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Occurrence of secular terms in the Carleman embedding

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Secular terms occur in many perturbative solutions of nonlinear equation systems. In this work, an investigation is made of which cases they may occur in as the result of the application of the linear Carleman embedding to a system of nonlinear equations. The solution for the embedded system is written in a form that makes it convenient to see how these terms originate. Their occurrence for the general case is discussed and the results are exemplified by working out the Hénon–Heiles system.

I. INTRODUCTION

Secular terms appear very often in connection with perturbative expansions of the solution of a system of nonlinear equations. These terms should be avoided when we look for approximate solutions over several revolutions of the system. Otherwise they will cause steadily growing amplitudes with time, in disagreement with the observed motion in the majority of cases. The anharmonic oscillator is a simple system where secular terms do appear if conventional straightforward perturbation expansion is performed.

The concepts of Carleman embedding (CE) and secular terms have been put together in a review article on the CE by Montroll and Helleman.[1] They employ the CE to recover the known exact solution of the logistic equation, and show how it can be used to develop a perturbation theory without secular terms. This last point is illustrated by the analysis of the anharmonic oscillator. Since this work, some attempts have been made to apply the CE to more complex systems. Steeb and Wilhelm,[2] have treated the two-dimensional Lotka–Volterra system in a first-order approximation, with results in agreement with the first term of an expansion of the limit cycle. In the context of the Lorenz model, Andrade and Rauh[3] show that any finite-order approximation given by the CE breaks down at the turbulent threshold.

The present work has been motivated by an analysis of the Hénon–Heiles system.[4,5] We wished to investigate how the CE would work near the transition to chaos in this model. Unlike the case of the Lorenz model, this transition is not associated with a stable fixed point that becomes unstable at a well-defined threshold value of a control parameter. In the Hénon–Heiles model, we have a large region of values of the energy where there are two kinds of coexisting trajectories, namely, those lying on the surface of the two-dimensional tori, and those which are chaotic. We have found that the approximate solutions are always similar, for all values of the energy, without any recognizable structural difference between a chaotic and a regular regime. Moreover, secular terms are present in the approximate solutions of order larger than 1. This behavior, of course, contrasts with the proposals of Montroll and Helleman,[1] who emphasize the absence of secular terms within the framework of the CE. A critical reading of the paper of Montroll and Helleman, however, reveals that the absence of secular terms is not due to the CE itself, but rather to a subtle expansion of the oscillation frequency which is carried out by the authors together with the embedding. Similar expansions of the frequency may be performed without any connection with the CE, and are related to the evaluation of the so-called Poincaré recurrence time.[6,7]

The main purpose of this work is to clear up these points. Also, we present a detailed discussion of the occurrence of secular terms when a given nonlinear system is treated by the CE only, without any extra approximations as in the paper of Montroll and Helleman. We think it is important to discuss the occurrence of the secular terms even if we wish to avoid them. This discussion provides a deeper insight of the method itself, and allows some comparisons between the CE and other methods which show the same kind of problem. In this paper we formally consider an autonomous system of P equations with quadratic nonlinearities and suppose, for the sake of simplicity, that it is written in a coordinate basis with a diagonal linear part. Section II is devoted to developing the formal CE solution of the system into a form which is particularly useful for the discussion of the occurrence of secular terms. This will be accomplished in Sec. III, where we show which terms may appear in each block of the infinite CE time evolution operator. In Sec. IV we illustrate the discussion of the preceding sections by the presentation of some results for the Hénon–Heiles system. Finally, we make some concluding remarks in Sec. V.

II. THE SOLUTION

We consider a P-dimensional system described by the vector $\mathbf{x}(t)$, whose equations of motion may be written as

$$\frac{d\mathbf{x}}{dt} = A\mathbf{x} + B\mathbf{x}^{[2]}, \tag{1}$$

where A and B are constant matrices of order $P\times P$ and $P\times P^2$, moreover A is supposed to be diagonal, and $\mathbf{x}^{[2]} = \mathbf{x}\otimes\mathbf{x}$ is a P^2-dimensional vector, where $\otimes$ denotes the Kronecker product.[2,8] After proceeding with the embedding of the original system, we are led to[2,8]

$$\frac{d}{dt}\begin{pmatrix}\mathbf{x}^{[1]}\\ \mathbf{x}^{[2]}\\ \vdots\\ \mathbf{x}^{[N]}\end{pmatrix} = \begin{pmatrix}A^1 & B^1 & 0 & 0 & \cdots\\ 0 & A^2 & B^2 & 0 & \cdots\\ 0 & 0 & \ddots & \ddots & \\ \vdots & \vdots & & A^N & B^N\end{pmatrix}\begin{pmatrix}\mathbf{x}^{[1]}\\ \mathbf{x}^{[2]}\\ \vdots\\ \mathbf{x}^{[N]}\end{pmatrix}, \tag{2}$$

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or, in shorthand notation

$$\frac{d}{dt}X = MX. \tag{2'}$$

In (2) we have

$$\begin{aligned} &\mathbf{x}^{[N]} = \mathbf{x}^{[N-1]} \otimes \mathbf{x}, \quad \mathbf{x}^{[1]} = \mathbf{x}, \\ &A^N = A^1 \otimes I^{N-1} + I^1 \otimes A^{N-1}, \quad A^1 = A, \\ &B^N = B^1 \otimes I^{N-1} + I^1 \otimes B^{N-1}, \quad B^1 = B, \end{aligned} \tag{3}$$

where I^N indicates the $P^N \times P^N$ identity matrix. Our intention is to write the solution of (2') as

$$X(t) = \exp(Mt)\,X(0) = T\exp(\widetilde{M}t)T^{-1}X(0), \tag{4}$$

where T is the matrix which transforms M into its diagonal form $\widetilde{M}$. We will write T in terms of its block components denoted by capital indices $T_{L,K}$. The dimension of such a block $T_{L,K}$ is $P^L \times P^K$. Due to the structure of M and to the fact that the A^1 (and hence all A^N) are diagonal matrices we have

$$T_{L,K} = 0, \quad L > K, \quad T_{K,K} = I^K. \tag{5}$$

The blocks of the inverse matrix $T^{-1} = U$ will be denoted by $U_{L,K}$ of order $P^L \times P^K$, and may be easily expressed in terms of the $T_{L,K}$ by

$$U_{L,K} = (-1)^{L+K}\,\mathrm{Det}(T')_{K,L}, \tag{6}$$

where $(T')_{K,L}$ is the matrix obtained from T by elimination of the Kth block line and the Lth block column. Now, $\mathrm{Det}(T')_{K,L}$ indicates a matrix of dimension $P^L \times P^K$ which is obtained by performing matrix multiplications and sums among the blocks of $(T')_{K,L}$ in the same way we calculate the determinant of a matrix. As a matter of fact, (6) is the block equivalent to the well-known expression for the elements of the inverse matrix. In the evaluation of (6) we must pay attention that the order of the factors $T_{L,K}$ in each term must be such that the several matrix multiplications are possible, but the product of an identity block by another identity block (or by a nonsquare block) does not afford them to be compatible in the sense of usual matrix multiplication. For instance, we have

$$\begin{aligned} &U_{L,L} = I^L, \quad U_{L,L+1} = -T_{L,L+1}, \\ &U_{L,L+2} = T_{L,L+1}T_{L+1,L+2} - T_{L,L+2}. \end{aligned} \tag{7}$$

The results above do indicate how we can bring (6) to the simpler form

$$U_{L,L+K} = -\sum_{M=J}^{J+K-1} U_{L,M}T_{M,L+K}. \tag{8}$$

The blocks $T_{L,K}$ and $U_{L,K}$ are to be determined from the condition $\widetilde{M} = UMT$, and as we have $\widetilde{M}_{L,K} = A^L\delta_{L,K}$ we get

$$A^L\delta_{L,K} = \sum_{M=L}^{K} U_{L,M}A^M T_{M,K} + \sum_{M=J}^{K-1} U_{L,M}B^M T_{M+1,K}. \tag{9}$$

When $L = K$, the above equation becomes an identity; when $L \neq K$, it gives the relations which determine the $T_{L,K}$. Making use of (8) we can reduce (9) to

$$\begin{aligned} \widetilde{M}_{L,K} = \sum_{M=L}^{L+K-1} U_{L,M}\{&A^M T_{M,K} \\ &- T_{M,K}A^K + B^M T_{M+1,K}\} = 0. \end{aligned} \tag{10}$$

Since (10) must be valid for any K, the $T_{M,K}$ will have to satisfy

$$A^M T_{M,K} - T_{M,K}A^K = -B^M T_{M+1,K}. \tag{11}$$

At this point we shall introduce a new notation for the blocks of T and U, which takes into account better the fact that the solution of (11) is dependent of the diagonal the block belongs to. So let

$$T^{L,K} = T_{L,L+K}, \quad U^{L,K} = U_{L,L+K}. \tag{12}$$

With this notation it becomes clearer that (11) gives a solution for the blocks of the Kth diagonal in terms of those of the $(K-1)$th diagonal. The components of this block are expressed as

$$T^{L,K}_{m,n} = \sum_j \frac{B^L_{m,j}T^{L+1,K-1}_{j,n}}{A^{L+K}_n - A^L_m}. \tag{13}$$

Now if we successively explicit the $T^{L,K-1}$ in terms of the $T^{L,K-2}$, $T^{L,K-3}$, and so on, we get the general result

$$T^{L,K}_{l_0,l_K} = \sum_{l_1,\ldots,l_{K-1}} \prod_{M=0}^{K-1} \frac{B^{L+M}_{l_M,l_{M+1}}}{A^{L+K}_{l_K} - A^{L+M}_{l_M}}. \tag{14}$$

The next task is to determine the $U^{L,K}_{l_0,l_K}$, starting from (8). We will not deduce it here, but we can easily see that if we insert the expression

$$U^{L,K}_{l_0,l_K} = \sum_{l_1,\ldots,l_{K-1}} \prod_{M=0}^{K-1} \frac{B^{L+M}_{l_M,l_{M+1}}}{A^L_{l_0} - A^{L+M+1}_{l_{M+1}}} \tag{15}$$

together with (14) into (8) we come to an identity.

Now we can finally write down the evolution operator $\exp(Mt)$. Since we are interested in the evolution of the first block component $\mathbf{x}^{[1]} = \mathbf{x}$ of X, we concentrate on the evaluation of the block components $(e^{Mt})_{1,K}$,

$$(e^{Mt})_{1,K} = \sum_{M=1}^{K} T_{1,M}e^{A^M t}U_{M,K}. \tag{16}$$

If we define $(e^{Mt})^{1,K} = (e^{Mt})_{1,K+1}$, and make use of the notation introduced in (12) we get

$$(e^{Mt})^{1,K}_{m,n} = \sum_{M=0}^{K} \sum_j T^{1,M}_{m,j}(e^{A^{M+1}t})_j\,U^{M,K-M}_{j,n}. \tag{17}$$

Now we insert expressions (14) and (15) into (17) to get the explicit form of the $(e^{Mt})^{1,K}_{l_0,l_K}$

$$(e^{Mt})^{1,K}_{l_0 l_K} = \sum_{M=0}^{K}\left\{\sum_{l_M}\left\{\sum_{l_1,\ldots,l_{M-1}}\prod_{N=0}^{M-1}\frac{B^{N+1}_{l_N,l_{N+1}}}{A^{M+1}_{l_M} - A^{N+1}_{l_N}}\right\}(e^{A^{M+1}t})_{l_M}\left\{\sum_{l_{M+1},\ldots,l_{K-1}}\prod_{N=0}^{K-M-1}\frac{B^{M+N}_{l_{M+N},l_{M+N+1}}}{A^M_{l_M} - A^{M+N+1}_{l_{M+N+1}}}\right\}\right\}. \tag{18}$$

We proceed one step further and bring (18) to a more convenient form for the analysis we will undertake in Sec. III,

$$(e^{Mt})^{1,K}_{l_0,l_K} = \sum_{l_0,\dots,l_{K-1}} \prod_{N=1}^{K-1} B^{N+1}_{l_N,l_{N+1}} \times \sum_{M=0}^{K} (e^{A^{M+1}t})_{l_M} \prod_{N=0}^{K} \frac{1-\delta_{N,M}}{A^{M+1}_{l_M} - A^{N+1}_{l_N}}, \tag{19}$$

where we consider that

$$\lim_{M\to N} \frac{1-\delta_{N,M}}{A^{M+1}_{l_M} - A^{N+1}_{l_N}} = 1. \tag{20}$$

III. DISCUSSION OF THE SECULAR TERMS

In this section we will discuss the conditions necessary for the secular terms to occur. If we consider (19) we see that it is much like the expansion coming from perturbation theory for the eigenvalues of a perturbed Hamiltonian $H = H_0 + \lambda H'$ in terms of the eigenvalues of H_0. It is well known that this expansion breaks down whenever you have degenerated states. A similar fact happens in (19) when we have

$$A^{M+1}_{l_M} = A^{N+1}_{l_N}. \tag{21}$$

In such a case the denominator in (19) goes to zero. However, due to the presence of the sum in M, we have two (or more) terms in (19) with the same denominator which will cancel each other, leading to an indetermination of the type 0/0 which is responsible for the secular terms. In order to see when (21) may occur, we have to consider that the eigenvalues A^M_m of A^M may be expressed in terms of the eigenvalues A^1_n of A^1 as[4,5]

$$A^M_m = \sum_{n=1}^{P} c_n A^1_n, \quad 0 < c_n \in \mathrm{N}, \quad \sum_{n=1}^{P} c_n = M. \tag{22}$$

So (22) indicates that (21) will be satisfied for large enough values of M and N provided

$$A^1_m / A^1_n = p/q, \quad p,q \in \mathbf{Z}, \tag{23}$$

for at least one pair of eigenvalues of A^1.

Before we start performing a detailed analysis of the occurrence of secular terms, we make simplifying changes in the notation and consider only the part of (19) that is relevant for the secular terms. So, for a given value for the set $\{l_\nu\}$ in (19) we consider the subset S^q_0 with $q+1$ elements of the set $\{A^{M+1}_{l_M}\}$ such that

$$S^q_0 = \{A^{M+1}_{l_M} | A^{M+1}_{l_M} = a_0\}. \tag{24}$$

We may consider, without loss of generality, that these elements are the $A^{M+1}_{l_M}$, $M = 0,1,\dots,q$, and will write henceforth

$$a_m = A^{M+1}_{l_M}. \tag{25}$$

Then the occurrence of secular terms for that particular choice of the $\{l_k\}$ will depend upon

$$Q^q_0 = \sum_{m=0}^{q} e^{a_m t} \prod_{n=0}^{K} \frac{1-\delta_{m,n}}{a_m - a_n}. \tag{26}$$

In (26) it is sufficient to take the sum until $m = q$, since the terms with $m = q+1, q+2,\dots,K$ do not contribute to the secular terms associated with the set S^q_0.

The evaluation of the Q^q_0 is performed by the usual limit procedures, e.g., by writing $a_n = a_0(1 + r_n)$, $n = 1,2,\dots,q$, and then taking the limit as $r_n \to 0$. As a result of the limit procedure we arrive at the expression

$$Q^q_0 = e^{a_0 t} \sum_{n=q+1}^{K} \frac{1}{a_0 - a_n} \sum_{s=0}^{q} \frac{t^s}{s!} \times \sum_{\substack{n_1,\dots,n_{q-s}=q+1 \\ n_1 > \dots > n_{q-s}}} \prod_{\alpha=1}^{q-s} \frac{1}{a_{n_\alpha} - a_0}. \tag{27}$$

We verify easily that (27) holds for low values of q, and for larger values we may proceed by induction to show that it is valid overall. This proof, though simple, is too lengthy to justify discussing the details here.

Now we recall the most important features, which indicate the number and the order of the secular terms that appear in any block $(e^{Mt})^{1,K}$. This time-evolution block is given by (19), in which several sums are to be taken over the set of indices $\{l_0, l_1,\dots,l_K\}$. For each set of values that these indices may assume, we ought to perform another sum over $M = 0,1,\dots,K$. We determine, for that particular choice of the $\{l_K\}$, the subsets $S^{q_0}_0, S^{q_1}_1,\dots,S^{q_t}_t$ of the set $\{A^{M+1}_{l_M}, M = 0,1,\dots,K\}$, such that all $q_n + 1$ eigenvalues belonging to a given $S^{q_n}_n$ are equal. Now in the sum over M we group together all those terms corresponding to the values of M for which the $A^{M+1}_{l_M}$ belong to the same set $S^{q_n}_n$, and call this group of terms $Q^{q_n}_n$. Each of the $Q^{q_n}_n$ will contain secular terms of maximal order t^{q_n}, whose general expression is given by (27). Now the highest-order secular term appearing in (19) for that particular choice of the $\{l_K\}$ is proportional to $t^{\bar{q}}$, where

$$\bar{q} = \max\{q_0, q_1,\dots,q_t\}. \tag{28}$$

The number of secular terms in $(e^{Mt})^{1,K}$ increases monotonically with the value of K. This block will contain all secular terms which had already appeared for lower K's and also new terms. These are due either to new eigenvalues that become equal, leading to secular terms associated with a new frequency, or to a larger number of equal eigenvalues already present in former blocks, which lead to a higher-order term associated with that frequency.

IV. EXAMPLE

We have undertaken an analysis of the Hénon–Heiles[4,5] model along the lines described in Sec. II and III. Several approximations for the trajectories have been evaluated, by considering different cutoffs of the matrix M. For each cutoff we determined the blocks $(e^{Mt})^{1,K}$, and then approximate the solution. The model we worked with is described by the following Hamiltonian:

$$H(q_1,q_2,p_1,p_2) = \tfrac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + q_1^2 q_2 - q_2^3/3. \tag{29}$$

This model is nonintegrable and the trajectories in the phase space are qualitatively different, depending upon the energy E of the system. In what follows we restrict the discussion to the cases where $E < \frac{1}{6}$. For energies far lower than $\frac{1}{6}$, the trajectories are confined to tori in the phase space. Increasing the energy until $E=\frac{1}{6}$ makes the trajectories leave the invariant tori and meander chaotically in the space among those most stable tori, which do exist until $E=\frac{1}{6}$. Despite the difference in the character of the trajectories for different values of E, all of them remain bounded in this range of energy.

If we write the equations of motion for the system described by (29), it turns out that the matrix A^1, which gives the linear part of the system is not diagonal, as the previous discussion affords it to be. We change then to a new coordinate basis in order that the matrix A^1 becomes a diagonal. In this new coordinate basis we have

$$Q_j = 2^{-1/2}(q_j - ip_j), \quad P_j = 2^{-1/2}(q_j + ip_j). \tag{30}$$

The eigenvalues of A^1 are $\pm i$, each one double degenerate. This indicates, according to (22), that the eigenvalues of A^M will be of the form

$$i(M-2m), \quad m = 0,1,\ldots,M. \tag{31}$$

The nonlinear part is described by the matrices B^N, as indicated in (2). It is originated by the cubic terms in the Hamiltonian.

Now we consider several approximations. An sth-order approximation takes into account the first $s+1$ blocks A^M and s blocks B^M. The zeroth-order approximation is that which considers no informations of the nonlinear part. The trajectories are the same as for the harmonic oscillator, and expressed by trigonometric funtions of t.

The first-order trajectories are still limit cycles, but now they contain harmonic contributions. There is still no secular term at this order, for there is no degeneracy between the eigenvalues of A^1 and those of A^2. We write below the time evolution for q_1 at this approximation

$$\begin{aligned} q_1^{(1)}(t) = {} & q_1^{(0)}(t) + (\tfrac{2}{3} q_1^0 q_2^0 + \tfrac{4}{3} p_1^0 p_2^0)\cos t \\ & - \tfrac{2}{3}(p_1^0 q_2^0 + p_2^0 q_1^0)\sin t + \tfrac{1}{3}(q_1^0 q_2^0 - p_1^0 p_2^0)\cos 2t \\ & + \tfrac{1}{3}(p_1^0 q_2^0 + q_1^0 p_2^0)\sin 2t - (q_1^0 q_2^0 + p_1^0 p_2^0), \end{aligned} \tag{32}$$

where superscript 0 indicates the values of the coordinates at $t=0$. In terms of the accuracy, this approximation is equivalent to that presented by Steeb[2] for the Lotka–Volterra model.

The second-order approximation gives trajectories which do contain secular terms of the type $t \sin t$ and $t \cos t$. Hence they are not limit cycles, but open orbits which revolute with increasing amplitude. The presence of these terms is due to the occurrence of the cases $A^1_{l_0} = A^3_{l_2} = \pm i$ in the sums of expression (19). The approximation also includes higher harmonic contributions, as becomes clear in the expression below for the $q_1(t)$ when $q_2^0 = p_2^0 = 0$:

$$\begin{aligned} q_1^{(2)}(t) = {} & q_1^{(1)}(t) + \tfrac{1}{48}(q_1^{03} - 3q_1^0 p_1^{02})\cos 3t \\ & + \tfrac{1}{9}(q_1^{03} + 4q_1^0 p_1^{02})\cos 2t \\ & + \tfrac{1}{144}(29q_1^{03} - 55q_1^0 p_1^{02})\cos t \\ & - q_1^{03}/3 + \tfrac{5}{12}(q_1^{03} + q_1^0 p_1^{02})t \sin t \\ & + \tfrac{1}{48}(3p_1^0 q_1^{02} - p_1^{03})\sin 3t \\ & + \tfrac{1}{9}(2p_1^{03} - p_1^0 q_1^{02})\sin 2t \\ & + \tfrac{1}{144}(5p_1^{03} + 65p_1^0 q_1^{02})\sin t \\ & - \tfrac{5}{12}(p_1^{03} + p_1^0 q_1^{02})t \cos t. \end{aligned} \tag{33}$$

The next approximation would consider four diagonal blocks. We have not worked out this case explicitly, but we are in a position to indicate which terms it will contain, based on the results of the previous sections. In the case of four blocks, besides those terms already present in (33), there would appear two more terms, which are linked with the cases $A^2_{l_1} = A^4_{l_3} = 0, \ \pm 2i$ in (19). Such analysis may be extended to higher-order approximations with the following general result: the blocks $(e^{Mt})^{1,K}$ will contain secular terms of maximal order L, when $K = 2L$ or $K = 2L + 1$.

We should consider two points about the presence of secular terms in the approximate solutions of the Hénon–Heiles system. The first has already been partially referred to in the Introduction; they indicate a growing amplitude, whereas the orbits are bounded for values of $E < \frac{1}{6}$.

The second is connected to other general aspects of the trajectories of the system. They are not limit cycles, and the time interval between two successive intersections with a plane in the phase space oscillates around 2π. If there were no secular terms, the approximate trajectories would be limit cycles with period 2π at any order considered, since all eigenvalues of M are of the form given by (31). That would not agree even qualitatively with the observed picture. So the presence of secular terms seems to be necessary and is, perhaps, the only way this method can display nonperiodicity and other nonlinear features of the solution of the system. An infinite number of such terms will certainly sum up to give the right solution, but as long as we are faced with a finite number of terms, the problems discussed above for the solution (33) will appear.

V. CONCLUSIONS

We have discussed the occurrence of the secular terms in the solution of a system of nonlinear equations using the method of the Carleman embedding without any concomitant perturbation expansion. We have obtained the formal CE solution of the system under consideration and brought it to a form particularly useful for the analysis of the occurrence of secular terms. If we concentrate on the blocks of the type $(e^{Mt})^{1,K}$, which are responsible for the description of the trajectories, we show that these terms will occur whenever we have two (or more) equal eigenvalues which belong to different diagonal blocks A^L and A^N of the matrix M, with $L,N \leqslant K$.

The occurrence of secular terms in the blocks $(e^{Mt})^{1,K}$ is cumulative, since these blocks, for a given K, will contain all secular terms already present in the blocks with lower K, in addition to new terms. These new terms are due to the fact that either new eigenvalues become equal or the number of equal eigenvalues already present for lower K have increased. Since there is a well-known recurrence relations for the eigenvalues of A^N in terms of the eigenvalues of the block A^1, it turns out that it is quite simple to see which terms will appear in a given order of approximation of the solution.

We have illustrated the use of the general results obtained in this paper by presenting our early expressions for the approximate solution of the Hénon–Heiles system. The occurrence of secular terms has been explicitly shown for a second-order cutoff, and a general discussion of the presence of other secular terms for higher-order truncations has been presented.

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