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A COMPUTER PROGRAM FOR INTEGRALS OF MOTION

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PROGRAM SUMMARY

Title of program: COSTANTI DEL MOTO

Catalogue number: ACYO

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: UNIVAC 1106; *Installation*: Centro di Calcolo dell' Università, Milano, Italy

Operating system: UNIVAC 1106 EXEC 8

Program language: FORTRAN

High speed storage required: 42 000 words

No. of bits in a word: 36

Overlay structure: none

No. of magnetic tapes required: none

Other peripherals used: Card reader, line printer, card punch

No. of cards in combined program and test deck: 800

Card punching code: IBM 026

Keywords: astrophysics, celestial mechanics, classical mechanics, stellar systems, integrals of motion

Nature of physical problem
The classical problem of constructing formal integrals for a Hamiltonian of harmonic oscillators coupled by polynomial interactions is considered.

Method of solution
An algorithm recently proposed [1] is applied which allows very fast computation of the integrals.

Restrictions on the complexity of the problem
The restrictions, imposed by array dimensions, are described in detail in the long write up, section 3.6.

Typical running time
The computation of one integral up to order 8 for a model with 2 degrees of freedom required an execution time of about 25 s on the UNIVAC 1106.

Reference
[1] A. Giorgilli and L. Galgani, Cel. Mech. 17 (1978) 267.

LONG WRITE-UP

1. Introduction

Consider a Hamiltonian system with n degrees of freedom and Hamiltonian

$$H(x, y) = H^{(2)}(x, y) + H^{(3)}(x, y) + \ldots, \tag{1}$$

where $H^{(s)}(x, y)$, $s = 2, 3, \ldots$, is a homogeneous polynomial of degree s in the canonical variables $x, y \in \mathbf{R}^n$, and let in particular

$$H^{(2)} = \sum_{l=1}^{n} \tfrac{1}{2}\omega_l (x_l^2 + y_l^2) \tag{2}$$

where $\omega_1, \ldots, \omega_n \in \mathbf{R}$ are not all vanishing.

It is well known that if one considers the unperturbed system with $H = H^{(2)}$ (i.e., the one obtained by neglecting terms of order greater than 2 in eq. (1)), then the system is integrable, being in fact a system of uncoupled harmonic oscillators with frequencies $\omega_1, \ldots, \omega_n$. On the other hand, it is also well known that the whole system (1) is generally nonintegrable, and formal solutions by means of formal series expansions are in general divergent [1].

On the other hand, despite this fact, a considerable number of numerical experiments performed on Hamiltonian systems of the type (1), as well as on different dynamical systems (billiards, particular mappings and so on) produced evidence that weakly perturbed integrable systems exhibit a nearly integrable behaviour. In particular, much work has been devoted to investigate whether formal series solutions can describe this nearly integrable behaviour [2–4]. The answer to this question appears to be in many cases positive, in spite of the divergence of the formal expansions, and it has even been conjectured that these series are, in fact, asymptotic series [3].

Computer programs have been developed in order to perform the computation of the coefficients in formal expansions, an horrendous task to be performed by hand. They use essentially two methods. The first was proposed by Whittaker [5] and Cherry [6], and improved by Contopoulos [2] who applied it to the computer. It consists in constructing integrals of motion for the Hamiltonian (1) by solving the equation

$$\{H, \Phi\} = 0 \tag{3}$$

where $\{\cdot, \cdot\}$ denotes the Poisson bracket and $\Phi = \Phi^{(2)} + \Phi^{(3)} + \ldots$ is a power series. Equating terms of the same order in eq. (3) and introducing the linear operator D by $D = \{H^{(2)}, \cdot\}$, one obtains

$$D\Phi^{(2)} = 0,$$

$$D\Phi^{(s)} = -\sum_{k=1}^{s-2} \{H^{(2+k)}, \Phi^{(s-k)}\}_{s=3,4,\ldots} \tag{4}$$

and the system of equations can be solved in an iterative way. The main difficulty of this method is that its consistency is not evident a priori. Indeed the solution of eq. (4) exists only if the r.h.s. belongs to R, the range of the operator D. The consistency can be established only by observing that at any order s the solution is determined only up to an arbitrary term $\tilde{\Phi}^{(s)}$, with $D\tilde{\Phi}^{(s)} = 0$, and that this term can be determined in such a way that the condition above for the existence of the solution is satisfied at successive orders. This implies a complicated backwards and forwards procedure in order to perform the explicit computation.

This difficulty is overcome by the second method, proposed by Birkhoff [7] and applied to the computer by Gustavson [4]. It consists in performing a canonical transformation

$$x = \xi + \frac{\partial W}{\partial y}, \qquad \eta = y + \frac{\partial W}{\partial \xi}, \tag{5}$$

where ξ, η are the new variables, and $W(\xi, y) = W^{(3)} + W^{(4)} + \ldots$ is the generating function. The problem consists in determining the generating function W in such a way that the new Hamiltonian $\Gamma(\xi, \eta) = H(x(\xi, \eta), y(\xi, \eta))$ takes a simple form, the so called normal form. The integrals of motion can then be immediately found in the form

$$\Phi(\xi, \eta) = \sum_{l=1}^{n} \alpha_l I_l,$$

where $\alpha_1, \ldots, \alpha_n \in \mathbf{R}$ are suitably chosen, and $I_l = \frac{1}{2}(\xi_l^2 + \eta_l^2)$, and they can be expressed as power series in the old variables x, y via the canonical transformation (5). The disadvantage of this method consists in the fact that it requires an inversion of a series in order to put the canonical transformation (5)

in an explicit form, a cumbersome and time-consuming procedure.

The aim of the present paper is to apply in a computer program a method of construction of formal integrals which avoids any inversion and, at the same time, does not require the complicated procedure of the Contopoulos approach. This last method was proposed by Giorgilli and Galgani [8], and will be described in the following section. A similar approach was also proposed by Hori [9] and Deprit [10].

2. Description of the method

The purpose of this section is to give a short account of the method applied in the program. To this end, only those features of the method will be illustrated here, which are essential to the understanding of the program. For more details and proofs, the reader is referred to ref. [8].

2.1. The basic algorithm

Let Π be the space of all polynomials in the $2n$ canonical variables $x_1, \ldots, x_n, y_1, \ldots, y_n$, and assume that one has assigned a formal power series $\chi = \chi^{(3)} + \chi^{(4)} + \ldots \in \Pi$, where, as in the introduction, $\chi^{(s)}$ denotes a homogeneous polynomial of order s. Define then the operator $T_\chi : \Pi \to \Pi$ via the recursive formula

$$T_\chi f = f_0 + f_1 + \ldots, \tag{6}$$

where $f \in \Pi$ and

$$f_0 = f, \quad f_r = \sum_{k=1}^{r} \frac{k}{r} \{\chi^{(2+k)}, f_{r-k}\}; \tag{7}$$

here subscripts are used because f, and thus also f_1, $f_2, \ldots$, have in general no definite order. It can be proven that T_χ is linear, and preserves products and Poisson brackets, i.e. $T_\chi(f \cdot g) = T_\chi f \cdot T_\chi g$, $T_\chi\{f, g\} = \{T_\chi f, T_\chi g\}$ for $f, g \in \Pi$. The latter property implies that χ is the generating function of a canonical transformation. In addition, T_χ is invertible so that, given $H \in \Pi$ as in eqs. (1) and (2), there exists a unique $Z \in \Pi$ satisfying the equation

$$T_\chi Z = H. \tag{8}$$

Let now $\tilde{\Phi}$ be an integral of motion for the Hamiltonian Z, i.e. $\{Z, \tilde{\Phi}\} = 0$; then one has also $\{H, T_\chi \tilde{\Phi}\} = 0$, so that $\Phi = T_\chi \tilde{\Phi}$ is an integral of motion for the Hamiltonian H. The problem is thus reduced to determining a suitable power series χ in such a way that Z has a simple form, for example Birkhoff's normal form, for which integrals of motion are easily found.

2.2. The equation for the normal form and the generating function

Put now in eq. (8): $Z = Z^{(2)} + Z^{(3)} + \ldots$. Then, making use of the definition and of the properties of T_χ, by straightforward manipulations one obtains the equations

$$Z^{(2)} = H^{(2)}, \tag{9}$$

$$Z^{(s)} - D\chi^{(s)} = H^{(s)} + Q^{(s)}, \quad s = 3, 4, \ldots, \tag{10}$$

where $D \cdot = \{H^{(2)}, \cdot\}$, as defined in section 1, and

$$Q^{(s)} = \begin{cases} 0, & s = 3 \\ -\sum_{k=1}^{s-3} Z_k^{(s-k)} - \sum_{k=1}^{s-3} \frac{k}{s-2} \{\chi^{(2+k)}, Z_{s-k-2}^{(2)}\}, & \\ & s = 4, 5, \ldots \end{cases} \tag{11}$$

$$Z_k^{(s)} = \begin{cases} Z^{(s)}, & k = 0;\ s = 2, 3, \ldots \\ \sum_{j=1}^{k} \frac{j}{k} \{\chi^{(2+j)}, Z_{k-j}^{(s)}\}, & k = 1, 2, \ldots; \\ & s = 2, 3, \ldots; \end{cases} \tag{12}$$

thus for a fixed order $s \geqslant 3$ the r.h.s. of eq. (10), involving terms of Z and χ only up to order $s-1$, is known. Eq. (10) is our main equation, which allows the generating function χ and the normal form Z to be determined. Indeed, consider first the equation for the third order

$$Z^{(3)} - D\chi^{(3)} = H^{(3)}. \tag{10a}$$

Performing the canonical transformation to complex variables q, p defined by

$$x_l = \frac{1}{\sqrt{2}} (q_l + \mathrm{i} p_l), \qquad y_l = \frac{\mathrm{i}}{\sqrt{2}} (q_l - \mathrm{i} p_l) \qquad (l = 1, \ldots, n) \tag{13}$$

one obtains that $H^{(2)}$, defined by eq. (2), takes the form

$$H^{(2)} = \mathrm{i}\sum_{l=1}^{n} \omega_l q_l p_l \tag{14}$$

so that one has

$$D = \mathrm{i}\sum_{l=1}^{n} \omega_l \left(p_l \frac{\partial}{\partial p_l} - q_l \frac{\partial}{\partial q_l} \right) . \tag{15}$$

On the other hand, a homogeneous polynomial of degree s in x, y is transformed by eq. (13) in a homogeneous polynomial of the same degree in q, p, so that

$$H^{(3)} = \sum_{\substack{j,k \\ |j|+|k|=3}} \alpha_{jk} q^j p^k , \tag{16}$$

(here the multi-index notation has been used, i.e. $j \equiv (j_1, \ldots, j_n)$, $|j| = |j_1| + \ldots + |j_n|$ and analogously for k; $q^j p^k \equiv q_1^{j_1} \cdot \ldots \cdot q_n^{j_n}\ p_1^{k_1} \cdot \ldots \cdot p_n^{k_n}$) with known coefficients α_{jk}. Put now

$$Z^{(3)} = \sum_{j,k} \beta_{jk} q^j p^k$$

$$\chi^{(3)} = \sum_{j,k} \gamma_{jk} q^j p^k \tag{17}$$

with unknown coefficients β_{jk}, γ_{jk}, and observe that

$$D q^j p^k = -\mathrm{i}\omega \cdot (j-k) q^j p^k , \tag{18}$$

where

$$\omega \cdot (j-k) = \sum_{l=1}^{n} \omega_l (j_l - k_l),$$

so that eq. (10a) reads

$$\sum_{j,k} \beta_{jk} q^j p^k + \mathrm{i}\sum_{j,k} \omega \cdot (j-k) \gamma_{jk} q^j p^k$$

$$= \sum_{j,k} \alpha_{jk} q^j p^k \tag{19}$$

and it is to be solved for β_{jk} and γ_{jk}. This can be done in the following way:

Rule A: if $\omega \cdot (j-k) = 0$ put $\beta_{jk} = \alpha_{jk}$, $\gamma_{jk} = 0$;

if $\omega \cdot (j-k) \neq 0$ put $\beta_{jk} = 0$,

$$\gamma_{jk} = -\mathrm{i}\alpha_{jk} / \omega \cdot (j-k) .$$

This simple rule works obviously also for any order s, and can be stated, more formally, in the following way. First one remarks that, via the canonical transformation (13), the operator D takes a diagonal form, and its domain Π splits into its range $R = \{q^j p^k : \omega \cdot (j-k) \neq 0\}$ and null space $N = \{q^j p^k : \omega \cdot (j-k) = 0\}$; then one solves eq. (10) with the supplementary condition that Z be in normal form, i.e., by definition, $Z \in N$. This condition immediately implies that

$$Z^{(s)} = (H^{(s)} + Q^{(s)})_{\mathrm{N}} ,$$

$$D\chi^{(s)} = (H^{(s)} + Q^{(s)})_{\mathrm{R}} , \tag{20}$$

where the subscripts N and R denote the null space part and the range part respectively; finally the solution for $\chi^{(s)}$ is made unique by requiring furthermore that $\chi^{(s)} \in R$. This is indeed the classical solution of Birkhoff and Gustavson.

Let me now recall what a resonance relation is. One says that among the frequencies ω there exists a resonance relation if there exist n integers $m_1, \ldots, m_n$, not all vanishing, such that

$$m \cdot \omega \equiv \sum_{l=1}^{n} m_l \omega_l = 0 . \tag{21}$$

Let me illustrate it with two typical examples with $n = 2$. If $\omega_1 = \sqrt{2}$, $\omega_2 = 1$, then eq. (21) holds only with $m_1 = m_2 = 0$, i.e. the frequencies are nonresonant. If instead $\omega_1 = 2$, $\omega_2 = 1$, then $\omega_1 - 2\omega_2 = 0$ holds. Now, the null space N depends critically on the existence of resonance relations. Thus in the first case a term $q^j p^k$ belongs to N if and only if $j = k$, so that for example no term of odd order belongs to N; in the second case instead one has that both $j = (1, 0)$, $k = (0, 2)$ and $j = (0, 2)$, $k = (1, 0)$ give $\omega \cdot (j-k) = 0$, so that both $q_1 p_2^2$ and $q_2 p_1^2$, of odd order, belong to N. The normal form then differs in the two cases, because by the first equation (20) one has $Z^{(3)} = 0$ in the first case and $Z^{(3)} \neq 0$ in general in the second case.

Let me now remark that other solutions are possible which bring Z into a simple form. Indeed observe that, in rule A, only the first part is necessarily required by eq. (10) (otherwise one would have a null denominator in γ_{jk}), while the second is arbitrary. In order to exploit this arbitrariness, while keeping the first part, let me introduce an n-tuple of real numbers $\mu \equiv (\mu_1, \ldots, \mu_n)$ which I call "pseudo-frequencies",

with the condition that they satisfy all the resonance relations satisfied by ω, i.e. that $m \cdot \omega = 0$ implies $m \cdot \mu = 0$. Thus for any such a μ one obtains a solution to eq. (10) if one simply changes rule A in the following:

Rule B: if $\mu \cdot (j-k) = 0$ put $\beta_{jk} = \alpha_{jk}, \gamma_{jk} = 0$

if $\mu \cdot (j-k) \neq 0$ put $\beta_{jk} = 0$,

$$\gamma_{jk} = -i\alpha_{jk}/\omega \cdot (j-k) .$$

Obviously, one must be sure that the denominator in γ_{jk} is never zero, but this is exactly the condition above that $m \cdot \omega = 0$ implies $m \cdot \mu = 0$.

This rule can be enunciated in a more formal way by introducing the null space $N_\mu = \{q^j p^k : \mu \cdot (j-k) = 0\}$ and the range $R_\mu = \{q^j p^k : \mu \cdot (j-k) \neq 0\}$ corresponding to the operator

$$D_\mu = i \sum_{l=1}^{n} \mu_l (p_l \partial/\partial p_l - q_l \partial/\partial q_l),$$

(so that N, R and D above should be denoted by N_ω, R_ω and D_ω for notational coherence) and by observing that if the relation $m \cdot \omega = 0$ implies $m \cdot \mu = 0$ then one has $N \subset N_\mu$. Thus the new rule consists in solving eq. (10) with the condition $Z \in N_\mu$, $\chi \in R_\mu$, i.e. by simply replacing in eq. (20) N by N_μ and R by R_μ.

In order to illustrate the usefulness of this new solution, consider again $n = 2$, $\omega_1 = 2$, $\omega_2 = \sqrt{1.001}$, so that the frequencies are nonresonant, but close to the resonance $\omega_1 - 2\omega_2 = 0$. If rule A is used, then in the expression for χ small denominators of the form $\omega_1 - 2\omega_2$ will appear. If however two numbers (pseudo-frequencies) $\mu_1 = 2$, $\mu_2 = 1$ are introduced and rule B is applied, then those small denominators will not appear, and Z will contain the same terms which would be generated if ω_1 and ω_2 were exactly resonant. In other words, the construction will be reminiscent of the quasi resonance, because it will be performed as if the system were resonant.

2.3. Construction of the integrals

Once the generating function χ and the normal form Z have been constructed, it is an easy matter to find integrals of motion, recalling that, if $\tilde{\Phi}$ is an integral for Z, i.e. one has $(\tilde{\Phi}, Z) = 0$, then $\Phi = T_\chi \tilde{\Phi}$ is an integral for the Hamiltonian $H = T_\chi Z$. Indeed, let $\mu \in \mathbf{R}^n$ be fixed (in particular one can take $\mu = \omega$, corresponding to rule A); then, as already observed, the condition $Z \in N_\mu$ amounts to say that Z contains only terms $q^j p^k$ for which $\mu \cdot (j-k) = 0$. Consider now an expression of the form

$$\tilde{\Phi} = i \sum_{l=1}^{n} \alpha_l q_l p_l \qquad \text{with } \alpha \in \mathbf{R}^n,$$

and observe that

$$\{\tilde{\Phi}, q^j p^k\} = -i\alpha \cdot (j-k) q^j p^k . \tag{22}$$

Then $\tilde{\Phi}$ is an integral of motion for Z if the expression (22) vanishes for all $q^j p^k \in N_\mu$, i.e. for all possible terms of Z. This is possible if $m \cdot \alpha = 0$ for all m for which $m \cdot \mu = 0$.

Thus the following result is obtained: if μ is nonresonant, there exist n independent integrals $\tilde{\Phi}$ for Z, namely the n quantities

$$\Phi_l^{(2)} = \tfrac{1}{2}(x_l^2 + y_l^2) , \qquad l = 1, \ldots, n; \tag{23}$$

if μ is resonant, and there exist r independent integer vectors $m \neq 0$ for which $m \cdot \mu = 0$, then one has $n - r$ independent integrals $\tilde{\Phi}$ for Z of the form

$$\Phi_i^{(2)} = \sum_{l=1}^{n} \tfrac{1}{2}\alpha_l^{(i)}(x_l^2 + y_l^2) \quad i = 1, \ldots, n-r, \tag{24}$$

where $\alpha^{(i)} \equiv (\alpha_1^{(i)}, \ldots, \alpha_n^{(i)}) \in \mathbf{R}^n$ are $n - r$ independent vectors such that $m \cdot \alpha = 0$ for all m for which $m \cdot \mu = 0$. Integrals of motion for H are finally obtained by computing

$$\Phi = T_\chi \tilde{\Phi} = \Phi^{(2)} + \Phi^{(3)} + \ldots, \tag{25}$$

where $\tilde{\Phi}$ is an integral for Z, and, according to the definition of T_χ given in eqs. (6), (7), one has

$$\Phi^{(2)} = \tilde{\Phi},$$

$$\Phi^{(s)} = \sum_{k=1}^{s-2} \frac{k}{s-2} \{\chi^{(2+k)}, \Phi^{(s-k)}\} , \quad s > 2 . \tag{26}$$

For example, consider again the case $n = 2$ with $\omega_1 = 2$, $\omega_2 = \sqrt{1.001}$. If the "nonresonant" construction (rule A) has been performed for Z and χ, then one can build two integrals starting from $\Phi_1^{(2)} = \frac{1}{2}(x_1^2 + y_1^2)$ and $\Phi_2^{(2)} = \frac{1}{2}(x_2^2 + y_2^2)$ respectively. Instead, if the "resonant" construction has been per-

formed with $\mu_1 = 2, \mu_2 = 1$, then only the integral can be built which starts from $\Phi^{(2)} = \frac{1}{2}\mu_1(x_1^2 + y_1^2) + \frac{1}{2}\mu_2(x_2^2 + y_2^2)$.

The three integrals so built are not independent, as will be explained in the following section. However, as explained above, the small denominators $\omega_1 - 2\omega_2$ which appear in the generating function χ in the non-resonant construction are absent in the resonant one, so that the latter integral also will be free from small denominators of the said type. The loss of an integral is the price paid for eliminating them.

2.4. A note on the number of independent integrals

For what concerns the nonresonant case, i.e. the case where the frequencies ω are nonresonant and rule A has been adopted, the procedure described in the preceding sections solves completely the problem of finding integrals for the Hamiltonian (1), because n independent formal integrals have been found which are in involution, i.e. with $\{\Phi_l, \Phi_k\} = 0$, ($l, k = 1, ..., n$), so that the system is formally integrable [11]. Obviously, other different integrals can be found, which however are not independent of $\Phi_1, ..., \Phi_n$. This is easily seen if one observes that the transformation T_χ defined in eqs. (6), (7) generates an integral if it is applied to any $\tilde{\Phi}$ such that $\{\tilde{\Phi}, Z\} = 0$. But the latter condition implies exactly that $\tilde{\Phi}$ is a formal series in the n quantities $\Phi_1^{(2)}, ..., \Phi_n^{(2)}$ above. Conversely, if Φ is an integral of motion for H, i.e. one has $\{\Phi, H\} = 0$, then, by the properties of the operator T_χ, there exists a $\tilde{\Phi}$ such that $\Phi = T_\chi\tilde{\Phi}$, and $\{\tilde{\Phi}, Z\} = 0$, i.e. $\tilde{\Phi}$ is a formal series in $\Phi_1^{(2)}, ..., \Phi_n^{(2)}$. For example, H itself is an integral of motion for H generated by $\tilde{\Phi} = Z$, as stated by eq. (8). This can be sufficient to justify the usefulness of the choice made above that the integrals built be a perturbation of second order terms. Moreover, an additional argument of interest for this particular choice is that the integrals thus built are just the action integrals of the system, as could be easily shown.

The discussion is not so simple in the resonant case. Indeed, choose a particular μ with r independent resonance relations. Then only $n - r$ integrals in involution can be built by the method described above. However, the energy integral can be added, since it is independent of the $n - r$ integrals above. This can be established by recalling the characterization given for N_μ in complex variables, from which it follows that Z contains terms $q^j p^k$ such that $\mu \cdot (j - k) = 0$ with $j \neq k$, and so it cannot be expressed as a power series in the $\Phi_l^{(2)}$'s given by eq. (24). For what concerns the existence of other integrals, one can observe that the $\Phi_l^{(2)}$'s have been so constructed that $\{\Phi_l^{(2)}, f\} = 0$ for any $f \in N$. This is obviously too strong a condition, which ensures the existence of $n - r$ independent integrals for a general Z, but does not ensure the nonexistence of other integrals independent of those above for a particular Z. But this is, to my knowledge, an open problem.

3. Computer code

3.1. Representation of polynomials

A machine representation of polynomials in several variables is obviously an essential device in performing the computations above. This is obtained in the following way: the coefficient $\alpha_{j_1,...,j_m}$ ($\alpha_{j_1,...,j_m} \in \mathbf{R}$, $j_1, ..., j_m$ non-negative integers) of the term $x_1^{j_1} \cdot ... \cdot x_m^{j_m}$ in a polynomial in the m variables $x_1, ..., x_m$ is stored in a one-dimensional array at the relative address $i(j_1, ..., j_m)$ given by the formula

$$i(j_1, ..., j_m) = \sum_{l=1}^{m} \binom{l - 1 + \sum_{k=0}^{l-1} j_{m-k}}{l}, \qquad (27)$$

where

$$\binom{k}{l} = \begin{cases} 0 & k < l \\ \dfrac{k!}{l!(k-l)!}, & k \geqslant l \end{cases}$$

is the binomial coefficient; this establishes a one-to-one correspondence between non-negative integers and m-tuples of exponents in a polynomial.

In the program this representation is afforded by three subprograms:

i. subroutine BINOM, which is called only once at the beginning of the program; it computes the table of the binomial coefficients and stores them in a common block. Its calling sequence is

   CALL BINOM(NLIB,NORD)

   where NLIB is the number of variables in the polynomials, and NORD the maximum order of the polynomials.

ii. function INDICE, which computes $i(j_1, ..., j_m)$ as given by eq. (27). Its FORTRAN reference is

i = INDICE(J,NLIB)

where J is the integer array of the exponents $j_1, ..., j_m$ and NLIB the number of variables.

iii. subroutine ESPON, which performs the inverse mapping of eq. (27), i.e., given i, computes $j_1, ..., j_m$. Its calling sequence is

CALL ESPON(I,J,NLIB)

where I, integer, is the relative address in the one-dimensional representation of the polynomial, NLIB is the number of independent variables and J is the integer array of the NLIB exponents which correspond to the index I, and are computed in the subroutine.

Since in the Hamiltonian case the variables x, y are canonically conjugate, they are ordered as $x_1, ..., x_n$, $y_1, ..., y_n$, so that one works with polynomials in $2n$ variables, where n is the number of degrees of freedom.

3.2. *Normal form and generating function*

The procedure described in section 2.2 for computing the normal form and the generating function is performed by subroutine NORGEN. Input to this subroutine are essentially:

i. the coefficients of the Hamiltonian, stored in the real array H;
ii. the harmonic frequencies ω, stored in the real array OMEGA;
iii. the vector μ which determines the subspace N_μ to which the normal form must belong, stored in the integer array MU.

Output from this subroutine are:

i. the normal form Z, whose coefficients are stored in the real array GAMMA;
ii. the generating function χ, whose coefficients are stored in the real array CHI.

This subprogram computes the r.h.s. of eq. (10) as given by eqs. (11) and (12). Then eq. (10) is solved by subroutine DMEN1 in two steps. First the canonical transformation (13) is performed which diagonalizes the operator D; then the terms of N_μ and R_μ are separated, and the quantities Z and χ computed by performing the inverse transformation of eq. (13).

The way in which the terms of N_μ and R_μ are separated requires some additional explanation. Indeed, two problems are involved, namely:

i. the possibility of choosing between rule A or B of section 2.2 in performing the construction;
ii. the fact that the concepts of exact resonance and nonresonance are meaningless for the computer; this is in fact the problem of deciding, with the floating arithmetics of the computer, if an expression of the form $m \cdot \mu$ vanishes or not.

The first problem has a trivial solution. It is sufficient to introduce, in addition to the set of frequencies ω which depend on the Hamiltonian, also the set of pseudo-frequencies μ which can be freely chosen by the programmer. The only important thing is to have in mind that the choice of μ is subject to the restriction that it must satisfy all the resonance relations satisfied by ω (see section 2.2). Thus, one can use rule A by choosing μ proportional to ω (or having exactly the same resonances); if however μ is chosen to be more resonant than ω, then rule B is used.

The second problem can be solved simply by using integer arithmetic instead of floating arithmetic, i.e. by defining μ as an integer vector. This technical trick obviously works in the completely resonant case (i.e. $n-1$ resonance relations for n degrees of freedom), because then there exists an n-tuple of integers proportional to ω. For what concerns the non-completely resonant case (in particular the non-resonant one), observe that, as previously noted, the resonant terms, i.e. the terms which belong to N_μ because of the resonance, are the terms $q^j p^k$, in complex variables diagonalizing D, for which $\mu \cdot (j-k) = 0$ with $j \neq k$. Define now, for a resonant μ, the order of resonance r as being $r = \inf_{m \cdot \mu = 0}^{m \neq 0} |m|$, with $m \in \mathbf{Z}^n$, where $|m| = |m_1| + |m_2| + ... + |m_n|$. Then it is evident that a resonant term cannot appear in a series expansion at an order lower than r. This means that, if the series are considered up to an order s, a resonance of order $r > s$ is equivalent to a nonresonance. So, for example, if $n = 3, s = 8$ and the ω's are nonresonant, choosing $\mu_1 = 1, \mu_2 = 10, \mu_3 = 100$ ensures that the system will be treated as if it were nonresonant. In an analogous way one proceeds in a case of partial resonance. For example, if $n = 3, s = 8, \omega_1 = 2, \omega_2 = 1, \omega_3 = \sqrt{1.001}$, one can choose $\mu_1 = 2, \mu_2 = 1, \mu_3 = 20$, using thus rule A; if one wants instead to use rule B one can take $\mu_1 = 2, \mu_2 = 1, \mu_3 = 1$.

3.3. Integrals of motion

Finally, the procedure described in section 2.3 is applied to generate the integrals of motion, by using the (already determined) generating function χ. This is performed by the subprogram SERIE. Input to this subprogram are the coefficients of the generating function and of the lowest order terms of the integral. Output are the coefficients of the expansion of the integral. The only nontrivial thing in this connection is the way in which the lowest order terms $\tilde{\Phi}$ of the integral must be chosen. According to the explanation in section 2.3, this depends on the choice made for μ. If a "nonresonant" μ (in the sense explained above) was chosen, then the lowest order term of the integral can be $\Phi_l^{(2)} = \frac{1}{2}(x_l^2 + y_l^2)$, $(l = 1, ..., n)$ and n independent integrals can be found. If however a μ was chosen which satisfies r independent resonance relations, then $n - r$ independent integrals can be built which start from

$$\Phi_i^{(2)} = \sum_{l=1}^{n} \tfrac{1}{2}\alpha_l^{(i)}(x_l^2 + y_l^2),$$

where the $\alpha^{(i)}$ are $n - r$ linearly independent vectors of $\mathbf{R}^n$ such that $m \cdot \mu = 0$ implies $m \cdot \alpha = 0$ for any $m \in \mathbf{Z}^n$.

3.4. Program input

Input to the program is on cards. They must be submitted in the following order:

Card 1: format (2I5)
NPART = number of the degrees of freedom;
NORD = maximum order in the series.

Card 2: format (10I8)
MU = integer array μ of the resonance relations, which determines the subspace N_μ to which the normal form must belong. Only the first NPART elements of MU are utilized in computation. The rules to fix these numbers are specified in section 3.2.

Group of cards 3: format (20I2, E25.10)
This is not a single card, but a group of several cards which contain the non-vanishing coefficients of the Hamiltonian, one coefficient per card. Note that the second order term of H must be as in formula (2). Any card must contain: J = integer array with dimension 20 of the exponents $j_1, ..., j_n, k_1, ..., k_n$ of the term $x_1^{j_1} \cdot ... \cdot x_n^{j_n} y_1^{k_1} \cdot ... \cdot y_n^{k_n}$ in the polynomial. The program reads 20 integers, but utilizes only the first 2×NPART of them. X = the real coefficient corresponding to the exponents J.
No restriction is imposed on the number of coefficients that can be read.

Card 4: a blank card
The program knows that there are no more coefficients for H when all the exponents read are zero. So this card stops the loop which reads the coefficients and allows execution to continue.

Card 5: format (2I5)
Print/punch flags for the generating function CHI. JST = 1 or 0. If JST = 1, then the coefficients of CHI are printed; if JST = 0 they are not printed. JSC = 1 or 0. If JSC = 1, then the nonvanishing coefficients of CHI are punched on cards; if JSC = 0 they are not punched.

Card 6: format (2I5)
Print/punch flags for the normal form GAMMA. See card 5.

Card 7: format (2I5)
Print/punch flags for an integral. See card 5.

Group of cards 8: format (20I2, E25.10)
Coefficients of the lowest order term of an integral, all of the same order (see section 3.3). The format is the same as for the Hamiltonian, cards 3.

Card 9: a blank card
See card 4.

The set of cards 7, 8, 9 must be repeated for any integral one wants to compute. There is no restriction on the number of integrals one can compute. The program stops when an attempt is made to read a nonexisting card 7. To this end, a facility of FORTRAN IV and V, i.e. transfer of control in a READ statement, is used.

All cards are read in the main program, apart from the set 2, 3, 4 which are read in subroutine HAMILT. The purpose of this subroutine is simply to define:

i. the real array of the harmonic frequencies OMEGA and the integer array of the resonance relations MU, stored in the common block/FREQ/;
ii. the coefficients of the Hamiltonian, stored in the array H.

Thus, if for example one has an analytical Hamiltonian not already expanded in power series as in eqs. (1), (2), one can replace this subroutine with a suitable

one which performs the expansion, and defines the arrays OMEGA, MU and H.

3.5. Program output

Output from the program is, optionally, on paper and/or cards, according to the flags specified in cards 5, 6, 7.

The coefficients of the various functions are printed by subroutine STAMPA in the same order as they are requested, in groups of at most 4 functions at a time. On every line the relative address in the array (i.e. the index i given by (27)), the exponents of $x_1, \ldots, x_n, y_1, \ldots, y_n$ and the corresponding coefficient(s) are printed. Lines of vanishing coefficients are omitted.

If an array is requested to be punched, then the subroutine SCHEDE is called which punches the relative address I and the corresponding coefficient F(I) in groups of 4 per card, with format (4(I5, E15.8)); only nonvanishing coefficients are punched. The cards containing the coefficients are preceded by a set of three blank cards, a card with asterisks and two blank cards, so that sets of coefficients corresponding to different arrays can be easily separated. Note that the exponents are not punched. So, in order to utilize these cards, it is necessary to use the routines BINOM and ESPON described in section 3.1.

3.6. Limitations of the program

The main limitation is imposed on the program by the amount of core required in order to store the polynomials. They are all stored in a unique array called F whose dimension is fixed in the main program. The dimension required for F depends on NPART and NORD according to the formula

$$N(n, k) = (k + 3)\binom{2n + k}{2n} - \binom{2n + k}{2n + 1} + 2n - 3 , \quad (28)$$

where n stands for NPART, k for NORD and N is the dimension of F. A table of the values of $N(n, k)$ for some current values of n and k is given in table 1. The dimension 30 000 given for F in the present program is sufficient for many interesting cases. If one changes the dimension of F, it is necessary to change also the DATA statement which initializes F with zeros. No other changes are required.

Other limitations imposed in the program are the following:

i) NPART cannot exceed 10;
ii) NORD cannot exceed 15;
iii) the quantity NORD + 2×NPART cannot exceed 25.

Changing these limits would require changing correspondingly various formats, dimensions and other features scattered through the program.

Table 1
Values of N(n, k) for some current values of n and k

k \ n	1	2	3	4	5	6	7	8	9	10
3	49	190	471	940	1645	2634	3955	5656	7785	10390
4	84	435	1353	3250	6650	12189	20615	32788	49680	72375
5	132	883	3369	9586	22666	47133	89159			
6	195	1639	7527	25030	67711					
7	275	2839	15447	59350						
8	374	4654	29604							
9	494	7294	53628							
10	637	11012	92667							
11	805	16108								
12	1000	22933								
13	1224	31893								
14	1479	43453								
15	1767	58141								

If the condition i) or iii) is violated the diagnostic "ERRORE SUB BINOM" is printed and the program stops. This is because the dimensions allowed for the table of the binomial coefficients would be exceeded. Another program stop could possibly occur with the diagnostic "ERRORE SUB ESPON". This means that an attempt has been made to find the exponents corresponding to an index i which exceeds the maximum one, implicitly fixed by NPART and NORD. This should not occur in the program, but can occur if improper use of this subroutine is made in other programs (for example programs utilizing the coefficients of the integrals).

3.7. Running time

The running time depends on various parameters (the degree NORD, the number of degrees of freedom, the number of nonvanishing coefficients generated, ...), and no typical running time can be indicated. However, for example, the computation of one integral up to order 8 for a model with 2 degrees of freedom required an execution time of about 25 s on the UNIVAC 1106 and 0.3 s on the CDC CY76; for 3 degrees of freedom and 3 integrals up to order 11 the time was about 70 s on the CDC CY76.

3.8. Test run

The test run computes one integral up to order six for the Hamiltonian

$$H(x, y) = \tfrac{1}{2}(x_1^2 + y_1^2) + \tfrac{1}{2}(x_2^2 + y_2^2) + x_1^2 x_2 - \tfrac{1}{3}x_2^3$$

with two degrees of freedom, and prints the coefficients of the generating function, the normal form and the integral whose lowest order term is

$$\Phi^{(2)} = \tfrac{1}{2}(x_1^2 + y_1^2) + \tfrac{1}{2}(x_2^2 + y_2^2) .$$

This is the only integral that can be constructed, according to what was said in section 2.3. The first column of coefficients corresponds to the generating function, the second to the normal form and the third to the integral.

Coming now to a short discussion of the results, one sees that, among the coefficients of the integral, the normal form and the generating function, one finds four coefficients of the order 10^{-8} or 10^{-9} (three at order 3 and one at order 5). These are due to numerical errors. Indeed, in the same computation performed in double precision, only these four terms did change, and they became of the order 10^{-18} or 10^{-19}.

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TEST RUN OUTPUT

```
 NUMBER OF DEGREES OF FREEDOM        2

 THE SERIES ARE TRUNCATED AT ORDER   6

 HARMONIC FREQUENCIES              RESONANCE RELATIONS

 1 .    1.000000+00                        1

 2 .    1.000000+00                        1

      C O E F F I C I E N T S   O F   O R D E R     2

 5   2  0  0  0     0.000000        5.000000-01     5.000000-01
 9   0  2  0  0     0.000000        5.000000-01     5.000000-01
12   0  0  2  0     0.000000        5.000000-01     5.000000-01
14   0  0  0  2     0.000000        5.000000-01     5.000000-01

      C O E F F I C I E N T S   O F   O R D E R     3

16   2  1  0  0     0.000000        0.000000        1.000000+00
18   2  0  0  1    -3.333333-01     0.000000        0.000000
20   1  1  1  0    -6.666667-01     0.000000        0.000000
23   1  0  1  1     0.000000        0.000000        1.490116-08
25   0  3  0  0     0.000000        0.000000       -3.333333-01
27   0  2  0  1     3.333333-01     0.000000        0.000000
28   0  1  2  0     0.000000        0.000000        7.450581-09
30   0  1  0  2     0.000000        0.000000       -1.490116-08
32   0  0  2  1    -6.666667-01     0.000000        0.000000
34   0  0  0  3     2.222222-01     0.000000        0.000000

      C O E F F I C I E N T S   O F   O R D E R     4

35   4  0  0  0     0.000000       -1.041667-01     1.041667-01
37   3  0  1  0     6.250000-02     0.000000        0.000000
39   2  2  0  0     0.000000       -2.083333-01     2.083333-01
41   2  1  0  1     6.250000-02     0.000000        0.000000
42   2  0  2  0     0.000000       -2.083333-01     2.083333-01
44   2  0  0  2     0.000000        3.750000-01    -3.750000-01
46   1  2  1  0     6.250000-02     0.000000        0.000000
49   1  1  1  1     0.000000       -1.166667+00     1.166667+00
51   1  0  3  0     1.041667-01     0.000000        0.000000
53   1  0  1  2     1.041667-01     0.000000        0.000000
55   0  4  0  0     0.000000       -1.041667-01     1.041667-01
57   0  3  0  1     6.250000-02     0.000000        0.000000
58   0  2  2  0     0.000000        3.750000-01    -3.750000-01
60   0  2  0  2     0.000000       -2.083333-01     2.083333-01
62   0  1  2  1     1.041667-01     0.000000        0.000000
64   0  1  0  3     1.041667-01     0.000000        0.000000
65   0  0  4  0     0.000000       -1.041667-01     1.041667-01
67   0  0  2  2     0.000000       -2.083333-01     2.083333-01
69   0  0  0  4     0.000000       -1.041667-01     1.041667-01
```

C O E F F I C I E N T S O F O R D E R 5

71	4	1	0	0	0.000000	0.000000	4.166666-01
73	4	0	0	1	4.503086-01	0.000000	0.000000
75	3	1	1	0	-8.530864-01	0.000000	0.000000
78	3	0	1	1	0.000000	0.000000	1.166667+00
80	2	3	0	0	0.000000	0.000000	2.777777-01
82	2	2	0	1	-1.753704+00	0.000000	0.000000
83	2	1	2	0	0.000000	0.000000	-7.499999-01
85	2	1	0	2	0.000000	0.000000	-1.916667+00
87	2	0	2	1	1.574075-02	0.000000	0.000000
89	2	0	0	3	-5.743827-01	0.000000	0.000000
91	1	3	1	0	1.485185+00	0.000000	0.000000
94	1	2	1	1	0.000000	0.000000	1.166667+00
96	1	1	3	0	-8.537037-01	0.000000	0.000000
98	1	1	1	2	-8.537037-01	0.000000	0.000000
101	1	0	3	1	0.000000	0.000000	7.777778-01
103	1	0	1	3	0.000000	0.000000	-2.333333+00
105	0	5	0	0	0.000000	0.000000	-1.388889-01
107	0	4	0	1	1.342593-01	0.000000	0.000000
108	0	3	2	0	0.000000	0.000000	1.027778+00
110	0	3	0	2	0.000000	0.000000	-1.388889-01
112	0	2	2	1	8.694444-01	0.000000	0.000000
114	0	2	0	3	2.793210-01	0.000000	0.000000
115	0	1	4	0	0.000000	0.000000	-7.777778-01
117	0	1	2	2	0.000000	0.000000	2.333333+00
119	0	1	0	4	0.000000	0.000000	-7.450581-09
121	0	0	4	1	-3.351852-01	0.000000	0.000000
123	0	0	2	3	-2.234568-01	0.000000	0.000000
125	0	0	0	5	1.117284-01	0.000000	0.000000

C O E F F I C I E N T S O F O R D E R 6

126	6	0	0	0	0.000000	2.922454-02	1.417824-02
128	5	0	1	0	-3.302083-01	0.000000	0.000000
130	4	2	0	0	0.000000	-7.873264-01	1.334201+00
132	4	1	0	1	6.239583-01	0.000000	0.000000
133	4	0	2	0	0.000000	8.767362-02	-5.407986-01
135	4	0	0	2	0.000000	-2.282986-01	-6.623263-01
137	3	2	1	0	1.247917+00	0.000000	0.000000
140	3	1	1	1	0.000000	-1.118055+00	5.493055+00
142	3	0	3	0	-4.495370-01	0.000000	0.000000
144	3	0	1	2	2.133333+00	0.000000	0.000000
146	2	4	0	0	0.000000	6.710069-01	-8.185763-01
148	2	3	0	1	-1.932639+00	0.000000	0.000000
149	2	2	2	0	0.000000	-1.015625+00	1.421875+00
151	2	2	0	2	0.000000	7.343749-01	-3.828124+00
153	2	1	2	1	-6.736111-01	0.000000	0.000000
155	2	1	0	3	4.861111-01	0.000000	0.000000
156	2	0	4	0	0.000000	8.767362-02	-7.352430-01
158	2	0	2	2	0.000000	-1.015625+00	4.921875+00
160	2	0	0	4	0.000000	6.336803-02	1.379340+00
162	1	4	1	0	-9.663194-01	0.000000	0.000000
165	1	3	1	1	0.000000	1.215278+00	-1.506944+00
167	1	2	3	0	2.133333+00	0.000000	0.000000
169	1	2	1	2	-5.615277+00	0.000000	0.000000
172	1	1	3	1	0.000000	-1.118055+00	4.861099-02
174	1	1	1	3	0.000000	1.215278+00	-8.506944+00
176	1	0	5	0	-1.371528-01	0.000000	0.000000
178	1	0	3	2	1.086806+00	0.000000	0.000000
180	1	0	1	4	-5.908565-01	0.000000	0.000000
182	0	6	0	0	0.000000	-6.799768-02	1.576967-01

184	0	5	0	1	-1.215278-02	0.000000	0.000000
185	0	4	2	0	0.000000	6.336803-02	-1.537326+00
187	0	4	0	2	0.000000	-2.039930-01	3.342013-01
189	0	3	2	1	4.861111-01	0.000000	0.000000
191	0	3	0	3	9.953703-02	0.000000	0.000000
192	0	2	4	0	0.000000	-2.282986-01	2.448785+00
194	0	2	2	2	0.000000	7.343749-01	-1.494792+00
196	0	2	0	4	0.000000	-2.039930-01	3.342014-01
198	0	1	4	1	5.434028-01	0.000000	0.000000
200	0	1	2	3	-1.181713+00	0.000000	0.000000
202	0	1	0	5	8.969907-02	0.000000	0.000000
203	0	0	6	0	0.000000	2.922454-02	-2.450810-01
205	0	0	4	2	0.000000	-7.873264-01	2.473090+00
207	0	0	2	4	0.000000	6.710069-01	-2.874132+00
209	0	0	0	6	0.000000	-6.799768-02	1.114005-01