

Quantum canonical transformations as integral transformations

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We discuss how the Hamiltonian changes in quantum canonical transformations. To the operator $\hat{\mathcal{H}}(\hat{p}, \hat{q})$ one can associate (in a given ordering rule) a c -number function $\mathcal{H}(p, q)$. It is this function that appears in the action of the phase-space path integral. A quantum canonical transformation $\hat{\mathcal{H}} \rightarrow \hat{\mathcal{H}}'$ can now be expressed as an integral transformation $\mathcal{H}'(\bar{p}, \bar{q}) = \int dp dq \mathcal{T}(\bar{p}, \bar{q}; p, q) \mathcal{H}(p, q)$. The kernel \mathcal{T} is constructed explicitly for point transformations and for the $p = -\bar{q}, q = \bar{p}$ reflection by studying changes of variables in the path integral. The ordering dependence of \mathcal{T} is displayed. The invariance of commutation rules is also discussed.

I. INTRODUCTION

The prospective uses of canonical transformations (CT's) in the functional integral quantization are numerous. Recently, CT's have been used, e.g., in the connection of quantizing classically integrable systems.¹

We know that in classical mechanics it is possible to make a CT to a coordinate system where the new Hamiltonian is identically zero.² It has been suggested that the same method could be used to solve quantum mechanics³; unfortunately such an approach does not work in general. We cannot use classical CT's in the c -number action function of the path-integral formalism because there will be additional purely quantum-mechanical effects.⁴ (These are usually of order \hbar^2 and in the semiclassical approximation they do not matter.¹) In fact only for point transformations and linear transformations do we know how the quantum CT's should be performed.⁵⁻⁸

In this paper we will discuss quantum CT's in terms of integral transformations. Our blanket assumption is that any quantum operator $\hat{\mathcal{H}}(\hat{p}, \hat{q})$ can be given by a c -number (but not necessarily classical) function $\mathcal{H}(p, q)$ through⁹

$$\hat{\mathcal{H}}(\hat{p}, \hat{q}) = \int d\tau d\theta dp dq (2\pi\hbar)^{-2} \mathcal{F}(\tau, \theta) \mathcal{H}(p, q) \times \exp \left[\frac{i}{\hbar} [\tau(\hat{p} - p) + \theta(\hat{q} - q)] \right], \tag{1.1}$$

where \mathcal{F} gives the ordering rule (see Sec. II A). With this representation transformations of operators can be expressed as transformations of the

corresponding c -number functions.

We now propose to describe the effects of a quantum CT in terms of an integral transformation kernel: If $\mathcal{H}'(p, q)$ results from a quantum CT applied to $\mathcal{H}(p, q)$, we write

$$\mathcal{H}'(\bar{p}, \bar{q}) = \int dp dq \mathcal{T}(\bar{p}, \bar{q}; p, q) \mathcal{H}(p, q). \tag{1.2}$$

The kernel \mathcal{T} is the main object of study in this paper. Previous studies on the CT's have usually discussed only the transformation of Hamiltonians that are either quadratic^{5,7} or at most finite polynomials⁶ in p . Now once \mathcal{T} is given we can apply it to any \mathcal{H} to obtain \mathcal{H}' , instead of deriving \mathcal{H}' from first principles in each case separately. Representation (1.2) allows us also to focus on \mathcal{T} and to study its properties without reference to specific Hamiltonians. (Transformation kernels in coordinate space have been discussed by Fanelli.⁸)

When CT's are represented by integral transformations according to (1.2) the natural composition is given by

$$\mathcal{T}_3(\bar{p}, \bar{q}; p, q) = \int dp' dq' \mathcal{T}_2(\bar{p}, \bar{q}; p', q') \times \mathcal{T}_1(p', q'; p, q). \tag{1.3}$$

This defines an associative product in the set of CT's as \mathcal{T}_3 is a CT whenever \mathcal{T}_2 and \mathcal{T}_1 are.

Let us note here that the representation (1.2) obviously works for classical CT's; if $p = p(\bar{p}, \bar{q}), q = q(\bar{p}, \bar{q})$ is a CT, then

$$T_{\text{class}}(\bar{p}, \bar{q}; p, q) = \delta(p - p(\bar{p}, \bar{q})) \delta(q - q(\bar{p}, \bar{q})), \tag{1.4}$$

corresponding to a direct substitution. Equation (1.3) gives the usual composition law for classical CT's.

In Sec. II B we construct the quantum transformation kernel \mathcal{S} for the point transformation $q=F(Q)$, $p=P/F'(Q)$ using the discrete form of the definition of path integral. The resulting kernel (2.23) is not of the form (1.4) although in the limit $\hbar \rightarrow 0$ it is obtained. A generalization to $q=F(Q)$, $p=[P+K'(Q)]/F'(Q)$ is made in Sec. II C, and the linear transformation $q=P$, $p=-Q$ is considered in Sec. II D.

All of these transformations can be written in the form (1.2) and this can be done for all orderings, although the kernel $\mathcal{S}^{(\mathcal{F})}$ does depend explicitly on the ordering function \mathcal{F} . The ordering dependence always enters in a similar fashion allowing us to define ordering-independent quantities (T) in Sec. III.

In Sec. IV we discuss the additional properties of normalization

$$\int dk dl T(\bar{k}, \bar{l}; k, l) = 1 \quad (1.5)$$

and unitarity

$$\int dk' dl' T(k', l'; \bar{k}, \bar{l})^* T(k', l'; k, l) = \delta(k - \bar{k}) \delta(l - \bar{l}). \quad (1.6)$$

The linear transformation kernel has these properties and for point transformations unitarity can be used to eliminate the additional freedom noticed by Kerler.⁶ We also observe in Sec. IV B that the composition (1.3) of two point transformations is again a point transformation.

In Sec. V we discuss the transformation kernels from the viewpoint that they must conserve commutation rules for operators. For the transformation kernel we derive from this requirement the equation

$$\int dk_1 dk_2 dl_1 dl_2 \sin \left[\frac{2}{\hbar} [(k - k_1)(l - l_2) - (k - k_2)(l - l_1)] \right] T(k_1, l_1; \bar{k}_1, \bar{l}_1) T(k_2, l_2; \bar{k}_2, \bar{l}_2) = \int d\bar{k} d\bar{l} T(k, l; \bar{k}, \bar{l}) \sin \left[\frac{2}{\hbar} [(\bar{k} - \bar{k}_1)(\bar{l} - \bar{l}_2) - (\bar{k} - \bar{k}_2)(\bar{l} - \bar{l}_1)] \right]. \quad (1.7)$$

It can be shown to hold for the kernels derived in Sec. II. With commutators the possible ordering dependence enters also in the standard form, which allows us to write the ordering-independent form (1.7) using definitions of Sec. III.

Finally in Sec. VI we discuss our results and some open problems.

II. DERIVATION OF THE TRANSFORMATION KERNEL FROM FUNCTIONAL INTEGRALS

A. Definition through discrete techniques

To derive the transformation kernels we will discuss the trace $\text{Tr} \{ \exp[-(i/\hbar) \hat{\mathcal{H}} T] \}$ rather than propagators, because this saves us from considering end-point effects which are not relevant when the Hamiltonian is transformed. The starting point in the functional-integral approach is the discrete procedure¹⁰

$$\text{Tr} \left[\exp \left[-\frac{i}{\hbar} \hat{\mathcal{H}}(\hat{p}, \hat{q}) T \right] \right] = \lim_{N \rightarrow \infty} \prod_{k=1}^N \int dq_k \langle q_{k+1}, t_{k+1} | q_k, t_k \rangle, \quad (2.1)$$

where $q_{N+1} = q_1$, $t_k = (k-1)\epsilon$, $\epsilon = T/N$, and

$$\langle q_{k+1}, t_{k+1} | q_k, t_k \rangle = \left\langle q_{k+1} \left| \exp \left[-\frac{i}{\hbar} \epsilon \hat{\mathcal{H}}(\hat{p}, \hat{q}) \right] \right| q_k \right\rangle. \quad (2.2)$$

Here and in the following we will explicitly write out the \hbar dependence, because we will later also discuss the classical limit $\hbar \rightarrow 0$. As a consequence all Fourier transforms will have a factor i/\hbar in the exponent (rather than i) unless otherwise stated. The i/\hbar multiplying \mathcal{H} has a different role from the other i/\hbar factors below and is irrelevant for us since the transformation (1.2) is linear.

When N is large we may approximate

$$\langle q_{k+1}, t_{k+1} | q_k, t_k \rangle \approx \left\langle q_{k+1} \left| 1 - \frac{i}{\hbar} \epsilon \hat{\mathcal{H}}(\hat{p}, \hat{q}) \right| q_k \right\rangle. \quad (2.3)$$

To calculate this matrix element we need the representation of operators by⁹

$$\hat{\mathcal{H}}(\hat{p}, \hat{q}) = \int d\tau d\theta dp dq (2\pi\hbar)^{-2} \mathcal{F}(\tau, \theta) \mathcal{H}(p, q) \exp \left[\frac{i}{\hbar} [\tau(\hat{p} - p) + \theta(\hat{q} - q)] \right]. \quad (2.4)$$

This equation has an arbitrary function $\mathcal{F}(\tau, \theta)$ which characterizes the quantum orderings. For any fixed quantum theory all operators are given by (2.4), but we may of course consider different theories characterized by different ordering functions. Note that a given operator can be expressed in different orderings if a corresponding change is made in the function $\mathcal{H}(p, q)$.

The function \mathcal{F} is arbitrary save for the following considerations:

(i) We require that the functions of one variable $f(p)$ and $g(q)$ are quantized by direct substitution $f(p) \rightarrow f(\hat{p}), g(p) \rightarrow g(\hat{q})$. This leads to

$$\mathcal{F}(0, \theta) = \mathcal{F}(\tau, 0) = 1. \quad (2.5a)$$

(ii) \mathcal{F} may depend on \hbar in a complicated manner but to obtain classical correspondence we need

$$\lim_{\hbar \rightarrow 0} \mathcal{F}(a\hbar, b\hbar) = 1. \quad (2.5b)$$

(iii) In the following we will also have to divide by \mathcal{F} , therefore we assume

$$\mathcal{F}(\tau, \theta) \neq 0, \quad \forall \tau, \theta \quad (2.5c)$$

to avoid singularities.

(iv) If we also have

$$\mathcal{F}(\tau, \theta)^* = \mathcal{F}(-\tau, -\theta), \quad (2.5d)$$

then the $\hat{\mathcal{H}}(\hat{p}, \hat{q})$ corresponding to a real $\mathcal{H}(p, q)$ will be Hermitian, but below we will not assume this. Typical examples are given by the so-called λ orderings

$$\mathcal{F}(\tau, \theta) = \exp \left[\frac{i}{\hbar} \left(\frac{1}{2} - \lambda \right) \tau \theta \right], \quad (2.5e)$$

which give the Weyl, standard ($\hat{q}^m \hat{p}^n$), and anti-standard ($\hat{p}^n \hat{q}^m$) orderings for $\lambda = \frac{1}{2}, 1$, and 0 , respectively. These orderings have the properties (i)–(iii) for any λ , but (iv) only for $\lambda = \frac{1}{2}$.

To calculate (2.3) with (2.4) we first note that

$$\left\langle q' \left| \exp \left[\frac{i}{\hbar} (\tau \hat{p} + \theta \hat{q}) \right] \right| q'' \right\rangle = \delta(\tau + q' - q'') \exp \left[\frac{i}{\hbar} \theta \frac{1}{2} (q' + q'') \right], \quad (2.6)$$

where we have used the canonical commutation rule

$$[\hat{q}, \hat{p}] = i\hbar. \quad (2.7)$$

We then obtain

$$\begin{aligned} \langle q' | \hat{\mathcal{H}}(\hat{p}, \hat{q}) | q'' \rangle &\equiv \bar{H}(q', q'') \\ &= \int d\theta dp dq (2\pi\hbar)^{-2} \mathcal{F}(q'' - q', \theta) \mathcal{H}(p, q) \exp \left[\frac{i}{\hbar} [\theta(-q + \frac{1}{2}(q'' + q')) + p(q' - q'')] \right], \end{aligned} \quad (2.8)$$

so that

$$\left\langle q_{k+1} \left| 1 - \frac{i}{\hbar} \epsilon \hat{\mathcal{H}}(\hat{p}, \hat{q}) \right| q_k \right\rangle = \int \frac{dp_k}{2\pi\hbar} \exp \left[\frac{i}{\hbar} [p_k(q_{k+1} - q_k)] \right] \left[1 - \frac{i}{\hbar} \epsilon \bar{H}(p_k, q_{k+1}, q_k) \right], \quad (2.9)$$

where

$$\bar{H}(p_k, q_{k+1}, q_k) = \int d\theta dq (2\pi\hbar)^{-1} \mathcal{F}(q_k - q_{k+1}, \theta) \mathcal{H}(p_k, q) \exp \left[\frac{i}{\hbar} [\theta(-q + \frac{1}{2}(q_{k+1} + q_k))] \right]. \quad (2.10)$$

We can now write (2.1) either as⁶

$$\text{Tr} \left[\exp \left[-\frac{i}{\hbar} \hat{\mathcal{H}}(\hat{p}, \hat{q}) T \right] \right] = \lim_{N \rightarrow \infty} \prod_{k=1}^N \left[\int dq_k \right] \prod_{l=1}^N \left[\delta(q_{l+1} - q_l) - \frac{i}{\hbar} \epsilon \bar{H}(q_{l+1}, q_l) \right], \quad (2.11)$$

using (2.8), or as^{10,11}

$$\text{Tr} \left[\exp \left[-\frac{i}{\hbar} \widehat{\mathcal{H}}(\widehat{p}, \widehat{q}) T \right] \right] = \lim_{N \rightarrow \infty} \prod_{k=1}^N \left[\int dq_k dp_k (2\pi\hbar)^{-1} \right] \exp \left[\frac{i}{\hbar} \sum_{l=1}^N [p_l(q_{l+1} - q_l) - \epsilon \widetilde{H}(p_l, q_{l+1}, q_l)] \right], \quad (2.12)$$

using (2.9) and (2.10).

In (2.8)–(2.12) $\mathcal{H}(p, q)$ is the primary dynamical quantity. After it is given we can for a specific ordering \mathcal{F} , compute $\widetilde{H}(q_{l+1}, q_l)$ from (2.8) or $\widetilde{H}(p_l, q_{l+1}, q_l)$ from (2.10) and obtain the above discrete definitions for the trace. For the particular case of λ orderings we obtain

$$\widetilde{H}(q', q'') = \int dp (2\pi\hbar)^{-1} \mathcal{H}(p, \lambda q' + (1-\lambda)q'') \exp \left[\frac{i}{\hbar} p(q' - q'') \right],$$

and

$$\widetilde{H}(p, q', q'') = \mathcal{H}(p, \lambda q' + (1-\lambda)q''), \quad (2.13)$$

as expected. The q_k 's introduced in (2.1) can be associated, if one so wishes, with the times t_k , then the dummy variables p_k are associated with the intervals (t_k, t_{k+1}) .^{10,11}

B. The point transformation $q = F(Q), p = P/F'(Q)$

We will now discuss the effects of a point transformation

$$q = F(Q), \quad (2.14a)$$

$$p = P/F'(Q) \quad (2.14b)$$

on the expression for the trace. We will assume that the function F is bijective.

Let us first consider the Eq. (2.11) as it only depends on the q_k 's. For each k we can use (2.14a) and obtain

$$\text{Tr} \left[\exp \left[-\frac{i}{\hbar} \widehat{\mathcal{H}} T \right] \right] = \lim_{N \rightarrow \infty} \prod_{k=1}^N \left[\int dQ_k |F'(Q_k)| \right] \prod_{l=1}^N \left\{ \delta(F(Q_{l+1}) - F(Q_l)) - \frac{i}{\hbar} \epsilon \widetilde{H}(F(Q_{l+1}), F(Q_l)) \right\}. \quad (2.15)$$

We now want to rewrite this in the form (2.11) with possibly a different \widetilde{H} .

Let us first take $\prod_k |F'(Q_k)|$ inside the curly brackets of the l -product. Because for each l both Q_{l+1} and Q_l appear, we have here some degree of freedom and can write⁶

$$\prod_{k=1}^N |F'(Q_k)| = \prod_{l=1}^N \alpha(Q_l) \beta(Q_{l+1}), \quad (2.16)$$

where the functions α and β are otherwise arbitrary except that

$$\alpha(Q) \beta(Q) = |F'(Q)|. \quad (2.17)$$

These functions are actually functionals of F , so if there is a possibility of confusion we will write $\alpha = \alpha(F; Q)$ etc. Now, since

$$\beta(Q_{l+1}) \delta(F(Q_{l+1}) - F(Q_l)) \alpha(Q_l) = \delta(Q_{l+1} - Q_l), \quad (2.18)$$

we can write (2.15) as

$$\text{Tr} \left[\exp \left[-\frac{i}{\hbar} \widehat{\mathcal{H}} T \right] \right] = \lim_{N \rightarrow \infty} \prod_{k=1}^N \left[\int dQ_k \right] \prod_{l=1}^N \left\{ \delta(Q_{l+1} - Q_l) - \frac{i}{\hbar} \epsilon \widetilde{H}'(Q_{l+1}, Q_l) \right\}, \quad (2.19)$$

where

$$\bar{H}'(Q_{l+1}, Q_l) = \alpha(Q_l) \beta(Q_{l+1}) \bar{H}(F(Q_{l+1}), F(Q_l)). \quad (2.20)$$

Only if \bar{H}' were related to some $\mathcal{H}'(P, Q)$ the same way \bar{H} was related to $\mathcal{H}(p, q)$ through (2.8) would the change of coordinates be meaningful. Such an $\mathcal{H}'(P, Q)$ can indeed be found as follows: substituting (2.8) in both sides of (2.20) gives

$$\begin{aligned} \int d\theta dp dq \mathcal{F}(Q'' - Q', \theta) \mathcal{H}'(p, q) \exp \left[\frac{i}{\hbar} [\theta(-q + \frac{1}{2}(Q'' + Q')) + p(Q' - Q'')] \right] \\ = \alpha(Q'') \beta(Q') \int d\theta dp dq \mathcal{F}(F(Q'') - F(Q'), \theta) \mathcal{H}(p, q) \\ \times \exp \left[\frac{i}{\hbar} \{ \theta(-q + \frac{1}{2}[F(Q') + F(Q'')]) + p(F(Q') - F(Q'')) \} \right] \end{aligned} \quad (2.21)$$

from which \mathcal{H}' can be solved by first taking a Fourier transform with respect to $\frac{1}{2}(Q'' + Q')$, dividing by \mathcal{F} , and then taking another pair of Fourier transforms. The result is

$$\begin{aligned} \mathcal{H}'(\bar{p}, \bar{q}) = \int dp dq d\theta du dv dw (2\pi\hbar)^{-3} \alpha(v - \frac{1}{2}u) \beta(v + \frac{1}{2}u) \\ \times \mathcal{F}(F(v - \frac{1}{2}u) - F(v + \frac{1}{2}u), \theta) [\mathcal{F}(-u, w)]^{-1} \\ \times \exp \left[\frac{i}{\hbar} \{ p[F(v + \frac{1}{2}u) - F(v - \frac{1}{2}u)] + \theta \frac{1}{2} [F(v + \frac{1}{2}u) + F(v - \frac{1}{2}u)] \right. \\ \left. - \theta q - vw - u\bar{p} + w\bar{q} \} \right] \mathcal{H}(p, q). \end{aligned} \quad (2.22)$$

This can clearly be written in the form of a transformation (1.2) where

$$\begin{aligned} \mathcal{F}_F^{(\mathcal{F})}(\bar{p}, \bar{q}; p, q) = \int dx dy d\theta dw (2\pi\hbar)^{-3} \alpha(x) \beta(y) \mathcal{F}(F(x) - F(y), \theta) [\mathcal{F}(x - y, w)]^{-1} \\ \times \exp \left[\frac{i}{\hbar} \{ p[F(y) - F(x)] + \theta \frac{1}{2} [F(x) + F(y)] - \theta q + w\bar{q} - w \frac{1}{2} (x + y) = \bar{p}(x - y) \} \right]. \end{aligned} \quad (2.23)$$

We have now obtained the kernel which can be used for quantum CT's corresponding to (2.14). Our regularity assumptions were (2.5a) and (2.5c) for the ordering function \mathcal{F} , and bijectivity for the function F . Thus under these assumptions a kernel can be constructed to transform Hamiltonians.

As an example let us consider the Weyl ordering $\mathcal{F} = 1$. After doing the θ, w , and y integrations we get

$$\begin{aligned} \mathcal{F}_F^{(1)} = \int dx (2\pi\hbar)^{-2} 2\delta(q - \frac{1}{2}[F(x + \bar{q}) + F(-x + \bar{q})]) \\ \times \alpha(x + \bar{q}) \beta(-x + \bar{q}) \exp \left[\frac{i}{\hbar} \{ p[F(-x + \bar{q}) - F(x + \bar{q})] + 2\bar{p}x \} \right]. \end{aligned} \quad (2.23')$$

With this kernel the Hamiltonian $\mathcal{H} = \frac{1}{2}p^2$ will be transformed to

$$\mathcal{H}'(\bar{p}, \bar{q}) = \frac{1}{2}\bar{p}^2 / F'(\bar{q})^2 - i\hbar\bar{p} \frac{1}{2} [\alpha'(\bar{q})\beta(\bar{q}) - \alpha(\bar{q})\beta'(\bar{q})] / F'(\bar{q})^3 + \frac{1}{2}\hbar^2 \alpha'(\bar{q})\beta'(\bar{q}) / F'(\bar{q})^3. \quad (2.24)$$

In particular if $\alpha = \beta = F'(q)^{1/2}$ ($F' > 0$) we get the usual result⁵⁻⁷

$$\mathcal{H}'(\bar{p}, \bar{q}) = \frac{1}{2}\bar{p}^2 / F'(\bar{q})^2 + \frac{1}{8}\hbar^2 F''(\bar{q})^2 / F'(\bar{q})^4. \quad (2.24')$$

Let us now check that, in the limit $\hbar \rightarrow 0$, (2.23) gives the classical result. Rather than comparing $\mathcal{F}_F^{(\mathcal{F})}$ directly with the distribution (1.4) we will compare their Fourier transforms (this time without the i/\hbar factor) with respect to p and q . After also scaling the w integration ($w = \bar{w}\hbar$) we find

$$\begin{aligned} \tilde{\mathcal{F}}_F^{(\mathcal{F})}(\bar{p}, \bar{q}; k, l) = \int dx dy d\bar{w} (2\pi)^{-1} \alpha(x) \beta(y) \delta(k\hbar + F(y) - F(x)) \mathcal{F}(\hbar k, \hbar l) [\mathcal{F}(x - y, \bar{w}\hbar)]^{-1} \\ \times \exp \{ i \{ l \frac{1}{2} [F(x) + F(y)] + \bar{p}(x - y) / \hbar + \bar{w} [\bar{q} - \frac{1}{2}(x + y)] \} \}. \end{aligned} \quad (2.25)$$

From the δ function we get

$$x - y = k\hbar/F'(x) + O(\hbar^2). \quad (2.26)$$

Therefore in the limit $\hbar \rightarrow 0$ the ordering functions \mathcal{F} go to 1 due to (2.5b). Then integrating over w we get

$$\begin{aligned} \tilde{\mathcal{F}}_F^{(\mathcal{F})}(\bar{p}, \bar{q}; k, l) &\approx \int dx dy \alpha(x)\beta(y)\delta(k\hbar + F'(x)(y-x))\delta(\bar{q} - \frac{1}{2}(x+y)) \\ &\times \exp(i\{\frac{1}{2}l[F(x)+F(y)] + \bar{p}k/F'(x)\}), \end{aligned}$$

which gives [recall (2.17)]

$$\tilde{\mathcal{F}}_F^{(\mathcal{F})}(\bar{p}, \bar{q}; k, l) \xrightarrow{\hbar \rightarrow 0} \tilde{T}_F^{\text{class}}(\bar{p}, \bar{q}; k, l) = \exp(i[lF(\bar{q}) + k\bar{p}/F'(\bar{q})]). \quad (2.27)$$

$\mathcal{F}_F^{(\mathcal{F})}$ of (2.23) also reduces to the classical substitution $q = F(Q)$ when we have to transform a function that only depends on q . According to (1.2) we then need only $\int dp \mathcal{F}_F^{(\mathcal{F})}(\bar{p}, \bar{q}; p, q)$, but integrating over p in (2.23) gives $\delta(x-y)/|F'(x)|$, and all ordering dependence goes away. The remaining integration can now be done giving

$$\int dp \mathcal{F}_F^{(\mathcal{F})}(\bar{p}, \bar{q}; p, q) = \delta(q - F(\bar{q})). \quad (2.28)$$

C. Extension to $q = F(Q)$, $p = (P + K'(Q))/F'(Q)$

The above derivation started with (2.11), where only q 's appeared. We therefore only needed to specify $q_k = F(Q_k)$ to continue, but finally we obtained the transformation rule for p as well. This is not surprising, for even if \bar{H} 's in (2.11) and (2.15) only depended on q 's, they are functionally dependent on the Hamiltonian $\mathcal{H}(p, q)$ through

$$\mathcal{H}'(P, \frac{1}{2}(Q' + Q'')) \stackrel{?}{=} \mathcal{H}(P[Q' - Q'']/[F(Q') - F(Q'')])\alpha(Q'')\beta(Q')$$

but here the left-hand side depends only on the sum $\frac{1}{2}(Q' + Q'')$ while the right-hand side depends both on the sum $\frac{1}{2}(Q' + Q'')$ and the difference $Q' - Q''$. However, when we keep the integration over P the differences $(Q' - Q'')$ can be converted to derivatives with respect to P through $\exp[(i/\hbar)P(Q' - Q'')]$, but this would give the same equations as in the previous derivation.

The above picture is still not quite complete because corresponding to (2.14a) there is in fact a family of classical CT's characterized by two functions F and K :

$$\begin{aligned} q &= F(Q), \\ p &= (P + K'(Q))/F'(Q). \end{aligned} \quad (2.30)$$

(2.8). Therefore we eventually obtained a transformation rule for Hamiltonians, for which the transformation of p 's is also needed.

We could also have started with (2.12) and then prescribed, e.g.,

$$p_l = P_l(Q_{l+1} - Q_l)/[F(Q_{l+1}) - F(Q_l)]. \quad (2.29)$$

This indicates how p_l is associated with the interval (t_l, t_{l+1}) rather than with either end point. In the limit $Q_{l+1} - Q_l \rightarrow 0$ we get $p = P/F'(Q)$ as required. The rule (2.29) guarantees that

$$p_l(q_{l+1} - q_l) = P_l(Q_{l+1} - Q_l),$$

so the form of (2.12) is preserved, but now we cannot equate $H(p, q', q'')$'s as we did with \bar{H} 's in (2.21). For example in the Weyl ordering ($\lambda = \frac{1}{2}$) we would get

For convenience we have chosen a derivative of the function K here.

What did we miss when we only obtained the $K' \equiv 0$ case? The tacit assumption in deriving (2.27) was that

$$\lim_{\hbar \rightarrow 0} [\alpha(x)\beta(x + O(\hbar))] = |F'(x)|, \quad (2.31)$$

but this need not be the case even if (2.17) holds.

Let us, e.g., assume that α and β depend on \hbar nonanalytically as follows:

$$\begin{aligned} \alpha(x) &= \bar{\alpha}(x) \exp\left[\frac{i}{\hbar}K(x)\right], \\ \beta(x) &= \bar{\beta}(x) \exp\left[-\frac{i}{\hbar}K(x)\right], \end{aligned} \quad (2.32)$$

where $\bar{\alpha}$ and $\bar{\beta}$ satisfy (2.17) and even (2.31). When we now take the $\hbar \rightarrow 0$ limit with (2.26) we get

$$\lim_{\hbar \rightarrow 0} [\alpha(x)\beta(x - \hbar k / F'(x) + O(\hbar^2))] = |F'(x)| \exp[ikK'(x)/F'(x)], \quad (2.33)$$

therefore with the choice (2.32) for \hbar dependence we indeed obtain the more general result

$$\tilde{T}_F^{\text{class}} = \exp\{i[IF(\bar{q}) + k(\bar{p} - K'(q))/(F'(q))]\} . \quad (2.34)$$

This demonstrates that the extra functions α and β are not idle decorations but determine a part of transformation. It is even more evident if we consider the classical CT

$$\begin{aligned} q &= Q, \\ p &= P + K'(Q), \end{aligned} \quad (2.35)$$

then the only thing we can do in (2.11) is to write

$$1 = \sum_{l=1}^N \frac{\alpha(Q_l)}{\alpha(Q_{l+1})} \quad (2.36)$$

and the choice (2.32) with $\beta = 1/\alpha$ gives the quantum CT corresponding to (2.35).

Thus in (2.23) we have the quantum transformation kernel corresponding to the general point transformation (2.30) with the above choice (2.32) for the functions α and β . However, (2.23) remains a well-defined transformation without any assumptions on the \hbar dependence of α, β , or F and can provide transformations with no classical counterpart. In Sec. IV we will discuss some further conditions on α and β .

D. The transformation $q = P, p = -Q$

To study the transformation

$$\begin{aligned} q &= P, \\ p &= -Q, \end{aligned} \quad (2.37)$$

we first go back to the definition (2.1). Instead of inserting eigenstates of the operator \hat{q} we could have used eigenstates of \hat{p} , i.e.,

$$\begin{aligned} \text{Tr} \left\{ \exp \left[-\frac{i}{\hbar} \hat{\mathcal{H}}(\hat{p}, \hat{q}) T \right] \right\} \\ = \lim_{N \rightarrow \infty} \prod_{k=1}^N \int dp_k \langle p_{k+1}, t_{k+1} | p_k, t_k \rangle, \end{aligned} \quad (2.38)$$

$$\begin{aligned} \langle p_{k+1}, t_{k+1} | p_k, t_k \rangle &= \left\langle p_{k+1} \left| \exp \left[-\frac{i}{\hbar} \epsilon \hat{\mathcal{H}}(\hat{p}, \hat{q}) \right] \right| p_k \right\rangle \\ &\approx \left\langle p_{k+1} \left| 1 - \frac{i}{\hbar} \epsilon \hat{\mathcal{H}}(\hat{p}, \hat{q}) \right| p_k \right\rangle. \end{aligned} \quad (2.39)$$

To compute these matrix elements with $\hat{\mathcal{H}}$ given as before by (2.4) we need

$$\begin{aligned} \left\langle p' \left| \exp \left[\frac{i}{\hbar} (\tau \hat{p} + \theta \hat{q}) \right] \right| p'' \right\rangle \\ = \delta(\theta + p'' - p') \exp \left[\frac{i}{\hbar} \tau \frac{1}{2} (p' + p'') \right]. \end{aligned} \quad (2.40)$$

Then we get, for example,

$$\begin{aligned} \langle p' | \hat{\mathcal{H}}(p, q) | p'' \rangle &\equiv \bar{H}_p(p', p'') \\ &= \int d\tau dp dq (2\pi\hbar)^{-2} \mathcal{F}(\tau, p' - p'') \mathcal{H}(p, q) \\ &\quad \times \exp \left[\frac{i}{\hbar} \left[-q(p' - p'') + \tau \left(-p + \frac{1}{2}(p' + p'') \right) \right] \right], \end{aligned} \quad (2.41)$$

$$\text{Tr} \left[\exp \left[-\frac{i}{\hbar} \hat{\mathcal{H}} T \right] \right] = \lim_{N \rightarrow \infty} \prod_{k=1}^N \left[\int dp_k \right] \prod_{l=1}^N \left[\delta(p_{l+1} - p_l) - \frac{i}{\hbar} \epsilon \bar{H}_p(p_{l+1}, p_l) \right] \quad (2.42)$$

corresponding to (2.8) and (2.11), respectively.

We now continue as in Sec. II by making the transformation $q = P$ in (2.11). It will then have the same form as (2.42), but to make sense out of this change of variables, we must insist that the function \bar{H} defined

by (2.8) from some Hamiltonian \mathcal{H} must be identical to a \overline{H}'_p arising from some other Hamiltonian \mathcal{H}' through (2.41). In equations

$$\int d\theta dp dq \mathcal{F}(p''-p', \theta) \mathcal{H}(p, q) \exp \left[\frac{i}{\hbar} [\theta(-q + \frac{1}{2}(p''+p')) + p(p'-p'')] \right] \\ = \int d\tau dp dq \mathcal{F}(\tau, p'-p'') \mathcal{H}'(p, q) \exp \left[\frac{i}{\hbar} [-q(p'-p'') + \tau(-p + \frac{1}{2}(p'+p''))] \right]. \quad (2.43)$$

Now we can solve for $\mathcal{H}'(p, q)$ the same way as from (2.21), and obtain

$$\mathcal{H}'(\overline{p}, \overline{q}) = \int dx dy dp dq (2\pi\hbar)^{-2} \mathcal{H}(p, q) \mathcal{F}(-y, x) [\mathcal{F}(x, y)]^{-1} \exp \left[\frac{i}{\hbar} [x(\overline{p}-q) + y(\overline{q}+p)] \right]. \quad (2.44)$$

This can again be written as a transformation (1.2) with

$$\mathcal{F}_{\text{refl}}^{(\mathcal{F})}(\overline{p}, \overline{q}; p, q) = \int dx dy (2\pi\hbar)^{-2} \mathcal{F}(-y, x) [\mathcal{F}(x, y)]^{-1} \exp \left[\frac{i}{\hbar} x(\overline{p}-q) + y(\overline{q}+p) \right]. \quad (2.45)$$

In particular for the λ orderings we get

$$\mathcal{F}_{\text{refl}}^{(\lambda)}(\overline{p}, \overline{q}; p, q) = [2\pi\hbar(1-2\lambda)]^{-1} \exp \left[\frac{i}{\hbar} [(\overline{q}+p)(\overline{p}-q)/(1-2\lambda)] \right], \quad (2.46)$$

which in the $\hbar \rightarrow 0$ limit (and for $\lambda = \frac{1}{2}$) reduces to the classical substitution

$$T_{\text{refl}}^{\text{class}}(\overline{p}, \overline{q}; p, q) = \delta(\overline{p}-q) \delta(\overline{q}+p). \quad (2.47)$$

It should be emphasized that (2.45) and (2.46) do not always reduce to the classical form (2.47) even though the reflection (2.37) is classically a linear CT. The possibility of ordering dependence in a linear transformation is not generally known and might lead one to conclude that the Weyl ordering is the only one possible. Our results show that any ordering is possible, but the naive substitution works only for orderings having the symmetry

$$\mathcal{F}(x, y) = \mathcal{F}(-y, x). \quad (2.48)$$

To get a feeling of what is going on let us consider as an example the case of

$$\mathcal{H} = p^2 q \quad (2.49a)$$

with λ orderings. Using (2.46) we get

$$\mathcal{H}' = q^2 p - 2(2\lambda - 1)i\hbar q. \quad (2.49b)$$

Corresponding to these we get from (2.4) the

operators

$$\widehat{\mathcal{H}}(\widehat{p}, \widehat{q}) = (1-\lambda)\widehat{p}^2 \widehat{q} + \lambda \widehat{q} \widehat{p}^2, \quad (2.50a)$$

$$\widehat{\mathcal{H}}'(p, q) = (1-\lambda)\widehat{p}^2 \widehat{q} + \lambda \widehat{q} \widehat{p}^2 - 2(2\lambda - 1)i\hbar \widehat{q}. \quad (2.50b)$$

Let us now check that $\widehat{\mathcal{H}}'$ results from $\widehat{\mathcal{H}}$ by the operator substitution $\widehat{q} \rightarrow \widehat{p}, \widehat{p} \rightarrow -\widehat{q}$. We get first

$$\widehat{\mathcal{H}}(-\widehat{q}, \widehat{p}) = (1-\lambda)\widehat{q}^2 \widehat{p} + \lambda \widehat{p} \widehat{q}^2,$$

but this is not in the canonical order. We have to commute \widehat{q}^2 and \widehat{p} , but then

$$\widehat{\mathcal{H}}(-\widehat{q}, \widehat{p}) = (1-\lambda)\widehat{p}^2 \widehat{q} + \lambda \widehat{q} \widehat{p}^2 \\ - (1-\lambda)[\widehat{p}, \widehat{q}^2] - \lambda[\widehat{q}^2, \widehat{p}] \\ = \widehat{\mathcal{H}}'(\widehat{p}, \widehat{q}). \quad (2.51)$$

Thus everything is in order and the diagram

$$\begin{array}{ccc} \mathcal{H} & \xrightarrow{(2.46)} & \mathcal{H}' \\ \downarrow (2.4) & & \downarrow (2.4) \\ \widehat{\mathcal{H}} & \xrightarrow{(2.51)} & \widehat{\mathcal{H}}' \end{array}$$

commutes in this example for every λ ordering.

III. ELIMINATING ORDERING DEPENDENCE

So far we have constructed the transformation kernels $\mathcal{F}^{(\mathcal{F})}$ for point transformations (2.23) and for the reflection (2.45). Both kernels depend explicitly on the ordering function \mathcal{F} , but in a similar manner. This suggests that we define an ordering-independent transformation kernel T by

$$\begin{aligned} \mathcal{F}^{(\mathcal{F})}(\bar{p}, \bar{q}; p, q) &= \int dx dy d\bar{x} d\bar{y} dk dl d\bar{k} d\bar{l} (2\pi\hbar)^{-4} \mathcal{F}(x, y) [\mathcal{F}(\bar{x}, \bar{y})]^{-1} \\ &\times \exp \left[\frac{i}{\hbar} [\bar{x}(\bar{p} - \bar{k}) + \bar{y}(\bar{q} - \bar{l}) - x(p - k) - y(q - l)] \right] T(\bar{k}, \bar{l}; k, l), \end{aligned} \quad (3.1a)$$

with the inverse transformation

$$\begin{aligned} T(\bar{k}, \bar{l}; k, l) &= \int dx dy d\bar{x} d\bar{y} dp dq d\bar{p} d\bar{q} (2\pi\hbar)^{-4} \mathcal{F}(\bar{x}, \bar{y}) [\mathcal{F}(x, y)]^{-1} \\ &\times \exp \left[\frac{i}{\hbar} [-\bar{x}(\bar{p} - \bar{k}) - \bar{y}(\bar{q} - \bar{l}) + x(p - k) + y(q - l)] \right] \mathcal{F}^{(\mathcal{F})}(\bar{p}, \bar{q}; p, q). \end{aligned} \quad (3.1b)$$

If $\mathcal{F} \equiv 1$ (Weyl ordering) (3.1) collapses to the identity and we can write

$$T(\bar{p}, \bar{q}; p, q) = \mathcal{F}^{(\text{Weyl})}(\bar{p}, \bar{q}; p, q). \quad (3.2)$$

For the kernel (2.23) we get

$$\begin{aligned} T_F(\bar{k}, \bar{l}; k, l) &= \int dx dy dw dz (2\pi\hbar)^{-3} \alpha(x) \beta(y) \\ &\times \exp \left\{ \frac{i}{\hbar} \left\{ w \left[\bar{l} - \frac{1}{2}(x + y) \right] + z \left[-l + \frac{1}{2}(F(x) + F(y)) \right] + \bar{k}(x - y) + k(F(y) - F(x)) \right\} \right\} \\ &= \int dx dy (2\pi\hbar)^{-1} \alpha(x) \beta(y) \delta(\bar{l} - \frac{1}{2}(x + y)) \delta(l - \frac{1}{2}[F(x) + F(y)]) \\ &\times \exp \left[\frac{i}{\hbar} [\bar{k}(x - y) + k(F(y) - F(x))] \right], \end{aligned} \quad (3.3)$$

and for the reflection,

$$T_{\text{refl}}(\bar{k}, \bar{l}; k, l) = \delta(\bar{k} - 1) \delta(\bar{l} + k), \quad (3.4)$$

i.e., the naive substitution, which is proper for linear transformations.

We can also define an order-giving operator $\mathcal{O}_{\mathcal{F}}(p, q; k, l)$ by

$$\begin{aligned} \mathcal{O}_{\mathcal{F}}(k, l; p, q) &= \int dx dy (2\pi\hbar)^{-2} \mathcal{F}(x, y) \\ &\times \exp \left[-\frac{i}{\hbar} [x(p - k) + y(q - l)] \right], \end{aligned} \quad (3.5a)$$

Its inverse is

$$\begin{aligned} \mathcal{O}_{\mathcal{F}}^{-1}(p, q; k, l) &= \int dx dy (2\pi\hbar)^{-2} [\mathcal{F}(x, y)]^{-1} \\ &\times \exp \left[\frac{i}{\hbar} [x(p - k) + y(q - l)] \right]. \end{aligned} \quad (3.5b)$$

Then (3.1) can be written as

$$\mathcal{F}^{(\mathcal{F})} = \mathcal{O}_{\mathcal{F}}^{-1} T \mathcal{O}_{\mathcal{F}}, \quad (3.1a')$$

$$T = \mathcal{O}_{\mathcal{F}} \mathcal{F}^{(\mathcal{F})} \mathcal{O}_{\mathcal{F}}^{-1}. \quad (3.1b')$$

It is evident that compositions (1.3) are preserved

in this transformation.

The operator $\mathcal{O}_{\mathcal{F}}$ is unitary if the ordering function is a pure phase, e.g., for the λ orderings (2.5e). For the Weyl ordering we have

$$\mathcal{O}_{\mathcal{F}} = 1. \tag{3.2'}$$

This result might suggest that the Weyl ordering is somehow special. It is true that many equations simplify in the Weyl ordering, but this does not mean that other orderings are eliminated. For this reason we have written the results in arbitrary orderings, and we make no claims as to which is the preferred one.

Corresponding to (3.1) we can also define a function H by

$$H = \mathcal{O}_{\mathcal{F}} \mathcal{H}, \tag{3.6a}$$

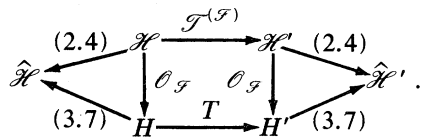
$$\mathcal{H} = \mathcal{O}_{\mathcal{F}}^{-1} H. \tag{3.6b}$$

When this is used in (2.4) we can write

$$\begin{aligned} \hat{\mathcal{H}}(\hat{p}, \hat{q}) &= \int dx dy dk dl (2\pi\hbar)^{-2} H(k, l) \\ &\times \exp \left[\frac{i}{\hbar} [x(q-l) + y(p-k)] \right], \end{aligned} \tag{3.7}$$

where now all ordering dependence (if any) is contained in $H(k, l)$.

With the above definitions, the following diagram commutes:



In the inner rectangle we have only c -number functions and possible ordering dependence. If we are only interested in the transformation rule of the operator $\hat{\mathcal{H}}$ into $\hat{\mathcal{H}}'$, we can either follow the upper route with explicit \mathcal{F} dependence in (2.4) and in the transformation $\mathcal{S}^{(\mathcal{F})}$ [(2.23) and (2.45)] or the lower route without such explicit dependence [see (3.7), (3.3), and (3.4)]. As far as the operator is concerned, both routes give the same operator transformation rule. From this viewpoint, it would appear that any ordering dependence is irrelevant, except that $H(k, l)$ in (3.7) might have some *impli-*

cit ordering dependence. However, this question is beyond the scope of this paper.

IV. ADDITIONAL STRUCTURE

A. Normalization and Unitarity

In this section we will introduce some general properties that the transformation kernels should have. First of all we should require that under any CT nothing happens to pure numbers. This can be put in the form of a normalization condition

$$\int dk dl T(\bar{k}, \bar{l}; k, l) = 1. \tag{4.1}$$

It is easy to see from (3.1') that this holds or fails for T and $\mathcal{S}^{(\mathcal{F})}$ simultaneously, also if it is true for T_1 and T_2 , it also holds for their composition T_3 (1.3). For the special transformation kernels derived in Sec. II property (4.1) can be shown easily for T_{refl} and also for T_F , e.g., from (3.3).

The other property that we will discuss here is unitarity

$$T^{-1}(\bar{k}, \bar{l}; k, l) = T(k, l; \bar{k}, \bar{l})^*,$$

i.e.,

$$\begin{aligned} \int dk' dl' T(k', l'; \bar{k}, \bar{l})^* T(k', l'; k, l) \\ = \delta(\bar{k} - k) \delta(\bar{l} - l). \end{aligned} \tag{4.2}$$

From (3.1') it follows that this also holds for T and $\mathcal{S}^{(\mathcal{F})}$ simultaneously and respects compositions (1.3).

The condition (4.2) differs from the one that is usually mentioned when one considers quantum CT's as unitary transformations.^{8,12} In this latter approach unitarity refers primarily to transformations of wave functions, i.e., unitarity in q space, while our unitarity (4.2) is in the (p, q) space. Here we will leave open questions whether either one or any such condition is necessary. We only use (4.2) to restrict the freedom in the functions α and β .

For T_{refl} (4.2) clearly holds, but for point transformations we get some conditions as follows: Substituting (3.3) to (4.2), integrating over k', l' , and using the resulting δ functions, we obtain

$$\begin{aligned} \int dk' dl' T_F(k', l'; \bar{k}, \bar{l})^* T_F(k', l'; k, l) &= \delta(l - \bar{l}) \int dx dy (2\pi\hbar)^{-1} |\alpha(x)\beta(y)|^2 \delta(l - \frac{1}{2}[F(x) + F(y)]) \\ &\times \exp \left[\frac{i}{\hbar} (k - k')[F(y) - F(x)] \right]. \end{aligned} \tag{4.3}$$

The double integral should be equal to $\delta(k - k')$. Changing variables to $u = \frac{1}{2}[F(x) + F(y)]$, $v = F(y) - F(x)$ we see that (4.2) holds if and only if

$$|\alpha(x)|^2 = |\beta(x)|^2 = |F'(x)|. \quad (4.4)$$

Using also (2.17) we obtain

$$\begin{aligned} \alpha(x) &= |F'(x)|^{1/2} \exp \left[\frac{i}{\hbar} K(x) \right], \\ \beta(x) &= |F'(x)|^{1/2} \exp \left[-\frac{i}{\hbar} K(x) \right], \end{aligned} \quad (4.5)$$

and

$$\begin{aligned} T_{F,K}(\bar{k}, \bar{l}; k, l) &= \int dx dy (2\pi\hbar)^{-1} |F'(x)|^{1/2} |F'(y)|^{1/2} \delta(l - \frac{1}{2}(x+y)) \delta(l - \frac{1}{2}[F(x) + F(y)]) \\ &\quad \times \exp \left[\frac{i}{\hbar} \{ \bar{k}(x-y) + k[F(y) - F(x)] + K(x) - K(y) \} \right]. \end{aligned} \quad (4.6)$$

The form (4.5) with $K \equiv 0$ has been adopted usually in discussions of point transformations, although the full freedom has been recognized.⁶ With the unitarity condition the freedom has been reduced so that now F and K have the classical interpretations of Sec. II C, if they are \hbar independent. However, in the derivation of Sec. II B it is not necessary to make any assumptions on the \hbar dependence of α , β , or F —a quantum CT is obtained in all cases.

B. Composition of point transformations

Of classical point transformations we know that the composition of two such transformations is also a point transformation.² We will now check what condition this would give to the functions α and β .

Owing to (3.1') we may just consider the ordering independent form and see whether (note the order)

$$\int dk' d_0 l' T_{F,K}(\bar{k}, \bar{l}; k', l') T_{G,L}(k', l'; k, l) = T_{G \circ F, K+L \circ F}(\bar{k}, \bar{l}; k, l), \quad (4.7)$$

where $(G \circ F)(x) = G(F(x))$, and we have also written out the extra freedom referred to in (2.30) and (4.5). Substituting (3.3) the left-hand side (LHS) becomes, after integrating over k' and l' ,

$$\begin{aligned} \text{LHS} &= \int dx_1 dy_1 dx_2 dy_2 (2\pi\hbar)^{-1} \alpha_{F,K}(x_1) \beta_{F,K}(y_1) \alpha_{G,L}(x_2) \beta_{G,L}(y_2) \\ &\quad \times \delta(\frac{1}{2}(x_2 + y_2) - \frac{1}{2}[F(x_1) + F(y_1)]) \delta(x_2 - y_2 - F(x_1) + F(y_1)) \\ &\quad \times \delta(\bar{l} - \frac{1}{2}(x_1 + y_1)) \delta(l - \frac{1}{2}[G(x_2) + G(y_2)]) \exp \left[\frac{i}{\hbar} \{ \bar{k}(x_1 - y_1) + k[G(y_2) - G(x_2)] \} \right]. \end{aligned}$$

Here the x_2 and y_2 integrations can be done and the results is of form (3.3) for $T_{G \circ F, K+L \circ F}$ provided that

$$\alpha_{G \circ F, K+L \circ F}(x) = \alpha_{F,K}(x) \alpha_{G,L}(F(x)) \quad (4.8)$$

with the same condition for β . This is a fairly strong condition, but it is compatible with the representation (4.5) obtained from unitarity, as can be

readily checked.

For classical CT's the inverse transformation is given by $G = F^{-1}$ and $L = -K \circ F^{-1}$. From (4.6) it is easy to check that

$$T_{F,K}(k, l; \bar{k}, \bar{l})^* = T_{F^{-1}, -K \circ F^{-1}}(\bar{k}, \bar{l}; k, l). \quad (4.9)$$

Finally we note that to obtain a point transformation

$$\begin{aligned} p &= F(P), \\ q &= Q/F'(P) \end{aligned} \quad (4.10)$$

in the p coordinate we can make first the reflection (2.37), then a point transformation [with $F(x) \rightarrow -F(-x)$], and finally the inverse of (2.37). The corresponding kernel is

$$\begin{aligned} T_{(4.10)}(\bar{k}, \bar{l}; k, l) &= T_{-F(-x)}(\bar{l}, -\bar{k}; l, -k) \\ &= T_F(\bar{l}, \bar{k}; l, k). \end{aligned} \quad (4.11)$$

V. CONSERVATION OF COMMUTATION RULES

A. Generalities

Usually canonical transformations are defined by the property that they leave commutation rules in-

variant.² In the previous sections we constructed the transformation kernels by changing variables in the path integral expression for the trace, Eq. (2.1). In this section we show that the kernels so obtained also conserve commutation rules.

Let us assume we have three operators related by a commutation rule

$$[\hat{\mathcal{A}}(\hat{p}, \hat{q}), \hat{\mathcal{B}}(\hat{p}, \hat{q})] = i\hbar \hat{\mathcal{C}}(\hat{p}, \hat{q}), \quad (5.1)$$

where the elementary commutation rule is

$$[\hat{q}, \hat{p}] = i\hbar. \quad (5.2)$$

As usual we assume that the operators are given by some c -number functions \mathcal{A} , \mathcal{B} , and \mathcal{C} according to (1.1). Substituting them in (5.1), using

$$\left[\exp \left[\frac{i}{\hbar} (\tau_1 \hat{p} + \theta_1 \hat{q}) \right], \exp \left[\frac{i}{\hbar} (\tau_2 \hat{p} + \theta_2 \hat{q}) \right] \right] = \exp \left[\frac{i}{\hbar} [(\tau_1 + \tau_2) \hat{p} + (\theta_1 + \theta_2) \hat{q}] \right] (-2i) \sin \left[\frac{1}{2\hbar} (\theta_1 \tau_2 - \tau_1 \theta_2) \right]. \quad (5.3)$$

and equating coefficients of the operators $\exp\{(i/\hbar)[\tau\hat{p} + \theta\hat{q}]\}$, we obtain an equation for the c -number functions. After taking Fourier transforms this equation can be written in the form [using (3.5)]

$$\begin{aligned} \int dk_1 dk_2 dl_1 dl_2 (2\pi\hbar)^{-2} (-8/\hbar) \sin \left[\frac{2}{\hbar} [(k_1 - k)(l_2 - l) - (k_2 - k)(l_1 - l)] \right] \{ (\mathcal{O}_{\mathcal{A}} \mathcal{A})(k_1, l_1) (\mathcal{O}_{\mathcal{B}} \mathcal{B})(k_2, l_2) \\ = (\mathcal{O}_{\mathcal{C}} \mathcal{C})(k, l) \}. \end{aligned} \quad (5.4)$$

Here again the order dependence appears in the standard way so we could as well go to the order-independent formalism by (3.6) and write

$$\int dk_1 dk_2 dl_1 dl_2 (2\pi\hbar)^{-2} (-8/\hbar) \sin \left[\frac{2}{\hbar} [(k_1 - k)(l_2 - l) - (k_2 - k)(l_1 - l)] \right] A(k_1, l_1) B(k_2, l_2) = C(k, l). \quad (5.5)$$

The Moyal-bracket formulation¹³ can be obtained from (5.5) by first writing it as

$$\begin{aligned} \int d\theta_1 d\theta_2 d\tau_1 d\tau_2 dk_1 dk_2 dl_1 dl_2 (2\pi\hbar)^{-4} \exp \left[\frac{i}{\hbar} [k(\tau_1 + \tau_2) + l(\theta_1 + \theta_2) - l_1\theta_1 - k_1\tau_1 - l_2\theta_2 - k_2\tau_2] \right] \\ \times (-2/\hbar) \sin \left[\frac{i}{2\hbar} (\theta_1 \tau_2 - \tau_1 \theta_2) \right] A(k_1, l_1) B(k_2, l_2) = C(k, l) \end{aligned} \quad (5.6)$$

and then converting θ_i and τ_i in the sine function to derivatives with respect to l_i and k_i . The result is

$$\frac{2}{\hbar} \sin \left[\frac{\hbar}{2} \left[\frac{\partial}{\partial q_A} \frac{\partial}{\partial p_B} - \frac{\partial}{\partial q_B} \frac{\partial}{\partial p_A} \right] \right] A(p, q) B(p, q) = C(p, q), \quad (5.7)$$

where, e.g.,

$$\frac{\partial}{\partial q_A} \frac{\partial}{\partial p_B} A(p, q) B(p, q) = \frac{\partial A(p, q)}{\partial q} \frac{\partial B(p, q)}{\partial p}. \quad (5.8)$$

In the limit $\hbar \rightarrow 0$ (5.7) reduces to the classical Poisson brackets.

Let us now discuss what happens in a CT. When we substitute the transformed quantities

$$A(k,l) = \int d\bar{k} d\bar{l} T(k,l;\bar{k},\bar{l}) A'(\bar{k},\bar{l}), \tag{5.9}$$

etc., to (5.5), we obtain

$$\int d\bar{k}_1 d\bar{k}_2 d\bar{l}_1 d\bar{l}_2 (2\pi\hbar)^{-2} (-8/\hbar) \left[\int dk_1 dk_2 dl_1 dl_2 \sin \left[\frac{2}{\hbar} [(k-k_1)(l-l_2) - (k-k_2)(l-l_1)] \right] \right. \\ \left. \times T(k_1,l_1;\bar{k}_1,\bar{l}_1) T(k_2,l_2;\bar{k}_2,\bar{l}_2) \right] A'(\bar{k}_1,\bar{l}_1) B'(\bar{k}_2,\bar{l}_2) \\ = \int d\bar{k} d\bar{l} T(k,l;\bar{k},\bar{l}) C'(\bar{k},\bar{l}). \tag{5.10}$$

Therefore the commutation relation (5.6) is invariant, provided that for all $\bar{k}_1, \bar{l}_1, \bar{k}_2, \bar{l}_2, k, l$,

$$\int dk_1 dk_2 dl_1 dl_2 \sin \left[\frac{2}{\hbar} [(k-k_1)(l-l_2) - (k-k_2)(l-l_1)] \right] T(k_1,l_1;\bar{k}_1,\bar{l}_1) T(k_2,l_2;\bar{k}_2,\bar{l}_2) \\ = \int d\bar{k} d\bar{l} T(k,l;\bar{k},\bar{l}) \sin \left[\frac{2}{\hbar} [(\bar{k}-\bar{k}_1)(\bar{l}-\bar{l}_2) - (\bar{k}-\bar{k}_2)(\bar{l}-\bar{l}_1)] \right]. \tag{5.11}$$

Equation (5.11) is the only condition for transformations to leave commutation rules invariant. One can now approach the problem of quantum CT's by constructing solutions of (5.11). It should be noted that (5.11) respects the composition law of CT's (1.3); this makes the set of canonical transformations a semigroup. Since the identity transformation

$$T(\bar{k},\bar{l};k,l) = \delta(\bar{k}-k)\delta(\bar{l}-l)$$

also satisfies (5.11) CT's actually form a monoid.

In Sec. IV A we discussed the additional conditions of normalization (4.1) and (phase-space) unitarity (4.2). As we mentioned earlier the normalization condition is natural as we do not want constants to change in CT's. Equation (4.1) is also independent of (5.11), for $T \equiv 0$ clearly satisfies (5.11) but not (4.1). It is not clear if (4.1) is enough to guarantee that the solutions of (5.11) form a group. The condition of (p,q) unitarity (4.2) is a strong additional restriction (although weaker than q unitarity of^{8,12}) and CT's having this property do

form a group.

The equation (5.11) was derived for the order-independent transformations. The corresponding equation for $\mathcal{S}^{(\mathcal{F})}$ can be derived directly from (5.4). Since the order dependence enters in the standard way it is easy to see that $\mathcal{S}^{(\mathcal{F})}$ satisfies its equations if and only if T [related to it by (3.1)] satisfies (5.11).

For classical CT's it is necessary and sufficient² that they leave the fundamental Poisson brackets

$$\{q,p\} = 1 \tag{5.12}$$

invariant. For quantum systems this would correspond to preserving (5.2), i.e., that (5.10) holds for the special case of

$$A'(\bar{k}_1,\bar{l}_1) = \bar{l}_1, \\ B'(\bar{k}_2,\bar{l}_2) = \bar{k}_2, \\ C'(\bar{k},\bar{l}) = 1.$$

This together with (4.1) gives the equation

$$\int dk_1 dl_1 dk_2 dl_2 d\bar{k}_1 d\bar{l}_1 d\bar{k}_2 d\bar{l}_2 (2\pi\hbar)^{-2} (-8/\hbar) \sin \left[\frac{2}{\hbar} [(k_1-k)(l_2-l) - (k_2-k)(l_1-l)] \right] \\ \times T(k_1,l_1;\bar{k}_1,\bar{l}_1) T(k_2,l_2;\bar{k}_2,\bar{l}_2) \bar{l}_1 \bar{k}_2 = 1, \tag{5.13}$$

for all k,l . This equation is then necessary while (5.11) with (4.1) is sufficient. Whether either one or perhaps something else is both necessary and sufficient we do not know. It is also not clear whether for two solutions of (5.13) also their composition (1.3) is a solution of (5.13). However, if T_1 satisfies (5.13) and T_2 (5.11) then $T_2 \circ T_1$ does satisfy (5.13). In the following we will only use (5.11).

B. Linear and point transformations

It is easy to see that the reflection (3.4) satisfies (5.11). In fact we can now do even better and con-

sider a general linear CT

$$q = \alpha Q + \beta P, \\ p = \gamma Q + \delta P. \tag{5.14}$$

Classically (5.14) is a CT if $\alpha\delta - \beta\gamma = 1$. Corresponding to this we define the transformation kernel of the quantum CT by

$$T_{\text{linear}}(\bar{k}, \bar{l}; k, l) = \delta(k - (\gamma\bar{l} + \delta\bar{k})) \times \delta(l - (\alpha\bar{l} + \beta\bar{k})). \quad (5.15)$$

It is easy to show that (5.15) satisfies (5.11), (4.1), and (4.2) provided only that $\alpha\delta - \beta\gamma = 1$. Linear quantum CT's are therefore given by the naive classical substitution in the order-independent formulation.

One can also show with a straightforward but lengthy calculation that (3.3) satisfies (5.11) with no restrictions on α and β in addition to the usual (2.17). This shows that the set of transformations leaving commutators invariant is larger than the set of unitary transformations.

IV. DISCUSSION

In this paper we have described quantum canonical transformations in terms of integral transformations. To each operator and ordering rule one associates by (1.1) a c -number function. The effects of a quantum CT can then be described by the transformation (1.2) on the c -number function. It is such a function, corresponding to the operator Hamiltonian, that appears in the exponent of the integrand in the path-integral formalism. If we want to change variables in the path integral the corresponding new c -number Hamiltonian is obtained by (1.2).

In Sec. II we constructed the needed transformation kernels for point transformations (II B–II C) and reflections $q = P$, $p = -Q$ (II D) by analyzing

changes of variables in the discrete definition of the path integral. The kernels were obtained for arbitrary ordering rules. (For the reflection, the kernel was found to be simple only for some of them.) In general the ordering dependence was shown in Sec. III to be of rather benign type and we were able to pass to the ordering-independent formalism.

By construction the bijective point transformations and reflections leave the spectrum of the Hamiltonian unchanged. However, not all transformations that leave commutation rules invariant are expressible as finite sequences of point transformations and reflections. These more general CT's might very well change the spectrum of the Hamiltonian. The construction and interpretation of them is still an open problem. A possible starting point could be to search for more general solutions of Eq. (5.11).

Note added. After finishing this work we found out about the work of Moshinsky *et al.* (Refs. 14–16 and references therein). In addition to linear transformations¹⁴ they have considered more general transformations.¹⁵ Their approach is different from ours as they aim to construct matrix elements of the corresponding x -space unitary operator by solving a differential equation. The paper in Ref. 16 is closest in spirit to the present work; however, none of these papers take the path integral as their starting point.

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Therefore, although classically it is true that in a CT $\int p\dot{q}dt = \int P\dot{Q}dt$, we have in general

$$\sum_i p_i(q_{i+1} - q_i) \neq \sum_i P_i(Q_{i+1} - Q_i),$$

and the difference will usually propagate everywhere. In the Lagrangian approach this corresponds to the observation that in non-Cartesian coordinates one should expand up to fourth order in $(Q_{i+1} - Q_i)$. See, e.g., B. S. DeWitt, Rev. Mod. Phys. **29**, 377 (1957); S. F. Edwards and Y. V. Gulyaev, Proc. R. Soc. London **A279**, 229 (1964); D. W. McLaughlin and L. S. Schulman, J. Math. Phys. **12**, 2520 (1971).

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