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**Gaussian Elimination Methods for
Calculating Classical Periodic
Trajectories in Two Dimensions**

K. T. R. Davies

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GAUSSIAN ELIMINATION METHODS FOR CALCULATING CLASSICAL
PERIODIC TRAJECTORIES IN TWO DIMENSIONS

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ABSTRACT

A Gaussian-elimination method for calculating classical periodic trajectories is formulated for a two-dimensional system. Two variants of the theory are obtained, one assuming that the *period* of the motion is fixed and the other assuming that the total *energy* is fixed. Comparisons are made between various approaches.

I. INTRODUCTION

A new algorithm was recently developed for calculating classical periodic trajectories.¹ It is based on the Monodromy matrix^{1,2} and has been particularly useful in calculations of *nonintegrable*, two-dimensional Hamiltonians.^{2–8} This Monodromy method^{1,2} involves 4×4 matrices, and one might ask whether it is possible to solve the problem in a two-dimensional space. Of course, the dimension of four in the method is just that of the phase space; alternatively, for a second-order differential equation (in time) one needs initially to specify two coordinates and two momenta. However, there is a certain amount of “overkill” in this approach since the periodic boundary conditions should, in principle, allow one to eliminate two degrees of freedom. In fact, for analogous one-dimensional problems (with a two-dimensional phase space) in which the boundary conditions are *fixed*, Gaussian elimination in one dimension allows one to solve very efficiently the equations of motion.⁹

In Section II of this report we generalize this Gaussian-elimination method to two dimensions and then, by introducing an additional recursion, treat the case of periodic boundary conditions. Two variations of the method are developed, one in which the period is fixed and the other in which the total energy is fixed. Also, in section II we compare this new Monodromy formulation with the original one,¹ concluding that the latter is probably preferable to the former, at least for most applications of interest. Nevertheless, the 2×2 method is important since it may provide valuable insights into various extensions of the theory, particularly when a large number of dimensions is required. Finally, another 2×2 method is being developed and it promises to be superior to any of the methods mentioned.¹⁰

II. GAUSSIAN ELIMINATION IN TWO DIMENSIONS

As in ref. 1, there are two variants of the method for calculating periodic trajectories. In the first one (MONOD.T) we fix the period of the trajectory, but the total energy changes in an unknown way. In the second method (MONOD.E) the energy is essentially fixed, but the period is unknown. We shall now discuss both methods and then compare various Monodromy-type approaches.¹

A. CONSTANT PERIOD FORMULATION (MONOD.T)

First, for a two-dimensional Hamiltonian system (with unit mass), the general equations of motion are

$$\ddot{x} + V_x(x, y) = 0 \tag{2.1}$$

$$\ddot{y} + V_y(x, y) = 0,$$

where a dot indicates time (t) differentiation and $V_x(x, y)$ and $V_y(x, y)$ are the partial derivatives with respect to x and y , respectively, of the potential energy function. For a trajectory with period τ we have

$$x(t + \tau) = x(t) ; y(t + \tau) = y(t). \tag{2.2}$$

We discretize Eqs. (2.1) and (2.2) with respect to time in the simplest possible way, obtaining¹

$$x_{j+1} - 2x_j + x_{j-1} + \epsilon^2 V_x(x_j, y_j) = 0 \tag{2.3}$$

$$y_{j+1} - 2y_j + y_{j-1} + \epsilon^2 V_y(x_j, y_j) = 0,$$

$$x_{j+N} = x_j ; y_{j+N} = y_j ; j = 0, 1, \dots, N, \tag{2.4}$$

and ϵ is the time step assumed. There are N time steps, with $\tau = N\epsilon$.

If we linearize Eqs. (2.3) in the vicinity of an approximate trajectory (with coordinates (x_j^0, y_j^0)), we find¹

$$\delta x_{j+1} - 2\delta x_j + \delta x_{j-1} + \epsilon^2 V_{xx}(x_j^0, y_j^0) \delta x_j + \epsilon^2 V_{xy}(x_j^0, y_j^0) \delta y_j = a_j \tag{2.5}$$

$$\delta y_{j+1} - 2\delta y_j + \delta y_{j-1} + \epsilon^2 V_{xy}(x_j^0, y_j^0) \delta x_j + \epsilon^2 V_{yy}(x_j^0, y_j^0) \delta y_j = b_j,$$

with the definitions

$$-a_j = x_{j+1}^0 - 2x_j^0 + x_{j-1}^0 + \epsilon^2 V_x(x_j^0, y_j^0) \tag{2.6}$$

$$-b_j = y_{j+1}^0 - 2y_j^0 + y_{j-1}^0 + \epsilon^2 V_y(x_j^0, y_j^0).$$

Eqs. (2.5) are rewritten as¹

$$X_{j+1} + X_{j-1} - P_j X_j = A_j, \quad (2.7)$$

where

$$X_j = \begin{pmatrix} \delta x_j \\ \delta y_j \end{pmatrix} \quad (2.8)$$

and

$$A_j = \begin{pmatrix} a_j \\ b_j \end{pmatrix} \quad (2.9)$$

are two-dimensional vectors and

$$P_j = \begin{pmatrix} 2 - \epsilon^2 V_{rr}(x_j^0, y_j^0) & -\epsilon^2 V_{ry}(x_j^0, y_j^0) \\ -\epsilon^2 V_{ry}(x_j^0, y_j^0) & 2 - \epsilon^2 V_{yy}(x_j^0, y_j^0) \end{pmatrix} \quad (2.10)$$

is a two-dimensional matrix.

Before considering the case of periodic trajectories, it is instructive to solve Eqs. (2.7) when we have zero boundary conditions, i.e.,

$$X_0 = 0 \quad (2.11a)$$

$$X_{N+1} = 0. \quad (2.11b)$$

The solution to Eqs. (2.7) and (2.11) is a simple generalization of the Gaussian-elimination method, as applied to one-dimensional problems.⁹ From Eqs. (2.7) and (2.11) it can easily be shown that

$$X_j = Q_j X_{j+1} + T_j, \quad (2.12)$$

where Q_j is a two-dimensional matrix and T_j is a two-component vector, which satisfy the recursions

$$Q_j = (P_j - Q_{j-1})^{-1} \quad (2.13)$$

$$T_j = Q_j (T_{j-1} - A_j). \quad (2.14)$$

We solve for the Q 's and T 's by *forward* recursion, starting with

$$Q_0 = 0 \quad (2.15a)$$

$$T_0 = 0, \quad (2.15b)$$

which follow from Eqs. (2.11a) and (2.12). (The right-hand-sides of Eqs. (2.15a) and (2.15b) are a null matrix and a zero vector, respectively.) Then, using Eq. (2.12), we evaluate the X 's by *backward* recursion starting from Eq. (2.11b). Of course, by rearranging the above equations one can also solve for the Q 's and T 's by backward recursion and for the X 's by forward recursion. Moreover, the method can be applied to other types of boundary conditions,⁹ e.g., if X_0 and X_N are fixed (but not necessarily zero) vectors or if all derivatives vanish on a boundary.

Now return to the periodic boundary condition, Eq. (2.4), which gives the *unknown* vector

$$X_0 = X_N, \quad (2.16)$$

and generalize Eq. (2.12) to

$$X_j = Q_j X_{j+1} + K_j X_N + T_j, \quad (2.17)$$

where K_j is another 2×2 matrix. Then, from Eqs. (2.7), (2.16), and (2.17) we find that the Q 's and T 's again satisfy Eqs. (2.13), (2.14), and (2.15), while the K 's obey the recursion

$$K_j = Q_j K_{j-1}, \quad (2.18)$$

with the initial condition

$$K_0 = 1, \quad (2.19)$$

whose right-hand-side is the unit matrix. Therefore, using Eqs. (2.13) (2.14), and (2.18), we construct the Q, T, K by *forward* recursions, starting with the boundary relations (2.15) and (2.19).

It is clear then that each X_j depends explicitly on the unknown X_N , i.e.,

$$X_j = S_j X_N + G_j, \quad (2.20)$$

where S_j is a matrix and G_j is a vector. From Eqs. (2.17) and (2.20) we obtain the relations

$$S_j = Q_j S_{j+1} + K_j, \quad (2.21)$$

$$G_j = Q_j G_{j+1} + T_j, \quad (2.22)$$

and

$$S_N = 1 \quad (2.23a)$$

$$G_N = 0, \quad (2.23b)$$

which allow us to determine the S 's and G 's by *backward* recursions. We next examine Eq. (2.7) for $j = N$, namely

$$X_{N+1} + X_{N-1} - P_N X_N = A_N. \quad (2.24)$$

Then, after substituting Eq. (2.20) into Eq. (2.24) and recalling from Eq. (2.4) that $X_{N+1} = X_1$, we find that

$$X_0 = X_N = (S_1 + S_{N-1} - P_N)^{-1} (A_N - G_1 - G_{N-1}). \quad (2.25)$$

Thus, with X_N finally determined, we can evaluate the remaining X 's from Eq. (2.17) by recursing *backwards*. Since Eqs. (2.5) were obtained by a linearization, we can construct a new trajectory from

$$\begin{aligned} x_j &= x_j^0 + \delta x_j \\ y_j &= y_j^0 + \delta y_j ; \quad j = 0, 1, \dots, N. \end{aligned} \quad (2.26)$$

This trajectory can, in turn, be used as a starting guess for the next iteration. For a reasonable initial trajectory, convergence is very rapid. Moreover, for each iteration this method gives results which are exactly the same as those obtained using the Monodromy matrix,¹ so the two approaches are identical. Notice too, from Eqs. (2.3), (2.6), and (2.8), that once we have calculated a periodic trajectory that satisfies the equations of motion, A_j is a null vector. Then, it is easily shown from Eqs. (2.14), (2.15b), (2.22), and (2.23b) that the vectors T_j and G_j also vanish whenever we achieve convergence. This vanishing of the converged vectors is always a general feature of the Monodromy method.¹

The total energy of the continuous Hamiltonian is, of course, conserved. However, because of our discretization, the energy is only approximately constant. Thus, it is useful to define an average energy¹

$$E_{AV} = \frac{1}{N} \sum_{j=0}^{N-1} E_j, \quad (2.27)$$

where E_j is the energy of the j^{th} “link”,

$$E_j = \frac{1}{2\epsilon^2} [(x_{j+1} - x_j)^2 + (y_{j+1} - y_j)^2] + \frac{1}{2} [V(x_{j+1}, y_{j+1}) + V(x_j, y_j)]. \quad (2.28)$$

We find that the maximum deviation of a single link from the average value is less than 1% for $N = 96$ and for a relatively simple trajectory. As the trajectory becomes more complicated (particularly for period multiplying branchings), we must increase the N value in order to achieve comparable accuracy.

B. CONSTANT ENERGY FORMULATION (MONOD_E)

Next, consider the case in which the energy in Eq. (2.27) is essentially constant, but the period (or ϵ) can change. We let $\epsilon^2 \rightarrow \epsilon_0^2 + \delta(\epsilon^2)$, and Eq. (2.7) is modified as follows¹

$$X_{j+1} + X_{j-1} - P_j X_j = A_j + B_j \delta(\epsilon^2), \quad (2.29)$$

where

$$B_j = \begin{pmatrix} -V_x(x_j^0, y_j^0) \\ -V_y(x_j^0, y_j^0) \end{pmatrix} \quad (2.30)$$

is a vector and P_j and A_j are defined as before with ϵ^2 replaced by ϵ_0^2 . Therefore, $A_j \rightarrow A_j + B_j \delta(\epsilon^2)$, and if we explicitly include $\delta(\epsilon^2)$ as an additional unknown in Eq. (2.17), we find that

$$X_j = Q_j X_{j+1} + K_j X_N + T_j + R_j \delta(\epsilon^2). \quad (2.31)$$

The two-component vector R_j satisfies

$$R_j = Q_j (R_{j-1} - B_j), \quad (2.32)$$

which can be constructed by *forward* recursion from the initial condition

$$R_0 = 0. \quad (2.33)$$

The Q 's, T 's, and K 's are evaluated in exactly the same way as in the previous subsection. We also modify Eq. (2.20) to include the $\delta(\epsilon^2)$ dependence, obtaining

$$X_j = S_j X_N + G_j + W_j \delta(\epsilon^2). \quad (2.34)$$

The S 's and G 's are calculated precisely as before, and W_j is a vector satisfying the relations

$$W_j = Q_j W_{j+1} + R_j, \quad (2.35)$$

and

$$W_N = 0. \quad (2.36)$$

Thus, we recurse *backwards* to construct the W 's from Eqs. (2.35) and (2.36).

We now have to determine three unknowns $(\delta x_N, \delta y_N, \delta \epsilon^2)$, which means that we need to solve three linear, simultaneous equations. From Eq. (2.29) (for $j = N$) and Eqs. (2.4) and (2.34), we obtain

$$(S_1 + S_{N-1} - P_N) X_N + (W_1 + W_{N-1} - B_N) \delta(\epsilon^2) = A_N - G_1 - G_{N-1}, \quad (2.37)$$

which gives two conditions. The third equation is obtained by demanding that the energy has a fixed value. In particular, we shall assume in Eq. (2.27) that the link E_0 is a constant.¹ (As remarked previously, this guarantees that $E_{AV} \approx E_0$.) Then, we linearize Eq. (2.28) for $j = 0$ to obtain

$$\begin{aligned} & \epsilon_0^2 [V_x(x_N^0, y_N^0) \delta x_N + V_y(x_N^0, y_N^0) \delta y_N + V_x(x_1^0, y_1^0) \delta x_1 + V_y(x_1^0, y_1^0) \delta y_1] \\ & + 2(x_1^0 - x_N^0)(\delta x_1 - \delta x_N) + 2(y_1^0 - y_N^0)(\delta y_1 - \delta y_N) \\ & + [-2E_0 + V(x_1^0, y_1^0) + V(x_N^0, y_N^0)] \delta(\epsilon^2) = \eta, \end{aligned} \quad (2.38)$$

with

$$\eta = 2\epsilon_0^2 E_0 (x_1^0 - x_N^0)^2 - (y_1^0 - y_N^0)^2 - \epsilon_0^2 [V(x_1^0, y_1^0) + V(x_N^0, y_N^0)]. \quad (2.39)$$

We rewrite Eq. (2.38) as

$$\tilde{\alpha} X_1 + \tilde{\beta} X_N + \kappa \delta(\epsilon^2) = \eta, \quad (2.40)$$

where

$$\kappa = -2E_0 + V(x_1^0, y_1^0) + V(x_N^0, y_N^0), \quad (2.41)$$

and $\tilde{\alpha}$ and $\tilde{\beta}$ are the *row* vectors

$$\tilde{\alpha} = \left([2(x_1^0 - x_N^0) + \epsilon_0^2 V_x(x_1^0, y_1^0)] , [2(y_1^0 - y_N^0) + \epsilon_0^2 V_y(x_1^0, y_1^0)] \right), \quad (2.42)$$

$$\tilde{\beta} = \left([2(x_1^0 - x_N^0) + \epsilon_0^2 V_x(x_N^0, y_N^0)] , [-2(y_1^0 - y_N^0) + \epsilon_0^2 V_y(x_N^0, y_N^0)] \right). \quad (2.43)$$

Finally, we combine Eqs. (2.34), (2.37), and (2.40) to obtain the 3×3 representation

$$\left(\begin{array}{c|c} F & \zeta \\ \hline -\frac{F}{\tilde{\gamma}} & \phi \end{array} \right) \left(\begin{array}{c} X_N \\ \hline \delta(\epsilon^2) \end{array} \right) = \left(\begin{array}{c} J \\ \hline \chi \end{array} \right), \quad (2.44)$$

with the definitions

$$F = S_1 + S_{N-1} - P_N \quad (2.45a)$$

$$\zeta = W_1 + W_{N-1} - B_N \quad (2.45b)$$

$$\tilde{\gamma} = \tilde{\alpha} S_1 + \tilde{\beta} \quad (2.45c)$$

$$\phi = \tilde{\alpha} W_1 + \kappa \quad (2.45d)$$

$$J = A_N - G_1 - G_{N-1} \quad (2.45e)$$

$$\chi = \eta - \tilde{\alpha} G_1. \quad (2.45f)$$

Eq. (2.44) can be easily inverted to evaluate X_N and $\delta(\epsilon^2)$, which are used to construct a new trajectory using the recursion (2.31) and then Eq. (2.26). The period of the trajectory is given by

$$\tau = N \sqrt{\epsilon_0^2 + \delta(\epsilon^2)}. \quad (2.46)$$

As before, we iterate until we obtain convergence.

C. COMPARISONS OF THE VARIOUS METHODS

MONOD.T and MONOD.E converge equally well for most cases of interest.¹ I.e., it usually doesn't matter very much whether we fix the period and let the energy come out of the calculation, or vice versa. In practice, in either method we have found that, for a reasonable starting trajectory, 4 – 10 iterations are required in order to achieve 8-figure accuracy for the final coordinates. However, In general MONOD.T works somewhat better than MONOD.E for cases in which the period is changing more rapidly than the energy, while MONOD.E is superior for the reverse situation.¹ In particular, if we are constructing a family (or sets of families) on a plot of the energy vs the period ($E - \tau$ plot), MONOD.T is better to use near horizontal tangents while MONOD.E is more useful near vertical

tangents. Also, it is important to use MONOD_E near the region of small oscillations about an equilibrium point,¹ where the period is almost constant over a range of energies. (In fact, there are many examples of families, originating from small oscillations, for which the period remains constant for *all* energies.^{2,3})

The most important result is that the 2×2 methods (MONOD_T and MONOD_E) give exactly the same results as those obtained using the analogous 4×4 Monodromy methods.¹ Thus, the 2×2 (“half-space”) formalism is completely equivalent to the earlier 4×4 (“full space”) theory. However, it is not very clear how to relate the two formalisms since the recursions are different in the two approaches. Moreover, there are major differences in the algorithms involved which may be significant numerically in various extensions of the work. (E.g., in nuclear TDHF studies.¹¹⁻¹⁹) The full-space method involves only one recursion (“once around the track”¹), while in the half-space method we must first recurse forward and then again backwards. Also, in the 2×2 method there is an inversion at every time step. In both methods, after we obtain the “end points” of the trajectory, we must perform an additional recursion in order to calculate the remaining coordinates.

A major disadvantage of this half-space approach is that it appears to give no information about stability, whereas in the full-space formalism the eigenvalues of the Monodromy matrix uniquely determine the stability of a trajectory.¹⁻³ Also, the eigenvectors of the Monodromy matrix (for its nonunity eigenvalues) are crucial for computing new families of trajectories which bifurcate from a parent family.^{1,2}

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