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LETTER TO THE EDITOR

Modulated kicks approximation in non-integrable classical and quantum systems

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Abstract. Time-dependent harmonic perturbation in dynamical systems is frequently approximated by a sequence of infinitely short pulses (so-called kicks) of alternating sign. In order to improve this approximation we increase the number of kicks per perturbation period. The validity of this method is tested numerically on an exemplary classical system: a particle in the Rosen-Morse potential well, driven by an external harmonic perturbation.

Dynamical systems with an unrealistic perturbation, in the form of a sequence of infinitely short pulses, have recently drawn a lot of attention. Such an approach greatly simplifies the analysis of a system, since the time evolution can be described in terms of the appropriate classical (or quantum) map. The well known kicked rotator model was investigated in the study of classical [1, 2] and quantum [3-5] chaos.

In the dynamical models of interaction of atoms with strong electromagnetic fields [6-9] the sinusoidal changes of field were simulated by a train of kicks of alternating sign. Not much is yet known about the validity of such an approximation. Leopold and Richards [6], however, reported significant differences between results obtained with impulsive and continuous perturbation.

In order to improve the alternated kicks approximation (AKA) and simulate the continuous perturbation in a better way we suggest increasing the number of pulses per wave period. In this letter the modulated kicks approximation (MKA) is defined and tested on an exemplary dynamical model. A correspondence is shown between the approximation of a continuous perturbation in a physical system by a train of infinitely short pulses and the numerical methods of solving the non-linear differential equations by the discretisation of time.

Consider an arbitrary smooth function $f(t)$ with period T. Let us define a sequence of distributions $\tilde{f}_N$

$$\tilde{f}_N(t) := A_N \sum_{i=0}^{N-1} f\left(\frac{iT}{N}\right)\delta\left(t-\frac{iT}{N}\right) \tag{1}$$

where N is a positive integer and the normalisation constant A_N is equal to

$$A_N = \left(\int_0^T f(t)\,\mathrm{d}t\right)\left[\sum_{i=0}^{N-1} f\left(\frac{iT}{N}\right)\right]^{-1} \tag{2}$$

in order to keep the integral constant

$$\int_0^T f(t)\,\mathrm{d}t = \int_0^T \tilde{f}_N(t)\,\mathrm{d}t.$$

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If the function $f(t)$ changes the sign, the normalisation is to be done separately in each interval between roots of $f(t)$. Function $\tilde{f}_N$, non-negative in one period only, can easily be generalised to

$$f_N(t) := \sum_{l=-\infty}^{l=\infty} \tilde{f}_N(t+lT). \tag{3}$$

Let L_f denote the distribution corresponding to the continuous function $f(t)$ and the distributions F_N correspond to $f_N(t)$. The modulated kicks approximation is based on the following corollary.

Corollary 1. In the limit $N \to \infty$ the series of distributions F_N converges pointwise to L_f.

This corollary, proved elsewhere [10], suggests that the continuous perturbations $f(t)$ may be replaced by the impulsive perturbation $f_N(t)$, provided N is large enough. Such an approximation (called the modulated kicks approximation) can be useful for different dynamical systems, since it enables us to write straightforwardly the classical (or quantum) map, instead of solving numerically the differential equation. Note that the MKA can also be applied for a generic (non-periodic) perturbation or a periodic one multiplied by a slowly varying envelope $C(t)$.

In the discussion of the dynamics of a Hamiltonian system, it is convenient to express the periodic perturbation in terms of the Fourier series. For an even function $f(t)$ we have

$$f(t) = \sum_{m=0}^{m=\infty} a_m \cos(m\omega t) \qquad \text{and} \qquad f_N(t) = \sum_{m=0}^{m=\infty} a_m^N \cos(m\omega t)$$

where $\omega = 2\pi/T$. The Fourier coefficients a_m of the perturbation determine the number and positions of the resonances in the phase space [1]. From corollary 1 it follows that

$$\forall m \in \mathbb{N}: \lim_{N\to\infty} a_m^N = a_m.$$

It means therefore that for sufficiently large N the structure of resonances in a system described by MKA is similar as in the corresponding system driven by a continuous perturbation.

As an illustration of the modulated kicks approximation we study the case of harmonic perturbation: $f(t) = \cos(\omega t)$. Hence, the definition (3) is

$$\begin{aligned} f_2(t) &= \sum_l A_2 \sum_{i=0}^{i=1} \cos(i\pi)\delta(t - iT/2 + lT) \\ &= (T/\pi) \sum_l \{\delta(t+lT) - \delta[t + T(l-\tfrac{1}{2})]\} \end{aligned} \tag{4}$$

where the normalisation constant A_2 is equal to T/π. Application of the function f_2 (and in this case also f_4) is thus equivalent to the well known alternated kicks approximation. The perturbation f_N consists of N kicks per one period, modulated by the cosine function $f(t)$. Figure 1 shows, in a schematic way, functions f_2, f_8, f_{16} and the function f_∞ represented by the sinusoidal wave.

To check numerically the accuracy of the approximation investigated we analyse an exemplary system: a single particle moving in the one-dimensional Rosen-Morse

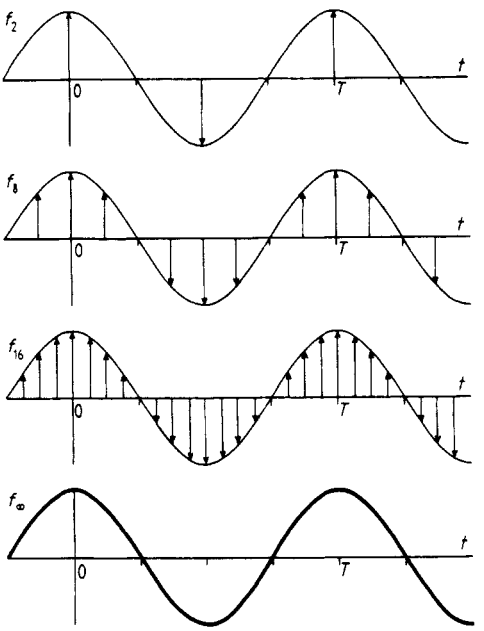

Figure 1. Schematic sketch of time-dependent perturbation—the harmonic wave represented by MKA with $N = 2$ (or 4), 8 and 16 kicks per period. In the limit $N \to \infty$ we recover the continuous wave (curve f_∞).

potential $V_0(x)$ driven by the harmonic field. This model was recently applied in a classical description of the above threshold ionisation [11]. The Hamiltonian is

$$H = H_0 + H_C = p^2/2 - U/\cosh^2(Ax) + V_C(x)\cos(\omega t) \tag{5}$$

where the mass of the particle is set to 1; two parameters U and A define the shape of the atomic potential $V_0(x)$. The interaction potential $V_C(x)$ is equal to Cx, where ω and C are perturbation frequency and strength respectively.

The motion of the system remains regular for small values of C and trajectories starting inside the potential well are trapped there for ever. For larger perturbation strengths the motion becomes chaotic and the particle can leave the potential well. This picture corresponds, in our simple model, to ionisation caused by an external field.

Time evolution of the non-integrable system (5) can be analysed by standard methods of numerical integration. On the other hand, the continuous perturbation in (5) can be replaced by the sequence of modulated kicks (3). It can be shown [10] that in the limit $N \to \infty$ the solution given by the classical (or quantum) map fulfills the differential equation originating from the system driven by the continuous perturbation. The simplest case of this approximation, where the system is driven by the train of alternated kicks (AKA) was analysed in [11]. To obtain the classical map it is enough to solve the equation of motion for the unperturbed system. It is more convenient to work in the canonical variables $\{P, Q\}$, where $P(t)$ remains constant between the kicks. The basic transformation R_j, $j = 0, \ldots, N-1$, consists of two terms: free evolution between kicks and infinitely short kicks represented by a change of momentum

$$R_j\begin{bmatrix} Q(t) \\ P(t) \end{bmatrix} = \begin{bmatrix} Q(t) + P(t)T/N \\ P(t) + F(jT/N)A_N\, \partial V_C(x)/\partial x \end{bmatrix}. \tag{6}$$

The full classical map M, which governs the evolution of the system during the perturbation period T is obtained as a composition of N transformations R_j:

$$M = \prod_{j=0}^{j=N-1} R_j. \tag{7}$$

In order to obtain the quantum map for the system analogous to (5) we expand the wavefunction in the basis of bound and free eigenstates of $\hat{H}_0$

$$|\Psi\rangle = \sum_m a_m(t)|m\rangle + \int_k b_k(t)|k\rangle \, \mathrm{d}k \tag{8}$$

where

$$\hat{H}_0|m\rangle = E_m|m\rangle \qquad E_m < 0$$

$$\hat{H}_0|k\rangle = E_k|k\rangle \qquad E_k > 0.$$

The transformation $\hat{R}_j$ in the quantum case maps the set of coefficients

$$\{a_m(t+jT/N),\, b_k(t+jT/N)\}$$

onto

$$\{a_m(t+(j+1)T/N),\, b_k(t+(j+1)T/N)\}.$$

For example

$$\hat{R}_j[a_m(t)] = a_m(t+T/N) = \sum_l a_l(t) \exp(-\mathrm{i}E_lT/hN)\, W^j_{ml}$$

$$+ \int_k b_k(t) \exp(-\mathrm{i}E_lT/\hbar N)\, W^j_{mk} \tag{9}$$

where the elements of N different matrices of the pulse are equal to

$$W^j_{mk} = \langle m|\exp[-\mathrm{i}V_C(x)F(t+jT/N)A_N/\hbar]|k\rangle \qquad j = 0, 1, \ldots, N-1. \tag{10}$$

In the analogy to the classical map M, the quantum map $\hat{M}$ consists of N elementary transformations $\hat{R}_j$. Applying the appropriate sequence of maps $\hat{R}_j$ to an arbitrary initial state $|\Psi(0)\rangle$ described by set $\{a_m(0), b_k(0)\}$ one can study the time evolution of the quantum system. To perform a numerical calculation according to the map (9) the appropriate energy cut-off in the integral term is necessary, as well as the method of discretisation of the continuum [9]. In both the classical and quantum calculations the computing time grows linearly with the number of kicks per perturbation period.

In order to check how the different kinds of impulsive perturbation approximate the continuous wave in the classical system, we calculated numerically the probability that a trajectory will leave the potential well. All initial points were taken randomly with the same negative initial energy E_0. Figure 2 presents the escape probability P after 200 perturbation periods (full saturation) against the perturbation strength C. Various kinds of perturbation were analysed: the continuous harmonic wave labelled as '∞', and impulsive perturbation MKA with 2, 6, 8 and 16 kicks per wave period. The AKA approximation significantly overestimates the probability of escape due to interaction with higher harmonics. The impulsive perturbation with larger N approximates the harmonic wave much better, and $N = 16$ MKA already gives quite accurate results.

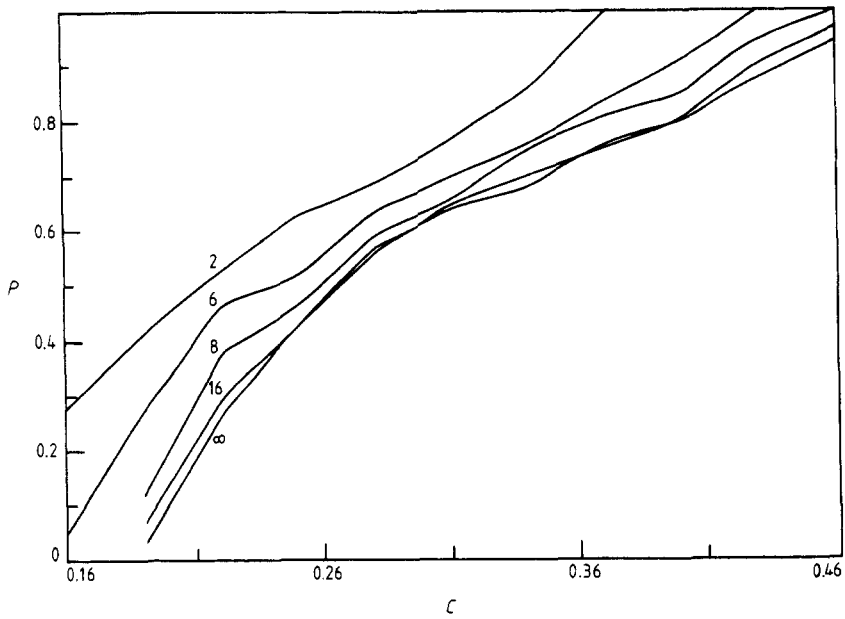

Figure 2. Escape probability P plotted against the field strength C, for parameters of the system $A = U = 1.0$, $\omega = 0.8$, $E_0 = 0.9$ (in atomic units). A number labelling each curve indicates the N kicks per period MKA, while '∞' denotes the harmonic wave. The alternating kicks perturbation ($N = 2$ curve) does not approximate the continuous wave well, whereas the $N = 16$ MKA does it much better.

In conclusion we have presented an effective method of analysis of the time-dependent Hamiltonian systems connected to the numerical integration of the equations of motion. In other words, the physical background for mathematical methods of numerical analyses is shown. We think that the MKA approximation can be used for a wide class of dynamical systems not necessary in the case of harmonic perturbation. Moreover, the same method may be applied for quantum models. Instead of solving the non-linear, partial Schrödinger equation, the problem reduces to construction of the appropriate quantum map. Some properties of the solutions can be found analytically by investigation of the map in the limit $N \to \infty$.

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