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The Campbell–Baker–Hausdorff expansion for classical and quantum kicked dynamics

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Abstract. A technique based on the Campbell-Baker-Hausdorff (CBH) formula is introduced to calculate the effective Hamiltonian for kicked dynamics, classical and quantum. An integrable example is exactly solved by this method. A non-integrable kicked spin dynamics is treated approximately up to seventh order in a perturbation parameter. The CBH expansion is evaluated in a transparent way with the help of a REDUCE program, thereby illustrating that the CBH expansion is asymptotic.

1. Introduction

The usefulness of Lie techniques in the investigation of dynamical systems is now well documented (Olver 1986, Finn 1986, Steinberg 1986). Symplectic maps also have been treated by these techniques (Dragt and Finn 1976). One of them is quite well known: the Birkhoff-Gustavson normal form transformation (for references see Lichtenberg and Lieberman (1983)). A somehow obscure role among these techniques is played by the so-called Campbell-Baker-Hausdorff (CBH) formula and in some sense the dual Zassenhaus formula. These formulae have been used to solve ordinary differential equations of the form: $\dot{Y} = AY$ with the linear operators $A(t)$ and $Y(t)$ depending on $t \in \mathbb{R}$ with the initial condition $Y(0) = I$, the identity (Magnus 1954). The idea of using the CBH formula for the construction of invariants of symplectic maps was put to work by Dragt and Finn (1976), but the practical use was quite limited.

The objective of this paper is to give a short introduction to these techniques from a practical point of view. I especially propose to show how the CBH formula gives the possibility of constructing an exact or approximate integral of a symplectic map (or its quantal counterpiece) depending on whether the map is integrable or only nearly integrable. Finally I shall demonstrate the CBH formula in an expanded form to be useful even for chaotic maps. It is now a tool for constructing local approximate integrals in the vicinity of elliptic orbits. This article gives a unified treatment of classical (symplectic) and quantum (unitary) maps thereby stressing the deep similarities between them. Of special importance among the constructed integrals is the effective Hamiltonian, the infinitesimal generator of the classical or quantum map.

The validity of the CBH expansion can be destroyed by resonances that show up in the classical as well as in the quantum case. This is studied in an example of an integrable map where at resonances there actually is no effective Hamiltonian. More interesting is the case of non-integrable maps where the effective Hamiltonian generates the flow in the smooth parts of the phase space approximately. For a non-integrable

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example it is shown how to calculate the CBH expansion up to seventh order in a perturbation parameter with the help of computer algebra.

2. The Campbell–Baker–Hausdorff formula

For reasons of being self-contained a short derivation of the CBH formula is given (Sattinger and Weaver 1987) and some conclusions are drawn. Suppose we have an algebra $\mathcal{A}$ of generally non-commuting quantities A, B, C, etc. By definition the commutator $[A, B] = AB - BA$ is an element of $\mathcal{A}$ too. Now for a shorthand notation introduce the elements $\hat{A}$, $\hat{B}$, $\hat{C}$, etc, of the adjoint algebra $\hat{\mathcal{A}}$ acting on the elements of $\mathcal{A}$ by

$$\hat{A}B = [A, B]. \tag{2.1}$$

Defining the exponential function of elements of $\hat{\mathcal{A}}$ by Taylor series we have the identity

$$B(t) := \exp(tA)B\exp(-tA) = \exp(t\hat{A})B. \tag{2.2}$$

The second equation can be easily proved by differentiating $B(t)$ with respect to t and noticing the initial condition $B(0) = B$. Now let A depend on t and define the function

$$B(s, t) := \exp(sA(t))\frac{\partial}{\partial t}\exp(-sA(t)). \tag{2.3}$$

Differentiating $B(s, t)$ with respect to s gives

$$\frac{\partial B}{\partial s} = [A, B] - \dot{A} = \hat{A}B - \dot{A} \qquad \left(\dot{A} = \frac{\mathrm{d}A}{\mathrm{d}t}\right) \tag{2.4}$$

with the solution

$$B(s, t) = \exp(s\hat{A}(t))B(0, t) - \int_0^s \mathrm{d}r\,\exp((s-r)\hat{A}(t))\dot{A}(t). \tag{2.5}$$

Noticing that $B(0, t)$ vanishes we get

$$\exp(A(t))\frac{\mathrm{d}}{\mathrm{d}t}\exp(-A(t)) = -f(\hat{A}(t))\dot{A}(t) \tag{2.6}$$

where $f(z) = (\exp(z) - 1)/z$.

Now for $A, B \in \mathcal{A}$ sufficiently close to 0 the element $C = \ln(\exp(A)\exp(B))$ is uniquely defined and we get the Campbell-Baker-Hausdorff (CBH) formula

$$C = B + \int_0^1 \mathrm{d}s\, g[\exp(s\hat{A})\exp(\hat{B})]A \tag{2.7}$$

where

$$g(z) = \ln(z)/(z-1) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)}(z-1)^n.$$

For a proof let $C(t) = \ln(\exp(tA)\exp(B))$ and we get with (2.6)

$$-A = \exp(C(t))\frac{\mathrm{d}}{\mathrm{d}t}\exp(-C(t)) = -f(\hat{C}(t))\dot{C}(t). \tag{2.8}$$

Noticing the identity $f(\ln z)g(z)=1$ and using (2.2) gives

$$\exp(\hat{C})D=\exp(C(t))D\exp(-C(t))=\exp(t\hat{A})\exp(\hat{B})D \tag{2.9}$$

for all $D\in\mathscr{A}$ and we finally get

$$\dot{C}(t)=g[\exp(t\hat{A})\exp(\hat{B})]A \tag{2.10}$$

which proves (2.7) when taking into account the initial condition $C(0)=B$. Writing $C=-\ln[\exp(-B)\exp(-A)]$ we get an alternative CBH formula

$$C=A+\int_0^1 ds\, g[\exp(-s\hat{B})\exp(-\hat{A})]B. \tag{2.7'}$$

Four special cases should be considered now.

(i) First let $\hat{A}\hat{B}A=\hat{B}^2A=0$. Then (2.7) simplifies considerably to

$$C=B+\int_0^1 ds\, g(1+s\hat{A}+\hat{B})A=B+A-\tfrac{1}{2}\hat{B}A \tag{2.11}$$

which gives the following well known formula if $[A,[A,B]]=[B,[A,B]]=0$

$$\exp(A)\exp(B)=\exp(A+B+\tfrac{1}{2}[A,B]). \tag{2.12}$$

(ii) Now we suppose only $\hat{A}\hat{B}^nA=0$ for all n. Then (2.7) simplifies to

$$C=B+g[\exp(\hat{B})]A=B+\hat{B}[\exp(\hat{B})-1]^{-1}A \tag{2.13}$$

and alternatively with $\hat{B}\hat{A}^nB=0$ for all n (2.7') gives

$$C=A+g[\exp(-\hat{A})]B=A-\hat{A}[\exp(-\hat{A})-1]^{-1}B \tag{2.13'}$$

showing the possibility of small denominators explicitly.

(iii) Suppose that A and B are linear combinations of three quantities $S_i(i=1,2,3)$ fulfilling the SU(2) commutation relations: $[S_j,S_k]=i\varepsilon_{jkl}S_l$. Then the CBH formula immediately tells us that C is also a linear combination of the S_i with the coefficients yet to be determined. This simply means that the succession of two rotations is a rotation.

(iv) For the last case we choose C of the form $C(\lambda)=-\ln[\exp(-\lambda B)\exp(-A)]$ and use

$$C(\lambda)=A+\int_0^1 ds\, g[\exp(-s\lambda\hat{B})\exp(-\hat{A})]\lambda B \tag{2.14}$$

which gives up to $O(\lambda^2)$

$$C(\lambda)=A+\lambda g[\exp(-\hat{A})]B+O(\lambda^2) \tag{2.15}$$

showing the possibility of small denominators as (2.13').

3. Quantum maps

Now we want to specify the algebra $\mathscr{A}$. For example, we might take the real (or complex) algebra of real (or complex) $N\times N$ matrices. Instead we look at the algebra H of Hermitian linear operators acting on the Hilbert space of some quantum system.

First we take the Hamilton operator of the system and define the unitary time evolution of some observable A in the Heisenberg picture

$$A(t) = \exp\left(\frac{\mathrm{i}}{\hbar} Ht\right) A(0) \exp\left(-\frac{\mathrm{i}}{\hbar} Ht\right) = \exp\left(\frac{\mathrm{i}}{\hbar} \hat{H}t\right) A(0) \tag{3.1}$$

with the ad operator $\hat{H}$ defined as in (2.1). For fixed t (3.1) defines a unitary quantum map. One might also look at the succession of two unitary maps, as it arises in connection with a kicked quantum system, for example the kicked rotator (Casati *et al* 1979) or kicked tops (Haake *et al* 1987a, b). Quantum maps of this kind look like

$$A_{n+1} = \exp\left(\frac{\mathrm{i}}{\hbar} t\hat{H}\right) \exp\left(\frac{\mathrm{i}}{\hbar} s\hat{V}\right) A_n \tag{3.2}$$

with H being the Hamiltonian of the unperturbed system and sV being the perturbation 'kicked in' at times nt with integer n. For an introduction to quantum maps see Berry *et al* (1979). For $[H, V] \neq 0$ the quantum map does not possess an integrable classical limit in general.

Comparison between (2.9) and (3.2) shows that the CBH formula should give an expression for the effective Hamiltonian operator H_{eff} defined as

$$\exp\left(\frac{\mathrm{i}}{\hbar} H_{\text{eff}}\right) = \exp\left(\frac{\mathrm{i}}{\hbar} tH\right) \exp\left(\frac{\mathrm{i}}{\hbar} sV\right). \tag{3.3}$$

For commuting H and V one gets of course $H_{\text{eff}} = tH + sV$. But generally with the help of (2.7) and (2.7′)

$$H_{\text{eff}} = sV + t \int_0^1 \mathrm{d}r\, g\left[\exp\left(\frac{\mathrm{i}}{\hbar} rt\hat{H}\right) \exp\left(\frac{\mathrm{i}}{\hbar} s\hat{V}\right)\right] H \tag{3.4}$$

$$H_{\text{eff}} = tH + s \int_0^1 \mathrm{d}r\, g\left[\exp\left(-\frac{\mathrm{i}}{\hbar} rs\hat{V}\right) \exp\left(-\frac{\mathrm{i}}{\hbar} t\hat{H}\right)\right] V. \tag{3.4'}$$

Supposing $\hat{V}\hat{H}^n V = 0$ for all n we get as in (2.13′)

$$H_{\text{eff}} = tH - \frac{\mathrm{i}}{\hbar} t\hat{H}\left[\exp\left(-\frac{\mathrm{i}}{\hbar} t\hat{H}\right) - 1\right]^{-1} sV. \tag{3.5}$$

Using (3.1) one finds in the eigenrepresentation of $H[H\,|\,n\rangle = E_n\,|\,n\rangle]$

$$\left\langle n \left| \exp\left(\frac{\mathrm{i}}{\hbar} t\hat{H}\right) A \right| m \right\rangle = \exp\left(\frac{\mathrm{i}}{\hbar}[E_n - E_m]t\right) A_{nm} \tag{3.6}$$

and in the special case (3.5)

$$\langle n|H_{\text{eff}}|m\rangle = tE_n\delta_{nm} - sV_{nm}\left(\frac{\mathrm{i}}{\hbar}[E_n - E_m]t\right)\left[\exp\left(-\frac{\mathrm{i}}{\hbar}[E_n - E_m]t\right) - 1\right]^{-1}. \tag{3.7}$$

From (3.7) we notice that starting at $t = 0$ and increasing t the given analytic continuation inevitably leads to resonances on account of small denominators, which destroy H_{eff} although for all non-resonant values of t the CBH formula (3.5) is exact in this special case. Resonances show up in the classical limit of quantum maps as well, as will be shown in the next section.

We conclude this section by stating a formula valid for unitary transformations of analytic functions of momentum and position operators

$$\exp\left(\frac{\mathrm{i}}{\hbar}\hat{H}\right)F(p,q)=F\left[\exp\left(\frac{\mathrm{i}}{\hbar}\hat{H}\right)p,\exp\left(\frac{\mathrm{i}}{\hbar}\hat{H}\right)q\right] \tag{3.8}$$

as can be proven immediately by Taylor expansion of F and use of (2.2).

4. Symplectic maps

In this section we want to use the CBH formula for the investigation of compositions of symplectic maps, the classical limit of unitary quantum maps.

We support the even-dimensional Euclidean vector space $\mathbb{R}^{2d}$ with cartesian coordinates $(p,q)=(p_1,\ldots,p_d,q_1,\ldots,q_d)$ and call it the phase space, p_i being momenta and q_i positions. Then we define the Poisson bracket (PB) for smooth phase space functions $F(p,q)$, $G(p,q)$ etc:

$$\{F,G\}=\sum_{k=1}^{d}\left(\frac{\partial F}{\partial q_k}\frac{\partial G}{\partial p_k}-\frac{\partial F}{\partial p_k}\frac{\partial G}{\partial q_k}\right). \tag{4.1}$$

The PB is bilinear, skew symmetric and fulfils the Jacobi identity (Arnol'd 1978)

$$\{\{F,G\},H\}+\{\{G,H\},F\}+\{\{H,F\},G\}=0. \tag{4.2}$$

Phase space functions commute with respect to simple multiplication. Therefore we cannot use the CBH formulae immediately. The classical analogue of the quantum commutator $[A,B]$ being the PB $\{F,G\}$ of two phase space functions F and G, the obviously useful analogue of the quantum operator $\hat{A}$ is the differential operator $\hat{F}$, a so-called Hamiltonian vector field:

$$\hat{F}=\sum_{k=1}^{d}\left(\frac{\partial F}{\partial q_k}\frac{\partial}{\partial p_k}-\frac{\partial F}{\partial p_k}\frac{\partial}{\partial q_k}\right) \tag{4.3}$$

acting on other phase space functions

$$\hat{F}G=\{F,G\}. \tag{4.4}$$

Vector fields are linear differential operators that do not commute generally. Defining $H=\{F,G\}$ for the moment and using the Jacobi identity (4.2) gives

$$\hat{H}K=\{\{F,G\},K\}=\hat{F}[\hat{G}K]-\hat{G}[\hat{F}K] \tag{4.5}$$

for all smooth functions K. Therefore

$$H=\{F,G\}\Rightarrow\hat{H}=[\hat{F},\hat{G}] \tag{4.6}$$

$[\hat{F},\hat{G}]$ denoting the commutator of the vector fields $\hat{F}$ and $\hat{G}$.

Now we look at the physical prototype of a Hamiltonian vector field: the vector field of the Hamiltonian $H(p,q)$ of a dynamical system. The time evolution of a phase space function $F(p,q)$ under the flow generated by H fulfils the differential equations (Arnol'd 1978)

$$\dot{F}=-\{H,F\}=-\hat{H}F. \tag{4.7}$$

For example, we get the Hamilton equations for the canonical coordinates

$$\begin{aligned}\dot{q}_k &= -\{H, q_k\} = \partial H/\partial p_k \\ \dot{p}_k &= -\{H, p_k\} = -\partial H/\partial q_k.\end{aligned} \tag{4.8}$$

For time-independent H we integrate (4.7) to give

$$F(t) = \exp(-\hat{H}t)F(0). \tag{4.9}$$

Since F has no explicit time dependence it changes only because its arguments p and q change in time and we get

$$\begin{aligned}\exp(-\hat{H}t)F(p(0), q(0)) &= F(p(t), q(t)) \\ &= F[\exp(-\hat{H}t)p(0), \exp(-\hat{H}t)q(0)].\end{aligned} \tag{4.10}$$

This should be compared with (3.8). For fixed t, (4.9) defines a symplectic classical map which should be compared with the unitary quantum map (3.1).

As in § 2 we now investigate the composition of maps, $V(p, q)$ being another phase space function and $\hat{V}$ the corresponding Hamiltonian vector field. Then we define the map

$$F_{n+1} = \exp(-t\hat{H}) \exp(-s\hat{V})F_n. \tag{4.11}$$

As in (3.2), H is the Hamiltonian of the unperturbed system and sV is the perturbation kicked in at times nt. As in § 2 we now construct an effective infinitesimal generator and the corresponding effective Hamiltonian vector field with the following property:

$$\exp(-\hat{H}_{\text{eff}}) = \exp(-t\hat{H}) \exp(-s\hat{V}). \tag{4.12}$$

Before we can use the CBH formula (2.7′) we have to define adjoint vector fields acting on vector fields in the obvious way

$$\tilde{\hat{F}}\hat{G} = [\hat{F}, \hat{G}]. \tag{4.13}$$

Again the Jacobi identity is fulfilled. We rewrite (4.6) and as in (4.5) we deduce

$$H = \hat{F}G \Rightarrow \hat{H} = \tilde{\hat{F}}\hat{G} = [\hat{F}, \hat{G}] \Rightarrow \tilde{H} = [\tilde{F}, \tilde{G}]. \tag{4.14}$$

Now we can use the CBH formula and find

$$\hat{H}_{\text{eff}} = t\hat{H} + \int_0^1 \mathrm{d}r\, g[\exp(rs\tilde{V}) \exp(t\tilde{H})]s\hat{V}. \tag{4.15}$$

The final question is whether $\hat{H}_{\text{eff}}$ is a Hamiltonian vector field. Formally we define the effective Hamiltonian

$$H_{\text{eff}}(p, q) = tH(p, q) + \int_0^1 \mathrm{d}r\, g[\exp(rs\hat{V}) \exp(t\hat{H})]sV(p, q) \tag{4.16}$$

$$H_{\text{eff}}(p, q) = sV(p, q) + \int_0^1 \mathrm{d}r\, g[\exp(-rt\hat{H}) \exp(-s\hat{V})]tH(p, q). \tag{4.16′}$$

Equation(4.14) guarantees the validity of the adjoint equation (4.15) if $H_{\text{eff}}(p, q)$ given by (4.16) exists. Otherwise, (4.16) should be read as a formula to generate an expansion in powers of s and t, the CBH expansion. The adjoint expansion can then formally be resummed to give (4.15). In this sense $\hat{H}_{\text{eff}}$ is the Hamiltonian vector field belonging

to $H_{\text{eff}}(p, q)$. $H_{\text{eff}}(p, q)$ is the infinitesimal generator of the map (4.11) and of course it is invariant under the map

$$\exp(-\hat{H}_{\text{eff}})H_{\text{eff}}(p, q) \equiv 0.$$

Using (4.10) this can be written in the form

$$H_{\text{eff}}(\exp(-t\hat{H})\exp(-s\hat{V})p, \exp(-t\hat{H})\exp(-s\hat{V})q) = H_{\text{eff}}(p, q) \tag{4.17}$$

for fixed s and t. If H_{eff} given by (4.16) does not exist as an analytic function then the CBH expansion in powers of s and t is invariant under the map (4.11).

Finally we state the analogue of (3.5). Supposing $\hat{V}\hat{H}^n V = 0$ for all n we get

$$H_{\text{eff}} = tH + t\hat{H}(\exp(t\hat{H}) - 1)^{-1} sV. \tag{4.18}$$

5. The classical limit of quantum maps

When comparing the last two sections we notice a correspondence between several quantities and formulae. The role of a classical Hamiltonian vector field $\hat{F}(p, q)$ is played by the adjoint quantum operator $-(\mathrm{i}/\hbar)\hat{F}$ leading to the well known correspondence

$$\{F, G\} \triangleq -(\mathrm{i}/\hbar)[F, G]. \tag{5.1}$$

With respect to this 'commutator' the classical functions $F(p, q)$ and $G(p, q)$ do not commute and the CBH formula (4.16) is a consequence of this.

Formally the classical (4.16) and the quantum (3.4) CBH formulae are identical (after making the identification (5.1)), but (3.4) contains more information (higher powers in $\hbar$) which cannot be restored from (4.16) by a unique quantisation prescription as simple examples show. This is reminiscent of the situation in the quantisation of normal forms (Wood and Ali 1987).

Although the validity of the CBH formula may be lost by resonances via small denominators in the classical as well as in the quantum case, it is always possible to associate an effective Hamilton operator with the unitary operator

$$U = \exp\left(\frac{\mathrm{i}}{\hbar} Ht\right)\exp\left(\frac{\mathrm{i}}{\hbar} Vs\right) = \int_0^{2\pi} \mathrm{d}\phi \exp(\mathrm{i}\phi)\rho(\phi)|\phi\rangle\langle\phi| \tag{5.2}$$

such that the phases ϕ become the energies of H_{eff}. We obviously have

$$H_{\text{eff}} = \frac{\hbar}{\mathrm{i}} \ln U = \int_0^{2\pi} \mathrm{d}\phi\, \hbar(\phi + 2\pi n(\phi))\rho(\phi)|\phi\rangle\langle\phi| \tag{5.3}$$

with arbitrary integers $n(\phi) = \mathrm{O}(1/\hbar)$ and spectral density $\rho(\phi)$. For an arbitrary choice of the phases $n(\phi)$, H_{eff} will not have a smooth classical limit. One possibility of choosing the $n(\phi)$ would be by analytic continuation starting with $H_{\text{eff}}(s = 0, t) = tH$ and increasing s. But this is not possible in general because H_{eff} is not analytic in both t and s as simple examples with discrete spectra show (Reed and Simon 1978). The reason lies in resonance phenomena called avoided level crossings that show up when two nearly degenerate eigenfunctions of $U(s, t)$ (or of $H(s, t) = tH + sV$) are strongly coupled by the perturbation V. This complicates the structure of their Wigner functions. The classical route into chaos is accompanied by 'overlapping' avoided level crossings coupling $\mathrm{O}(1/\hbar)$ or more eigenfunctions on the energy shell leading to more and more

'irregular' eigenfunctions that cannot be approximated by semiclassical quantisation procedures. The criterion of Hose and Taylor (1983) gives a first hint how to construct the quantum numbers $n(\phi)$ for nearly integrable (i.e. weakly perturbed) cases. For strongly perturbed dynamics 'good quantum numbers' may only exist for parts of the spectrum.

The given arguments show that even the last integral H_{eff} of a kicked dynamics may be lost in the classical limit, in contrast to autonomous dynamics, where the Hamiltonian $H(p, q)$ is always a global single-valued analytic integral of motion. This clearly shows that integrable autonomous dynamics with one degree of freedom can become non-integrable through periodically kicked perturbations: H, the last and only integral of the motion is lost, first locally near hyperbolic orbits, and globally for stronger perturbations.

6. An integrable example

First we want to show the power of the CBH formula for integrable systems. We choose $d=1$, $s=\alpha$, $t=\beta$, $H=p$ and $V(q)=V(q+2\pi)$ leading to the vector fields

$$\hat{H}=-\frac{\partial}{\partial q}=\hat{p} \qquad \hat{V}=V'(q)\frac{\partial}{\partial p}=V'(q)\hat{q}. \tag{6.1}$$

This generates the map

$$\begin{pmatrix}p\\q\end{pmatrix}\to\exp\left(\beta\frac{\partial}{\partial q}\right)\exp\left(-\alpha V'(q)\frac{\partial}{\partial p}\right)\begin{pmatrix}p\\q\end{pmatrix}=\begin{pmatrix}p-\alpha V'(q+\beta)\\q+\beta\end{pmatrix}. \tag{6.2}$$

This map has been investigated by Grempel *et al* (1982) and by Berry (1984). The vector fields $\hat{H}$ and $\hat{V}$ fulfil the condition $\hat{V}\hat{H}^n V=0$ for all n and with (4.18) we find

$$H_{\text{eff}}(p, q)=\beta p+\beta\hat{p}[\exp(\beta\hat{p})-1]^{-1}\alpha V(q). \tag{6.3}$$

After Fourier expansion of $V(q)$

$$V(q)=\operatorname{Re}\left(\sum_{m=1}^{\infty}c_m\exp(\mathrm{i}mq)\right) \qquad (c_m\in\mathbb{C}) \tag{6.4}$$

and noticing

$$f(\hat{p})\exp(\mathrm{i}mq)=f(-\mathrm{i}m)\exp(\mathrm{i}mq) \tag{6.5}$$

we get for the effective Hamiltonian

$$H_{\text{eff}}=\beta p+\tfrac{1}{2}\alpha\beta\operatorname{Re}\left(\sum_{m=1}^{\infty}mc_m\exp[\mathrm{i}m(q+\beta/2)]/\sin(m\beta/2)\right). \tag{6.6}$$

First we want to check that the integration of the Hamiltonian flow generated by H_{eff} from $t=0$ to $t=1$ leads to the map (6.2):

$$\begin{aligned}\dot{q}&=\frac{\partial}{\partial p}H_{\text{eff}}=\beta\\ \dot{p}&=-\frac{\partial}{\partial q}H_{\text{eff}}.\end{aligned} \tag{6.7}$$

Integration gives

$$\begin{aligned} q_{n+1} &= q_n + \beta \\ H_{\text{eff}}(p_{n+1}, q_{n+1}) &= H_{\text{eff}}(p_n, q_n) \end{aligned} \tag{6.8}$$

and finally from the last equation

$$p_{n+1} - p_n = -\alpha \frac{\partial}{\partial q_{n+1}} V(q_{n+1}) \tag{6.9}$$

which is equivalent to the map (6.2).

Obviously H_{eff} given by (6.6) is destroyed by resonances at $m\beta = 2\pi n$ if $c_m \neq 0$. But even then formula (6.6) still can be used to construct the invariant curves for the resonant map taken at the resonant value $\beta_0 = 2\pi n_0 / m_0$ with n_0 and m_0 relatively prime. The rescaled H_{eff} is an integral of the map (6.2), too:

$$I = \lim_{\beta \to \beta_0} H_{\text{eff}} \sin(\beta m_0/2) = \alpha \pi n_0 \operatorname{Re}\left(\sum_{\mu=1}^{\infty} c_{\mu m_0} \exp[\mathrm{i}\mu(m_0 q + n_0 \pi)] \right). \tag{6.10}$$

This involves only q and we see that the invariant sets are systems of lines parallel to the p axis.

Now look at the corresponding effective Hamiltonian of the quantum map. As in the classical case the condition $\hat{V}\hat{H}^n V = 0$ is fulfilled and with (3.5) we find

$$H_{\text{eff}} = \beta p - \frac{\mathrm{i}}{\hbar} \beta \hat{p} \left[\exp\left(-\frac{\mathrm{i}}{\hbar} \hat{p} \right) - 1 \right]^{-1} \alpha V. \tag{6.11}$$

Since no products of p and q remain in the formula, there are no ordering problems. Therefore (6.6) is true for the quantum case, too. In q representation we get for non-resonant and non-vanishing β:

$$H_{\text{eff}} = -\mathrm{i}\hbar\beta \frac{\partial}{\partial q} + \tfrac{1}{2}\alpha\beta \operatorname{Re}\left(\sum_{m=1}^{\infty} m c_m \exp[\mathrm{i}m(q + \beta/2)] / \sin(m\beta/2) \right). \tag{6.12}$$

The eigenfunctions of H_{eff} are Bloch waves with wavevector K

$$\begin{aligned} H_{\text{eff}} \psi_n(q, K) &= E_n(K) \psi_n(q, K) \\ \psi_n(q, K) &= \exp(\mathrm{i}Kq) u_n(q, K) \end{aligned} \tag{6.13}$$

with the 2π-periodic function $u_n(q, K) = u_n(q + 2\pi, K)$. Solving the eigenvalue equation leads to

$$\begin{aligned} u_n(q, K) &= c \exp\left(\frac{\mathrm{i}}{\hbar\beta} (q[E_n(K) - \beta\hbar K] + v(q)) \right) \\ v(q) &= -\tfrac{1}{2}\alpha\beta \operatorname{Im}\left(\sum_{m=1}^{\infty} c_m \exp(\mathrm{i}m\beta/2)[\exp(\mathrm{i}mq) - 1] / \sin(m\beta/2) \right). \end{aligned} \tag{6.14}$$

The periodicity of u_n implies the quantisation condition

$$E_n(K) = \beta\hbar(n + K) \qquad n \text{ integer.} \tag{6.15}$$

By the method of stationary phases one can show for $\hbar \to 0$ that the eigenfunctions are localised along the classical integral curves for the given quantised energy $E_n(K) = H_{\text{eff}}(p, q)$. For a given wavevector K the spectrum of the quasi-energy $\varphi_n(K) \equiv E_n(K)/\hbar \pmod{2\pi}$ is dense in $[0, 2\pi)$ if β/π is irrational. Because of the localisation

of the eigenfunctions along the integral curves only $O(1/\sqrt{\hbar})$ eigenfunctions are appreciably excited by a coherent state $|p, q\rangle$ in the semiclassical limit. This is in contrast with the case of non-integrable strongly chaotic maps where the number of excited 'irregular' eigenfunctions is $O(1/\hbar)$ (Haake *et al* 1987a).

7. A non-integrable example

Replacing p by $p^2/2$ in the unperturbed Hamiltonian of the last section's example we get the so-called kicked rotator (Casati *et al* 1979) which leads to a non-integrable map

$$\hat{H} = -\frac{\partial H}{\partial p}\frac{\partial}{\partial q} = -p\frac{\partial}{\partial q} \qquad \hat{V} = V'(q)\frac{\partial}{\partial p} \tag{7.1}$$

$$\begin{pmatrix} p \\ q \end{pmatrix} \to \exp\left(\beta p \frac{\partial}{\partial q}\right) \exp\left(-\alpha V'(q)\frac{\partial}{\partial p}\right)\begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} p - \alpha V'(q+\beta p) \\ q + \beta p \end{pmatrix}. \tag{7.2}$$

$\hat{H}$ and $\hat{V}$ do not fulfil any of the simplifying conditions mentioned at the end of § 2. The iterated Poisson brackets of $p^2/2$ and $V(q)$ generate products of higher and higher powers of p and q as soon as $V'(q)$ is non-linear. In general then there is no possibility of evaluating the CBH formula immediately and one has to calculate the CBH expansion and try to resum it.

Previous investigations tried to calculate the CBH expansion with the help of computer algebraic programs in the most general form (Richtmyer and Greenspan 1965). But then the calculation of the iterated Poisson brackets is still left, and if they do not show any simple building law, as is usually the case, for this evaluation one has to use the computer once again. Therefore it is reasonable to calculate the CBH expansion in one step. This section shows how to do that for a simple non-integrable classical example.

The formulae to start with are (4.16) or (4.16'). With the definition of $g(z)$ after (2.7) formula (4.16) can be expanded in the form

$$H_{\text{eff}} = tH + \sum_{n=0}^{\infty} \frac{1}{n+1} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \int_0^1 \mathrm{d}r [\exp(rs\hat{V}) \exp(t\hat{H})]^k sV. \tag{7.3}$$

Sums and integrals have been interchanged because (7.3) will be evaluated only asymptotically for $s, t \to 0$. The expression under the integral is nothing but a k-fold map acting on V. Therefore H_{eff} can be calculated up to a wanted power in s and t by calculating the mapped V up to the required accuracy. This is a straightforward computer algebraic job.

As an example I choose the dynamics of a kicked top (Haake *et al* 1987b) with

$$H = L_y^2/2 \qquad V = L_x^2/2 \tag{7.4}$$

with the components of the angular momentum vector $\boldsymbol{L}$ fulfilling the PB relations

$$\{L_x, L_y\} = L_z \qquad \text{and cyclically in } x, y \text{ and } z. \tag{7.5}$$

One might make this Poissonian structure to a symplectic structure. First we notice from (7.5) that the scalar $\boldsymbol{L}^2 = L_x^2 + L_y^2 + L_z^2$ is unchanged under a Lie transformation generated by any function of $\boldsymbol{L}$, because $\{\boldsymbol{L}^2, \boldsymbol{L}\} \equiv (0, 0, 0)$. So we might choose $\boldsymbol{L}^2 = 1$. For reasons of convenience we write x instead of L_x, etc. Finally we introduce the polar angle ϕ by expressing x, y, z in polar coordinates: $x + \mathrm{i}y = (1 - z^2)^{1/2} \exp(\mathrm{i}\phi)$.

States of the system are thus represented by points on the unit sphere. Defining the PB in the canonical way by identifying ϕ as the angle and z as the action variable we can reproduce the Poissonian structure (7.5): $\{x, y\} = z$ (and cyclically). Actually for calculating H_{eff} only the Poissonian structure is needed and several symplectic structures leading to the same Poissonian structure give the same result.

Coming back to the non-integrable example, we put it in the form

$$\exp(-\varepsilon \hat{H}_{\text{eff}}) = \exp(-\varepsilon t \hat{H}) \exp(-\varepsilon \hat{V}) = \exp(-\varepsilon t y \hat{y}) \exp(-\varepsilon x \hat{x}). \tag{7.6}$$

This generates the map $(x, y, z) \to (x', y', z')$

$$\begin{aligned} x' &= \bar{x} \\ y' &= \bar{y} \cos(\varepsilon \bar{x}) - \bar{z} \sin(\varepsilon \bar{x}) \\ z' &= \bar{z} \cos(\varepsilon \bar{x}) + \bar{y} \sin(\varepsilon \bar{x}) \end{aligned} \tag{7.7}$$

with

$$\begin{aligned} \bar{x} &= x \cos(\varepsilon t y) + z \sin(\varepsilon t y) \\ \bar{y} &= y \\ \bar{z} &= z \cos(\varepsilon t y) - x \sin(\varepsilon t y). \end{aligned}$$

We want to calculate H_{eff} only for $t = 1$ but to do this we need the map (7.7) for $t \in [0, 1]$. With the definition (7.4) of H and V (4.16′) gives

$$H_{\text{eff}} = \tfrac{1}{2} x^2 + \int_0^1 \mathrm{d}t \, g[\exp(-\varepsilon t \hat{H}) \exp(-\varepsilon \hat{V})] \tfrac{1}{2} y^2. \tag{7.8}$$

$$H_{\text{eff}} = \tfrac{1}{2} x^2 + \sum_{n=0}^{\infty} \frac{(-1)^n}{n+1} \int_0^1 \mathrm{d}t [\exp(-\varepsilon t \hat{H}) \exp(-\varepsilon \hat{V}) - 1]^n \tfrac{1}{2} y^2. \tag{7.9}$$

To calculate H_{eff} up to Nth order in ε we only have to take the Taylor expansion of sin and cos in (7.7) up to Nth order. The n-fold iteration of this truncated map acting on y can be calculated by the computer and will be named

$$y_n(\varepsilon, t) = [\exp(-\varepsilon t \hat{H}) \exp(-\varepsilon \hat{V})]^n y + \mathrm{O}(\varepsilon^{N+1}). \tag{7.10}$$

From (7.9) we see that we only have to sum up for $n \leqslant N$

$$H_{\text{eff}} = \tfrac{1}{2} x^2 + \tfrac{1}{2} \sum_{n=0}^{N} \frac{1}{n+1} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \int_0^1 \mathrm{d}t \, y_n^2(t, \varepsilon) + \mathrm{O}(\varepsilon^{N+1}). \tag{7.11}$$

The expression on the right-hand side has been summed up by REDUCE for $N = 7$. The first few terms are

$$\begin{aligned} H_{\text{eff}} = {} & \tfrac{1}{2}(x^2 + y^2) + \tfrac{1}{2} \varepsilon x y z + \tfrac{1}{12} \varepsilon^2 (x^4 - x^2 + 4x^2 y^2 + y^4 - y^2) \\ & + \tfrac{1}{12} \varepsilon^3 (1 - 2x^2 - 2y^2) x y z + \mathrm{O}(\varepsilon^4). \end{aligned} \tag{7.12}$$

Figures 1-4 allow us to compare the integral curves $H_{\text{eff}} = \text{constant}$ with the map (7.7). Two different views of the unit sphere are shown: one of the northern hemisphere $z \geqslant 0$ projected on the xy plane and one from the equator for $x \geqslant 0$ projected on the yz plane. For $\varepsilon < 2$ the two poles $z = \pm 1$ are elliptic fixed points and the CBH expansion gives quite reasonable results in their vicinity. For $\varepsilon > 2$ these poles are hyperbolic fixed points and the CBH expansion in their vicinities breaks down although around

the four elliptic fixed points on the equator (only one is fully visible) the approximation is still useful even for $\varepsilon > 2$.

8. Discussion

The main result of this paper is that the Campbell-Baker-Hausdorff (CBH) formula allows an asymptotic expansion for an approximate integral of non-integrable maps—classical as well as quantum.

In the classical case several situations have to be distinguished.

If the map has elliptic fixed points surrounded by regions of regular motion the CBH formula allows the construction of an effective Hamiltonian H_{eff}. This Hamiltonian generates a flow which, after integration for integer times, resembles the original map in the vicinity of the elliptic fixed points. Therefore H_{eff} not only gives the approximate integral curves but also allows us to calculate winding numbers.

If the map has elliptic n-cycles ($n > 1$) or jumps between unconnected integral curves, no effective Hamiltonian exists. But as the integrable example in § 6 shows, the CBH formula might still give an (approximate) integral of the map.

If the map is nearly integrable the CBH formula gives an approximate integral that can be used to calculate the separatrices connecting hyperbolic orbits along which the chaos starts to show up (cf figure 1(b)).

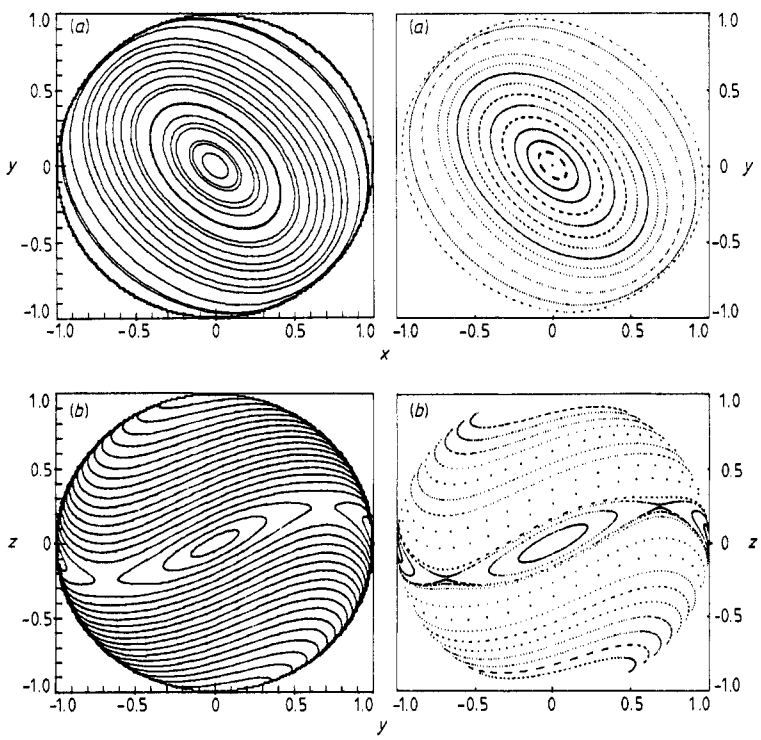

Figure 1. Lines of constant H_{eff} given by the CBH expansion (7.12) up to $O(\varepsilon^7)$ (LHS) compared with classical iteration (7.7) (RHS) for (a) $\varepsilon = 1$ on the northern hemisphere ($z > 0$) and (b) around the equator ($x > 0$). Note that the CBH expansion is globally reliable in this nearly integrable case.

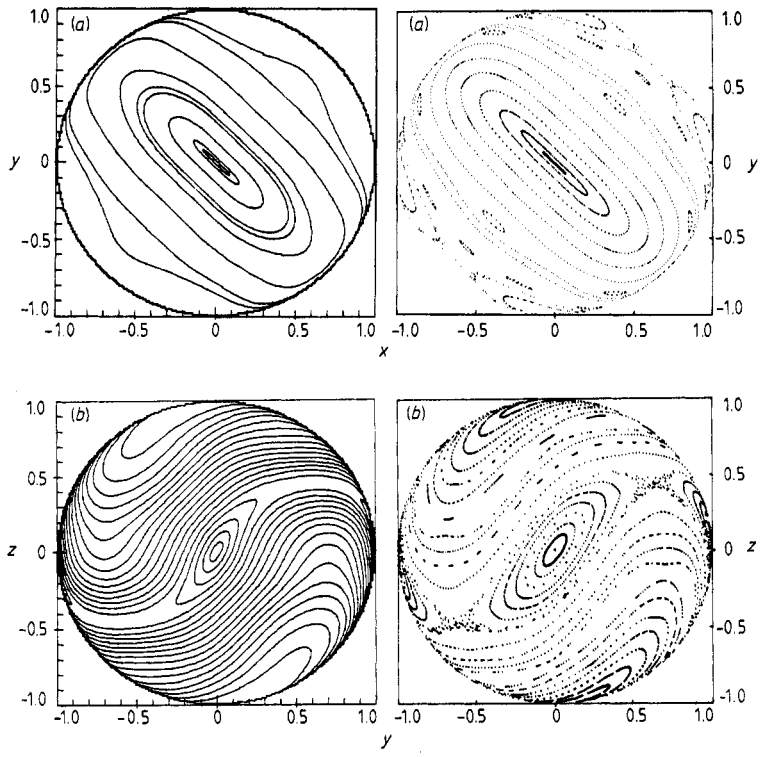

Figure 2. The same as figure 1 for $\varepsilon = 2$. Note that the CBH expansion still faithfully reproduces all regular structures, even though the elliptic fixed points at the poles $z = \pm 1$ are now just marginally stable.

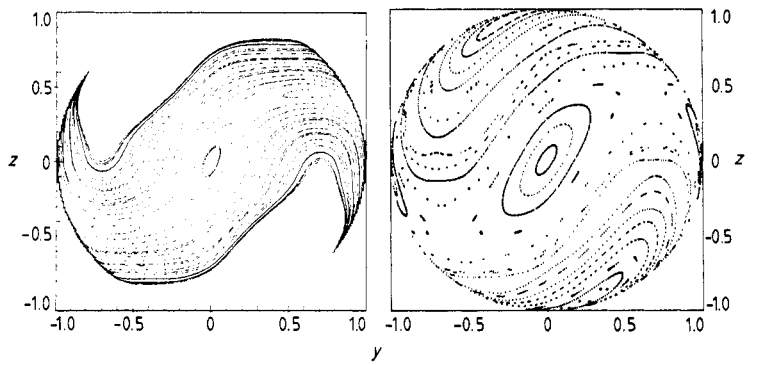

Figure 3. Lines of constant $H_{\text{eff}}(p, q)$ given by the CBH expansion (7.12) up to $O(\varepsilon^7)$ (LHS) compared with classical iteration (7.7) (RHS) for $\varepsilon = 2.1$ around the equator ($x > 0$). In contrast to the now chaotic behaviour of the iteration near the poles the equatorial behaviour is still dominantly regular and well represented by the CBH expansion.

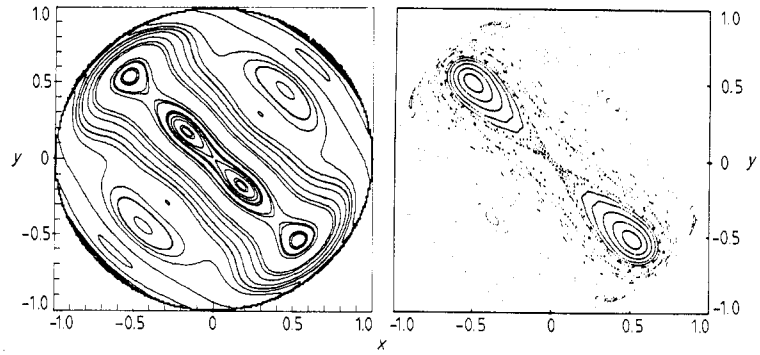

Figure 4. The same as figure 3 but for $\epsilon = 2.5$ on the northern hemisphere ($z > 0$). With the last KAM trajectory between the poles destroyed, the CBH expansion bears little resemblance to the exact dynamics. Only symmetries are respected and the most prominent regular islands are recognisable from the H_{eff} curves.

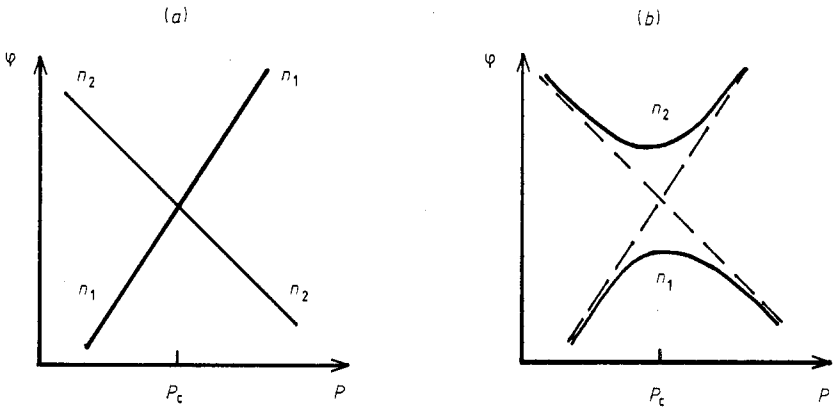

Figure 5. Dependence of two representative eigenenergies $E_j = \hbar[\phi_j(P) + 2\pi n_j]$ ($j = 1, 2$) of the effective Hamilton operator upon a perturbation parameter P near an (avoided) degeneracy: (a) for an integrable case showing level crossing (the n_j of the spectrum are chosen in such a way that H_{eff} possesses a smooth classical limit); (b) for a nearly integrable case showing avoided level crossings (the energies are determined by analytic continuation). The results are different thereby illustrating the non-existence of a smooth classical limit for phase choices of the form (b) in contrast to figure 1.

For non-integrable maps like the one presented in figures 1–4 the CBH expansion can at best be asymptotic and, as numerical evidence shows, it actually is. As is typical for asymptotic expansions there is an optimal choice for the order of the expansion depending on the parameters and on the phase space region to be approximated. For strongly chaotic maps the approximations fail badly.

In the quantum case an effective Hamilton operator for the map always exists as was shown in § 5. But there are eigenvalue ambiguities. The CBH expansion resolves these ambiguities in such a way that the eigenvalues are given by analytic continuation upon increasing the perturbation. Actually the CBH expansion fails at avoided level crossings where the eigenphases of H_{eff} have to jump in order to allow a smooth classical limit for stronger perturbations (see figure 5). But this failure only concerns

that part of the Hilbert space which is involved in avoided level crossings. (Further details will be published in Scharf (1988).)

As a conclusion I make some general remarks. The CBH formula was constructed for 'A and B sufficiently close to 0'. This restriction has been shown to be important for integrable as well as non-integrable kicked dynamics. For integrable ones it might happen that there actually is no H_{eff} at localised resonances, as the example in § 6 has shown. The investigation of other kicked dynamics along the lines just presented is straightforward.

The big advantage in investigating symplectic maps via the CBH expansion is we have non-commutativity of the generators only with respect of the Lie product. After calculating the PB no ordering problems exist and expansions become comparatively easy to resum. When calculating H_{eff} in the quantum case this advantage is lost and one has to run the calculations with non-commuting quantities (and of course with the exact quantum map). This exceeds the computer capacity much earlier than the corresponding classical calculations. But if one is only interested in the semi-classical correction, i.e. terms of $O(\hbar)$, again this is simple to manage.

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