilde{G}(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2})}\rho'\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right) \tag{14}$$

Replacing (14) in (11), after lengthy calculations evaluating the action of the consecutive terms, we obtain the following equation for the primed density matrix:

$$\Bigg[\frac{i\hbar}{m}\sum_l \frac{\partial}{\partial s_l}\frac{\partial}{\partial x_l} + \frac{i\hbar}{2m}\sum_{l;\,k,m\neq l}\left(\frac{\partial\tilde{G}_m}{\partial x_l}\frac{\partial\tilde{G}_k}{\partial x_l}\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - \frac{\partial\tilde{G}_m}{\partial x_l}\frac{\partial\tilde{G}_k}{\partial x_l}\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right) + \frac{1}{i\hbar}\left(V\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - V\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right)\Bigg]\rho'\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)$$
$$= e^{-i\tilde{G}}\frac{\partial e^{i\tilde{G}}\rho'\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right)}{\partial t} \tag{15}$$

We achieved to a large extend our goal to reformulate the equation into a convenient form for numerical treatment. Indeed, both, the second term in the first line of (15) and the time derivative of $\tilde{G}$, have the same structure as the potential term and can formally be associated to it:

$$V' = V - \frac{\hbar^2}{2m}\sum_{l;\,k,m\neq l}\frac{\partial\tilde{G}_m}{\partial x_l}\frac{\partial\tilde{G}_k}{\partial x_l} + \hbar\sum_m\frac{\partial G_m}{\partial t} \tag{16}$$

Now the Wigner–Weyl transform of V' provides the Wigner potential. From a numerical point of view the assignment (16) demonstrates the full computational equivalence between the derived equation and the standard Wigner equation. Any particular numerical technique used to solve the standard equation can be applied for finding the solution of (15). Moreover this holds true for a generic solution of Eq. (9). The analysis of this equation and the analysis of the vector function G is beyond the scope of this work. We continue by specifying the concrete form of G in (9) with the help of a line integral. This allows to derive a well known formulation of the Wigner picture in the presence of a vector potential, which in particular demonstrates the correctness of the proposed approach.

3 The line integral formulation of $\tilde{G}$

We consider the standard formulation of G in terms of a line integral defined by the curve $\mathbf{y} = \mathbf{y}(\xi)$, $\xi \in R$:

$$G_m(\mathbf{r}) = \frac{e}{\hbar}\int_a^b A_m(y_1(\xi),y_2(\xi),y_3(\xi))\frac{dy_m}{d\xi}d\xi;$$
$$\mathbf{y}(a) = \mathbf{o}\ \text{arbitrary point};\quad \mathbf{y}(b) = \mathbf{r} \tag{17}$$

Defined in such a way by a stationary vector potential $\mathbf{A} \neq \mathbf{A}(t)$, G satisfies (9):

$$\nabla G(\mathbf{r}) = \frac{e}{\hbar}\mathbf{A}(\mathbf{r}); \qquad \text{or} \qquad \frac{\partial G_m(\mathbf{r})}{\partial r_k} = \frac{e}{\hbar}\delta_{mk}A_k(\mathbf{r}) \tag{18}$$

Furthermore, with the help of (10), $\tilde{G}$ can be expressed as:

$$\tilde{G} = \frac{e}{\hbar}\int_{\mathbf{r}-\frac{\mathbf{s}}{2}}^{\mathbf{r}+\frac{\mathbf{s}}{2}} \mathbf{A}(\mathbf{y})\cdot d\mathbf{y} = \frac{e}{\hbar}\int_{-1/2}^{1/2} \mathbf{A}(\mathbf{r}+\mathbf{s}\tau)\cdot \mathbf{s}d\tau \qquad (19)$$

We note that **A** must be a rotationless quantity in order for the definition to be independent of the line path, which is in accordance with the considered case of a zero magnetic field. As asserted by (18), the derivative of G_m with respect to a differential increment along the k direction is zero.

Accordingly, the second term in (15) becomes zero. In particular, after the Wigner–Weyl transform we obtain the zero vector potential gauge Wigner picture:

$$f'_w(\mathbf{x},\mathbf{k}) = \frac{1}{(2\pi)^3}\int d\mathbf{s}e^{-i\mathbf{k}\cdot\mathbf{s}}\rho'\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right); \qquad (20)$$

$$\frac{\partial f'_w(\mathbf{x},\mathbf{k})}{\partial t} + -\frac{\hbar}{m}\mathbf{k}\cdot\nabla_{\mathbf{x}} f'_w(\mathbf{x},\mathbf{k}) = \int d\mathbf{k}' V_w\left(\mathbf{x},\mathbf{k}-\mathbf{k}'\right) f'_w\left(\mathbf{x},\mathbf{k}'\right); \qquad (21)$$

$$V_w(\mathbf{x},\mathbf{k}) = \frac{1}{i\hbar(2\pi)^3}\int d\mathbf{s}e^{-i\mathbf{s}\cdot(\mathbf{k}-\mathbf{k}')}\left(V\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right) - V\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\right) \qquad (22)$$

This links the vector potential Wigner function to the solution of the standard (scalar potential) Wigner equation by a unitary transform defined by the particular $\tilde{G}$ (19). This equation is well known from a computational point of view. A variety of stochastic and deterministic techniques for finding f'_w have been developed in the last three decades [12–16].

Finally, we rewrite Eq. (20) by using (14) and take the concrete form of $\tilde{G}$ in (19) into account to obtain the following definition of the Wigner function:

$$f'_w(\mathbf{x},\mathbf{k}) = \frac{1}{(2\pi)^3}\int d\mathbf{s}e^{-i\mathbf{s}\cdot\left(\mathbf{k}+\frac{e}{\hbar}\int_{-1/2}^{1/2}\mathbf{A}(\mathbf{x}+\mathbf{s}\tau)d\tau\right)} \times\rho\left(\mathbf{x}+\frac{\mathbf{s}}{2},\mathbf{x}-\frac{\mathbf{s}}{2}\right) \qquad (23)$$

This result is equivalent to the transform giving rise to a gauge invariant Wigner function suggested sixty years ago by Stratonovich [8] and represents the main expression in theories considered by Serimaa et al. [10] and Haas et al. [9]. It has the following meaning: The unitary transform $e^{-i\tilde{G}}$ as applied to the vector potential density matrix ρ on the left of (14) gives rise to a transition to f', which is the *gauge invariant* Wigner function due to the lack of dependence on the vector potential. As imposed by the trace operation, in the transition from wave to phase space quantum mechanics, the phase space functions corresponding to the physical quantities are also modified in this transition. This is especially convenient, if expectation values of gauge-invariant operators must be evaluated. Such operators, e.g., functions of kinetic momentum, transfer into the well known counterparts of the scalar potential Wigner picture.

4 Summary

The presented analysis of the Wigner equation in the presence of electromagnetic potentials enables three computational strategies: (i) To develop numerical approaches for the solution of (11), where most concepts of the existing numerical techniques to the Wigner equation can be reused; (ii) To use the existing numerical approaches to solve (15), which, with the help of (16), formally resembles the standard Wigner theory. Here, a generic function $\tilde{G}$, solution of (9) may be considered. (iii) To specify $\tilde{G}$ as a line integral and to use (23). The phase space formulation of the problem offers an insight about the role of the gauge transforms in quantum mechanics. Indeed, one can see that V' (16) appears in the same way for the two gauges (3). Then, by using the fact that for up to quadratic potentials the action of the Wigner potential is equivalent to the action of a force term, usually known as the classical limit of the Wigner equation [11]. We conclude about the equivalence of the two gauge approaches.

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