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On dynamical properties in a Moyal quantization

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Abstract. Dynamical properties of classical Hamiltonian systems and their Moyal quantizations are related.

1. Introduction

Moyal's quantization concept [1] has been the focus of renewed interest in the past two decades for mainly two reasons. One is a general revival of the phase-space picture of quantum mechanics as initiated by Weyl and Wigner (see for example [2–17]). Another one is the rapidly developing theory of deformation algebras, for which Moyal quantization has become a standard example (see [18–31]). This was first elucidated in a fundamental paper by Bayen *et al* [18] which supports arguments by which Moyal's quantization concept seems to be the most natural way to pass from quantum to classical mechanics (see also [32] ch 8.3g). This point of view will be emphasized by the examples presented here. We shall begin with a short review of the general concept. For reasons explained in detail in [33] we prefer a regular Hilbert space, i.e. a phase-space representation of a Moyal quantization.

2. Hilbert space (phase-space) representation of a Moyal quantization

Let $a(p,q), (p,q) \in \mathbb{R}^{2N}$, be a real- or complex-valued function (observable) on a $2N$-dimensional phase space, and let $R(a(p,q))$ and $R^{\times}(a(p,q))$ denote its left- and right-regular representation in a Moyal quantization on a state space $L^2(\mathbb{R}^{2N})$ of functions $f(p,q)$. That is, if $\widehat{f}(x,y)$ denotes the Fourier transform of $f(p,q)$ and '$\circ_\hbar$' the Moyal product then [33]

$$R(a(p,q))f(p,q) \equiv a(p,q) \circ_\hbar f(p,q)$$
$$= (1/2\pi)^N \int_{\mathbb{R}^{2N}} \widehat{f}(x,y) a(p+\hbar y/2, q-\hbar x/2) \exp[i(xp+yq)]\, d(x,y)$$
$$R^{\times}(a(p,q))f(p,q) \equiv f(p,q) \circ_\hbar a(p,q)$$
$$= (1/2\pi)^N \int_{\mathbb{R}^{2N}} \widehat{f}(x,y) a(p-\hbar y/2, q+\hbar x/2) \exp[i(xp+yq)]\, d(x,y).$$

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This may be symbolically written as

$$R(a(p,q)) = a(p - \mathrm{i}\hbar\partial_q/2, q + \mathrm{i}\hbar\partial_p/2)$$

$$R^\times(a(p,q)) = a(p + \mathrm{i}\hbar\partial_q/2, q - \mathrm{i}\hbar\partial_p/2)$$

where $\partial_p = \mathrm{grad}_p$, $\partial_q = \mathrm{grad}_q$. Let $h(p,q) = p^2/2 + V(q)$ be a Hamilton function. Then the corresponding time evolution operators of the Moyal quantized system are $\exp(\mathrm{i}t\delta_h)$, $t \in \mathbb{R}$, where

$$\mathrm{i}\delta_h = \mathrm{i}[R(h(p,q)) - R^\times(h(p,q))] = \hbar p\partial_q + \mathrm{i}(V(q+\mathrm{i}\hbar\partial_p/2) - V(q-\mathrm{i}\hbar\partial_p/2)).$$

Expanding the last expression in a formal Taylor series yields

$$\mathrm{i}\delta_h = \hbar p\partial_q - 2\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}((\hbar\partial_q/2)^{2n+1}V(q))\partial_p^{2n+1}. \tag{1}$$

It is easily seen that

$$\lim_{\hbar\to 0}(\mathrm{i}\delta_h/\hbar) = p\partial_q - (\partial_q V(q))\partial_p \equiv L_h \tag{2}$$

is the Liouville operator, that is the operator which generates the time evolution operators $\exp(tL_h)$, $t \in \mathbb{R}$, of the classical system. To compare classical with quantum time evolution let us introduce the operators $\alpha_t = \exp(\mathrm{i}t\delta_h/\hbar)$ and $\beta_t = \exp(tL_h)$, $t \in \mathbb{R}$. It follows from (2) that

$$\alpha_t(A\circ_\hbar B\circ_\hbar\ldots) = (\alpha_t A)\circ_\hbar(\alpha_t B)\circ_\hbar\ldots \to \beta_t(A\cdot B\cdot\ldots) = (\beta_t A)\cdot(\beta_t B)\cdot\ldots \qquad \text{for } \hbar\to 0.$$

If $V(q)$ is, at most, quadratic then $\mathrm{i}\delta_h/\hbar = L_h$ and therefore $\alpha_t = \beta_t$ for all $t \in \mathbb{R}$. If $V(q)$ is not at most quadratic then it nevertheless can happen that $\alpha_t a(p,q) = \beta_t a(p,q)$ for all $t \in \mathbb{R}$ and non-trivial $a(p,q) \neq h(p,q)$. We will show below that this is the case for $V(q) = k/q^2, q \in \mathbb{R}$, where k is arbitrary real. Apart from such probably rare cases there are, however, numerous examples in which $\alpha_t a(p,q)$ approaches $\beta_t a(p,q)$ if either $t \to \infty$ or if the energy $E \to \infty$ (or if some other parameter tends to some fixed finite or infinite value), provided $a(p,q)$ satisfies certain growth conditions. In any of these cases one may consider the Liouville operator L_h as a first approximation of the operator $\mathrm{i}\delta_h/\hbar$. In some cases this can be expressed by a suitably adapted version [34] of the Duhamel formula, whose first-order approximation reads here as

$$\alpha_t(a(p,q)) = \beta_t(a(p,q)) + (\hbar^2/4!)\int_0^t \beta_{t-s}[\partial_q^3 V(q)\partial_p^3\beta_s(a(p,q))]\,\mathrm{d}s + \mathrm{o}(\hbar^4). \tag{3}$$

However, contrary to a certain folklore, approximations of this kind do not always work, as will be demonstrated by the example $V(q) = k/q^2$ (see appendix A.1). Another method is to use a Taylor expansion of $\alpha_t = \exp(\mathrm{i}t\delta_h/\hbar)$ in powers of t combined with analytic continuation. Although rigorous statements on the respective convergence are not available, the invariance of the energy or the (p,q)-commutator under time translations provides a sufficiently good estimate of the quality of such an approximation. We have applied this method to the (one-dimensional) potential $V(q) = q^4/4$ by using a *Mathematica* program generally developed for Moyal quantization. The results are presented in appendix A.2.

Both the methods just described will yield a global approximation for such systems only when $\beta_t q$ is periodic or at least stays bounded. For escaping trajectories it remains to study the asymptotic properties in the sense explained above. This will be demonstrated in section 2. The examples given there are typical for a large class of similiar systems with an arbitrary finite number of degrees of freedom.

Classical and Moyal time evolution can be related in a very compact form, which exhibits some interesting common global features of both evolutions. Let $a(p, q, t) \equiv \beta_t a(p, q)$ and $A(p, q, t) \equiv \alpha_t a(p, q)$. Then

$$(\partial_t - \mathrm{i}\delta_h/\hbar)A(p, q, t) = 0$$

and

$$(\partial_t - L_h)a(p, q, t) = 0.$$

Setting

$$\hbar^2 C_h := \mathrm{i}\delta_h/\hbar - L_h = (\mathrm{i}/\hbar)[V(q + \mathrm{i}\hbar\partial_p/2) - V(q - \mathrm{i}\hbar\partial_p/2) - \mathrm{i}\hbar\partial_q V(q)\partial_p]$$

the first of the two preceding equations can be written as

$$(\partial_t - L_h)A(p, q, t) = \hbar^2 C_h A(p, q, t).$$

So if $G_h(p, q, t)$ is a Green function of the last equation, that is if

$$(\partial_t - L_h)G_h(p, q, t) = \delta(t)\delta(p)\delta(q) \tag{4}$$

then ('$*$' denotes convolution)

$$A(p, q, t) = A_0(p, q, t) + \hbar^2(G_h * (C_h A))(p, q, t) \tag{5}$$

where $A_0(p, q, t)$ is an arbitrary function satisfying $(\partial_t - L_h)A_0(p, q, t) = 0$. By choosing $A_0(p, q, t) = a(p, q, t)$ we get

$$A(p, q, t) = a(p, q, t) + \hbar^2(G_h * (C_h A))(p, q, t). \tag{6}$$

Thus $A(p, q, t) \rightarrow a(p, q, t)$ for $\hbar \rightarrow 0$ as required. Writing $(K_h A)(p, q, t) \equiv (G_h * (C_h A))(p, q, t)$ we finally obtain

$$(I - \hbar^2 K_h)A(p, q, t) = a(p, q, t) \tag{7}$$

and hence, assuming the existence of $(I - \hbar^2 K_h)^{-1}$,

$$A(p, q, t) = (I - \hbar^2 K_h)^{-1} a(p, q, t). \tag{8}$$

As to the inverse of $I - \hbar^2 K_h$, note the following. It is easily seen that C_h is skew-symmetric, and the same is true for K_h if G_h is real-valued. Since we may, in addition, assume K_h to be densely defined and closed, it follows that in this case $(I - \hbar^2 K_h)^{-1}$ is a bounded operator with a norm not exceeding 1. To what extent this last relation can be constructively used for calculating $A(p, q, t)$ if $a(p, q, t)$ is known remains to be investigated. Apart from this relation (8) might be useful for statements on properties, which are commom to $A(p, q, t)$ and $a(p, q, t)$. An important example is the following statement:

If $a(p,q,t) \equiv \beta_t a(p,q)$ is periodic with respect to t, say modulo T, then the same is true for $A(p,q,t) \equiv \alpha_t a(p,q)$ (and vice versa).

It is obvious that relation (8) will also allow us to make statements concerning, for example, asymptotic, oscillatory or singular behaviour, which hold simultaneously for $A(p,q,t)$ and $a(p,q,t)$. A Green function $G_h(p,q,t) = G_h^{(0)}(p,q,t)+G_h^{(1)}(p,q,t)$, where $G_h^{(0)}$ satisfies $(\partial_t - L_h)G_h^{(0)}(p,q,t) = 0$ but is otherwise arbitrary, can be constructed as follows. Let $(\delta_\varepsilon(p,q))_{\varepsilon>0}$ be a sequence (of smooth functions) converging to $\delta(p,q) \equiv \delta(p)\delta(q)$, and let $g_\varepsilon(p,q,t) = (\mathrm{sign}(t) + c_0)\beta_t\delta_\varepsilon(p,q)/2$, where c_0 is an arbitrary (real) constant and $\beta_t = \exp(tL_h)$. Then, because of $\partial_t\,\mathrm{sign}(t)/2 = (1/\pi)\partial_t \lim_{k\to 0}\tan^{-1}(t/k) = \delta(t)$,

$$(\partial_t - L_h)g_\varepsilon(p,q,t) = \delta(t)\beta_t\delta_\varepsilon(p,q) = \delta(t)\delta_\varepsilon(p,q)$$

and the right-hand side converges to $\delta(t)\delta(p)\delta(q)$ for $\varepsilon \to 0$. Hence we may define $G_h^{(1)} = \lim_{\varepsilon\to 0} g_\varepsilon$ (in the distribution sense). If in particular $h(p,q) = p^2/2 + V(q)$, where $\lim_{|q|\to 0} V(q)/|q| = 0$, then $L_h\delta(p,q) = 0$ and therefore $\beta_t\delta_\varepsilon(p,q) \to \delta(p,q)$ for $\varepsilon \to 0$. That is, in this case $G_h^{(1)}(p,q,t) = (\mathrm{sign}(t) + c_o)\delta(p,q)/2$. In all other cases $G_h^{(1)}(p,q,t)$ could yield a complicated distribution.

As to expectation values in a phase-state space the situation is as follows. Let $u(p,q)$ and $v(p,q)$ be functions in $L^2(\mathbb{R}^{2N})$. Then $\langle \mathbf{1}, \overline{u} \circ_\hbar v\rangle = \langle u, v\rangle$ where $\langle.,.\rangle$ denotes the inner product [18]. This extends to dual pairs of functions. That is, if $f(p,q)$ is in the domain of $R(a(p,q))$, and if $\rho \equiv f \circ_\hbar \overline{f}$, then

$$\begin{aligned}\langle f, R(a(p,q))\rangle &= \int_{\mathbb{R}^{2N}} \overline{f(p,q)}(a(p,q) \circ_\hbar f(p,q))\,\mathrm{d}(p,q)\\ &= \int_{\mathbb{R}^{2N}} a(p,q) \circ_\hbar (f(p,q) \circ_\hbar \overline{f(p,q)})\,\mathrm{d}(p,q)\\ &= \int_{\mathbb{R}^{2N}} a(p,q)\rho(p,q)d(p,q) \equiv \langle a\rangle_\rho.\end{aligned}$$

That is, the Moyal quantum expectation value of $R(a(p,q))$ with respect to a state $f(p,q) \in L^2(\mathbb{R}^{2N})$ is equal to the classical expectation value of $a(p,q)$ with respect to the 'density' $\rho = f \circ_\hbar \overline{f}$. We note that ρ can be negative (this has been extensively studied in the context of *Wigner functions*, see [2–17]). The Heisenberg uncertainty principle is, by the way, reflected by the fact [33] that there is no sequence $(f_\varepsilon)_{\varepsilon>0}$ such that $f_\varepsilon \circ_\hbar \overline{f_\varepsilon}$ converges for $\varepsilon \to 0$ to a Dirac distribution or its derivatives. Therefore comparing α_t and β_t, or rather calculating $(\alpha_t - \beta_t)a(p,q)$ for some observable $a(p,q)$, has finally to be translated into a phase-space expectation value. Since the α_t share with the β_t the property of preserving the phase-space volume [18], $\langle\alpha_t a(p,q)\rangle_\rho = \langle\alpha_{-t}f, R(a(p,q))\alpha_{-t}f\rangle$ where $\rho = f \circ_\hbar \overline{f}$ holds.

3. Examples

In the first two examples, both with one degree of freedom, we shall discuss asymptotic properties of α_t applied to suitable functions $a(p,q)$. The basic idea is to make a canonical transformation $(p,q) \to (E,\tau)$, where

$$E = h(p,q) = p^2/2 + V(q) \tag{9}$$

and

$$\tau = \int^q \frac{\mathrm{d}x}{\sqrt{(2h(p,q) - 2V(x))}}. \tag{10}$$

In this way the operator $\mathrm{i}\delta_h$ becomes a differential operator which depends on E, τ, ∂_E and ∂_τ. Since τ is the phase of an autonomous system, the limit $\tau \to \infty$ is equivalent to the limit $t \to \infty$ and hence allows us to make statements in the case of escaping trajectories if t tends to infinity. The limit $E \to \infty$ will be of interest both for escaping and closed phase-space trajectories.

3.1. The potential k/q^2, $0 \neq k \in \mathbb{R}$

Let $E \equiv h(p,q) = p^2/2 + k/q^2$, $(p,q) \in \mathbb{R}^2$, $0 \neq k \in \mathbb{R}$. Then by (1)

$$\begin{aligned}(i\delta_h/\hbar)^2(q^2) &= (\mathrm{i}/2\hbar)((p - \mathrm{i}\hbar\partial_q/2)^2 - (p + \mathrm{i}\hbar\partial_q/2)^2)^2 q^2 \\ &= (\mathrm{i}\delta_h/\hbar)(2pq) = 2p^2 + 4k/q^2 = 4E.\end{aligned}$$

Since $\delta_h E = 0$ it follows

$$\alpha_t(q^2) = (1 + t(\mathrm{i}\delta_h/\hbar)/1! + t^2(\mathrm{i}\delta_h/\hbar)^2/2!)q^2 = q^2 + 2pqt + 2Et^2 \tag{11}$$

$$\alpha_t(pq) = pq + 2Et^2. \tag{12}$$

The classical solution of our Hamiltonian system follows from

$$t = \int^q \mathrm{d}x/\sqrt{2E - 2k/x^2} = \sqrt{2Eq^2 - 2k}/2E.$$

Thus

$$\beta_t q = \sqrt{q^2 + 2pqt + 2Et^2} \tag{13}$$

$$\beta_t(q^2) = (\beta_t q)^2 = q^2 + 2pqt + 2Et^2 \tag{14}$$

$$\beta_t(pq) = pq + 2Et. \tag{15}$$

By comparing (11) with (14) and (12) with (15) we conclude that $\alpha_t(q^2) = \beta_t(q^2)$ and $\alpha_t(pq) = \beta_t(pq)$ for all $t \in \mathbb{R}$. Thus the classical and the quantum phase-space expectation values with respect to a density $\rho = f \circ_\hbar \overline{f}$ coincide for the observables q^2 and pq for all times. Note that by (11) and (12) we can calculate the quantum time evolution for q^{2m}, $(pq)^n$, m and n arbitrary natural, and all observables which are obtained as Moyal products of these expressions. Using (11) yields for example

$$\alpha_t(q^4) = \alpha_t(q^2) \circ_\hbar \alpha_t(q^2) = \beta_t(q^4) - 6k\hbar^2 t^4/q^4.$$

However, these coincidences between classical and quantum time evolution for non-quadratic Hamiltonians can be expected to be the rare exceptions.

Let us now consider asymptotic properties. For $E > 0$ the potential k/q^2 classically yields only escaping trajectories regardless of the sign of k. By introducing the energy E and the phase τ as new (canonical) variables we obtain

$$q = \sqrt{2E\tau^2 + k/E} \qquad p = 2E\tau/\sqrt{2E\tau^2 + k/E}.$$

From the identity $\partial_p = (\partial E/\partial p)\partial_E + (\partial\tau/\partial p)\partial_\tau$ it then follows that

$$\begin{aligned}\partial_p/q &= (1 + k/2E^2\tau^2)^{-1}(\partial_E/\tau - (1 - k/2E^2\tau^2)\partial_\tau/2E) \\ &= (-1/2E + \mathrm{o}(E^{-3}\tau^{-2}))\partial_\tau + (1/\tau + \mathrm{o}(E^{-2}\tau^{-3}))\partial_E.\end{aligned}$$

Using this relation, after a short calculation, we obtain from (1)

$$\begin{aligned}\mathrm{i}\delta_h/\hbar &= L_h + (2k/q^2)\sum_{n=1}^{\infty}(n+1)(\mathrm{i}\hbar/2)^{2n}(\partial_p/q)^{2n+1} \\ &= L_h + k(1/E\tau^2 + \mathrm{o}(E^{-3}\tau^{-4}))\sum_{n=1}^{\infty}(n+1)(\mathrm{i}\hbar/2)^{2n}((-1/2E + \mathrm{o}(E^{-3}\tau^{-2}))\partial_\tau \\ &\quad + (1/\tau + \mathrm{o}(E^{-2}\tau^{-3}))\partial_E)^{2n+1}.\end{aligned}$$

It thus finally follows that

$$\lim_{E\to\infty}(\alpha_t - \beta_t)f(E,\tau) = 0 \qquad \text{only if} \qquad \lim_{E\to\infty}|f(E,\tau)E^{-4}| = 0$$

$$\lim_{t\to\infty}(\alpha_t - \beta_t)f(E,\tau) = 0 \qquad \text{only if} \qquad \lim_{t\to\infty}|f(E,\tau)\tau^{-5}| = 0.$$

This statement can be generalized to a large class of potentials (with an arbitrary finite number of degrees of freedom) which vanish at infinity. We shall consider this elsewhere.

3.2. The potential $q^4/4$

Let $h(p,q) = p^2/2 + q^4/4$, $(p,q) \in \mathbb{R}^2$. This system has classical solutions $q(t) \equiv \beta_t q = \lambda\mathrm{cn}(\lambda(t+\tau))$, $p(t) \equiv \beta_t p = \partial(\beta_t q)/\partial\tau = \partial(\beta_q)/\partial t$, $t \in \mathbb{R}$, $\tau \in \mathbb{R}$, where $\lambda = (4E)^{1/4}$ and 'cn' denotes the *cosinus amplitudinis* (with module $1/\sqrt{2}$). Since we have closed trajectories $(\beta_t p, \beta_t q)$, the limit $t \to \infty$ makes no sense. It remains to consider whether $\alpha_t - \beta_t$ tends to zero if E tends to infinity. Inverting the Jacobian $\partial(p,q)/\partial(\lambda,\tau)$ we get

$$\partial_p = \lambda^{-4}(-(q+\tau p)\partial_\tau + \lambda p\partial_\lambda) \qquad \partial_q = \lambda^{-4}(2p - \tau q^3)\partial_\tau + \lambda q^3\partial_\lambda).$$

It follows with these equations ($\mathrm{sn} = \sqrt{1-\mathrm{cn}^2}$, $\mathrm{dn} = \sqrt{(1+\mathrm{cn}^2)/2}$)

$$\begin{aligned}\mathrm{i}\delta_h/\hbar &= L_h - (\hbar^2/4)q\partial_p{}^3 \\ &= L_h - (q\hbar^2/4)[-(q+\tau p)\partial_\tau + p\tau\partial_\lambda]^3 \\ &= L_h - (\hbar^2/4)(4E)^{-11/4}\mathrm{cn}((4E)^{1/4})\{-[(4E)^{1/4}\mathrm{cn}((4E)^{1/4}\tau) \\ &\quad +2\tau E^{1/2}\mathrm{sn}((4E)^{1/4}\tau)\mathrm{dn}(4E)^{1/4}\tau)]\partial_\tau + 8E^{3/2}\mathrm{sn}((4E)^{1/4}\tau)\mathrm{dn}((4E)^{1/4}\tau)\partial_E\}^3.\end{aligned}$$

It is not difficult to see that $q\partial_p{}^3 g(E,\tau) \to 0$ for $E \to 0$ if $|g(E,\tau)|$ increases with respect to E less than $E^{5/4}$, and fails to do so otherwise. Consequently,

$$\lim_{E\to\infty}(\alpha_t - \beta_t)g(E,\tau) = 0 \qquad \text{only if} \qquad \lim_{E\to\infty}|g(E,\tau)\,E^{-5/4}| = 0.$$

In particular

$$\lim_{E\to\infty}(\alpha_t - \beta_t)(q^m p^n) = 0 \qquad \text{if} \qquad m + 2n < 5.$$

3.3. Constants of motion: periodic potentials, Toda potential

We conclude with two examples which demonstrate that classical constants of motion (first integrals) do not need to have quantum counterparts and vice versa.

3.3.1. Periodic potentials. Let $h(p,q) = p^2/2 + V(q)$, $(p,q) \in \mathbb{R}^{2N}$, where $V(q \pm z) = V(q)$ for some constant vector $z \in \mathbb{C}^N$. Let $k \in \mathbb{Z}$, and let $\chi(k,p) = \exp[2ik(zp)/\hbar]$. Then

$$\begin{aligned}\delta_\hbar \chi(k,p) &= (V(q + i\hbar\partial_p) - V(q - i\hbar\partial_p))\chi(k,p) \\ &= (V(q - kz) - V(q + kz))\chi(k,p) = 0.\end{aligned}$$

Hence $\alpha_t \chi(k,p) = \chi(k,p)$ for all $t \in \mathbb{R}$. This extends to arbitrary elements of the linear space spanned by the $\chi(k,p)$, $k \in \mathbb{Z}$. However, $L_\hbar \chi(k,p) \neq 0$ for $k \neq 0$. Thus the $\chi(k,p)$, $k \in \mathbb{Z}$ (and their linear combinations) are constants of motion quantum mechanically but not classically. This example has an analogue in the Heisenberg picture. It is based on the following, easy to prove statement (omitting any finesse on domains of operators). For any two operators A, B satisfying $[A,B] = i\mathbb{1}$, $[\exp(\mu A), \exp(2ik\pi B/\mu)] = 0$ for arbitrary complex $\mu \neq 0$ and arbitrary $k \in \mathbb{Z}$ holds. Then let $A = P$, $B = Q$ where (P,Q) is a Heisenberg couple. The property $V(Q \pm 2\pi i/\mu) = V(Q)$ determines a symmetry group with *inner* automorphisms $\sigma : f(Q) \to Sf(Q)S^{-1} = f(Q + 2\pi i/\mu)$ where $S = \exp(2\pi i P/\hbar\mu)$. It is easily seen that S commutes with the corresponding Hamiltonian in the Heisenberg picture. Now, classically by $V(q \pm 2\pi i/\mu) = V(q)$ we also have a symmetry group. The corresponding automorphisms are $\tilde{\sigma} = \exp(2\pi i\partial_q/\mu)$, and they leave the Hamilton function $h(p,q)$ invariant. However, since these automorphisms are *outer*, there is no function (= constant of motion) $s(p,q)$ such that $\tilde{\sigma}a(p,q) = s(p,q)a(p,q)$, $a(p,q) \not\equiv 0$ or 1.

3.3.2. Toda potential. Let $h(p,q) = p^2/2 + V(q)$, $(p,q) \in \mathbb{R}^6$, where

$$V(q) = \exp(q_1 - q_2) + \exp(q_2 - q_3) + \exp(q_3 - q_1).$$

It is known [35] that $h(p,q)$ and the following expressions are in involution (meaning that their mutual Poisson brackets vanish):

$$a(p) = \sum_{j \bmod 3} p_j$$

$$b(p,q) = \prod_{j \bmod 3} (p_j + p_{j+1} - 2p_{j+2}) \sum_{j \bmod 3} (p_j + p_{j+1} - 2p_{j+2}) \exp(q_j - q_{j+1}).$$

if we write $H = R(h(p,q))$, $A = R(a(p,q))$ and $B = R(b(p,q))$. Then

$$[H,A] = 0 \qquad [A,B] = 0 \qquad [H,B] = \hbar R(c(p,q))$$

where

$$c(p,q) \equiv \sum_{j \bmod 3} (p_j^2 + 2p_{j+1}p_{j+2})[\exp(q_j - q_{j+1}) - \exp(q_{j+1} - q_{j+2})].$$

Thus the Moyal operators corresponding to $h(p,q)$, $a(p,q)$ and $b(p,q)$ are not all in involution in contrast to the classical case. This raises the question of whether there exists a 'complete' set of mutually commuting Moyal operators at all.

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Appendix

The numerical calculations presented in the following are based either on a Taylor series expansion of $\alpha_t = \exp(it\delta_h/\hbar)$ in powers of t combined with analytic continuation or on the modified Duhamel formula (3). As to the first method it means that we start with a Taylor expansion $\alpha_{t,n} = \sum_{j=0}^{n}(it\delta_h/\hbar)^j q/j!$ of α_t for some interval $[0, t_1)$ and an energy E. A value for t_1 can be fixed as follows. Let $\Delta E(t,n) = h(\alpha_{t,n}p, \alpha_{t,n}q)$ be the deviation of the energy from the initial energy $E = h(p,q)$ caused by our approximation. Allowing a certain error $\Delta E(t,n)$ we define $t_1 > 0$ as the bound for t in accordance with this error. We proceed then by analytic continuation. That is, we calculate $\alpha_{t,n}a(p,q)$ (if $a(p,q)$ is the observable in which we are interested) on $[t_1, t_2)$ for initial values $p_1 = \alpha_{t_1,n}p$ and $q_1 = \alpha_{t_1,n}q$ (where p and q were the intial values at $t = 0$). t_2 could then be fixed in the same way as t_1 was. By periodicity with respect to t we can expect to get in this fashion a finite covering of the interval of periodicity. The final result can then be checked by calculating the maximal energy deviation on the global interval using the approximations obtained by the preceding calculations. Although this scheme lacks (due to considerable technical difficulties) rigour as concerns convergence, we think that the estimates based on the energy deviation will suffice.

A.1. The potential k/q^2

Writing (3) as

$$\alpha_t(a(p,q)) = \alpha_t^{(2)}(a(p,q)) + o(\hbar^4)$$

it follows by a short calculation that

$$\alpha_t{}^{(2)}(q) - \beta_t(q) = \hbar^2 k^2 t^6 q^{-6}(q^2 + 2pqt + 2Et^2)^{-5/2}.$$

Hence

$$\lim_{t\to\infty}[(\alpha_t{}^{(2)}(q) - \beta_t(q))/t] = \hbar^2 k^2 q^{-6}(2E)^{-5/2}.$$

This is in contrast to $\lim_{t\to\infty}[(\alpha_t(q) - \beta_t(q))/t] = 0$, as shown in section 3. Further

$$\lim_{E\to\infty}[\alpha_t{}^{(2)}(q) - \beta_t(q)] = 0.$$

Thus the Duhamel formula yields an approximation only if E is large, regardless of the values for t. Let us compare this with a rough estimate by a Taylor expansion. One has

$$\alpha_{t,n}(q) \equiv \sum_{j=0}^{n}(it\delta_h/\hbar)^j q/j!$$
$$= q + pt + kt^2/q^3 + kpt^3/q^4 + k(-k + 2p^2q^2)t^4/q^7 + \cdots$$

We now substitute $(2E\tau^2 + k/E)^{1/2}$ for q and $2E\tau(2E\tau^2 + k/E)^{-1/2}$ for p, and consider τ as the initial value of t. That is, $\tau \to \infty$ is equivalent to $t \to \infty$. The powers of E and τ in (16) decrease strictly monotonically with increasing powers of t. From $\beta_t(q) = \sqrt{2E(t-\tau)^2 + k/E}$ it therefore follows by an easy calculation that

$$\lim_{t\to\infty}[\alpha_{t,n}(q) - \beta_t(q)] = \lim_{t\to\infty}[\alpha_{t,1}(q) - \beta_t(q)] = 0$$

$$\lim_{E\to\infty}[\alpha_{t,n}(q) - \beta_t(q)] = \lim_{E\to\infty}[\alpha_{t,1}(q) - \beta_t(q)] = 0.$$

That is, for this example a Taylor expansion yields a better all round approximation than the Duhamel formula.

A.2. The potential $q^4/4$

Setting $\hbar = 1$ we have calculated $Q(t) = \alpha_t(q)$ and $q(t) = \beta_t(q)$ for energies $E = 1$, $E = 10$, and $E = 100$, all with initial values $P(0) = p(0) = 0$, $Q(0) = q(0) = (4E)^{1/4}$ with the Taylor expansion explained above. The order of these expansions was in all cases 12. The intervals $[t_j, t_{j+1})$, $t_0 = 0$, $0 \leqslant j \leqslant N(E)$, were given a uniform 'steplength' $\Delta t = t_{j+1} - t_j$ (depending on E) such that the relative deviation of energy, $|\Delta E(t)/E|$, is below 0.5% at the first step. This is achieved with $\Delta t = 0.4$, $\Delta t = 0.2$ and $\Delta t = 0.12$ for $E = 1$, $E = 10$ and $E = 100$ respectively. The corresponding intervals of periodicity are $T = 5.24$, $T = 2.95$ and $T = 1.66$, which means 13 steps in each case. The maximal absolute values of $\Delta Q(t)/Q_0 \equiv (Q(t) - q(t))/Q(0)$ and $\Delta E(t)/E \equiv (P(t)^2/2 + Q(t)^4/4)/E - 1$ on the corresponding intervals of periodicity are given in table A1. We have further listed the values of $\Delta Q(T)/Q_0$ to demonstrate that $Q(T)$ is periodic in the same way that the classical position $q(t)$ is, namely modulo $T = \Gamma(1/4)^2(2\pi)^{-1/2}(E)^{-1/4}$ (cf a corresponding statement in section 2)†. Calculations based on the Duhamel formula have been omitted. Compared with a Taylor expansion they are highly unsatisfactory as to efficiency and accuracy.

Table A1.

E	1	10	100
T	5.24	2.95	1.66
$\lvert\Delta Q(t)/Q_0\rvert_{max}$	0.38%	0.0078%	0.0016%
$\Delta Q(T)/Q_0$	0.067%	0.0013%	0.0006%
$\lvert\Delta E(t)/E\rvert_{max}$	0.37%	0.0071%	0.0015%

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† The calculation time (including plots for all functions listed above) was, by the way, about 7 min on an i486 DX2/66 (8 MB RAM) PC with a program running under *Mathematica* for Windows, version 2.1, ©Wolfram Research, Inc., 1992.

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