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Quantum canonical invariance—a Moyal approach

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Abstract. The quasiclassical generalised Moyal quantisation procedure is applied to the problem of quantum canonical invariance. Simple new formulae for the Moyal bracket corresponding to various correspondence rules are given, and are used to calculate the 'additional potential terms' arising from a point canonical transformation made on a free Hamiltonian. The status of canonical transformations in other equivalent quantum phase space formulations is also reviewed.

1. Introduction

Canonical invariance is an important example of an anomalous symmetry—it plays a vital part in the Hamiltonian formulation of classical mechanics, but does not survive any standard 'canonical' quantisation procedure intact. This is most familiar in the context of the standard Dirac quantisation algorithm (where classical Poisson brackets are replaced by quantum commutators). The Groenwald–Van Hove theorem (Groenwald 1946, Van Hove 1951) proves that this quantisation procedure cannot be fully implemented, even when the phase space is \mathbb{R}^{2n} . Consequently, the canonical invariance of the classical Poisson brackets does not carry over to the quantum commutators. This same problem arises, in other guises, in other phase space formulations of quantum theories. Gervais and Jevicki (1976) studied the effects of a point canonical transformation in a phase space path integral and showed that the stochastic nature of the path integral is responsible for the loss of canonical invariance. This loss is signalled by the presence of 'additional potential terms' in the transformed Hamiltonian.

In this paper I apply the methods of Moyal quantisation to the question of quantum canonical invariance. In this context, the loss of canonical invariance is easily understood as being due to the deformation of the classical Poisson bracket algebra. I also review, and clarify, various other manifestations of the loss of canonical invariance, giving an explicit four-way equivalence between the situation in the operator theory, the discretised path integral theory, the non-linear perturbative path integral theory and the Moyal approach. By bringing together results from these different methods one can show, for example, that the claim made in the literature (see, e.g., Gervais and Jevicki (1976) § 2) that 'making a formal nonlinear point canonical transformation within a phase space path integral results in a different quantum theory' must be re-evaluated.

In § 2 I discuss the operator ordering problem and then the generalised Moyal approach to quantisation, giving some new simple formulae for the Moyal bracket applicable to certain correspondence rules. In § 3 I discuss the above-mentioned

equivalent manifestations of the breaking of canonical invariance. In § 4 I use the Moyal methods to calculate the 'additional potential terms' arising from a more general class of point canonical transformations. Finally, I conclude with some discussion concerning the extension of the Moyal ideas to more complicated phase space systems, and indeed to the canonical quantisation of field theories.

2. Correspondence rules and Moyal quantisation

For our purposes, the essential ingredients of classical mechanics are

- (i) the phase space \mathcal{S} , the points of which represent the classical states;
- (ii) the algebra \mathcal{A} of smooth functions on \mathcal{S} , the elements of which represent the physical observables;
- (iii) the Poisson bracket which gives \mathcal{A} a Lie algebra structure

$$\{f, g\} = \frac{\partial f}{\partial \xi^i} \omega^{ij} \frac{\partial g}{\partial \xi^j} \quad (2.1)$$

where ω is the symplectic 2-form ($= -d\Theta$ where Θ is the Liouville form) on \mathcal{S} , the ξ^i are local coordinates on \mathcal{S} , and $f, g \in \mathcal{A}$. A canonical transformation is simply a diffeomorphism φ of \mathcal{S} which preserves the symplectic structure

$$\varphi^* \omega = \omega$$

i.e. Poisson brackets are preserved.

Dirac's canonical quantisation prescription can be thought of as a mapping D from \mathcal{A} into the space of operators on a Hilbert space \mathcal{H} (to which the quantum states belong)

$$D: f \mapsto \hat{f}$$

such that

$$D(i): \quad D: (\alpha f + \beta g) \mapsto \alpha \hat{f} + \beta \hat{g}$$

$$D(ii): \quad D: 1 \mapsto \hat{1}$$

$$D(iii): \quad D: \{f, g\} \mapsto \frac{1}{i\hbar} [\hat{f}, \hat{g}].$$

The replacement of Poisson brackets with operator commutators is an appealing idea and has had many well known successes, not least of which is the fact that it allows much of Hamilton's formalism for mechanics to be generalised to quantum theories. However, it was shown many years ago by Van Hove (1951) and Groenwald (1946) that such a quantisation procedure cannot be applied to the whole classical algebra \mathcal{A} (at least if the quantum representation is required to be irreducible). This may be easily understood in the conventional operator formalism of quantisation in which a 'correspondence rule' Ω must be chosen so that we know (unambiguously) how to order the non-commuting operators \hat{p} and \hat{q} in the operator $\hat{f}(\hat{p}, \hat{q})$ corresponding to the classical function $f(p, q)$. But then, if f, g and $\{f, g\}$ are all quantised according to the same correspondence rule Ω , we find in general that

$$\Omega(\{f, g\}) \neq \frac{1}{i\hbar} [\Omega(f), \Omega(g)] \quad (2.2)$$

(see, e.g., Abraham and Marsden 1978, Guillemin and Sternberg 1984), which contradicts $D(iii)$. Note that there is no problem if we restrict f and g to the basic observables p and q ; the problems arise when f and g are more complicated functions of p and q . One special case of interest is when f and g are bilinear functions, corresponding to field theoretical currents in the infinite-dimensional case.

Some approaches to quantisation (such as geometric quantisation) proceed by relaxing the requirement of irreducibility or the condition $D(ii)$ (see, e.g., Abraham and Marsden (1982) and references therein). However, we will retain these requirements, which means that $D(iii)$ must be relaxed to

$$\Omega : \{f, g\} \mapsto \frac{1}{i\hbar} [\hat{f}, \hat{g}] + O(\hbar)$$

where the precise form of the $O(\hbar)$ ‘corrections’ depends on the particular correspondence rule chosen. The generalised Moyal procedure discussed here provides an elegant way of computing these $O(\hbar)$ ‘corrections’ simply in terms of classical functions and partial derivatives. This procedure involves explicitly constructing a new classical Lie algebra (strictly, a deformation of the Poisson bracket algebra, with deformation parameter \hbar) which is isomorphic to the quantum Lie algebra of operators with the Dirac commutator $(1/i\hbar)[\ , \]$. To achieve this, we define a new Ω -dependent product $*_{\Omega}$ (called the generalised Moyal product) for the algebra \mathcal{A} . It is defined so that

$$f *_{\Omega} g = \Omega^{-1}(\Omega(f)\Omega(g)) \tag{2.3}$$

for all $f, g \in \mathcal{A}$, where the product on the RHS is the usual multiplication of operators. This definition means that $f *_{\Omega} g$ is that classical function which, when quantised according to the rule Ω , gives the product of the Ω -quantised operators corresponding to the classical functions f and g . Note that the Moyal product is non-commutative, due to the non-commutativity of operator multiplication. Next we define the generalised Moyal bracket $\{\{ \ , \ \}_{\Omega}$ to be

$$\{\{f, g\}\}_{\Omega} = \frac{1}{i\hbar} (f *_{\Omega} g - g *_{\Omega} f) \tag{2.4}$$

for all $f, g \in \mathcal{A}$.

The Moyal product $*_{\Omega}$ is clearly associative (associativity being inherited from the associativity of operator multiplication), and so the commutator-style definition of the Moyal bracket ensures that $\{\{ \ , \ \}_{\Omega}$ satisfies the Jacobi identity:

$$\{\{f, \{\{g, h\}\}_{\Omega}\}\}_{\Omega} + \{\{g, \{\{h, f\}\}_{\Omega}\}\}_{\Omega} + \{\{h, \{\{f, g\}\}_{\Omega}\}\}_{\Omega} = 0.$$

Notice that, by construction, we have ensured that

$$\Omega : \{\{f, g\}\}_{\Omega} \mapsto \frac{1}{i\hbar} [\Omega(f), \Omega(g)] \tag{2.5}$$

for all $f, g \in \mathcal{A}$. This means that Ω now sets up an isomorphism between the quantum Lie algebra, with bracket being the commutator, and the quasiclassical Lie algebra resulting from equipping \mathcal{A} with the Moyal bracket. Also note that, for any Ω ,

$$\{\{ \ , \ \}_{\Omega} = \{ \ , \ \}_{PB} + O(\hbar) \tag{2.6}$$

where the $O(\hbar)$ terms can be computed wholly within the classical regime using the Moyal bracket.

The usual Moyal bracket (Moyal 1949, Bayen *et al* 1978) corresponds to the case where Ω is Weyl ordering, W :

$$W: q^n p^m \mapsto \frac{1}{2^n} \sum_{k=0}^n \binom{n}{k} \hat{q}^{n-k} \hat{p}^m \hat{q}^k. \quad (2.7)$$

Then an explicit formula for the Moyal bracket is

$$\{\{f, g\}\}_W = \frac{1}{i\hbar} \sum_{n=0}^{\infty} (\frac{1}{2}i\hbar)^n (f(\bar{P})^n g - g(\bar{P})^n f) \quad (2.8)$$

where \bar{P} is the bidifferential operator

$$\left(\frac{\bar{\partial}}{\partial q} \frac{\bar{\partial}}{\partial p} - \frac{\bar{\partial}}{\partial p} \frac{\bar{\partial}}{\partial q} \right).$$

However, Weyl ordering is just one particular ordering rule—general correspondence rules have been studied in great detail in the literature (Argawal and Wolf 1970, Cohen 1966, Dowker 1976). Following Argawal and Wolf (1970) and Cohen (1966), we may characterise a large class of orderings by

$$\Omega: f(p, q) \mapsto \hat{f}(\hat{p}, \hat{q}) = \iint d\xi d\eta \exp[i(\hat{p}\xi + \hat{q}\eta)] \tilde{f}(\xi, \eta) \Omega(\xi, \eta) \quad (2.9)$$

where \tilde{f} is the Fourier transform of f , and the 'weight function' $\Omega(\xi, \eta)$ is a C^∞ function from \mathbb{R}^2 to \mathbb{C} , satisfying the following conditions:

(i) $\Omega(0, \eta) = \Omega(\xi, 0) = 1$; ensuring that $\Omega: q^n \mapsto \hat{q}^n$ and $\Omega: p^n \mapsto \hat{p}^n$;

(ii) $\Omega^*(\xi, \eta) = \Omega(-\xi, -\eta)$ if Ω is a Hermitian ordering.

The inverse Ω^{-1} can be defined and is given by

$$\Omega^{-1}: \hat{f}(\hat{p}, \hat{q}) \mapsto f(p, q) = \frac{1}{\sqrt{2\pi}} \bar{\Omega} \left(i \frac{\partial}{\partial q}, i \frac{\partial}{\partial p} \right) \exp(ipq) \langle p | \hat{f}(\hat{p}, \hat{q}) | q \rangle$$

where

$$\bar{\Omega}(\xi, \eta) \equiv [\Omega(-\xi, -\eta)]^{-1} \exp(\frac{1}{2}i\xi\eta). \quad (2.10)$$

Then, using the defining relation (2.3), the generalised Moyal product is (Bakas and Kakas 1987a)

$$f *_\Omega g = \int d\xi d\eta \int d\xi' d\eta' \tilde{f}(\xi, \eta) \tilde{g}(\xi', \eta') \omega(\xi, \eta; \xi', \eta') \\ \times \exp\{i[\hat{p}(\xi + \xi') + \hat{q}(\eta + \eta')]\}$$

where

$$\omega(\xi, \eta; \xi', \eta') \equiv \frac{\Omega(\xi, \eta) \Omega(\xi', \eta')}{\Omega(\xi + \xi', \eta + \eta')} \exp[(\frac{1}{2}i\hbar(\xi\eta' - \xi'\eta)]. \quad (2.11)$$

Some examples of the more common correspondence rules and their associated Ω weight functions are

Weyl as in (2.7); $\Omega = 1$

standard $S: q^m p^n \mapsto \hat{q}^m \hat{p}^n$ (2.12)

$$\Omega(\xi, \eta) = \exp(\frac{1}{2}i\xi\eta)$$

antistandard AS: $q^m p^n \mapsto \hat{p}^n \hat{q}^m$ (2.13)

$$\Omega(\xi, \eta) = \exp(-\frac{1}{2}i\xi\eta)$$

normal N: $z^m z^{*n} \mapsto (a^+)^n a^m$ (2.14)

$$\Omega(\xi, \eta) = \exp[\frac{1}{4}(\xi^2 + \eta^2)]$$

antinormal AN: $z^m z^{*n} \mapsto a^m (a^+)^n$ (2.15)

$$\Omega(\xi, \eta) = \exp[-\frac{1}{4}(\xi^2 + \eta^2)]$$

where in the last two cases, $z \equiv (1/\sqrt{2\hbar})(q + ip)$ and $z^* \equiv (1/\sqrt{2\hbar})(q - ip)$.

We now present a simple method for deriving more manageable formulae for the generalised Moyal product $*_{\Omega}$, and hence the generalised Moyal bracket $\{\{, \}\}_{\Omega}$, for these correspondence rules. Consider first of all the standard correspondence rule (2.12), and let

$$\hat{f} \equiv \hat{q}^m \hat{p}^n \quad \hat{g} \equiv \hat{q}^r \hat{p}^s$$

so that \hat{f} and \hat{g} are already standard ordered. In order to compute $*_S$ all we have to do is reorder the product $\hat{f}\hat{g}$, using the basic commutation relation $[\hat{q}, \hat{p}] = i\hbar \hat{1}$, until it is also standard ordered. This involves calculating $[\hat{p}^n, \hat{q}^r]$ which can be done easily by representing \hat{q} by x and \hat{p} by $-i\hbar d/dx$, and using Leibniz's formula,

$$\left(\frac{d}{dx}\right)^n (fg) = \sum_{k=0}^n \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}}$$

Then

$$\hat{f}\hat{g} = \hat{q}^{m+r} \hat{p}^{n+s} + \hat{q}^m [\hat{p}^n, \hat{q}^r] \hat{p}^s = \sum_{k=0}^n (-i\hbar)^k \binom{n}{k} r(r-1) \dots (r-k+1) \hat{q}^{m+r-k} \hat{p}^{n+s-k}$$

We can invert the standard ordering map and find that

$$f *_S g = \sum_{k=0}^n \frac{(-i\hbar)^k}{k!} \left(\frac{\partial}{\partial p}\right)^k f \left(\frac{\partial}{\partial q}\right)^k g \tag{2.16}$$

where $f \equiv \Omega^{-1}(\hat{f}) = q^m p^n$ and $g \equiv \Omega^{-1}(\hat{g}) = q^r p^s$. Now the bilinearity of the product $*_{\Omega}$ means that this result generalises to all f and g which can be expanded as power series in p and q . Then (2.16) becomes

$$f *_S g = \sum_{k=0}^{\infty} \frac{(-i\hbar)^k}{k!} \left(\frac{\partial}{\partial p}\right)^k f \left(\frac{\partial}{\partial q}\right)^k g. \tag{2.17a}$$

The corresponding Moyal bracket is

$$\begin{aligned} \{\{f, g\}\}_S &= \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} (i\hbar)^{k-1} \left[\left(\frac{\partial}{\partial p}\right)^k f \left(\frac{\partial}{\partial q}\right)^k g - \left(\frac{\partial}{\partial p}\right)^k g \left(\frac{\partial}{\partial q}\right)^k f \right] \\ &= \{f, g\}_{PB} + \frac{1}{2}i\hbar \left(\frac{\partial^2 f}{\partial p^2} \frac{\partial^2 g}{\partial q^2} - \frac{\partial^2 g}{\partial p^2} \frac{\partial^2 f}{\partial q^2} \right) + O(\hbar^2). \end{aligned} \tag{2.17b}$$

This simple procedure can clearly also be applied to other correspondence rules, yielding, for example the following:

antistandard

$$f *_{AS} g = \sum_{k=0}^{\infty} \frac{(i\hbar)^k}{k!} \left(\frac{\partial}{\partial q}\right)^k f \left(\frac{\partial}{\partial p}\right)^k g \tag{2.18a}$$

$$\begin{aligned} \{\{f, g\}\}_{\text{AS}} &= \sum_{k=0}^{\infty} \frac{1}{k!} (i\hbar)^{k-1} \left[\left(\frac{\partial}{\partial q} \right)^k f \left(\frac{\partial}{\partial p} \right)^k g - \left(\frac{\partial}{\partial q} \right)^k g \left(\frac{\partial}{\partial p} \right)^k f \right] \\ &= \{f, g\}_{\text{PB}} + \frac{1}{2} i\hbar \left(\frac{\partial^2 f}{\partial q^2} \frac{\partial^2 g}{\partial p^2} - \frac{\partial^2 g}{\partial q^2} \frac{\partial^2 f}{\partial p^2} \right) + \mathcal{O}(\hbar^2) \end{aligned} \quad (2.18b)$$

normal

$$f^{*_{\text{N}}} g = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{\partial}{\partial z} \right)^k f \left(\frac{\partial}{\partial z^*} \right)^k g \quad (2.19a)$$

$$\begin{aligned} \{\{f, g\}\}_{\text{N}} &= \frac{1}{i\hbar} \sum_{k=0}^{\infty} \frac{1}{k!} \left[\left(\frac{\partial}{\partial z} \right)^k f \left(\frac{\partial}{\partial z^*} \right)^k g - \left(\frac{\partial}{\partial z} \right)^k g \left(\frac{\partial}{\partial z^*} \right)^k f \right] \\ &= \{f, g\}_{\text{PB}} + \hbar \left(\frac{\partial^2 f}{\partial q^2} \frac{\partial^2 g}{\partial p \partial q} - \frac{\partial^2 f}{\partial q \partial p} \frac{\partial^2 g}{\partial q^2} + \frac{\partial^2 f}{\partial q \partial p} \frac{\partial^2 g}{\partial p^2} - \frac{\partial^2 f}{\partial p^2} \frac{\partial^2 g}{\partial q \partial p} \right) + \mathcal{O}(\hbar^2) \end{aligned} \quad (2.19b)$$

antinormal

$$f^{*_{\text{AN}}} g = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \left(\frac{\partial}{\partial z^*} \right)^k f \left(\frac{\partial}{\partial z} \right)^k g \quad (2.20a)$$

$$\begin{aligned} \{\{f, g\}\}_{\text{AN}} &= \frac{1}{i\hbar} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \left[\left(\frac{\partial}{\partial z^*} \right)^k f \left(\frac{\partial}{\partial z} \right)^k g - \left(\frac{\partial}{\partial z^*} \right)^k g \left(\frac{\partial}{\partial z} \right)^k f \right] \\ &= \{f, g\}_{\text{PB}} - \hbar \left(\frac{\partial^2 f}{\partial q^2} \frac{\partial^2 g}{\partial p \partial q} - \frac{\partial^2 f}{\partial q \partial p} \frac{\partial^2 g}{\partial q^2} + \frac{\partial^2 f}{\partial q \partial p} \frac{\partial^2 g}{\partial p^2} - \frac{\partial^2 f}{\partial p^2} \frac{\partial^2 g}{\partial q \partial p} \right) + \mathcal{O}(\hbar^2). \end{aligned} \quad (2.20b)$$

There are some natural generalisations of these formulae.

(i) It is straightforward to generalise these formulae to the case when the phase space is \mathbb{R}^{2n} , for example for symmetric ordering,

$$\begin{aligned} \{\{f, g\}\}_{\text{S}} &= \sum_{k=0}^{\infty} (-1)^k \frac{(i\hbar)^{k-1}}{k!} \left(\frac{\partial^k f}{\partial p^{\alpha_1} \dots \partial p^{\alpha_k}} \frac{\partial^k g}{\partial q_{\alpha_1} \dots \partial q_{\alpha_k}} \right. \\ &\quad \left. - \frac{\partial^k g}{\partial p^{\alpha_1} \dots \partial p^{\alpha_k}} \frac{\partial^k f}{\partial q_{\alpha_1} \dots \partial q_{\alpha_k}} \right) \end{aligned}$$

where summation (from 1 to n) over repeated α_j is understood.

(ii) We can also consider the fermionic case, where the creation and annihilation operators satisfy anticommutation relations

$$[b^m, b^{+n}]_+ = \delta^{mn}$$

(characteristic of a Clifford algebra) rather than the commutation relations

$$[a^m, a^{+n}] = \delta^{mn}$$

(characteristic of the Heisenberg algebra). Then, for example, the Moyal bracket for normal ordering of fermionic creation and annihilation operators is (for f and g even elements of the classical Grassmann algebra)

$$\{\{f, g\}\}_{\text{N}} = \frac{1}{i\hbar} \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{\partial^k f}{\partial b^{\alpha_1} \dots \partial b^{\alpha_k}} \frac{\partial^k g}{\partial b_{\alpha_1}^* \dots \partial b_{\alpha_k}^*} - (-1)^k \frac{\partial^k g}{\partial b^{\alpha_1} \dots \partial b^{\alpha_k}} \frac{\partial^k f}{\partial b_{\alpha_1}^* \dots \partial b_{\alpha_k}^*} \right)$$

$$= \{f, g\}_{\text{PB}}^+ + \frac{1}{2i\hbar} \left(\frac{\partial^2 f}{\partial b^\alpha \partial b^\beta} \frac{\partial^2 g}{\partial b_\alpha^* \partial b_\beta^*} - \frac{\partial^2 f}{\partial b_\alpha^* \partial b_\beta^*} \frac{\partial^2 g}{\partial b^\alpha \partial b^\beta} \right) + \dots$$

where $\{, \}^+_{\text{PB}}$ is the generalised Poisson bracket for a Grassmann phase space (Casalbuoni 1976).

(ii) We also comment here that equations (2.19) and (2.20) for the normal and antinormal orderings are particularly relevant to coherent state path integrals (Faddeev 1976, Klauder and Skagerstam 1985), where the normal (respectively antinormal) symbol of a commutator is not simply the Poisson bracket of the two normal (respectively antinormal) symbols, but has corrections given by (2.19*b*) (respectively (2.20*b*)). Coherent state path integrals provide a good example of a formulation in which particular operator orderings (namely normal and antinormal) are especially convenient.

(iv) These formulae can also be extended to the case of quantising a classical Hamiltonian field theory. This can be achieved by considering the system to be in a (large) spatial box, so that we have a countably infinite number of modes. Alternatively, one can consider all classical functions to be (spatially) smeared with arbitrary smearing functions so that the generalisation of the Moyal formulae to Hamiltonian field theory consists of replacing all partial derivatives with functional derivatives (the smearing being introduced as a means of handling the spatial delta functions). For example, defining

$$F(u) \equiv \int d^3x f(x) u(x)$$

$$G(v) \equiv \int d^3y g(y) v(y)$$

then

$$\begin{aligned} \{\{F, G\}\}_{\text{N}} = \{F, G\}_{\text{PB}} + \frac{1}{2i\hbar} \iint d^3x d^3y \left(\frac{\delta^2 F}{\delta z(x) \delta z(y)} \frac{\delta^2 G}{\delta z^*(x) \delta z^*(y)} \right. \\ \left. - \frac{\delta^2 G}{\delta z(x) \delta z(y)} \frac{\delta^2 F}{\delta z^*(x) \delta z^*(y)} \right) + \dots \end{aligned}$$

Such a generalised formula, for the case of normal ordering of anticommuting phase space variables, is required for the Moyal calculation of the chiral anomaly as an anomalous commutator (Bakas *et al* 1988).

(v) These methods suggest various ways of approaching the problem of quantising classical systems with more complicated phase spaces than \mathbb{R}^2 or \mathbb{R}^{2n} . The associativity of the generalised Moyal product requires ω in equation (2.11) to satisfy a 2-cocycle condition (Bakas and Kakas 1987*a*), which suggests that for non-trivial phase space systems we could follow the procedure of Isham (1984) and look for general 2-cocycles in the canonical group action. Another very different approach is to look for deformations of the general Poisson bracket (2.1) on the curved space (Bayen *et al* 1978).

However, for our purposes here the main point of the Moyal structure is that even for simple flat phase spaces (bosonic and Grassmann) it provides a simple quasiclassical formalism in which to analyse the deformation of the classical Poisson bracket algebra (and hence the classical canonical invariance) under quantisation.

3. Canonical transformations in quantum theories

Having introduced the idea of Moyal quantisation, we now give a brief review of the various manifestations of the loss of canonical invariance during quantisation. This is most familiar in the conventional operator formulation of the quantum theory. Consider a classical system with (globally defined) phase space coordinates p and q , and a given correspondence rule Ω mapping these to the basic self-adjoint operators \hat{p} and \hat{q} of the quantum system. Now consider making an infinitesimal canonical transformation, generated by $G(p, q)$, in the classical system, and the infinitesimal canonical transformation generated by $\hat{G}(\hat{p}, \hat{q})$ (where $\hat{G} \equiv \Omega(G)$) in the quantum system:

Classical	Quantum
$q' = q + \varepsilon\{G, q\}$	$\hat{q}' = \hat{q} + (\varepsilon/i\hbar)[\hat{G}, \hat{q}] \equiv \hat{U}\hat{q}\hat{U}^\dagger$
$p' = p + \varepsilon\{G, p\}$	$\hat{p}' = \hat{p} + (\varepsilon/i\hbar)[\hat{G}, \hat{p}] \equiv \hat{U}\hat{p}\hat{U}^\dagger$
$f'(p', q') = f(p, q) + \varepsilon\{G, f\}$	$\hat{f}'(\hat{p}', \hat{q}') = f(\hat{p}, \hat{q}) + (\varepsilon/i\hbar)[\hat{G}, \hat{f}]$

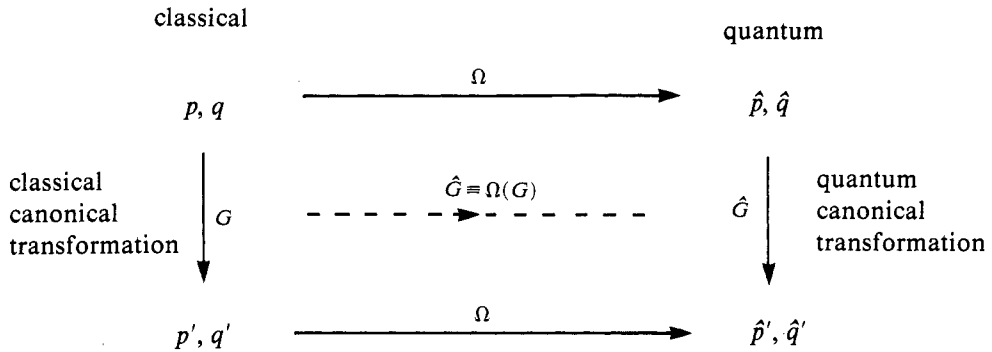
But now, by (2.2),

$$\Omega(\{G, f\}) \neq (1/i\hbar)[\hat{G}, \hat{f}]$$

in general, which means that

$$\Omega(f'(p', q')) \neq \hat{f}'(\hat{p}', \hat{q}')$$

i.e. the following diagram is non-commutative.



Manifestation 1. It is incorrect to use the same correspondence rule to relate an operator theory and classical theory before and after a (non-linear) canonical transformation.

This can be seen very elegantly in the generalised Moyal approach where it is not the Poisson bracket, but the Moyal bracket, which is directly related to the quantum commutator by the mapping Ω . This Moyal bracket, together with the corresponding Moyal product, can be used to define a pseudomechanics which reduces to classical mechanics in the limit $\hbar \rightarrow 0$. This pseudomechanics has a non-commutative product and has its dynamics defined by the Moyal bracket:

$$\hat{f}(p, q) \equiv \{\{H, f\}\}_\Omega.$$

It does not possess canonical invariance as only the first term of the Moyal bracket (i.e. the usual Poisson bracket) is a symplectic invariant. Thus, for $\hbar > 0$ we have a classical representation of the loss of canonical invariance in the corresponding quantum operator theory.

Manifestation 2. In the Moyal approach, where one is committed to a chosen correspondence rule, the dynamics is governed by the Moyal bracket $\{\{, \}\}_\Omega$ which is not a canonical invariant—only its $O(\hbar^0)$ term, which is the Poisson bracket, is canonically invariant.

The equivalence of this to manifestation 1 follows from the fact that the $O(\hbar)$ and higher terms arise from the operator reorderings necessary to impose the defining relation (2.3).

To discuss the loss of canonical invariance in phase space path integrals it is necessary to establish the equivalence between operator correspondence rules and path integral discretisations. This has been studied in great detail in the literature (for an excellent discussion see Langouche *et al* (1982)), so I will only state the important results here. If the phase space path integral

$$I = \int Dq Dp \exp\left(\frac{i}{\hbar} \int_{t''}^{t'} dt (p\dot{q} - H(p, q))\right)$$

is 'defined'/constructed (following Katz (1965)) using the short-time propagators

$$\langle q_{k+1} t_{k+1} | q_k t_k \rangle = \langle q_{k+1} | \exp[(-i\varepsilon/\hbar) \hat{H}^\Omega] | q_k \rangle \tag{3.1}$$

$$= \int dp_{k+1/2} \exp\{i/\hbar [p_{k+1/2}(q_{k+1} - q_k) - \varepsilon h^\Omega(p_{k+1/2}, q_{k+1}, q_k)]\} \tag{3.2}$$

then the ambiguity in the discretisation (i.e. the exact dependence of h^Ω on both q_k and q_{k+1}) corresponds precisely to the ambiguity in ordering the non-commuting operators in \hat{H}^Ω . This follows trivially from the fact that getting from (3.1) to (3.2) involves inserting momentum resolutions of the identity at appropriate points inside \hat{H}^Ω . Note that there is no such ambiguity for Hamiltonians of the form $\frac{1}{2}p^2 + V(q)$. In particular, for phase space path integrals, we have the following correspondences:

Weyl ordering	\longleftrightarrow	midpoint discretisation
$\hat{H} = W(H(p, q))$		$h^W(p, q_{k+1}, q_k) = H[p, (q_{k+1} + q_k)/2]$
standard ordering	\longleftrightarrow	postpoint discretisation
$\hat{H} = S(H(p, q))$		$h^S(p, q_{k+1}, q_k) = H(p, q_{k+1})$
antistandard ordering	\longleftrightarrow	prepoint discretisation
$\hat{H} = AS(H(p, q))$		$h^{AS}(p, q_{k+1}, q_k) = H(p, q_k)$

It is a simple matter to verify that these correspondences hold. Given these correspondences, we immediately arrive at the following.

Manifestation 3. It is incorrect to make a formal (non-linear) canonical transformation within a phase space path integral while retaining the same discretisation rule before and after the transformation. The equivalence of this to manifestations 1 and 2 follows directly from the equivalence between discretisations and operator ordering rules.

This is a reflection of the fact that path integrals are not Riemann–Lebesgue integrals but stochastic integrals. The earliest warning against making formal non-linear transformations within a path integral came in a beautiful paper by Edwards and Gulyaev (1964), in which they showed that a formal change of variables from cartesian to polar coordinates in the configuration space path integral for the two-dimensional free non-relativistic particle leads to the wrong answer. They showed that, within the path integral, one must respect the appropriate stochastic calculus (e.g., for the Itô calculus, $(\Delta x(t))^2 \sim O(\Delta t)$; a result familiar from the theory of Brownian motion (Arthurs 1975)) rather than the conventional rules of differential calculus. Gervais and Jevicki (1976) used this result of Edwards and Gulyaev to show that it is possible to make a point canonical transformation in the midpoint discretised form of the path integral provided one keeps all terms to $O((\Delta Q)^4)$ (since $(\Delta Q)^4/\Delta t \sim \Delta t$). The key point was that the original Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^n p_i^2 + V(q) \quad (3.3)$$

acquired an ‘additional potential term’

$$\Delta V = \frac{1}{8} \hbar^2 \Gamma_{ij}^i(Q) \Gamma_{im}^j(Q) g^{lm}(Q) \quad (3.4)$$

after the point canonical transformation

$$q_a(t) = F^a(Q(t)) \quad p_a(t) = F_{,i}^a(Q(t)) g^{ij}(Q(t)) P_j(t). \quad (3.5)$$

In this notation

$$g_{ij}(Q) \equiv \sum_{a=1}^n F_{,i}^a(Q) F_{,j}^a(Q)$$

and Γ_{ij}^i are the Christoffel symbols corresponding to g_{ij} and its inverse g^{ij} . The presence of these ‘additional potential terms’ signals the breaking of canonical invariance. It is clear that the precise form of ΔV will depend on the particular ordering/discretisation chosen. We will show in the next section how this additional potential term, as well as the additional potential terms corresponding to other discretisations, may be calculated in a simple manner using the generalised Moyal product.

It was also claimed by Gervais and Jevicki (1976) that performing the formal transformation (3.5) in the phase space path integral gave a perturbatively different theory. However, this claim must be re-evaluated in the light of the fourth manifestation of the loss of canonical invariance under quantisation, namely canonical invariance in non-linear perturbation expansions. Making the transformation (3.5) formally, the Hamiltonian (3.3) becomes

$$H' = \frac{1}{2} g^{ij}(Q) P_i P_j + V(F(Q))$$

the kinetic part of which is of the form of the kinetic part of the Hamiltonian for a particle in a curved background with metric $g_{ij}(Q)$. Now a time-splitting ambiguity arises in the perturbation expansion for such a non-linear quantum theory. Using Schwinger’s method of sources (Schwinger 1951), we write the generating functional as

$$Z[J, K] = \exp \left[\frac{-i}{\hbar} \int dt H_{\text{int}} \left(\frac{1}{i\hbar} \frac{\delta}{\delta K(t)}, \frac{1}{i\hbar} \frac{\delta}{\delta J(t)} \right) \right] Z_0[J, K] \quad (3.6)$$

where J and K are sources coupled to Q and P , respectively, Z_0 is the free generating functional, and H_{int} is

$$H_{\text{int}} = H - H_{\text{free}}.$$

Now to make the perturbation expansion one must choose some time-splitting rule Ω to avoid the problems of functionally differentiating at the same time argument. But if H_{int} involves terms containing both P and Q factors then we will get different answers in our perturbation expansion depending on our choice of ordering for the time-splitting of the action of $\delta/\delta K$ and $\delta/\delta J$. This ambiguity corresponds precisely to the ambiguity in the operator ordering in H_{int} and to the ambiguity in the phase space path integral discretisation, as can be seen from the fact that

$$\langle \hat{P}^n(t) \hat{Q}^m(t) \rangle_0 = \lim_{\epsilon \rightarrow 0^+} \frac{\delta}{\delta J(t)} \frac{\delta}{\delta J(t+\epsilon)} \cdots \frac{\delta}{\delta J(t+m\epsilon)} \frac{\delta}{\delta K(t+(m+1)\epsilon)} \cdots$$

$$\times \frac{\delta}{\delta K(t+(n+m)\epsilon)} \ln Z_0[J, K] \Big|_{J=K=0}.$$

Once this choice is made, instead of (3.6) we have

$$Z[J, K] = \exp \left[-\frac{i}{\hbar} \int dt H_{\text{int}}^\Omega \left(\frac{1}{i\hbar} \frac{\delta}{\delta K(t)}, \frac{1}{i\hbar} \frac{\delta}{\delta J(t)} \right) \right] Z_0[J, K]$$

where H_{int}^Ω is understood to have been written as a sum of multiplicative terms in which the action of the $\delta/\delta J(t)$ and $\delta/\delta K(t')$ has been time split in a well defined manner.

Then $H_{\text{int}}^\Omega = H_{\text{int}} + \Delta H^\Omega$, and the ΔH^Ω represents the ‘corrections’ to the formal classical expression for H_{int} due to the choice of the particular time-splitting rule Ω . Such perturbation expansions have been treated in the context of non-linear quantum theories in some classic papers by Leschke *et al* (1978) and Langouche *et al* (1979), who find that in the perturbation expansion arising from (3.6) there are

- (i) new Ω -dependent vertices from the correction term, and
- (ii) Ω -dependent equal-time contractions appearing in closed loops

and that while individual Feynman diagrams are Ω dependent, to any given order in \hbar the sum of all diagrams is independent of the choice of Ω . Thus we have the following.

Manifestation 4. It is incorrect to make a formal (non-linear) point canonical transformation within a path integral while retaining the same perturbative expansion and Feynman rules. The equivalence of this to the above-mentioned manifestations follows easily from the equivalence of the time splitting of the functional derivative operators $\delta/\delta K(t)$ and $\delta/\delta J(t')$ to a choice of ordering for the non-commuting Q and P factors in $H_{\text{int}}(Q, P)$.

Applying these results to the problem of making a point canonical transformation in a path integral, we see that one can in fact make such a transformation, provided one realises that the resulting theory will (in general) be non-linear and so will require a new choice of perturbation expansion. Indeed, in the case of Weyl ordering (which we recall corresponds to a midpoint discretised path integral), Leschke *et al* found an additional two-loop contribution

$$\frac{1}{8} \hbar^2 (F'')^2$$

which matches exactly the ‘discrepancy’ found by Gervais and Jevicki (in the case with phase space = \mathbb{R}^2).

Thus, a more precise way to state the initial claim made by Gervais and Jevicki in § 2 of their 1976 paper is that the original quantum theory is changed by the retention

of the initial perturbation expansion after the formal canonical transformation, rather than by the formal transformation itself. A careful examination of the generating functional (3.6) shows that it is, in fact, impossible to retain the initial perturbation expansion. Proceeding as suggested by the lead-up to ‘manifestation 4’ of this section, we see that the transformed theory is not perturbatively different (i.e. to any given order, the contributions agree), although it does require a new perturbation expansion.

4. Moyal calculation of ‘additional potential terms’

In this last section we use the Moyal methods discussed earlier to calculate the ‘additional potential terms’ resulting from a non-linear point canonical transformation, for three common quantum phase space orderings: Weyl, standard and antistandard. This method is more general than the discretised path integral calculation in the sense that we do not need to assume a particular Taylor expansion for the potentials or the transformation functions. After making a point canonical transformation of the form in (3.3) and (3.5), the kinetic part of the Hamiltonian becomes

$$H = \frac{1}{2}g^{ij}(Q)P_i(t)P_j(t). \tag{4.1}$$

In the operator quantum theory, the kinetic term should be written in its Hermitian form

$$\hat{H} = \frac{1}{2}g(\hat{Q})^{-1/4}\hat{P}_i g^{ij}(\hat{Q})g(\hat{Q})^{1/2}\hat{P}_j g(\hat{Q})^{-1/4} \tag{4.2}$$

as this corresponds to the covariant Laplace operator in the curved configuration space with metric g_{ij} (De Witt 1952). Now consider the Moyal Ω deformation of the classical theory with Hamiltonian (4.1). In the Moyal formulation, the classical phase space functions do not change their character (i.e. they do not become operators), but the ordinary classical product operation does change its character and becomes the non-commutative quasiclassical $*_{\Omega}$ product. So we must decide on an ordering of the (classical!) functions appearing in H . In analogy to (4.2) we choose

$$H^{\Omega} \equiv \frac{1}{2}g(Q)^{-1/4} *_{\Omega} P_i *_{\Omega} g^{ij}(Q) *_{\Omega} g(Q)^{1/2} *_{\Omega} P_j *_{\Omega} g(Q)^{-1/4}. \tag{4.3}$$

Then we have by construction that

$$\hat{H} = \Omega(H^{\Omega})$$

and that

$$H^{\Omega} = \frac{1}{2}g^{ij}(Q)P_iP_j + O(\hbar). \tag{4.4}$$

In the limit $\hbar \rightarrow 0$, the Moyal product $*_{\Omega}$ reduces to the ordinary product of functions so H^{Ω} reduces to (4.1).

These $O(\hbar)$ ‘quantum corrections’ in (4.4) are just the additional potential terms found in the operator formalism by re-ordering the Hamiltonian (4.2) into Ω -ordered form, in the discretised path integral by retaining stochastic terms throughout the transformation, and in the non-linear perturbative approach by choosing a time-splitting Ω in $g^{ij}(\delta/\delta J(t))K_i(t)K_j(t)$. We see here that these extra terms may be calculated using formulae (2.16a)–(2.20a), which simply involves differentiating and multiplying ordinary classical functions.

For the cases when Ω is Weyl, standard and antistandard ordering (corresponding to midpoint, prepoint and postpoint discretisation in the path integral respectively), the quantum corrections to the classical Hamiltonian are

$$\Delta H^W = \frac{1}{8}\hbar^2(F'')^2/(F')^4$$

$$\Delta H^S = i\hbar PF''/(F')^3 + \frac{1}{8}\hbar^2[2F'''/(F')^3 - 5(F'')^2/(F')^4]$$

$$\Delta H^{AS} = -i\hbar PF''/(F')^3 + \frac{1}{8}\hbar^2[2F'''/(F')^3 - 5(F'')^2/(F')^4]$$

where for simplicity of writing the formulae we have considered a two-dimensional phase space and where ' means d/dQ .

Now notice that if we specialise to the case considered by Leschke *et al* (1978) and Gervais and Jevicki (1976), where $F(Q)$ is expanded in a Taylor series about $Q=0$ with $F'(0)=1$, then the above formulae become

$$\Delta H^W = \frac{1}{8}\hbar^2(F''(0))^2$$

$$\Delta H^S = i\hbar P[F''(0) - 3Q(F''(0))^2 + QF'''(0)] + \frac{1}{8}\hbar^2[-5(F''(0))^2 + 2F'''(0)]$$

$$\Delta H^{AS} = -i\hbar P[F''(0) - 3Q(F''(0))^2 + QF'''(0)] + \frac{1}{8}\hbar^2[-5(F''(0))^2 + 2F'''(0)].$$

These agree precisely with the results of Leschke *et al* (1978).

5. Conclusion and discussion

In this short paper, we have introduced the notion of Moyal quantisation to the very general problem of quantum canonical invariance. This somewhat unfamiliar formulation of the quantum phase space theory is seen to be particularly well suited to discussing the deformation of the classical Poisson bracket algebra after quantisation. In the generalised Moyal theory the dynamics is described by c -number phase space functions together with a non-commutative product $*_{\Omega}$ and a Lie product given by the Moyal bracket $\{\{ , \}\}_{\Omega}$. In the classical limit $\hbar \rightarrow 0$, this product $*_{\Omega}$ reduces to the usual commutative product of functions, and the bracket $\{\{ , \}\}_{\Omega}$ reduces to the usual Poisson bracket $\{ , \}_{PB}$. But for $\hbar > 0$, only the lowest order (in \hbar) term of the Moyal bracket is invariant under canonical transformations (except for the trivial linear canonical transformations which leave the whole Moyal bracket invariant). The 'failure' of classical point canonical invariance is signalled by the appearance in the formally transformed Hamiltonian of 'additional potential terms' which are purely quantum effects. Given the equivalence with other quantum phase space formulations discussed in § 3, we see that in any such theory a general non-linear canonical transformation must not be made purely formally, but must be accompanied by an 'appropriate' quantum correction, the form of this correction being determined by the particular formulation.

The repercussions of this loss of classical canonical invariance go far beyond the loss of the convenient classical device of making canonical transformations to simplify a given problem. We see that the process of quantisation deforms the whole canonical structure of classical mechanics and classical field theory. In the Hamiltonian formulation of classical theories the time evolution, symmetries and constraints are all described in terms of the Poisson bracket Lie algebra structure on phase space (Dirac 1967). Even the subtleties involved in the Hamiltonian description of a relativistic theory can be handled within a (generalised) Poisson bracket framework if we extend our notion

of phase space to include Grassmann variables (see, e.g., Henneaux 1985). But in the standard Hamiltonian (often called 'canonical') quantisation procedure we are tied to a particular operator ordering—normal ordering—because of the Fock space formulation on which conventional quantum theory is based. Given this commitment to a specific correspondence rule, it is clear from the straightforward discussion in this paper that, after quantisation according to the normal ordering rule, general Poisson bracket relations will not map exactly to the corresponding operator commutation relations but will be deformed to some extent. Moreover, using equation (3.19*b*), the Moyal formulation provides a simple way of calculating the deformation of a given Poisson bracket relation.

There are two cases of particular interest in quantum field theory. Firstly, given a set of first-class classical constraints φ_α with (closed) Poisson bracket Lie algebra

$$\{\varphi_\alpha, \varphi_\beta\} = C_{\alpha\beta}{}^\gamma \varphi_\gamma$$

after quantisation we expect (if the φ_α are non-linear) the corresponding quantum Lie algebra (with Lie product now the normal-ordered Moyal bracket) to be deformed:

$$\{\{\varphi_\alpha, \varphi_\beta\}\}_N = C_{\alpha\beta}{}^\gamma \varphi_\gamma + O(\hbar)$$

so that the quantum Lie algebra is no longer closed. This deformation term corresponds precisely to the 'anomalous commutators' in the quantum Lie algebra found by other quantum methods. Bakas and Kakas (1987*b*) have applied the Moyal methods to the Virasoro constraint algebra in the bosonic string theory to calculate the Schwinger term in the quantum commutation relations of the normal-ordered Virasoro generators L_n . A second case of special interest is that of classical currents which, being bilinear in the basic 'canonical' field variables, will have their classical Poisson bracket relations deformed by the normal ordering quantisation procedure. Further work along these lines will be presented elsewhere (Bakas *et al* 1988).

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