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Quantum maps, adiabatic invariance and the semiclassical limit

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Abstract. An exact adiabatic invariance principle for quantum maps acting in an (effectively) finite-dimensional Hilbert space is derived and is used to construct effective Hamilton operators which generate the corresponding maps. It is shown that for classically non-integrable quantum maps these effective Hamilton operators do not possess any smooth classical limit even for the nearly integrable case. The equivalence of the effective Hamilton operators given by adiabatic switching and by the quantum Campbell-Baker-Hausdorff formula is proved. Moreover a diabatic invariance principle is formulated that leads to effective Hamilton operators with a smooth classical limit for nearly integrable dynamics via 'slipping over resonances'. These effective Hamiltonians are compared with the Hamiltonians given by the classical Campbell-Baker-Hausdorff formula. It is explained how the last integral of quantum maps—the effective Hamilton operator—is destroyed in the classical limit.

1. Introduction

Kicked Hamiltonian quantum dynamics (or quantum maps) with finite-dimensional Hilbert space are integrable even if their classical limit, a kicked classical dynamics, is not. The quantum dynamics can be 'integrated' by solving the eigenvalue problem (i.e. by diagonalisation) which is only an algebraic procedure. The classical counterpart of this procedure would be to find a canonical transformation that puts the map in normal form locally: after a suitable choice of canonical coordinates (I, φ) the map would then act as a twist map in the vicinity of fixed points $(\varphi \to \varphi + \omega(I),\ I \to I)$. (See, for example, Eckhardt (1986) for classical and quantum normal forms.) Generically this strategy fails because the construction of the appropriate canonical transformation is plagued by resonances in the form of small denominators. Kicked classical dynamics are non-integrable generically and no smooth canonical transformation can make them look like twist maps, even locally. But there is hope left that the 'smooth parts' of the phase space, containing only a negligible measure of chaotic trajectories, may be smoothly approximated with the help of a perturbative procedure (Izrailev and Sokolov 1985). The Campbell-Baker-Hausdorff expansion (Scharf 1988) is a recent example. It allows for a straightforward construction of an approximate integral of the map.

As kicked quantum maps with finite-dimensional Hilbert space are integrable the question arises whether there exists some adiabatic invariance that allows the comparison of different quantum maps, that evolve smoothly into each other by increasing a perturbation parameter adiabatically. For autonomous dynamics, classical as well

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as quantum, some interesting features of adiabatic switching are well known; for example, Berry's phase accompanying adiabatic changes in quantum systems (Berry 1984a) and the possibility of adiabatic semiclassical quantisation when Einstein-Brillouin-Keller quantisation fails (Reinhardt and Dana 1987). It is known that the adiabatic and semiclassical limits do not commute when avoided degeneracies of (quasi) energy levels show up in the course of the adiabatic switching (Berry 1984b). These avoided degeneracies or avoided level crossings result from tunnelling between eigenfunctions that are either (i) exponentially localised in phase space leading to a tunnel splitting of the order $\exp(-1/\hbar)$ in the semiclassical limit or (ii) delocalised along chaotic regions in phase space leading to a much stronger splitting of the order $\hbar^f$, which is comparable to the mean level spacing of a system with f degrees of freedom. While (i) can happen for all quantum dynamics, (ii) is typical for quantum dynamics with a chaotic classical limit showing trajectories that cover appreciable parts of the (compact) energy surface. For quantum dynamics with a non-integrable classical limit near-degeneracies of the type (ii) are the rule rather than the exception. Therefore it is a big surprise that adiabatic semiclassical quantisation works so well for these dynamics. A possible explanation is that if the adiabatic process is slow compared to the frequencies occurring in the dynamics but fast enough to 'slip over' the chaotic regions then the non-adiabatic influence of the chaos is negligible (Berry 1984b) and semiclassical quantisation still gives good results (Reinhardt and Dana 1987). The question arises as to what corresponds to the slipping over narrow classical chaotic regions in the case of switching of a quantum dynamics. It will be shown to be jumping over avoided level crossings.

Adiabatic switching was used in investigating a kicked classical dynamics, the standard map (Dana and Reinhardt 1987). It was shown up to second order in the kicking parameter that tori adiabatically evolving out of KAM tori are KAM tori, too. As the map is area preserving, even during the adiabatic process, families of KAM tori with the same action are constructed. A semiclassical quantisation procedure follows straightforwardly.

In this paper I will show that there exists an exact adiabatic principle for kicked quantum maps with finite-dimensional Hilbert space (or a finite-dimensional part of the Hilbert space being of practical relevance for physical initial conditions): it is possible to generate the eigenstates of one quantum map out of the eigenstates of another one by adiabatic switching between the two maps and acting on the initial eigenstates with the corresponding propagators successively. This adiabatic switching is equivalent to analytical continuation of the quasienergies and eigenstates of the kicked dynamics upon increasing a real perturbation parameter (for example, the kick strength). Moreover this is shown to be equivalent to constructing an effective Hamilton operator for the kicked quantum dynamics with the help of the Campbell-Baker-Hausdorff formula (Scharf 1988). As soon as avoided level crossings show up in the spectra the so-constructed effective Hamilton operators do not possess a smooth classical limit. The mentioned slipping over the chaotic regions in the classical case of adiabatic switching is shown to have its quantum analogue in jumping over avoided level crossings (Noid *et al* 1983) leading now to effective Hamilton operators that do possess smooth (approximate) effective Hamiltonians as their classical limit in the case of nearly integrable maps. This non-adiabatic switching (which will be called diabatic in the following) with jumping over avoided level crossings gives reasonable results for eigenvalues and eigenvectors of the unitary propagator of the quantum map only far away from the avoided level crossings. A necessary condition for that is that the

level splitting of the near-degeneracies is much smaller than the mean level spacing. As soon as a finite part of the eigenfunctions are coupled strongly by the kick and therefore show strong level repulsion the jumping over fails. This is just the case for kicked dynamics with a strongly non-integrable classical limit. Their spectra show level spacings following one of three universal distributions with linear, quadratic or quartic level repulsion (depending on their antiunitary symmetries) on a scale of the mean level spacing (Robnik and Berry 1986, Scharf *et al* 1988).

As the exact adiabatic switching presupposes a switching frequency small compared to all frequencies occurring in the quantum map, problems show up especially for weakly perturbed maps with a nearly integrable classical limit. As already mentioned in this case quasienergies can come very close ($\Delta E \sim \exp(-1/\hbar)$) leading to extremely small frequencies. In contrast to that the adiabatic switching of the classical map works especially well in the nearly integrable case as does the diabatic switching of the quantum map. In practical calculations for the quantum map one always does diabatic switching, not taking into account the exponentially small near-degeneracies but jumping over them.

There are two timescales for the changing of the parameters that must be well separated in the case of successfully applying diabatic switching. The changing of the parameters must be slow enough to be adiabatic in the smooth regions of the classical phase space or to follow the eigenvalues and eigenvectors, changing slowly with the parameters far away from avoided level crossings. But on the other hand it must be fast enough to slip over narrow chaotic regions or avoided level crossings, respectively, to minimise their (non-adiabatic) influence.

2. Level dynamics and analytic continuation

Following an idea of Pechukas (1983) and Yukawa (1985) I write the equations of motion for the eigenvectors and eigenvalues of a perturbed quantum map with respect to the perturbation parameter K. The unitary operator that generates the quantum map will be chosen in the form

$$U(K) = U(0)\exp(\mathrm{i}KV/\hbar) = \exp(\mathrm{i}H_0/\hbar)\exp(\mathrm{i}KV/\hbar) \tag{2.1}$$

with the parts $U(0)$ and $\exp(\mathrm{i}KV/\hbar)$ generating maps which possess integrable classical limits. K is a real perturbation parameter and V the perturbation potential. $U(K)$ is acting in a d-dimensional Hilbert space. The eigenvalue problem of $U(K)$ will be written as

$$U(K)|\varphi_n(K)\rangle = \exp(\mathrm{i}\varphi_n(K))|\varphi_n(K)\rangle \qquad n = 1, \ldots, d. \tag{2.2}$$

The change of $\varphi_n(K)$ and $|\varphi_n(K)\rangle$ with K can be written in the form of equations of motion for an integrable many-particle system on a circle with repulsive two-particle interactions and internal degrees of freedom. It is conveniently called 'generalised Sutherland-Moser dynamics' (Kuś *et al* 1987, Nakamura and Mikeska 1987). First we look at the change of eigenvectors and eigenvalues upon increasing K, which will from now on be called level dynamics:

$$\begin{aligned}
|\varphi_n(K+\delta K)\rangle &= |\varphi_n(K)\rangle + \delta K|\psi_n(K)\rangle + \mathrm{O}(\delta K^2) \\
|\psi_n(K)\rangle &= \sum_{m\neq n} \frac{\mathrm{i}V_{mn}(K)/\hbar}{\exp[\mathrm{i}(\varphi_n-\varphi_m)]-1}|\varphi_m(K)\rangle \\
\varphi_n(K+\delta K) &= \varphi_n(K) + \delta K V_{nn}(K)/\hbar + \mathrm{O}(\delta K^2)
\end{aligned} \tag{2.3}$$

with $V_{mn}(K)=\langle\varphi_m(K)|V|\varphi_n(K)\rangle$. Starting at $K_0=0$ equation (2.3) can be used to determine the $|\varphi_n(K)\rangle$ in a given representation; for example, the one spanned by the states $|\varphi_n(K_0)\rangle$. For non-vanishing couplings $V_{mn}(K)$ in the vicinity of a near-degeneracy $\varphi_m\approx\varphi_n$ the resonant denominator in (2.3) ultimately leads to a repulsion of the eigenphases and inhibits crossing: degeneracies are avoided generically (Berry 1985).

As one of the main objectives of this paper is to construct an effective Hamiltonian $H_{\text{eff}}(K)$ with the property

$$U(K)=\exp[(\mathrm{i}/\hbar)H_{\text{eff}}(K)] \tag{2.4}$$

the first question is how to express $H_{\text{eff}}(K+\delta K)$ in terms of $H_{\text{eff}}(K)$ and V up to first order in δK with the help of the level dynamics. Using (2.3) we write

$$\begin{aligned}H_{\text{eff}}(K+\delta K)&=\sum_{n=1}^{d}\hbar\varphi_n(K+\delta K)|\varphi_n(K+\delta K)\rangle\langle\varphi_n(K+\delta K)|\\&=H_{\text{eff}}(K)+\delta K\sum_{n=1}^{d}V_{nn}(K)|\varphi_n(K)\rangle\langle\varphi_n(K)|\\&\quad+\delta K\sum_{n=1}^{d}\hbar\varphi_n(K)\{|\varphi_n(K)\rangle\langle\psi_n(K)|+\text{HC}\}+\mathrm{O}(\delta K^2)\end{aligned} \tag{2.5}$$

where HC denotes the Hermitian conjugate. Finally we get up to order δK:

$$\langle\varphi_m(K)|H_{\text{eff}}(K+\delta K)|\varphi_n(K)\rangle=\hbar\varphi_n(K)\delta_{nm}+\delta K\frac{\mathrm{i}(\varphi_n(K)-\varphi_m(K))V_{mn}(K)}{\exp[\mathrm{i}(\varphi_n(K)-\varphi_m(K))]-1}. \tag{2.6}$$

For $n=m$ the second term should be replaced by its limit for $\phi_n\to\varphi_m$, i.e. by $\mathrm{i}\delta KV_{nn}(K)$. Integration of the level dynamics (2.3) up to a given K gives the same result as diagonalising $U(K)$. Construction of $H_{\text{eff}}(K)$ with the help of (2.6) means continuation of the phases φ_n, which are then no longer confined to the interval $[0,2\pi)$. This has important consequences for the spectrum of the effective Hamilton operator. For an example look at the unitary operator $\exp(\mathrm{i}KJ_z)$, J_z denoting the z component of the angular momentum operator J with the eigenstates $|j,m\rangle$ $(m=-j,-j+1,\ldots,j)$: $J_z|j,m\rangle=m|j,m\rangle$ and $J^2|j,m\rangle=j(j+1)|j,m\rangle$. Upon increasing K the eigenphases (modulo 2π) of $U(K)$ intersect and continuation of the spectrum with the help of level dynamics leads to the right $H_{\text{eff}}(K)$:

$$H_{\text{eff}}(K)=\hbar KJ_z\qquad\hbar=\mathrm{O}(1/j). \tag{2.7}$$

But look at the slightly different unitary operator

$$U(K,\varepsilon)=\exp(\mathrm{i}\varepsilon H_0/\hbar)\exp(\mathrm{i}KJ_z) \tag{2.8}$$

with H_0 being a non-linear function of the J components and $[H_0,J_z]\neq0$ (for example: $H_0=\hbar(J_x+J_y^2/j)$), and ε arbitrarily small but positive. Now the quantum map given by $U(K,\varepsilon)$ does not possess an integrable classical limit as numerical evidence shows. That means for $\varepsilon>0$ and $K>0$ there does not exist an exact smooth phase-space invariant (although there might be a good approximate invariant for small enough ε). Conservation of J^2 leads to a two-dimensional phase space in the form of a sphere with action $z=\cos\theta$ and angle variable φ (θ,φ denoting polar and azimuthal angle,

respectively) (Haake and Shepelyansky 1988). An additional invariant would imply the integrability of the classical map. In contrast to that the quantum map always possesses an additional integral, H_{eff}. Consequently H_{eff} cannot possess a globally smooth classical limit in the classically non-integrable case.

For $\varepsilon > 0$ upon increasing K the eigenvalues $\exp(i\varphi_n(K))$ of $U(K)$ move around on the unit circle and repel each other as (2.3) shows because of the now non-vanishing couplings V_{mn}. In addition to that there is no mean rotation of the phases upon increasing K as the trace of J_z vanishes. Therefore all phases $\varphi_n(K)$ are clamped to the interval $(-2\pi, 2\pi)$ for arbitrary K, because if one phase moves further than $\pm 2\pi$ it has to push all other phases in positive or negative direction thereby leading to a non-vanishing mean rotation of the phases. Continuation of the phases therefore leads in the limit $\varepsilon \to 0^+$ to an $H_{\text{eff}}(K, 0^+)$ of the form

$$H_{\text{eff}} = \hbar[KJ_z(\text{mod } 4\pi)] = \hbar \sum_{m=-j}^{j} |j, m\rangle\langle j, m|[Km(\text{mod } 4\pi)]. \tag{2.9}$$

Noting that $\hbar = O(1/j)$ equation (2.9) leads to a vanishing classical limit of H_{eff} in strong contrast to (2.7). Moreover (2.9) shows strong relative oscillations in the semiclassical limit. Expressing the projector $|j, m\rangle\langle j, m|$ in the form

$$|j, m\rangle\langle j, m| = \prod_{\substack{\mu=-j \\ (\mu \neq m)}}^{j} \frac{J_z - \mu}{m - \mu} \tag{2.10}$$

shows that H_{eff} can be written as a polynomial in J_z of the order $2j$. The semiclassical limit of the scaled $H_{\text{eff}}/\hbar$ vanishes typically on a number of circles ($z = \cos\theta = \text{constant}$) that is of $O(j)$, implying the non-existence of a smooth classical limit.

3. Level dynamics and the Campbell–Baker–Hausdorff formula

With the help of the level dynamics it is easy to show that the Campbell-Baker-Hausdorff (CBH) formula (Scharf 1988) for non-degenerate kicked quantum systems with finite-dimensional Hilbert space converges. This is important because kicked dynamics are generically non-integrable in the classical limit (see Berry *et al* 1979) and their classical CBH expansion cannot converge in the non-integrable case but only gives asymptotic results near $K = 0$ (see Scharf 1988). How this failure of the CBH expansion in the classical limit can be understood and why it is the best that can happen will be explained in the next sections.

In a previous paper (Scharf 1988) it was shown that $H_{\text{eff}}(K)$ can be written with the help of the CBH formula

$$H_{\text{eff}}(K) = H_0 + K \int_0^1 dr\, g\left[\exp\left(-\frac{i}{\hbar} rK\hat{V}\right) \exp\left(-\frac{i}{\hbar}\hat{H}_0\right)\right] V. \tag{3.1}$$

The function $g(z) = \ln(z)/(z-1)$ is analytic near $z = 1$ and has the Taylor expansion

$$g(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n+1} (z-1)^n \qquad \text{for } |z-1| < 1. \tag{3.2}$$

$\hat{V}$ and $\hat{H}_0$ denoting adjoint operators acting on operators A like V and H_0 as $\hat{V}A = [V, A] = VA - AV$. It easily follows that

$$\exp\left(-\frac{\mathrm{i}}{\hbar} K\hat{V}\right) \exp\left(-\frac{\mathrm{i}}{\hbar} \hat{H}_0\right) A$$

$$= \exp\left(-\frac{\mathrm{i}}{\hbar} KV\right) \exp\left(-\frac{\mathrm{i}}{\hbar} H_0\right) A \exp\left(\frac{\mathrm{i}}{\hbar} H_0\right) \exp\left(\frac{\mathrm{i}}{\hbar} V\right)$$

$$= \exp\left(-\frac{\mathrm{i}}{\hbar} \hat{H}_{\mathrm{eff}}(K)\right) A. \tag{3.3}$$

As a consequence of (3.1) we have with the substitution $s = r(1 + \delta K/K)$:

$$H_{\mathrm{eff}}(K + \delta K) = H_0 + K \int_0^{1+\delta K/K} \mathrm{d}s\, g\left[\exp\left(-\frac{\mathrm{i}}{\hbar} sK\hat{V}\right) \exp\left(-\frac{\mathrm{i}}{\hbar} \hat{H}_0\right)\right] V$$

$$= H_{\mathrm{eff}}(K) + K \int_1^{1+\delta K/K} \mathrm{d}s\, g\left[\exp\left(-\frac{\mathrm{i}}{\hbar} sK\hat{V}\right) \exp\left(-\frac{\mathrm{i}}{\hbar} \hat{H}_0\right)\right] V. \tag{3.4}$$

Up to order δK we get

$$H_{\mathrm{eff}}(K + \delta K) = H_{\mathrm{eff}}(K) + \delta K g\left[\exp\left(-\frac{\mathrm{i}}{\hbar} K\hat{V}\right) \exp\left(-\frac{\mathrm{i}}{\hbar} \hat{H}_0\right)\right] V. \tag{3.5}$$

Using the definition of $g(z)$ we can finally show up to order δK

$$\langle \varphi_m(K) | H_{\mathrm{eff}}(K + \delta K) | \varphi_n(K) \rangle$$

$$= \langle \varphi_m(K) | H_{\mathrm{eff}}(K) | \varphi_n(K) \rangle + \delta K \frac{\mathrm{i}(\varphi_n(K) - \varphi_m(K)) V_{mn}(K)}{\exp[\mathrm{i}(\varphi_n(K) - \varphi_m(K))] - 1}. \tag{3.6}$$

Comparison with the level dynamical result (2.6) shows that both are identical. The CBH formula therefore gives the correct $H_{\mathrm{eff}}(K)$ as long as no degeneracies of the form $\varphi_n = \varphi_m$ for $n \neq m$ and $V_{mn} \neq 0$ occur. Otherwise it might happen that no well defined $H_{\mathrm{eff}}(K)$ exists (see Scharf 1988). Leaving aside the case of exact degeneracy the quantum CBH expansion for finite-dimensional Hilbert space therefore converges to the correct effective Hamilton operator.

4. Adiabatic invariance for kicked quantum dynamics

Dana and Reinhardt (1987) have shown that the idea of adiabatic switching of a perturbation to find adiabatic invariants works quite well for the near-integrable standard map. For $K \ll 1$ they proved up to second order in K that an exact invariant torus of given action coincides with the one constructed via adiabatic switching. For $K \approx 1$ occurrence of global chaos and disappearance of the last KAM torus finally destroys adiabatic invariance. Then the two above-mentioned conditions, i.e. to slip over separatrices or chaotic regions quickly but to change K slowly enough (adiabatically) compared with the intrinsic frequencies of the dynamics, cannot be fulfilled at the same time.

First I show that for kicked quantum dynamics with (effectively) finite-dimensional Hilbert space there is an exact adiabatic invariance. This is intuitive because finite-dimensional (or infinite-dimensional but localised) kicked quantum dynamics are

'integrable', as was mentioned before. Their level dynamics is completely integrable (Wojciechowski 1985, Kuś 1988) and as long as no degeneracies occur the classical adiabatic principle (Arnol'd 1978) should hold for the level dynamics.

Starting with the exact eigenstate $|\varphi_n(K)\rangle$ of $U(K)$ adiabatic switching from K to $K+\delta K$ means the generation of a state vector

$$|\Phi_n(K)\rangle = \left(\prod_{s=1}^{N} U[K+\delta K(N-s)/N]\right) U(K)^{-N}|\varphi_n(K)\rangle \tag{4.1}$$

for some $N \gg 1$, acting with the $s=N$ term in the product on the state vector first. $U(K)^{-N}$ has been added for convenience to get rid of a large dynamical phase factor. Up to order δK we get with the help of (2.1)

$$\begin{aligned}\langle\varphi_m(K)|\Phi_n(K)\rangle &= \exp(-\mathrm{i}N\varphi_n(K))\left\langle \varphi_m(K)\left|\left(\prod_{s=1}^{N} U(K+\delta K(N-s)/N]\right)\right|\varphi_n(K)\right\rangle \\ &= \delta_{nm} + \mathrm{i}\delta K\left\langle \varphi_m\left|\left[\sum_{s=1}^{N} U(K)^{s}\left(\frac{N-s}{N}\right)\frac{V}{\hbar}U(K)^{-s}\right]\right|\varphi_n(K)\right\rangle. \end{aligned}\tag{4.2}$$

And finally:

$$\begin{aligned}&\langle\varphi_m(K)|\Phi_n(K)\rangle \\ &\quad = \delta_{nm}[1+\tfrac{1}{2}\mathrm{i}(N-1)V_{nn}\delta K/\hbar] + \mathrm{i}\delta K(1-\delta_{nm})\frac{V_{mn}/\hbar}{\exp[\mathrm{i}(\varphi_n-\varphi_m)]-1} \\ &\qquad \times\left(1-\frac{\exp[\mathrm{i}N(\varphi_n-\varphi_m)]-1}{\exp[\mathrm{i}(\varphi_n-\varphi_m)]-1}\frac{\exp[\mathrm{i}(\varphi_n-\varphi_m)]}{N}\right). \end{aligned}\tag{4.3}$$

As long as $|N\delta K V_{nn}(K)/\hbar| \ll 1$ (but $N \gg 1$) equation (4.3) gives for $m=n$

$$\langle\varphi_n(K)|\Phi_n(K)\rangle = \exp[\tfrac{1}{2}\mathrm{i}NV_{nn}\delta K/\hbar] + \mathrm{O}(\delta K^2). \tag{4.4}$$

This should be compared with the result (2.3) of the level dynamics

$$\langle\varphi_n(K)|\varphi_n(K+\delta K)\rangle = 1 + \mathrm{O}(\delta K^2). \tag{4.5}$$

For $n \neq m$ and $\varphi_n \neq \varphi_m$ equation (4.3) gives

$$\begin{aligned}\langle\varphi_m(K)|\Phi_n(K)\rangle &= \mathrm{i}\delta K\frac{V_{mn}/\hbar}{\exp[\mathrm{i}(\varphi_n-\varphi_m)]-1} \\ &\quad\times\left(1-\frac{\exp[\mathrm{i}N(\varphi_n-\varphi_m)]-1}{\exp[\mathrm{i}(\varphi_n-\varphi_m)]-1}\frac{\exp[\mathrm{i}(\varphi_n-\varphi_m)]}{N}\right). \end{aligned}\tag{4.6}$$

For $N \gg |\sin[N(\varphi_n-\varphi_m)/2]\sin[(\varphi_n-\varphi_m)/2]^{-1}|$ the second term in (4.6) can be dropped and the result is in accordance with the level-dynamical one

$$\langle\varphi_m(K)|\varphi_n(K+\delta K)\rangle = \mathrm{i}\delta K V_{mn}\hbar^{-1}\{\exp[\mathrm{i}(\varphi_n-\varphi_m)]-1\}^{-1}. \tag{4.7}$$

Besides an unimportant phase factor the state vectors $|\Phi_n(K)\rangle$ and $|\varphi_n(K+\delta K)\rangle$ are equal up to terms of order δK as long as the mentioned conditions on $N|\delta K|$ and N are fulfilled. Then adiabatic switching from K to $K+\Delta K$ with ΔK of the order 1 replacing the small δK in (4.1) is nothing else but numerical integration of the level

dynamics. The errors can be made as small as one likes by taking large enough N as long as no degeneracies occur ($\varphi_n \neq \varphi_m$ for $V_{nm} \neq 0$). In this case the adiabatic principle for kicked quantum systems is exact:

$$|\varphi_n(K+\Delta K)\rangle = \lim_{N\to\infty}\left(\prod_{s=1}^{N} U[K+\Delta K(N-s)/N]\right)U(K)^{-N}|\varphi_n(K)\rangle. \tag{4.8}$$

5. The semiclassical limit and the jumping over resonances

As the simple near-integrable example in § 2 has illustrated, the continuation of the eigenphases does not lead to reasonable effective Hamilton operators as soon as (even exponentially small) level repulsion appears. If the strength of the level repulsion is so small that colliding levels can come orders of magnitude closer to each other than the mean level spacing then the correct choice of the quasienergies $\hbar\varphi$ is only achieved by jumping over the near-degeneracies (see figure 1) such that $\lim_{\varepsilon\to 0^+}\varphi(K,\varepsilon)=\varphi(K,0)$ outside a small region around the avoided level crossing. For K far away from a near-degeneracy the two eigenstates involved have decoupled again and it is obvious that the physical successors of the initially decoupled states are then given not by analytic continuation but by jumping over the region of strong coupling (Noid *et al* 1983). As long as the states decouple sufficiently before they are involved in new avoided level crossings with other states it is possible to follow the fate of each state upon increasing the perturbation parameter K as if it did not take part in couplings with other states. If the state carried some good quantum numbers initially at $K=0$ it is natural to attach the same quantum numbers to its successor at arbitrary K as long as K stays well outside the coupling regions. But as soon as these coupling regions or resonances start to overlap it is no longer possible to find a successor for each state unambiguously and the 'near-good' quantum numbers begin to vanish in the haze. In the case of quantum maps with one near-integral in the classical limit (the energy) at best, it now becomes clear how this integral can be destroyed already in the semiclassical limit, although an effective Hamilton operator, gained via continuation of the eigenphases, always exists (see figure 2). Only the eigenphases $\varphi_i = O(1)$ are known but to reconstruct the eigenenergies $E_i = \hbar(\varphi_i + 2\pi n_i) = O(1)$ the integers

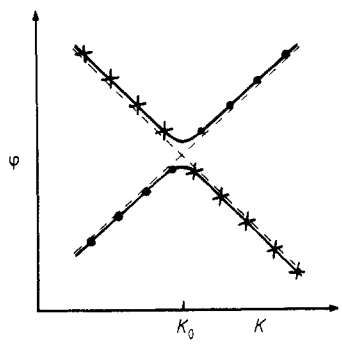

Figure 1. Typical dependence of two eigenphases φ_i of a quantum map upon a perturbation parameter K that show a degeneracy in the integrable case (broken lines), which is avoided in the near-integrable case (full lines). Eigenphases of initially uncoupled states ($K < K_0$) and their successors after decoupling again ($K > K_0$) are marked by dots and crosses.

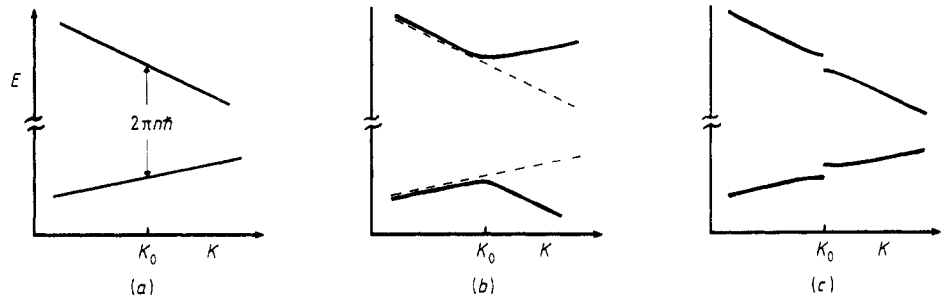

Figure 2. Typical dependence of two energies $E_i = \hbar(\varphi_i + 2\pi n_i)$ of the effective Hamilton operator (2.4) upon a perturbation parameter K (*a*) for the integrable case (see figure 1, broken lines); (*b*) for the near-integrable case with continuation of the eigenphases $\varphi = E/\hbar$ (mod 2π) (see figure 1, full lines), (*c*) with jumping over the avoided crossings of the eigenphases (see figure 1, dots and crosses). While the jumping of the phases gives a result (*c*) that comes as close as possible to the integrable case, the exact continuation (*b*) gives completely wrong energies after the avoided level crossing has happened.

$n_i = O(1/\hbar)$ have to be determined, too. The n_i, which are the quantum numbers in this non-autonomous case, can be attached to each eigenstate unambiguously only for $K = 0$, where the energies E_i are actually known. But as long as each of the states $|\varphi_i(K = 0)\rangle$ possesses a successor $|\varphi_i(K \neq 0)\rangle$ that decouples sufficiently from all other states the integers n_i are still good quantum numbers. The correct way to determine these successors is, of course, by jumping over the avoided level crossings and adiabatic switching between them.

As was shown in § 4 exact adiabatic switching follows the eigenphases of the quantum map closely (as does the quantum Campbell-Baker-Hausdorff result). Numerical calculations work with a finite step size δK by which K is increased from kick to kick during the switching process. To give a good approximation to the results of exact adiabatic switching this step size has to be chosen at least so small that the smallest details in the $\varphi(K)$ curves with large curvature can be resolved. If these curves have two well separated size scales, one for structures far away from avoided level crossings and the other, much smaller one, for the avoided level crossings

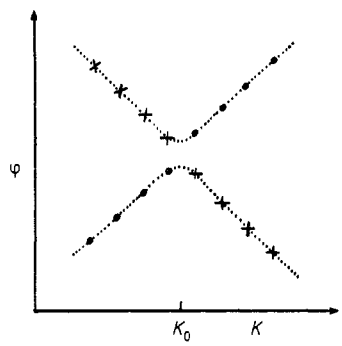

Figure 3. Schematic dependence of two eigenphases upon a perturbation parameter K near an avoided crossing determined with the help of adiabatic switching with small step size (small dots) following the two hyperbolae (exact K dependence), and with the help of diabatic switching with larger step size (larger dots and crosses) jumping over the avoided crossing but nevertheless following the hyperbolae in the asymptotic regions quite closely.

themselves, then jumping over the near-degeneracies can be achieved by choosing a δK well between the two scales. As numerical examples in the next paragraph show, the $\varphi(K)$ curves are then followed as closely as possible well away from the avoided level crossings, but these regions of near-degeneracy and strong coupling are ignored by jumping over them (see figure 3). As soon as the near-degeneracies show level splitting no longer small compared to the mean spacing the diabatic switching no longer gives reasonable results. Of course further decreasing δK leads back to exact adiabatic switching that works perfectly but does not jump over the near-degeneracies and is therefore of no value for the construction of an effective Hamilton operator possessing a classical limit.

6. An example

The difference between adiabatic and diabatic switching processes for quantum maps and their connection with the CBH formula will now be illustrated with a kicked spin dynamics (Frahm and Mikeska 1986, Nakamura *et al* 1986) that has been investigated previously (Scharf 1988). It is generated by the unitary operator

$$U(K, K') = \exp\left(\frac{\mathrm{i}K}{2j} J_x^2\right) \exp\left(\frac{\mathrm{i}K'}{2j} J_y^2\right). \tag{6.1}$$

This dynamics is non-integrable in the classical limit and shows a transition into global chaos for $K = K' \approx 2.5$.

First one might ask how good an approximation are the eigenvalues gained via diabatic switching compared to the exact ones. For that question I chose $j = 10$ (21 eigenvalues), determined the eigenvalues and eigenvectors of $U(K, 0)$ and then switched them from $K' = 0$ to $K' = K$ in N steps as indicated by (4.8). It turns out that for $N = 1000$ the largest and the mean relative errors are 0.01 and 0.001 respectively for $K = 1$, and 0.1 and 0.02 respectively for $K = 2$. Step number $N = 1000$ still means diabatic switching with jumping over near-degeneracies as shown in figure 3. Further increase of N first leads to larger errors (for $N = 8000$ and $K = 2$ the relative errors are 1.0 and 0.2, respectively) until for even larger N the switching becomes adiabatic and follows the level dynamics closely without jumping.

A look at the classical maps explains why this happens (Haake *et al* 1987a, Scharf 1988). For $K = 1$ the map is near-integrable and the eigenvalues of U can be determined semiclassically by torus quantisation. For $K = 2$ the classical map shows the instability of two primary resonances and the eigenvalues of the quantum map start to repel each other appreciably (Frahm and Mikeska 1986, Haake *et al* 1987b). For $K = 3$ the classical map is globally chaotic and the quantum map shows strong level repulsion leading to splittings of the order of the mean level spacing.

As the diabatic switching gives approximations $\tilde{\varphi}_n$ and $|\tilde{\varphi}_n\rangle$ for both the eigenphases φ_n and the eigenvectors $|\varphi_n\rangle$ of U an approximation $\tilde{H}_{\mathrm{eff}}$ to the effective Hamilton operator H_{eff} (2.4) can be constructed:

$$\tilde{H}_{\mathrm{eff}} = \sum_n |\tilde{\varphi}_n\rangle \tilde{E}_n \langle\tilde{\varphi}_n| \tag{6.2}$$

with the energies $\tilde{E}_n = \hbar\tilde{\varphi}_n$ which are typically of order 1 because the phases $\tilde{\varphi}$ are of order $j = 1/\hbar$, in strong contrast to the exact phases which are only known modulo 2π.

To compare H_{eff} and $\tilde{H}_{\text{eff}}$ with the classical phase space structures, expectation values with angular momentum coherent states $|\theta, \varphi; j\rangle$ are calculated (see Perelomov (1986) for an introduction) with spherical angles θ and φ

$$\begin{aligned} H_{\text{eff}}(\theta, \varphi; j) &= \langle \theta, \varphi; j | H_{\text{eff}} | \theta, \varphi; j \rangle \\ \tilde{H}_{\text{eff}}(\theta, \varphi; j) &= \langle \theta, \varphi; j | \tilde{H}_{\text{eff}} | \theta, \varphi; j \rangle. \end{aligned} \tag{6.3}$$

The effective Hamilton operators and their expectation values (6.3) are j dependent. From the simple example (2.8) one expects that $H_{\text{eff}}(\theta, \varphi; j)$ will not have a smooth classical limit neither for eigenphases restricted to the interval $[0, 2\pi)$ nor for continuation of the eigenphases upon increasing K', because phases (of the same $\exp(i\pi J_z)$ eigenspace) repel each other, as was the case in the example (2.8). For finite j the function $H_{\text{eff}}(\theta, \varphi; j)$ will already show strong oscillations perpendicular to the phase

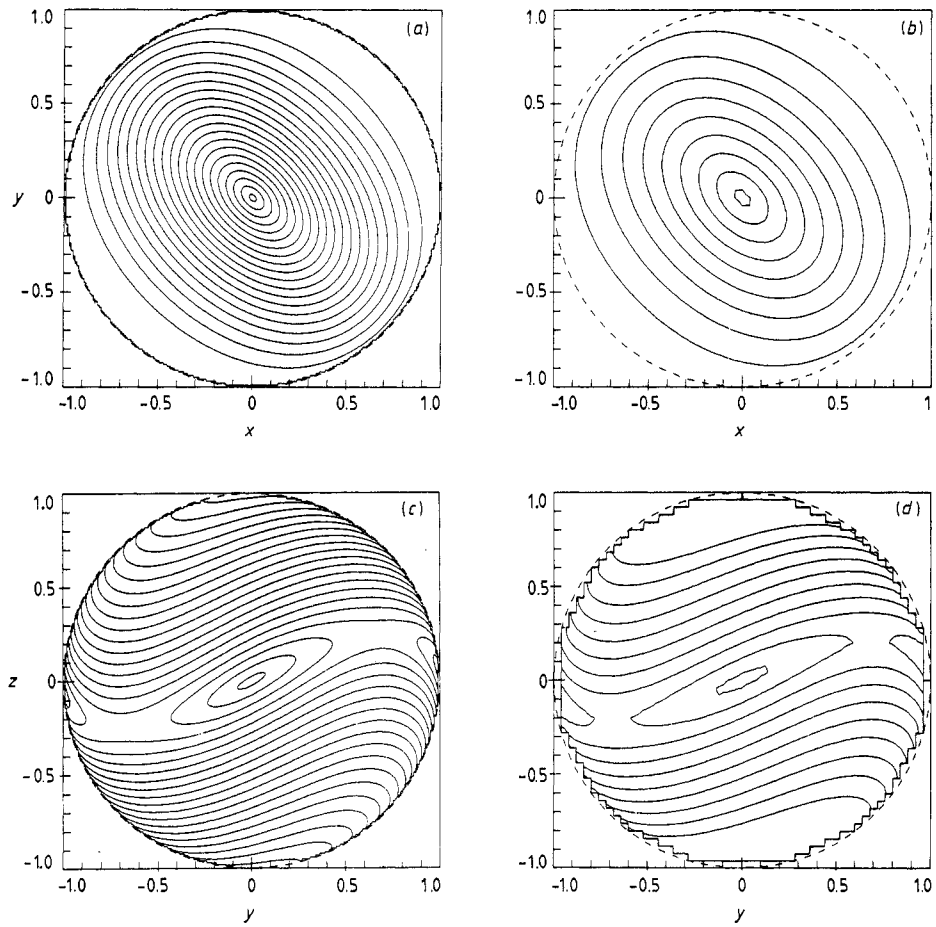

Figure 4. (a, c) Lines of constant $H_{\text{eff}} = H_{\text{CBH}}$ given by the CBH formula (3.1) up to $O(K^7)$ (for details, see Scharf (1988)) compared with (b, d) lines of constant expectation values of the diabatically ($N = 1000$) gained $\tilde{H}_{\text{eff}}$ ($j = 10$) for (a, b) $K = 1$ on the northern hemisphere ($z > 0$) and (c, d) around the equator ($x > 0$). Although $\hbar = 1/j = 0.1$ is still large the classical quasi-integral H_{CBH} and its diabatic counterpiece $\tilde{H}_{\text{eff}}(j = 10)$ resemble each other strongly.

space curves $H_{\text{eff}}(\theta, \varphi; j) = E$, although these curves will follow KAM tori closely in the near-integrable case. But the strong oscillations make it increasingly difficult for growing j to use these curves as approximate integral curves of the classical map.

In contrast to H_{eff} we expect $\tilde{H}_{\text{eff}}$ to possess a smooth classical limit in the near-integrable case and therefore $\tilde{H}_{\text{eff}}(\theta, \varphi; j)$ to be a well behaved approximate integral of the classical map for large enough j. It turns out that $j = 10$ is already large enough to see the difference between $H_{\text{eff}}(\theta, \varphi; j)$ and $\tilde{H}_{\text{eff}}(\theta, \varphi; j)$ and to see that the latter is a good approximate integral of the classical map.

For $K = 1$ and $K = 2$ phase space pictures of the classical map were already given and an approximate effective Hamiltonian $H_{\text{CBH}}(\theta, \varphi)$ was constructed via the CBH expansion (Scharf 1988). It was found to be a good approximate integral of the classical map in the smooth parts of the phase space near the primary resonances. In the following picture the diabatically gained $\tilde{H}_{\text{eff}}(\theta, \varphi; j = 10)$ and $H_{\text{CBH}}(\theta, \varphi)$ are compared for $K = 1$ (see figure 4) and $K = 2$ (see figures 5 and 6) on the spherical phase space with cartesian coordinates x, y and z for an optimal choice for the number

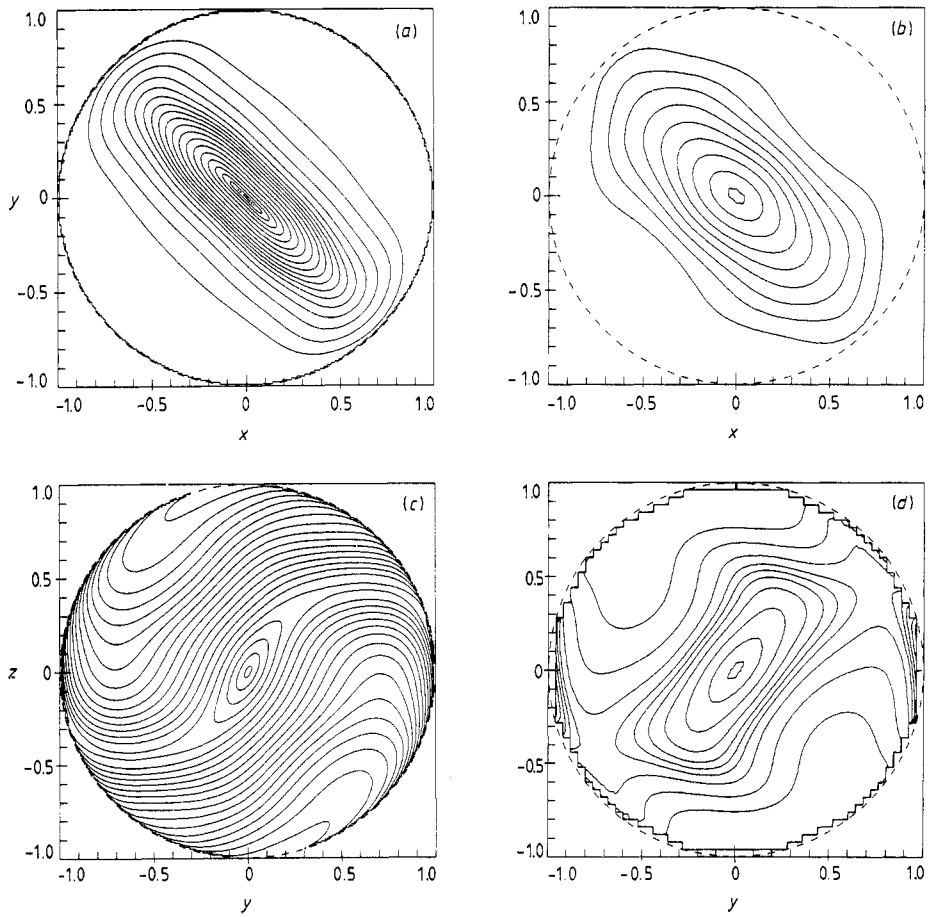

Figure 5. The same as figure 4 for $K = 2$. Now the diabatic approximation starts to fail near the poles $x = y = 0$ which are marginally stable classically. Near the equator the resemblance between H_{CBH} and $\tilde{H}_{\text{eff}}(j = 10)$ is stronger and the results should be compared with the classical iteration (see figure 6).

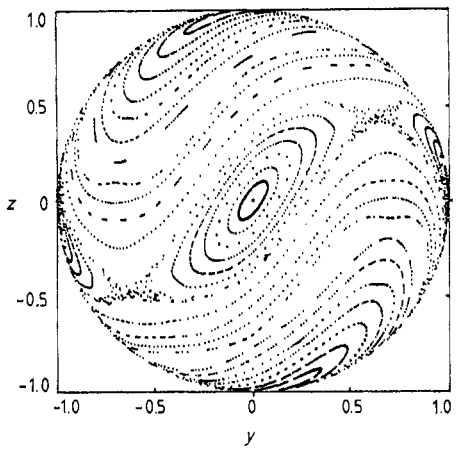

Figure 6. Classical iteration for $K = 2$ around the equator ($x > 0$), to be compared with figure 5(c, d).

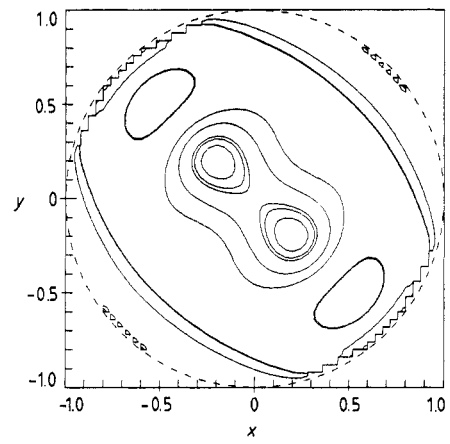

Figure 7. Lines of constant expectation values of the exact $H_{\text{eff}}(j = 10)$ with eigenenergies determined from the eigenphases of U restricted to $[0, 2\pi)$ for $K = 2$ on the northern hemisphere ($z > 0$). Notice that there is almost no resemblance with the diabatic and CBH results (see figure 5(a, b)).

of steps ($N = 1000$). The conformity is convincing for $K = 1$ and satisfactory for $K = 2$ besides the polar regions ($\theta = 0$ and $\theta = \pi$). Further increase of the step number N in the diabatic process leads to worse results, as was already mentioned for the eigenvalues.

These results have to be contrasted with pictures for $H_{\text{eff}}(\theta, \varphi; j = 10)$ constructed from the eigenvectors and eigenvalues of U, the latter ones either confined to $[0, 2\pi)$ or continued upon increasing K'. As soon as these eigenvalues disagree clearly with the diabatically gained ones the phase space functions $H_{\text{eff}}(\theta, \varphi; j)$ show strong oscillations that lead to numerical artefacts in the contour plots $H_{\text{eff}}(\theta, \varphi; j) = E$ for finite j (see figure 7) and to the non-existence of a smooth classical limit.

7. Discussion

In this paper I have investigated how several methods for calculating effective Hamiltonians and Hamilton operators for classical and quantum maps, respectively, compare with each other. It was shown that exact diagonalisation of the unitary quantum propagator, the introduced level dynamics, adiabatic switching and the Campbell-Baker-Hausdorff construction lead to the same effective Hamilton operator, which does not possess a smooth classical limit generically, even in the near-integrable case (first $\hbar \to 0$, then perturbation $\to 0$). On the other hand numerical results show that diabatic switching may lead to Hamilton operators that do possess a smooth classical limit. These smooth Hamiltonians are approximate integrals of the classical maps and correspond to Hamiltonians constructed with the classical Campbell-Baker-Hausdorff formula evaluated asymptotically in the perturbation parameter for near-integrable classical maps. As was briefly mentioned adiabatic switching of the near-integrable classical standard map also leads to approximate phase space invariants.

If there are no exact accidental degeneracies in the quantum spectrum then the CBH formula leads to the exact effective Hamilton operator, which may also be constructed from the exact eigenvectors and the continued eigenphases. In particular the CBH formula converges in the quantum case. In strong contrast to that, the classical CBH formula can be used in the non-integrable case only asymptotically for small perturbations. The reason seems to be the same as in the case of normal forms, which may be convergent in the quantum case but divergent in the classical case (Robnik 1986). For $\hbar \neq 0$ accidental degeneracies leading to vanishing denominators are suppressed. Then the quantum normal form and the quantum CBH expression converge but do not possess a classical limit. For $\hbar = 0$ resonances are not suppressed in both cases and the results are only asymptotic in the perturbation. That resonances really show up for diabatic switching can be seen in figure 3: diabatically constructed eigenphases cross. As the number of avoided or real level crossings in a fixed perturbation interval grows like $\hbar^{-2}$ upon decreasing $\hbar$ (level density times level velocity = $O(j^2) = O(1/\hbar^2)$) then for the mentioned kicked angular momentum dynamics the resonances grow dense along the real perturbation strength axis. In the classical limit the perturbation expansions, whether CBH or normal forms, therefore diverge but may be still useful asymptotically.

As the effective Hamiltonian of a classical map generates a continous phase space flow, which is only stroboscopically equivalent with the map, it cannot generate n-cycles for $n > 1$. Therefore one has to take n-fold iterates of the classical map making n-cycles to fixed points in order to construct effective Hamiltonians. The same trick is also used in the quantum case. Actually the unitary propagator in the example (4.8) is the square of a previously investigated operator (Nakamura *et al* 1986). With this method approximate integrals of classical maps may be constructed near n-cycles.

Acknowledgments

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