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Wigner distribution functions and the representation of a non-bijective canonical transformation in quantum mechanics

R Dirl†, P Kasperkovitz† and M Moshinsky‡§

† Technische Universitat Wien, Vienna, Austria

‡ Instituto de Física, Universidad Nacional Autonoma de Mexico, Apdo Postal 20-364, México, DF 01000, México

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Abstract. In a previous paper, with a similar title, we showed that for bijective (i.e. one-to-one onto) canonical transformations we can obtain their quantum mechanical representations in the form of a kernel in the phase space of Wigner distribution functions and recover our classical expectation for this kernel in the limit $\hbar \to 0$. For non-bijective canonical transformations the situation is more complex as the phase space acquires either a Riemann surface structure or requires the introduction of the concept of an ambiguity group. By discussing the non-bijective canonical transformation taking us from an oscillator of frequency κ^{-1}, where κ is an integer, to one of unit frequency, we see how the kernel is generalised to include the indices associated with the irreducible representations of the ambiguity group, i.e. the ambiguity spins. We obtain the kernel explicitly and show that in the limit $\hbar \to 0$ we recover the form that we expect in the Riemann surface picture of our phase space. While we illustrate our analysis through the representation in Wigner distribution phase space of a specific non-bijective canonical transformation, the procedure is clearly extendable to the representations of general canonical transformations of this type.

1. Introduction and summary

One of the authors (MM) and his collaborators have discussed extensively the representations in quantum mechanics of non-linear and non-bijective canonical transformations (Mello and Moshinsky 1975, Kramer *et al* 1978, Moshinsky and Seligman 1978, 1979, Deenen *et al* 1980, Flores *et al* 1986). The representations, to be denoted by U, were given in definite Hilbert spaces like, for example, the one associated with the coordinate q; thus the matrix elements $\langle q|U|q'\rangle$ associated with specific canonical transformations were derived explicitly. It is not easy though to see in this picture the quantum modifications to the canonical transformations, as the latter are formulated in phase space rather than in Hilbert space. Thus García-Calderón and Moshinsky (1980) discussed the representation of bijective (i.e. one-to-one onto) canonical transformations in the phase space version of quantum mechanics developed originally by Wigner (1932). In the present article we will extend the analysis to non-bijective canonical transformations through the specific example relating an oscillator of unit frequency with another one of frequency κ^{-1}, where κ is an integer. This example is sufficiently general to characterise the main features of the problem.

§ Member of El Colegio Nacional.

We proceed now to outline the main steps of our analysis. In § 2 we briefly review the work of García-Calderón and Moshinsky (1980) so as to derive the kernel, to be denoted by K, that serves as the representation of the canonical transformation in phase space, i.e. we determine explicitly the matrix element $\langle q'p'|K|qp\rangle$ in terms of that of $\langle q|U|q'\rangle$. In § 3 we discuss the non-bijective canonical transformation relating the action and angle of an oscillator of frequency 1 with the one of frequency κ^{-1}, where κ is integer, and give the corresponding representation $\langle q|U|q'\rangle$. In § 4 we derive $\langle q'p'|K|qp\rangle$ for the canonical transformation mentioned, while in § 5 we discuss its limit when $\hbar\to 0$ so as to recover the explicit classical limit of $\langle q'p'|K|qp\rangle$ mentioned in § 2. Finally in § 6 we indicate how we can proceed from our specific example to the general problem of representations of non-bijective canonical transformations in Wigner distribution space.

2. Representation of canonical transformations in the phase space of Wigner distribution functions

We begin by recalling the definition of the Wigner distribution function $f(q,p)$ for a given wavefunction $\psi(q)$, i.e.

$$f(q,p)=(\pi\hbar)^{-1}\int_{-\infty}^{\infty}\langle\psi|q+y\rangle\langle q-y|\psi\rangle\exp(\mathrm{i}2py/\hbar)\,\mathrm{d}y \tag{2.1}$$

where we use Dirac's notation $\langle q|\psi\rangle=\psi(q)$, $\langle\psi|q\rangle=\psi^*(q)$, and restrict ourselves to a single degree of freedom. As is well known (Wigner 1932), the integration of $f(q,p)$ with respect to p or q gives respectively the probability density for the state $|\psi\rangle$ in configuration or momentum space.

We consider now a canonical transformation

$$\begin{aligned}&Q=Q(q,p)\qquad P=P(q,p)\\&\{Q,P\}=\frac{\partial Q}{\partial q}\frac{\partial P}{\partial p}-\frac{\partial Q}{\partial p}\frac{\partial P}{\partial q}=1\end{aligned} \tag{2.2}$$

under which a *classical* distribution function $f(q,p)$ would of course transform into $F(q,p)$ given by

$$F(q,p)=f(Q(q,p),P(q,p)). \tag{2.3}$$

In quantum mechanics, however, the state $|\psi\rangle$ transforms (Mello and Moshinsky 1975, Kramer *et al* 1978, Moshinsky and Seligman 1978, 1979, Deenen *et al* 1980) into

$$|\psi\rangle\to|\Psi\rangle=U|\psi\rangle \tag{2.4}$$

and thus

$$\begin{aligned}F(q,p)&=(\pi\hbar)^{-1}\int_{-\infty}^{\infty}\langle\Psi|q+y\rangle\langle q-y|\Psi\rangle\exp(2\mathrm{i}py/\hbar)\,\mathrm{d}y\\&=(\pi\hbar)^{-1}\iiint_{-\infty}^{\infty}\mathrm{d}z_+\,\mathrm{d}y\,\mathrm{d}z_-[\langle\psi|z_+\rangle\langle z_+|U^\dagger|q+y\rangle\\&\qquad\times\langle q-y|U|z_-\rangle\langle z_-|\psi\rangle\exp(\mathrm{i}2py/\hbar)].\end{aligned} \tag{2.5}$$

Writing $z_\pm = q' \pm y'$ when it is associated with ψ, and $z_\pm = q' \pm \bar{y}'$ when it is associated with U, and integrating over q', y', $\bar{y}'$, y with the extra factor

$$\delta(y'-\bar{y}') = (\pi\hbar)^{-1}\int_{-\infty}^{\infty} \exp[2\mathrm{i}p'(y'-\bar{y}')/\hbar]\,\mathrm{d}p' \tag{2.6}$$

we immediately arrive at the relation

$$F(q,p) = \iint_{-\infty}^{\infty} \mathrm{d}q'\,\mathrm{d}p'\,f(q',p')\langle q'p'|K|qp\rangle \tag{2.7}$$

in which the kernel K is given by

$$\langle q'p'|K|qp\rangle = 2(\pi\hbar)^{-1}\iint_{-\infty}^{\infty} \mathrm{d}y\,\mathrm{d}y'\,\langle q'+y'|U^{+}|q+y\rangle\langle q-y|U|q'-y'\rangle$$
$$\times \exp[\mathrm{i}(2py-2p'y')/\hbar] \tag{2.8}$$

whereas from (2.3) we expect that in the classical limit, i.e. when $\hbar\to 0$, we should obtain

$$\lim_{\hbar\to 0}\langle q'p'|K|qp\rangle = \delta(q'-Q(q,p))\delta(p'-P(q,p)). \tag{2.9}$$

The above derivation of $\langle q'p'|K|qp\rangle$ is the one given by García-Calderón and Moshinsky (1980) and implicitly presupposes that the canonical transformation (2.2) is bijective (i.e. one-to-one onto) so that the representation $\langle q|U|q'\rangle$ has no ambiguity spin indices (Kramer *et al* 1978, Moshinsky and Seligman 1981). Furthermore the classical limit (2.9) holds in this case as the phase space has only one sheet. In the next section we consider a particular non-bijective canonical transformation and the way it affects the kernel (2.8) and its limit (2.9).

3. Non-bijective canonical transformations relating two oscillators of different frequencies and their representation in quantum mechanics

Among the simplest of the non-linear and non-bijective canonical transformations is the one that relates an oscillator of frequency κ^{-1}, with κ integer, with another one of unit frequency.

Denoting by q, p the coordinates and momenta of the oscillator of frequency κ^{-1}, and taking units in which the mass of the particle becomes unity, the Hamiltonian takes the form

$$\tfrac{1}{2}(p^2+\kappa^{-2}q^2). \tag{3.1}$$

It is convenient to carry out the dilation transformation

$$q\to\kappa^{1/2}q \tag{3.2a}$$

$$p\to\kappa^{-1/2}p \tag{3.2b}$$

to convert (3.1) into

$$\kappa^{-1}\tfrac{1}{2}(p^2+q^2)\equiv\kappa^{-1}j \tag{3.3a}$$

where j is the action variable of the oscillator (Moshinsky and Seligman 1978). The canonically conjugate variable to (3.3a) is given by

$$\kappa\varphi\equiv\kappa\tan^{-1}(p/q) \tag{3.3b}$$

where φ is the angle variable, and we have have the Poisson bracket relation

$$\{j, \varphi\}_{q,p} = \frac{\partial j}{\partial q}\frac{\partial \varphi}{\partial p} - \frac{\partial j}{\partial p}\frac{\partial \varphi}{\partial q} = 1. \tag{3.4}$$

Turning now our attention to the oscillator of unit frequency whose coordinates and momenta will be denoted by (Q, P) the corresponding action and angle variables are defined by (Moshinsky and Seligman 1978)

$$J = \tfrac{1}{2}(P^2 + Q^2) \tag{3.5a}$$

$$\Phi = \tan^{-1}(P/Q) \tag{3.5b}$$

where in this case the action J coincides with the Hamiltonian of the oscillator and we still have

$$\{J, \Phi\}_{Q,P} = 1. \tag{3.6}$$

The canonical transformation relating these two oscillators is just a dilation in the action–angle phase space, i.e.

$$\kappa^{-1} j = J \tag{3.7a}$$

$$\kappa\varphi = \Phi. \tag{3.7b}$$

To obtain the corresponding expression for Q, P as functions of q, p we notice that

$$Q = (2J)^{1/2}\cos\Phi = (2j/\kappa)^{1/2}\cos\kappa\varphi \tag{3.8a}$$

$$P = (2J)^{1/2}\sin\Phi = (2j/\kappa)^{1/2}\sin\kappa\varphi \tag{3.8b}$$

and using the development of $\cos(\kappa\varphi)$, $\sin(\kappa\varphi)$ in terms of powers of $\cos\varphi$, $\sin\varphi$ (Gradshteyn and Ryzhik 1965, p 27) together with the fact that

$$q = (2j)^{1/2}\cos\varphi \tag{3.9a}$$

$$p = (2j)^{1/2}\sin\varphi \tag{3.9b}$$

we get the non-linear canonical transformation (Moshinsky and Seligman 1981)

$$Q = \kappa^{-1/2}(q^2+p^2)^{(1-\kappa)/2}\sum_s \binom{\kappa}{2s} q^{\kappa-2s}(-1)^s p^{2s} \tag{3.10a}$$

$$P = \kappa^{-1/2}(q^2+p^2)^{(1-\kappa)/2}\sum_s \binom{\kappa}{2s+1} q^{\kappa-2s-1}(-1)^s p^{2s+1}. \tag{3.10b}$$

The mapping between the phase spaces (q, p) and (Q, P) is illustrated in figure 1 where clearly, from (3.7b), a sector of angle $(2\pi/\kappa)$ in the (q, p) plane of figure 1(a)

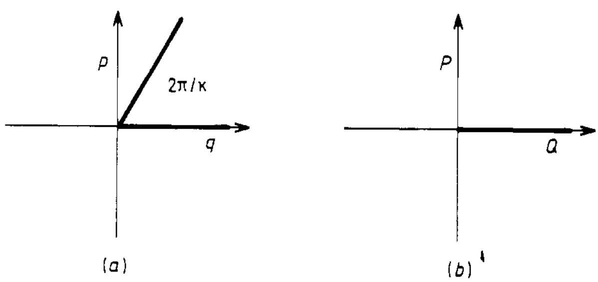

Figure 1. A sector $2\pi/\kappa$ in the (q, p) phase space of (a) is mapped on the full (Q, P) plane of (b) by the canonical transformation (3.10). The cut connecting the different sheets in the (Q, P) plane is marked by a bold line in (b).

is mapped on the full plane (Q, P) of figure 1(*b*). Thus the canonical transformation is non-bijective and to retrieve bijectivity (i.e. a mapping one-to-one onto) the phase plane (Q, P) must have κ sheets (Moshinsky and Seligman 1981) connected along the cut in the positive real axis Q as indicated by the bold line in figure 1(*b*).

In the previous paragraph bijectivity was recovered by associating a Riemann-type structure with the phase plane (Q, P). Alternatively this objective can be achieved by noting that the linear canonical transformation

$$\begin{aligned} q_\lambda &= q\cos(2\pi\lambda/\kappa) - p\sin(2\pi\lambda/\kappa) \\ p_\lambda &= q\sin(2\pi\lambda/\kappa) + p\cos(2\pi\lambda/\kappa) \end{aligned} \qquad \lambda = 0, 1, \ldots, \kappa-1 \tag{3.11}$$

implies $j_\lambda = j$, $\varphi_\lambda = \varphi + (2\pi\lambda/\kappa)$ and thus, from (3.8), gives us all points (q_λ, p_λ), $\lambda = 0, 1, \ldots, \kappa-1$ that map on a single point (Q, P). Because of this property the group of linear canonical transformations (3.11), which is isomorphic to the cyclic group C_κ, was called the ambiguity group (Kramer *et al* 1978, Moshinsky and Seligman 1981). Then, instead of a Riemann surface structure for the (Q, P) plane, we can retain it as a single sheet, but characterise the functions $f(Q, P)$ in it by irreducible representations (irreps), of the group C_κ, of which there are κ which again can be represented by an index λ taking the values $\lambda = 0, 1, \ldots, \kappa-1$ (Moshinsky and Seligman 1981). This index received the name of ambiguity spin and it proved fundamental for the definition and determination of the representation in quantum mechanics of non-bijective canonical transformations.

For the oscillators of frequency κ^{-1} and 1 the canonical transformation (3.10) has the ambiguity group (3.11), and thus its representation U in quantum mechanics must have an ambiguity spin index $\lambda = 0, 1, \ldots, \kappa-1$ associated with the irreps of this group. The matrix representation can then be written as $\langle q|U^\lambda|q'\rangle$ and its explicit form is given by (Kramer *et al* 1978, equation (6.9))

$$\langle q|U^\lambda|q'\rangle = \sum_{n=0}^{\infty} \phi_n(q)\phi^*_{n\kappa+\lambda}(q') \tag{3.12}$$

where $\phi_n(q)$ are the normalised solutions of the Schrödinger equation for an oscillator of unit mass and frequency

$$\frac{1}{2}\left(-\hbar^2\frac{\partial^2}{\partial q^2} + q^2\right)\phi_n(q) = \hbar(n+\tfrac{1}{2})\phi_n(q) \tag{3.13}$$

given by

$$\phi_n(q) = [(\pi\hbar)^{1/2}2^n n!]^{-1/2} H_n(q\hbar^{-1/2})\exp(-q^2/2\hbar) \tag{3.14}$$

where H_n are Hermite polynomials. Note that we keep Planck's constant $\hbar$ in our analysis as one of our main objectives will be to recover the classical picture when $\hbar \to 0$.

While the reader is referred to the paper of Kramer *et al* (1978) for the explicit derivation of (3.12) it is worthwhile to understand it intuitively. Dirac (1958) indicates that a canonical transformation that takes a given Hamiltonian into another, when both of them have continuous spectra in the interval $-\infty$ to ∞, would have the unitary representation

$$\langle q|U|q'\rangle = \int_{-\infty}^{\infty} \psi_E(q)\phi^*_E(q')\,\mathrm{d}E \tag{3.15}$$

where $\psi_E(q)$, $\phi_E(q)$ are the normalised eigenstates of the two Hamiltonians. This $\langle q|U|q'\rangle$ would have precisely the property of transforming the eigenstate $\phi_E(q)$ of one of the Hamiltonians into the eigenstate $\psi_E(q)$ of the other.

The expression (3.15) also holds for two Hamiltonians that have the same discrete spectra (Mello and Moshinsky 1975) except that a sum then replaces the integral.

In the case of Hamiltonians of oscillators of frequency κ^{-1} and 1, the spectra are not the same and in fact the former has κ levels in the interval in which the latter has only one. If we designate by ν the number of quanta of the oscillator of frequency κ^{-1}, we can write $\nu \equiv \lambda \bmod \kappa$, i.e. $\nu = n\kappa + \lambda$ where $\lambda = 0, 1, \ldots, \kappa - 1$. In this case for each value of λ we have only one level for the oscillator of frequency κ^{-1} in the interval where there is one level for the oscillator of frequency 1. The expression (3.12) for $\langle q|U^{\lambda}|q'\rangle$ establishes then a one-to-one correspondence between the states $\phi_{n\kappa+\lambda}(q)$ and $\phi_n(q)$ corresponding to these levels.

As the representation of the non-bijective canonical transformation (3.10) in ordinary Hilbert space carries the ambiguity spin index λ, i.e. $\langle q|U^{\lambda}|q'\rangle$, we see from (2.8) that the kernel K will carry two of these indices as we now have to write

$$\langle q'p'|K^{\lambda'\lambda}|qp\rangle = (2/\pi\hbar) \iint_{-\infty}^{\infty} \mathrm{d}y\, \mathrm{d}y' \langle q+y|U^{\lambda}|q'+y'\rangle^* \langle q-y|U^{\lambda'}|q'-y'\rangle \times \exp[\mathrm{i}(2py - 2p'y')/\hbar] \tag{3.16}$$

where we have made use of the fact that $\langle q'|U^{\dagger}|q\rangle = \langle q|U|q'\rangle^*$ in which * stands for conjugate.

In the next section we determine the explicit form of $\langle q'p'|K^{\lambda'\lambda}|qp\rangle$ and discuss its properties.

4. The matrix representation of the kernel K in the Wigner distribution phase space

The matrix $\langle q'p'|K^{\lambda'\lambda}|qp\rangle$, which carries the ambiguity spin indices $\lambda', \lambda = 0, 1, \ldots, \kappa - 1$ is given by (3.16). Substituting in it the value $\langle q|U^{\lambda}|q'\rangle$ of (3.12) we immediately obtain that

$$\langle q'p'|K^{\lambda'\lambda}|qp\rangle = (2\pi\hbar) \sum_{n,n'=0}^{\infty} f_{nn'}(q,p) f^*_{n\kappa+\lambda, n'\kappa+\lambda'}(q',p') \tag{4.1}$$

where

$$f_{nn'}(q,p) = (\pi\hbar)^{-1} \int_{-\infty}^{\infty} \phi^*_n(q+y)\phi_{n'}(q-y) \exp(\mathrm{i}2py/\hbar)\, \mathrm{d}y \tag{4.2}$$

and a similar definition holds for $f_{n\kappa+\lambda, n'\kappa+\lambda'}(q',p')$ where the * appearing in (4.1) and (4.2) implies conjugation.

To determine then $\langle q'p'|K^{\lambda'\lambda}|qp\rangle$ we require first the explicit expression of $f_{nn'}(q,p)$ of (4.2) where the function $\phi_n(q)$ is given by (3.14). Substituting y in (4.2) by

$$y = \mathrm{i}p + \hbar^{1/2}x \tag{4.3}$$

and taking into account the explicit expression of $\phi_n(q)$ given by (3.14), we see that $f_{nn'}(q,p)$ takes the form

$$f_{nn'}(q,p) = (-1)^{n'} \exp[-(q^2+p^2)/\hbar]\pi^{-1}\hbar^{-1/2}A_nA_{n'} \times \int_{-\infty}^{\infty} H_n(x+z)H_{n'}(x-z^*) \exp(-x^2)\, \mathrm{d}x \tag{4.4}$$

where

$$A_n = (\pi\hbar)^{-1/4}(2^n n!)^{-1/2} \tag{4.5}$$

and

$$z = [(q + \mathrm{i}p)/\hbar^{1/2}] \tag{4.6}$$

with z^* being its conjugate.

The last integral in (4.4) is given in Gradshteyn and Ryzhik (1965, p 838, formula 7.377) and introducing the notation

$$r = (q^2 + p^2)^{1/2} \tag{4.7a}$$

$$\varphi = \tan^{-1}(p/q) \tag{4.7b}$$

as well as

$$\rho = (2zz^*)^{1/2} = (2/\hbar)^{1/2} r \tag{4.7c}$$

one obtains for $f_{nn'}(q, p)$ the expression

$$f_{nn'}(q, p) = \pi^{-1/2}\hbar^{-1} R_{\nu|m|}(\rho)(2\pi)^{-1/2}\exp(\mathrm{i}m\varphi) \tag{4.8}$$

where $R_{\nu|m|}$ is the normalised radial function of the two-dimensional oscillator given by

$$R_{\nu|m|}(\rho) = [2(\nu!)/(\nu + |m|)!]^{-1/2}(-1)^\nu L_\nu^{|m|}(\rho)\rho^{|m|}\exp(-\rho^2/2) \tag{4.9}$$

with $L_\nu^{|m|}$ being a Laguerre polynomial. The ν, m in (4.8) are related to n, n' by

$$2\nu + |m| = n + n' \qquad m = n - n'. \tag{4.10}$$

The expression (4.8) is well known, having been derived, among others, by Krüger and Poffyn (1977) who, besides evaluating it directly, used the fact that $f_{nn'}(q, p)$ satisfies the (quantum) Liouville equation, and the eigenvalue equation for the energy in phase space, which are precisely those of a two-dimensional oscillator and its angular momentum.

As later we will have to carry out integrations over the phase space whose volume element is $\mathrm{d}q\,\mathrm{d}p$ we note that it becomes

$$r\,\mathrm{d}r\,\mathrm{d}\varphi = (\hbar/2)\rho\,\mathrm{d}\rho\,\mathrm{d}\varphi \tag{4.11}$$

if we use the coordinates (4.7).

To determine now explicitly the $\langle q'p'|K^{\lambda'\lambda}|qp\rangle$ of (4.1) we need the $f_{n\kappa+\lambda,n'\kappa+\lambda'}(q', p')$ in terms of the polar coordinates

$$\rho' = (2/\hbar)^{1/2}(q'^2 + p'^2)^{1/2} \qquad \varphi' = \tan^{-1}(p'/q'). \tag{4.12}$$

The function will again have the form (4.8) but with radial and angular quantum numbers ν', m' given by

$$2\nu' + |m'| = (n\kappa + \lambda) + (n'\kappa + \lambda') = (2\nu + |m|)\kappa + (\lambda + \lambda') \tag{4.13a}$$

$$m' = (n\kappa + \lambda) - (n'\kappa + \lambda') = m\kappa + (\lambda - \lambda'). \tag{4.13b}$$

While the m' is given explicitly by (4.13b), to determine ν' we need to discuss separately the cases $m > 0$, $m < 0$ and $m = 0$. If $m > 0$ we note that $m' > 0$ as $|\lambda - \lambda'| < \kappa$ and thus from (4.13) we have

$$\nu' = \nu\kappa + \lambda'. \tag{4.14a}$$

If $m<0$ then $m'<0$ again because $|\lambda-\lambda'|<\kappa$, and thus from (4.13) we have

$$\nu'=\nu\kappa+\lambda. \tag{4.14b}$$

If $m=0$ and $\lambda>\lambda'$ then $m'>0$ and $\nu'=\nu\kappa+\lambda'$, while if $\lambda<\lambda'$ then $m'<0$ and $\nu'=\nu\kappa+\lambda$. Both possibilities for $m=0$ are summarised by

$$\nu'=\nu\kappa+\min(\lambda,\lambda'). \tag{4.14c}$$

The expression (4.1) for $\langle q'p'|K^{\lambda'\lambda}|qp\rangle$ involves summations over the indices n, $n'=0,1,2,\ldots$. Through the relation (4.10) we can transform it to a summation over ν, m where $\nu=0,1,2,\ldots$ while $m=0,\pm1,\pm2,\ldots$. From the discussion of the previous paragraph it is convenient to separate the summation over m into m positive, m negative (where we change the sign of m) and $m=0$. We thus have

$$\begin{aligned}\langle q'p'|K^{\lambda'\lambda}|qp\rangle &= (\pi\hbar)^{-1}\exp[\mathrm{i}(\lambda'-\lambda)\varphi'] \\ &\quad\times\sum_{\nu=0}^{\infty}\Bigg(\sum_{m=1}^{\infty}[R_{\nu m}(\rho)\exp(\mathrm{i}m\varphi)R_{\nu\kappa+\lambda',m\kappa+\lambda-\lambda'}(\rho')\exp(-\mathrm{i}m\kappa\varphi')] \\ &\quad+\sum_{m=1}^{\infty}[R_{\nu m}(\rho)\exp(-\mathrm{i}m\varphi)R_{\nu\kappa+\lambda,m\kappa-\lambda+\lambda'}(\rho')\exp(\mathrm{i}m\kappa\varphi')] \\ &\quad+R_{\nu0}(\rho)R_{\nu\kappa+\min(\lambda,\lambda'),|\lambda-\lambda'|}(\rho')\Bigg).\end{aligned} \tag{4.15}$$

A check on the expansion (4.8) is provided when $\kappa=1$ in which case we see from (3.10) that we have the identity canonical transformation, i.e.

$$Q=q \qquad P=p \tag{4.16}$$

for which there are no ambiguity spin indices as $\lambda=\lambda'=0$. The kernel then must be (García-Calderón and Moshinsky 1980)

$$\begin{aligned}\langle q'p'|K|qp\rangle &= \delta(q-q')\delta(p-p') \\ &= \frac{1}{r'}\delta(r-r')\delta(\varphi-\varphi') \\ &= \left(\frac{2}{\hbar}\right)\frac{1}{\rho'}\delta(\rho-\rho')\delta(\varphi-\varphi').\end{aligned} \tag{4.17}$$

On the other hand from (4.15) we see that for $\kappa=1$ the kernel becomes

$$\begin{aligned}\langle q'p'|K|qp\rangle &= (2/\hbar)\sum_{\nu=0}^{\infty}\sum_{m=-\infty}^{\infty}[R_{\nu|m|}(\rho)(2\pi)^{-1/2}\exp(\mathrm{i}m\varphi)] \\ &\quad\times[R_{\nu|m|}(\rho')(2\pi)^{-1/2}\exp(\mathrm{i}m\varphi')]^* \\ &= (2/\hbar)(1/\rho')\delta(\rho-\rho')\delta(\varphi-\varphi')\end{aligned} \tag{4.18}$$

as the $[R_{\nu|m|}(\rho)(2\pi)^{-1/2}\exp(\mathrm{i}m\varphi)]$, $\nu=0,1,\ldots$, $m=0,\pm1,\ldots$, give a complete and orthonormal set of states in the ρ, φ space. We see that (4.17) and (4.18) coincide.

5. The kernel K in the classical limit

For bijective canonical transformations that take us from q, p to $[Q(q,p), P(q,p)]$, the expected classical limit of the kernel $\langle q'p'|K|qp\rangle$ is given by the product of δ functions appearing in (2.9), which transforms a Wigner distribution function $f(q,p)$ into $F(q,p)=f[Q(q,p), P(q,p)]$ as one would expect.

For the non-bijective case, such as the example discussed in § 3 of this paper, the classical limit is more complex, as the phase space (Q, P) has κ-sheets or, equivalently, the functions $f(Q, P)$ in it must be characterised by irreducible representation of the ambiguity group C_κ of (3.11).

Rather than guess the form of the classical limit as we could do it in the bijective case, we shall derive it from the limit of $\langle q'p'|K^{\lambda'\lambda}|qp\rangle$ when $\hbar\to 0$, and then show that the result agrees with what we would expect intuitively if we used the κ-sheeted Riemann surface structure of the Q, P phase space.

To achieve our purpose we first must analyse the behaviour of the radial function

$$R_{\nu|m|}(\rho)=R_{\nu|m|}[(2/\hbar)^{1/2}r] \tag{5.1}$$

when $\hbar\to 0$. We note from the definitions (4.7) and (4.9) that

$$\int_0^\infty (2/\hbar)(R_{\nu|m|}(\rho))^2 r\,\mathrm{d}r=1. \tag{5.2}$$

Furthermore as $\rho=(2/\hbar)^{1/2}r$ tends to ∞ when $\hbar\to 0$ we can replace in this limit the Laguerre polynomial in (4.9) by its highest power, i.e. (Gradhsteyn and Ryzhik, 1965, p 1037) by

$$(-1)^\nu L_\nu^{|m|}(\rho^2)\simeq(\rho^{2\nu}/\nu!) \tag{5.3}$$

so we can write when $h\to 0$ that

$$(2/\hbar)[R_{\nu|m|}(\rho)]^2\simeq(4/\hbar)[\nu!(\nu+|m|)!]^{-1}(\rho^2)^{2\nu+|m|}\exp(-\rho^2). \tag{5.4}$$

The right-hand side, considered as a function of ρ^2, has clearly a maximum at $\rho^2=2\nu+|m|$ for which

$$(2/\hbar)(R_{\nu|m|}(\rho))^2_{\max}\simeq(4/\hbar)[\nu!(\nu+|m|)!]^{-1}(2\nu+|m|)^{2\nu+|m|}\exp[-(2\nu+|m|)] \tag{5.5}$$

and thus, when $\hbar\to 0$, the maximum of this function tends to ∞. From (5.2) and (5.5) we conclude that, when $\hbar\to 0$, then

$$(2/\hbar)[R_{\nu|m|}(\rho)]^2\simeq(4/\hbar)\delta[\rho^2-(2\nu+|m|)] \tag{5.6}$$

since the right-hand side also has a maximum at $\rho^2=2\nu+|m|$ and its integral with respect to the volume element $r\,\mathrm{d}r$ is 1.

We now turn our attention to the terms $R_{\nu\kappa+\lambda',m\kappa+\lambda-\lambda'}(\rho')$, $R_{\nu\kappa+\lambda,m\kappa-\lambda+\lambda'}(\rho')$ and $R_{\nu\kappa+\min(\lambda,\lambda'),|\lambda-\lambda'|}(\rho')$ appearing in (4.15). A similar analysis indicates that for $m>0$ in the limit $\hbar\to 0$ we can write

$$\begin{aligned}(2/\hbar)(R_{\nu\kappa+\lambda,m\kappa-\lambda+\lambda'}(\rho'))^2&\simeq(2/\hbar)(R_{\nu\kappa+\lambda',m\kappa+\lambda-\lambda'}(\rho'))^2\\&\simeq(4/\hbar)\delta\{\rho'^2-[(2\nu+m)\kappa+(\lambda+\lambda')]\}\\&\simeq(4/\hbar)\delta[\rho'^2-(2\nu+m)\kappa]\end{aligned} \tag{5.7a}$$

while for $m=0$ we have

$$\begin{aligned}(2/\hbar)(R_{\nu\kappa+\min(\lambda,\lambda'),|\lambda-\lambda'|}(\rho'))^2&\simeq(4/\hbar)\delta[\rho'^2-(2\nu\kappa+\lambda+\lambda')]\\&\simeq(4/\hbar)\delta(\rho'-2\nu\kappa).\end{aligned} \tag{5.7b}$$

We note that $\rho'^2=(2/\hbar)r'^2$ and thus tends to ∞ when $\hbar\to 0$. This implies contributions from the δ functions only when ν, $|m|$ become very large and thus we can disregard the $\lambda+\lambda'$ appearing there as indicated on the right-hand side of (5.7*a*, *b*).

We now note from a similar analysis that when $\hbar\to 0$ we have

$$\{(2/\hbar)[\kappa^{-1/2}R_{\nu|m|}(\rho'\kappa^{-1/2})]^2\simeq(4/\hbar)\delta[\rho'^2-(2\nu+|m|)\kappa] \tag{5.8}$$

so clearly in the limit $\hbar\to 0$ all the radial functions appearing in (5.7) can be replaced by $\kappa^{-1/2}R_{\nu|m|}(\rho'\kappa^{-1/2})$ and thus substituting in (4.15) we obtain

$$\begin{aligned}\langle q'p'|K^{\lambda'\lambda}|qp\rangle\\ &\simeq\exp[\mathrm{i}(\lambda'-\lambda)\varphi'](2/\hbar)\sum_{m=-\infty}^{\infty}\left(\sum_{\nu=0}^{\infty}(R_{\nu|m|}(\rho)\kappa^{-1/2}R_{\nu|m|}(\rho'\kappa^{-1/2})\right.\\ &\quad\left.\times(2\pi)^{-1}\exp[im(\varphi-\kappa\varphi')]\right).\end{aligned} \tag{5.9}$$

For a fixed $|m|$ the $R_{\nu|m|}(\rho)$ constitute a complete set of orthonormal states where the volume element is $\rho\,\mathrm{d}\rho$ so that the summation over ν gives $(1/\rho')\delta(\rho-\rho'\kappa^{-1/2})$. This then leaves the summation

$$(2\pi)^{-1}\sum_{m=-\infty}^{\infty}\exp[im(\varphi-\kappa\varphi')]=\delta(\varphi-\kappa\varphi') \tag{5.10}$$

as is obvious from the Fourier expansion of the δ function. Thus we finally obtain

$$\lim_{\hbar\to 0}\langle q'p'|K^{\lambda'\lambda}|qp\rangle=\exp[\mathrm{i}(\lambda'-\lambda)\varphi'](1/r')\delta(r-r'\kappa^{-1/2})\delta(\varphi-\kappa\varphi') \tag{5.11}$$

where we made use of the fact that $\delta(ax)=a^{-1}\delta(x)$ to replace the ρ by r.

The expression (5.11) already resembles what we expect classically if we note that in action-angle phase space (j,φ) the canonical transformation (3.10) becomes just the dilation (3.7) and that furthermore $r=(2j)^{1/2}$. We notice though that the appearance of $\exp[\mathrm{i}(\lambda'-\lambda)\varphi']$ in (5.11) gives us a non-diagonal matrix in the indices λ, λ' as is to be expected in a picture in which the kernel is characterised by the irreps λ, λ' of the ambiguity group (Moshinsky and Seligman 1981).

In the Riemann surface picture of figure 1(*b*), we would expect the classical kernel to be diagonal in λ, λ' and to reflect the change in the relations between φ and φ' as we go from one sheet of the Riemann surface to another.

The analysis of Moshinsky and Seligman (1981) shows how we can transform operators from the ambiguity group picture to the Riemann surface picture for the canonical transformation (3.10) with the help of a unitary matrix whose elements are

$$V_{\lambda\mu}=\kappa^{-1/2}\exp(\mathrm{i}\lambda\varphi/\kappa)\exp(\mathrm{i}2\pi\lambda\mu/\kappa)\qquad\lambda,\mu=0,1,\ldots,\kappa-1. \tag{5.12}$$

With it we can write the kernel, to be denoted by $\bar{K}$, in the Riemann surface picture in the form

$$\langle q'p'|\bar{K}^{\mu'\mu}|qp\rangle=\sum_{\lambda',\lambda=0}^{\kappa-1}V^{+}_{\mu'\lambda'}\left(\lim_{\hbar\to 0}\langle q'p'|K^{\lambda'\lambda}|qp\rangle\right)V_{\lambda\mu} \tag{5.13}$$

where $^{+}$ denotes the Hermitian conjugate and thus $V^{+}_{\mu'\lambda'}=V^{*}_{\lambda'\mu'}$.

Before substituting (5.11) and (5.12) in (5.13) we notice that

$$\delta(\varphi-\kappa\varphi')=\kappa^{-1}\sum_{\tau=0}^{\kappa-1}\delta\{[(\varphi+2\pi\tau)/\kappa]-\varphi'\} \tag{5.14}$$

as

$$(2\pi)^{-1}\sum_{m=-\infty}^{\infty}\exp[im(\varphi-\kappa\varphi')]$$
$$=(2\pi)^{-1}\kappa^{-1}\sum_{\tau=0}^{\kappa-1}\sum_{M=-\infty}^{\infty}\exp\{iM[(\varphi+2\pi\tau)/\kappa-\varphi']\} \tag{5.15}$$

where (5.15) follows from the fact that

$$\kappa^{-1}\sum_{\tau=0}^{\kappa-1}\exp[i2\pi\tau M/\kappa]=\begin{cases}1 & \text{if } M=m\kappa\\ 0 & \text{otherwise.}\end{cases} \tag{5.16}$$

We then have that

$$\langle q'p'|\bar{K}^{\mu'\mu}|qp\rangle$$
$$=(1/r')\delta(r-r'\kappa^{-1/2})\kappa^{-2}\sum_{\lambda,\lambda',\tau=0}^{\kappa-1}\{\exp[i(\lambda'-\lambda)(\varphi'-\varphi\kappa^{-1})]$$
$$\times\exp(-i2\pi\mu'\lambda'/\kappa)\delta[(2\pi\tau/\kappa)-(\varphi'-\varphi\kappa^{-1})]\exp(i2\pi\mu\lambda/\kappa)\}$$
$$=(1/r)\delta(\kappa^{1/2}r-r')\sum_{\tau=0}^{\kappa-1}\left(\kappa^{-1}\sum_{\lambda'=0}^{\kappa-1}\exp[i2\pi(\tau-\mu')\lambda'/\kappa]\right)$$
$$\times\left(\kappa^{-1}\sum_{\lambda=0}^{\kappa-1}\exp[i2\pi(\mu-\tau)\lambda/\kappa]\right)\delta[\kappa^{-1}(\varphi+2\pi\tau)-\varphi'] \tag{5.17}$$

where the right-hand side was obtained with the help of the δ function, and in which the large round brackets give $\delta_{\mu'\tau}$, $\delta_{\mu\tau}$ so we finally get

$$\langle q'p'|\bar{K}^{\mu'\mu}|qp\rangle=(1/r)\delta(\kappa^{1/2}r-r')\delta[\kappa^{-1}(\varphi+2\pi\mu)-\varphi']\delta_{\mu'\mu}. \tag{5.18}$$

The expression (5.18) is now the classical limit of the kernel that agrees with our intuition about the canonical transformation (3.7) in the action–angle phase space. The action which is $(r'^2/2)$ goes into $\kappa(r^2/2)$, but the angle φ' does not go into φ/κ but into $(\varphi+2\pi\mu)/\kappa$ depending which sheet we are in the (Q, P) Riemann surface of figure 1.

We have thus not only obtained explicitly the quantum kernel given by (4.15) but have also shown that it gives the correct classical limit (5.18) in the Riemann surface picture.

So far our discussion was restricted to the specific non-bijective canonical transformation relating the oscillators of frequency κ^{-1} and 1. In the next section we outline the procedure for arbitrary non-bijective canonical transformations.

6. Conclusion

For general non-bijective canonical transformations in classical mechanics we have shown that bijectivity can be recovered, either by introducing a Riemann-type sheet structure in the phase plane, or by the concept of the ambiguity group (Kramer *et al* 1978, Moshinsky and Seligman 1981). The latter is more convenient as it can be incorporated in quantum mechanics through the concept of ambiguity spin.

Thus, in principle, we can always obtain the representation, in the ordinary Hilbert spaces of quantum mechanics, of a non-bijective canonical transformation, but now this representation will also contain ambiguity spin indices.

The translation to the Wigner distribution phase space is then given by (3.16) and the kernel K will have not one but two sets of ambiguity spin indices, reflecting the fact that we are in (q, p) rather than in q or p space.

The kernel can be calculated either directly, as is done for the canonical transformation (3.10) in (4.1) and (4.15), or a quantum Liouville equation and an eigenvalue equation for the energy of the type discussed by Kruger and Poffyn (1977) can be obtained for terms appearing in the kernel, and thus it could be determined from these equations as was indicated in the paragraph following (4.10).

Once we have our kernel K in the Wigner distribution phase space we can pass to its classical limit by taking $\hbar \to 0$. This limit gives the kernel in the picture associated with the ambiguity group. The passage from this picture to the Riemann surface one is a purely classical problem whose general features have been outlined by Moshinsky and Seligman (1981).

Thus the procedures discussed in this and previous papers can be extended to the analysis of kernels in Wigner distribution phase space associated with arbitrary non-bijective canonical transformations.

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