Wigner Distribution Functions and the Representation of Canonical Transformations in Time-Dependent Quantum Mechanics

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Abstract. For classical canonical transformations, one can, using the Wigner transformation, pass from their representation in Hilbert space to a kernel in phase space. In this paper it will be discussed how the time-dependence of the uncertainties of the corresponding time-dependent quantum problems can be incorporated into this formalism.

Key words: canonical transformations; Wigner function; time-dependent quantum mechanics; quantum uncertainties

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1 Introduction

In classical Hamiltonian mechanics the time-evolution of a physical system is described by canonical transformations in phase space that keep the Poisson brackets of the transformed coordinate and momentum with respect to the initial ones unchanged. This transformation in phase space can be described (for a one-dimensional problem in physical space and, therefore, a two-dimensional one in phase space, to which we will restrict ourselves in the following) by the so-called two-dimensional real symplectic group $Sp(2,\mathbb{R})$, represented by 2×2 matrices with determinant equal to 1. (In order to compare our new results with earlier ones for the time-independent case, we only consider the homogeneous symplectic group without translations, not the inhomogeneous symplectic group $ISp(2,\mathbb{R})$.) It has been shown in [1] how it is possible to obtain the representation of the group of linear canonical transformations in time-independent quantum mechanics via the determination of the configuration space representation of the unitary operator that connects quantum mechanically the transformed variables x and p with the initial ones, x' and p'. A subsequent Wigner transformation shows explicitly that for the time-independent problems considered by this method, essentially the classical results are reproduced. This agrees with the fact that at least for quadratic Hamiltonians, the Wigner function evolves as $W(x',p',t) = W(x_M(x',p',-t), p_M(x',p',-t), 0)$, where x_M and p_M are the Moyal time evolution of position and momentum which, again for quadratic Hamiltonians, coincide with the classical evolution [2, 3, 4, 5].

In a different study [6] it has been shown that, for time-dependent quantum systems, characteristic differences compared with the classical situation arise, in particular, when the time-dependence of the quantum mechanical uncertainties of position and momentum are taken into

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account. One such difference can already be found for the most simple physical system, the free motion.

In classical mechanics, the dynamics of a system may not only be described by its trajectory but, particularly for systems with many degrees of freedom, a statistical description in terms of virtual ensembles or distribution functions in phase space (also called Γ-space in this context) is possible. These density-type functions $\varrho_\Gamma(x,p,t)$ must be globally conserved, which is guaranteed if they fulfil a kind of conservation law in the form of a continuity equation in phase space that connects the explicit change in time of the density function ϱ_Γ with the divergence of a current $\vec{j}_\Gamma = \varrho_\Gamma \vec{v}_\Gamma$. If the system obeys Hamilton's equations of motion, the divergence of the velocity field $\vec{v}_\Gamma$ always vanishes, $\nabla_\Gamma \vec{v}_\Gamma = 0$ (where ∇_Γ is the nabla-operator in phase space). In a hydrodynamical description, this would mean that ϱ_Γ describes an incompressible medium. In this probabilistic context, this corresponds to Liouville's theorem that, from all possible transformations of phase space, selects only those where a phase extension always retains its volume during motion. Making use of the concepts of measure theory, this statement can be made even more precise in the formulation that the measure of point-sets is an invariant of the time-evolution of the virtual ensemble.

It can be shown straightforwardly that the quantum mechanical density $\varrho(x,t)=\Psi^*(x,t)\Psi(x,t)$, corresponding to the complex solution $\Psi(x,t)$ of the time-dependent Schrödinger equation also fulfils a continuity equation (now in position- or configuration space). In this case, however, the divergence of the corresponding vector field is proportional to the relative change in time of the mean square deviation of position (position uncertainty) $\langle \tilde{x}^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$, i.e., $\nabla_x \vec{v} = \frac{1}{2} \frac{d}{dt} \langle \tilde{x}^2 \rangle / \langle \tilde{x}^2 \rangle$. So, $\nabla_x \vec{v}$ only vanishes if $\langle \tilde{x}^2 \rangle$ is constant which, e.g. for a Gaussian wave packet, would correspond to a constant width of this wave packet. It is, however, well known that already for the free motion, the wave packet width is not constant but spreading with increasing time. If one would consider the wave packet width as a kind of measure for the "volume" of our quantum system, it certainly would not be conserved under time-evolution. This situation also does not change if one tries to include the momentum aspect by also taking into account the corresponding mean-square deviation $\langle \tilde{p}^2 \rangle$ and then considering the product of $\langle \tilde{x}^2 \rangle$ and $\langle \tilde{p}^2 \rangle$ as an adequate measure for the "volume" of the system; since $\langle \tilde{p}^2 \rangle$ is constant for the free motion, therefore, the product with $\langle \tilde{x}^2 \rangle$ still grows in time. (For a more detailed discussion, see also [6].) A more consistent approach for a comparison with the classical case could, however, make use of the phase-space formulation of quantum mechanics in the form of the time-dependent Wigner function which shall be done in this paper.

Unlike in the time-independent situation where the quantum mechanical results mainly reproduce the classical ones, in the time-dependent case there are obviously, at least, formal differences between the classical and the quantum mechanical descriptions of the system even already for such simple ones like the free motion. These differences are intimately connected with the time-dependence of the typical quantum mechanical aspect of the system, namely, the uncertainties of position and momentum. Therefore, in this paper, we will investigate the influence of the time-dependence of the quantum system, in particular of the uncertainties, on the representation of the group of linear canonical transformations in quantum mechanics.

For this purpose, in Section 2, we briefly summarize the main results of the time-independent quantum mechanical case. In Section 3 we then consider the time-dependent case and discuss the characteristic differences compared with the time-independent situation, in particular the role of the time-dependence of the quantum uncertainties. In order to be on the safe side of systems with exact analytic solutions, we restrict our discussion to systems with at most quadratic Hamiltonians, in particular, to the harmonic oscillator (with possibly time-dependent frequency) and the free motion. Possible ways of overcoming these limitations and of extending our method to further problems will be mentioned in Section 4 where the results will also be summarized and some perspectives will be mentioned.

2 Time-independent case

The time-evolution in classical Hamiltonian mechanics is described by canonical transformations in phase space that can be represented by

$$\begin{pmatrix} x \\ p \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x' \\ p' \end{pmatrix}, \tag{1}$$

where a, b, c, d are real and the determinant of the 2×2 matrix is 1, i.e., $ad - bc = 1$. The group of transformations represented by the 2×2 matrices is the so-called two-dimensional real symplectic group $Sp(2, \mathbb{R})$.

Following [1] (see Chapter 35 and references cited therein), it is possible to obtain the representation of the group of linear canonical transformations (1) in quantum mechanics. Referring to [1, 7], the main objective is to determine the configuration space representation

$$\langle x|U|x'\rangle = K(x, x')$$

of the unitary operator U that provides the quantum mechanical relation between x, p and x', p', according to

$$x = Ux'U^{-1}, \qquad p = Up'U^{-1}. \tag{2}$$

With the help of the kernel $K(x, x')$, the effect of any canonical transformation (1) can be described as

$$\Psi(x) = \int_{-\infty}^{+\infty} dx'\, K(x, x')\Psi(x').$$

The integral kernel $K(x, x')$ has been derived taking into consideration the fact that it must satisfy the following two differential equations [8, 9]

$$\left(ax + b\frac{\hbar}{i}\frac{\partial}{\partial x}\right) K(x, x') = x' K(x, x'), \tag{3}$$

$$\left(cx + d\frac{\hbar}{i}\frac{\partial}{\partial x}\right) K(x, x') = -\frac{\hbar}{i}\frac{\partial}{\partial x'} K(x, x'). \tag{4}$$

An exponential ansatz, bilinear in x and x', finally leads to $K(x, x')$ in the form

$$K(x, x') = \left(\frac{1}{2\pi b}\right)^{\frac{1}{2}} \exp\left\{-\frac{i}{2b}\left[ax^2 - 2xx' + dx'^2\right]\right\}. \tag{5}$$

This kernel $K(x, x')$, related with the specific canonical transformation, is formulated in configuration space, whereas, the corresponding classical canonical transformation is formulated in phase space. Therefore, it is interesting to discuss the representation of this canonical transformation in the phase space version of quantum mechanics that was developed by Wigner [10] with the help of the corresponding distribution function. This distribution function $W(x, p)$ can be obtained from a given wave function $\Psi(x)$ in configuration space via the so-called Wigner transformation

$$W(x, p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dy\, e^{ipy/\hbar} \Psi^* \left(x + \frac{y}{2}\right) \Psi \left(x - \frac{y}{2}\right). \tag{6}$$

Applying this transformation to the kernel (5) leads to the phase space kernel in the form [7]

$$K(x, x', p, p') = \delta[x' - (ax + bp)]\delta[p' - (cx + dp)],$$

showing that, for this linear canonical transformation, the kernel coincides with its classical limit. So, the quantum mechanical problem mainly reproduces the classical situation without any additional specific quantum mechanical aspect.

3 Time-dependent case

Now we will investigate how far this is still true in the case of specific quantum dynamical aspects entering the problem. So, considering time-dependent problems in quantum mechanics in terms of the time-dependent Schrödinger equation or equivalent formulations, one finds that not only classical position and momentum change in time (in a way that can be described by canonical transformations) but, also the typical quantum mechanical degrees of freedom, like position- and momentum-uncertainties, may be time-dependent (corresponding, e.g., to wave packets with time-dependent width). For certain problems with exact analytical solutions in form of Gaussian wave packets, it has been shown (see, e.g., [11] and references cited therein) how the transition from initial position and time (in configuration space) to any later position and time can be achieved with the help of a time-dependent kernel (or propagator) $K(x,x',t,t')$ according to

$$\Psi(x,t) = \int_{-\infty}^{+\infty} dx'\, K(x,x',t,t')\Psi(x',t'). \tag{7}$$

The integral kernel $K(x,x',t,t')$ can be obtained in different ways, e.g., via Feynman's path integral method [12], or, for kernels quadratic in x and x', similar to the discussion in the time-independent case [7] in the form

$$K(x,x',t,t'=0) = \left(\frac{m}{2\pi i\hbar\alpha_0\hat{z}}\right)^{\frac{1}{2}} \exp\left\{\frac{im}{2\hbar\hat{z}}\left[\dot{\hat{z}}x^2 - 2x\left(\frac{x'}{\alpha_0}\right) + \hat{u}\left(\frac{x'}{\alpha_0}\right)^2\right]\right\}, \tag{8}$$

where $\alpha_0 = \sqrt{\frac{2m\langle\tilde{x}^2\rangle_0}{\hbar}}$ is proportional to the initial position uncertainty, or initial mean square deviation in space, $\langle\tilde{x}^2\rangle_0 = \langle x^2\rangle_0 - \langle x\rangle_0^2$ (where $\langle\cdots\rangle$ denotes mean values calculated according to $\langle\cdots\rangle = \int_{-\infty}^{+\infty}\Psi^*\cdots\Psi\,dx'$). We choose this form of the kernel because of the explicit appearance of α_0 and, therefore, the initial position uncertainty. This quantity is essential for the time-evolution of the quantum uncertainties. As has been shown in [11], already for the simple example of the harmonic oscillator, the time-evolution of the position uncertainty and, hence, the width of the Gaussian wave packet solution of this problem, behaves qualitatively very different if the initial position uncertainty corresponds to that of the ground state (constant width) or differs from it (oscillating width) where the latter represents the general solution which, in the limit $\omega \to 0$, provides the free motion wave packet, whereas, the former only leads to a plane wave solution in this limit (for further details see [11]). The time-dependence enters this kernel explicitly via the parameters $\hat{z}(t)$ and $\hat{u}(t)$. In the limit $t \to 0$, the kernel turns into a delta function.

Since, according to (7), the dependence of $\Psi(x,t)$ on x and t enters only via $K(x,x',t,t')$, this kernel also must fulfil the time-dependent Schrödinger equation. Inserting K, in the form given in (8), into this equation shows that the parameters $\hat{z}(t)$ and $\hat{u}(t)$ both fulfil the equation of motion for the corresponding classical problem (e.g., the free motion or the harmonic oscillator with possibly time-dependent frequency), however, they are not independent of each other but are coupled via the relation

$$\dot{\hat{z}}\hat{u} - \dot{\hat{u}}\hat{z} = 1. \tag{9}$$

This resembles the condition that the determinant of the entries of the 2×2 matrix of the linear canonical transformation (1) must fulfil.

Inserting (8) into (7) with an initial Gaussian wave packet $\Psi_{\mathrm{WP}}(x',t')$ of the form

$$\Psi_{\mathrm{WP}}(x',t'=0) = \left(\frac{m\beta_0}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left\{\frac{im}{2\hbar}\left[i\left(\frac{x'}{\alpha_0}\right)^2 + 2\frac{p_0}{m}x'\right]\right\}$$

leads to a Gaussian wave packet

$$\Psi_{\mathrm{WP}}(x,t) = \left(\frac{m}{\pi\hbar}\right)^{\frac{1}{4}} \left(\frac{1}{\hat{u}+i\hat{z}}\right)^{\frac{1}{2}} \exp\left\{\frac{im}{2\hbar}\left[\frac{\dot{\hat{z}}}{\hat{z}}x^2 - \frac{(x-\frac{p_0\alpha_0}{m}\hat{z})^2}{\hat{z}(\hat{u}+i\hat{z})}\right]\right\}, \tag{10}$$

whose maximum follows the classical trajectory $\eta(t)$, which is, therefore, up to a constant, proportional to $\hat{z}$, i.e.,

$$\hat{z} = \frac{m}{\alpha_0 p_0}\langle x\rangle(t) = \frac{m}{\alpha_0 p_0}\eta(t) \tag{11}$$

with initial momentum p_0 and mean value of position $\langle x\rangle$ which is, according to Ehrenfest's theorem, identical with the classical trajectory $\eta(t)$.

The coefficient of the term quadratic in x in the exponent of the Gaussian can be expressed via the complex quantity

$$\frac{2\hbar}{m}y = \frac{\dot{\hat{z}}}{\hat{z}} - \frac{1}{\hat{z}(\hat{u}+i\hat{z})} = \frac{\dot{\lambda}}{\lambda}, \tag{12}$$

where $\hat{u}$ and $\hat{z}$ have been combined to form the complex variable

$$\lambda = \hat{u} + i\hat{z}. \tag{13}$$

The quantity $\frac{2\hbar}{m}y$ fulfils the complex nonlinear Riccati equation (here given for the harmonic oscillator)

$$\frac{2\hbar}{m}\dot{y} + \left(\frac{2\hbar}{m}y\right)^2 + \omega^2 = 0, \tag{14}$$

which can be linearized, using equation (12), to a complex Newtonian equation

$$\ddot{\lambda} + \omega^2\lambda = 0 \tag{15}$$

for the variable λ (for details see [11, 13]). The complex quantity $\lambda(t)$ can also be expressed in polar coordinates as

$$\lambda = \alpha e^{i\varphi} = \alpha\cos\varphi + i\alpha\sin\varphi, \tag{16}$$

where relation (9) turns into

$$\dot{\varphi} = \frac{1}{\alpha^2}, \tag{17}$$

which has similarities with the conservation of angular momentum but, here, for the motion of $\lambda(t)$ in the *complex* plane.

Through equations (13), (15) and (11) it is obvious that the imaginary part of equation (15), up to a constant factor, is just the Newtonian equation of motion for the wave packet maximum. The width of the wave packet (10), or its position uncertainty $\langle\tilde{x}^2\rangle = \langle x^2\rangle - \langle x\rangle^2$, respectively, is connected with the imaginary part of $\left(\frac{2\hbar}{m}y\right)$ via $\frac{2\hbar}{m}y_I = \frac{\hbar}{2m\langle\tilde{x}^2\rangle}$. From λ in polar coordinates (see equation (16)) and pursuing equation (12) and (17) it follows that the variable of the complex Riccati equation (14) can be written as

$$\left(\frac{2\hbar}{m}y\right) = \frac{\dot{\lambda}}{\lambda} = \frac{\dot{\alpha}}{\alpha} + i\dot{\varphi} = \frac{\dot{\alpha}}{\alpha} + i\frac{1}{\alpha^2} = \left(\frac{2\hbar}{m}y_R\right) + i\left(\frac{2\hbar}{m}y_I\right),$$

with $\alpha^2 = 2m\langle\tilde{x}^2\rangle/\hbar$. The imaginary part of equation (14) agrees with equations (17) and (9). The real part of equation (14) with the above-mentioned results leads, however, to a real nonlinear differential equation for the position uncertainty $\alpha(t)$,

$$\ddot{\alpha} + \omega^2(t)\alpha = \frac{1}{\alpha^3}. \tag{18}$$

It is well-known in the literature [14, 15] that a pair of differential equations consisting of the Newtonian equation of motion (15), but now only for $\eta(t)$, and the nonlinear equation (18), possesses a dynamical invariant, the so-called Ermakov invariant,

$$I_L = \frac{1}{2}\left[(\dot{\eta}\alpha - \eta\dot{\alpha})^2 + \left(\frac{\eta}{\alpha}\right)^2\right] = \text{const} = \frac{1}{2}\left(\frac{\alpha_0 p_0}{m}\right)^2, \tag{19}$$

that connects the classical position and momentum (or velocity) and their uncertainties. This becomes even more obvious if one realizes that, with the help of α, φ and λ and their time-derivatives (denoted by overdots), the quantum mechanical uncertainties can now be expressed in the following forms

$$\langle\tilde{x}^2\rangle = \frac{\hbar}{2m}\alpha^2 = \frac{\hbar}{2m}\lambda\lambda^*, \tag{20}$$

$$\langle\tilde{p}^2\rangle = \frac{\hbar m}{2}(\dot{\alpha}^2 + \alpha^2\dot{\varphi}^2) = \frac{\hbar m}{2}(\dot{\lambda}\dot{\lambda}^*), \tag{21}$$

$$\langle[\tilde{x},\tilde{p}]_+\rangle = \langle\tilde{x}\tilde{p} + \tilde{p}\tilde{x}\rangle = \hbar\dot{\alpha}\alpha = \frac{\hbar}{2}\frac{\partial}{\partial t}(\lambda\lambda^*), \tag{22}$$

where $\tilde{x} = x - \langle x\rangle$, $\tilde{p} = p - \langle p\rangle$.

In order to compare the time-dependent kernel (8) with the kernel $K(x,x')$ in (5), one must take into account that $K(x,x')$ has been obtained via equations (3) and (4) which describe the transformation of x and p into the initial values x' and p', whereas, $K(x,x',t,t')$ in (8) describes the inverse transformation from x' to x. This is expressed, e.g., by the different signs in the exponents of (5) and (8). In order to make a direct comparison, one must therefore take the inverse transformation of (8), obtained by changing the sign in the exponent, and interchanging $\dot{\hat{z}}$ and $\hat{u}$. Inserting this kernel into equations (3) and (4), one obtains the corresponding equations for the time-dependent problem,

$$\dot{\hat{z}}x - \hat{z}\frac{p}{m} = \frac{x'}{\alpha_0}, \tag{23}$$

$$-\dot{\hat{u}}x + \hat{u}\frac{p}{m} = -\frac{\alpha_0 p'}{m} \tag{24}$$

or, in matrix notation,

$$\begin{pmatrix} \frac{x'}{\alpha_0} \\ -\frac{\alpha_0 p'}{m} \end{pmatrix} = \begin{pmatrix} \dot{\hat{z}} & -\hat{z} \\ -\dot{\hat{u}} & \hat{u} \end{pmatrix}\begin{pmatrix} x \\ \frac{p}{m} \end{pmatrix} = \mathbf{M}\begin{pmatrix} x \\ \frac{p}{m} \end{pmatrix}. \tag{25}$$

Again, the transformation matrix $\mathbf{M}$ has the determinant $\dot{\hat{z}}\hat{u} - \dot{\hat{u}}\hat{z} = 1$, which corresponds, according to (17), to a kind of conservation of angular momentum (in a complex plane). However, different from the time-independent case, the initial state is not only characterized by the initial position x' and momentum p' but, also, by the corresponding initial uncertainties since $\alpha_0 = (\frac{2m}{\hbar}\langle\tilde{x}^2\rangle_0)^{1/2}$ is proportional to the initial position uncertainty and (for a minimum uncertainty wave packet with $\langle\tilde{x}\rangle_0^2\langle\tilde{p}^2\rangle_0 = \hbar^2/4$) the inverse $\frac{1}{\alpha_0} = (\frac{2}{m\hbar}\langle\tilde{p}^2\rangle_0)^{1/2}$ is proportional to the initial momentum uncertainty, i.e., $\frac{x'}{\alpha_0} \propto \frac{x'}{\sqrt{\langle\tilde{x}^2\rangle_0}}$, $\frac{\alpha_0 p'}{m} \propto \frac{p'}{\sqrt{\langle\tilde{p}^2\rangle_0}}$.

Following the procedure for the inverted propagator (8) outlined in [7], by applying the Wigner transformation (6), one arrives at a similar result. The kernel $K(x,x',p,p',t,t')$ (being time-dependent via $\hat{z}(t)$ and $\hat{u}(t)$), which provides the Wigner function $W(x,p,t)$ via

$$W(x,p,t) = \int_{-\infty}^{+\infty} dx'dp'\, K(x,x',p,p',t,t')W(x',p',t'=0)$$

with

$$\begin{aligned} W(x',p',t'=0) &= \frac{1}{\pi\hbar}\exp\left\{-\frac{x'^2}{2\langle\tilde{x}^2\rangle_0} - \frac{p'^2}{2\langle\tilde{p}^2\rangle_0}\right\} \\ &= \frac{1}{\pi\hbar}\exp\left\{-\frac{m}{\hbar}\left[\left(\frac{x'}{\alpha_0}\right)^2 + \left(\frac{\alpha_0 p'}{m}\right)^2\right]\right\}, \end{aligned} \tag{26}$$

(see, e.g., [11]), is given by the product of two delta functions where now, however, x' is replaced by $\frac{x'}{\alpha_0}$ and p' is replaced by $\frac{\alpha_0 p'}{m}$ and the transformed variables in the delta functions are determined by (23), (24), i.e.,

$$K(x,x',p,p',t,t'=0) = \delta\left[\left(\frac{x'}{\alpha_0}\right) - \left(\dot{\hat{z}}x - \hat{z}\frac{p}{m}\right)\right]\delta\left[\left(\frac{\alpha_0 p'}{m}\right) - \left(\hat{u}\frac{p}{m} - \dot{\hat{u}}x\right)\right].$$

Applying this kernel to the initial Wigner distribution function (26) yields the function $W(x,p,t)$ as

$$W(x,p,t) = \frac{1}{\pi\hbar}\exp\left\{-\frac{m}{\hbar}\left[\left(\dot{\hat{z}}x - \hat{z}\frac{p}{m}\right)^2 + \left(\hat{u}\frac{p}{m} - \dot{\hat{u}}x\right)^2\right]\right\}.$$

Using the definitions (13) and (16) of λ and its relation to the uncertainties as given in equations (20)–(22), finally allows one to write

$$W(x,p,t) = \frac{1}{\pi\hbar}\exp\left\{-\frac{2}{\hbar^2}\left[\langle\tilde{p}^2\rangle x^2 - \langle[\tilde{x},\tilde{p}]_+\rangle xp + \langle\tilde{x}^2\rangle p^2\right]\right\}, \tag{27}$$

where the time-dependence of the uncertainties is determined totally by the time-dependence of $\hat{z}(t)$ and $\hat{u}(t)$. In the case of time-dependent Gaussian wave packets, the classical time-dependence is expressed by the fact that the maximum of the wave packet follows the classical trajectory. This is taken into account by shifting the variables of position and momentum from x to $\tilde{x} = x - \langle x\rangle$ and p to $\tilde{p} = p - \langle p\rangle$. Since $\langle x\rangle$ and $\langle p\rangle$ are purely time-dependent quantities, $\tilde{x}$ and $\tilde{p}$ can replace x and p in equations (3), (4) since these equations only contain derivatives with respect to space, not time. So, x and p in (27) would be replaced by $\tilde{x}$ and $\tilde{p}$ which would lead to the result obtained in [16] showing the connection between the exponent of the time-dependent Wigner function and the dynamical Ermakov invariant that is connected with the parameters $\hat{z}$ and $\hat{u}$ of the time-dependent kernel $K(x,x',t,t')$ and has been defined in equation (19) (for details see also [11]).

In the quantum mechanical phase space picture according to Wigner, this results not only in changing initial position- and momentum-uncertainties into their values at time t but, also, an additional contribution occurs from the time-change of $\langle\tilde{x}^2\rangle$, or α^2, respectively, expressed by the term proportional to $\langle[\tilde{x},\tilde{p}]_+\rangle$, or $\dot{\alpha}\alpha$, respectively, in the exponent of $W(x,p,t)$.

All these quantum dynamical aspects are contained in the time-dependent parameters $\hat{z}$ and $\hat{u}$, entering the transformation matrix in (25). In particular, the change of the position uncertainty (proportional to α) is taken into account by the parameter $\hat{u}$, which can be expressed as [11]

$$\hat{u} = \dot{\hat{z}}\alpha^2 - \hat{z}\dot{\alpha}\alpha = \left(\frac{m}{\alpha_0 p_0}\right)[\dot{\eta}\alpha^2 - \eta\dot{\alpha}\alpha]. \tag{28}$$

For constant uncertainty $\alpha = \alpha_0$, $\hat{u}$ is simply proportional to the classical velocity $\dot{\eta}(t)$, for $\dot{\alpha} \neq 0$, however, the situation can become quite different. As an example the free motion shall be discussed briefly, since there $\alpha = \alpha(t)$, which is expressed in the spreading of the corresponding wave packet solution. For this purpose, also $\dot{\hat{u}}$ is now given in terms of η and $\dot{\eta}$ where the equations of motion (15) (for $\eta(t)$) and (18) (for $\alpha(t)$) are applied. So it follows from (28) that

$$\dot{\hat{u}} = \left(\frac{m}{\alpha_0 p_0}\right)\left[\dot{\eta}\dot{\alpha}\alpha - \eta\left(\dot{\alpha}^2 + \frac{1}{\alpha^2}\right)\right].$$

For constant $\alpha = \alpha_0$, all terms proportional to $\dot{\alpha}$ vanish and the transformation matrix in (25) can be written as

$$\mathbf{M} = \begin{pmatrix} \dot{\hat{z}} & -\hat{z} \\ -\dot{\hat{u}} & \hat{u} \end{pmatrix} = \left(\frac{m}{\alpha_0 p_0}\right)\begin{pmatrix} \dot{\eta} & -\eta \\ \frac{1}{\alpha_0^2} & \alpha_0^2\dot{\eta} \end{pmatrix}.$$

For the harmonic oscillator with constant width (note: there is another solution with oscillating width) $\alpha = \alpha_0 = \frac{1}{\sqrt{\omega}}$ and $\eta(t) = \frac{v_0}{\omega}\sin\omega t$ ($\eta(0) = 0$), $\dot{\eta} = v_0 \cos\omega t$ ($\dot{\eta}(0) = v_0 = \frac{p_0}{m}$), $\mathbf{M}$ turns into

$$\mathbf{M}_{\mathrm{HO}} = \left(\frac{m}{\alpha_0 p_0}\right)\begin{pmatrix} v_0\cos\omega t & -\frac{v_0}{\omega}\sin\omega t \\ v_0 \sin\omega t & \frac{v_0}{\omega}\cos\omega t \end{pmatrix} = \begin{pmatrix} \frac{1}{\alpha_0}\cos\omega t & -\alpha_0\sin\omega t \\ \frac{1}{\alpha_0}\sin\omega t & \alpha_0\cos\omega t \end{pmatrix},$$

i.e., (up to the constant α_0 that also occurs in the column vectors) just the classical result is reproduced.

However, for the free motion with $\eta(t) = v_0 t$, $\dot{\eta}(t) = v_0$, for constant $\alpha = \alpha_0$, one would obtain

$$\tilde{\mathbf{M}}_{\mathrm{fr}} = \left(\frac{m}{\alpha_0 p_0}\right)\begin{pmatrix} v_0 & -v_0 t \\ \frac{1}{\alpha_0^2}v_0 t & \alpha_0^2 v_0 \end{pmatrix},$$

that is different from the classical situation where the matrix element in the first column and second row would be zero. The consequence for a free motion wave packet with constant width would be that the transformation matrix would no longer describe a canonical transformation, since its determinant would no longer be equal to 1 but

$$\det(\tilde{\mathbf{M}}_{\mathrm{fr}}) = \left[1 + \left(\frac{t}{\alpha_0^2}\right)^2\right],$$

which just describes the time-dependence of the wave packet spreading.

For $\dot{\alpha} \neq 0$, the well-known time-dependence of the wave packet width, given by $\alpha^2(t) = \alpha_0^2\left[1 + \left(\frac{t}{\alpha_0^2}\right)^2\right]$ and obtained as a solution of equation (18) for $\omega = 0$, leads to the correct transformation matrix

$$\mathbf{M}_{\mathrm{fr}} = \left(\frac{m}{\alpha_0 p_0}\right)\begin{pmatrix} v_0 & -v_0 t \\ 0 & \alpha_0^2 v_0 \end{pmatrix}, \tag{29}$$

with $\det(\mathbf{M}_{\mathrm{fr}}) = 1$. This shows explicitly the influence of the time-dependence of the uncertainty α on the transformation describing the dynamics of the system.

It should also be mentioned that the determinant of $\mathbf{M}$, written in terms of η, $\dot{\eta}$, α and $\dot{\alpha}$ takes just the form of the Ermakov invariant, i.e.,

$$\mathbf{M} = \left(\frac{m}{\alpha_0 p_0}\right)\begin{pmatrix} \dot{\eta} & -\eta \\ -\dot{\eta}\dot{\alpha}\alpha + \eta\left(\dot{\alpha}^2 + \frac{1}{\alpha^2}\right) & \dot{\eta}\alpha^2 - \eta\dot{\alpha}\alpha \end{pmatrix} \tag{30}$$

yields

$$\det(\mathbf{M}) = \left(\frac{m}{\alpha_0 p_0}\right)^2 \left[\dot{\eta}^2\alpha^2 - 2\eta\dot{\eta}\alpha\dot{\alpha} + \eta^2\left(\dot{\alpha}^2 + \frac{1}{\alpha^2}\right)\right]$$

$$= \left(\frac{m}{\alpha_0 p_0}\right)^2 \left[(\dot{\eta}\alpha - \dot{\alpha}\eta)^2 + \left(\frac{\eta}{\alpha}\right)^2\right]. \tag{31}$$

At this point it appears appropriate to discuss some differences characteristic of our method in comparison with other approaches that try to find a quantum analogue to the classical canonical transformations in the case of time-dependent quantum systems, particularly, when the Wigner phase space formulation is applied.

So in [17, 18] the Wigner function for the free motion and Gaussian-shaped distribution function is given by ($\hbar = 1$)

$$W(x,p,t) = \frac{1}{\pi}\exp\left\{-\left[\frac{1}{b}\left(x - \frac{p}{m}t\right)^2 + bp^2\right]\right\}$$

with constant parameter b (that would, in our notation, correspond to $b = \frac{2}{\hbar^2}\langle\tilde{x}^2\rangle_0 = \frac{\alpha_0^2}{m\hbar} = \frac{\hbar^2}{2\langle\tilde{p}^2\rangle_0}$ (for a minimum uncertainty wave packet)). The equivalence to the conserved volume element in classical phase space is intended to be established by the statement: "this distribution is concentrated within the region where the exponent is less than 1 in magnitude" and, for the choice of a coordinate system where $b = 1$, "the above phase space distribution function is a circle at $t = 0$. As time progresses, the circle becomes a tilted ellipse while preserving its area." This elliptic deformation is a canonical transformation that corresponds to our transformation (29) but, in the case of these authors' description, the time-dependence in their transformation only originates from the classical dynamics, transforming the initial position x into $x - \frac{p}{m}t$ (with constant p). The correct spreading Gaussian wave packet for the free motion, however, obviously has a time-dependent width, corresponding to a time-dependent parameter b in the notation of the references quoted. This still holds if one considers the corresponding Wigner function. However, if the width in position space is time-dependent, in our notation $\dot{\alpha} \neq 0$, a third term in the exponent of the Wigner function, namely, the one taking into account the position-momentum-correlations (see equations (22) and (27)), must occur. This term is missing in the above-mentioned approach.

In another approach [19], a relation between the Wigner function for two-photon coherent states and the one for Glauber coherent states has been established that looks quite similar to our transformations (1) or (25). However, this method is based on combinations of creation and annihilation operators. It has been shown recently [20] that the Ermakov invariant (that is, up to a constant factor, equivalent to the determinant of our transformation matrix (25); see also (31)), can be factorized into two terms that are a kind of (complex) generalization of the creation and annihilation operators and turn into these for $\dot{\alpha} = 0$ (for further details, see [20]). Therefore, also in the approach [19] based on the usual creation and annihilation operators, the time-dependence of the uncertainties expressed by $\dot{\alpha} \neq 0$ is not taken into account.

It is also known in the literature that quantum uncertainties are related with classical error margins and that, particularly for quadratic Hamiltonians, the classical error margins satisfy the classical Hamiltonian equations [21]. Furthermore, in our case, it can even be shown that the quantum uncertainties obey equations of motion that can be derived from a quantum-uncertainty Hamiltonian function that now provides the time-evolution of the quantum uncertainties in a canonical formalism. This Hamiltonian is nothing but the ground state energy or, respectively, the energy contribution of the momentum and position fluctuations to the overall energy of the Gaussian wave packet solution for the system. To make these formal aspects obvious, we write the energy of the system, calculated as the mean value of the Hamiltonian operator using the

Gaussian wave packet solutions of the corresponding time-dependent Schrödinger equation, in the form (for the harmonic oscillator)

$$\begin{aligned}\langle H_{\text{op}}\rangle &= \frac{1}{2m}\langle p^2\rangle + \frac{m}{2}\omega^2\langle x^2\rangle = \left(\frac{1}{2m}\langle p\rangle^2 + \frac{m}{2}\omega^2\langle x\rangle^2\right) + \left(\frac{1}{2m}\langle \tilde{p}^2\rangle + \frac{m}{2}\omega^2\langle \tilde{x}^2\rangle\right)\\ &= \left(\frac{m}{2}\dot{\eta}^2 + \frac{m}{2}\omega^2\eta^2\right) + \left[\frac{\hbar}{4}\left(\dot{\alpha}^2 + \alpha^2\dot{\varphi}^2\right) + \frac{\hbar}{4}\omega^2\alpha^2\right]\\ &= E_{\text{cl}} + \tilde{E} = (T_{\text{cl}} + V_{\text{cl}}) + (\tilde{T} + \tilde{V}).\end{aligned}$$

In order to establish a Lagrangian/Hamiltonian formalism for the uncertainties, we assume that a corresponding Lagrangian $\tilde{\mathcal{L}}$ can be written as the difference between kinetic and potential energy fluctuations, but now expressed in terms of the variables α, φ and the corresponding velocities $\dot{\alpha}$, $\dot{\varphi}$, i.e.

$$\tilde{\mathcal{L}}(\alpha,\dot{\alpha},\varphi,\dot{\varphi}) = \tilde{T} - \tilde{V} = \frac{\hbar}{4}\left(\dot{\alpha}^2 + \alpha^2\dot{\varphi}^2 - \omega^2\alpha^2\right).$$

The corresponding Euler–Lagrange equations are then

$$\frac{d}{dt}\frac{\partial\tilde{\mathcal{L}}}{\partial\dot{\varphi}} - \frac{\partial\tilde{\mathcal{L}}}{\partial\varphi} = 0, \qquad \frac{d}{dt}\frac{\partial\tilde{\mathcal{L}}}{\partial\dot{\alpha}} - \frac{\partial\tilde{\mathcal{L}}}{\partial\alpha} = 0.$$

From the first equation follows $\frac{d}{dt}(\frac{\hbar}{2}\alpha^2\dot{\varphi}) = 0$, or, $\alpha^2\dot{\varphi} = \text{const}$, in agreement with equation (17); from the second equation follows $\ddot{\alpha} + \omega^2\alpha = \dot{\varphi}^2\alpha = \frac{\text{const}}{\alpha^3}$, equivalent to equation (18) (for const $= 1$).

The corresponding canonical momenta are then given by

$$\frac{\partial\tilde{\mathcal{L}}}{\partial\dot{\varphi}} = \frac{\hbar}{2}\alpha^2\dot{\varphi} = p_\varphi, \qquad \frac{\partial\tilde{\mathcal{L}}}{\partial\dot{\alpha}} = \frac{\hbar}{2}\dot{\alpha} = p_\alpha.$$

With the help of these definitions, the quantum energy contribution $\tilde{E} = \tilde{T} + \tilde{V}$ can be written in a Hamiltonian form as

$$\tilde{\mathcal{H}}(\alpha,p_\alpha,\varphi,p_\varphi) = \frac{p_\alpha^2}{\hbar} + \frac{p_\varphi^2}{\hbar\alpha^2} + \frac{\hbar}{4}\omega^2\alpha^2.$$

It is straightforward to show [13] that the corresponding Hamiltonian equations of motion again reproduce the results (17) and (18), only now expressed with the help of the canonical momenta. An interesting point is that because of relation (17), i.e. $\dot{\varphi} = \frac{1}{\alpha^2}$, the canonical "angular momentum" p_φ has the constant value $p_\varphi = \frac{\hbar}{2}$, a value that does not usually describe an orbital angular momentum but the non-classical angular momentum-type quantity spin.

Finally, using these results, the uncertainty product can be expressed as

$$U = \langle\tilde{x}^2\rangle\langle\tilde{p}^2\rangle = p_\varphi^2 + (\alpha p_\alpha)^2.$$

In this context it should be mentioned that some authors (e.g., [22, 23, 24]) assume that the role of the phase space volume in quantum mechanics is played by the square root of the so-called "invariant uncertainty product" $\langle\tilde{x}^2\rangle\langle\tilde{p}^2\rangle - \frac{1}{4}\langle[\tilde{x},\tilde{p}]_+\rangle^2 = \frac{\hbar^2}{4}$, which is definitely a constant of motion since it is equivalent to our quantity p_φ^2. So, this square root would just be $p_\varphi = \frac{\hbar}{2}\alpha^2\dot{\varphi}$ which, due to the equivalence between equations (9) and (17), leads back to the requirement for the determinant of our transformation matrix (25) to be equal to 1.

4 Conclusions and perspectives

In classical mechanics, canonical transformations can be characterized by certain properties, like the conservation of a volume element in phase space under these transformations, corresponding to Liouville's theorem that can easily be checked by calculating the Wronskian determinant of the transformation that should be equal to 1.

In quantum mechanics, this conservation law appears to have its correspondence in the conservation of a so-called "invariant uncertainty product" that holds for systems with time-dependent and time-independent quantum uncertainties since any explicit time-dependence of the uncertainties is compensated for by subtracting a term proportional to $\langle[\tilde{x},\tilde{p}]_+\rangle^2$. The remaining conserved quantity corresponds to the conservation of p_φ, the "angular momentum" for the motion of $\lambda(t)$ in the complex plane. Due to the equivalence of equations (9) and (17), this conservation law is identical with the requirement that the determinant of our transformation matrix (25) for the time-dependent quantum problem must be equal to 1. From equations (30) and (31), it finally follows that this requirement is identical with the existence of a dynamical invariant for the system, the so-called Ermakov invariant.

Another major result of our analysis is that, in the time-dependent quantum mechanical problem, the transformation (25) corresponding to the classical linear canonical transformation (1) and its time-independent quantum mechanical analogue (3), (4) does not only transform the *initial position* and *momentum* into its values at a later time but, also, does the same *simultaneously* with the *corresponding uncertainties*! In how far this is connected with the existence of a Lagrangian/Hamiltonian formulation of the dynamics of the quantum uncertainties will be further investigated.

So far, the discussion of the time-dependent case included only systems where the potential is at most quadratic in its variables. This might not be as restrictive as it seems at first sight since one may sometimes perform canonical transformations to reduce a given Hamiltonian to a quadratic form [25] which has been shown explicitly by Sarlet for some polynomial Hamiltonians. To what extent this method can also be applied in our case requires more detailed studies.

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