Exercises

Exercise 29.1 **Kustaanheimo–Stiefel transformation.** *Check the Kustaanheimo–Stiefel regularization for collinear helium; derive the Hamiltonian (29.10) and the collinear helium equations of motion (29.11).*

Exercise 29.2 **Helium in the plane.** *Starting with the helium Hamiltonian in the infinite nucleus mass approximation $m_{he} = \infty$, and angular momentum $L = 0$, show that the three body problem can be written in terms of three independent coordinates only, the electron-nucleus distances r_1 and r_2 and the inter-electron angle Θ, see fig. 29.1.*

Exercise 29.3 **Helium trajectories.** *Do some trial integrations of the collinear helium equations of motion (29.11). Due to the energy conservation, only three of the phase space coordinates (Q_1, Q_2, P_1, P_2) are independent. Alternatively, you can integrate in 4 dimensions and use the energy conservation as a check on the quality of your integrator.*

The dynamics can be visualized as a motion in the original configuration space (r_1, r_2), $r_i \geq 0$ quadrant, or, better still, by an appropriately chosen 2-d Poincaré section, exercise 29.4. Most trajectories will run away, do not be surprised - the classical collinear helium is unbound. Try to guess approximately the shortest cycle of fig. 29.4.

Exercise 29.4 **A Poincaré section for collinear Helium.** *Construct a Poincaré section of fig. 29.3b that reduces the helium flow to a map. Try to delineate regions which correspond to finite symbol sequences, that is initial conditions that follow the same topological itinerary in the fig. 29.3a space for a finite number of bounces. Such rough partition can be used to initiate 2–dimensional Newton-Raphson method searches for helium cycles, exercise 29.5.*

Exercise 29.5 **Collinear helium cycles.** *The motion in the (r_1, r_2) plane is topologically similar to the pinball motion in a 3-disk system, except that the motion is in the Coulomb potential.*

Just as in the 3-disk system the dynamics is simplified if viewed in the fundamental domain, *in this case the region between r_1 axis and the $r_1 = r_2$ diagonal. Modify your integration routine so the trajectory bounces off the diagonal as off a mirror. Miraculously, the symbolic dynamics for the survivors again turns out to be binary, with 0 symbol signifying a bounce off the r_1 axis, and 1 symbol for a bounce off the diagonal. Just as in the 3-disk game of pinball, we thus know what cycles need to be computed for the cycle expansion (29.23).*

Guess some short cycles by requiring that topologically they correspond to sequences of bounces either returning to the same r_i axis or reflecting off the diagonal. Now either Use special symmetries of orbits such as self-retracing to find all orbits up to length 5 by a 1-dimensional Newton search.

Exercise 29.6 **Collinear helium cycle stabilities.** *Compute the eigenvalues for the cycles you found in exercise 29.5, as described in sect. 29.1.4. You may either integrate the reduced 2×2 matrix using equations (29.13) together with the generating function l given in local coordinates by (29.14) or integrate the full 4×4 Jacobian matrix, see sect. 17.1. Integration in 4 dimensions should give eigenvalues of the form $(1, 1, \Lambda_p, 1/\Lambda_p)$; The unit eigenvalues are due to the usual periodic orbit invariances; displacements along the orbit as well as perpendicular to the energy manifold are conserved; the latter one provides a check of the accuracy of your computation. Compare with table 29.1.4; you should get the actions and Lyapunov exponents right, but topological indices and stability angles we take on faith.*

Exercise 29.7 **Helium eigenenergies.** *Compute the lowest eigenenergies of singlet and triplet states of helium by substituting cycle data into the cycle expansion (29.23) for the symmetric and antisymmetric zeta functions (29.22). Probably the quickest way is to plot the magnitude of the zeta function as function of real energy and look for the minima. As the eigenenergies in general have a small imaginary part, a contour plot such as fig. 15.1, can yield informed guesses. Better way would be to find the zeros by Newton method, sect. 15.1.4. How close are you to the cycle expansion and quantum results listed in table 29.2? You can find more quantum data in ref. [29.3].*