Isochronous systems are not rare

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Abstract

A (classical) dynamical system is called *isochronous* if it features an *open* (hence *fully dimensional*) region in its phase space in which *all* its solutions are *completely periodic* (i. e., periodic in *all* degrees of freedom) with the *same* fixed period (independent of the initial data, provided they are inside the *isochrony* region). When the isochrony region coincides with the *entire* phase-space one talks of *entirely isochronous* systems. A trick is presented associating to a dynamical system a modified system depending on a parameter so that when this parameter vanishes the original system is reproduced while when this parameter is *positive* the modified system is *isochronous*. This technique is applicable to large classes of dynamical systems, justifying the title of this talk. An analogous technique (introduced with **François Leyvraz**), even more widely applicable -- for instance, to *any* translation-invariant (classical) many-body problem – transforms a real autonomous *Hamiltonian* system into an *entirely isochronous* real autonomous *Hamiltonian* system. The modified system is of course no more translation-invariant, but in its centre-of-mass frame it generally behaves quite similarly to the original system over times much shorter than the isochrony period *T* (which may be chosen at will). Hence, when this technique is applied to a "realistic" many-body Hamiltonian yielding, in its centre of mass frame, *chaotic* motions with a natural time-scale much smaller than (the chosen) *T*, the corresponding modified Hamiltonian shall yield a chaotic behavior (implying statistical mechanics, thermodynamics with its second principle, etc.) for quite some time before the *entirely isochronous* character of the motion takes over hence the system returns to its initial state, to repeat the cycle over and over again. We moreover show that the quantized versions of these modified Hamiltonians feature infinitely degenerate *equispaced* spectra.

Analogous techniques are applicable to nonlinear evolution PDEs, but in this talk there will be no time to cover this aspect. Although the material reported in my 264-page monograph entitled *Isochronous systems*---just published (February 2008) by Oxford University Press---is a synthesis of work done over the last 10 years with several collaborators, *all* the results presented below are joint work with **François Leyvraz**. Some of the additional results obtained very recently with him are also presented at the end of this talk.

Main references

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A trick to transform a Hamiltonian into an *isochronous* Hamiltonian

$$\left[\ H\left(\underline{p},\underline{q}\right),\Theta\left(\underline{p},\underline{q}\right)\ \right]=1$$

Isochronous Hamiltonian:

$$\tilde{H}\left(\underline{p},\underline{q};\Omega\right)=\frac{1}{2}\left\{\left[H\left(\underline{p},\underline{q}\right)\right]^2+\Omega^2\left[\Theta\left(\underline{p},\underline{q}\right)\right]^2\right\};\quad T=\frac{2\pi}{\Omega}$$

“Isochronous Hamiltonian systems are not rare”

A remarkable example ("transient chaos")

We write as follows the (simplest version of the) Hamiltonian characterizing the standard nonrelativistic *N*-body problem:

$$H\left(\underline{p},\underline{q}\right)=\frac{1}{2}\sum_{n=1}^{N}\left[p_n^2\right]+V\left(\underline{q}\right),\ V(\underline{q}+a)=V(\underline{q}).$$

Let us now review some standard related developments, trivial as they are.

We hereafter denote with P the total momentum, and with Q the (canonically-conjugate) centre-of-mass coordinate:

$$P=\sum_{n=1}^{N} p_n\,,\ Q=\frac{1}{N}\sum_{n=1}^{N} q_n\,.$$

Thanks to the translation invariance property

$$\left[H,P\right]=0$$

Here and hereafter the Poisson bracket $[F,G]$ of two functions $F\left(\underline{p},\underline{q}\right)$ and $G\left(\underline{p},\underline{q}\right)$ of the canonical variables is defined as follows:

$$[F,G]=\sum_{n=1}^{N}\left[\frac{\partial F\left(\underline{p},\underline{q}\right)}{\partial p_n}\frac{\partial G\left(\underline{p},\underline{q}\right)}{\partial q_n}-\frac{\partial G\left(\underline{p},\underline{q}\right)}{\partial p_n}\frac{\partial F\left(\underline{p},\underline{q}\right)}{\partial q_n}\right].$$

And let us recall that the evolution of any function $F\left(\underline{p},\underline{q}\right)$ of the canonical coordinates is determined by the equation

$$F\,'=\left[H\,,F\,\right],$$

where the appended prime denotes differentiation with respect to the "timelike" variable corresponding to the evolution induced by the Hamiltonian *H*.

It is now convenient to introduce the "relative coordinates" x_n and the "relative momenta" y_n via the standard definitions

$$x_n = q_n - Q, \; y_n = p_n - \frac{P}{N} .$$

Note that these are not canonically conjugated quantities, since $[y_n, x_m] = \delta_{nm} - 1/N$, and they are not independent since obviously their sum vanishes:

$$\sum_{n=1}^{N} y_n = 0, \; \sum_{n=1}^{N} x_n = 0.$$

It is moreover convenient to introduce the "relative-motion" Hamiltonian $h(\underline{y}, \underline{x})$ via the formula

$$h(\underline{y}, \underline{x}) = \frac{1}{2} \sum_{n=1}^{N} y_n^2 + V(\underline{x}) = \frac{1}{4N} \sum_{n,m=1}^{N} (p_n - p_m)^2 + V(\underline{q})$$

so that

$$H(\underline{p}, \underline{q}) = \frac{P^2}{2N} + h(\underline{y}, \underline{x}) .$$

Note that this definition of the relative-motion Hamiltonian $h(\underline{y}, \underline{x})$ entails that it Poisson commutes with both *P* and *Q* :

$$[P, h] = 0, \; [Q, h] = 0.$$

For completeness and future reference let us also display the equations of motion implied by the original Hamiltonian $H(\underline{p},\underline{q})$:

$$q_n' = p_n\,,\;\; p_n' = -\partial V(\underline{q})/\partial q_n\,,\;\; q_n'' = -\partial V(\underline{q})/\partial q_n\,,$$

where (for reasons that will be clear below) we denote as τ the independent variable corresponding to this Hamiltonian flow and with appended primes the differentiations with respect to this variable:

$$q_n \equiv q_n(\tau),\;\; p_n \equiv p_n(\tau),\;\; q_n' \equiv \partial q_n(\tau)/\partial\tau\,,\;\; p_n' \equiv \partial p_n(\tau)/\partial\tau\,.$$

Hence

$$Q' = \frac{P}{N}\,,\;\; P' = 0$$

yielding

$$Q(\tau) = Q(0) + \frac{P(0)}{N}\tau\,,\;\; P(\tau) = P(0),$$

as well as

$$x_n' = y_n = \frac{\partial h(\underline{y},\underline{x})}{\partial y_n}\,,\;\; y_n' = -\frac{\partial V(\underline{x})}{\partial x_n} = -\frac{\partial h(\underline{y},\underline{x})}{\partial x_n}\,.$$

Note that these equations have the standard Hamiltonian form even though, as mentioned above, x_n and y_n are not canonically conjugated variables.

This ends the review of quite standard results for the classical nonrelativistic many-body problem. Let us also emphasize that, above and below, the restriction to unit-mass particles, and to one-dimensional space, is merely for simplicity: generalizations – also of the following results – to the more general case with *different* masses and *arbitrary* space dimensions is quite elementary, essentially trivial.

The isochronous Hamiltonian

The Ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$ is now defined by the formula

$$\tilde{H}(\underline{p},\underline{q};\Omega)=\frac{1}{2}\left\{\left[P+\frac{h(\underline{y},\underline{x})}{b}\right]^2+\Omega^2\,Q^2\right\},$$

where *b* is an arbitrary constant (introduced for dimensional reasons: it has the dimensions of a momentum, hence of the square-root of an energy) and Ω is a *positive* constant. Let us emphasize that hereafter the evolution of the various quantities is that caused by this new Ω-modified Hamiltonian (which does not quite reduce to the original Hamiltonian when Ω vanishes – more about this below); the corresponding independent variable is hereafter denoted as *t* (and interpreted as "time"), and differentiations with respect to this variable will be denoted, as usual, by superimposed dots, and of course, for any function $F\equiv F(\underline{p},\underline{q})$ of the canonical variable its time evolution will be determined by the standard equation

$$\dot{F}=\left[\tilde{H},F\right].$$

It is now easily seen that there hold the following Poisson commutation formulas:

$$\left[\tilde{H},Q\right]=P+\frac{h(\underline{y},\underline{x})}{b},\;\;\left[\tilde{H},P\right]=-\Omega^2\,Q,\;\;\left[\tilde{H},h\right]=0,$$

so that the quantities *Q*, *P* and *h* evolve as follows under the flow induced by the Ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$:

$$\dot{Q}=P+\frac{h(\underline{y},\underline{x})}{b},\;\;\dot{P}=-\Omega^2\,Q,\;\;\dot{h}=0,$$

entailing

$$Q(t)=Q(0)\cos(\Omega t)+\dot{Q}(0)\frac{\sin(\Omega t)}{\Omega}=bC\,\frac{\sin[\Omega(t-t_0)]}{\Omega},$$

$$P(t)=P(0)\cos(\Omega t)+\dot{P}(0)\frac{\sin(\Omega t)}{\Omega}+\frac{h[\underline{y}(0),\underline{x}(0),]}{b}[\cos(\Omega t)-1],$$

$$h[\underline{y}(t),\underline{x}(t)]=h[\underline{y}(0),\underline{x}(0)].$$

It is moreover plain that the total momentum *P* and the centre-of-mass coordinate *Q* Poisson-commute with the relative-motion momenta and coordinates y_n and x_n hence as well with any function of these variables, hence the evolution equations of the relative-motion coordinates and momenta x_n and y_n under the flow induced by the Ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$ read

$$\dot{x}_n=\frac{1}{b}\left[P+\frac{h(\underline{y},\underline{x})}{b}\right]\frac{\partial h(\underline{y},\underline{x})}{\partial y_n}=\frac{\dot{Q}}{b}\,\frac{\partial h(\underline{y},\underline{x})}{\partial y_n},$$

$$\dot{y}_n=-\frac{1}{b}\left[P+\frac{h(\underline{y},\underline{x})}{b}\right]\frac{\partial h(\underline{y},\underline{x})}{\partial x_n}=-\frac{\dot{Q}}{b}\,\frac{\partial h(\underline{y},\underline{x})}{\partial x_n},$$

namely

$$\dot{x}_n=C\cos[\Omega(t-t_0)]\frac{\partial h(\underline{y},\underline{x})}{\partial y_n}\,,\quad \dot{y}_n=-C\cos[\Omega(t-t_0)]\frac{\partial h(\underline{y},\underline{x})}{\partial x_n}\,,$$

$$C=\left(2\tilde{H}\right)^{1/2}/b,\ \sin(\Omega t_0)=-\Omega Q(0)\left(2\tilde{H}\right)^{-1/2}.$$

It is now crucial to observe -- by comparing these evolution equations caused by the Ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$ with the analogous ones caused by the original Hamiltonian $H(\underline{p},\underline{q})$ -- that it is justified to conclude that

$$\tilde{x}_n(t)=x_n(\tau),\;\;\tilde{y}_n(t)=y_n(\tau),$$

where (changing for convenience notation) we now denote as $\tilde{x}_n,\tilde{y}_n$ the canonical variables whose time evolution is determined by the Ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$ and as x_n,y_n the canonical variables whose time evolution is determined by the original, un-modified Hamiltonian $H(\underline{p},\underline{q})$. Here clearly (and most importantly)

$$\tau\equiv\tau(t)=C\,\frac{\sin[\Omega(t-t_0)]}{\Omega}=\frac{Q(t)}{b}\;,$$

where the two constants are given by simple explicit formulas in terms of the initial values of the centre-of-mass of the system and of the Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$ (which is of course a constant of motion). The crucial observation is that $\tau(t)$ is a (real, nonsingular) periodic function of *t* with period

$$T=2\pi/\Omega\;.$$

In this manner the dynamics of the canonical coordinate and momenta evolving according to our Ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$ are finally obtained, and due to the periodic behaviour under this flow of the collective coordinates *Q* and *P*, as well as the remarkable relation we just found among the time evolution of the "relative motion" variables of the Ω-modified Hamiltonian and those of the original unmodified Hamiltonian, it is now plain that the dynamics yielded by the Ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$ is *isochronous* with period *T* (for arbitrary initial data): indeed the time evolution due to the original Hamiltonian is generally, for arbitrary initial data, uniquely well-defined for all real time -- unless it runs into singularities, which should not be the case for physically sound models, and in any case should only happen exceptionally.

The Ω=0 limit and the behaviour of the *isochronous* system over time scales much shorter than *T*

When Ω vanishes, the Ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\Omega)$ does not quite reduce to the unmodified Hamiltonian $H(\underline{p},\underline{q})$; but it is plain that the dynamics yielded by the Hamiltonian $\tilde{H}(\underline{p},\underline{q};0)$ differs only marginally from that yielded by the original Hamiltonian $H(\underline{p},\underline{q})$. To illustrate this point we now display the version that the most relevant formulas written above take when Ω vanishes, Ω=0.

Let us consider firstly the evolution of the centre-of-mass *Q* and the total momentum *P* yielded by the Hamiltonian $\tilde{H}(\underline{p},\underline{q};0)$,

$$Q(t)=Q(0)+\left\{P(0)+\frac{h\left[\underline{y}(0),\underline{x}(0)\right]}{b}\right\}t=Q(0)+b\,C\,t,\;\; P(t)=P(0),$$

to be compared with the analogous evolution yielded by the Hamiltonian $H(\underline{p},\underline{q})$,

$$Q(t)=Q(0)+\frac{P(0)}{N}t,\;\; P(t)=P(0).$$

Next, let us make an analogous comparison for the evolution of the "relative-motion" variables. The relevant formula is of course always

$$\tilde{x}_n(t)=x_n(\tau),\;\; \tilde{y}_n(t)=y_n(\tau),$$

but now with

$$\tau=C\,t+Q(0)/b\;.$$

These formulas confirm the assertion that the dynamics yielded by the Hamiltonian $\tilde{H}(\underline{p},\underline{q};0)$ differs only marginally from that yielded by the original Hamiltonian $H(\underline{p},\underline{q})$.

In fact an analogous relationship -- entailing that $\tau = \tau(t)$ on a sufficiently short time scale varies linearly in *t* holds generally, since in the neighborhood of any time $\bar{t}$ -- except when $\dot{Q}(\bar{t})$ vanishes –

$$\tau(t) = \frac{Q(\bar{t}) + \dot{Q}(\bar{t})(t-\bar{t})}{b} + O\left[\left(\frac{t-\bar{t}}{T}\right)^2\right].$$

Transient chaos

One therefore finds that – essentially throughout the time evolution -- the Ω-modified dynamics differs from the unmodified one solely by a time rescaling -- by a possibly negative coefficient -- and by a time shift. The coefficient and the shift are time-independent over a time scale much smaller than the isochrony period *T*=2π/Ω, but vary periodically with period *T*. A peculiar state of affairs arises, however, whenever $\dot{Q}(\bar{t})$ vanishes, namely when $d\tau/dt$ changes its sign: this of course happens twice within every time period *T*, this being in fact a consequence of the periodicity of $\tau(t)$, which itself is the cause of the isochrony. These aspects are apparent in the two figures displayed in the examples reported below.

It is interesting to speculate on the application of this Ω-modification technique to any Hamiltonian describing a "realistic" translation-invariant many-body problem featuring, in its centre-of-mass system, "chaotic" motions with a natural time scale T_C. Then -- provided the constant Ω is assigned so that the isochrony period $T = 2\pi/\Omega$ is much larger than this time scale, $T >> T_C$ -- the Ω-modified problem shall exhibit some kind of *chaotic* behavior for quite some time before the *isochronous* character of all its motions takes over, causing thereafter a recurrent evolution. This phenomenology -- qualitative rather than quantitative as it necessarily is, since a precise definition of *chaos* requires generally that a system displaying it be observed for *infinite* time -- is nevertheless remarkable.

A simple example

I now display, with minimal comments, the findings obtained by applying our Ω-modification technique to the very simple Hamiltonian describing a couple of equal mass one-dimensional particles interacting pairwise with a force proportional to their mutual distance; when this force is attractive this model corresponds of course, in the centre-of-mass system, to the standard "harmonic" oscillator model. (We write "harmonic" under inverted commas to emphasize that the entirely isochronous Ω-modified Hamiltonians yielded by our technique all yield motions deserving to be called harmonic, inasmuch as they are characterized by just a single frequency of oscillation: in the case of many-body problems the term "nonlinear harmonic oscillators", introduced together with Inozemtsev, is perhaps the most appropriate to describe the corresponding dynamics...).

The original Hamiltonian:

$$H\left(p_1, p_2; q_1, q_2\right) = \frac{1}{2}\left(p_1^{\ 2} + p_2^{\ 2}\right) + \frac{\omega^2}{4}\left(q_1 - q_2\right)^2 \ .$$

Some standard definitions and related formulas:

$$x_1 = q_1 - Q = \frac{q_1 - q_2}{2}, \ \ x_2 = q_2 - Q = \frac{q_2 - q_1}{2}, \ x_1 + x_2 = 0 \ ,$$

$$y_1 = p_1 - \frac{P}{2} = \frac{p_1 - p_2}{2}, \ \ y_2 = p_2 - \frac{P}{2} = \frac{p_2 - p_1}{2}, \ y_1 + y_2 = 0 \ ,$$

$$h\left(x_1, x_2; y_1, y_2\right) = \frac{1}{2}\left(y_1^{\ 2} + y_2^{\ 2}\right) + \frac{\omega^2}{4}\left(x_1 - x_2\right)^2 \ ,$$

$$H\left(p_1, p_2; q_1, q_2\right) = \frac{1}{4}P^2 + h\left(y_1 y_2; x_1 x_2\right) ;$$

$$x_n\left(t\right) = x_n\left(0\right)\cos\left(\omega t\right) + y_n\left(0\right)\frac{\sin\left(\omega t\right)}{\omega} \ , \ \ y_n\left(t\right) = y_n\left(0\right)\cos\left(\omega t\right) - \omega\, x_n\left(0\right)\frac{\sin\left(\omega t\right)}{\omega} \ , n = 1,2 \ .$$

The Ω-modified Hamiltonian

$$\tilde{H}(p_1 p_2; q_1 q_2; \Omega) = \frac{1}{2}\left\{\left[P + \frac{h(y_1 y_2; x_1, x_2)}{b}\right]^2 + \Omega^2\left(\frac{q_1+q_2}{2}\right)^2\right\}$$

$$= \frac{1}{2}\left\{\left[p_1 + p_2 + \frac{(p_1-p_2)^2}{4b}\right]^2 + \frac{\omega^2}{2b}\left[p_1 + p_2 + \frac{(p_1-p_2)^2}{4b}\right](q_1-q_2)^2 + \left(\frac{\omega^2}{4b}\right)^2 (q_1-q_2)^4 + \Omega^2\left(\frac{q_1+q_2}{2}\right)^2\right\}$$

The *isochronous* motions yielded by this Ω-modified Hamiltonian:

$$x_n(t) = x_n(0)\cos\left\{\omega C\frac{\sin[\Omega(t-t_0)]+\sin(\Omega t_0)}{\Omega}\right\} + \frac{y_n(0)}{\omega}\sin\left\{\omega C\frac{\sin[\Omega(t-t_0)]+\sin(\Omega t_0)}{\Omega}\right\},\ n=1,2,$$

$$y_n(t) = y_n(0)\cos\left\{\omega C\frac{\sin[\Omega(t-t_0)]+\sin(\Omega t_0)}{\Omega}\right\} - \omega x_n(0)\sin\left\{\omega C\frac{\sin[\Omega(t-t_0)]+\sin(\Omega t_0)}{\Omega}\right\},\ n=1,2\ ,$$

with C and t_0 defined in terms of the initial data.

The entirely isochronous character of this motion, with period $T=2\pi/\Omega$, is evident; and note that this outcome obtains even if ω is purely imaginary, ω=iα with α real, in which case the original Hamiltonian H and the Ω-modified Hamiltonian $\tilde{H}$, as well of course as the corresponding solutions, are nevertheless *all real*.

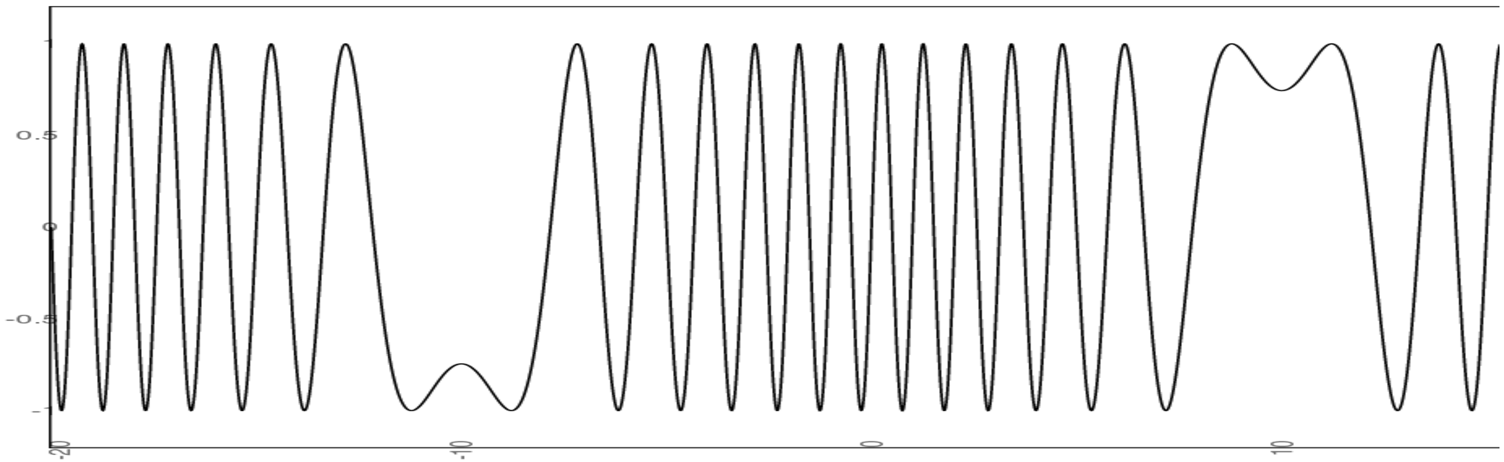

Figure 1: Graph (over almost one time period) of $x_n(t)$ for
$x_n(0)=0,\ \ y_n(0)=\omega=40\Omega=2\pi,\ \ \Omega=\pi/20,\ \ C=1,\ \ t_0=0.$

Note the overall periodicity with period $T=2\pi/\Omega=40$, the large regions where the behaviour is nearly periodic with the original period $2\pi/\omega=1$ of the solutions of the unmodified Hamiltonian, and the transition regions around the times *t*=10 and *t*=30 when $\dot{\tau}(t)$.

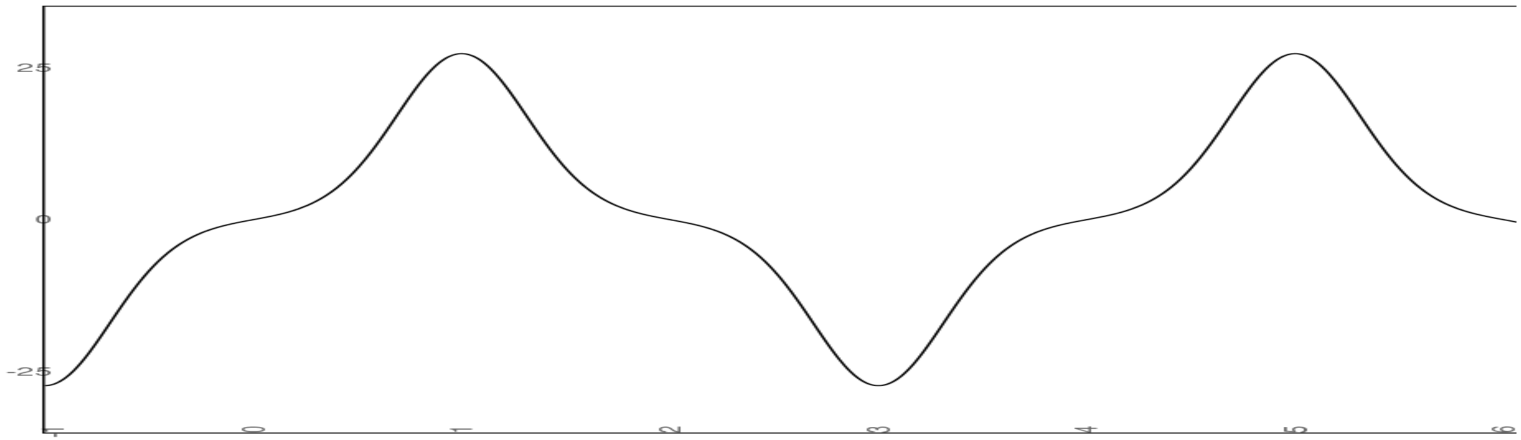

Figure 2: Graph (over almost two time periods) of $x_n(t)$ for
$x_n(0)=0,\ \ y_n(0)=\omega=4i\Omega=2\pi i,\ \ \Omega=\pi/2,\ \ C=1,\ \ t_0=0.$

Note the overall periodicity with period $T=2\pi/\Omega=4$, the regions where the time evolution resembles the original $\sin(\omega t)/i=\sinh(2\pi t)$ behaviour of the corresponding solution of the unmodified Hamiltonian, and the transition regions around the times *t*=-1,1,3,5,7 when $\dot{\tau}(t)$ vanishes.

The quantum case

Finally we tersely show that, in a quantal context, our Ω-modified Hamiltonian

$$\tilde{H}\left(\underline{p},\underline{q};\Omega\right)=\left\{\left[P+h\left(\underline{y},\underline{x}\right)/b\right]^{2}+\Omega^{2}Q^{2}\right\}/2,$$

features an (infinitely degenerate) equispaced spectrum with spacing $\hbar\Omega$.

This spectrum consists of the eigenvalues E_k of the stationary Schrödinger equation

$$\frac{1}{2}\left\{\left[-i\hbar\frac{\partial}{\partial Z}+\frac{\lambda}{b}\right]^{2}+\Omega^{2}Z^{2}\right\}\psi_{k}(Z;\lambda)=E_{k}\,\psi_{k}(Z;\lambda),$$

obtained from this Hamiltonian via the standard quantization rule

$$P\Rightarrow -i\hbar\,\partial/\partial Z,\;\; Q\Rightarrow Z,$$

and by identifying λ as an eigenvalue of the quantized version of the relative-motion Hamiltonian $h\left(\underline{y},\underline{x}\right)$. Indeed this Schrödinger equation is obtained by assuming that the eigenfunctions of the quantized version of the Hamiltonian $\tilde{H}\left(\underline{p},\underline{q};\Omega\right)$ factor into the product of an eigenfunction, $\psi_k(Z;\lambda)$, depending on the variable *Z* and on which acts the differential operator *∂/∂Z* , and of the eigenfunction corresponding to the eigenvalue λ of the quantized version of the relative-motion Hamiltonian $h\left(\underline{y},\underline{x}\right)$. The justification for this factorization is in the commutativity of the operators representing the quantal versions of the canonical variables *P* and *Q* , see above, with the operator representing the quantal version of the relative-motion Hamiltonian $h\left(\underline{y},\underline{x}\right)$ -- a commutativity reflecting the Poisson-commutativity of the corresponding quantities in the classical context.

It is now plain that the above Schrödinger equation features the spectrum and eigenfunctions

$$E_k=\hbar\Omega\left(k+1/2\right),\;\; k=0,1,2,\ldots,$$

$$\psi_k(Z;\lambda)=\exp\left(\frac{i\lambda z}{b\sqrt{\hbar\Omega}}-\frac{z^2}{2}\right)H_k(z),\;\; z=Z\sqrt{\frac{\Omega}{\hbar}}\;,$$

where $H_k(z)$ denotes the standard Hermite polynomial of order *k*.

This spectrum is of course equispaced with spacing $\hbar\Omega$, and it is infinitely degenerate inasmuch as it does not feature any dependence on the eigenvalues λ.

Oscillatory and isochronous chemical reactions

A set of chemical reactions:

$$U+U \Rightarrow U \text{ with rate } \alpha ,$$

$$U+W \Rightarrow U \text{ with rate } \beta ,$$

$$W+W \Rightarrow U \text{ with rate } \gamma ,$$

$$W+W \Rightarrow W+W+W \text{ with rate } \delta + 2\gamma .$$

Here and hereafter α, β, γ and δ are 4 positive constants. Hereafter we indicate with *u≡u(t)* and *w≡w(t)* the amounts (say, the number of molecules) of the chemicals *U* and *W* contained in the reactor at time t. Hence we model the chemical kinetics via the following system of two nonlinear ODEs:

$$\dot{u} = -\alpha u^2 + \gamma w^2 , \quad \dot{w} = -\beta u w + \delta w^2 = \left(-\beta u + \delta w\right) w .$$

Note that, while the second of these two ODEs guarantees that, if *w*(0)>0, then *w*(*t*)>0 for all (subsequent) time, the first ODE does not seem to guarantee automatically that, if *u*(0)>0, then *u*(*t*)>0 for all (subsequent) time; although this is indeed the case, as we now show.

Assumptions and definition:

$$\gamma\beta^2 > \alpha\delta^2 , \; 2\beta\gamma > \delta^2 ; \; \eta^2 = \left(\gamma\beta^2 - \alpha\delta^2\right)/\alpha .$$

The qualitative/quantitative behavior of this model is then characterized by the following two Propositions.

Proposition 1. For arbitrary initial data (of course positive, $u(0)>0$, $w(0)>0$), the dependent variables $u(t)$ and $w(t)$ solution of this system of ODEs remain *positive* and *finite* for all (positive) time (i. e., no blow-up) and both *vanish asymptotically*,

$$u(\infty)=0, \; w(\infty)=0.$$

Proposition 2. In the specially interesting case characterized by the equality

$$\beta = 2\alpha, \text{ entailing } \eta^2 = 4\alpha\gamma - \delta^2 ,$$

the solution of the initial-value problem of this model can be exhibited explicitly:

$$u(t) = \frac{C}{\alpha\eta} \frac{\delta + \eta C(t - t_0)}{1 + C^2 (t - t_0)^2}, \quad w(t) = \frac{2C}{\eta^2} \frac{1}{1 + C^2 (t - t_0)^2},$$

$$C = [\eta w(0)/2]\left\{1 + [\delta - 2\alpha u(0)/w(0)]^2/\eta^2\right\},$$

$$Ct_0 = [\delta - 2\alpha u(0)/w(0)]/\eta .$$

It appears therefore that the chemical reactions described above lead to the eventual (asymptotic) *disappearance* of both chemicals, *U* and *W*. Let us now discuss two variants of this model.

Firstly, we suppose that there occurs additionally a constant decay of the chemical *U*---say, caused by a fifth chemical reaction,

$$U \Rightarrow Z \ \text{ with rate } \theta \, ,$$

with the neutral chemical *Z* giving no further reaction---or, equivalently, caused by an outflow of the chemical *U* from the reactor, proportional to the quantity of this chemical contained in it. Common sense might suggest that the disappearance of both chemicals---or at least of *U*---should continue to be the final (asymptotic) outcome of this process. But this is not the case, as we now show.

The modeling of the process is now provided by the system

$$\dot{u} = -\theta\, u - \alpha\, u^2 + \gamma\, w^2 \, ,$$

$$\dot{w} = -\beta\, u\, w + \delta\, w^2 = \left(-\beta u + \delta w\right) w \, .$$

A qualitative description of the behavior of the system is then provided by the following proposition.

Proposition 3. This system of two nonlinear ODEs features the equilibrium configuration

$$u(t) = \bar{u} = \frac{\theta\,\delta^2}{\alpha\,\eta^2}\ ,\ \ w(t) = \bar{w} = \frac{\theta\,\beta\,\delta}{\alpha\,\eta^2}\ ,$$

which is clearly inside the first quadrant of the *u-w* (phase-space) Cartesian plane. Then---from any initial configuration---the solution of this system tends asymptotically to this equilibrium configuration or oscillates around it, depending whether the quantity

$$\rho = \gamma\,\beta^2 + (\alpha - \beta)\,\delta^2 = \alpha\,\eta^2 + (2\,\alpha - \beta)\,\delta^2\ ,$$

is positive (*stable* equilibrium) or negative (*unstable* equilibrium).

Note that this result entails that, if $\rho>0$ (which is certainly the case if $2\,\alpha>\beta$, all solutions are either periodic or approach a limit cycle. For a more complete analysis one must perform numerical simulations: we have not been able to find any explicit (nontrivial) solution of this model.

Another interesting variant of the original model obtains if a *constant* flow of the chemical U is siphoned out of the reactor tank, at a steady rate independent of its quantity present in it (presumably the chemical engineer in charge knows out to do it: via an appropriate faucet that lets out only a constant flux of the chemical U, or a constant flux of the mixture of the two chemicals U and W that gets then infinitely quickly separated into U and W, putting back W in the reactor). Again, common sense might suggest that the disappearance of both chemicals, U and W---or at least of U---should continue to be the final (asymptotic) outcome of this process, but this is not what happens.

The natural modeling of the chemical process now reads

$$\dot{u} = -f - \alpha u^2 + \gamma w^2 ,$$

$$\dot{w} = -\beta u w + \delta w^2 = (-\beta u + \delta w) w .$$

A description of the behavior of this system is then provided by the following two propositions.

Proposition 4. This system of two nonlinear ODEs features, in the first quadrant of the *u*-*w* (phase-space) Cartesian plane, the single equilibrium configuration

$$u(t)=\bar{u}=(\delta/\eta)\sqrt{f/\alpha}\ ,\ \ w(t)=\bar{w}=(\beta/\eta)\sqrt{f/\alpha}\ ,$$

This configuration is stable if $\beta<2\alpha$, it is unstable if $\beta>2\alpha$. If the initial data $u(0)>0$, $w(0)>0$ are sufficiently close to this equilibrium configuration, the trajectory of the dependent variables $u(t)$, $w(t)$ shall *approach* it asymptotically (exponentially in time) if $\beta<2\alpha$; it shall instead *rotate* around it (clockwise) if $\beta>2\alpha$, with both $u(t)$ and $w(t)$ remaining *positive* throughout their cyclic evolution. For *arbitrary* initial data (however far from the equilibrium configuration) the system gives rise to no blow-up; on the other hand the dependent variable $u(t)$ might eventually become *negative*, signifying a breakdown of the chemical significance of this model.

Proposition 5. In the case characterized by the equality $\beta=2\alpha$ the solution of the initial-value problem of this model can be exhibited explicitly:

$$u(t) = \sqrt{\frac{f}{\alpha}\,\frac{1}{\eta}}\;\frac{\delta\left(1-A^2\right)-2\eta A\sin\left(\omega t+\phi\right)}{1+A^2+2A\cos\left(\omega t+\phi\right)}\;,$$

$$w(t) = \sqrt{\frac{f}{\alpha}\,\frac{1}{\eta}}\;\frac{2\alpha\left(1-A^2\right)}{1+A^2+2A\cos\left(\omega t+\phi\right)}\;,$$

$$A=\sqrt{\frac{\left[2\alpha u(0)-\delta w(0)\right]^2+\left[\eta w(0)+\omega\right]^2}{\left[2\alpha u(0)-\delta w(0)\right]^2+\left[\eta w(0)-\omega\right]^2}}\;,$$

$$\phi=-\arcsin\left[\frac{2\omega\left[2\alpha u(0)-\delta\delta(0)\right]}{\sqrt{\left[2\alpha u(0)-\delta w(0)\right]^4+2\left[2\alpha u(0)-\delta\delta(0)\right]^2 V_+ + V_-^2}}\right],$$

$$V_{\pm}=\eta^2\left[w(0)\right]^2\pm\omega^2$$

Clearly, for arbitrary initial data $u(0)>0$, $w(0)>0$, this solution is *nonsingular* and *isochronous*, traveling clockwise around the equilibrium configuration with the period $T=\pi / \sqrt{(f\,\alpha)}$ (independent of the initial data, and remarkably also of the two rates γ and δ). The trajectory of the system in the *u*-*w* (phase-space) Cartesian plane is the ellipse defined by the equation

$$4\alpha^2\left(\overline{w}u-\overline{u}w\right)^2+\omega^2\left(w-\overline{w}-A^2\left[w+\overline{w}\right]\right)^2=\left(A\omega^2/\eta\right)^2 ,$$

which shrinks to the equilibrium point if the initial data coincide with the equilibrium configuration. This trajectory remains *inside* the first quadrant of the *u*-*w* (phase-space) Cartesian plane provided the initial data $u(0)>0$, $w(0)>0$ are *inside* the ellipse (enclosing of course the equilibrium point defined by the equation

$$4\,\alpha\,u\left(\alpha\,u-\delta\,w\right)^2+\left(2\sqrt{\alpha\gamma}\,w-\omega\right)^2=0 .$$