

Programs of Modelling and Visualization of Trajectories of Particles with Variable Mass in the Field of a Massive Geoid

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Abstract. We describe algorithms and tutor programs for simulation and visualization of the trajectory sets of a few-body system including a movement of the carrier rocket taking account of basic forces forming pathways. We consider typical examples of visualization of movement of a classical particle with variable mass in the field of a massive geoid. We also study dynamics of a semiclassical few-body model and trajectory sets of two negative charged particles in the field of a positive charged surface. The symbolic computation system MAPLE is applied to generate computer codes using numerical integrators for solving the Cauchy problem and to simplify visualization tasks.

1 Introduction

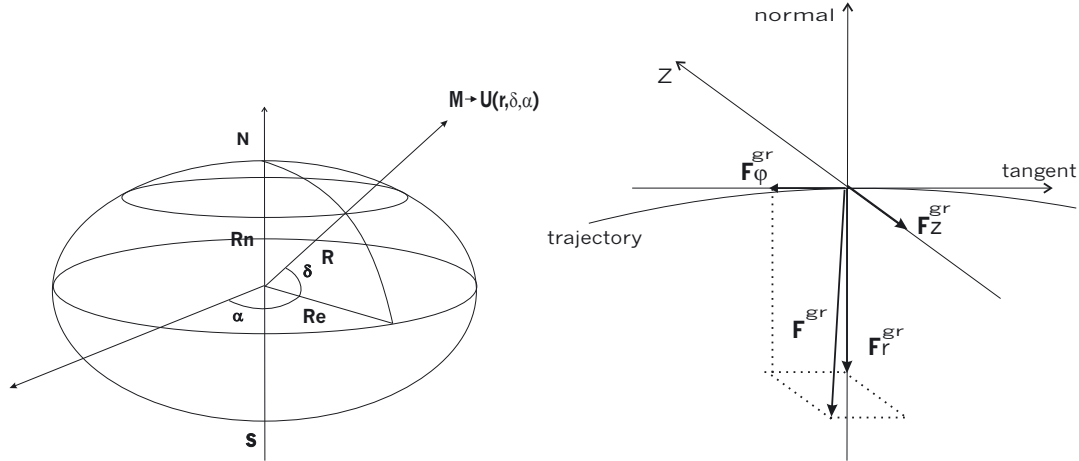
The applications of symbolic computing in the study of the classical and quantum few-body problem dynamics and the visualization of corresponding trajectories are the subject of recent papers[1–3]. Note that a quantum few-body problem with the pair Coulomb interactions can be treated via the semiclassical capture and ionization models of atomic and molecular targets[4–7]. In these models a semiclassical character of the trajectory set is approximated by the velocity dependent pseudopotentials or variable mass of particles [8].

In the first part of the talk we consider the problem of simulating the launching and tracing flight paths of satellites that was solved half a century ago, but its detailed description and visualization is rather a cumbersome task [9–13]. Nevertheless such a modelling problem is of interest as a standard module for the automatic information and control systems [14, 15]. We remind that the stationary trajectory of a satellite is well described by the Kepler laws, while a description of an active part of trajectory requires the solution of a system of differential equations with the account of basic forces acting on the carrier [9, 10]. The technique of the construction of the model, algorithm and visualization of a flight path and of a tutor program 'Sputnik', simulating the motion of the satellite on an active and passive parts of the flight path, is considered. In particular, for the 2D visualization the carrier rocket is viewed as a material point and the equations of motion are integrated in a system of cylindrical coordinates. All characteristic parameters are bound to the Earth surface by means of the geographic coordinates of a subsatellite point. The position of the carrier rocket is figured in the delivery plane of a launching, and the position of a subsatellite point is introduced as an authentic projection of the Earth surface [13].

In the second part of the talk we consider a visualization problem of a family of the hyperbolic paths by Maple in a semiclassical model of the double ionization processes of a helium atom [3], where two electrons are ejected on the hyperbolic paths via a surface of the order of atomic unit with some initial data generated either by the elliptic orbits of the internal region [6] or the corresponding quantum mechanical calculations [16, 17].

We apply Maple with aim to have a useful tool both to generate different codes for a numerical simulation adopted to different methods [18] and modifications of the task and to have a visualization tutoring experience by a more simple way. The latter is oriented to the further solution of some kind of inverse problems, in particular, fitting a set of the initial conditions, which yield a particle orbited on given elliptic or hyperbolic paths.

The talk is organized as follows. Section 2 deals with the basic steps and equations of the algorithm. Section 3 gives a description of the basic modules of the program, typical initial data map points of world space-vehicle launching sites and some examples of the computer 3D visualization of the position and slope of a launching orbit. The run of the program SPUTNIK is demonstrated on an example of imitation of flight of the carrier such as ARIANA [13]. The given program is implemented for the 2D and 3D visualization cases by means of PASCAL and MAPLE, respectively. In section 4 we consider an application of the 2D visualization of classical trajectories of electrons in the semiclassical model of the double ionization of a helium atom by a fast electron, allowing one to fit experimental data in view of



we use an approximation of the potential of a massive rotational ellipsoid up to within the terms of the same order in $\kappa = (R_e - R_n)/R_e$:

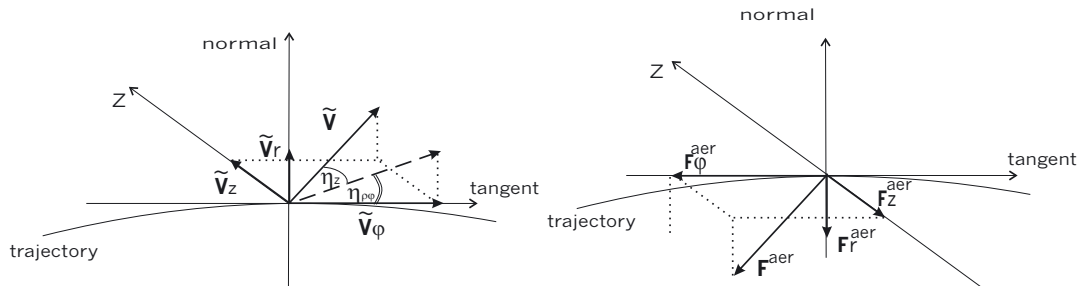
$$U(r, \delta) = - \left[\left(1 - \frac{2\kappa}{2 - \kappa} \cos^2 \delta \right) \left(\frac{R_e}{r} \right)^2 + \dots \right] \frac{GM}{r},$$

where R_e and R_n are the equatorial and polar radii of the Earth, M is the mass of the Earth, G is the gravity constant, r is a distance from the center of the Earth to the satellite, δ is a geographic latitude of the subsatellite point.

4. *The aerodynamic forces.* If the projections of the relative (to the atmosphere) velocity $\tilde{\mathbf{v}}$ are preset, the aerodynamic forces \mathbf{F}^{aer} are defined via the formulas

$$F_r^{aer} = -\frac{1}{2}\rho|\tilde{v}|(c_x S_{\perp} \tilde{v}_r - c_y S_{\parallel} \tilde{v}_{\varphi}), \quad F_{\varphi}^{aer} = -\frac{1}{2}\rho|\tilde{v}|(c_y S_{\parallel} \tilde{v}_r + c_x S_{\perp} \tilde{v}_{\varphi}), \quad F_z^{aer} = -\frac{1}{2}\rho|\tilde{v}|c_z S_z \tilde{v}_z,$$

where $S_{\parallel} = S_{\parallel}(\beta)$, $S_{\perp} = S_{\perp}(\beta)$, $S_z = S_z(\beta)$ are the areas of the carrier seen from normal, from tangent,



and from z -direction,

$$\tilde{v}_{\rho} = \dot{r}, \quad \tilde{v}_{\varphi} = r\dot{\varphi} - \omega\tau r \cos i, \quad \tilde{v}_z = \dot{z} - \omega\tau r \sin i, \quad |\tilde{v}| = (\tilde{v}_{\rho}^2 + \tilde{v}_{\varphi}^2 + \tilde{v}_z^2)^{1/2},$$

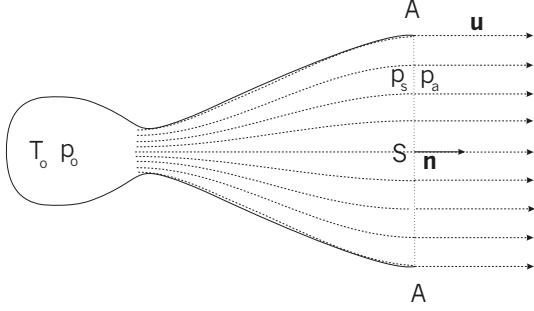
are components of the relative (to the atmosphere) velocity $\tilde{\mathbf{v}}$, ω is the angular velocity of rotation of the Earth, $\tau \in [0, 1]$ is the atmosphere friction coefficient, i is the inclination angle. For dependence of an atmosphere density $\rho = \rho(h, t, \mu, \delta, \alpha)$ and temperature $T = T(h, \delta, \alpha)$ of altitude h , we use the following approximations, which agree well with experimental data:

$$\rho = \rho_0 \exp(-|\dot{m}|gh/R_b T), \quad T = T(h) = T_0(\alpha_T \exp(\gamma_T h) + \beta_T). \\ h = r - R, \quad R = R_e \sqrt{1 - (1 - 1/(1 + \kappa)^2) \sin^2 \varphi \sin^2 i},$$

Here $\alpha_T = 0.95$, $\beta_T = 0.05$, $\gamma_T = 1.67 \cdot 10^{-4}$, and the aerodynamical coefficients c_x , c_y and c_z are supposed to be constants.

5. *The tractive force* A tractive force \mathbf{F}^{tr} is considered to be a sum of two items: one item appears at the expense of momentum carried away by a gas jet, and the second item appears because of a difference of pressure till both sides of outflow section of a nozzle

$$\mathbf{F}^{tr} = |\dot{m}|\mathbf{u} + (p_s - p_a)S\mathbf{n},$$



where \dot{m} is the second propellant consumption, \mathbf{u} is the velocity of its outflow, S is the area of the nozzle cross section, p_s is the pressure inside the nozzle, and p_a is an atmospheric pressure. For the reasons a module of the tractive force $F^{tr} = |\mathbf{F}^{tr}|$ is specified by means of the so-called specific pulse I_s , which is defined as a traction resulting from the combustion of one kilogram of the fuel within one second, i.e. $F^{tr} = |\dot{m}|gI_s$. As two components of the tractive force have a different nature, the specific pulse can be subdivided into two parts $I_s = I_c + \delta I_a$, where $I_c = u/g$ and $\delta I_a = (p_s - p_a)S/(|\dot{m}|g)$.

The values I_c and δI_a are defined from a thermodynamical model of the nozzle flow of a gas jet with the invariable structure, i.e. a model "of the frozen flow":

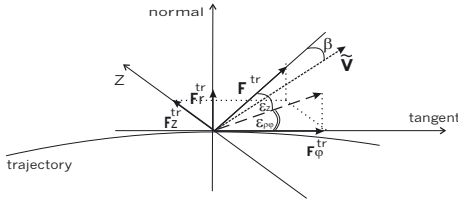
$$I_c = I_0 \sqrt{1 - (p_c/p_0)^{(\gamma-1)/\gamma}}, \quad \delta I = \frac{\gamma - 1}{2\gamma} \frac{(p_c/p_0)^{(\gamma-1)/\gamma}}{1 - (p_c/p_0)^{(\gamma-1)/\gamma}} I_c,$$

where I_0 is a limiting specific pulse, and γ is the parameter of an adiabat of the products of combustion with molar mass μ_g . An atmospheric pressure changes with altitude h in accordance with the barometric height formula, therefore, for the specific pulse I_s we have:

$$I_s = I_s(h) = I_{sv}(1 - q \exp(-|\dot{m}|gh/R_bT)), \\ I_{sv} = I_c(1 + \bar{k}), \quad q = (1 - p_0/p_{cp} \cdot \bar{k}/(1 + \bar{k})), \quad \bar{k} = \delta I/I_c,$$

where p_0 is the atmospheric pressure on the Earth surface. The projections of a vector of the tractive force \mathbf{F}^{tr} are set by means of projective angles as follows:

$$F_r^{tr} = |\dot{m}|I_s g \cos \varepsilon_z(t) \sin \varepsilon_{\rho\varphi}(t), \quad F_\varphi^{tr} = |\dot{m}|I_s g \cos \varepsilon_z(t) \cos \varepsilon_{\rho\varphi}(t), \quad F_z^{tr} = |\dot{m}|I_s g \sin \varepsilon_z(t).$$



Here $\varepsilon_z(t)$ is an angle of the directional control and $\varepsilon_{\rho\varphi}(t)$ is an angle of the control at the pitch. The control of the traction is made with zero angle of an attack $\beta = 0$, i.e. the vector of the tractive force \mathbf{F}^{tr} is parallel to the vector of the relative velocity $\tilde{\mathbf{v}}$.

6. *Equations of motion: fissile flight.* On a fissile flight segment at compiling differential equations of motion we take into consideration following conditions:

a) the gravity forces act in three directions; considering, that the movement occurs only in a plane $z = 0$, we shall obtain that one of equations of motion is transformed to an equation for determination of an angle of directional control $\varepsilon_z(t)$. Thus it appears that the angle $\varepsilon_z(t)$ is so small that in the given approximation it is possible to assume that $\sin \varepsilon_z(t) \approx 0$ and $\cos \varepsilon_z(t) \approx 1$;

b) since a control at a pitch in the plane of the motion is realized with the zero angle of attack, then $\sin \varepsilon_{\rho\varphi}(t) = \tilde{v}_r/|\tilde{v}|$ and $\cos \varepsilon_{\rho\varphi}(t) = \tilde{v}_\varphi/|\tilde{v}|$;

c) Considering that the gravity potential is created by a massive body with a surface of a rotation ellipsoid, the components of potential gradient are set by the following formulas:

$$\text{grad}_r U(r, \delta) = [1 - 3(\sin^2 \varphi \sin^2 i - 1)K(\kappa)(R_e/r)^2] GM/r^2, \\ \text{grad}_\varphi U(r, \delta) = [0 - \sin 2\varphi \sin^2 i K(\kappa)(R_e/r)^2] GM/r^2, \\ K(\kappa) = \kappa/(1 - \kappa/2);$$

d) a current weight of the launcher $m(t)$ is expressed via its initial mass m_0 , a second propellant consumption \dot{m} , and the flight time t :

$$m(t) = m_0 - |\dot{m}|t, \quad |\dot{m}| = \text{const}.$$

As a result we have a system of differential equations

$$\begin{aligned}\ddot{r} &= -\operatorname{grad}_r U(r, \delta) + r\dot{\varphi}^2 - \frac{\rho|\tilde{v}|}{2m(t)} (c_x S_{\perp} \tilde{v}_r - c_y S_{\parallel} \tilde{v}_{\varphi}) + \frac{|\dot{m}|}{m(t)} \bar{I}_s g \frac{\tilde{v}_r}{|\tilde{v}|}, \\ r\ddot{\varphi} &= -\operatorname{grad}_{\varphi} U(r, \delta) - 2\dot{r}\dot{\varphi} - \frac{\rho|\tilde{v}|}{2m(t)} (c_y S_{\parallel} \tilde{v}_r + c_x S_{\perp} \tilde{v}_{\varphi}) + \frac{|\dot{m}|}{m(t)} \bar{I}_s g \frac{\tilde{v}_{\varphi}}{|\tilde{v}|},\end{aligned}$$

with the initial conditions

$$r(0) = R_{st}, \quad \dot{r}(0) = 0, \quad \varphi(0) = \varphi_{st}, \quad \dot{\varphi}(0) = \omega\tau \cos i.$$

This system of equations is solved by the Runge-Kutta numerical integrator of the fourth order; applying other numerical integrators with the analytical Taylor expansions of the right-hand side terms of those like in [18] is also possible.

7. *Equations of motion: passive flight.* The passive part of flying is described by differential equations in the absence of traction. Thus, it is assumed that the flying of the satellite takes place in vacuum in Newtonian gravitation potential, i.e. the equations of motion are given by

$$\ddot{r} = -GM/r^2 + r\dot{\varphi}^2, \quad r\ddot{\varphi} = -2\dot{r}\dot{\varphi}.$$

The solutions of these equations are known:

$$r = \frac{p}{1 + \varepsilon \cos(\varphi - \varphi_x)}, \quad p = \frac{L^2}{GM}, \quad \varepsilon = \left(1 + \frac{4EL^2}{(GM)^2}\right)^{1/2},$$

where E is an energy of the satellite, L is its moment and the unknown value φ_x is defined by final values of the dynamic parameters of an active part of flying. The dependence of time t via coordinate φ is determined by means of a series

$$t - t_k = \frac{T}{2\pi} [(\varphi - \varphi_k) - 2\varepsilon \sin(\varphi - \varphi_k) + \frac{3}{4}\varepsilon^2 \sin 2(\varphi - \varphi_k) + \dots],$$

where t_k is a time of exit into an orbit, φ_k is the coordinate of the satellite at a given moment of time, and T is a period of rotation of satellite determined from the third Kepler law.

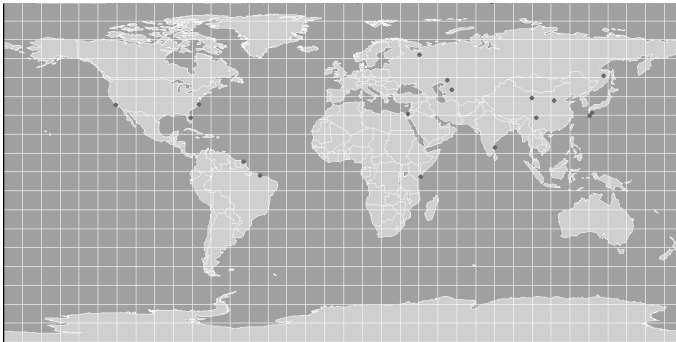


Fig. 1. Points on the map are the world space-vehicle launching sites positions [13]

3 Description of the Program

The proposed program SPUTNIK consists of three module and the program of management of the system menu:

- module 1 contains the routines for the calculation and display on the screen of parameters of an orbit and the characteristics of movement of the satellite at the given moment of time and visualization of its motion; the allocation of this part simplifies adaptation of various mathematical means for the solution of different physical problems;
- module 2 contains the constants, the data about carriers, space-vehicle launching sites, and parameters of orbits that simplify the creation of the new versions in different languages; in this case the text is given as files of textual type, but if necessary it is possible to set the text as a file or database;

- module 3 contains the procedures for management of the menu as well as the procedure of input and output of the textual and graphic information on the screen, that allows to quickly remake this program for the study of other physical processes;
- the basic program `sputnik` administers the system menu. After a display of title page on the screen the menu containing 5 items is obtained: the theoretical part (contains the theoretical items of information); the instructions (instructions necessary for work with the program); the choice of the rocket-carrier (it is possible to choose a type of the rocket-carrier and to look at its characteristics); the choice of the space-vehicle launching site (it is possible to choose the space-vehicle launching site, look at points in Fig. 1; and to look at the location and inclination of an orbit of started rocket-carrier); the model of flight (the model of flight is demonstrated for the chosen configuration of a rocket and space-vehicle launching site: the first movement of the carrier on an active part of flight is shown, then the location of a subsatellite point on a surface of the Earth on a passive part of flight, see examples in Figs. 2, 3; thus, the basic parameters of movement are displayed on the screen).

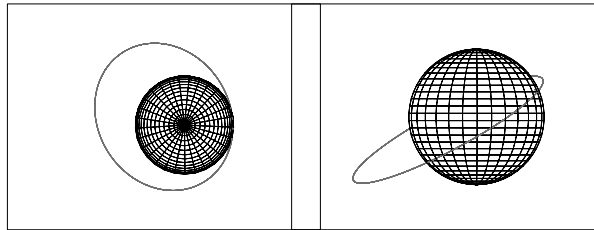


Fig. 2. An example of the computer visualization of the position and slope of a started launcher orbit in a fixed coordinate system

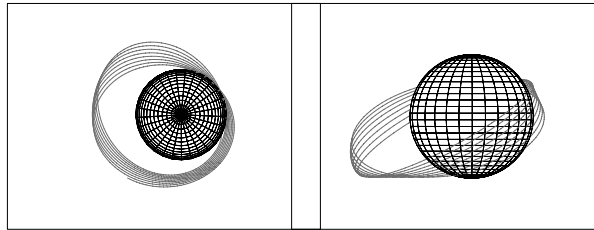


Fig. 3. An example of computer visualization of passive part of the launcher orbit in rotation coordinate system

The work of the program SPUTNIK is demonstrated on an example of the imitation of flight of the carrier such as ARIANA [13]. The given program has been implemented by means PASCAL 7.0 and MAPLE 7.

4 Visualization of Trajectories of Ejected Electrons in a Semiclassical Model of Helium Atom

Here we consider an application of the two-dimensional visualization of classical trajectories of electrons in the semiclassical model of double ionization of a helium atom by fast electron, allowing to fit experimental data in view of deviations from rectilinear trajectories of electrons to take into account the Coulomb interaction in the exit channel [3]. In general case, the classical model of an N electron atom of atomic number Z is described by the Hamiltonian [8] (in atomic units)

$$H_{cl} = T + V_Z + V_{ij} = \sum_{i=1}^N \left[\frac{p_i^2}{2} - \frac{Z}{r_i} \right] + \sum_{i < j} \frac{1}{r_{ij}},$$

where \mathbf{r}_i and \mathbf{p}_i are the positions and momenta of the atomic electrons relative to the fixed nucleus and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ are the coordinates of electron pairs. The semiclassical, Kirschbaum–Wilets version of this

model is described by

$$H_{sc} = H_{cl} + V_H + V_P = H_{cl} + \sum_{i=1}^N V_H(r_i, p_i) + \sum_{i<j} V_P(r_{ij}, p_{ij}),$$

where

$$V_H(r_i, p_i) = \frac{\xi_H}{4a_H r_i^2} \exp(a_H(1 - (r_i p_i / \xi_H)^4))$$

is a Heisenberg-type pseudopotential which stabilizes the atom by preventing the collapse of the atomic electrons into the nucleus, while

$$V_P(r_{ij}, p_{ij}) = \frac{\xi_H}{4a_P r_{ij}^2} \exp(a_H(1 - (r_{ij} p_{ij} / \xi_P)^4)) \delta_{s_i s_j}$$

is Pauli-type pseudopotential which separates identical electron pairs in phase space, resulting in an electronic structure. The semiclassical model of an atom can be minimized to find a stable ground state in which the electrons, while at rest, have nonzero momenta in the presence of momentum dependent potentials; this process has been reviewed by Cohen, who calculated the ground states up to $Z = 38$ with fixed parameters defined in the pseudopotentials [7]. The model is used to study the collision systems in dependence of both the ground states of electron distributions and of the collision dynamics versus the pseudo potential parameters a and ξ .

Below we present the simulation of the double ionization of helium atom ($N=2$) by a fast electron with the initial momentum $\mathbf{p}_0 \gg 1$. The visualization of the classical trajectories of the two ejected electrons with momenta $\mathbf{p}_1, \mathbf{p}_2$ are given in a plane of their motion in coordinate system shown in Fig. 4 beyond a "surface" with characteristic atomic size $r_0 \sim 1$. Here r_1, r_2 are the distances between atomic nucleus with charge $Z = 2$ and the electrons, and θ_1, θ_2 are the angles between a transferred momentum $\mathbf{Q} = \mathbf{p}_s - \mathbf{p}_0 \approx -\mathbf{p}_1 - \mathbf{p}_2$ and radius-vectors of electrons, where \mathbf{p}_s is the scattering momentum of a fast electron (projectile particle). We assume for definiteness that $0 < \theta_1 < 180^\circ$ and $-180^\circ < \theta_2 < 0$, and count of angle θ_1 from axis \mathbf{Q} counter-clockwise while angle θ_2 counter-clock. The distance s between electrons is

$$s = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta_1 - \theta_2)}, \quad (1)$$

and the angular moment M_i of each electron $i = 1, 2$ is defined as

$$M_i = r_i^2 \dot{\theta}_i. \quad (2)$$

In these notations, the equations of motion take the form

$$\ddot{r}_1 = \frac{M_1^2}{r_1^3} - \frac{2}{r_1^2} + \frac{r_1 - r_2 \cos(\theta_1 - \theta_2)}{s^3}, \quad \ddot{r}_2 = \frac{M_2^2}{r_2^3} - \frac{2}{r_2^2} + \frac{r_2 - r_1 \cos(\theta_1 - \theta_2)}{s^3}, \quad (3)$$

$$\dot{M}_1 = \frac{r_1 r_2 \sin(\theta_1 - \theta_2)}{s^3}, \quad \dot{M}_2 = \frac{r_1 r_2 \sin(\theta_2 - \theta_1)}{s^3}. \quad (4)$$

Equation (4) shows that the full angular moment $M = M_1 + M_2$ is the integral of motion, in the same way as the total energy $E_f = E_1 + E_2$ of the ejected electrons

$$H = E_f = \frac{\dot{r}_1^2}{2} + \frac{\dot{r}_2^2}{2} + \frac{M_1^2}{2r_1^2} + \frac{M_2^2}{2r_2^2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{s}. \quad (5)$$

The latter is calculated by formula $E_f = E_0 - E_i - p_s^2/2$, where $E_0 = p_0^2/2$ and $E_i = E_0^{He}$ is the energy of the initial bound state of a helium atom. Let $E_f = 0.74$ and the initial conditions for the system of equations (3), (4) are

$$r_1(0) = r_2(0) = r_0 = 1, \theta_1(0) = \theta_{10}, \theta_2(0) = \theta_{20}, M_1(0) = M_2(0) = 0, |\dot{r}_1(0)| = |\dot{r}_2(0)|. \quad (6)$$

The corresponding plot of asymptotic values of angle $\theta = (\theta_1 - \theta_2)/2$ versus the values of angle $\theta_0 = (\theta_{10} - \theta_{20})/2$ at time $t = 0$ is shown in Fig. 4. For a set of initial data $\theta_{10} \in (0, 180)$ and $\theta_{20} \in (-180, 0)$ the plots of asymptotic isolines of angles θ_1 and θ_2 versus the values of angles θ_{10} and θ_{20} at time $t = 0$ are shown in Fig. 5. One can see from these figures that the electrons from two angular domains of an

atomic "surface" of radius r_0 can reach the same detector. To compare the calculations with experiment we have at the first stage to find for each couple of measured plane angles the emitting angles using the plots. After this we calculate using, say, the close-coupling technique the differential cross section with the angles θ_{10} and θ_{20} and the function $|f(x)|^2$ which is the coefficient of penetration through the external potential barrier. One can insert all obtained data in the differential cross-section formula [3]

$$\frac{d^5\sigma(\theta_1, \theta_2)}{dE_1 dE_2 d\Omega_1 d\Omega_2 d\Omega_s} = \frac{1}{2} \sum_{i=1}^2 |f(x_i)|^2 \left(\frac{d^5\sigma(\theta_{10}, \theta_{20})_i}{dE_1 dE_2 d\Omega_1 d\Omega_2 d\Omega_s} \right)_{in}. \quad (7)$$

and compare the result with the experiment at the angles of observation θ_1 and θ_2 [16,17]. Here E_1 and E_2 are the energies, and Ω_1, Ω_2 are the solid angles of emitted electrons and Ω_s is solid angle of scattering fast electron, summation means that the arrival angle θ_i of an electron corresponds to two emitting angles θ_{10}, θ_{20} , the function $f(x_i)$ is dependent on θ_{10}, θ_{20} and the radius r_0 playing a role of adjusting parameters of the model [3].

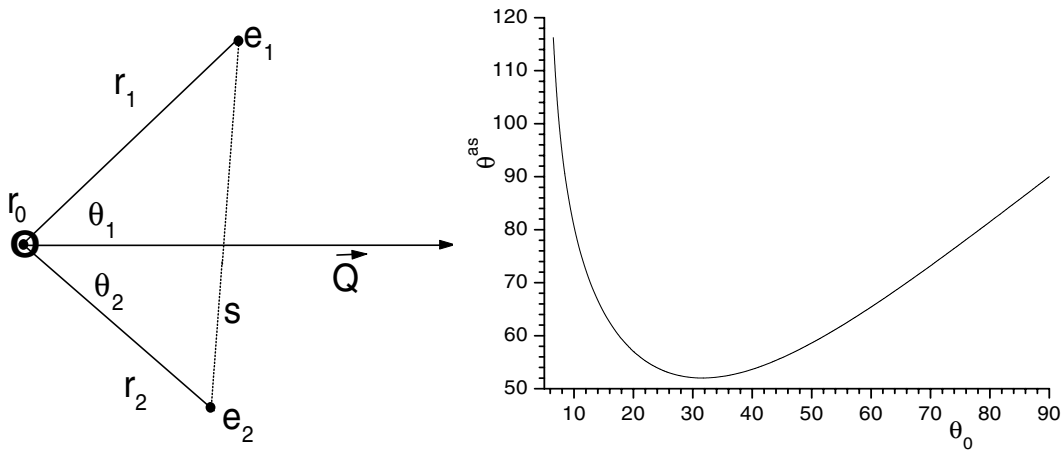


Fig. 4. Coordinate frame and asymptotic values of angle $\theta^{as} = (\theta_1^a - \theta_2^a)/2$ versus initial value θ_0

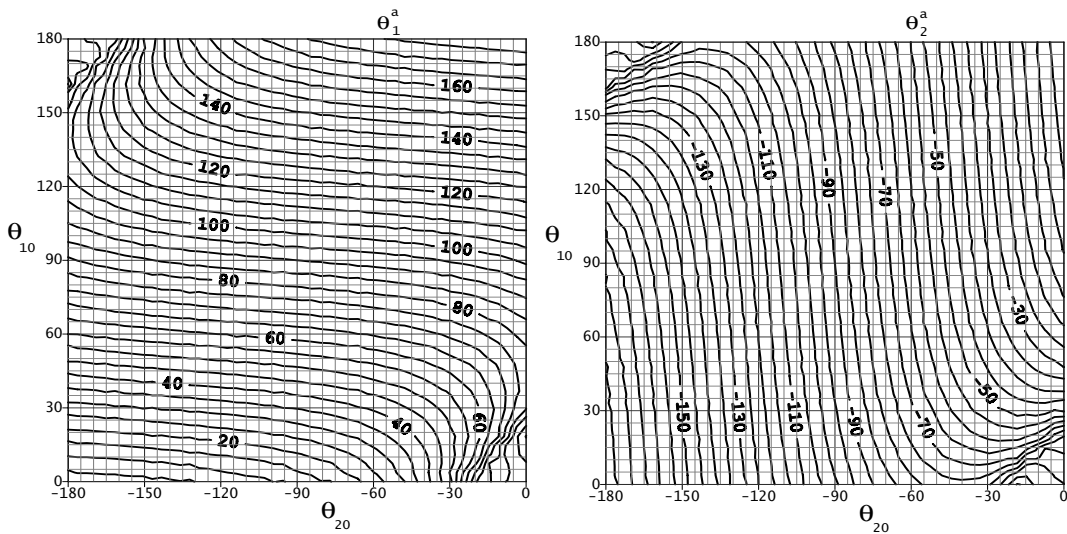


Fig. 5. Asymptotic isolines of angles θ_1^a and θ_2^a versus initial angles $\theta_{20} = \theta_2(0), \theta_{10} = \theta_1(0)$

5 Conclusion

We show the efficiency of symbolic computer systems in the study of the classical and quantum few-body problem dynamics and visualization of corresponding trajectories on typical examples. We see further perspective of applications of symbolic computation system MAPLE in generating the needed computer codes compatible with FORTRAN and C++ applied for the numerical integration of Cauchy problem together with solving some kind of inverse problems and simplifying the visualization tasks under consideration.

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