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Quantum mechanical representations of canonical transformations given by a generating function

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Abstract. Quantization of canonical transformations is greatly simplified by the use of generating functions. A number of well-known results about linear canonical transformations and gauge transformations appear "automatically". A new way to discuss time measurements in quantum mechanics is applied to the free fall motion. Energy-time variables are more difficult to introduce in the free particle case but using the concept of ambiguity group associated to the transformation we obtain essentially the same results as Moshinsky and Seligman. Finally we give the quantum representations of the dynamical group of $H = QPQ$ and explain the freedom associated with the extensions of this operator.

1. Introduction

A series of recent papers written by Moshinsky and coworkers [1–4] on representations of general canonical transformations is at the origin of the present paper. The central point is the discussion of the ambiguities related to the lack of bijectivness of these transformations, which are given in some implicit way.

Starting with two phase spaces E and $\bar{E}$, a n-tuple of relations

$$F_k(q, p, \bar{q}, \bar{p}) = G_k(q, p) - G_k(\bar{q}, \bar{p}) = 0 \qquad (q, p) \in E(\bar{q}, \bar{p}) \in \bar{E}$$

may define locally some canonical transformations, if standard conditions on Poisson bracket holds. Clearly the submanifold of $F = 0$ does not generally define the graph of a mapping. In order to restore unicity, Moshinsky and Seligman introduce "sheets" into the phase space like Riemann's sheets in the theory of analytic functions. Eventually this elaboration leads to canonical mappings of $\mathbb{R}_{2n}$ to $\mathbb{R}_{2n}$.

Instead of the Poisson bracket condition, we prefer to give the classical transformation with the help of a generating function [5]. The kernel of the corresponding unitary transformation is then automatically given by Van Vleck's formula [6]. The classical interpretation of the determinant as a transversality measure of the chosen coordinate system allows a better understanding of the unitary kernel singularities. Our point of view is identical with Maslov's asympotic method [7] which allows the use of concepts from catastrophe theory [8].

The link between generating functions and unitary transformations introduces a great conceptual and computational simplification into the subject. Although we do not succeed in the search of a general relation between the ambiguity group of Moshinsky et al. and singularities of generating functions, we are convinced that it is the most important mathematical question about the structure of quantum mechanics. The goal of the few examples given here is to convince the reader of its importance.

2. Generating functions

Canonical transformations are mappings of phase spaces which preserve the Poisson bracket. This condition is complicated but corresponds to a rather simple geometrical fact. As pointed out by Abraham [9], the graph of a canonical map is a Lagrangian manifold in the symplectified Cartesian product of the two spaces. As a consequence, the transformation is essentially given by the gradient of some function called "generating function" [5].

Let ϕ be the canonical map of E on $\bar{E}$

$$\phi : E \ni (q, p) \mapsto (\bar{q}, \bar{p}) \in \bar{E} \tag{2.1}$$

We define four generating functions of ϕ by the following differentials

$$dW = p \cdot dq - \bar{p} \cdot d\bar{q} \tag{2.2a}$$

$$dG = -q \cdot dp + \bar{q} \cdot d\bar{p} \tag{2.2b}$$

$$dS = p \cdot dq + \bar{q} \cdot d\bar{p} \tag{2.2c}$$

$$dF = -q \cdot dp - \bar{p} \cdot d\bar{q} \tag{2.2d}$$

Each generating function gives ϕ by means of an implicit equation system. This system has a unique solution iff the corresponding functional determinant is non-vanishing:[1])

$$J = \det\left(\frac{\partial^2 W}{\partial q\, \partial \bar{q}}\right) \neq 0 \tag{2.3}$$

and analogously for G, S and F. This is clearly a transversality condition. If a generating function is such that $J \neq 0$ everywhere, then it unfolds the graph of the map. We say simply that this function "unfold the transformation". It is a big chance if a single generating function (globally) unfolds, but we want to limit ourselves to this simple case.

Obviously the functions W, G, S, F are related by Legendre transformations [10], and the result is not unique, unless some convexity relations holds.

Writing the generating function of the inverse map ϕ^{-1} with a dash, we have obviously

$$\begin{aligned} \bar{W}(\bar{q}, q) &= -W(q, \bar{q}) \\ \bar{G}(\bar{p}, p) &= -G(p, \bar{p}) \\ \bar{S}(\bar{q}, p) &= -F(p, \bar{q}) \\ \bar{F}(\bar{p}, q) &= -S(q, \bar{p}) \end{aligned} \tag{2.4}$$

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[1]) J is the Jacobian of the mappings $q\bar{q} \to qp$ and $q\bar{q} \to \bar{q}\bar{p}$. In the sequel we call it simply "the Jacobian". (It is *not* the Hessian.)

More generally, the composition

$$\phi = \phi_2 \circ \phi_1 \tag{2.5}$$

of two canonical maps ϕ_1 and ϕ_2 is related to generating functions W, G, S or F obtained by the following construction from the corresponding W_1 and W_2, etc. Let us define

$$\begin{aligned} w(q, \bar{q}, \bar{\bar{q}}) &= W_1(q, \bar{q}) + W_2(\bar{q}, \bar{\bar{q}}) \\ g(p, \bar{p}, \bar{\bar{p}}) &= G_1(p, \bar{p}) + G_2(\bar{p}, \bar{\bar{p}}) \\ s(q, \bar{p}, \bar{q}, \bar{\bar{p}}) &= S_1(q, \bar{p}) + S_2(\bar{q}, \bar{\bar{p}}) - \bar{p} \cdot \bar{q} \\ f(p, \bar{q}, \bar{p}, \bar{\bar{q}}) &= F_1(p, \bar{q}) + F_2(\bar{p}, \bar{\bar{q}}) + \bar{p} \cdot \bar{q} \end{aligned} \tag{2.6}$$

and look for variations with respect to the once barred variables. Denoting the critical point with a subscript 0, the corresponding critical value gives a generating function for ϕ

$$\begin{aligned} W(q, \bar{\bar{q}}) &= w(q, \bar{q}_0, \bar{\bar{q}}) \\ G(p, \bar{\bar{p}}) &= g(p, \bar{p}_0, \bar{\bar{p}}) \\ S(q, \bar{\bar{p}}) &= s(q, \bar{p}_0, \bar{q}_0, \bar{\bar{p}}) \\ F(p, \bar{\bar{q}}) &= f(p, \bar{q}_0, \bar{p}_0, \bar{\bar{q}}) \end{aligned} \tag{2.7}$$

This construction exhibits all differential geometric difficulties of the subject. The critical points do not need to exist or to be unique. If W_1 and W_2 unfold, we have no guaranty that W unfolds. For this subject, catastrophe theory is certainly very helpful [8].

Given a canonical map, a generating function which unfolds the transformation is defined up to a constant additive term. If the generating function is piecewise continuous having several branches, each branch is defined up to a constant. In sections 6 to 10 typical examples are given.

3. Van Vleck's canonical formula

Let us assume that a canonical transformation is given globally by its generating function W. $W(q, \bar{q})$ is differentiable on $\mathbb{R}^n \times \mathbb{R}^n$ and the J is non-vanishing.

$$J = \det\left(\frac{\partial^2 W}{\partial q\, \partial \bar{q}}\right) \neq 0, \qquad q, \bar{q} \in \mathbb{R}^n \tag{3.1}$$

Then, the canonical transformation is uniquely defined by

$$p_k - \frac{\partial W}{\partial qk}(q, \bar{q}) = 0 \qquad k = 1, \ldots, n \tag{3.2a}$$

and

$$\bar{p}_k + \frac{\partial W}{\partial \bar{q}^k}(q, \bar{q}) = 0 \qquad k = 1, \ldots, n \tag{3.2b}$$

Equations (3.2a) define implicitely $\bar{q}^k(q, p)$ and (3.2b) gives $q^k(\bar{q}, \bar{p})$. For a quantum mechanical problem, we want to calculate the unitary kernel $\langle q \mid \bar{q} \rangle$ which diagonalizes $\bar{q}_{op}$.

$$\langle q | \bar{q}_{op} | \bar{q} \rangle = \bar{q} \langle q \mid \bar{q} \rangle \tag{3.3}$$

Here is the first difficulty. We have to construct the quantum mechanical operator $\bar{q}_{op}$ corresponding to the implicitly defined classical $\bar{q}$. Disregarding all problems related with the non-commutativity, replacing p in (3.2a) by its Schroedinger operator

$$\langle q \mid p_k^{op} \cdots = \frac{\hbar}{i} \frac{\partial}{\partial q^k} \langle q \mid \cdots \tag{3.4}$$

we obtain

$$\frac{\hbar}{i} \frac{\partial}{\partial q^k} \langle q \mid \bar{q} \rangle = \frac{\partial W}{\partial q^k} \cdot \langle q \mid \bar{q} \rangle$$

whose integration is trivial

$$\langle q \mid \bar{q} \rangle = N \exp \frac{i}{\hbar} W(q, \bar{q})$$

This crude approximation is interesting. Complex conjugation is equivalent to a change of sign of W; it gives the inverse transformation in the same approximation. Moreover, this expression is reminiscent to the stationary wave function in the first *WKB* approximation.

Now we calculate the next approximation which is the Van Vleck's result [6]. Our calculation method allows, at least in principle, to compute higher corrections. These higher order terms go to zero with $\hbar$. They are not uniquely defined and without geometrical interpretation.

In order to perform the calculation of $\bar{q}_{op}$, we first have to define $\bar{q}(q, p)$ explicitly. For this purpose, we look at an expansion of W in $\varepsilon = \bar{q} - \bar{q}_0$, around an arbitrary point $\bar{q}_0$. We have[2])

$$W(q, \bar{q}) = W(q, \bar{q}_0) + \frac{\partial W}{\partial \bar{q}_0^k} \varepsilon^k + \frac{1}{2} \frac{\partial^2 W}{\partial \bar{q}_0^k \partial \bar{q}_0^l} \varepsilon^k \varepsilon^l + \cdots \tag{3.5}$$

Introducing this expansion into (3.2a) we obtain

$$p_k - \frac{\partial W}{\partial q^k} - \frac{\partial^2 W}{\partial q^k \partial \bar{q}_0^l} \varepsilon^l - \frac{1}{2} \frac{\partial^3 W}{\partial q^k \partial \bar{q}_0^l \partial \bar{q}_0^m} \varepsilon^l \varepsilon^m - \cdots = 0 \tag{3.6}$$

Because of (3.1) it is possible, in principle, to obtain $\varepsilon_{\bar{q}_0}^k(q, p)$ as a power series in p. Here we restrict ourselves to the linear term. This approximate calculation would be exact for a W linear in $\bar{q}$ or quadratic in q and $\bar{q}$, for example. In this linear approximation, we have

$$\varepsilon^l = (\Omega^{-1})^{lk} \left(p_k - \frac{\partial W}{\partial q^k} \right)$$

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[2]) By $\frac{\partial W}{\partial \bar{q}_0^k}$ we mean $\frac{\partial W}{\partial \bar{q}^k}(q, \bar{q}_0)$.

with

$$\Omega_{kl}=\frac{\partial^2 W}{\partial q^k\,\partial \bar{q}_0^l} \tag{3.7}$$

Condition (3.1) ensures existence and uniqueness of the inverse matrix Ω^{-1} everywhere, and ε is well defined as a function of p and q for each value of $\bar{q}_0$. The construction of the corresponding Hermitian operator family requires to take half the anticommutator of p_{op} with Ω^{-1}. Defining

$$\varepsilon^l_{\text{op}}=\bar{q}^l_{\text{op}}-\bar{q}^l_0\mathbb{1} \tag{3.8}$$

we have in the linearized symmetrical approximation

$$\begin{aligned}\varepsilon^l_{\text{op}}&=\tfrac{1}{2}\{(\Omega^{-1})^{lk},p^{\text{op}}_k\}-(\Omega^{-1})^{lk}\frac{\partial W}{\partial q^k}\\&=(\Omega^{-1})^{lk}\left(p^{\text{op}}_k-\frac{\partial W}{\partial q^k}\right)+\frac{\hbar}{2i}\frac{\partial(\Omega^{-1})^{lk}}{\partial q^k}\end{aligned}$$

But we have the identity

$$\frac{\partial}{\partial q^k}(\Omega^{-1})^{lk}=-(\Omega^{-1})^{lk}\frac{\partial}{\partial q^k}\log|\det\|\Omega\||\tag{3.9}$$

valid for matrices of the form (3.7). It follows, recalling the definition (3.1)

$$\varepsilon^l_{\text{op}}=(\Omega^{-1})^{lk}\left[p^{\text{op}}_k-\frac{\partial}{\partial q^k}\left(W+\frac{\hbar}{2i}\log|J|\right)\right]\tag{3.10}$$

For each value of $\bar{q}^k_0$ we find a common eigenfunction of eigenvalue 0 for each $\varepsilon^l_{\text{op}}$. Namely

$$\psi_{\bar{q}_0}(q)=c(\bar{q}_0)\,|J|^{1/2}\exp\frac{i}{\hbar}W(q,\bar{q}_0)$$

is obviously a solution of

$$\varepsilon^l_{\text{op}}\psi_{\bar{q}_0}=0\qquad\forall\, l$$

In this approximation, the matrix-elements $\langle q\mid\bar{q}\rangle$ take the form given by Van Vleck [6]

$$\langle q\mid\bar{q}\rangle\simeq\psi_{\bar{q}}(q)=\frac{1}{(2\pi\hbar)^{n/2}}\left|\det\left(\frac{\partial^2 W}{\partial q\,\partial\bar{q}}\right)\right|^{1/2}\exp\frac{i}{\hbar}W(q,\bar{q})\tag{3.11}$$

Here the coefficient c was chosen in analogy with the standard normalization of the plane waves. That it is independent of $\bar{q}$ is obvious from the symmetry in q and $\bar{q}$ of the problem. The normalization (3.11) ensures unitarity as we shall see in the next paragraph. The formula (3.11) is exact if the second derivatives of W in $\bar{q}$ vanish. Otherwise it is asymptotically exact for $\hbar=0$.

In (3.11) phase and argument have precise classical meanings. The phase is a generating function and the argument is the square root of the Jacobian which tells the possibility to solve the implicit relations (3.2). It is a transversality measure of the coordinate system in $E\times\bar{E}$ (associated with the generating function) with respect to the graph of the map.

Finally, the freedom of an additive constant in W (for the same transformation) manifests itself in the freedom of a general phase factor in quantum mechanics.

4. Unitarity

The kets $|q\rangle$ being normalized to fulfil

$$\langle q \mid q'\rangle = \delta^{(n)}(q-q') \tag{4.1}$$

we expect the same to hold for $|\bar{q}\rangle$ if unitarity of $\langle q \mid \bar{q}\rangle$ holds. From (3.11) we have

$$\begin{aligned}\langle \bar{q} \mid \bar{q}'\rangle &= \int \langle \bar{q} \mid q\rangle\, d^n q \langle q \mid \bar{q}'\rangle = \int \langle q \mid \bar{q}\rangle^* \langle q \mid \bar{q}'\rangle\, d^n q \\ &= \frac{1}{(2\pi\hbar)^n} \int \left| \det\left(\frac{\partial^2 W}{\partial q\, \partial \bar{q}}(q, \bar{q})\right) \det\left(\frac{\partial^2 W}{\partial q\, \partial \bar{q}'}\right)\right|^{1/2} \\ &\quad \times \exp \frac{i}{\hbar}(W(q, \bar{q}) - W(q, \bar{q}'))\, d^n q\end{aligned} \tag{4.2}$$

If in particular W is a polynomial of second degree in q and $\bar{q}$ or first degree in either q or $\bar{q}$, (3.11) gives at least formally an exact result (cf. section 3) and the integral (4.2) can be performed exactly yielding (4.1) for the kets $|\bar{q}\rangle$.

Generally, unitarity does not hold exactly. We show below that

$$\lim_{\hbar \to 0} \langle \bar{q} \mid \bar{q}'\rangle = \delta^{(n)}(\bar{q}-\bar{q}'). \tag{4.3}$$

If unitarity holds, (3.11) is an exact expression. If not, the lack of unitarity is an inverse measure for the quality of (3.11).

The phase

$$\psi(q, \bar{q}, \bar{q}') = W(q, \bar{q}) - W(q, \bar{q}') \tag{4.4}$$

of the integrand in (4.2) vanishes for all q if $\bar{q} = \bar{q}'$, forcing the integral to diverge. For $\bar{q} \neq \bar{q}'$, this phase has no stationary point. The gradient never vanishes

$$\frac{\partial \psi}{\partial q} = \frac{\partial W}{\partial q}(q, \bar{q}) - \frac{\partial W}{\partial q}(q, \bar{q}') = p(q, \bar{q}) - p(q, \bar{q}') \tag{4.5}$$

because (3.1) is assumed to hold. Therefore, the integral (4.2) is vanishingly small except in a neighbourhood $\bar{q}' \sim \bar{q}$. For $\bar{q}'$ arbitrary close to $\bar{q}$ we can write

$$\begin{aligned}&\psi \simeq (\bar{q} - \bar{q}')^k \frac{\partial W}{\partial \bar{q}^k}(q, \bar{q}) = -(\bar{q} - \bar{q}') \cdot \bar{p} \\ &\det\left(\frac{\partial^2 W}{\partial q\, \partial \bar{q}}(q, \bar{q}')\right) \cong \det\left(\frac{\partial^2 W}{\partial q\, \partial \bar{q}}(q, \bar{q})\right)\end{aligned} \tag{4.6}$$

Changing the integration variable from q to $\bar{p}$, the integral (4.2) becomes

$$\langle \bar{q} \mid \bar{q}'\rangle = \int \frac{d^n \bar{p}}{(2\pi\hbar)^n} \exp -\frac{i}{\hbar}(\bar{q} - \bar{q}')\bar{p} = \delta^{(n)}(\bar{q} - \bar{q}') \tag{4.7}$$

This result is independent of $\hbar$.

In regions where (4.6) does not hold, the integral is in general $\hbar$-dependent but vanishes (in distribution sense) for $\hbar \to 0$. This last fact follows from

$$\frac{1}{\hbar^n} \exp \frac{i}{\hbar} \psi(q, \bar{q}, \bar{q}') \underset{\hbar \to 0}{\longrightarrow} 0 \qquad \bar{q} \neq \bar{q}' \in \mathbb{R}^n$$

when ψ has no stationary point in q. This achieves the proof of (4.3).

5. Four useful representations

The kernel (3.11) intertwines the two Hilbert spaces $L^2(\mathbb{R}^n, d^n q)$ and $L^2(\mathbb{R}^n, d^n \bar{q})$. It is well known that appropriate Fourier transforms lead to the momentum spaces $L^2(\mathbb{R}^n, d^n p)$ and $L^2(\mathbb{R}^n, d^n \bar{p})$. The transformation to the momentum representation is also canonical and unitary. For this reason, all kernels are of the same asymptotic form as (3.11) provided we use the appropriate generating function.

$$\langle q \mid \bar{q} \rangle = \frac{1}{(2\pi\hbar)^{n/2}} \left| \det \left(\frac{\partial^2 W}{\partial q \, \partial \bar{q}} \right) \right|^{1/2} \exp \frac{i}{\hbar} W(q, \bar{q}) \tag{5.1}$$

$$\langle q \mid \bar{p} \rangle = \frac{1}{(2\pi\hbar)^{n/2}} \left| \det \left(\frac{\partial^2 S}{\partial q \, \partial \bar{p}} \right) \right|^{1/2} \exp \frac{i}{\hbar} S(q, \bar{p}) \tag{5.2}$$

$$\langle p \mid \bar{q} \rangle = \frac{1}{(2\pi\hbar)^{n/2}} \left| \det \left(\frac{\partial^2 F}{\partial p \, \partial \bar{q}} \right) \right|^{1/2} \exp \frac{i}{\hbar} F(p, \bar{q}) \tag{5.3}$$

$$\langle p \mid \bar{p} \rangle = \frac{1}{(2\pi\hbar)^{n/2}} \left| \det \left(\frac{\partial^2 G}{\partial p \, \partial \bar{p}} \right) \right|^{1/2} \exp \frac{i}{\hbar} G(p, \bar{p}) \tag{5.4}$$

Here the functions W, S, F and G are just the generating functions of section 2. The Fourier transforms lead to Legendre transformations for the exponents in the stationary phase approximation.

A good generating function has to obey the transversality condition (3.1). Once a good generating function has been found, the other kernels are Fourier transforms and, as a rule, do not have the simple form (5.1)–(5.4). The Legendre transformations may have many solutions or branches. Outside the bifurcation sets, the stationary phase method holds and we have to add the exponential terms of all branches. The important point is the determination of the appropriate relative phases. This problem was first recognized and solved by Maslov [7].

The composition of kernels of type (5.1)–(5.4) may be evaluated in the stationary phase approximation, leading to expressions of the same type but with generating functions obtained by the rule (2.6), (2.7).

Instead of going into more details of the general theory, we prefer to discuss some examples.

6. Linear canonical transformations

Moshinsky and Quesne [11] solved this problem explicitly already in 1971, without reference to the generating function formalism. These authors use the

$W(q, \bar{q})$ representation. To obtain a linear transformation, W has to be a polynomial of second degree. Using notations similar to Ref. [11] we put

$$W = \tfrac{1}{2}(-\tilde{q}B^{-1}Aq + 2\tilde{q}B^{-1}\bar{q} - \bar{q}^{\sim}DB^{-1}\bar{q}) \tag{6.1}$$

where capitals denote $n \times n$ matrices, and $\tilde{q}, \tilde{\bar{q}}$ are transposed vectors of q and $\bar{q}$. Condition (3.1) gives

$$J = \det B^{-1} = \text{const.} \neq 0 \tag{6.2}$$

and B exists. Canonical equations give

$$p = \nabla_q W = -B^{-1}Aq + B^{-1}\bar{q}$$
$$\bar{p} = -\nabla_{\bar{q}} W = -\tilde{B}^{-1}q + DB^{-1}\bar{q}$$

and we can reorganize

$$\begin{pmatrix} \bar{q} \\ \bar{p} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} \tag{6.3}$$

where

$$C = DB^{-1}A - \tilde{B}^{-1} \tag{6.4}$$

In equation (6.1), $B^{-1}A$ and DB^{-1} are symmetrical matrices. This ensures with (6.4) all canonicity relations. Insertion of the expression (6.1) into (5.1) gives a unitary kernel. This is the key result of Moshinsky and Quesne. By composition of such unitary kernels, the stationary phase method gives an exact result, provided the resulting generating function (2.7) exists and unfolds.

But, in the case of symplectic transformations, no generating function unfolds for all elements of the group. This is due to the topology of the group. Phase factors appear which means that we are dealing with the metaplectic representation, i.e. a representation of the universal covering of the symplectic group as has been carefully discussed by by J. Leray [12].

We want to point out that the representation $W(q, \bar{q})$ fails to unfold the identity map. As a consequence, it is difficult to discuss some very simple problems in these variables. On the other hand, using $S(q, \bar{p})$ we can answer all questions about the neighbourhood of the identity map. Putting

$$S(q, \bar{p}) = \tfrac{1}{2}(-\tilde{q}D^{-1}Cq + 2\tilde{q}D^{-1}\bar{p} + \bar{p}^{\sim}BD^{-1}\bar{p}) \tag{6.5}$$

we obtain from (2.2c)

$$p = \nabla_q S = -D^{-1}Cq + D^{-1}\bar{p}$$
$$\bar{q} = \nabla_{\bar{p}} S = \tilde{D}^{-1}q + BD^{-1}\bar{p}$$

A trivial calculation gives

$$\begin{pmatrix} \bar{q} \\ \bar{p} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} \tag{6.6}$$

with

$$A = \tilde{D}^{-1} + BD^{-1}C \tag{6.7}$$

This time D needs to be non-singular and this condition does not exclude the unity matrix as (6.2) does.

Inserting (6.5) in (5.2) one obtains

$$\langle q\,|\bar{p}\rangle=\frac{1}{(2\pi\hbar)^{n/2}}\frac{1}{|\det D|^{1/2}}\exp\frac{i}{2\hbar}(-\tilde{q}D^{-1}Cq+2\tilde{q}D^{-1}\bar{p}+\bar{p}^{\sim}BD^{-1}\bar{p}) \tag{6.8}$$

For the identity map $A=D=\mathbb{1}$, $B=C=0$, we have simply the plane wave, which has nice analytical properties in the complex domain of the group parameters. For example, let us consider the transformation group associated with the motion of the harmonic oscillator

$$H=\frac{p^2}{2m}+\frac{m\omega^2}{2}q^2 \tag{6.9}$$

We have

$$\begin{pmatrix} q(t)\\ p(t)\end{pmatrix}=\begin{pmatrix}\cos\omega t & \dfrac{1}{m\omega}\sin\omega t\\ -m\omega\sin\omega t & \cos\omega t\end{pmatrix}\begin{pmatrix}\bar{q}\\ \bar{p}\end{pmatrix} \tag{6.10}$$

where $\bar{q}$, $\bar{p}$ stand for the initial condition. Using (6.5) and (6.6) we find a family of generating functions

$$S_t(q,\bar{p})=\frac{1}{2\cos\omega t}\left(m\omega q^2\sin\omega t+2q\bar{p}+\frac{\bar{p}^2}{m\omega}\sin\omega t\right) \tag{6.11}$$

All quantities have a precise meaning in the domain $|\mathrm{Re}\,\omega t|<\pi/2$. Writing

$$|\;\rangle_t=\exp-\frac{i}{\hbar}Ht\,|\;\rangle \tag{6.12}$$

we obtain from (6.8)

$$\begin{aligned}\langle q|\exp\frac{i}{\hbar}Ht\,|\bar{p}\rangle={}_t\langle q\mid\bar{p}\rangle&=(2\pi\hbar)^{-1/2}\,|\cos\omega t|^{-1}\exp\frac{i}{2\hbar\cos\omega t}\\&\quad\times\left(m\omega q^2\sin\omega t+2q\bar{p}+\frac{\bar{p}^2}{m\omega}\sin\omega t\right)\end{aligned} \tag{6.13}$$

Now, let us consider purely imaginary "time" $t=i\hbar\beta$. We obtain the equilibrium state operator from (6.13). The normalized limit $\beta\to\infty$ is a projector onto the ground state $|0\rangle\langle 0|$

$$\lim_{\beta\to\infty}N\langle q|\,e^{-\beta H}\,|\bar{p}\rangle\propto\exp\frac{-1}{2\hbar}\left(m\omega q^2+\frac{\bar{p}^2}{m\omega}\right) \tag{6.14}$$

The result is a product. Obviously, after normalization, we obtain

$$\langle q\mid 0\rangle=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp-\frac{m\omega}{2\hbar}q^2 \tag{6.15a}$$

$$\langle 0\mid\bar{p}\rangle=\left(\frac{1}{\pi\hbar m\omega}\right)^{1/4}\exp-\frac{\bar{p}^2}{2\hbar m\omega} \tag{6.15b}$$

which are the well known wave functions of the ground state of the harmonic oscillator in configuration and momentum spaces respectively. Instead of time parameter, we can complexify the phase space itself. In doing so, we can introduce the normal modes. The transformation

$$\begin{pmatrix} \bar{q} \\ \bar{p} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -\dfrac{i}{m\omega} \\ -im\omega & 1 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} \tag{6.16}$$

is useful in the sense that it is symplectic and that the variables $\bar{q}$ and $\bar{p}$ undergo a very simple transformation with time. Namely

$$\bar{q}(t) = \bar{q}(0) \exp i\omega t \qquad \bar{p}(t) = \bar{p}(0) \exp -i\omega t \tag{6.17}$$

For q and p real, we have $\bar{p} = -im\omega\bar{q}^*$ and the full information is contained in the complex variable $\bar{p} = z \in \mathbb{C}$. The integral kernel corresponding to (6.16) is

$$\langle q \mid z \rangle = \frac{2^{1/4}}{(2\pi\hbar)^{1/2}} \exp -\frac{1}{\hbar}\left[\frac{1}{2}\left(m\omega q^2 - \frac{z^2}{m\omega}\right) + i\sqrt{2}\, qz\right] \tag{6.18}$$

Here, q is real and z is complex. For $z = 0$ we have essentially (6.15a), namely the ground state of the harmonic oscillator. Otherwise (6.18) is a coherent state of Glauber.

7. Gauge transformations

These transformations are the most general ones which do not change the configuration space coordinates. Obviously $S(q, \bar{p})$ and $F(p, \bar{q})$ unfold, W does not exist and G is a multivalued Legendre transform of S. We have

$$\bar{q}^k = \frac{\partial S}{\partial \bar{p}_k} = q^k \tag{7.1}$$

and the most general solution is

$$S = q^k \bar{p}_k + s(q) \tag{7.2}$$

which leads to

$$p_k = \bar{p}_k + \frac{\partial s}{\partial q^k} \tag{7.3}$$

This type of parametrization is useful each time we encounter conserved quantities. The result (7.3) indicates to what extent conjugate variables $\bar{p}$ are defined.

Condition (3.1) is satisfied.

$$\det \left\| \frac{\partial^2 S}{\partial q^k\, \partial \bar{p}_l} \right\| = 1 \tag{7.4}$$

and the corresponding Van Vleck's formula is exact

$$\langle q \mid \bar{p} \rangle = \frac{1}{(2\pi\hbar)^{n/2}} \exp \frac{i}{\hbar} (q \cdot \bar{p} + s(q)) \tag{7.5}$$

Simple Fourier transforms give

$$\langle q \mid \bar{q}\rangle = \delta(q-\bar{q}) \exp \frac{i}{\hbar} s(q) \tag{7.6}$$

$$\langle p \mid \bar{q}\rangle = \frac{1}{(2\pi\hbar)^{n/2}} \exp \frac{i}{\hbar}(-p\cdot\bar{q}+s(\bar{q})) \tag{7.7}$$

$$\langle p \mid \bar{p}\rangle = \frac{1}{(2\pi\hbar)^{n}} \int d^n q \exp \frac{i}{\hbar}(q\cdot(\bar{p}-p)+s(q)) \tag{7.8}$$

The four expressions (7.5–8) are exact, and obviously (7.8) is the most complicated. If necessary (7.8) may be asymptotically evaluated in stationary phase approximation. In this case we have to take all stationary points into account, and in some cases we have to expect delta function singularities on caustics.

Among transformations of type (7.3) we have passive Galilei transformations or elements of the Newton group in the terminology of Giovannini and Piron [13]. In potential scattering theory, the S-matrix is also of the form (7.5) in action angle variables [14], and s is $\hbar$ times the phase shift.

8. Energy time variables for the free fall

Let us consider the one dimensional motion of a particle submitted to a constant force $F_0 \neq 0$ and let us try to describe the phase space orbits with energy and time variables. For this purpose, we chose the turning point as time origin.

$$\bar{q} = E = \frac{p^2}{2m} - F_0 q \tag{8.1}$$

$$\bar{p} = -T = -\frac{p}{F_0} \tag{8.2}$$

This transformation is clearly canonical and the generating function S unfolds

$$S(q,\bar{p}) = \frac{F_0^2\bar{p}^3}{6m} - F_0 q\bar{p} \tag{8.3}$$

$$p = \frac{\partial S}{\partial q} = -F_0\bar{p} \qquad \bar{q} = \frac{\partial S}{\partial \bar{p}} = \frac{\bar{p}^2 F_0^2}{2m} - qF_0$$

We have the exact relation

$$\langle q \mid \bar{p}\rangle = \sqrt{\frac{|F_0|}{2\pi\hbar}} \exp \frac{i}{\hbar} F_0\left(\frac{F_0}{6m}\bar{p}^3 - q\bar{p}\right)$$

Writing T instead of $-\bar{p}$, we have

$$\langle q \mid T\rangle = \sqrt{\frac{|F_0|}{2\pi\hbar}} \exp -\frac{i}{\hbar} F_0\left(\frac{F_0}{6m}T^3 - qT\right) \tag{8.4}$$

In this case, T is eigenvalue of a time operator which is unitarily equivalent to the position operator. Looking at the time evolution, we can study the quantity

$$\varphi_q(t) = \int \langle q \mid T+t \rangle g(T)\, dT \tag{8.5}$$

This is the probability amplitude to find the system at time t at the position q. Conversely, it is the probability amplitude to obtain a "click" at time t if the detector is at position q. We have an interchange between two different description possibilities. Here, q is the superselection rule as proposed by Piron [15].

In fact, the explicit expression (8.5) is a solution of Piron's equation

$$-i\hbar \frac{\partial}{\partial q} \varphi = \pi \varphi \tag{8.6}$$

with

$$\pi = \sqrt{2m\left(i\hbar \frac{\partial}{\partial t} + F_0 q\right)} \tag{8.7}$$

The reader needs simply to compare the action of π^2 on φ with the q-derivative. The advantage of the explicit relation (8.5) is that we avoid the ill-defined operator (8.7). We can also discuss precisely the meaning of such a time probability amplitude, which displays caustics and tunnelling in the time coordinate.

As superselection rule, q has no "thickness" and the corresponding detector formulates the event "jump over the point q".

9. Time-energy description of the one-dimensional free motion

At first sight, we would expect the free motion to be simpler to discuss than the free fall. This is not the case because the transformation to energy-time variables is not one-to-one. For this reason, we introduce the dichotomic variable $\varepsilon = \pm 1$ which tells the sign of p if we give the energy E.

The map

$$\begin{array}{lcl} q = \varepsilon\sqrt{\dfrac{2E}{m}}\,T & & T = \dfrac{mq}{p} \\ p = \varepsilon\sqrt{2mE} & \longleftrightarrow & E = \dfrac{p^2}{2m} \\ & & \varepsilon = \dfrac{p}{|p|} \end{array} \tag{9.1}$$

is one-to-one and canonical in the two domains $p > 0$ and $p < 0$ separately. We have the choice between 3 generating functions where, in some way, the variable ε must appear.

We have

$$W(q, T) = \frac{mq^2}{2T} \tag{9.2}$$

$$\frac{\partial^2 W}{\partial q\, \partial T} = -\frac{mq}{T^2} \tag{9.3}$$

or

$$F(p, T) = -\frac{p^2 T}{2m} \tag{9.4}$$

$$\frac{\partial^2 F}{\partial p\, \partial T} = -\frac{p}{m} \tag{9.5}$$

or

$$S(q, E, \varepsilon) = \varepsilon\sqrt{2mE}q \tag{9.6}$$

$$\frac{\partial^2 S}{\partial q\, \partial E} = \varepsilon\sqrt{\frac{m}{2E}} \tag{9.7}$$

Before writing the Van Vleck formula, we have to define the functional space we use. Clearly, the space of functions of $E > 0$ is not large enough. For this reason, we try to define kets $|E, \varepsilon\rangle$. Taking (9.6) we obtain a meaningful expression

$$\langle q \mid E, \varepsilon\rangle = \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{m}{2E}\right)^{1/4} \exp\frac{i}{\hbar}\varepsilon\sqrt{2mE}\, q \tag{9.8}$$

The definition of the "time" kets does obviously not follow from the use of (9.4). Probability amplitude in time must be of positive frequency and the time coordinate has to be supplemented by the knowledge of ε. For this reason we put

$$\langle p \mid T, \varepsilon'\rangle = \frac{\delta_{\varepsilon\varepsilon'}}{\sqrt{2\pi\hbar}}\sqrt{\frac{|p|}{m}} \exp -\frac{i}{\hbar}\frac{p^2 T}{2m} \tag{9.9}$$

where ε is the sign of p. Combining (9.8) and (9.9) we obtain

$$\langle T, \varepsilon \mid E, \varepsilon'\rangle = \frac{\delta_{\varepsilon\varepsilon'}}{\sqrt{2\pi\hbar}} \exp\frac{i}{\hbar}ET \tag{9.10}$$

With this notation the energy time formalism is complete and we can use it equally well as the standard one. But, for all problems which are symmetrical for the right-left interchange, it may be better to diagonalize the parity operator with eigenvalue π. But parity operator acts on ε in the energy time description of states.

$$|E, \pi\rangle = \frac{1}{\sqrt{2}}(|E, \varepsilon = +1\rangle + \pi\, |E, \varepsilon = -1\rangle)$$

$$|T, \pi\rangle = \frac{1}{\sqrt{2}}(|T, \varepsilon = +1\rangle + \pi\, |T, \varepsilon = -1\rangle) \tag{9.11}$$

We have here projections onto the two irreducible representations of the ambiguity related to the incompleteness of E and T.

For the scattering in one dimension by a symmetrical potential independent of time and zero outside a finite range, the asymptotic states are of the form (9.11) with the same energy and parity.

We are in the situation of a gauge transformation in the two separate subspaces of parity ± 1. Denoting the final quantum state number by a dash, we have

$$\langle \bar{T}, \bar{\pi} \mid E, \pi \rangle = \frac{\delta_{\bar{\pi},\pi}}{\sqrt{2\pi\hbar}} \exp \frac{i}{\hbar} (E\bar{T} + 2\hbar\delta_{\pi}(E)) \tag{9.12}$$

The generating function of the time delay is written here in conventional units, namely as a phase shift δ [16]. The time delay has a complete classical meaning for the two separate subspaces. We think of two indistinguishable particles coming symmetrically from infinity against the potential. After collision, we have again two particles going back symmetrically to infinity. Because of the indistinguishability, we cannot distinguish between a cross-over of the particles or a repulsion. Parity + states behave like a boson pair and parity − like a fermion pair. In order to construct an incident packet, we have to go back to the ε variable and the fundamental quantum effect of tunnelling appears as a consequence of the difference in time delays of the two parity states for the same energy. Going back to the $|E, \varepsilon\rangle$ basis, we obtain

$$\langle \bar{E}, \bar{\varepsilon} \mid E, \varepsilon \rangle = \delta(E - \bar{E})[\tau\delta_{\bar{\varepsilon},\varepsilon} + \rho\delta_{\bar{\varepsilon},-\varepsilon}] \tag{9.13}$$

with

$$\left.\begin{aligned} \tau &= \tfrac{1}{2}(e^{2i\delta_+} + e^{2i\delta_-}) \\ \rho &= \tfrac{1}{2}(e^{2i\delta_+} - e^{2i\delta_-}) \end{aligned}\right. \tag{9.14}$$

We recognize the reflexion and transmission coefficients.

10. Unitary transformations generated by *QPQ*

This example is chosen to explain a paradoxal fact. The study of polynomial observables is a standard subject in the beginning of all textbooks on quantum mechanics. The commutator Lie algebra works without difficulties or ambiguities. On the other hand, from the point of view of functional analysis, polynomials in Q and P are unbounded operators which are usually not self-adjoint or essentially self-adjoint.

We take $h = q^2 p$ as classical Hamilton function. This function corresponds exactly to the operator QPQ in the Weyl–Wigner correspondence [17]. A related Hamilton function arises in the Coulomb problem in parabolic coordinates.

The canonical equations are easy to integrate and we obtain a family of canonical transformations parametrized by the "time" t.

$$\begin{aligned} q &\mapsto \bar{q} = \frac{q}{1 - qt} \\ p &\mapsto \bar{p} = (1 - qt)^2 p \end{aligned} \tag{10.1}$$

A discussion of this map which leaves the configuration space invariant may be found in [5]. Here we first look at the four generating functions which correspond to such transformations.

Clearly $W_t(q, \bar{q})$ does not exist because q and $\bar{q}$ are not independent. The function $G_t(p, \bar{p})$ has two branches

$$G_t^{(\pm)}(p, \bar{p}) = -\frac{1}{t}[p + \bar{p} \pm 2\sqrt{p\bar{p}}] \tag{10.2}$$

and

$$\frac{\partial^2 G}{\partial p\, \partial \bar{p}} = \frac{\mp 1}{2t\sqrt{p\bar{p}}} \tag{10.3}$$

The function G is well defined but not really appropriate because it develops singularities. Considering $S_t(q, \bar{p})$, we find the solution

$$S_t(q, \bar{p}) = \frac{q\bar{p}}{1 - qt} \tag{10.4}$$

and

$$\frac{\partial^2 S}{\partial q\, \partial \bar{p}} = \frac{1}{(1 - qt)^2} \tag{10.5}$$

This function is appropriate for the use in Van Vleck's expression because the determinant does not depend on $\bar{p}$. The construction of §4 is exact. For the function F we have a similar situation. Inserting (10.4) in (5.2) and using the notation of the transformation group

$$|\bar{p}\rangle = U_t\,|p'\rangle \tag{10.6}$$

we obtain

$$\langle q|\, U_t\,|p'\rangle = \frac{1}{2\pi\hbar}\frac{1}{|1 - qt|}\exp\frac{i}{\hbar}\frac{qp'}{1 - qt}$$

This expression is a natural solution of the problem, but not the most general. The very rapidly oscillating behaviour for $1 - qt \approx 0$ separates the two domains $1 - qt > 0$ and $1 - qt < 0$ in such a way that the phase relation between them is necessarily lost. We have the freedom to multiply this function by an arbitrary phase factor in each domain independently. For $1 - qt < 0$ point q moves to $\bar{q}$ through infinity and for $1 - qt > 0$ point q moves continuously (in t) to $\bar{q}$.

From the point of view of functional analysis we have the freedom of an arbitrary relative phase factor, but from geometrical considerations, we can reduce this liberty in a natural way. Putting

$$\langle q|\, U_t^{(\alpha)}\,|p'\rangle = \frac{1}{2\pi\hbar}\frac{\exp i\alpha\theta(1 - tq)}{1 - tq}\exp\frac{i}{\hbar}\frac{qp'}{1 - tq} \tag{10.7}$$

we obtain by a Fourier transform

$$\langle q|\, U_t^{(\alpha)}\,|q'\rangle = \frac{\exp i\alpha\theta(qq')}{qq'}\,\delta\!\left(\frac{1}{q} - \frac{1}{q'} - t\right) \tag{10.8}$$

Using the Wigner isomorphism in a direct way to

$$\bar{P} = UPU^+ \quad \text{and} \quad \bar{Q} = UQU^+ \tag{10.9}$$

we recover (10.1) for each real value of α. This result comes out in a distribution sense. Looking in the same way at the differential $\bar{p}\, d\bar{q}$, we obtain

$$\bar{p}\, d\bar{q} = p\, dq - \hbar\alpha t\, \delta(1-tq)\, dq \tag{10.10}$$

which corresponds to

$$\bar{p}(q, p) = (1-tq)^2(p - \hbar\alpha t\, \delta(1-tq)) \tag{10.11}$$

In ordinary calculations the second term is put equal to zero as $x^2\delta(x) = 0$. But the differential $d\bar{q}$ contains a pole of second order in $(1-tq)$ which cancels the coefficient in (10.10). We think that this result suggests the need of non-standard analysis for a clean formulation of quantum mechanics in phase space.

From the above considerations, the requirement of strict canonicity of $\bar{q}, \bar{p}$ implies $\alpha = 0$. In this case U_t is an unitary representation of a one parameter group. Going to the infinitesimal elements we obtain explicitly the properties of an unique extension of the generator QPQ.

11. Conclusion

In the present paper we have looked at the quantum transformation theory in exact analogy with finite classical canonical maps. The key of all considerations is the transversality condition of the generating function.

If a generating function exists which globally unfolds the map, the WKB approximation scheme works well and the Van Vleck's exponential gives a meaningful approximation. The exponent is a generating function of the canonical map properly normalized by Planck's constant. This seems to be the most general formulation of the discovery of the wave mechanics by de Broglie [18]. On the other hand, the norm factor has an equally well defined geometrical meaning as a transversality measure of the graph of the map with respect to the manifold of independent variables. At this point, the language of catastrophe theory is appropriate.

In spite of the limitations given by the unfolding condition, we obtain interesting results for the definition of the time operator for the free fall and also a procedure for the choice of some extension of non self-adjoint operators based on the correspondence principle. Proper quantum effects, however, arise by superposition of exponential terms. This phenomena appears for example if a physical process imposes the choice of non transverse independent variables. In this case we have to write the transformation in integral form as proposed by Maslov. The asymptotic evaluation of such integral transforms is a well known subject in optics [8].

Another source of interferences lays in the topology of the classical canonical map itself. In order to enforce mappings of $\mathbb{R}^{2n}$ onto $\mathbb{R}^{2n}$ for non-linear canonical transformations, (action-angle variables) Moshinsky and Seligman introduce sheeted phase spaces and the important notion of the ambiguity group. Projection onto irreducible representations of the ambiguity group leads to interferences between different sheets, i.e. different exponential terms. We used explicitly this method in order to discuss the one dimensional scattering.

In spite of the abovementioned success, the method is not a universal remedy for all possible ambiguities associated either with non-essentially self-adjoint operators or to the order of non-commuting operators. The same ambiguities arise here also, but in a different context. It is nevertheless helpful to look at such problems from different points of view in order to choose the physically pertinent extension.

Finally we want to point out that our results are very close in spirit to the method of Feynman path integral.

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