Calculations of periodic orbits: The monodromy method and application to regularized systems

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We describe a numerical method for calculating periodic orbits, which is a generalization of the monodromy method by Baranger et al. to the case of an arbitrary autonomous dynamical system. Two variants of the method are developed, using the midpoint and the Runge–Kutta discretization of equations of motion, respectively. Particularly, we adapt the first variant for calculating periodic orbits of Hamiltonian systems when the period or the energy is given a priori. Finally, we consider the application of the monodromy method to the case of regularized mechanical systems and demonstrate the use by two examples. © 1999 American Institute of Physics.

I. INTRODUCTION

Calculations of periodic orbits (trajectories) and analysis of their features (stability properties, etc.) is very important for investigation of purely classical systems as well as for the semiclassical quantization. Our motivation for studying this problem came mostly from the latter. The semiclassical techniques for nonintegrable systems are usually based on the periodic-orbit theory of Gutzwiller where the quantum level density is expressed in terms of contributions of classical periodic orbits. Regular motion, i.e. the motion confined to invariant tori, can be quantized also applying EBK rules to the geometry of the tori (torus quantization). In that case, beside the periodic orbits, we deal with the so-called quasi-periodic orbits filling irrational tori. However, since infinite set of periodic orbits (although of measure zero) is everywhere dense, in fact, we calculate relevant quantities (action integral, winding numbers, etc.) for quasi-periodic orbits by interpolating the values of nearby periodic orbits.

One can use generally two methods for the numerical calculation of periodic orbits. The first is the method of propagation and closure, which consists in integrating equations of motion from given initial conditions for an expected period, and then in varying the initial conditions until the trajectory becomes closed. The second is monodromy method which starts from an approximate periodic orbit and iteratively, using a variant of the Newton–Raphson method, finds an exact periodic orbit. In this paper we shall describe a few variants of the monodromy method. There are at least two reasons why we prefer this method: (a) If the periodic orbit is highly unstable, the nearby trajectories are chaotic and it is difficult to find initial conditions which provide a closure. (b) By using the monodromy method, we calculate the periodic orbit and its monodromy matrix at the same time, which is required for stability analysis (calculations of Lyapunov exponents and winding numbers). The first method will be used only for calculating an approximate periodic orbit necessary to start the monodromy method.

The original monodromy method has been developed by Baranger et al. and used for calculating periodic orbits for a particle in a number of two-dimensional potentials. The corresponding equations of motion have been the Newton’s equations for system with two degrees of freedom. In this paper, besides the extension to higher dimensionality, we generalize the method to be applicable for calculating peri-
Generally, equations of motion for variations—The midpoint variant

II. THE GENERAL MONODROMY METHOD

Let us consider an autonomous dynamical system in $D$-dimensional phase space. It is defined by a set of $D$ first-order differential equations in $D$ variables $\mathbf{x} = (x_1, \ldots, x_D)$,

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}).$$

(1)

Generally, equations of motion (1) are not integrable and cannot be solved analytically. In order to perform numerical calculations, these equations must be discretized to give the corresponding difference equations. A solution of the difference equations is a series of the phase-space points $\mathbf{x}_n = (x_{1,n}, \ldots, x_{D,n})$, which represents a solution of equations (1) in discretized time, i.e., $\mathbf{x}_n = \mathbf{x}(t_n)$. Difference equations are usually given in the form of recursive relations, enabling, for a given initial condition $\mathbf{x}(0) = \mathbf{x}_0$, a calculation of the discretized trajectory step-by-step (this is not always the case, however).

We look for a solution of (1) with a given period $T$. Let the trajectory be represented by $N$ points equally spaced in time $\mathbf{x}_n, n = 1, \ldots, N$, with the time step $\Delta t = T/N$. Periodicity is then expressed by the condition

$$\mathbf{x}_{n+1} = \mathbf{x}_1.$$  

(2)

Suppose that an approximate periodic solution $\mathbf{x}_0^n, n = 1, \ldots, N$ is given. It can be an exact periodic solution with a slightly different period, previously obtained using the monodromy method, or some approximately closed orbit obtained using any other method. Then, we look for an improved solution in the form

$$(x_{1,n}, \ldots, x_{D,n}) = (x_0^{n} + \delta x_{1,n}, \ldots, x_0^{D,n} + \delta x_{D,n}).$$

(3)

**A. Equations for variations—The midpoint variant**

Discretization can be realized in a number of different ways. One of the most simple is the midpoint method, which is a variant of the Euler–Cauchy method, where derivatives $x_i$ are replaced by ratios $(x_{i,n+1} - x_{i,n})/\Delta t$. We attach these values to the values of $x_i$ in the middle of intervals $(x_{i,n}, x_{i,n+1})$ rather than at the ends,

$$(x_i)_{n+1/2} = \frac{x_{i,n+1} - x_{i,n}}{\Delta t}.$$  

(4)

Then, if we write equations of motion (1) at the midpoint of each of the intervals,

$$(x_i)_{n+1/2} = f_i(x_{n+1/2}),$$

(5)

where

$$x_{i,n+1/2} = \frac{x_{i,n+1} + x_{i,n}}{2},$$

(6)

after applying (4) we obtain the following difference equations:

$$x_{i,n+1} = x_{i,n} + \Delta t f_i \left( \frac{x_{n+1} + x_n}{2} \right), \quad i = 1, \ldots, D,$$

(7)

which is one of the possible discretization of Eqs. (1). Note that $x_{n+1}$ variables are not explicitly expressed in terms of $x_n$, so expression (7) in this form cannot be used directly for the step-by-step integration.

Substituting (3) in Eqs. (7) and linearizing them in the vicinity of the approximate solution, we obtain the following system of linear equations for variations $(\delta x_{1,n}, \ldots, \delta x_{D,n})$:

$$\delta x_{i,n+1} = \delta x_{i,n} + \Delta t \sum_{j=1}^{D} \left( \frac{\partial f_i}{\partial x_j} \right) x_{j,n+1/2} \delta x_{j,n} + c'_{i,n},$$

(8)

where

$$c'_{i,n} = -x_{i,n+1}^{0} + x_{i,n}^{0} + \Delta t f_i(x_{n+1/2}^{0}).$$

(9)

and $x_{n+1/2}^{0} = (x_{n+1}^{0} + x_{n}^{0})/2$. System (8) is a set of $D \times N$ linear equations for $D \times N$ variables $\delta x_{i,n}$. When we solve it, we use the improved solution (3) as a new approximate solution and start the next iteration. Note that the improved solution is, although approximate, closed at each iteration. If iterative process converges, a few iterations are sufficient to obtain an exact (sufficiently accurate) periodic solution. This is the Newton–Raphson method. In the following we show that solving the system of linear equations (8) for all $D \times N$ variations is not necessary. If we apply the so-called ‘‘once-around-the-trajectory’’ procedure, it is sufficient to do that for one of $N$ points (i.e., for $D$ variations), usually for $n = 1$. Then we are referring to the monodromy method.

Let us write the system (8) in the matrix form

$$A_{n+1/2} \delta \mathbf{x}_n + B_{n+1/2} \delta \mathbf{x}_n + c'_n,$$

(10)

where $A$ and $B$ are $D \times D$ matrices, given by the matrix elements
\[ A_{ij,n+1/2} = \delta_{ij} - \frac{\Delta t}{2} \left( \frac{\partial f_i}{\partial x_j} \right) x = x_n^{0,1/2} , \]
\[ B_{ij,n+1/2} = \delta_{ij} + \frac{\Delta t}{2} \left( \frac{\partial f_i}{\partial x_j} \right) x = x_n^{0,1/2} , \]
respectively, whereas \( \delta x_n \) and \( c_n' \) are D-vectors,
\[ \delta x_n = \left( \begin{array}{c} \delta x_{1,n} \\ \vdots \\ \delta x_{D,n} \end{array} \right) , \quad c_n' = \left( \begin{array}{c} c_{1,n}' \\ \vdots \\ c_{D,n}' \end{array} \right) . \]
By multiplying matrix equation (10) from the left with matrix \( A_{n+1/2}^{-1} \), which is an inverse matrix of the matrix \( A_{n+1/2} \), we obtain
\[ \delta x_{n+1} = U_n \delta x_n + c_n , \]
where
\[ U_n = A_{n+1/2}^{-1} B_{n+1/2} , \]
and
\[ c_n = A_{n+1/2}^{-1} c_n' . \]
When the system of linear equations for variations is taken in the matrix form (13), the remainder of the procedure of the monodromy method is identical to those by Baranger et al.\(^5,6\) (the ‘once-around-the-trajectory’ procedure—see Sec. II C). The problem in applying this variant of the monodromy method for an arbitrary dynamical systems may be the evaluation of the inverse matrix \( A_{n+1/2}^{-1} \). This problem is avoided in the Runge–Kutta variant of the method.

### B. Equations for variations—The Runge–Kutta variant

One widely used more accurate method for solving the systems of ordinary first-order differential equations is the (fourth-order) Runge–Kutta method.\(^1\) Now, if we use this method instead of the midpoint method, the system of difference equations (7) is replaced by
\[ x_{i,n+1} = x_{i,n} + \Delta x_{i,n} , \quad i = 1, \ldots, D , \]
where
\[ \Delta x_n = (k_{1,n}^{(1)} + 2k_{1,n}^{(2)} + 2k_{1,n}^{(3)} + k_{1,n}^{(4)})/6 . \]
The k-coefficients are given by
\[ k_{1,n}^{(1)} = \Delta t f_i(x_n) , \]
\[ k_{2,n}^{(1)} = \Delta t f_i(x_n^{1/2}) , \]
\[ k_{3,n}^{(1)} = \Delta t f_i(x_n^{2/3}) , \]
\[ k_{4,n}^{(1)} = \Delta t f_i(x_n^{3/4}) , \]
where four D-vectors \( k_n \) have corresponding k-coefficients for the components. Difference equations (16) [with expressions (17) and (18)] are usually used for the step-by-step numerical integration of equations of motion (1), starting from an initial point. However, here we shall use these equations to develop another variant of the monodromy method.

Substituting (3) in Eqs. (16) and linearizing them in the vicinity of the approximate solution, we obtain the following system of linear equations for variations (\( \delta x_{1,n} , \ldots, \delta x_{D,n} \)):
\[ \delta x_{i,n+1} = \delta x_{i,n} + \delta \Delta x_{i,n} + c_{i,n} , \]
where
\[ c_{i,n} = -x_{i,n}^{0} + x_{i,n}^{0} + \Delta x_{i,n}^{0} , \]
and
\[ \delta \Delta x_n = (\delta k_{1,n}^{(1)} + 2\delta k_{1,n}^{(2)} + 2\delta k_{1,n}^{(3)} + \delta k_{1,n}^{(4)})/6 , \]
\[ \delta k_{1,n}^{(1)} = \Delta t \frac{\partial f_i}{\partial x_j} x = x_n^{0} , \]
\[ \delta k_{1,n}^{(2)} = \Delta t \frac{\partial f_i}{\partial x_j} x = x_n^{0,1/2} , \]
\[ \delta k_{1,n}^{(3)} = \Delta t \frac{\partial f_i}{\partial x_j} x = x_n^{0,2/3} , \]
\[ \delta k_{1,n}^{(4)} = \Delta t \frac{\partial f_i}{\partial x_j} x = x_n^{0,3/4} , \]
where \( x_n^{0,r} , \quad r = 1, 2, 3 \) are defined as in eqs. (18), replacing everywhere \( x_n \) with \( x_n^{0} \).

Further, in order to solve Eqs. (19), the variations \( \delta \Delta x_{i,n} \) have to be expressed explicitly in terms of \( \delta x_{i,n} \). After multiple mutual substitution of \( \delta k \) expressions (22) and then inserting them into (21), system (19) reduces directly to the matrix form (13). The matrix elements of the system matrix \( U_n \) are, in this case,
\[ U_{ij,n} = \delta_{ij} + \frac{\Delta t}{6} \left( A_{ij}^{(1)} + \Delta t \sum_{k=1}^{D} A_{ijk}^{(2)} + \frac{\Delta t^2}{2} \sum_{k=1}^{D} \sum_{l=1}^{D} A_{ijkl}^{(3)} \right) , \]

where indices 0, 1, 2, 3 of the partial derivatives in (24) denote \( x = x_n^{0} , \quad x_n^{0,1}, \quad x_n^{0,2}, \quad x_n^{0,3} \), respectively.
The $D$-vector $c_n$ is here
\begin{equation}
\mathbf{c}_n = \begin{pmatrix} c_{1,n} \\ \vdots \\ c_{D,n} \end{pmatrix}.
\end{equation}

Further, except in the forms of matrix $\mathbf{U}_n$ and vector $c_n$, the following procedure is identical to that used in the previous variant.

C. The “once-around-the-trajectory” procedure

Successive applications of relation (13) give
\begin{equation}
\delta x_{n+1} = A_{n+1} \delta x_1 + \Gamma_{n+1},
\end{equation}
where $A_n$ and $\Gamma_n$ are the $D \times D$ matrix and $D$-vector, respectively, defined by recursive relations,
\begin{align}
A_{n+1} &= U_n A_n, \\
\Gamma_{n+1} &= U_n \Gamma_n + c_n,
\end{align}
with initial conditions
\begin{equation}
A_1 = 1, \quad \Gamma_1 = 0,
\end{equation}
where $\mathbf{0}$ denotes here the $D$-vector having all components equal to zero. When $n = N + 1$ (i.e., after having gone once-around-the-trajectory completely), relation (26) gives the connection between initial variations and variations after one period:
\begin{equation}
\delta x_{N+1} = A_{N+1} \delta x_1 + \Gamma_{N+1}.
\end{equation}

By the use of the periodicity condition for improved solution, $\delta x_{N+1} = \delta x_1$, it gives
\begin{equation}
(1 - A_{N+1}) \delta x_1 = \Gamma_{N+1}.
\end{equation}
The last equation is a $D \times D$ matrix equation determining unknown vector $\delta x_1$. When we determine $\delta x_1$, using (13) or (26), we calculate all $\delta x_n$ and obtain an improved solution from (3), which we use to start a new iteration. If an iterative process converges, it approaches the exact solution after a few iterations.

The criterion for stopping the iteration process should be a function of $c_{i,n}$ values, which decreases if the process converges (for an exact solution these values should be equal to zero). The most simple criterion is
\begin{equation}
\sum_{n=1}^{N} \sum_{i=1}^{D} c_{i,n}^2 < \epsilon,
\end{equation}
where $\epsilon$ is some small number (comparable to the machine double precision).

The monodromy method gives (discretized) solutions of Eqs. (1) identical to those which could be obtained after solving $D \times N$ linear equations (13) by the Newton–Raphson method. An important difference is that the monodromy method is much faster [in this case one solves $D$ linear equations (31), i.e., only for variation $\delta x_1$], and, what is of particular interest, it provides the monodromy matrix determining the stability of the calculated periodic orbit.

We emphasize at this point that in many cases an exact periodic solution need not necessarily exist in the vicinity of a given approximate periodic solution. In this case the iteration process diverges (what usually leads to a jump to another class of periodic solutions) or eventually, by taking $\epsilon$ which is not sufficiently small, it can converge to a closed path, which is not an exact solution, and diverges again after taking $\epsilon$ smaller. Such a “solution” can also be recognized by the nonconservance of corresponding integrals of motion along the path (e.g., energy for the Hamiltonian systems).

D. The discretized monodromy matrix

The monodromy matrix $\mathbf{M}$ of a periodic orbit connects arbitrary infinitesimal variations in the initial conditions $\delta \mathbf{x}(0)$ with corresponding changes after one period $\delta \mathbf{x}(T)$,
\begin{equation}
\delta \mathbf{x}(T) = \mathbf{M} \delta \mathbf{x}(0).
\end{equation}
For a discretized periodic solution $\mathbf{x}_n$, monodromy matrix $\mathbf{M}_1$ is defined by
\begin{equation}
\delta \mathbf{x}_{N+1} = \mathbf{M}_1 \delta \mathbf{x}_1.
\end{equation}

$D$-dimensional vector $\delta \mathbf{x}_1$ consists of arbitrary infinitesimal variations in the initial conditions, which, in general, can destroy the periodic structure of the trajectory, while $D$-vector $\delta \mathbf{x}_{N+1}$ consists of the corresponding variations in the coordinates and momenta after one period.

While using the monodromy method for calculating a periodic orbit, we also obtain its monodromy matrix $\mathbf{M}_1$ at the end of the iterative procedure. If the convergence is ensured, $\Gamma_{N+1} \rightarrow \mathbf{0}$ and $A_{N+1}$ is identical to monodromy matrix $\mathbf{M}_1$ [see Eqs. (30) and (34)].

\begin{equation}
\mathbf{M}_1 = A_{N+1} = U_1 U_2 \cdots U_N.
\end{equation}

We note that the discretized monodromy matrix can be defined in $N$ different ways, depending on the starting point of the trajectory, which is varied,
\begin{equation}
\mathbf{M}_n = U_{n-1} U_{n-2} \cdots U_2 U_1 U_N U_{N-1} \cdots U_{n+1} U_n.
\end{equation}
The matrices $\mathbf{M}_n$ are different for different $n$, but they have the same eigenvalues. Note that at least one of these eigenvalues has to be very close to unity, corresponding to the eigenvector with variations along the orbit $\delta \mathbf{x}_1 = \mathbf{x}_{N+1} - \mathbf{x}_n$. The eigenvalues of the monodromy matrix, as it is well known, determine stability of the periodic orbit, i.e., they give the corresponding Lyapunov exponents and winding numbers (see, e.g., Ref. 12).

Finally, we mention the problem of the possible singularity of the matrix on the left-hand side of Eq. (31). Namely, since $A_{N+1}$ converges to the monodromy matrix and it has the unit eigenvalues corresponding to the eigenvectors $\delta \mathbf{x}_1$, it might seem that $1 - A_{N+1}$ is a singular matrix. However, when using the monodromy method this problem has never arisen, which can be explained by the orthogonality $\Sigma_{n=1}^{N} \sum_{i=1}^{D} \delta x_{i,n}^* c_{i,n}^* = 0$ (see the Appendix in Ref. 5).
III. THE MONODROMY METHOD AND HAMILTONIAN SYSTEMS

In this section we adapt the midpoint variant of the monodromy method for applying to Hamiltonian systems. In this case the dynamics is described by the Hamilton’s equations,

\[
\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad i = 1, \ldots, F,
\]

with a Hamiltonian function, which we write in the form

\[
H = \sum_{i=1}^{F} \frac{p_i^2}{2m_i} + V(q),
\]

where the potential energy \( V \) is a function of \( F \) generalized coordinates \( q = (q_1, \ldots, q_F) \), \( p = (p_1, \ldots, p_F) \) are \( F \) conjugated momenta and \( m_i \) are the masses. \( F \) is the number of degrees of freedom and the phase space is \( 2F \)-dimensional. (For a fully three-dimensional few-body problem \( m_i = m_{i+1} = m_{i+2} \) for \( i = 3k-2, k = 1, \ldots, K \), where \( K \) is the number of bodies. Then \( F = 3K \).

If we write

\[
x_i = q_i, \quad x_{i+F} = p_i, \quad i = 1, \ldots, F,
\]

Eqs. (37) determine the vector field components in (1), which are in this case

\[
f_i = \frac{p_i}{m_i}, \quad f_{i+F} = -V_i, \quad i = 1, \ldots, F,
\]

where \( V_i = \partial V/\partial q_i \).

A. Calculations of periodic orbits with a given period

For the components (40) difference equations (7) become

\[
q_{i,n+1} = q_{i,n} + (\Delta t/m_i) p_{i,n+1/2},
\]

\[
p_{i,n+1} = p_{i,n} - \Delta t V_i(q_{i,n+1/2}), \quad i = 1, \ldots, F,
\]

where \( q_{n+1/2} = \frac{(q_{n+1} + q_{n})}{2} \) and \( p_{n+1/2} = \frac{(p_{n+1} + p_{n})}{2} \). Equations for the variations \( \delta q_{i,n}, \delta p_{i,n}, \delta q_{F,n}, \delta p_{F,n} \) can be obtained in the form (10) directly after specifying the matrix elements of \( A_{n+1/2} \) and \( B_{n+1/2} \), by inserting the first derivatives of the vector field components (40), which are

\[
\frac{\partial f_i}{\partial j} = 0, \quad \frac{\partial f_i}{\partial p_j} = \frac{\delta f_i}{\delta q_j} = 0, \quad \frac{\partial f_{i+F}}{\partial q_j} = -V_{ij},
\]

\[
\frac{\partial f_{i+F}}{\partial p_j} = 0, \quad i, j = 1, \ldots, F,
\]

into Eqs. (11). However, since the evaluation of inverse matrix \( A_{n+1/2}^{-1} \) is not trivial in this case, it is difficult to obtain equations for the variations in the form (13), which is necessary for applying the “once-around-the-trajectory” procedure.

However, if we adopt the new momenta labeling \( p_{n+1/2} \rightarrow p_n \), then instead of Eqs. (41), we have

\[
q_{i,n+1} = q_{i,n} + (\Delta t/m_i) p_{i,n},
\]

Linearized equations for variations are then

\[
\delta q_{i,n+1} = \delta q_{i,n} + \frac{\Delta t}{m_i} \delta p_{i,n} + c'_{i,n},
\]

\[
\delta p_{i,n+1} = \delta p_{i,n} - \Delta t \sum_j V_{ij}(q_{i,n+1}) \delta q_{j,n+1} + c'_{i+F,n},
\]

where

\[
c'_{i,n} = -q_{i,n+1}^0 + q_{i,n}^0 + (\Delta t/m_i) p_{i,n}^0,
\]

\[
c'_{i+F,n} = -p_{i,n+1}^0 + p_{i,n}^0 - \Delta t V_i(q_{i,n+1}).
\]

System (44) can be written in the matrix form

\[
A_{n+1} \delta q_{n+1} = B \delta x_n + c_n',
\]

where matrices \( A_{n+1} \) and \( B \), written in terms of \( F \times F \) blocks, are

\[
A_{n+1} = \begin{pmatrix} 1 & 0 \\ \Delta t P_{n+1} & 1 \end{pmatrix},
\]

\[
B = \begin{pmatrix} 1 & \Delta t Q \\ 0 & 1 \end{pmatrix},
\]

where

\[
Q = \begin{pmatrix} m_1^{-1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & m_F^{-1} \end{pmatrix},
\]

\[
P_n = \begin{pmatrix} V_{11,n} & \cdots & V_{1F,n} \\ \vdots & \ddots & \vdots \\ V_{F1,n} & \cdots & V_{FF,n} \end{pmatrix},
\]

\[
V_{ij,n} = \left( \frac{\partial^2 V}{\partial q_i \partial q_j} \right)_{q=q_n^0}.
\]

Since the inverse matrix of matrix \( A_{n+1} \), having form (47), is

\[
A_{n+1}^{-1} = \begin{pmatrix} 1 & 0 \\ -\Delta t P_{n+1} & 1 \end{pmatrix},
\]

matrix equation (13) follows after multiplying Eq. (46) from the left with \( A_{n+1}^{-1} \), where the system matrix \( U_n \) and vector \( c_n \) are

\[
U_n = A_{n+1}^{-1} B = \begin{pmatrix} 1 & \Delta t Q \\ -\Delta t P_{n+1} & 1 - \Delta t^2 P_{n+1} \end{pmatrix},
\]

\[
c_n = A_{n+1}^{-1} \begin{pmatrix} c'_{1,n} \\ \vdots \\ c'_{F,n} \end{pmatrix} = \begin{pmatrix} -\Delta t \sum_i V_{1i}(q_{i,n+1}) c'_{i,n} + c'_{F+1,n} \\ \vdots \\ -\Delta t \sum_i V_{Fi}(q_{i,n+1}) c'_{i,n} + c'_{2F,n} \end{pmatrix}.
\]
Now, we can apply the "once-around-the-trajectory" procedure, described in Sec. II C. The criterion for stopping the iteration process can be (32). However, since \((c_{i,n+1} - c_{i,n})/\Delta t - c_{i,F,n}/m_i\), here we use the criterion
\[
\sum_{n=1}^{N} \sum_{i=1}^{F} \left( c_{i,n+1} - c_{i,n} + \frac{\Delta t}{m_i} c_{i,F,n} \right)^2 < \varepsilon.
\] (52)

Due to the numerical errors, the energy may not be always rigorously constant along the orbit (e.g., for insufficiently large \(N\)), so we take the average value
\[
E = \frac{1}{N} \sum_{n=1}^{N} E_n,
\] (53)
where \(E_n\) are the energy values at each point of the periodic orbit,
\[
E_n = \sum_{i=1}^{F} p_{i,n}^2 + V \left( \frac{q_{i,n} + q_{i,n+1}}{2} \right).
\] (54)

We notice that the variant of the monodromy method given in this subsection is the generalization of the monodromy method for Hamiltonian systems with two degrees of freedom, described by Baranger et al.\(^{5,6}\) to the case with arbitrary degrees of freedom. Also, there is a difference in formulation, since the present method is formulated in the phase space in contrast to the original method, which is formulated in the configuration space.

B. Calculations of periodic orbits with a given energy

It is sometimes essential to be able to calculate periodic orbits of a system determined by a Hamiltonian (38) giving the energy \textit{a priori}, and letting the period come out. To do that, we have to allow at each iteration also the change of period \(T\), i.e., allow for the variable step \(\Delta t = \Delta t_0 + \delta \Delta t\), and add one more linear equation connecting \(\delta \Delta t\) with other variations at a given energy.

Then, instead of Eqs. (44) we have
\[
\begin{align*}
\delta q_{i,n+1} &= \delta q_{i,n} + \frac{\Delta t_0}{m_i} \delta p_{i,n} + \frac{p_{i,n}^0}{m_i} \delta \Delta t + c_i', \\
\delta p_{i,n+1} &= \delta p_{i,n} + \Delta t_0 \sum_{j=1}^{F} V_{ij}(q_{i,n+1}) \delta q_{j,n+1} - V_i(q_{i,n+1}) \delta \Delta t + c_i',
\end{align*}
\] (55)
where
\[
\begin{align*}
c_i' &= -q_{i,n+1}^0 + q_{i,n} + (\Delta t_0/m_i) p_{i,n}^0, \\
c_i'_{i+F,n} &= -p_{i,n}^0 + p_{i,n} - \Delta t_0 V_i(q_{i,n+1}).
\end{align*}
\] (56)

System (55) can be written in the matrix form
\[
A_{n+1} \delta x_{n+1} = B \delta x_n + d'_n \delta \Delta t + c'_n,
\] (57)
where matrices \(A_{n+1}\) and \(B\) are given by (47) and
\[
\begin{pmatrix}
p_{1,n+1}^0/m_1 \\
\vdots \\
p_{F,n+1}^0/m_F \\
-V_1(q_{n+1}^0) \\
\vdots \\
-V_F(q_{n+1}^0)
\end{pmatrix}
\] (58)

After multiplying Eq. (57) from the left with \(A_{n+1}^{-1}\), we obtain
\[
\delta x_{n+1} = U_n \delta x_n + d_n \delta \Delta t + c_n,
\] (59)
where system matrix \(U_n\) and vector \(c_n\) are given by (50) and (51), whereas
\[
d_n = A_{n+1}^{-1} d'_n.
\]

Subsequently, we apply the "once-around-the-trajectory" procedure similar to those described in Sec. II C. A successive application of relation (59) gives
\[
\delta x_{n+1} = \Lambda_n \delta x_1 + \Delta_n \delta \Delta t + \Gamma_n,
\] (60)
where \(\Lambda_n\) is \(2F \times 2F\) matrix and \(\Delta_n\) and \(\Gamma_n\) are \(2F\)-vectors, defined by recursive relations,
\[
\begin{align*}
\Lambda_{n+1} &= U_n \Lambda_n, \\
\Delta_{n+1} &= U_n \Delta_n + d_n, \\
\Gamma_{n+1} &= U_n \Gamma_n + c_n,
\end{align*}
\] (62) (63) (64)
with initial conditions
\[
\L_1 = 1, \quad \Delta_1 = 0, \quad \Gamma_1 = 0.
\] (65)
For the \(n = N+1\) relation (61) gives the connection between initial variations and variations after one period,
\[
\delta x_{N+1} = \Lambda_{N+1} \delta x_1 + \Delta_{N+1} \delta \Delta t + \Gamma_{N+1},
\] (66)
what, using the periodicity condition for the improved solution, \(\delta x_N = \delta x_1\), gives
\[
(1 - \Lambda_{N+1}) \delta x_1 - \Delta_{N+1} \delta \Delta t = \Gamma_{N+1}.
\] (67)
This matrix equation gives \(2F\) linear equations for \(2F + 1\) unknown variations. An additional equation follows from the energy condition (54) for \(n = 1\), which according to (43) can be written in the form
\[
E_1 = \sum_{i=1}^{F} \frac{p_{i,1}^2}{2m_i} + V \left( q_1 + \frac{\Delta t}{2} Q p_1 \right).
\] (68)
giving a linearized equation for variations,
\[
\sum_{i=1}^{F} \left[ \frac{p_{i,1}^0}{m_i} \delta p_{i,1} + V_i(q_{1/2}^0) \delta q_{i,1} + \frac{\Delta t_0}{2m_i} \delta p_{i,1} + \frac{p_{i,1}^0}{2m_i} \delta \Delta t \right] = \eta, \tag{69}
\]
where \( q_{1/2}^0 = (q_1^0 + q_2^0)/2 = q_0^0 + \Delta t_0 Q p_1^0/2 \) and
\[
\eta = E_1 - \sum_{i=1}^{F} \frac{p_{i,1}^0}{2m_i} - V(q_{1/2}^0). \tag{70}
\]

Equation (69) can be written in the concise form
\[
(\Xi, \delta \xi) + \xi_0 \delta \Delta t = \eta, \tag{71}
\]
where \((\Xi, \delta \xi)\) denotes the scalar product. The vector \(\xi = (\xi_1, \ldots, \xi_{2F})\) has the components
\[
\xi_i = V_i(q_{1/2}^0), \quad \xi_{i+F} = \frac{p_{i,1}^0}{m_i} + \frac{\Delta t_0}{2m_i} V_i(q_{1/2}^0), \quad i = 1, \ldots, F
\]
and
\[
\xi_0 = \frac{1}{2} \sum_{i=1}^{F} \frac{p_{i,1}^0}{m_i} V_i(q_{1/2}^0). \tag{73}
\]

If we express \( \delta \Delta t \) from (71) and then insert into (67), we obtain
\[
\left( 1 - \Lambda_{N+1} + \frac{1}{\xi_0} (\Delta_{N+1}, \Xi) \right) \delta \xi_1 = \Gamma_{N+1} + \frac{\eta}{\xi_0} \Lambda_{N+1}, \tag{74}
\]
where the diadic product \((\Delta_{N+1}, \Xi)\) is used in order to keep the matrix form \((\Delta_{N+1}, \Xi)_i = (\Delta_{N+1}), \xi_i \). This equation is a \(2F \times 2F\) matrix equation, which fully determines unknown variations \( \delta \xi_1 \) and, together with (71), \( \delta \Delta t \) also. Then, using (61) we calculate all \( \delta \xi_n \) and obtain an improved solution \( \xi_n = \xi_0^0 + \delta \xi_n \), which we use to start a new iteration with the new time step \( \Delta t = \Delta t_0 + \delta \Delta t \). If the iterative process converges, it approaches the periodic solution (orbit) with energy \( E_1 \) after a few iterations. The criterion for stopping the iterative process can be (52) or alternatively \( \eta < \epsilon \), where \( \epsilon \) is some small number.

IV. APPLICATIONS TO THE REGULARIZED SYSTEMS

In the previous section we have described the method for calculating periodic orbits for a class of Hamiltonian systems determined by a Hamiltonian function (38). However, in many cases of physical interest potential function \( V(q) \) has one or more singularities. Thus, the accuracy of the computations depends to a great extent on how close the periodic orbit passes the singularity. In a drastic case of orbits passing through the singularity, the monodromy method, as well as any other numerical method, appears completely nonapplicable. Typical examples for such systems are the few-body systems with Coulombic or gravitational interactions between the constituents, which are of particular interest in atomic and molecular physics and in celestial mechanics, respectively. In this situation the most successful method for avoiding the singularities is the regularization of differential equations of motion, before they are solved numerically.

Regularization of a three-dimensional Coulomb (Kepler) problem can be done by the so-called Kustaanheimo–Stiefel (KS) transformations. This method is based on the fact that the three-dimensional Coulomb/Kepler problem is equivalent to a pair of coupled two-dimensional harmonic oscillators in a four-dimensional space. These problems in two-dimensions (planar cases) can be regularized also by the transition to semiparabolic coordinates. By applying two KS transformations Aarseth and Zare succeeded to regularize a three-body problem in celestial mechanics.15

An important feature of the transformations used to regularize the above problems is that they are canonical, which means that equations of motion preserve the canonical form (37) with a new time variable \( \tau \) and a new Hamiltonian function \( \bar{H} \) of the new coordinates and momenta \((\bar{q}, \bar{p})\).
\[
\frac{d\bar{q}_i}{d\tau} = \frac{\partial \bar{H}}{\partial \bar{p}_i}, \quad \frac{d\bar{p}_i}{d\tau} = -\frac{\partial \bar{H}}{\partial \bar{q}_i}, \quad i = 1, \ldots, F. \tag{75}
\]
The new Hamiltonian function may have a form different from (38) and, although it is a constant of motion, it usually does not express the energy of the system. This constant is sometimes called the pseudo-energy \( \bar{E} \). Thus, keeping the pseudo-energy constant through the iterative process is an essential condition to be satisfied while applying the monodromy method to regularized systems. Otherwise, the iterative process converges to a periodic solution for a system different from that we are starting with. Thus, the best way in this case is using a variant of the monodromy method which keeps the pseudo-energy constant by varying the step \( \Delta \tau \). If the regularized Hamiltonian function has the form (38), i.e.,
\[
\bar{H} = \sum_{i=1}^{F} \frac{p_{i,1}^2}{2m_i} + \bar{V}(\bar{q}; E) = \bar{E}, \tag{76}
\]
we can use for this purpose the variant for the calculation of periodic orbits with a given energy, described in Sec. III B, for nonregularized systems, by replacing \( q \rightarrow \bar{q}, \, p \rightarrow \bar{p}, \, t \rightarrow \tau, \, V \rightarrow \bar{V} \) and \( E_1 \rightarrow \bar{E} \).

If we apply the variant for the calculation of periodic orbits with a given period, in order to keep the pseudo-energy constant, it is necessary to take the period of the exact solution to be the same as the period of the approximate orbit. More precisely, we have to find the period providing the same values of \( \bar{E} \) before starting the iterative process and after convergence, which can be slightly different from the period of the approximate orbit due to the numerical error.

Note also that an approximate solution for starting the first iteration must be some approximate periodic orbit calculated in regularized coordinates, with constant new-time-variable step \( \Delta \tau \). The approximate periodic orbits can be obtained using any method of propagation and closure (step-by-step), applied to the regularized system.

In the following, we give two examples where the calculations of periodic orbits for regularized systems is described in more details, the first one where \( \bar{H} \) has the form (76) and the other one where it is not the case.
A. One-electron atoms in external fields

Here we demonstrate the use of the monodromy method for calculating periodic orbits of an electron moving in the Coulomb field of an (infinitely heavy) nucleus of charge $Z$ and at the same time in a constant external field. If the $z$-axis is taken to be the direction of an external field, the Hamiltonian of this system, making use of the atomic units ($m_e = e = 1$) and cylindrical coordinates $(\rho, \phi, z)$, reads

\[ H = \frac{p^2}{2} - \frac{Z}{r} + F(\rho,z), \tag{77} \]

where $r = (\rho^2 + z^2)^{1/2}$ is the electron–nucleus distance, $p^2 = p_\rho^2 + p_z^2$ is the electromagnetic momentum and $F(\rho,z)$ is the potential of the electron in the external field. Due to the cylindrical symmetry, the $z$-component of angular momentum is conserved and the $\phi$-motion is separated from that in the $(\rho,z)$ plane. Thus, the system is reduced to the problem with two degrees of freedom. Here we consider the $l_z = 0$ case. In this case the Hamiltonian function (77) has the form (38), which enables us to use the variants of monodromy method, given in Sec. III.

However, if we want to calculate the orbits passing through or closely to the nucleus (the singularity), this system must be regularized. For this purpose we introduce semiparabolic coordinates $u, v$,

\[ u = \sqrt{r + z}, \quad v = \sqrt{r - z}, \tag{78} \]

and conjugated momenta,

\[ p_u = \frac{du}{d\tau}, \quad p_v = \frac{dv}{d\tau}, \tag{79} \]

where the new time variable $\tau$ is defined by the transformation

\[ d\tau = 2rd\tau = (u^2 + v^2) d\tau. \tag{80} \]

The singularity in the Hamiltonian (77), when the old variables $(\rho, z, p_\rho, p_z, t)$ are expressed in terms of the new ones $(u, v, p_u, p_v, \tau)$, can be removed by the transformation

\[ \tilde{H} = 2r (H' - E) + 2Z = 2Z, \tag{81} \]

where $r = (u^2 + v^2)/2$, $H'$ is a Hamiltonian function (77) expressed in terms of regularized variables and $E$ is the total energy of the system. The fixed pseudo-energy ($\tilde{E} = 2Z$) is necessary in order to retain the canonical form of the regularized equations of motion. The regularized Hamiltonian also has the form (76), i.e.,

\[ \tilde{H} = \frac{p_u^2 + p_v^2}{2} + \tilde{V}(u,v;E) = 2Z, \tag{82} \]

where

\[ \tilde{V} = 2r (V - E) + 2Z = -E (u^2 + v^2) + (u^2 + v^2) F\left(u,v,\frac{u^2 - v^2}{2}\right) \tag{83} \]

is the quasi-potential. Therefore, the method described in Sec. III B, can be applied to this regularized system, if we write $q_1 = u$, $q_2 = v$, $p_1 = p_u$, $p_2 = v$ and replace $t \rightarrow \tau$, $\tilde{E} \rightarrow \tilde{E}$, $V \rightarrow \tilde{V}$.

Let us consider now the case when the external field is a uniform magnetic field. As usually in this case, we use the scaled Hamiltonian, which does not depend explicitly on the field strength, but only on the scaled energy $E_{sc}$. \(^{12}\) The function $F(\rho,z)$ is then

\[ F = \frac{p^2}{8}, \tag{84} \]

and a regularized Hamiltonian is (82) with $E_{sc}$ instead of $E$ and

\[ \tilde{V} = -E_{sc} (u^2 + v^2) + (u^2 + v^2) u^2 v^2. \tag{85} \]

In order to construct the matrix $\mathbf{U}_n$ and the vectors $\mathbf{c}_n$ and $\mathbf{d}_n$, we have to evaluate the first and the second derivatives of the quasi-potential (85) $\tilde{V}_u, \tilde{V}_v, \tilde{V}_{uu}, \tilde{V}_{uv}, \tilde{V}_{vv} = \tilde{V}_{vu}$, and apply relations (48) (here $\mathbf{Q} = 1$), (50), (51), (56), and (60). Then, we can start the iterative procedure, by solving the $4 \times 4$ matrix equation (74) at each iteration. The matrix $\Lambda_{N+1}$, vectors $\Gamma_{N+1}, \Delta_{N+1}$ and $\Xi$, and parameters $\eta$ and $\xi_0$, used here, are given by the relations (62)–(65), (70), (72), and (73).

An illustrative example is the calculation of the straight-line periodic orbit of an electron in the hydrogen atom ($Z = 1$), perpendicular to the direction of the magnetic field (labeled by $I_1$). \(^{12}\) Since one of the turning points of the orbit is located at the nucleus (the singularity of the real potential), this calculation cannot be performed without regularization. The approximate orbit can be obtained by the numerical integration (e.g., the Runge–Kutta method) of the Hamilton’s equations (75) for a regularized Hamiltonian (82) with pseudo-potential (85), using constant step $\Delta \tau$. As an initial position of the electron for starting the integration we can use the other turning point, which is for scaled energy $E_{sc} = -0.1$ located at $(\rho,z) = (1.8668770,0)$. By taking $\Delta \tau = 10^{-2}$, the (first) approximate closure of orbit appears after 240 steps. The integration of relation (80) for this number of steps gives the period $T_0 \approx 3.85$. If we want to find the “exact” $I_1$ periodic orbit and its monodromy matrix, we have to apply the monodromy method, using the orbit obtained above for starting the first iteration (i.e., as an approximate periodic solution). However, since the $I_1$ orbit expressed in regularized coordinates becomes closed after two $T_0$ periods, it is necessary to take for the “approximate” periodic solution the $I_1$ orbit of doubled period ($2T_0 \approx 7.70$), which consists of $N = 480$ points for $\Delta \tau = 10^{-2}$. There appears also another problem while using this orbit for starting the monodromy method. Namely, since we have calculated the orbit starting from the turning point with zero velocity, it is also $p_{u,0} = p_{v,0} = 0$ and due to (73) $\xi_0 = 0$. Thus, we have division by zero in Eq. (74). This difficulty, however, can be simply overcome by performing cyclic permutation of all points of the approximate periodic orbit $(x_0^0, x_{N+1}^0)$.

The monodromy method (the variant for regularized systems with a given pseudo-energy) then attains the “exact”
where the planar motion of the system, since it covers all possible three-body configurations with total angular momentum \( L = 0 \) and also some of the important configurations with \( L \neq 0 \). The Hamiltonian function (86) has the form (38), which enables us to use of the variant of the monodromy method, given in Sec. III.\textsuperscript{16,17} However, as noted above, because of the singular character of the Coulomb interaction, the accuracy of the computations depends on how close the periodic orbit passes the singularity.\textsuperscript{18} Therefore, especially in the case of orbits passing through the singularity, regularization of the system appears essential.

Here we follow procedure of Arseth and Zeze\textsuperscript{15} to regularize planar motion of the system given by the Hamiltonian (86) and introduce the regularized coordinates and momenta \( Q_i, P_i, \quad i = 1, 2, 3, 4 \), instead of \( r_1 = (x_1, y_1), \quad r_2 = (x_2, y_2), \quad p_1 = (p_{x1}, p_{y1}), \quad p_2 = (p_{x2}, p_{y2}), \) by means of the transformations\textsuperscript{19,20}

\[
\begin{align*}
x_1 &= Q_1^2 - Q_2^2, & y_1 &= 2Q_1Q_2, \\
x_2 &= Q_1^2 - Q_3^2, & y_2 &= 2Q_3Q_4, \\
p_{x1} &= \frac{Q_1P_1 - Q_2P_2}{2r_1}, & p_{y1} &= \frac{Q_2P_1 + Q_1P_2}{2r_1}, \\
p_{x2} &= \frac{Q_3P_3 - Q_4P_4}{2r_2}, & p_{y2} &= \frac{Q_4P_3 + Q_3P_4}{2r_2},
\end{align*}
\]

and the new time variable \( \tau \) by

\[
d\tau = r_1r_2 d\tau,
\]

where \( r_1 = Q_1^2 + Q_2^2, \quad r_2 = Q_3^2 + Q_4^2 \).

It can be shown that if \( H \) is replaced by

\[
\tilde{H} = r_1r_2(H' - E) = 0,
\]

where \( H' \) is Hamiltonian function (86) expressed in terms of regularized variables and \( E \) is the total energy of the system, equations of motion preserve the canonical form (37), i.e.,

\[
\frac{dQ_i}{d\tau} = \frac{\partial \tilde{H}}{\partial P_i}, \quad \frac{dP_i}{d\tau} = -\frac{\partial \tilde{H}}{\partial Q_i}, \quad i = 1, \ldots, 4.
\]

Such a transformed Hamiltonian \( \tilde{H} \) is regular when \( r_1 \to 0 \) or \( r_2 \to 0 \) and has the explicit form

\[
\tilde{H} = \frac{r_2P_1^2}{8} + \frac{r_1P_2^2}{8} + \tilde{V}(r_1, r_2, r_{12}; E),
\]

where \( \tilde{V} = (P_1, P_2), \quad P_2 = (P_3, P_4) \) and

\[
\tilde{V} = r_1r_2(V - E) = -Z(r_1 + r_2) + r_1r_2\left(\frac{1}{r_{12}} - E\right),
\]

where

\[
r_{12} = [(Q_1^2 - Q_2^2 - Q_3^2 + Q_4^2)^2 + 4(Q_1Q_2 - Q_3Q_4)^2]^{1/2}.
\]

Then, equations of motion (90) read as

\[
\begin{align*}
\frac{dQ_1}{d\tau} &= \frac{r_2P_1}{4}, & \frac{dP_1}{d\tau} &= -\frac{P_2^2Q_1}{4} - \tilde{V}_1, \\
\frac{dQ_2}{d\tau} &= \frac{r_1P_2}{4}, & \frac{dP_2}{d\tau} &= -\frac{P_1^2Q_2}{4} - \tilde{V}_2, \\
\frac{dQ_3}{d\tau} &= r_1P_3, & \frac{dP_3}{d\tau} &= -\frac{P_1^2Q_3}{4} - \tilde{V}_3, \\
\frac{dQ_4}{d\tau} &= r_2P_4, & \frac{dP_4}{d\tau} &= -\frac{P_2^2Q_4}{4} - \tilde{V}_4,
\end{align*}
\]
where \( \overline{V}_i = \partial \overline{V} / \partial Q_i, \ i = 1, \ldots , 4 \) (for the explicit expressions of \( \overline{V}_i \), see Ref. 20). Although the case \( R_{12} \rightarrow 0 \) is still singular, expression (92) suggests that close triple encounters may be integrated numerically, because the critical term \( r_1 r_2 / r_{12} \) is numerically well behaved even for small values of \( r_{12} \).

Note that Hamiltonian function (91) has not the form (38), which makes the variants of the monodromy method, given in Sec. III, inadequate for this case. As mentioned above, an application of the midpoint variant of the monodromy method described in Sec. II A, is connected with the nontrivial task of finding \((8 \times 8)\) inverse matrix \( A_{n-1}^{-1} \). In this case, the most suitable appears to be the Runge–Kutta variant of the monodromy method.

If we go back to the unique labeling of the phase-space variables: \( x_i = Q_i, x_{i+4} = P_i, i = 1, \ldots , 4, \) Eqs. (93) take the form (1) with the following components of the vector field \( f \):

\[
\begin{align*}
  f_1 &= \frac{(x_3^2 + x_2^2)x_5}{4}, \quad f_5 = -\frac{(x_7^2 + x_8^2)x_1}{4} - \overline{V}_1(x_1, x_2, x_3, x_4), \\
  f_2 &= \frac{(x_3^2 + x_2^2)x_6}{4}, \quad f_6 = -\frac{(x_7^2 + x_8^2)x_2}{4} - \overline{V}_2(x_1, x_2, x_3, x_4), \\
  f_3 &= \frac{(x_7^2 + x_8^2)x_7}{4}, \quad f_7 = -\frac{(x_5^2 + x_6^2)x_3}{4} - \overline{V}_3(x_1, x_2, x_3, x_4), \\
  f_4 &= \frac{(x_7^2 + x_8^2)x_8}{4}, \quad f_8 = -\frac{(x_5^2 + x_6^2)x_4}{4} - \overline{V}_4(x_1, x_2, x_3, x_4).
\end{align*}
\]

In order to apply the monodromy method (Runge–Kutta variant), it is necessary to find all derivatives \( df_i / dx_j \) and determine the system matrix \( U_n \) using Eqs. (23), (24).

Here we present the calculation of the asymmetric stretch (AS) collinear periodic orbit of the classical helium atom. The orbit can be obtained by the propagation method, starting with the electrons from initial positions \( r_1 = (3.52651, 0), r_2 \approx (0, 0) \) at the total energy \( E = -1 \), using numerical (Runge–Kutta) integration of regularized equations of motion (93) with constant step \( \Delta \tau \). By taking \( \Delta \tau = 10^{-2} \), the (first) closure of the trajectory appears after 266 steps. Integration of relation (88) for this number of steps gives the period \( T_0 = 11.491 \). However, if we want to find an “exact” AS periodic orbit and its monodromy matrix, we have to apply the monodromy method, taking the orbit obtained by the propagation method for starting the first iteration (i.e., as an approximate periodic solution). Since the AS orbit expressed in regularized coordinates becomes closed after two \( T_0 \) periods, it is necessary to take for an “approximate” periodic orbit the AS periodic orbit of a doubled period (\( 2T_0 = 22.982 \)), which consists of \( N = 532 \) points for \( \Delta \tau = 10^{-2} \). In this case, we obtain an “exact” periodic solution with the pseudo-energy \( \overline{E} = 10^{-3} \), after two iterations (criterion for stopping: \( \varepsilon = 10^{-15} \)). However, for slightly changed step \( \Delta \tau = 1.0002 \times 10^{-2} \) and \( N = 532 \), we reach a more exact periodic solution with \( \overline{E} = 10^{-5} \) and \( 2T = 22.984 \), after three iterations. The eigenvalues of the monodromy matrix for the last solution are \( \mu_1 = 11.077, \mu_2 = 0.09027, \mu_{3,4} = 0.55143 \pm i0.83422 \) and \( \mu_{5,6,7,8} = 1 \). Two real eigenvalues \( \mu_{1,2} \) give the nonvanishing Lyapunov exponents, indicating that one (radial) oscillatory mode of the AS orbit is unstable. On the other hand, two complex conjugate eigenvalues \( \mu_{3,4} = \exp(\pm 2\pi i \gamma) \) are associated with stable (bending) mode of an orbit in the vicinity of this periodic orbit. Possible values for the frequency ratio (winding number) of bending and radial modes are then \( \gamma = 0.15697 + k, k = 0, \pm 1, \pm 2, \ldots \). Note that the present results hold for the AS orbit with a doubled period, which implies that \( \gamma_{AS} = \gamma / 2 \). An analysis of the nearby periodic orbits using the surface of section technique indicates that \( 1 \leq \gamma_{AS} < 13/12 \) and, consequently, it must be \( k = 2 \), i.e., \( \gamma_{AS} \approx 1.0785 \). This result and the results for other values of the nuclear charge \( Z \) are shown in Fig. 2. The results for \( Z = 1 \) and 2 are still used by the author for calculating semiclassical energy spectra of the hydrogen negative ion and the helium atom, respectively.

V. CONCLUDING REMARKS

In this paper we have presented a numerical method for calculating periodic orbits applicable for an arbitrary dynamical system, with the variants of the method adapted for
the Hamiltonian systems and, particularly, the application for calculations of periodic orbits of Hamiltonian systems with singular potentials, i.e., when the equations of motion must be regularized.

The general monodromy method is a generalization and reformulation (in phase space) of the monodromy method by Baranger et al. 5,6 used originally to calculate periodic orbits for a particle in various two-dimensional potentials. Two variants of the method—the midpoint variant and the Runge–Kutta variant—are developed, starting from two types of discretization of equations of motion. FORTRAN programs which implement two variants of the method are tested and it is found that the second variant is somewhat slower. However, this variant is universally applicable and we use it whenever the midpoint variant fails. Of course, variants based on other discretization methods may be developed. Particularly, the midpoint variant of the method, adapted for Hamiltonian systems, given in Sec. III, is a direct generalization of the original monodromy method to many degrees of freedom (with a reformulation in phase space). As in the original method, versions for the calculation of periodic orbits with a given period and with a given energy are developed.

An inconvenience when we use the monodromy method for the calculation of periodic orbits is that we must calculate first an approximate periodic orbit by the use of some other method. Thus, in fact, we have to do two jobs. However, the advantage of the monodromy method versus propagation step-by-step methods is that it determines immediately the monodromy matrix for calculated periodic orbit, which gives Lyapunov exponents and winding numbers of stable modes, which is necessary in most applications. Also, as it has been shown in Sec. IV A, the last paragraph, if we find an exact periodic solution for one choice of parameters of the system, we are in a position to find very quickly the whole class of orbits of a given type for different parameters, by using each previous exact solution as an approximate one for the next calculation with (not too much) changed parameters. For example, calculating the class of 47 periodic orbits \( I_1 \) with scaled energies \( -0.13 \leq E_c \leq 0.1 \), in Sec. IV A, consumes 2–3 s on the Silicon Graphics Work Station 180 MHz/IP32 Processor (we have used the MIPS F77 optimizing compiler).

However, the principal motivation to develop the method for calculation of periodic orbits applicable for arbitrary dynamical systems (i.e. besides the generalization to many degrees of freedom, generalization to the systems with equations of motion which are not Newton’s) has been because of the difficulties arising while applying the original method to the mechanical systems with singular potentials (e.g. Coulomb and gravitational interaction). The equations of motion for a regularized three body Coulomb (or gravitational) system are not Newton’s equations, as it has been demonstrated in the previous section. An application of the Runge–Kutta variant of monodromy method to regularized two-electron atomic systems has been extensively tested, and it is found very reliable. Also, other variants are tested in applying to appropriate mechanical systems and all of them converge to exact solution, if the orbits avoid eventual singularities.

There are, however, nonsingular cases when the variant of monodromy method for the calculations of periodic orbits with given periods that does not work. This appears, for example, in the case of the harmonic oscillator, where all periodic orbits have the same period. Then, after convergence, we obtain a usually trivial periodic orbit which consists of a single point. This difficulty, however, does not appear when using versions of the monodromy method which do not keep the period constant, but other physical quantities, as the energy or, in the case of regularized system, the pseudo-energy.

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1 M. C. Gutzwiller, Chaos in Classical and Quantum Mechanics (Springer-Verlag, New York, 1990).
12 This is not the most general form of Hamiltonian function [see e.g., regularized Hamiltonian function (91) in Sec. IV B]. The form (38) covers the class of mechanical systems, sometimes called the Newtonian, because in this case the Hamilton’s equations are equivalent to the Newton’s equations of motion.
21 N. S. Simonović, Facta Universitatis, Series: Physics, Chemistry and Technology (Niš, Yugoslavia) 1, 13 (1998).