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Wavefunctions on phase space

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Abstract

Theories of Torres-Vega and Fredrick (1993 *J. Chem. Phys.* **98** 3103), Harriman (1994 *J. Chem. Phys.* **100** 3651) and of Ban (1998 *J. Math. Phys.* **39** 1744), in which phase space points (p, q) are used as configurational variables to formulate quantum mechanics are considered from the standpoint of a class of quantization schemes associating phase space functions with operators. The connection between these schemes and the theories given in Torres-Vega and Fredrick (1993 *J. Chem. Phys.* **98** 3103), Harriman (1994 *J. Chem. Phys.* **100** 3651), Dirac (1930 *The Principles of Quantum Mechanics* (Oxford: Oxford University Press)), Møller, Jørgensen and Torres-Vega (1997 *J. Chem. Phys.* **106** 7228), Klauder and Skagerstam (1985 *Coherent States: Applications in Physics and Mathematical Physics* (Singapore: World Scientific)), Li, Wei and Lü (2004 *Phys. Rev.* A **70** 022105), Ban (1998 *J. Math. Phys.* **39** 1744) is made by means of augmented wavefunctions $\psi_\sigma^{(\lambda)}(p, q; t)$, where $\lambda = 0$ corresponds to the ordering of Wigner and Weyl. For that case we use these functions to define a family of positive operator-valued measures for the phase angle of an harmonic oscillator.

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1. Introduction

The usual formulation of quantum mechanics in phase space is that of Weyl's association [1, 2] of operators $\hat{A}$ with functions $A(p, q)$ and Wigner's equivalent association [3] of the density matrix $\hat{\rho}$ with his function $W(p, q, t)$. As discussed by Cohen [4], the Wigner–Weyl association is but one of an infinite number of possibilities.

It is natural to wonder whether one can also find associations between wavefunctions $|\psi\rangle$ and phase space functions. To try to achieve this Torres-Vega and co-workers [5] and, independently, Harriman [6] have hypothesized a phase space representation which they write as $|\Gamma\rangle = |p, q\rangle$ corresponding to 'eigenstates' of some (unspecified) operator $\hat{\Gamma}$ so that,

$$\hat{\Gamma}|\Gamma'\rangle = \Gamma'|\Gamma'\rangle \qquad \text{and} \qquad \langle\Gamma'|\Gamma''\rangle = \delta(\Gamma' - \Gamma''). \tag{1}$$

In this formalism, it is suggested that any state $|\psi\rangle$ in Hilbert space, can be represented by $\psi(\Gamma) = \langle\Gamma|\psi\rangle$ and that closure obtains, so that

$$\int |\Gamma\rangle \, \mathrm{d}\Gamma \langle\Gamma| = 1, \tag{2}$$

although the details of this measure are not defined. In this theory the actions of the usual position and momentum operators on $\langle\Gamma|$ take the general forms

$$\langle\Gamma|\hat{q}|\psi\rangle = \left(\alpha q + \mathrm{i}\hbar\beta\frac{\partial}{\partial p}\right)\psi(\Gamma) \tag{3}$$

and

$$\langle\Gamma|\hat{p}|\psi\rangle = \left(\gamma p + \mathrm{i}\hbar\delta\frac{\partial}{\partial q}\right)\psi(\Gamma), \tag{4}$$

where (to preserve canonicality between $\hat{p}$ and $\hat{q}$) the real dimensionless parameters α, β, γ and δ must obey the relation

$$\beta\gamma - \alpha\delta = 1. \tag{5}$$

The actions of $\hat{p}$ and $\hat{q}$ are well known of course [7]. For example, the product of $\langle\Gamma|$ with 'eigenstates' of the position operator follows from (3) and (4), which give

$$\langle\Gamma|q'\rangle q' = \left(\alpha q + \mathrm{i}\hbar\beta\frac{\partial}{\partial p}\right)\langle\Gamma|q'\rangle \qquad \text{and} \qquad \mathrm{i}\hbar\frac{\partial}{\partial q'}\langle\Gamma|q'\rangle = \left(\gamma p + \mathrm{i}\hbar\delta\frac{\partial}{\partial q}\right)\langle\Gamma|q'\rangle.$$

These have the solution [11]

$$\langle\Gamma|q'\rangle = G\left(q' + \frac{q}{\delta}\right)\mathrm{e}^{-\mathrm{i}\frac{p}{\hbar\beta}(q'-\alpha q)}, \tag{6}$$

where G is an arbitrary function.

The formalism in equations (1)–(4) was suggested ([5], [8]) by the properties of coherent states. In their generalized form these are [9]

$$|p, q; \sigma\rangle \equiv \hat{D}[p, q]|\sigma\rangle, \tag{7}$$

where $|\sigma\rangle$ is any 'fiducial state,' and

$$\hat{D}[p, q] = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p\hat{q} - q\hat{p})}. \tag{8}$$

By using the relations

$$\exp[\mathrm{i}(\xi\hat{q} + \eta\hat{p})] = \exp\left(\mathrm{i}\frac{\hbar}{2}\xi\eta\right)\exp(\mathrm{i}\xi\hat{q})\exp(\mathrm{i}\eta\hat{p}) = \exp\left(-\mathrm{i}\frac{\hbar}{2}\xi\eta\right)\exp(\mathrm{i}\eta\hat{p})\exp(\mathrm{i}\xi\hat{q}) \tag{9}$$

and differentiating with respect to parameters, it is easy to show that

$$\langle p, q; \sigma|\hat{q} = \left(\frac{q}{2} + \mathrm{i}\hbar\frac{\partial}{\partial p}\right)\langle p, q; \sigma| \qquad \text{and} \qquad \langle p, q; \sigma|\hat{p} = \left(\frac{p}{2} - \mathrm{i}\hbar\frac{\partial}{\partial q}\right)\langle p, q; \sigma|,$$

corresponding to the choices $\alpha = \gamma = 1/2$ and $\beta = 1 = -\delta$ in equations (3) and (4). The generalized coherent states are over-complete [9] so they satisfy equation (2) with $\mathrm{d}\Gamma = \mathrm{d}p\,\mathrm{d}q/h$,

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}|p, q; \sigma\rangle\langle p, q; \sigma| = 1, \tag{10}$$

but they do not obey an orthogonality relation like that in equation (1). Indeed, using relations (9) gives the result

$$\langle p', q'; \sigma|p, q; \sigma\rangle = \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}(pq' - p'q)}\langle\sigma|p - p', q - q'; \sigma\rangle,$$

which is quite smooth in its p and q dependence. Difficulties along this line have been indicated by Li *et al* [10].

It appears that working with ordinary coherent states in Hilbert space cannot satisfy both requirements (1) and (2). But the fact that the pair (p, q) lies in $R \otimes R$, suggests working in a larger Hilbert space. For example, Ban [11] has developed his 'relative-state' formalism in an extended Hilbert space $\widetilde{H} = H \otimes H_{\rm r}$, where H and $H_{\rm r}$ are 'relevant' and 'reference' Hilbert spaces, respectively. Using his notation, and with his choice of $\hbar = 1$, a complete (but not over-complete) orthonormal set of state vectors in the augmented space $\widetilde{H}$ are $\{|\omega(r, k; s)\rangle; r, k \epsilon R\}$, where s is a real parameter, and

$$|\omega(r, k; s)\rangle = \frac{1}{\sqrt{2\pi}} \, \mathrm{e}^{-\frac{\mathrm{i}}{2}(1+s)kr} \int_{-\infty}^{\infty} \mathrm{d}x |x\rangle \otimes |x - r\rangle_r \, \mathrm{e}^{\mathrm{i}kx}. \tag{11}$$

Here $|x + r\rangle$ and $|x\rangle_r$ are position 'eigenstates' for H and $H_{\rm r}$, s is a real parameter, r and k are position and momentum variables, and a 'phase space' completeness relation like equation (1) is satisfied:

$$\langle\langle\omega(r'k'; s)|\omega(r, k; s)\rangle\rangle = \delta(r - r')\delta(k - k').$$

In this formalism, one ultimately seeks the behaviour of states in the relevant system by choosing some state $\phi(x)$ in the reference system and projecting $|\omega(r, k; s)\rangle$ onto it, so obtaining a state in H, namely

$$|\omega(r, k; s)\rangle = \frac{1}{\sqrt{2\pi}} \, \mathrm{e}^{-\frac{\mathrm{i}}{2}(1+s)kr} \int_{-\infty}^{\infty} \mathrm{d}x |x\rangle \phi^*(x - r) \, \mathrm{e}^{\mathrm{i}kx}, \tag{12}$$

which are over-complete in H, so that

$$\int_{-\infty}^{\infty} \mathrm{d}r \, \mathrm{d}k |\omega(r, k; s)\rangle\langle\omega(r, k; s)| = 1. \tag{13}$$

For a given s, the representation of an arbitrary state $|\psi\rangle$ in H is then the phase space function

$$\psi_s(r, k) \equiv \langle\omega(r, k; s)|\psi\rangle, \tag{14}$$

which is normalized

$$\int_{-\infty}^{\infty} \mathrm{d}r \, \mathrm{d}k |\psi_s(r, k)|^2 = 1. \tag{15}$$

Among many other properties, Ban shows, where $\hat{q}$ and $\hat{p}$ are the usual position and momentum operators in H, that

$$\langle\omega(r, k; s)|\hat{q}|\psi\rangle = \left[\frac{1}{2}(1 + s)r + \mathrm{i}\frac{\partial}{\partial k}\right] \psi_s(r, k), \tag{16}$$

and

$$\langle\omega(r, k; s)|\hat{p}|\psi\rangle = \left[\frac{1}{2}(1 - s)k - \mathrm{i}\frac{\partial}{\partial r}\right] \psi_s(r, k). \tag{17}$$

This scheme is consistent with equations (3) and (4) by, for example, making the associations $\hbar k = 2p$, $r = 2q$, $\beta = 1/2$, $(s + 1) = \alpha = \gamma$ and $\delta = 1/2$.

Equations (13), (16) and (17) suggest a formulation of quantum mechanics in phase space with points (r, k). For instance, with a Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \tag{18}$$

one can write the usual Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial}{\partial t}|\psi, t\rangle = \hat{H}|\psi, t\rangle \tag{19}$$

in Ban's notation as

$$\mathrm{i}\frac{\partial}{\partial t}\psi_s(r,k;t) = H\left(\frac{(1+s)}{2}r + \mathrm{i}\frac{\partial}{\partial k}, \frac{(1-s)}{2}k - \mathrm{i}\frac{\partial}{\partial r}\right)\psi_s(r,k;t) \tag{20}$$

and calculating expectations of operators $A(\hat{p},\hat{q})$, when there is no ambiguity concerning order, as

$$\langle\psi,t|A(\hat{q},\hat{p})|\psi,t\rangle = \int_{-\infty}^{\infty}\mathrm{d}r\,\mathrm{d}k\psi_s^*(r,k;t)A\left(\frac{(1+s)}{2}r + \mathrm{i}\frac{\partial}{\partial k}, \frac{(1-s)}{2}k - \mathrm{i}\frac{\partial}{\partial r}\right)\psi_s(r,k;t). \tag{21}$$

Very recently, de Gosson [12] has discussed some mathematical aspects of the case $\alpha = 1 = \beta, \gamma = 0, \delta = -1$ (in equations (3) and (4)) from the standpoint of the Weyl calculus. The approach I shall follow here is also to start with the Wigner–Weyl picture and then consider alternatives.

Section 2 formally describes the phase space picture of Wigner and Weyl, uses it to define the phase space wavefunction $\psi_\sigma(p,q;t)$, and discusses its time propagation for a Hamiltonian $H(p,q) = p^2/2m + V(q)$. The system configuration is labelled by phase space points (p,q), so there are two independent canonical operator pairs, $(\hat{\mathbf{p}}_1, \hat{\mathbf{q}}_1)$ and $(\hat{\mathbf{p}}_2, \hat{\mathbf{q}}_2)$. A parallel is drawn between this theory and that of Ban [11]. The formulation of section 2 is completely consistent with the prescription of equations (1)–(4). Section 3 considers matrix elements with respect to augmented wavefunctions, and in particular the phase angle (roughly speaking, $\arctan(p/q)$), which gives rise to a family of positive operator-valued measures which are consistent with the notion that the distribution of phase angle for an harmonic oscillator in a pure number state ought to be random. Section 4 looks at the formalism from the standpoint of orderings [4] different from that of Wigner and Weyl. These orderings lead to a family of momentum and position operators satisfying (3) and (4). Section 5 is a discussion.

2. Wigner–Weyl picture

The commonest phase space description of quantum mechanics is given by the Weyl transform [13]. Here I shall adopt a formal but efficient notation [14]. The Weyl correspondence of an operator $\hat{A}$ with a function $A(p,q)$ is given by

$$A(p,q) = \mathrm{Tr}(\hat{A}\hat{\Delta}(p,q)) \tag{22}$$

and

$$\hat{A} = \int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}A(p,q)\hat{\Delta}(p,q), \tag{23}$$

where

$$\begin{aligned}\hat{\Delta}(p,q) &= \int_{-\infty}^{\infty}\frac{\mathrm{d}p'\,\mathrm{d}q'}{h}\exp\left[-\frac{\mathrm{i}}{\hbar}(p'q - q'p)\right]\hat{D}[p',q'] \\ &= \int_{-\infty}^{\infty}\mathrm{d}x\exp\left(\frac{\mathrm{i}}{\hbar}px\right)\left|q+\frac{x}{2}\right\rangle\left\langle q-\frac{x}{2}\right|.\end{aligned} \tag{24}$$

Formally $\hat{\Delta}$ has the properties that its trace is unity, that

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}\hat{\Delta}(p,q) = 1, \tag{25}$$

and that

$$\mathrm{Tr}(\hat{\Delta}(p,q)\hat{\Delta}(p',q')) = h\delta(p-p')\delta(q-q'). \tag{26}$$

From these properties one can show that, for two operators $\hat{A}$ and $\hat{B}$,

$$\mathrm{Tr}(\hat{A}\hat{B}) = \int_{-\infty}^{\infty} \frac{\mathrm{d}p\,\mathrm{d}q}{h} A(p,q)B(p,q), \tag{27}$$

and that the Weyl transform of the product is

$$(\hat{A}\hat{B})(p,q) = A(p,q)\exp\left[\frac{\mathrm{i}\hbar}{2}\left(\frac{\partial^*}{\partial q}\frac{\partial}{\partial p} - \frac{\partial^*}{\partial p}\frac{\partial}{\partial q}\right)\right]B(p,q), \tag{28}$$

where the starred operators act to the left on $A(p,q)$. The Wigner function for a quantum system is defined as the Weyl transform of the density matrix divided by h.

Henceforth I shall restrict the discussion to Hamiltonians of the form (18), which, by equation (28) has the Weyl transform

$$H(p,q) = \frac{p^2}{2m} + V(q). \tag{29}$$

The evolution from an initial state $|\psi\rangle$ is given by

$$|\psi;t\rangle = \hat{U}_t|\psi\rangle, \qquad \text{where} \quad \hat{U}_t = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}t\right). \tag{30}$$

Taking the matrix element of $\hat{\Delta}$ between any state $|\psi\rangle$ and some chosen background or 'drone' state, $|\sigma\rangle$ gives, by (22), the phase space wavefunction

$$\begin{aligned}\psi_\sigma(p,q) &\equiv \langle\sigma|\hat{\Delta}(p,q)|\psi\rangle = (|\psi\rangle\langle\sigma|)(p,q)\\ &= \int_{-\infty}^{\infty} \frac{\mathrm{d}p\,\mathrm{d}q}{h}\exp\left[-\frac{\mathrm{i}}{\hbar}(p'q - q'p)\right]\langle p',q';\sigma|\psi\rangle.\end{aligned} \tag{31}$$

Generally, if $|\psi\rangle$ and $|\mu\rangle$ are any two states, then, by (31) and (27)

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p\,\mathrm{d}q}{h}\psi_\sigma^*(p,q)\mu_\sigma(p,q) = \langle\psi|\mu\rangle, \tag{32}$$

independent of $|\sigma\rangle$. In particular, ψ_σ is normalized with respect to the phase space integral.

$\psi_\sigma(p,q)$ is the Weyl symbol of $|\psi\rangle\langle\sigma|$. It can be closely related to Ban's formalism, equations (11), (12) and (14). To see this, use equations (24) and (31) to get

$$\begin{aligned}\psi_\sigma(p,q) &= \int_{-\infty}^{\infty} \mathrm{d}x\,\exp\left(-\frac{2\mathrm{i}}{\hbar}px\right)\sigma^*\left(q+\frac{x}{2}\right)\psi\left(q-\frac{x}{2}\right)\\ &= 2\exp\left(\frac{2\mathrm{i}}{\hbar}pq\right)\int_{-\infty}^{\infty}\mathrm{d}x\,\exp\left(-\frac{2\mathrm{i}}{\hbar}px\right)\psi(x)\sigma^*(2q-x),\end{aligned} \tag{33}$$

corresponding, for instance, to the choices $\sigma^*(-x) = \phi(x)$, $k = 2p/\hbar$, $r = 2q$ and $s = 0$ in equation (12). So these ψ_σ are essentially equivalent to a special case of Ban's states $\psi_s(r,k)$, equation (14). And, by analogy with $|\omega(r,k;s)\rangle$, equation (11), we can write

$$\psi_\sigma(p,q) = \langle(p,q)|\psi\rangle_\sigma, \tag{34}$$

where the new notation indicates that $\langle(p,q)|$ is not a product $\langle p|\langle q|$, although $(p,q) \in R\otimes R$.

Formally, from (31) with (30), (22) and (27), the time evolution of ψ_σ (with $|\sigma\rangle$ fixed) is

$$\begin{aligned}\psi_\sigma(p,q;t) &= \mathrm{Tr}(\hat{\Delta}(p,q)\hat{U}(t)|\psi\rangle\langle\sigma|)\\ &= \int_{-\infty}^{\infty}\frac{\mathrm{d}p'\,\mathrm{d}q'}{h}(\hat{\Delta}(p,q)\hat{U}(t))(p',q')(|\psi\rangle\langle\sigma|)(p',q')\\ &= \int_{-\infty}^{\infty}\mathrm{d}p'\,\mathrm{d}q'R(p,q,t|p',q',0)\psi_\sigma(p',q';0),\end{aligned} \tag{35}$$

where

$$R(p,q,t|p',q',t') = \frac{1}{h}\mathrm{Tr}(\hat{\Delta}(p,q)\hat{U}(t-t')\hat{\Delta}(p',q')). \tag{36}$$

Equation (26) shows that, as $t - t' \to 0$, $R(p,q,t|p',q',t') \to \delta(p-p')\delta(q-q')$, and equations (22)–(36) can be used to show that it is a propagator, obeying the equation

$$\int_{-\infty}^{\infty} \mathrm{d}p'\,\mathrm{d}q' R(p,q,t|p',q',t')R(p',q',t'|p_0,q_0,t_0) = R(p,q,t|p_0,q_0,t_0). \tag{37}$$

Another property of $R(p,q,t|p',q',t')$ is that its integral over p and q (or p' and q') generates the Weyl transform of $\hat{U}_{t-t'}$. For instance, by (25)

$$\int_{-\infty}^{\infty} \mathrm{d}p'\,\mathrm{d}q' R(p,q,t|p',q',t') = \mathrm{Tr}(\hat{\Delta}(p,q)\hat{U}(t-t')) = U(p,q,t-t'). \tag{38}$$

The equation of motion obeyed by R is easy to find when it is driven by the Hamiltonian (18): use

$$\mathrm{i}\hbar\frac{\partial}{\partial t}(\hat{U}_t\hat{\Delta}(p',q')) = \hat{H}\hat{U}_t\hat{\Delta}(p',q'),$$

and apply (28). Collecting terms give

$$\mathrm{i}\hbar\frac{\partial}{\partial t}R(p,q,t|p',q',0) = \hat{\mathbf{h}}_1 R(p,q,t|p',q',0), \tag{39}$$

where

$$\hat{\mathbf{h}}_1 = \frac{1}{2m}\hat{\mathbf{p}}_1^2 + V(\hat{\mathbf{q}}_1) \tag{40}$$

is a Hamiltonian acting in the configuration (phase) space with operators

$$\hat{\mathbf{p}}_1 = p + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial q} \qquad \text{and} \qquad \hat{\mathbf{q}}_1 = q - \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}. \tag{41}$$

Note that $\hat{\mathbf{p}}_1$ and $\hat{\mathbf{q}}_1$ are conjugate to each other when acting on functions in phase space, so that $[\hat{\mathbf{p}}_1, \hat{\mathbf{q}}_1] = -\mathrm{i}\hbar$. The 'doubled up' space with configurational states $|(p,q)\rangle$ has two degrees of freedom, so we can define two independent operators, $\hat{\mathbf{p}}_2$ and $\hat{\mathbf{q}}_2$, which commute with the pair $(\hat{\mathbf{p}}_1, \hat{\mathbf{q}}_1)$ and are themselves canonical. They are

$$\hat{\mathbf{p}}_2 = -p + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial q} \qquad \text{and} \qquad \hat{\mathbf{q}}_2 = q + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}. \tag{42}$$

In view of the form of equations (39) and (40), we can write

$$R(p,q,t|p',q',0) = \langle (p,q)|\hat{\mathbf{U}}_1(t)|(p',q')\rangle, \tag{43}$$

where

$$\hat{\mathbf{U}}_1(t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{h}}_1 t\right). \tag{44}$$

$|(p,q)\rangle$ cannot, of course, be mutual 'eigenstates' of any canonical position and momentum. On the other hand, we can represent them, for instance, by means of mutual 'eigenstates' of the commuting pair $(\hat{\mathbf{p}}_1, \hat{\mathbf{q}}_2)$. If (p_1', q_2') are their corresponding 'eigenvalues', then their mutual 'eigenstates' are $|p_1', q_2'\rangle = |p_1'\rangle|q_2'\rangle$, and solving the equations

$$\langle (p,q)|\hat{\mathbf{p}}_1|p_1',q_2'\rangle = \left(p + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial q}\right)\langle (p,q)|p_1',q_2'\rangle = p_1'\langle (p,q)|p_1',q_2'\rangle$$

and

$$\langle (p,q)|\hat{\mathbf{q}}_2|p_1',q_2'\rangle = \left(q + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}\right)\langle (p,q)|p_1',q_2'\rangle = q_2'\langle (p,q)|p_1',q_2'\rangle$$

gives

$$\langle (p,q)|p_1',q_2'\rangle = \frac{2}{h}\exp\left(-\frac{2\mathrm{i}}{\hbar}pq\right)\exp\left(\frac{2\mathrm{i}}{\hbar}(q_2'p+p_1'q)\right)\exp\left(-\frac{\mathrm{i}}{\hbar}p_1'q_2'\right). \tag{45}$$

Similarly

$$\langle (p,q)|q_1',p_2'\rangle = \frac{2}{h}\exp\left(\frac{2\mathrm{i}}{\hbar}pq\right)\exp\left(\frac{2\mathrm{i}}{\hbar}(-q_1'p+p_2'q)\right)\exp\left(-\frac{\mathrm{i}}{\hbar}p_2'q_1'\right). \tag{46}$$

Note that states $|p_1',q_2'\rangle$, $|q_1',p_2'\rangle$ and $|(p,q)\rangle$ lie in a product space of two dimensions in a way analogous to Ban's states $||\omega(r,k;s)\rangle$ (equation (11)).

The final phase factors in these two expressions have been chosen so that the actions of $(\hat{\mathbf{q}}_1,\hat{\mathbf{p}}_2)$ on $|p_1',q_2'\rangle = |p_1'\rangle|q_2'\rangle$ and of $(\hat{\mathbf{p}}_1,\hat{\mathbf{q}}_2)$ on $|q_1',p_2'\rangle = |q_1'\rangle|p_2'\rangle$ are correct. For instance, we require that

$$\langle (p,q)|\hat{\mathbf{q}}_1|p_1',q_2'\rangle = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_1'}\langle (p,q)|p_1',q_2'\rangle = \left(q - \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}\right)\langle (p,q)|p_1',q_2'\rangle.$$

With (45) and (46) it is easy to show that

$$\int_{-\infty}^{\infty} \mathrm{d}p_1'\,\mathrm{d}q_2'\langle (p,q)|p_1',q_2'\rangle\langle p_1',q_2'|(p',q')\rangle = \delta(p-p')\delta(q-q'), \tag{47}$$

$$\int_{-\infty}^{\infty} \mathrm{d}p\,\mathrm{d}q\,\langle p_1',q_2'|(p,q)\rangle\langle (p,q)|p_1,q_2\rangle = \delta(p_1'-p_1)\delta(q_2'-q_2), \tag{48}$$

and

$$\begin{aligned}\langle q_1',p_2'|p_1',q_2'\rangle &= \int_{-\infty}^{\infty} \mathrm{d}p\,\mathrm{d}q\,\langle q_1',p_2'|(p,q)\rangle\langle (p,q)|p_1',q_2'\rangle \\ &= \frac{1}{h}\exp\left(\frac{\mathrm{i}}{\hbar}q_1'p_1'\right)\exp\left(-\frac{\mathrm{i}}{\hbar}q_2'p_2'\right).\end{aligned} \tag{49}$$

Note that in this doubled up space, any operator of the form

$$\hat{\Gamma} = \int_{-\infty}^{\infty} \mathrm{d}p\,\mathrm{d}q\,\Gamma(p,q)|(p,q)\rangle\langle (p,q)| \tag{50}$$

is diagonal in the manner of equation (1). Equations (40), (41), (47), (48) and (50) provide an expression of the full proposal of Torres-Vega *et al* [5] for the cases $\alpha = 1 = \gamma$, $\beta = 1/2 = -\delta$ and $\alpha = 1 = \gamma$, $\beta = -1/2 = \delta$.

The operators $\hat{\mathbf{p}}_2$ and $\hat{\mathbf{q}}_2$ do not figure in the motion of $R(p,q,t|p',q',t')$, but it is possible to construct another propagator for which they do. It is

$$Q(p,q,t|p',q',t') = \frac{1}{h}\mathrm{Tr}\left(\hat{\Delta}(p,q)\hat{U}\left(\frac{t-t'}{2}\right)\hat{\Delta}(p',q')\hat{U}\left(\frac{t-t'}{2}\right)\right). \tag{51}$$

Using the content of equations (22)–(27), $Q(p,q,t|p',q',t')$ is seen to approach $\delta(p-p')\delta(q-q')$ as $t-t'\to 0$ and to propagate in the manner of equation (37). Also, just as for (38), one sees that

$$\int_{-\infty}^{\infty} \mathrm{d}p'\,\mathrm{d}q'\,Q(p,q,t|p',q',t') = U(p,q,t-t'), \tag{52}$$

and similarly for the integral of $Q(p,q,t|p',q',t')$ over $\mathrm{d}p\,\mathrm{d}q$.

Propagator Q was defined, and discussed in [15] in the semi-classical limit. $Q(p,q,t|p',q',0)$ is the Weyl transform of $(1/h)$ times $\hat{U}_{t/2}\hat{\Delta}(p',q')\hat{U}_{t/2}$, which obeys the equation of motion

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}(\hat{U}_{t/2}\hat{\Delta}(p',q')\hat{U}_{t/2}) = \frac{1}{2}\{\hat{H},\hat{U}_{t/2}\hat{\Delta}(p',q')\hat{U}_{t/2}\}, \tag{53}$$

where the curly brackets indicate an anti-commutator. Then, using equation (28), and its complex conjugate, and collecting terms gives

$$\mathrm{i}\hbar\frac{\partial}{\partial t}Q(p,q,t|p',q',0) = \frac{1}{2}(\hat{\mathbf{h}}_1+\hat{\mathbf{h}}_2)Q(p,q,t|p',q',0), \tag{54}$$

where $\hat{\mathbf{h}}_1$ is given by (40) and

$$\hat{\mathbf{h}}_2 = \frac{1}{2m}\hat{\mathbf{p}}_2^2 + V(\hat{\mathbf{q}}_2). \tag{55}$$

Hamiltonians $\hat{\mathbf{h}}_1$ and $\hat{\mathbf{h}}_2$ commute. In the manner of (43) we can write Q, for example, as

$$\begin{aligned} Q(p,q,t|p_0,q_0,0) &= \langle(p,q)|\exp\left(-\frac{\mathrm{i}}{\hbar}(\hat{\mathbf{h}}_1+\hat{\mathbf{h}}_2)\frac{t}{2}\right)|(p_0,q_0)\rangle \\ &= \int_{-\infty}^{\infty}\mathrm{d}p'\,\mathrm{d}q'\langle(p,q)|\hat{\mathbf{U}}_1(t/2)|(p',q')\rangle\langle(p',q')|\hat{\mathbf{U}}_2(t/2)|(p_0,q_0)\rangle, \end{aligned} \tag{56}$$

where

$$\hat{\mathbf{U}}_2(t/2) = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{h}}_2\frac{t}{2}\right),$$

and similarly for $\hat{\mathbf{U}}_1(t/2)$. The first propagator in the second line of equation (56) is just $R(p,q,t/2|p',q',0)$, equation (43), while the second is $R(-p',q',t/2|-p_0,q_0,0)$.

Apart from the fact that it can be used to generate $U(p,q,t)$, from the derivation of its equation of motion, equation (53), it can be seen that Q intrinsically generates the motion under the action of the anti-commutator with the Hamiltonian. On the other hand, the Wigner propagator, $P(p,q,t|p',q',t')$ follows propagation by the commutator with $\hat{H}$. It propagates the Weyl transform of the density matrix (the Wigner function times h), and is given [14] by

$$P(p,q,t|p',q',t') = \frac{1}{h}\mathrm{Tr}(\hat{U}^\dagger(t-t')\hat{\Delta}(p,q)\hat{U}(t-t')\hat{\Delta}(p',q')). \tag{57}$$

Both Q and P are propagators. It is easy to show that they can be combined to construct the generally non-propagating two-time function

$$\begin{aligned} C(p,q,t|p',q',t') &= \frac{1}{h}\mathrm{Tr}(\hat{\Delta}(p,q)\hat{U}(t)\hat{\Delta}(p',q')\hat{U}^\dagger(t')) \\ &= \int_{-\infty}^{\infty}\mathrm{d}p''\,\mathrm{d}q''\,Q(p,q,t|p'',q'',t')P\left(p'',q'',\frac{1}{2}(t+t')|p',q',0\right). \end{aligned}$$

3. Matrix elements: the phase angle

The pairs $(\hat{\mathbf{p}}_1,\hat{\mathbf{q}}_1)$ and $(\hat{\mathbf{p}}_2,\hat{\mathbf{q}}_2)$ commute and are independent, and this is reflected by their matrix elements with respect to the phase space wavefunctions. For instance, using definitions (24), (31) and (41), with some algebra, shows that

$$\begin{aligned} {}_\sigma\langle\psi|\hat{\mathbf{p}}_1^m\hat{\mathbf{q}}_1^n|\mu\rangle_\sigma &= \int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}\psi_\sigma^*(p,q)\left(p+\frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial q}\right)^m\left(q-\frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}\right)^n\mu_\sigma(p,q) \\ &= \langle\psi|\hat{p}^m\hat{q}^n|\mu\rangle, \end{aligned} \tag{58}$$

but that

$$ {}_\sigma\langle\psi|\hat{\mathbf{p}}_2^m\hat{\mathbf{q}}_2^n|\mu\rangle_\sigma = \langle\sigma|\hat{q}^n(-\hat{p})^m|\sigma\rangle\langle\psi|\mu\rangle. \tag{59}$$

So operator functions only of $\hat{\mathbf{p}}_1$ and $\hat{\mathbf{q}}_1$ are treated in the usual way, independent of the drone states, but $\hat{\mathbf{p}}_2$ and $\hat{\mathbf{q}}_2$ act only with respect to drone states in a 'twisted' manner.

If, however, one asks for matrix elements of phase space functions with respect to the wavefunctions $\psi_\sigma(p,q)$ then states $|\psi\rangle$ and $|\sigma\rangle$ both contribute. For instance, one can show that

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p\,\mathrm{d}q}{h} \psi_\sigma^*(p,q) p^m q^n \mu_\sigma(p,q) = \langle\psi,\sigma| \left(\frac{\hat{q}_1+\hat{q}_2}{2}\right)^n \left(\frac{\hat{p}_1+\hat{p}_2}{2}\right)^m |\mu,\sigma\rangle, \tag{60}$$

where the state $|\psi,\sigma\rangle = |\psi\rangle|\sigma\rangle$ is the Cartesian product, and $(\hat{p}_1,\hat{q}_1)$ and $(\hat{p}_2,\hat{q}_2)$ are the usual momentum and position operators, the former pair acting on $|\psi\rangle$ and $|\mu\rangle$, but the latter on $|\sigma\rangle$.

A more interesting example of this mutual contribution is the phase angle of an harmonic oscillator, which relates to the modes of a quantized electromagnetic field [13]. The Weyl transform of the creation operator, $\hat{a}^\dagger = \frac{1}{\sqrt{2}}\big(\alpha\hat{q} - \mathrm{i}\frac{\hat{p}}{\alpha\hbar}\big)$, is easily shown from equations (22) and (24) to be $a^*(p,q) = \frac{1}{\sqrt{2}}\big(\alpha q - \mathrm{i}\frac{p}{\alpha\hbar}\big)$. It is most efficient to define dimensionless variables $(x,y) = \big(\frac{p}{\hbar\alpha}, \alpha q\big)$, so that the Weyl transform of $\hat{a}^\dagger$ is $\frac{-\mathrm{i}}{\sqrt{2}} R\,\mathrm{e}^{\mathrm{i}\phi}$, where $R^2 = x^2 + y^2$ and $\phi = \arctan(y/x)$. For an harmonic oscillator of mass m, $\alpha^2 = m\omega/\hbar$ and the Hamiltonian, $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2$, has a Weyl transform given by $H(p,q) = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 = \frac{\hbar\omega}{2}R^2$. In order that the phase angle ϕ be unique we need to choose a cut in the x–y plane to complete its definition. If we agree to choose the negative x-axis for this, then ϕ is limited to the range $(-\pi,\pi]$. With these variables, $\mathrm{d}p\,\mathrm{d}q/h = R\,\mathrm{d}R\,\mathrm{d}\phi/2\pi$, and in the Wigner–Weyl picture, ϕ and its corresponding operator, $\hat{\phi}$, are related [16] by

$$\phi = \mathrm{Tr}(\hat{\phi}\hat{\Delta}(R,\phi)) \qquad \text{and} \qquad \hat{\phi} = \int_0^\infty \mathrm{d}R\,R \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi}\phi\hat{\Delta}(R,\phi), \tag{61}$$

where we now consider $\hat{\Delta}$ as a function of plane polar coordinates R and ϕ.

This angle operator, $\hat{\phi}$, is the quantization of the phase angle in the Weyl picture. Many of its properties have been studied rigorously [13, 17]. In particular, it is bounded and self-adjoint, and it has the particularly attractive property that the Weyl transform of its commutator with $\hat{H}$ is identical to the classical commutator of ϕ with $H(p,q)$. For our choice of cut in the phase plane, the matrix elements of $\hat{\phi}$ with respect to the energy eigenstates $|h_n\rangle$, $(n \geqslant 0)$ of the harmonic oscillator, with energies $(n+1/2)\hbar\omega$, are given by

$$\langle h_m|\hat{\phi}|h_n\rangle = \int_0^\infty \mathrm{d}R\,R \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi}\phi\langle h_m|\hat{\Delta}(R,\phi)|h_n\rangle, \tag{62}$$

where

$$\langle h_m|\hat{\Delta}(R,\phi)|h_n\rangle = 2(-1)^n \mathrm{i}^{|m-n|} 2^{\frac{|m-n|}{2}} \sqrt{\frac{n_\ell!}{n_g!}}\, \mathrm{e}^{\mathrm{i}(n-m)\phi} R^{|m-n|}\,\mathrm{e}^{-R^2} L_{n_\ell}^{|m-n|}(2R^2) \tag{63}$$

$n_\ell(n_g)$ is the lesser (greater) of the pair (m,n), and L_a^b is the Laguerre polynomial [18]. When (63) is used in (62) one finds after some manipulation [13, 17] that

$$\langle h_m|\hat{\phi}|h_n\rangle = (1-\delta_{m,n})\frac{\mathrm{i}^{n-m+1}}{m-n} g_{m,n}, \tag{64}$$

where $g_{m,n}$ is the symmetric matrix

$$g_{m,n} = 2^{-\frac{|m-n|}{2}} \frac{\Gamma\big(\frac{n_\ell}{2}+s_\ell\big)}{\Gamma\big(\frac{n_g}{2}+s_\ell\big)} \sqrt{\frac{n_g!}{n_\ell!}}, \tag{65}$$

with

$$s_\ell = \begin{cases} 1/2 & n_\ell \text{ even} \\ 1 & n_\ell \text{ odd.} \end{cases} \tag{66}$$

Operator $\hat{\phi}$ is an observable in the usual interpretation of quantum mechanics. There are other candidates for this rôle too [13, 19]. All of them must bow to the fact that no phase operator can be canonical with the number operator $\hat{n} = \hat{a}^\dagger\hat{a}$. This 'no-go' theorem was pointed out by Louisell [20] and follows directly by contradiction: If it *were* true that $[\hat{\phi}, \hat{n}] = \mathrm{i}$, then taking diagonal matrix elements of this equation with respect to the ground state $|h_0\rangle$ would imply that $0 = \mathrm{i}$. The no-go theorem notwithstanding, the attraction of some sort of complementarity between $\hat{\phi}$ and $\hat{n}$ is compelling. For instance there is the 'acid test' [19], which would require that the standard deviation of a phase-angle with respect to the number states $\{|h_n\rangle; n \geqslant 0\}$ should be characteristic of a *random* distribution over its range of values (here $(-\pi, \pi]$). The acid test is not satisfied by any well-defined candidate phase operator on a Hilbert space known to the author, but it is satisfied by the prescription of Pegg and Barnett [21], based on a limiting technique and shown [22, 23] to be equivalent, for phase angle calculations, to a positive operator-valued measure (POM).

We can consider the present formalism from this viewpoint by examining matrix elements with respect to the augmented wavefunctions $\psi_\sigma(p, q)$. Suppose we have any function of ϕ only, say $f(\phi)$. Then, defining

$$M_\sigma(f; \psi, \mu) \equiv \int_0^\infty \mathrm{d}R\, R \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi} \psi_\sigma^*(R, \phi) f(\phi) \mu_\sigma(R, \phi), \tag{67}$$

we can choose oscillator energy eigenstates to get

$$M_{h_\sigma}(f; h_m, h_n) = \int_0^\infty \mathrm{d}R\, R \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi} f(\phi) \langle h_m | \hat{\Delta}(R, \phi) | h_\sigma \rangle \langle h_\sigma | \hat{\Delta}(R, \phi) | h_n \rangle. \tag{68}$$

The diagonal elements are given by choosing $n = m$. Using equation (63) then gives

$$M_{h_\sigma}(f; h_m, h_m) = \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi} f(\phi) \left\{ \frac{n_\ell!}{n_g!} \int_0^\infty 4R\, \mathrm{d}R (2R^2)^{|m-\sigma|}\, \mathrm{e}^{-2R^2} \left(L_{n_\ell}^{|m-\sigma|}(2R^2) \right)^2 \right\}.$$

The integral over R is standard [18], and the quantity in curly brackets is unity, so we are left with

$$M_{h_\sigma}(f; h_m, h_m) = \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi} f(\phi). \tag{69}$$

This is characteristic of a uniform angle distribution over the range $(-\pi, \pi]$, so that the choice of any drone state from the set of oscillator eigenstates meets the 'acid test'. In particular, $M_{h_\sigma}(\phi; h_m, h_m) = 0$ and $M_{h_\sigma}(\phi^2; h_m, h_m) = \pi^2/3$.

$M_\sigma(f; \psi, \mu)$ defines a POM. For example, with respect to the phase angle ϕ, equation (68) can be written as

$$M_{h_\sigma}(f; h_m, h_m) = \int_{-\pi}^{\pi} f(\phi) \mathrm{Tr}\big(|h_m\rangle\langle h_m|\, \mathrm{d}\hat{\Pi}_{h_\sigma}(\phi) \big),$$

where

$$\mathrm{d}\hat{\Pi}_{h_\sigma}(\phi) = \frac{\mathrm{d}\phi}{2\pi} \int_0^\infty \mathrm{d}R\, R \hat{\Delta}(R, \phi) |h_\sigma\rangle\langle h_\sigma| \hat{\Delta}(R, \phi)$$

obeys the usual requirements [24] to be a POM on the interval $(-\pi, \pi]$. As a non-projective POM, M shares with the formalism of Barnett and Pegg [21] the property that it defines no single operator for phase; the expectation of the operator corresponding to functions of ϕ is *not* the same function of the operator corresponding to ϕ itself. For example,

$$M_\sigma(\phi^2; h_m, h_m) \neq \sum_{n\geqslant 0} M_\sigma(\phi; h_m, h_n) M_\sigma(\phi; h_n, h_m).$$

For an isolated oscillator mode, the natural choice for the drone state is the vacuum, $|h_0\rangle$. In that case, referring to definition (68) and utilizing equation (63), one finds

$$\begin{aligned} M_{h_0}(f; h_m, h_n) &= \mathrm{i}^{m-n} \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi} f(\phi)\, \mathrm{e}^{\mathrm{i}(n-m)\phi} \frac{2^{\frac{m+n+4}{2}}}{\sqrt{n!m!}} \int_0^\infty \mathrm{d}R\, R^{m+n+1}\, \mathrm{e}^{-2R^2} \\ &= \mathrm{i}^{m-n} \frac{\Gamma\left(\frac{m+n}{2}+1\right)}{\sqrt{m!n!}} \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi} f(\phi)\, \mathrm{e}^{\mathrm{i}(n-m)\phi}, \end{aligned} \tag{70}$$

which reduces to equation (69) when $n = m$.

Another interesting case, still with a vacuum drone state, is that of a coherent state, namely

$$|\psi_s\rangle = \mathrm{e}^{-\frac{1}{2}|s|^2} \sum_{m\geqslant 0} \frac{s^m}{\sqrt{m!}} |m\rangle, \tag{71}$$

where s is complex. Then a little juggling with (63) and (71) gives

$$\psi_{h_0}(R, \phi; s) = \langle h_0|\hat{\Delta}(R, \phi)|\psi_s\rangle = 2\,\mathrm{e}^{-\frac{1}{2}|s|^2} \mathrm{e}^{-\mathrm{i}\sqrt{2}sR\,\mathrm{e}^{-\mathrm{i}\phi}} \mathrm{e}^{-R^2}.$$

It is convenient to let $s = \rho\,\mathrm{e}^{\mathrm{i}(\frac{\pi}{2}-\theta)}$ and $r = \sqrt{2}R$ to get

$$\begin{aligned} M_{h_0}(f; h_n, h_n) &= \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{\pi} f(\phi) \int_0^\infty \mathrm{d}r\, r \exp\left(-[r^2 + \rho^2 - 2r\rho\cos(\phi-\theta)]\right) \\ &= \int_{-\pi}^{\pi} \frac{\mathrm{d}\phi}{2\pi} f(\phi) P(\phi; \rho, \theta), \end{aligned} \tag{72}$$

where the angle distribution in this case is $P(\phi; \rho, \theta)/2\pi$, where

$$P(\phi; \rho, \theta) = \mathrm{e}^{-\rho^2} + \rho\cos(\phi-\theta)\sqrt{\pi}\,\mathrm{e}^{-\rho^2\sin^2(\phi-\theta)}[1 + \mathrm{Erf}(\rho\cos(\phi-\theta))], \tag{73}$$

and where $\mathrm{Erf}(z) = \frac{2}{\pi}\int_0^z \mathrm{d}t \exp(-t^2)$ is the error function [18].

When $|s| = \rho$ approaches zero, so $|\psi_s\rangle$ approaches the vacuum state, and P approaches unity. In that limit we have a random distribution of angle, but in the other extreme (ρ large) P approaches a delta function centred at $\phi = \theta$. If the angle θ is not too close to the cut at $\phi = -\pi$, then we can (by setting $f(\phi)$ equal to ϕ and ϕ^2) ask for the mean and standard deviation squared of phase angle as a function of ρ. The former is θ and the latter is a smooth monotonically decreasing function of ρ, starting at a value $\pi^2/3$ at $\rho = 0$ and dropping to zero as $(2\rho^2)^{-1}$ for large ρ. For the coherent state, equation (71), the expectation of the number operator $\hat{n} = \hat{a}^\dagger\hat{a}$ is $\overline{n} = \rho^2$, so the large $\overline{n}$-dependence of the standard deviation squared is $(2\overline{n})^{-1}$.

4. Other orderings

The Wigner–Weyl correspondence treats momentum and position even handedly. For instance, as follows from (22) and (24),

$$(\mathrm{e}^{\mathrm{i}(\xi\hat{q}+\eta\hat{p})})(p, q) = \mathrm{e}^{\mathrm{i}(\xi q+\eta p)}, \tag{74}$$

where ξ and η are real parameters. With this rule, functions of $\hat{p}$ only transform to the same functions of p, and similarly for q, but, for example, $(\hat{p}\hat{q} + \hat{q}\hat{p})/2$ transforms to pq, whereas the transform of $\hat{p}\hat{q}$ is $pq - \mathrm{i}\hbar/2$ and that of $\hat{q}\hat{p}$ is $pq + \mathrm{i}\hbar/2$. As discussed by Cohen [4], there are an infinite number of other possible correspondences between operators and functions on phase space. We shall write Cohen's scheme as [25]

$$(\mathrm{e}^{\mathrm{i}(\xi\hat{q}+\eta\hat{p})})^f(p,q) = \frac{1}{f(\xi,\eta)}\,\mathrm{e}^{\mathrm{i}(\xi q+\eta p)} = f^{-1}(-\mathrm{i}\partial_q, -\mathrm{i}\partial_p)\,\mathrm{e}^{\mathrm{i}(\xi q+\eta p)}, \tag{75}$$

where by f^{-1} we mean $1/f$, and $f = 1$ gives the Wigner–Weyl case. If one requires that functions of p only transform to the same functions of $\hat{p}$ only, and similarly for q, then we must require that

$$f(0,\eta) = 1 = f(\xi,0). \tag{76}$$

For an ordering characterized by f, then, equation (75) would generalize to

$$A^f(p,q) = f^{-1}(-\mathrm{i}\partial_q, -\mathrm{i}\partial_p)A(p,q), \tag{77}$$

where $A(p,q)$ is the Wigner–Weyl transform of some operator $\hat{A}$. It is possible to preserve much of the latter formalism. For instance the generalization of equation (22) is

$$A^f(p,q) = \mathrm{Tr}(\hat{A}\hat{\Delta}^f(p,q)), \tag{78}$$

where we define the operator

$$\hat{\Delta}^f(p,q) = f^{-1}(-\mathrm{i}\partial_q, -\mathrm{i}\partial_p)\hat{\Delta}(p,q). \tag{79}$$

We can invert (78) to get $\hat{A}$ provided we can find something similar to equation (26). This follows by multiplying equation (79) by $\hat{\Delta}(p',q')$ and taking the trace:

$$\begin{aligned}\mathrm{Tr}(\hat{\Delta}^f(p,q)\hat{\Delta}(p',q')) &= hf^{-1}(-\mathrm{i}\partial_q, -\mathrm{i}\partial_p)\delta(p-p')\delta(q-q')\\ &= hf^{-1}(\mathrm{i}\partial_{q'}, \mathrm{i}\partial_{p'})\delta(p-p')\delta(q-q').\end{aligned}$$

Then defining

$$\hat{\Delta}_f(p,q) = f(\mathrm{i}\partial_q, \mathrm{i}\partial_p)\hat{\Delta}(p,q) \tag{80}$$

shows that

$$\mathrm{Tr}(\hat{\Delta}_f(p,q)\hat{\Delta}^f(p',q')) = \mathrm{Tr}(\hat{\Delta}^f(p,q)\hat{\Delta}_f(p',q')) = h\delta(p-p')\delta(q-q'). \tag{81}$$

From this, generalizing equation (23),

$$\hat{A} = \int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}A^f(p,q)\hat{\Delta}_f(p,q) = \int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}A_f(p,q)\hat{\Delta}^f(p,q). \tag{82}$$

By the same token, the generalization of equation (27) is

$$\mathrm{Tr}(\hat{A}\hat{B}) = \int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}A_f(p,q)B^f(p,q) = \int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}A^f(p,q)B_f(p,q), \tag{83}$$

where, for example,

$$B_f(p,q) = \mathrm{Tr}(\hat{B}\hat{\Delta}_f(p,q)).$$

Let us now specialize to the class of orderings characterized by

$$f(\xi,\eta;\lambda) = \mathrm{e}^{\mathrm{i}\frac{\hbar}{2}\lambda\xi\eta}, \tag{84}$$

where λ is a real parameter [26]. To see what orderings this choice implies, hark back to equation (75), which can be written in this case as

$$(\mathrm{e}^{\mathrm{i}(\xi\hat{q}+\eta\hat{p})})^{(\lambda)}(p,q) = \mathrm{e}^{-\mathrm{i}\frac{\hbar}{2}\lambda\xi\eta}\,\mathrm{e}^{\mathrm{i}(\xi q+\eta p)}.$$

Referring to equation (9), evidently the choice $\lambda = -1$ corresponds to the ordering

$$(\mathrm{e}^{\mathrm{i}\xi\hat{q}}\,\mathrm{e}^{\mathrm{i}\eta\hat{p}})^{(-1)}(p,q) = \mathrm{e}^{\mathrm{i}(\xi q+\eta p)},$$

called 'standard' or 'p' ordering, and the case $\lambda = 1$ corresponds to the 'anti-standard' scheme

$$(\mathrm{e}^{\mathrm{i}\eta\hat{p}}\,\mathrm{e}^{\mathrm{i}\xi\hat{q}})^{(1)}(p,q) = \mathrm{e}^{\mathrm{i}(\xi q+\eta p)}.$$

Choosing $\lambda = 0$, gives the Wigner–Weyl ordering.

The family given by (84) obeys the requirements of equation (76), so that equations (77)–(83) hold good, but it has the further property—not obeyed by all orderings satisfying (76)—that, when $\xi\eta$ is real,

$$f^*(\xi,\eta;\lambda) = f^{-1}(\xi,\eta;\lambda). \tag{85}$$

This property permits the generalization of equations (31) and (32), for, by (84) and (79), we can define

$$\psi_\sigma^{(\lambda)}(p,q) = \langle\sigma|\hat{\Delta}^{(\lambda)}(p,q)|\psi\rangle = \mathrm{e}^{\mathrm{i}\frac{\hbar}{2}\lambda\partial p\partial q}\psi_\sigma(p,q), \tag{86}$$

so that (integrating by parts)

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}\big(\psi_\sigma^{(\lambda)}(p,q)\big)^*\mu_\sigma^{(\lambda)}(p,q) = \int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}\psi_\sigma^*(p,q)\mu_\sigma(p,q) = \langle\psi|\mu\rangle,$$

and the same applies to

$$\psi_{\sigma,(\lambda)}(p,q) = \langle\sigma|\hat{\Delta}_{(\lambda)}(p,q)|\psi\rangle = \mathrm{e}^{-\mathrm{i}\frac{\hbar}{2}\lambda\partial p\partial q}\psi_\sigma(p,q). \tag{87}$$

The propagation of $\psi_\sigma^{(\lambda)}(p,q)$ in time is given by

$$\begin{aligned}\psi_\sigma^{(\lambda)}(p,q;t) &= f^{-1}(-\mathrm{i}\partial_q,-\mathrm{i}\partial_p;\lambda)\psi_\sigma(p,q;t) = \mathrm{e}^{\mathrm{i}\frac{\hbar}{2}\lambda\partial_p\partial_q}\psi_\sigma(p,q;t)\\ &= \mathrm{Tr}(\hat{\Delta}^{(\lambda)}(p,q)\hat{U}(t)|\psi\rangle\langle\sigma|)\\ &= \int\frac{\mathrm{d}p'\,\mathrm{d}q'}{h}(\hat{\Delta}^{(\lambda)}(p,q)\hat{U}(t))_{(\lambda)}(p',q')(|\psi\rangle\langle\sigma|)^{(\lambda)}(p',q')\\ &= \int\frac{\mathrm{d}p'\,\mathrm{d}q'}{h}R^{[\lambda]}(p,q,t|p',q',0)\psi_\sigma^{(\lambda)}(p',q';0),\end{aligned} \tag{88}$$

where the propagator is

$$\begin{aligned}R^{[\lambda]}(p,q,t|p',q',t') &= \frac{1}{h}\mathrm{Tr}(\hat{\Delta}^{(\lambda)}(p,q)\hat{U}(t-t')\hat{\Delta}_{(\lambda)}(p',q'))\\ &= \mathrm{e}^{\mathrm{i}\frac{\hbar}{2}\lambda\partial_p\partial_q}\,\mathrm{e}^{-\mathrm{i}\frac{\hbar}{2}\lambda\partial_{p'}\partial_{q'}}R(p,q,t|p',q',t')\end{aligned} \tag{89}$$

with $R(p,q,t|p',q',t')$ given by equation (36).

Similarly

$$\psi_{\sigma;(\lambda)}(p,q;t) = \int\frac{\mathrm{d}p'\,\mathrm{d}q'}{h}R_{[\lambda]}(p,q,t|p',q',0)\psi_{\sigma;(\lambda)}(p',q';0), \tag{90}$$

where

$$\begin{aligned}R_{[\lambda]}(p,q,t|p',q',t') &= \mathrm{e}^{-\mathrm{i}\frac{\hbar}{2}\lambda\partial_p\partial_q}\,\mathrm{e}^{\mathrm{i}\frac{\hbar}{2}\lambda\partial_{p'}\partial_{q'}}R(p,q,t|p',q',t')\\ &= R^{[-\lambda]}(p,q,t|p',q',t').\end{aligned} \tag{91}$$

$R^{[\lambda]}$ and $R_{[\lambda]}$ both propagate in the manner of equation (37), and corresponding to (38) we have

$$\int_{-\infty}^{\infty}\mathrm{d}p'\,\mathrm{d}q'R^{[\lambda]}(p,q,t|p',q',t') = U^{(\lambda)}(p,q,t-t'), \tag{92}$$

and similarly for $R_{[\lambda]}$.

The equation of motion, say for $R^{[\lambda]}$, follows by using equation (89) to convert equation (39), to get

$$\mathrm{i}\hbar\frac{\partial}{\partial t}R^{[\lambda]}(p,q,t|p',q',0) = \hat{\mathbf{h}}_{1,\lambda}R^{[\lambda]}(p,q,t|p',q',0). \tag{93}$$

Here

$$\hat{\mathbf{h}}_{1,\lambda} = \frac{1}{2m}(\hat{\mathbf{p}}_{1,\lambda})^2 + V(\hat{\mathbf{q}}_{1,\lambda}), \tag{94}$$

with the canonical pair

$$\hat{\mathbf{p}}_{1,\lambda} = p + \frac{\hbar}{2\mathrm{i}}(1-\lambda)\frac{\partial}{\partial q} \qquad \text{and} \qquad \hat{\mathbf{q}}_{1,\lambda} = q - \frac{\hbar}{2\mathrm{i}}(1+\lambda)\frac{\partial}{\partial p}. \tag{95}$$

From these results, we can write (cf equation (43))

$$R^{[\lambda]}(p,q,t|p',q',0) = \langle (p,q)|\hat{\mathbf{U}}_{1,\lambda}(t)|(p',q')\rangle, \tag{96}$$

where

$$\hat{\mathbf{U}}_{1,\lambda}(t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{h}}_{1,\lambda}t\right). \tag{97}$$

Also, from equation (91), $R_{[\lambda]}$ is given by the substitution $\lambda \to -\lambda$. The propagator Q of the Wigner–Weyl picture, equation (56), generalizes to $Q_{[\lambda]}$ and $Q^{[\lambda]}$, where, for instance,

$$Q^{[\lambda]}(p,q,t|p',q',t') = \frac{1}{h}\mathrm{Tr}\left(\hat{\Delta}^{(\lambda)}(p,q)\hat{U}\left(\frac{t-t'}{2}\right)\hat{\Delta}_{(\lambda)}(p',q')\hat{U}\left(\frac{t-t'}{2}\right)\right) \tag{98}$$

$$\int_{-\infty}^{\infty} \mathrm{d}p'\,\mathrm{d}q'\,Q^{[\lambda]}(p,q,t|p',q',t') = U^{(\lambda)}(p,q,t-t'). \tag{99}$$

The equation of motion for $Q^{[\lambda]}$ follows from (54) and definition (98); it is

$$\mathrm{i}\hbar\frac{\partial}{\partial t}Q^{[\lambda]}(p,q,t|p',q',0) = \frac{1}{2}(\hat{\mathbf{h}}_{1,\lambda} + \hat{\mathbf{h}}_{2,\lambda})Q^{[\lambda]}(p,q,t|p',q',0), \tag{100}$$

where

$$\hat{\mathbf{h}}_{2,\lambda} = \frac{1}{2m}(\hat{\mathbf{p}}_{2,\lambda})^2 + V(\hat{\mathbf{q}}_{2,\lambda}), \tag{101}$$

and $\hat{\mathbf{p}}_{2,\lambda}$ and $\hat{\mathbf{q}}_{2,\lambda}$ are the second, independent, canonical pair

$$\hat{\mathbf{p}}_{2,\lambda} = -p + \frac{\hbar}{2\mathrm{i}}(1+\lambda)\frac{\partial}{\partial q} \qquad \text{and} \qquad \hat{\mathbf{q}}_{2,\lambda} = q + \frac{\hbar}{2\mathrm{i}}(1-\lambda)\frac{\partial}{\partial p}. \tag{102}$$

It is also possible to evaluate matrix elements for the quantization schemes characterized by the choice (84). For instance, noting that

$$\mathrm{e}^{\mathrm{i}\frac{\hbar}{2}\lambda\partial_p\partial_q}(\hat{\mathbf{p}}_1,\hat{\mathbf{q}}_1,\hat{\mathbf{p}}_2,\hat{\mathbf{q}}_2)\,\mathrm{e}^{-\mathrm{i}\frac{\hbar}{2}\lambda\partial_p\partial_q} = (\hat{\mathbf{p}}_{1,\lambda},\hat{\mathbf{q}}_{1,\lambda},\hat{\mathbf{p}}_{2,\lambda},\hat{\mathbf{q}}_{2,\lambda})$$

we can see, for example, that

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}\left(\psi_\sigma^{(\lambda)}(p,q)\right)^*(\hat{\mathbf{p}}_{1,\lambda})^m(\hat{\mathbf{q}}_{1,\lambda})^n\mu_\sigma(p,q) = \langle\psi|\hat{p}^m\hat{q}^n|\mu\rangle, \tag{103}$$

just as for equation (58), so that if all quantities are transformed then the matrix elements are unchanged. On the other hand, after some algebra one finds (compare equation (60))

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}&\left(\psi_\sigma^{(\lambda)}(p,q)\right)^* p^m q^n \mu_\sigma^{(\lambda)}(p,q)\\ &= \int_{-\infty}^{\infty}\frac{\mathrm{d}p\,\mathrm{d}q}{h}\psi_\sigma^*(p,q)\left(p+\lambda\frac{\hbar}{2\mathrm{i}}\partial_q\right)^m\left(p+\lambda\frac{\hbar}{2\mathrm{i}}\partial_p\right)^n\mu_\sigma(p,q)\\ &= \langle\psi,\sigma|\left(\frac{1+\lambda}{2}\hat{q}_1+\frac{1-\lambda}{2}\hat{q}_2\right)^n\left(\frac{1-\lambda}{2}\hat{p}_1+\frac{1+\lambda}{2}\hat{p}_2\right)^m|\mu,\sigma\rangle.\end{aligned} \tag{104}$$

5. Discussion

A main goal for this paper was to show that the quantum structure envisioned by Torres-Vega and co-workers [5] and by Harriman [6], equations (1)–(4), can be realized by 'lifting' the usual formalism with coherent states up a dimension. Then over-completeness (equation (10)) becomes simple completeness in the augmented space (equations (47) and (48)). The formal construction of Ban [11] also achieves this (equation (13)), and we have shown that there is a close resemblance between his theory and that of this paper (equations (12) and (33)). Our theory is based directly on the standard calculus of the Weyl transform, focusing especially on the Weyl symbol, $\psi_\sigma(p,q)$, of the generally off-diagonal operator $|\psi\rangle\langle\sigma|$, where σ is any fixed state. Were σ not fixed, but equal to ψ then the corresponding Weyl symbol would be h times the Wigner function for the pure state $|\psi\rangle\langle\psi|$. In our case $|\sigma\rangle$ is fixed and $\psi_\sigma(p,q)$ develops in time through the propagator $R(p,q,t|p',q',t')$, equation (43). In the augmented space any operator of the form (50) satisfies condition (1) of diagonality with respect to *both* p and q.

As we have seen (equations (41) and (42)) this analysis is a special case of the prescription of equations (1)–(4) with $\alpha = 1 = \gamma, \beta = 1/2 = -\delta$ and $\alpha = 1 = \gamma, \beta = -1/2 = \delta$. As an illustration, we gave in section 3 several examples of matrix elements with respect to the augmented wavefunctions, dwelling especially on functions of the phase angle $\phi = \arctan(p/m\omega q)$ leading to a family of positive operator-valued measures on the interval $(-\pi,\pi]$, any one of which implies randomness in angle distribution for an oscillator in any pure number state. Between them, equations (16) and (17) of Ban, and the action of our operators $\hat{\mathbf{p}}_{1,\lambda}$ and $\hat{\mathbf{q}}_{1,\lambda}$ of equation (95), include a wide range of the relations hypothesized in equations (3) and (4). Furthermore, making the identifications $\lambda = -s$, $q = (1-\lambda)r/2$, and $p = (1+\lambda)k/2$ in (95) rescales $\hat{\mathbf{p}}_{1,\lambda}$ and $\hat{\mathbf{q}}_{1,\lambda}$ to two new canonical operators

$$\hat{\mathbf{P}}_{1,s} = \left(\frac{1-s}{2}\right)k - \mathrm{i}\hbar\frac{\partial}{\partial r} \qquad \text{and} \qquad \hat{\mathbf{Q}}_{1,s} = \left(\frac{1+s}{2}\right)r + \mathrm{i}\hbar\frac{\partial}{\partial k},$$

whose actions match (16) and (17).

Note that if one makes the formal identification of $|\psi\rangle$ in equation (33) with the position 'eigenstate' $|q'\rangle$, one finds

$$\psi_{q'}(p,q) = 2\,\mathrm{e}^{\frac{2\mathrm{i}}{\hbar}p(q-q')}\sigma^*(2q-q'),$$

which is a special case of (6).

We chose to develop the theory in a consistent way around the Weyl symbol $\psi_\sigma(p,q) = \langle\sigma|\hat{\Delta}(p,q)|\psi\rangle$. However, from equation (24), one can write

$$\hat{D}[p,q] = \int_{-\infty}^{\infty} \mathrm{d}q' \exp\left(\frac{\mathrm{i}}{\hbar}pq'\right)\left|q' + \frac{q}{2}\right\rangle\left\langle q' - \frac{q}{2}\right|,$$

and, by taking matrix elements of this with respect, say, to position 'eigenstates' $|x\rangle$ and $|y\rangle$ it is easy to derive the known result that $\hat{\Delta}(p,q) = 2\hat{D}(2p,2q)\hat{\Pi}$, where $\hat{\Pi}$ is the parity operator, so that a formulation in terms of $\hat{D}$ would also be possible.

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