The spectrum of Helium obtained by periodic orbit theory.

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Contents

0.1 Purpose and a short overview.

As can be inferred from the title, the aim of this report is to find eigenenergies of the quantum mechanical Helium atom by an application of periodic orbit theory. From here the purpose is twofold.

1° To make a more or less clear line of reasoning from Gutzwiller's trace formula to the zeroes of the dynamical zeta function.

2° To implement all necessary routines on a computer in order to find periodic orbits, to calculate stability eigenvalues, action, etc. to expand the zeta function in a sixth order curvature expansion, inserting the relevant quantities and finally end up with the spectrum of Helium (in a certain range).

Re 1° Attention will be paid to the symmetry of the system, showing that careful use of this greatly improves and reduces formulae (section 2.1 and 3.2). Furthermore a thorough treatment of smooth coordinate transformations will be given to justify that all quantities of interest can equally well be calculated in the transformed coordinates (section 2.2). With the right symmetry and transformations at hand, I introduce the so called fundamental domain (section 3.2.2)and show how this constitutes the best domain for all numerical work (section 3.2.4 and 3.2.5). A fully desymmetrized version of the dynamical zeta function is presented. Explicit expressions will be derived for all quantities entering the zeta function (section 3.3-3.5).

Re 2° Comparison will be made with numerical results found in the same way in [1]. I will implement a fourth order Runge-Kutta method for integration, a (single point) Newton-Raphson search method for short orbits and a multiple shooting method for an exhausting search for orbits up to length six. Zeroes of the zeta function will be found by built-in routines from IDL.

1 Periodic orbit theory in a glimpse.

In this section a very short review of Gutzwiller's trace formula and the dynamical zeta function is given and, assuming that all eigenvalues are hyperbolic, the zeta function is rewritten to a more convenient form.

1.1 From Gutzwiller's trace formula to the dynamical zeta function.

Starting from Gutzwiller's trace formula it is shown how one is led to the dynamical zeta function. According to [1] the trace formula (regularized version) can be written as

$$\mathrm{Tr}G(E) := \sum_n \frac{1}{E-E_n} = -i\pi\bar{d}(E) + \frac{1}{i}\sum_{p\in P} T_p \sum_{r=1}^{\infty} \frac{exp(ir(S_p(E)/\hbar - \pi\alpha_p/2))}{|\det(1-\mathbf{J}_p^r)|^{1/2}},$$

where P is the set of prime cycles, T_p is the period of the cycle, S_p is the action along the cycle, α_p is the topological index (counting the number of sign changes of $\det \mathbf{J}_p^r$ along the orbit), J_p is the stability matrix and $\bar{d}(E)$ is the density of states.

As can be seen from the definition of $\mathrm{Tr}G(E)$ poles must be found along the real axis in points equal to eigenenergies of the system. Numerically it is easier to search for roots than for poles and this motivates the definition of another function $\Delta(E)$ given by

$$\begin{aligned}
\Delta(E) &= \exp\left(-\int_{E_0}^{E} dE \mathrm{Tr} G(E)\right) \\
&= e^{i\pi\bar{N}(E)} \exp\left(-\frac{1}{i}\sum_{p\in P}\sum_{r=1}^{\infty}\int_{E_0}^{E} dE\cdot T_p(E)\frac{e^{ir(S_p(E)/-\alpha_p\pi/2)}}{|\det(1-\mathbf{J}_p^r)|^{1/2}}\right) \\
&= e^{i\pi\bar{N}(E)} \exp\left(-\frac{1}{i}\sum_{p\in P}\sum_{r=1}^{\infty}\int_{S(E_0)}^{S(E)} dS\frac{e^{ir(S_p-\alpha_p\pi/2)}}{|\det(1-\mathbf{J}_p^r)|^{1/2}}\right) \\
&= e^{i\pi\bar{N}(E)} \exp\left(-\sum_{p\in P}\sum_{r=1}^{\infty}\frac{1}{r}\frac{e^{ir(S_p(E)-\alpha_p\pi/2)}}{|\det(1-\mathbf{J}_p^r)|^{1/2}}\right).
\end{aligned}$$

Here the relation $d(S(E)) = T(E)dE$ for periodic orbits has been exploited, and the accumulated density $\bar{N}(E)$ has been introduced. Furthermore, since we eventually only will need the roots of $\Delta(E)$, we left out the constant factor obtained by evaluating the integrand in E_0. Alternatively we could simply assume that E_0 is chosen such that the integrand has a root.

As conjectured in [4] (these things are apparently difficult to prove) the eigenvalues of the stability matrix for any periodic orbit are hyperbolic in the case of Helium[1]; in the collinear plane, real; perpendicular to the collinear plane, complex with unit norm. Thus the eigenvalues, $\Lambda_{||}$ and $\Lambda_\perp$, in and perpendicular to the plane can be written,

$$\Lambda_{||} = \epsilon e^{-\lambda} \text{ with } \lambda > 0 \text{ and } \epsilon = \mathrm{sgn}\Lambda_{||}; \Lambda_\perp = e^{i2\pi\sigma} \text{ with } \sigma \in \mathbb{R}.$$

Next, by exploiting $e^{-\lambda} < 1$ and that $1-\epsilon e^{\lambda}$ has the same sign as ϵ, we note,

$$\begin{aligned}
|\det(\mathbf{1}-\mathbf{J})| &= |(1-\epsilon e^{-\lambda})|\cdot|(1-\epsilon e^{\lambda})|\cdot|(1-e^{i2\pi\sigma})(1-e^{-i2\pi\sigma})| \\
&= (1-\epsilon e^{-\lambda})\cdot\epsilon(1-\epsilon e^{\lambda})\cdot|(1-e^{i2\pi\sigma})(1-e^{i2\pi\sigma})^*| \\
&= (1-\epsilon e^{-\lambda})\cdot\epsilon(1-\epsilon e^{\lambda})\cdot(1-e^{i2\pi\sigma})(1-e^{i2\pi\sigma})^* = \epsilon\det(\mathbf{1}-\mathbf{J}).
\end{aligned}$$

In the second last equation it was used that for any complex number z it holds that $zz^* > 0$. Now we can continue with,

$$\begin{aligned}
|\det(1-\mathbf{J}^r)|^{-1/2} &= \epsilon^{-1/2}\frac{\Lambda_{||}^{r/2}}{1-\Lambda_{||}^r}\frac{\Lambda_\perp^{r/2}}{1-\Lambda_\perp^r} \\
&= \epsilon^{-1/2}\Lambda_\perp^{r/2}\Lambda_{||}^{r/2}\sum_{k=0}^{\infty}\Lambda_\perp^{rk}\sum_{m=0}^{\infty}\Lambda_{||}^{mr} \\
&= \epsilon^{-1/2}\sum_{k,m=0}^{\infty}\Lambda_\perp^{r(k+1/2)}\Lambda_{||}^{r(m+1/2)}.
\end{aligned}$$

By recognizing that $\ln(1-x) = -\sum_{n=1}^{\infty}\frac{x^n}{n}$ we can perform the sum over r in the semi-

[1] A set of eigenvalues are set to be hyperbolic if they occur in pairs being each others inverse.

classical zeta function,

$$\begin{aligned}
\Delta(E) &= e^{i\pi\bar{N}(E)} \prod_{k,m=0}^{\infty} \prod_{p\in P} \exp\left[-\sum \frac{1}{r}(e^{i(S_p(E)-\alpha_p\pi/2)}\Lambda_{\perp}^{k+1/2}\epsilon^{-1/2}\Lambda_{||}^{m+1/2})^r\right] \\
&= e^{i\pi\bar{N}(E)} \prod_{k,m=0} \prod_{p\in P} \exp\ln(1-e^{i(S_p(E)-\alpha_p\pi/2)}\Lambda_{\perp}^{k+1/2}\epsilon^{-1/2}\Lambda_{||}^{m+1/2}) \\
&= e^{i\pi\bar{N}(E)} \prod_{k,m=0} \prod_{p\in P} \left[1-e^{i(S_p(E)-\alpha_p\frac{\pi}{2})+(k+\frac{1}{2})i2\pi\sigma_p-(m+1/2)\lambda_p}\epsilon^{m+\frac{1}{2}}\epsilon^{-\frac{1}{2}}\right] \\
&\equiv e^{i\pi\bar{N}(E)} \prod_{k,m=0}^{\infty} \zeta_{k,m}^{-1}(E).
\end{aligned}$$

Here we have finally reached the dynamical zeta function

$$\begin{aligned}
\zeta_{k,m}^{-1}(E) &= \prod_{p\in P}(1-t_{k,m}^{p}(E)) \text{ with} \\
t_{k,m}^{p}(E) &= \epsilon^m \exp(i(S_p(E)-\alpha_p\pi/2+2\pi(k+1/2)\sigma)-(m+1/2)\lambda_p)
\end{aligned}$$

According to [1] k, m can be related to the quantum numbers of Helium. The aim for this report is to obtain a range of the spectrum corresponding to $k = m = 0$. Hence hereafter we will suppress k and m and simply write $\zeta^{-1}(E)$ and $t^p(E)$.

1.2 Symbolic dynamics.

As seen in the last section, the problem of finding the spectrum of Helium has been reduced to that of finding roots in a complex function, which is a product over the set of periodic orbits. For practical purposes we need an expansion of the zeta function with finitely many terms, and in order to choose these wisely, we will need some appropriate way of labeling the orbits, i.e. we need some correspondence between periodic orbits and some appropriate set. Let $\{0,1\}^{\mathbb{Z}}$ denote the set of doubly infinite strings of 0's and 1's. Whereas this set is actually uncountable, the set $\{0,1\}^{\mathbb{Z}}_{per}$ of strings with a period is actually countable. A mapping from the set of trajectories into $\{0,1\}^{\mathbb{Z}}$ such that periodic trajectories are mapped into $\{0,1\}^{\mathbb{Z}}_{per}$ is denoted a (binary) *symbolic dynamic* (or symbolic representation) of the system.[2]

A symbolic dynamic which maps the set of periodic trajectories bijectively into $\{0,1\}^{\mathbb{Z}}_{per}$, is said to be complete. As will be mentioned in section 3.4, a wisely chosen complete symbolic dynamic can lead to a super-convergent expansions of the zeta function.

1.3 The curvature expansion.

Consider again the dynamical zeta function,

$$\zeta^{-1}(z) = \prod_{p\in P}(1-t_p(z)).$$

In general, infinite products are not too well studied and, I think, the convergence of this entity is not guaranteed in the general case. Nevertheless one can make a meaningful approximation based on physical insight contained in the following idea:

[2] There might be other natural conditions to be fulfilled; for instance the symbolic dynamics should map "similar" trajectories into "similar" strings. However, the definition given here is good enough for our purposes.

A long orbit p gives a contribution which is almost canceled by the contributions from the shorter orbits being decompositions of the long ones.

To be more precise let us introduce the following notation: Given a symbolic string p, the set $\{s^{(1)}, \ldots, s^{(n)}\}$ of symbolic strings is said to be a *decomposition* of p if the concatenation $s = s^{(1)} \cdots s^{(n)}$ is equal to p. Let $\mathcal{S}_p$ denote the set of all decompositions of p. The above idea can now be stated as follows: The term $t_p(z)$, which depends solely on the quantities S_p, λ_p, σ_p and α_p, will be nearly equal (with opposite sign) to the quantity,

$$\sum_{s \in \mathcal{S}_p} (-1)^n t_{s^{(1)}} \cdots t_{s^{(n)}}.$$

One says that the longer orbits are *shadowed* by the shorter ones. According to [1] complete shadowing implies super-exponential convergence of the curvature expansion (the error goes something like e^{-n^2} where n is the order of approximation.) In section 3.5 we will make a curvature expansion for the Helium atom.

2 General features in dynamical systems.

2.1 Symmetry.

As always in physics, symmetry is a great source of trickery. Both in the sense that care should be taken to draw the right conclusions and that short cuts can be found to ease life in general.

To put it simply, I want to find out what consequences symmetries in a Hamiltonian have on trajectories, stability matrices etc. Among the exciting (and well known I guess) features are (for a certain set of symmetries):

1) The symmetry operation and the flow commutes.

2) The set of trajectories becomes symmetric with respect to this symmetry.

3) The stability matrices for symmetric trajectories are equal (modulo symmetry).

The following three sections give precise formulations and proofs of these features.

2.1.1 Symmetries of H commutes with the corresponding flow.

In this section I will study the general question of which symmetries in the Hamiltonian are inherited by the flow.

In the following H denotes a Hamiltonian on a 2d-dimensional phase space (in effect it is just a smooth real mapping on $\mathbb{R}^{2d}$), $f^t(\xi)$ is the flow induced by Hamiltons equations of motion, $\mathbf{S}$ is a linear symmetry on $\mathbb{R}^{2d}$, that is, $\mathbf{S}$ is a $2d \times 2d$ matrix for which $\mathbf{S}^T = \mathbf{S}^{-1}$.

I want to find sufficient conditions on $\mathbf{S}$ such that for any time t and any initial point ξ we have $f^t(\mathbf{S}\xi) = \mathbf{S}f^t(\xi)$. Whether these conditions are necessary will be of no concern here.

The first condition on $\mathbf{S}$ is that $H(\mathbf{S}\xi) = H(\xi)$ for all ξ, i.e. H is invariant under $\mathbf{S}$. Now we can show that $\mathbf{S}$ commutes with $\frac{\partial H}{\partial \xi}$ in the following sense:

$$\frac{\partial H}{\partial \xi}(\mathbf{S}\xi_0) = \mathbf{S}\frac{\partial H}{\partial \xi}(\xi_0).$$

This follows because for any column unit vector $\hat{e}$ it holds,

$$\begin{aligned}
\hat{e}^T \cdot \frac{\partial H}{\partial \xi}(\mathbf{S}\xi_0) &= \lim_{\epsilon \to 0} \frac{1}{\epsilon}(H(\mathbf{S}\xi_0 + \epsilon\hat{e}) - H(\mathbf{S}\xi_0)) \\
&= \lim_{\epsilon \to 0} \frac{1}{\epsilon}(H(\xi_0 + \epsilon\mathbf{S}^T\hat{e}) - H(\xi_0)) \\
&= (\mathbf{S}^T\hat{e})^T \cdot \frac{\partial H}{\partial \xi}(\xi_0) \\
&= \hat{e}^T \cdot \mathbf{S}\frac{\partial H}{\partial \xi}(\xi_0)
\end{aligned}$$

The next step is to find some conditions on $\mathbf{S}$ such that it commutes with the symplectic matrix $\mathbf{w}$. We have

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} = \begin{pmatrix} -\mathbf{B} & \mathbf{A} \\ -\mathbf{D} & \mathbf{C} \end{pmatrix}$$

and

$$\begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} = \begin{pmatrix} \mathbf{C} & \mathbf{D} \\ -\mathbf{A} & -\mathbf{B} \end{pmatrix}.$$

If these are to be equal we must have $-\mathbf{B} = \mathbf{C}$ and $\mathbf{A} = \mathbf{D}$. Thus $\mathbf{S}$ commutes with $\mathbf{w}$ if and only if it can be written on the form

$$\mathbf{S} = \begin{pmatrix} \mathbf{S}_0 & \mathbf{S}_1 \\ -\mathbf{S}_1 & \mathbf{S}_0 \end{pmatrix}.$$

Putting on $\mathbf{S}$ this additional condition we finally have

$$\mathbf{w}\frac{\partial H}{\partial \xi}(\mathbf{S}\xi_0) = \mathbf{S}\mathbf{w}\frac{\partial H}{\partial \xi}(\xi_0).$$

Now for small time steps Δt, we must have

$$\begin{aligned}
f^{\Delta t}(\mathbf{S}\xi_0) &\approx \mathbf{S}\xi_0 + \Delta t\mathbf{w}\frac{\partial H}{\partial \xi}(\mathbf{S}\xi_0) \\
&= \mathbf{S}(\xi_0 + \Delta t\mathbf{w}\frac{\partial H}{\partial \xi}(\xi_0)) \\
&= \mathbf{S}f^{\Delta t}(\xi_0).
\end{aligned}$$

In the limit $\Delta t \to 0$ this is exact. Generalizing this to any time is done as follows,

$$\begin{aligned}
f^t(\mathbf{S}\xi_0) &= \lim_{N \to \infty} (f^{t/N})^N(\mathbf{S}\xi_0) \\
&= \mathbf{S} \lim_{N \to \infty} (f^{t/N})^N(\xi_0) = \mathbf{S}f^t(\xi_0).
\end{aligned}$$

Thus it has been proved that the flow commutes with the symmetry $\mathbf{S}$ if :

I: $\mathbf{S}$ is linear and has the block structure given above.

II: H is invariant under $\mathbf{S}$.

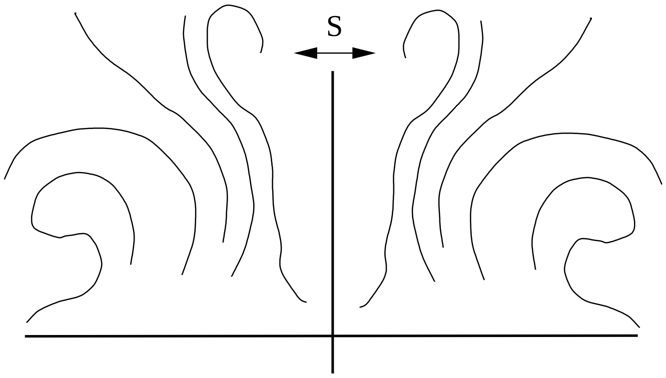

Figure 1: If the Hamilton has a symmetry $\mathbf{S}$ which fulfills condition I and II, the set of trajectories become symmetric with respect to $\mathbf{S}$. In this figure $\mathbf{S}$ is illustrated as a reflection through an axis.

2.1.2 The set of trajectories inherits symmetries from H.

In this section a short comment is given on the symmetries of the set of trajectories.

Assuming $\mathbf{S}$ is a symmetry of the Hamiltonian (fulfilling condition I and II) the claim is as follows:

For any time t_0 and any initial point ξ it holds that the trajectory starting in ξ and ending in $f^{t_0}(\xi)$ is symmetrically equal to the trajectory starting in $\mathbf{S}\xi$ and ending in $f^{t_0}(\mathbf{S}\xi)$. In other words, the trajectory $\mathcal{T}_1 = \{f^t(\xi) \in \mathbb{R}^d | 0 < t < t_0\}$ is mapped into the trajectory $\mathcal{T}_2 = \{f^t(\mathbf{S}\xi) \in \mathbb{R}^d | 0 < t < t_0\}$ under the action of $\mathbf{S}$.

To prove this is straightforward. Simply let $\mathbf{S}$ act on every point in $\mathcal{T}_1$ and exploit that $\mathbf{S}$ and $f^t(\cdot)$ commutes for every t.

This result is illustrated in figure 1.

2.1.3 Correspondence between stability matrices from symmetric trajectories.

In this section I will derive a formula connecting the stability matrices for two trajectories which are equal modulo symmetries of H. A general definition of stability matrices is given in section 2.2.1

The setup is as follows: H is a Hamiltonian on a d-dimensional phase space, $f^t(\xi)$ is the induced flow and $\mathbf{S}$ is a linear symmetry on $\mathbb{R}^d$ fulfilling condition I and II from section 2.1.1. Pick some initial point $\xi \in \mathbb{R}^d$ and some evolution time t_0. In the following we will sometimes suppress t and write $f(\cdot)$ instead of $f^t(\cdot)$.

Let $\delta\xi$ be any infinitesimal vector. Then $\mathbf{S}\delta\xi$ will also be infinitesimal (in fact $||\mathbf{S}\delta\xi|| \leq ||\mathbf{S}|| \cdot ||\delta\xi|| = ||\delta\xi||$). Now, as explained in figure 2 we must have,

$$f(\mathbf{S}\xi) + \mathbf{J}_f(\mathbf{S}\xi) \cdot \mathbf{S}\delta\xi = \mathbf{S}(f(\xi) + \mathbf{J}_f(\xi) \cdot \delta\xi).$$

Exploiting $f(\mathbf{S}\xi) = \mathbf{S}f(\xi)$ and recalling that $\delta\xi$ was arbitrarily chosen we finally end up with

$$\mathbf{J}_f(\mathbf{S}\xi) \quad = \quad \mathbf{S}J_f(\xi)\mathbf{S}^{-1}. \tag{1}$$

The argument can be made for any pair of symmetric trajectories, and (1) then says that the stability matrices can be calculated equally well for symmetric trajectories, and obtaining one from the other is simply obtained by a change of basis ($\mathbf{S}$ is in particular orthogonal).

This will be of great use later on, because it allows us to perform all numerical calculations in the so called fundamental domain.

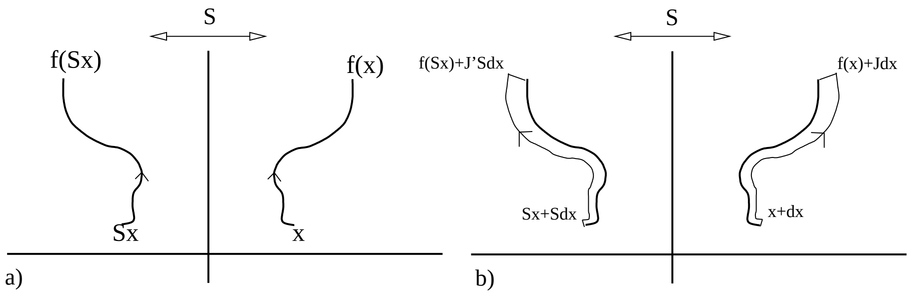

Figure 2: Trajectories in a phase space. $\mathbf{S}$ is some symmetry (indicated as a reflection), $f(\cdot)$ is the flow (suppressing time dependence) induced by a Hamiltonian which is invariant under $\mathbf{S}$. Part a: illustrates that the symmetry of H is inherited by the shape of trajectories, thus the trajectories starting in ξ and $\mathbf{S}\xi$ are equal modulo $\mathbf{S}$. In part b: we have made a small displacement of ξ into $\xi + \delta\xi$. This initial point evolves to to the terminal point $f(\xi) + \mathbf{J}_f(\xi)\delta\xi$. The trajectory with initial point $\mathbf{S}(\xi + \delta\xi)$ (which is equal to $\mathbf{S}\xi + \mathbf{S}\delta\xi$) will evolve to $f(\mathbf{S}\xi) + \mathbf{J}_f(\mathbf{S}\xi)\mathbf{S}\delta\xi$. Now, because $\mathbf{S}\xi + \mathbf{S}\delta\xi$ and $\xi + \delta\xi$ are equal modulo $\mathbf{S}$, their trajectories will be equal modulo $\mathbf{S}$, in particular their termination points will be equal modulo $\mathbf{S}$. In other words, $f(\mathbf{S}\xi) + \mathbf{J}_f(\mathbf{S}\xi) \cdot \mathbf{S}\delta\xi = \mathbf{S}(f(\xi) + \mathbf{J}_f(\xi) \cdot \delta\xi)$.

2.2 Smooth coordinate transformations.

Just as well as symmetries, clever coordinate transformations can greatly improve the performance of numerical routines (for instance in connection with removal of singularities in the equations of motion). In this section I will derive some central results in this connection. We need them to justify that certain quantities entering Gutzwiller's trace formula are conserved under coordinate transformations. In particular we will show that the stability eigenvalues and the topological index is conserved under smooth coordinate transformations.

At first we need some general concepts. Assume f is a flow and g is a smooth invertible mapping on the phase space. Then $h^t(\xi) = g \circ f^t \circ g^-1(\xi)$ is denoted the *transformed flow*. This is appropriate because trajectories of f is mapped by g into trajectories of h,

$$\begin{aligned} g\{f^t(\xi)|t_0 \leq t \leq t_1\} &= \{g \circ f^t \circ g^{-1}(\xi')|t_0 \leq t \leq t_1\} \\ &= \{h^t(\xi')|t_0 \leq t \leq t_1\}, \end{aligned}$$

where we put $\xi' = g(\xi)$.[3] We can think of these trajectories as *corresponding* to each other (one is the transformed of the other). Usually we will also denote ξ and $g(\xi)$ as *corresponding* points.

[3]If the coordinate transformation involves a transformation of time as well (this is perfectly acceptable), we would need to adjust the limits of t.

2.2.1 The stability matrix.

Let f be a smooth mapping from $\mathbb{R}^d$ into $\mathbb{R}^d$. We define the *stability* or *monodromy* matrix of f as the coordinate dependent $d \times d$ matrix $\mathbf{J}_f(x)$ satisfying

$$\mathbf{J}_f(x) \cdot \hat{e}_i = \lim_{\epsilon \to 0} \frac{1}{\epsilon}(f(x + \epsilon \hat{e}_i) - f(x)),$$

for all unit vectors $\hat{e}_i$.[4] Clearly this is a generalization of the usual concept of differentiation. An equivalent but more loose definition is that for infinitesimal vectors δx it holds,

$$\mathbf{J}_f(x)\delta x \approx f(x + \delta x) - f(x).$$

Accepting this sloppy version, it is simple to show the chain rule for stability matrices. Let g be another smooth mapping from $\mathbb{R}^d$ into $\mathbb{R}^d$. For any matrix A (of finite dimension) it holds that $||A|| < \infty$ where $|| \cdot ||$ is the operator norm. From this it follows that if δx is an infinitesimal vector, then $A\delta x$ is as well because $||A\delta x|| \le ||A|| \cdot ||\delta x||$. Using the above definition twice we derive the stability of f composed with g.

$$\begin{aligned}
\mathbf{J}_{f \circ g}(x)\delta x &\approx f(g(x + \delta x)) - f(g(x)) \approx f(g(x) + \mathbf{J}_g(x)\delta x) - f(g(x)) \\
&\approx f(g(x)) + \mathbf{J}_f(g(x)) \cdot \mathbf{J}_g(x)\delta x - f(g(x)) = \mathbf{J}_f(g(x)) \cdot \mathbf{J}_g(x) \cdot \delta x.
\end{aligned}$$

Thus

$$\mathbf{J}_{f \circ g}(x) = \mathbf{J}_f(g(x)) \cdot \mathbf{J}_g(x).$$

2.2.2 Conservation of stability eigenvalues.

Now we want to interpret f as the flow of some dynamical system evaluated at some time t (usually one would write $f^t(x)$ but for simplicity we will suppress t); g will be interpreted as a coordinate transformation. For g we thus additionally have to assume that g is invertible, that is $g \circ g^{-1} = \text{id}$. As explained above $h \equiv g \circ f \circ g^{-1}$ defines the flow in the new coordinates. It is straightforward to verify that $h(x') = x'$ if and only if $f(x) = x$ with $x' = g(x)$. In other words any fixpoint x for the original flow transforms to the fixpoint x' for the transformed flow. We will say that the fixpoints correspond to each other.

The following calculation shows the promised result: Stability eigenvalues of h and f are equal in corresponding fixpoints.

Assume $x' = g(x)$, i.e. $g^{-1}(x') = x$ and that $f(x) = x$. The central trick is given by the following identity which holds for any y in the phase space,

$$\mathbf{1} = \mathbf{J}_{\text{id}} = \mathbf{J}_{g \circ g^{-1}}(y) = \mathbf{J}_g(g^{-1}(y)) \cdot \mathbf{J}_{g^{-1}}(y).$$

With this,

$$\begin{aligned}
\det(\Lambda - \mathbf{J}_h(x')) &= \det[\Lambda - \mathbf{J}_g(f(g^{-1}(x'))) \cdot \mathbf{J}_f(g^{-1}(x')) \cdot \mathbf{J}_{g^{-1}}(x')] \\
&= \det[\Lambda - \mathbf{J}_g(f(x)) \cdot \mathbf{J}_f(x) \cdot \mathbf{J}_{g^{-1}}(x')] \\
&= \det[\Lambda - \mathbf{J}_g(x) \cdot \mathbf{J}_f(x) \cdot \mathbf{J}_{g^{-1}}(x')] \\
&= \det[\mathbf{J}_g(g^{-1}(x')) \cdot (\Lambda - \mathbf{J}_f(x)) \cdot \mathbf{J}_{g^{-1}}(x')] \\
&= \det[\mathbf{J}_g(g^{-1}(x')) \cdot \mathbf{J}_{g^{-1}}(x') \cdot (\Lambda - \mathbf{J}_f(x))] \\
&= \det[\Lambda - \mathbf{J}_f(x)].
\end{aligned}$$

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[4] We will not be conserved with existence and uniqueness of $\mathbf{J}_f(x)$ from this definition. Alternatively one could alternatively define $\mathbf{J}_f$ in the usual way by partial derivatives, $(\mathbf{J}_f(x_0))_{ij} = (\frac{\partial f}{\partial x_j})_i|_{x_0}$.

This equation says that Λ is an eigenvalue of $\mathbf{J}_h(x')$ if and only if Λ is an eigenvalue of $\mathbf{J}_f(x)$. Thus the eigenvalues are conserved under the transformation.

2.2.3 Conservation of the topological index.

Now we turn to prove the other assertion of conservation of topological index. To be precise, I will show that $\alpha_{\mathcal{T}}$ calculated for a trajectory of the original flow f is equal to $\alpha_{\mathcal{T}'}$ calculated for the corresponding trajectory of the transformed flow h.

As before, assume f and g are smooth mappings $\mathbb{R}^d \to \mathbb{R}^d$, g is invertible and h is the transformed flow,

$$h = g \circ f \circ g^{-1}.$$

We now show (putting $x' = g(x)$),

$$\det \mathbf{J}_h(x') = 0 \text{ if and only if } \det \mathbf{J}_f(x) = 0.$$

Assuming the latter equality one finds,

$$\det \mathbf{J}_h(x') = \det \mathbf{J}_g(fg^{-1}(x')) \cdot \det \mathbf{J}_f(x) \cdot \det \mathbf{J}_{g^{-1}}(x') = 0.$$

Next assume the former equation. Exploiting that g is invertible, hence $\mathbf{J}_g$ has a non-vanishing determinant (similarly for g^{-1}), one finds by factorizing the determinant as $\det \mathbf{AB} = \det \mathbf{A} \cdot \det \mathbf{B}$ that $\det \mathbf{J}_h$ can vanish only if $\det \mathbf{J}_f$ vanishes.

Ignoring for now those cases of saddle points where the determinant vanishes but does not change sign, we have shown that $\mathbf{J}_h$ and $\mathbf{J}_f$ changes sign in corresponding points. This justifies that α_p is conserved under smooth coordinate transformations.

3 Application of the theory to the Helium atom.

3.1 Equations of motion.

This section follows [3] and [4].

We are considering the Helium atom with an infinitely massive nucleus and charge eZ, surrounded by two electrons with charge e and mass m. Naturally, only Coulomb forces will be taken into account and for this setup it is well known that the Hamiltonian becomes

$$H(\bar{r}_1, \bar{r}_2, \bar{p}_1, \bar{p}_2) = \frac{\bar{p}_1^2}{2m} + \frac{\bar{p}_2^2}{2m} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}},$$

with $r_i = |\bar{r}_i|$ and $r_{12} = |\bar{r}_1 - \bar{r}_2|$. Explicit time independence implies that H is constant along any trajectory determined from Hamiltons equation of motion. According to [3] trajectories of positive energy will eventually have both electrons wandering off to infinity, whereas those of negative energy at most allows the ionization of a single electron and at least makes the existence of doubly bound periodic orbits possible. Thus we are interested in orbits for which $H = -E, (E > 0)$.

Now, it is seen that three hyper surfaces of singularities exist in H; namely $r_1 = 0$, $r_2 = 0$ and $r_{12} = 0$. Two of them correspond to collisions between one electron and the nucleus and the last one corresponds to the triple collision between both electrons and the nucleus. As shown next, the former kind of singularity can be removed by some clever transformations.

3.1.1 Performing a clever coordinate transformation.

At first we make a simple scaling (using the same variable names),

$$\bar{r}_i \equiv \bar{r}_i \frac{e^2}{E}, \bar{p}_i \equiv \frac{\bar{p}_i}{\sqrt{m_e E}}, i = 1,2, t \equiv \frac{e^2\sqrt{m}}{E^{3/2}} t$$

resulting in a Hamiltonian

$$H'(\bar{r}_1, \bar{r}_2, \bar{p}_1, \bar{p}_2) = \frac{\bar{p}_1^2}{2} + \frac{\bar{p}_2^2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} - \frac{1}{|\bar{r}_1 - \bar{r}_2|}.$$

Note that E has been divided out, thus $H' = -1$, constantly.

Later on we will restrict ourselves to the case of zero angular momentum. For orbits found in this $L = 0$ plane we need to find stability values not only for displacements in this plane, but also for displacements perpendicular to the plane (recall that our task is still to determine eigenvalues for the full three-dimensional Helium atom). It should be clear from $y_i \leftrightarrow z_i, p_i^y \leftrightarrow p_i^z$-symmetry that stability eigenvalues (measuring degree of stretching and twisting) for y- and z-displacements should be equal. Thus it is enough if we derive equations of motion for either y or z. We will choose y and thus put $z_i = 0$ and $p_i^z = 0$, $i = 1,2$. Following [3] we now perform a Kustaanheimo and Stiefel (KS) transformation,

$$\begin{array}{lll} x_1 = Q_1^2 - Q_2^2, & y_1 = 2Q_1Q_2, & r_1 = R_1^2 = Q_1^2 + Q_2^2, \\ x_2 = Q_3^2 - Q_4^2, & y_2 = 2Q_3Q_4, & r_1 = R_2^2 = Q_3^2 + Q_4^2, \\ p_1^x = \frac{Q_1P_1 - Q_2P_2}{2R_1^2}, & p_1^y = \frac{Q_2P_1 + Q_1P_2}{2R_1^2} & \\ p_2^x = \frac{Q_3P_3 - Q_4P_4}{2R_2^2}, & p_2^y = \frac{Q_4P_3 + Q_3P_4}{2R_2^2}. & \end{array}$$

In [5] it is explicitly shown to be canonical.

At last it is observed that in general, for a time independent Hamiltonian $H(q,p)$, a transformation of the time differential $dt = f(q,p)d\tau$ preserves the dynamics if a new Hamiltonian is introduced as $H'(q,p) = f(q,p)(H(q,p) - E)$. Namely it holds,

$$\begin{aligned} \frac{dH'(q,p)}{dq} &= \frac{df(q,p)}{dq}(H(q,p) - E) + f(q,p)\frac{dH(q,p)}{dq} = -f(q,p)\frac{dp}{dt} \\ &= -f(q,p)\frac{dp}{d\tau}\frac{d\tau}{dt} = -\frac{dp}{d\tau}. \end{aligned}$$

Similarly it is shown that $\frac{dH(q,p)}{dp} = \frac{dq}{d\tau}$, i.e. with respect to the transformed time τ, the equations of motion of q and p is obtained from the Hamiltonian H'. Here we will use the transformation $\frac{dt}{d\tau} = r_1 r_2$.

This together with the KS-transformation yields,

$$\begin{aligned} K(Q_1, Q_2, Q_3, Q_4, P_1, P_2, P_3, P_4) &= \frac{1}{8}R_2^2(P_1^2 + P_2^2) + \frac{1}{8}R_1^2(P_3^2 + P_4^2) \\ &\quad -Z(R_2^2 + R_1^2) + R_1^2 R_2^2 (1 + \frac{1}{R_{12}^2}). \end{aligned}$$

Here we have put

$$R_{12}^2 = [(Q_1^2 + Q_2^2)^2 + (Q_3^2 + Q_4^2)^2 - 2(Q_1Q_3 + Q_2Q_4)^2 + 2(Q_1Q_4 - Q_2Q_3)^2]^{1/2}.$$

Now, for the original Hamiltonian we note that

$$H(\mathcal{R}(\bar{r}_1, \bar{r}_2, \bar{p}_1, \bar{p}_2)) = H(\bar{r}_1, \bar{r}_2, \bar{p}_1, \bar{p}_2)$$

for any rotation $\mathcal{R}$ around origo (i.e. H has rotational symmetry). It is concluded that the angular momentum must be constant along any flow. In order to reduce the number of dimensions in the problem, we restrict ourselves to flows with zero angular momentum (Other choices of L would make the numerical work far more complicated). By an appropriate choice of basis, we can thus put $y_i = 0$ and $p_i^y = 0$ for $i = 1, 2$. In effect we have reduced the phase space from

$$\mathcal{F} = \{(x_1, y_1, x_2, y_2, p_1^x, p_1^y, p_2^x, p_2^y) \in \mathbb{R}^8\}$$

to the collinear plane, which is the subspace

$$\mathcal{F}_{co} = \{(x_1, 0, x_2, 0, p_1^x, 0, p_2^x, 0) | x_1, x_2, p_1^x, p_2^x \in \mathbb{R}\} \equiv \{(x_1, x_2, p_1^x, p_2^x) \in \mathbb{R}^4\}.$$

We will typically use η to denote points in the full 8-dimensional phase space $\mathcal{F}$, i.e

$$\eta = (x_1, y_1, x_2, y_2, p_1^x, p_1^y, p_2^x, p_2^y)$$

in the old coordinates or

$$\eta = (Q_1, Q_2, Q_3, Q_4, P_1, P_2, P_3, P_4)$$

in the new ones; and use ξ to denote points in the 4-dimensional reduced phase space $\mathcal{F}_{co}$, i.e.

$$\xi = (x_1, y_1, p_1^x, p_1^y) \text{ or } \xi = (Q_1, Q_4, P_1, P_4).$$

It is not difficult explicitly to verify that any trajectory starting in $\mathcal{F}_{co}$ indeed will stay in there. For instance

$$\frac{dp_i^y}{dt}|_{\eta \in \mathcal{F}_{co}} = -\frac{\partial H}{\partial y_i}(\eta)|_{\eta \in \mathcal{F}_{co}} = -\frac{1}{2}\frac{Ze^2}{|r_i|^3} 2y_i|_{y_i=0} = 0.$$

In other words, $\mathcal{F}_{co}$ is an invariant (with respect to the dynamics) subspace. Furthermore, as noted in [3], at least for cycles of length less than or equal to six, motion off the collinear plane is meta-stable in the sense that initial infinitesimal deviations from $\mathcal{F}_{co}$ at most oscillates but never grows in size (eigenvalues for the stability perpendicular to $\mathcal{F}_{co}$ are complex with norm unity).

Besides the $L = 0$ assumption we will at this point restrict ourselves to the case where the electrons start at different sides of the nucleus (for a general discussion see [3]). Regarding the nucleus as impenetrable we expect the electrons to bounce back at collisions, thus the electrons will forever stay at different sides and we can choose once and for all $x_1 > 0$ and $x_2 < 0$. Insisting on real phase space coordinates, one can infer from the KS-transformation that in $\mathcal{F}_{co}$ one has

$$\begin{array}{lll} |x_1| = x_1 = Q_1^2, & Q_2 = 0, & r_1 = R_1^2 = Q_1^2 \\ |x_2| = -x_2 = Q_4^2, & Q_3 = 0 & r_2 = R_2^2 = Q_4^2 \\ p_1^x = P_1/2Q_1, & P_2 = 0 & \\ p_2^x = -P_4/2Q_4, & P_3 = 0. & \end{array}$$

With these comments we finally write the Hamiltonian as

$$K_{co}(Q_1, Q_4, P_1, P_4) = K|_{\mathcal{F}_{co}} = \frac{1}{8}Q_4^2P_1^2 + \frac{1}{8}Q_1^2P_4^2 - Z(Q_1^2 + Q_4^2) + Q_1^2Q_4^2(1 + \frac{1}{Q_1^2 + Q_4^2}).$$

Having gone through all the dirty work, the equations of motion are right ahead of us. As emphasized already we know that trajectories initially in $\mathcal{F}_{co}$ will stay there, i.e. $\dot{Q}_i = \dot{P}_i = 0$

for $i = 2, 3$. Hence we only need to calculate time derivatives of Q_1, Q_4, P_1 and P_4. The result is

$$\begin{aligned}
\frac{dQ_1}{d\tau} &= Q_4^2 P_1/4, \\
\frac{dQ_4}{d\tau} &= Q_1^2 P_4/4, \\
\frac{dP_1}{d\tau} &= 2Q_1 \left[Z - P_4^2/8 - Q_4^2(1 + \frac{Q_4^2}{(Q_1^2 + Q_4^2)^2}) \right], \\
\frac{dP_4}{d\tau} &= 2Q_2 \left[Z - P_4^2/8 - Q_1^2(1 + \frac{Q_1^2}{(Q_1^2 + Q_4^2)^2}) \right]. \qquad (2)
\end{aligned}$$

3.2 Symmetry.

3.2.1 The symmetry group of K.

We consider the Hamiltonian as derived in section 3.1,

$$K_{co}(Q_1, Q_4, P_1, P_4) = K|_{\mathcal{F}_{co}} = \frac{1}{8}Q_4^2 P_1^2 + \frac{1}{8}Q_1^2 P_4^2 - Z(Q_1^2 + Q_4^2) + Q_1^2 Q_4^2 (1 + \frac{1}{Q_1^2 + Q_4^2}).$$

In this section we find those symmetries of H that fulfills the conditions I and II derived in section 2.1.1.

First of all, because all variables occur squared in K_{co} we can immediately see that negation of any number of them will leave K_{co} unchanged. The general negation matrix has the form

$$\begin{pmatrix} \pm 1 & & & \\ & \pm 1 & & \\ & & \pm 1 & \\ & & & \pm 1 \end{pmatrix}.$$

Condition I in section 2.1.1 now reduces this to three possible negations

$$\mathbf{S}_{n,1} = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix} \text{ and } \mathbf{S}_{n,2} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix},$$

and the composition of these two. $\mathbf{S}_{n,i}$ corresponds to a reflection of particle i through origo, in particular if $Q_i = 0$ it corresponds to a reflection of particle i ($P_i \mapsto -P_i$). The composition of $\mathbf{S}_{n,1}$ and $\mathbf{S}_{n,2}$ corresponds to inversion through origo.

The other symmetry we will need is exchange of particles corresponding to $Q_1 \leftrightarrow Q_4, P_1 \leftrightarrow P_4$, which has the correct block structure

$$\mathbf{S}_{ex} = \begin{pmatrix} 0 & 1 & & \\ 1 & 0 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix}.$$

Now the set $\mathcal{S}_K$ of compositions of $\mathbf{S}_{n,1}, \mathbf{S}_{n,2}$ and $\mathbf{S}_{ex}$ constitutes a group; this is denotes the *symmetry group* of K_{co}. It is straightforward to verify that the group generated by $\mathbf{S}_{n,1}, \mathbf{S}_{n,2}, \mathbf{S}_{ex}$ has 8 elements, thus the symmetry group has order 8. In particular any element of $\mathcal{S}_K$ must have order 1,2,4 or 8.

3.2.2 The fundamental domain.

In this section I will argue that all periodic orbits can be found by restricting the integrations to the so-called fundamental domain defined as,

$$\mathcal{F}_{fund} = \{(Q_1, Q_4, P_1, P_4) \in \mathcal{F}_{co} | 0 \le Q_4 \le Q_1\}.$$

See figure 3 for an illustration. Let $\mathcal{P}_1$ and $\mathcal{P}_2$ denote the planes defined by $Q_4 = 0$ and $Q_1 = Q_4$ respectively. Clearly $\mathcal{F}_{fd}$ is exactly bounded by $\mathcal{P}_1$ and $\mathcal{P}_4$.

Now given an initial point $\xi_0 \in \mathcal{F}_{fd}$, one can start integrating the equations of motion. In order to keep the trajectory in $\mathcal{F}_{fd}$ we adopt the following integration scheme:

1° When we hit $\mathcal{P}_1$, apply $\mathbf{S}_{n,2}$.

2° When we hit $\mathcal{P}_2$, apply $\mathbf{S}_{ex}$.

Let us see why this will keep the trajectory inside $\mathcal{F}_{fd}$. We have $\dot{Q}_4 = Q_1^2 P_4/4$ and $\dot{Q}_1 = Q_4^2 P_1/4$. Thus when hitting $\mathcal{P}_1$, i.e. $Q_4 = 0$, an application of $\mathbf{S}_{n,2}$ sending P_4 to $-P_4$, will reverse the velocity of Q_4, thus keeping the trajectory in $\mathcal{F}_{fd}$.[5] In the other case, hitting plane $\mathcal{P}_2$ from inside $\mathcal{F}_{fd}$, we must have $\dot{Q}_4 > 0$ and $\dot{Q}_1 < 0$. From here we see that $P_1 < 0$ and $P_2 > 0$. Now applying $\mathbf{S}_{ex}$ mapping $P_1 \leftrightarrow P_4$, implies that the velocities of both Q_1 and Q_4 are reversed.

3.2.3 Fixpoints can be found in the fundamental domain.

Next I want to show that any periodic orbit can be found in the fundamental domain.

Assume the integration scheme 1° and 2° from above has been adopted. Let $\xi_0 \in \mathcal{F}_{fd}$ be any point on a periodic orbit (with respect to the integration scheme). Start integrating and assume that we hit plane i_1 (i_1 is either 1 or 2) at time t_1, plane i_2 at time $t_1 + t_2$,..., and that finally we are back at ξ_0 after time $T = t_1 + t_2 + \cdots + t_k + t_{k+1}$. With $f^t(\xi)$ denoting the flow, we thus have the identity,

$$\xi_0 = f^{t_{k+1}} \mathbf{S}_{(k)} f^{t_k} \cdots \mathbf{S}_{(2)} f^{t_2} \mathbf{S}_{(1)} f^{t_1}(\xi_0).$$

Here $\mathbf{S}_{(m)} = \mathbf{S}_{n,2}, \mathbf{S}_{ex}$ depending on whether $i_m = 1, 2$. Now both $\mathbf{S}_{n,2}$ and $\mathbf{S}_{ex}$ are in the symmetry group of K_{co}, thus the flow commutes with them. This gives us,

$$\xi_0 = \mathbf{S}_0 f^T(\xi_0),$$

where we have put $\mathbf{S}_0 = \mathbf{S}_{(1)} \mathbf{S}_{(2)} \cdots \mathbf{S}_{(k)}$. Now, it is easy to verify that $\mathbf{S}_{n,2}$ and $\mathbf{S}_{ex}$ actually generates the whole symmetry group of K_{co}. Thus $\mathbf{S}_0$ can be any element of this group, in particular it must have order r=1,2,4 or 8. We can repeat the integration r times and still come back to ξ_0; this gives us

$$\begin{aligned}\xi_0 &= \left[f^{t_{k+1}} \mathbf{S}_{(k)} f^{t_k} \cdots \mathbf{S}_{(2)} f^{t_2} \mathbf{S}_{(1)} f^{t_1}\right]^r (\xi_0) \\ &= \mathbf{S}_0^r f^{rT}(\xi_0) = f^{rT}(\xi_0).\end{aligned}$$

Thus ξ_0 is a point on a periodic orbit with respect to integration in the full space $\mathcal{F}_{co}$.

For the other way around, pick an arbitrary orbit in the full space. If this has no intersection with $\mathcal{F}_{fd}$, we can at least find an orbit symmetric to this which does intersect $\mathcal{F}_{fd}$ (cf. section 2.1.2 on symmetry of trajectories). Now, pick an initial point on the orbit in $\mathcal{F}_{fd}$ and start integrating according to the integration scheme above. Because we can uniquely

[5] $\mathbf{S}_{n,2}$ also sends $Q_4 \to -Q_4$ but this clearly have no effect when $Q_4 = 0$.

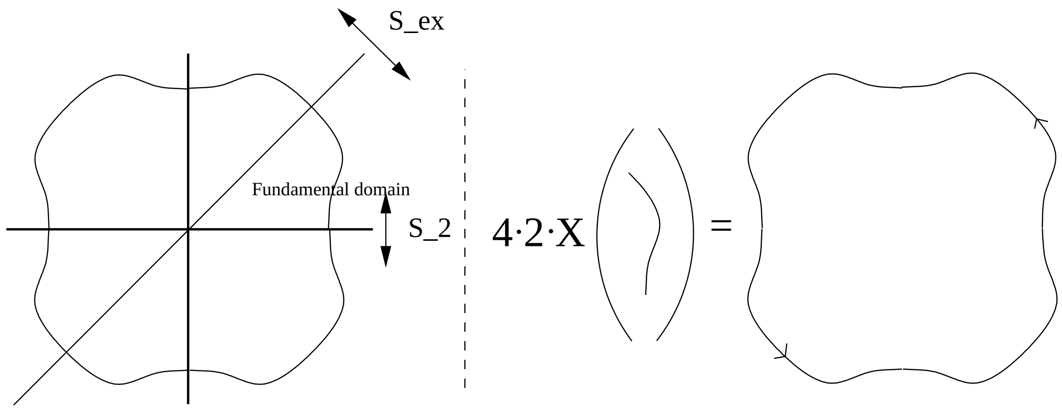

Figure 3: An example of an orbit with degree of symmetry $r = 4$. Left: Following the orbit back and forth in the fundamental domain involves (depending on where you start) symmetry actions $\mathbf{S}_{n,2}$ and $\mathbf{S}_{ex}$ and then you are back. The order of $\mathbf{S}_0 = \mathbf{S}_{n,2}\mathbf{S}_{ex}$ can explicitly be verified to be 4. Right: Illustrates that the complete orbit is made up of 8 symmetric pieces. I write $4 \cdot 2$ to emphasize that integration in the fundamental domain will take us both back and forth, thus the complete orbit is only $r = 4$ times as long as the orbit in the fundamental domain.

unfold the orbit from the fundamental domain to the full domain (simply by reversing all symmetry operations), and the orbit is assumed to be closed in the full domain, naturally it will also be closed in the fundamental domain, hence it is a periodic orbit with respect to integration in the fundamental domain.

It has thus been shown that any periodic orbit can be found in the fundamental domain. Furthermore we have assigned a number r being a degree of symmetry. The meaning of this number is illustrated by figure 3.

3.2.4 The action and the topological index can be calculated in the fundamental domain.

In this section I want to justify (loosely) that the action and the topological index as needed in Gutzwiller's trace formula, can actually be found by doing all the integrations in the fundamental domain.

As mentioned later on, the action is found as twice the period of the orbit. Recalling that $dt = \frac{1}{-E}Q_1^2Q_4^2d\tau$, we see that dt is invariant under all the symmetries $\mathbf{S}_{n,1}, \mathbf{S}_{n,2}, \mathbf{S}_{ex}$; thus integrating dt along symmetric parts of the trajectories will yield equal contributions. As illustrated in figure 3, an orbit with degree of symmetry r will consist of $2r$ symmetrical parts of trajectories. By integrating dt up along the orbit in the fundamental domain, we will only get the contribution from 2 of these parts. Thus, the action S_p in the full domain is related to the action S_P^{fd} in the fundamental domain by

$$S_p = r \cdot S_p^{fd}.$$

Next we turn to the topological index. I will only give a loose treatment of this point. According to [1] it can be defined as the number of times the neighborhood twists. Because the set of trajectories is completely symmetric, symmetric trajectories (i.e. equal modulo one of the symmetries in K_{co}) will have symmetric neighborhoods. In particular topological properties such as number of twists must be the same for both trajectories. By the same argument as above we must have that

$$\alpha_p = r \cdot \alpha_p^{fd}.$$

3.2.5 The stability can be calculated in the fundamental domain.

According to section 2.1.3 the stability matrices from symmetric trajectories are equal modulo a change of basis (in fact, the basis change induced by the symmetry). Consider now a trajectory in the fundamental domain. Recall that this was obtained by acting with a symmetry $\mathbf{S}$ every time one of the planes $\mathcal{P}_1$ or $\mathcal{P}_2$ is hit. Now

$$\dot{\mathbf{J}}(\xi(t)) = \mathbf{A}(\xi(t))\mathbf{J}(\xi(t)),$$

but $\mathbf{A}(\xi)$ is in general not invariant under $\mathbf{S}$, namely

$$\mathbf{A}(\mathbf{S}\xi) = \mathbf{w}\partial^2 K(\mathbf{S}\xi) = \mathbf{S}\mathbf{w}\partial^2 K(\xi) = \mathbf{S}\mathbf{A}(\xi) \text{ cf. section 2.1.1.}$$

In order to get the right result for the stability matrix, we have to unfold the trajectory in the following sense:

Let ξ_0 be the initial points. Assume we hit plane $\mathcal{P}_i$ at time t_i, thus we apply a symmetry $\mathbf{S}^{(i)}$ at time t_i. For every time t we can back trace the point $\eta(t)$ where the trajectory would have been at time t if no symmetries had been applied. That is

$$\eta(t) = \mathbf{S}^{(t)}\xi(t),$$

where

$$\mathbf{S}^{(t)} = \prod_{i:t_i \leq t} S^{(i)}$$

is the product of all symmetries applied so far. Then we simply integrate $\mathbf{J}$ along the unfold trajectory according to the equation

$$\dot{\mathbf{J}}(t) = \mathbf{A}(\eta(t)) \cdot \mathbf{J}(t).$$

Having integrated $\mathbf{J}_{p,fd}$ along an orbit with degree of symmetry r in the fundamental domain, we have to remember that in the full space we have only gone a fraction $\frac{1}{r}$ of the full way (see figure 3). The stability matrix for the full orbit becomes $\mathbf{J}_{p,fd}^r$, that is the eigenvalues are raised to the r'th power, hence the logarithm of the eigenvalues (i.e. λ_p and $2\pi i\sigma_p$) get multiplied by r.

Remark: If this technique of unfolding is not applied while integrating $\mathbf{J}$ and instead integration is performed according to $\dot{\mathbf{J}}(t) = \mathbf{A}(\xi(t)) \cdot \mathbf{J}(t)$, then one will find a different stability matrix. However the set of eigenvalues might be equal in either way. I could not find an argument for this but if it is true, the above prescription to find $\mathbf{J}$ is not relevant, though still correct.

3.2.6 Further reduction of $\zeta^{-1}(z)$ by symmetry in K.

In this section I will reduce the zeta function exploiting the symmetry of the system.

As shown in the previous section, all periodic orbits can be found in the fundamental domain. Furthermore, we saw that a degree of symmetry r could be assigned to any orbit such that all the quantities λ_p, σ_p and α_p can be found by integration in the fundamental domain. Assuming that some orbit p has degree of symmetry r, we can now see,

$$\begin{aligned} t^p(E) &= \exp\left[i(S_p(E) - \alpha_p\pi/2 + \pi\sigma_p) - \frac{1}{2}\lambda_p\right] \\ &= \exp\left[i(rS_p^{fd}(E) - r\alpha_p^{fd}\pi/2 + \pi r\sigma_p^{fd}) - \frac{1}{2}r\lambda_p^{fd}\right] \\ &= \exp\left[i(S_p(E)^{fd} - \alpha_p^{fd}\pi/2 + \pi\sigma_p^{fd}) - \frac{1}{2}\lambda_p^{fd}\right]^r . \\ &\equiv (t^p_{fd})^r \end{aligned}$$

Thus we have expressed the term t^p corresponding to p in terms of quantities found solely in the fundamental domain.

Now, any orbit p will have a degeneracy D_p assigned to it in the sense that there in total exists D_p distinct orbit all being equal to orbit p modulo some symmetry of the system. This follows from the general symmetry of the set of trajectories.[6] Just as the case with the symmetry degree, D can only take on the values $1, 2, 4, 8$. As shown in section 2.2.2 and 2.2.3, trajectories which are equal modulo symmetries will have the same values of S_p, λ_p, σ_p and α_p, thus $t^p(E)$ is the same for all these trajectories. Hence in general we can write

$$\zeta^{-1}(z) = \prod_{r,D=1,2,4,8} \prod_{p\in\mathcal{P}_{r,D}} (1 - (t^p_{fd})^r)^D,$$

where $\mathcal{P}_{r,D}$ denotes the set of orbits with degree of symmetry r and degeneracy D. (To be precise, $\mathcal{P}_{r,d}$ denotes the set of equivalence classes (modulo symmetries), thus one has to remember only to include one representation of each class in the above product). Now according to [1] there are two cases $(r, D) = (2, 1)$ and $(r, D) = (1, 2)$, yielding

$$\zeta^{-1}(E) = \prod_{p\in\mathcal{P}_{1,2}} (1 - t^p_{fd})^2 \prod_{p\in\mathcal{P}_{2,1}} (1 - (t^p_{fd})^2) \equiv \zeta_+^{-1}(E)\cdot\zeta_-^{-1}(E),$$

with

$$\zeta_+^{-1} = \prod_{p\in\mathcal{P}_{1,2}} (1 - t^p_{fd}) \prod_{p\in\mathcal{P}_{2,1}} (1 - t^p_{fd}) = \prod_{p\in\mathcal{P}} (1 - t^p_{fd}),$$

and

$$\zeta_-^{-1}(E) = \prod_{p\in\mathcal{P}_{1,2}} (1 - t^p_{fd}) \prod_{p\in\mathcal{P}_{2,1}} (1 + t^p_{fd}).$$

Now roots in ζ_+^{-1} and ζ_-^{-1} correspond to two different ranges of the Helium spectrum [1]. Here we are only interested in the one corresponding to ζ_+^{-1}.

A few last corrections to ζ_+^{-1} comes from the following remarks:

[6] The symmetry of the set of trajectories can be formulated as: For any trajectory $\mathcal{T}$, and any symmetry $\mathbf{S}$ in the symmetry group of K, there will exist a trajectory equal to $\mathbf{S}\mathcal{T}$. (This might be equal to $\mathcal{T}$). The number of different trajectories obtained by applying all these symmetries, is called the degeneracy of $\mathcal{T}$.

As mentioned in section 3.1.1, page 12 the winding number σ_p is (the logarithm of) the stability eigenvalue perpendicular to the collinear plane in both the y and z directions. Although we have suppressed this fact all along and made all arguments for only one perpendicular eigenvalue, inclusion of a second copy of σ_p would simply have resulted in a factor 2 in the formulas where σ_p appears. Furthermore it is common to measure the action in units of 2π. At last, as will be seen in section 3.6.2 the action has been scaled such that S in the transformed coordinates, and S_0 in the original coordinates are related as $S_0 = \frac{S}{\sqrt{E}}$. Putting $z = \frac{1}{\sqrt{E}}$ we finally arrive at the expression,

$$\zeta_+^{-1}(z) = \prod_{p \in \mathcal{P}} (1 - t^p_{fd}),$$

with

$$t^p_{fun} = \exp\left[2\pi i(\frac{S_p^{fd}}{2\pi} z + \sigma_p^{fd}) - \frac{1}{2}\lambda_p^{fd} - \alpha_p^{fd}\frac{\pi}{2}\right].$$

Apart from a minus in front of σ_p this is the same expression as given in [4]. In order to find the zeroes of the zeta function I actually used the expression from [4].

Remark: The above argument, dividing all cases of degeneracy and degree of symmetry into (2,1) and (1,2) does not seem to fit on the general orbit. I have found several other valid pairs, for instance $(r, D) = (4, 1)$ for orbit $\bar{0}$, $(r, D) = (2, 4)$ for orbit $\overline{01}$, $(r, D) = (2, 4)$ for orbit $\overline{100}$ etc. Maybe there is an argument missing.

3.3 Equations for the stability matrix.

According to [1], ch. 5, the stability matrix $\mathbf{J}(\xi(\tau))$ for a given trajectory is governed by the equation of motion

$$\frac{d\mathbf{J}}{d\tau} = \mathbf{A}(\xi(\tau))\mathbf{J}(\tau),$$

with the initial condition $\mathbf{J}(0) = \mathbf{1}$. Here $\mathbf{A}$ is defined by

$$\mathbf{A}_{ij} = \frac{\partial \dot{\eta}_i}{\partial \eta_j}.$$

As we saw in section 2.2.1, we are free to use the transformed coordinates to find $\mathbf{J}$. Thus $\eta = (Q_i, P_i | i = 1, \ldots, 4)$ and the flow is induced by the transformed Hamiltonian $K(\eta)$.

Using the symplectic matrix

$$\mathbf{w} = \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}$$

we have the equations of motion in the convenient form

$$\dot{\eta} = \mathbf{w}\frac{\partial K}{\partial \eta}.$$

Hence

$$A_{ij} = \frac{\partial}{\partial \eta_j}(w_{ik}\frac{\partial K}{\partial \eta_k}) = w_{ik}\frac{\partial^2 K}{\partial \eta_j \partial \eta_k} \text{ or } \mathbf{A} = \mathbf{w}\frac{\partial^2 K}{\partial \eta^2}.$$

3.3.1 The stability matrix decouples into $\mathbf{J}_{||}$ and $\mathbf{J}_{\perp}$.

It is noted that K has eight variables, thus $\mathbf{A}$ is an 8×8 matrix. By choosing a specific order of its elements, namely $\mathcal{O} = (1,4,5,8,2,3,6,7)$, we can argue that it separates into two 4×4 matrices. Let $x \in \{Q_1, Q_4, P_1, P_4\}$ and $y \in \{Q_2, Q_3, P_2, P_3\}$, then $\frac{\partial^2 K}{\partial x \partial y} = \frac{\partial^2 K}{\partial y \partial x} = 0$ as explained by an example, say $x = Q_4, y = P_2$. We can interpret

$$\frac{\partial}{\partial Q_4}(\frac{\partial K}{\partial P_2})|_{\eta \in \mathcal{F}_{co}} = \frac{\partial}{\partial Q_4}(\dot{Q}_2)|_{\eta \in \mathcal{F}_{co}}$$

as the variation in $\dot{Q}_2$ when displacing the point of the trajectory along the Q_4-direction. But such a displacement will still leave η in $\mathcal{F}_{co}$, thus $\dot{Q}_2 = 0$ with or without the displacement, that is, the variation in $\dot{Q}_2$ is zero, that is $\frac{\partial^2 K}{\partial Q_4 \partial P_2} = 0$. Because of the continuity of K (up to at least second order derivatives) we have equality between mixed derivatives, hence also $\frac{\partial}{\partial P_2}\left(\frac{\partial K}{\partial Q_4}\right) = 0$.[7]

Hence we can write

$$\frac{\partial^2 K(\eta)}{\partial(Q_1, Q_4, P_1, P_4, Q_2, Q_3, P_2, P_3)^2}|_{\mathcal{F}_{co}} = \partial^2 K_{||} \otimes \partial^2 K_{\perp}$$

where

$$\partial^2 K_{||} = \frac{\partial^2 K_{co}(Q_1, Q_4, P_1, P_4)}{\partial(Q_1, Q_4, P_1, P_4)^2} \text{ and } \partial^2 K_{\perp} = \frac{\partial^2 K(Q_1, Q_4, P_1, P_4, Q_2, Q_3, P_2, P_3)}{\partial(Q_2, Q_3, P_2, P_3)^2}|_{\mathcal{F}_{co}}.$$

With respect to the basis ordered according to $\mathcal{O}$ it is straightforward to verify that

$$\mathbf{w} = \mathbf{w} \otimes \mathbf{w},$$

where $\mathbf{w}$ on the right hand side is the 4×4 symplectic matrix. Thus we have,

$$\mathbf{A} = A_{||} \otimes A_{\perp}$$

with

$$A_{||} = \mathbf{w} \cdot \partial^2 K_{||} \text{ and } A_{\perp} = \mathbf{w} \cdot \partial^2 K_{\perp}.$$

Recalling how $\mathbf{J}$ is found by integrating contributions on the form $\mathbf{AJ}$ and taking into account that $\mathbf{J}$ initially is separable $\mathbf{J}(0) = \mathbf{1} = \mathbf{1} \otimes \mathbf{1}$, we conclude that $\mathbf{J}$ inherits this block structure.

3.3.2 Differential equations of the stability matrix.

In order to get the derivatives for $i = 2, 3$ we are forced to use the Hamiltonian K defined on the full phase space, but things are simplified for $i = 1, 4$ because in this case we can use K_{co}. A complete list of the second derivatives occurring in $\partial^2 K_{||}$ and $\partial^2 K_{\perp}$ is given below. Because we put on the restriction that trajectories should lie in the collinear plane, we will immediately evaluate all expressions with $Q_2 = Q_3 = P_2 = P_3 = 0$. Also, because of equality between mixed partial these are represented only once. We put $R = Q_1^2 + Q_2^2$. The results are listed in Table 1 These are the elements to be used in the integration of the monodromy matrix.

[7] What about the triple collision point corresponding to $Q_1^2 + Q_4^2 = 0$? Surely K is not continuous here and the argument does not hold. Indeed, according to [4] and [3] it is exactly the triple collision that induces the fully chaotic behavior of the system. Any trajectory reaching this point will have no unique continuation (and then we are really in bad trouble). However, for any finite time T, the set of trajectories reaching the triple point within time T will (I think) be vanishing (i.e. it has zero measure); thus we simply count on whatever starting point we choose and whatever time scale we work at, the triple collision will not occur in practice (although we might get arbitrarily close).

$$
\begin{aligned}
\frac{\partial^2 K_{co}}{\partial Q_1 \partial Q_1} &= -2(Z - P_4^2/8 - Q_4^2(1 + \frac{Q_4^4 - 3Q_1^2 Q_4^2}{R^3})) \\
\frac{\partial^2 K_{co}}{\partial Q_4 \partial Q_1} &= 4Q_1 Q_4 (1 + 2\frac{Q_1^2 Q_4^2}{R^3}) \\
\frac{\partial^2 K_{co}}{\partial P_1 \partial Q_1} &= 0 \\
\frac{\partial^2 K_{co}}{\partial P_4 \partial Q_1} &= \frac{1}{2} Q_1 P_4 \\
\frac{\partial^2 K_{co}}{\partial Q_4 \partial Q_4} &= -2(Z - P_1^2/8 - Q_1^2(1 + \frac{Q_1^4 - 3Q_1^2 Q_4^2}{R^3})) \\
\frac{\partial^2 K_{co}}{\partial P_1 \partial Q_4} &= \frac{1}{2} Q_4 P1 \\
\frac{\partial^2 K_{co}}{\partial P_4 \partial Q_4} &= 0 \\
\frac{\partial^2 K_{co}}{\partial P_1 \partial P_1} &= \frac{1}{4} Q_4^2 \\
\frac{\partial^2 K_{co}}{\partial P_4 \partial P_1} &= 0 \\
\frac{\partial^2 K_{co}}{\partial P_4 \partial P_4} &= \frac{1}{4} Q_1^2 \\
\frac{\partial^2 K}{\partial Q_2 \partial Q_2} &= \frac{1}{4} P_4^2 - 2Z + 2Q_4^2(1 + \frac{1}{R}) - 2\frac{Q_4^2 Q_1^2 (Q_1^2 - Q_4^2)}{R^3}, \\
\frac{\partial^2 K}{\partial Q_2 \partial Q_3} &= 4\left(\frac{Q_1 Q_4}{R}\right)^3, \\
\frac{\partial^2 K}{\partial Q_2 \partial P_2} &= 0, \\
\frac{\partial^2 K}{\partial Q_2 \partial P_3} &= 0, \\
\frac{\partial^2 K}{\partial Q_3 \partial Q_3} &= \frac{1}{4} P_1^2 - 2Z + 2Q_1^2(1 + \frac{1}{R}) - 2\frac{Q_1^2 Q_4^2 (Q_4^2 - Q_1^2)}{R^3}, \\
\frac{\partial^2 K}{\partial Q_3 \partial P_2} &= 0, \\
\frac{\partial^2 K}{\partial Q_3 \partial P_3} &= 0, \\
\frac{\partial^2 K}{\partial P_2 \partial P_2} &= \frac{1}{4} Q_4^2, \\
\frac{\partial^2 K}{\partial P_2 \partial P_3} &= 0, \\
\frac{\partial^2 K}{\partial P_3 \partial P_3} &= \frac{1}{4} Q_1^2.
\end{aligned}
$$

Table 1: All second derivatives of K.

3.4 Symbolic dynamics for Helium.

Finding a proper symbolic dynamics is in general a hard problem; no generic rules can be given. Here we will follow other peoples advice; in particular we will adopt the symbolic dynamics given in [4]. The symbolic string $s = \cdots s_{-2}s_{-1}s_0s_1s_2\cdots$ corresponding to a given trajectory is prescribed as follows:

> Let $\cdots i_{-2}i_{-1}i_0i_1i_2\cdots$ be a recording of electron collisions such that $i_k = 1, 2$ depending on whether electron 1 or 2 hits the nucleus in the k'th collision. In practice this is found simply by integrating Hamiltons equations of motion back and forth in time and by noticing in which order the trajectory hits the plane $r_1 = 0$ and $r_2 = 0$. Now s_k is defined by
>
> $$s_k = \begin{cases} 0 \text{ if } i_{k-1} \neq i_k \\ 1 \text{ if } i_{k-1} = i_k \end{cases}$$

Thus for instance $s = \bar{0}$ denotes a trajectory where the electrons keep hitting the nucleus in turn. In [4] it is conjectured that this symbolic dynamics is complete with only one missing point, namely: a trajectory is mapped into $\bar{1}$ if and only if one electron is going to infinity (ionized). Thus we have found a periodic symbolic string which is not the image of a periodic trajectory, thus the symbolic dynamics is not onto, hence it is not complete.

3.5 The curvature expansion for Helium.

Looking a bit ahead, the prime cycles of table 3 of section 4.2 can be compared with any standard table of binary prime cycles (for instance table 3.1 of [1]) and from this it is concluded that the pruning of the symbolic dynamics up to prime cycles of length six, includes only one inadmissible cycle, namely 1 (corresponding to one electron going to infinity). For pruned symbolic dynamics in general, the shadowing will not be complete simply because the set of decompositions is incomplete (cf. the discussion in section 1.3). For instance, the lack of orbit with symbolic dynamics $p = 1$ makes the shadowing of t_{01} by $-t_0t_1$ fail.

In the following we will make the expansion of the zeta function up to products with total cycle length six. Reference is made to [1], table 10.1 where it has been done to the order we need. By inserting a 0 everywhere t_1 occurs as a factor, we can write the expansion as given in Table 2 As can be seen, only six out of twenty shadows are complete. Thus the super exponential convergence fails. Nevertheless as we shall see, quite nice results are obtained anyway.

3.6 What to do in practice.

3.6.1 How to find periodic orbits? (Multiple shooting).

Different methods can and should in general be applied to find periodic orbits for a given dynamical system. Starting with some simple integrations from arbitrary initial points and for arbitrary time periods, performing arbitrary projections on different 2- or 3-dimensional subspaces, one should get a minimum of understanding of the basic features of the topology of the flow. For systems like Helium which allows single ionization, finding orbits which does not go to infinity is difficult in itself (difficult might not be the right word, one has to be either patient or lucky). When a basic understanding has been achieved, one can start looking for periodic orbits. This is in no way trivial (to put it gently). Ultimately some very systematic methods should be applied. Although a simple one-parameter bisection method is

$$
\begin{array}{rlllll}
\zeta^{-1} \approx & 1 - t_0 - 0 & & & & \\
& -t_{01} & +t_0 \cdot 0 & & & \\
& -t_{001} & +t_{01} t_0 & & & \\
& -t_{011} & +t_{01} \cdot 0 & & & \\
& -t_{0001} & +t_{001} \cdot 0 & & & \\
& -t_{0011} & +t_{001} \cdot 0 & +t_{011} t_0 & -t_0 t_{01} \cdot 0 & \\
& -t_{0111} & +t_{011} \cdot 0 & & & \\
& -t_{00001} & +t_0 t_{0001} & & & \\
& -t_{00011} & +t_0 t_{0011} & +t_{0001} \cdot 0 & -t_0 t_{001} \cdot 0 & \\
& -t_{00101} & +t_{001} t_{01} & & & \\
& -t_{01011} & +t_{01} t_{011} & & & \\
& -t_{00111} & +t_0 t_{0111} & +t_{0011} \cdot 0 & -t_0 t_{011} \cdot 0 & \\
& -t_{01111} & +t_{0111} \cdot 0 & & & \\
& -t_{000001} & +t_0 t_{00001} & & & \\
& -t_{000011} & +t_{00011} t_0 & +t_{00001} \cdot 0 & -t_0 t_{0001} \cdot 0 & \\
& -t_{000101} & +t_0 t_{00101} & +t_{0001} t_{01} & -t_0 t_{001} t_{01} & \\
& -t_{000111} & +t_0 t_{00111} & +t_{00011} \cdot 0 & -t_0 t_{0011} \cdot 0 & \\
& -t_{001011} & -t_{110100} & +t_{00101} \cdot 0 & +t_0 t_{01011} & +t_{0011} t_{01} \\
& & & +t_{001} t_{011} & -t_0 t_{01} t_{011} & -t_{001} t_{01} \cdot 0 \\
& -t_{010111} & +t_{01011} \cdot 0 & +t_{01} t_{0111} & -t_{01} t_{011} \cdot 0 & \\
& -t_{001111} & +t_{00111} \cdot 0 & +t_0 t_{01111} & -t_0 t_{0111} \cdot 0 & \\
& -t_{011111} & +t_{01111} \cdot 0. & & &
\end{array}
$$

Table 2: The curvature expansion of the zeta function to sixth order. Because of the lack of an orbit with symbolic dynamics $\bar{1}$ a zero is explicitly inserted everywhere t_1 should have occurred. This clearly shows where the shadowing fails.

sufficient to find orbits up to length five (cf. [1] ch. 19) and a two-parameter search method successfully has been applied to find all orbits up to length six (cf. [2]), I have nevertheless used a different more complicated method called multiple shooting. The following section gives a short review of this.

Multiple shooting. This section follows [1] ch. 6.

Let $\mathcal{P}_1, \dots, \mathcal{P}_k$ be some planes in a d-dimensional phase space. A periodic orbit passing through these in the given order starting and ending in $\xi_1' \in \mathcal{P}_1$, will along the way pass through points $\xi_i' \in \mathcal{P}_i, i = 1, \dots, k$. Letting $f^t(\xi)$ denote the flow of the dynamics, we clearly have that $(\xi_1', \dots, \xi_k')$ will be a root of the mapping

$$F : \bigotimes_{i=1}^{k} \mathbb{R}^d \to \mathbb{R}^{dk}$$

given by

$$F(\xi_1, \dots, \xi_k) = \begin{bmatrix} f^{(k)}(\xi_k) - \xi_1 \\ f^{(1)}(\xi_1) - \xi_2 \\ \vdots \\ f^{(k-1)}(\xi_{k-1}) - \xi_k \end{bmatrix}.$$

Here we have defined $f^{(i)}(\cdot) = f^{\Delta t_i}(\cdot)$ and Δt_i is the time of flight from ξ_i to ξ_{i+1}. Recall that for a smooth mapping $f : \mathbb{R} \to \mathbb{R}$, Newton-Raphson iteration gives x_n a correction δx_n satisfying

$$f'(x_n)\delta x_n = -f(x_n).$$

Generalizing this we define a correction $(\delta\xi_1, \dots, \delta\xi_k)$ to any point $(\xi_1, \dots, \xi_k)$ near the root $(\xi_1', \dots, \xi_k')$ implicitly by the equation

$$\mathbf{J}_F(\xi_1, \dots, \xi_k) \cdot \begin{bmatrix} \delta\xi_1 \\ \delta\xi_2 \\ \vdots \\ \delta\xi_k \end{bmatrix} = - \begin{bmatrix} f^{(k)}(\xi_k) - \xi_1 \\ f^{(1)}(\xi_1) - \xi_2 \\ \vdots \\ f^{(k-1)}(\xi_{k-1}) - \xi_k \end{bmatrix}.$$

By exploiting that

$$\frac{\partial f^{(j)}(\xi_j)}{\partial \xi_i} = \delta_{ij} \mathbf{J}_j(\xi_i) \quad (\text{ putting } \mathbf{J}_j \equiv \mathbf{J}_{f^{(j)}}(\xi_j)),$$

and that $\frac{\partial \xi_i}{\partial \xi_j} = \delta_{ij}\mathbf{1}$ one finds

$$\mathbf{J}_F(\xi_1, \dots, \xi_k) = \begin{bmatrix} \mathbf{-1} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{J}_k \\ \mathbf{J}_1 & \mathbf{-1} & \mathbf{0} & & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2 & \mathbf{-1} & & \mathbf{0} \\ & & & \ddots & \vdots \\ & & & & \mathbf{-1} \end{bmatrix}$$

By inverting $\mathbf{J}_F$ one can find the correction $\delta\xi$ and in general this can point in any direction. Thus an initial guess with $\xi_1, \dots, \xi_k$ lying in the planes $\mathcal{P}_1, \dots, \mathcal{P}_k$ respectively, can be corrected to a sequence of phase space points lying outside the planes. In principle this should cause no problems; the method should anyway converge to a sequence of points lying nicely in the appropriate planes. Nevertheless, numerically one would typically need all integrations to start exactly from the intended planes. In order to deal with this we will add some constraints, namely that $\delta\xi \cdot a_i = 0$ where a_i is a vector normal to plane $\mathcal{P}_i$. In general one ends up with a system of equations with no solution. Approximate solutions (such as those obtained by singular value decomposition, cf. [6]) could be applied. However, according to [1] ch. 6, this can be resolved by introducing small time steps $\delta T_1, \dots, \delta T_k$ and velocity vectors along the flow $v_j = \mathbf{w} \cdot \frac{\partial K}{\partial \xi}(f^{(j)}(\xi_j))$, setting it all up in an extended matrix equation,

$$\begin{bmatrix} -\mathbf{1} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{J}_k & v_1 & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{J}_1 & -\mathbf{1} & \mathbf{0} & & \mathbf{0} & \mathbf{0} & v_2 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2 & -\mathbf{1} & & \mathbf{0} & \mathbf{0} & \mathbf{0} & v_3 & \cdots & \mathbf{0} \\ \vdots & & \ddots & \ddots & \vdots & \vdots & & & \ddots & \vdots \\ \mathbf{0} & \cdots & \cdots & \mathbf{J}_{k-1} & -\mathbf{1} & \mathbf{0} & \cdots & \cdots & \cdots & v_k \\ a_1 & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \cdots & \cdots & \cdots & \mathbf{0} \\ \mathbf{0} & a_2 & \mathbf{0} & & \vdots & \vdots & \ddots & & & \vdots \\ \mathbf{0} & \mathbf{0} & a_3 & & \vdots & \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots & \vdots & & & \ddots & \vdots \\ \mathbf{0} & \cdots & \cdots & \cdots & a_k & \mathbf{0} & \cdots & \cdots & \cdots & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \delta\xi_1 \\ \delta\xi_2 \\ \vdots \\ \delta\xi_k \\ \delta T_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \delta T_k \end{bmatrix} = - \begin{bmatrix} f^{(k)}(\xi_k) - \xi_1 \\ f^{(1)}(\xi_1) - \xi_2 \\ \vdots \\ f^{(k-1)}(\xi_{k-1}) - \xi_k \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 0 \end{bmatrix}$$

From here $\delta\xi_1, \cdots, \delta\xi_k$ are determined by iteration starting from a wisely chosen initial guess.

3.6.2 How to find the quantities $\lambda_p, S_p, \sigma_p, \alpha_p$.

In this section I will discuss and explicitly state how to find the quantities entering the dynamical zeta function. To recapitulate, we need for each periodic orbit the Lyapunov exponent λ_p, the winding number σ_p, the action S_p and the topological index α_p. For now we will assume that the periodic orbits have been found, an appropriate routine for numerical integration has been implemented and we are ready to go.

λ_p and σ_p are related to the stability eigenvalues in and perpendicular to the collinear plane by

$$\Lambda_{||} = e^{\lambda_p} \text{ and } \Lambda_{\perp} = e^{2\pi i \sigma_p}.$$

As explained in the previous section the stability in the plane is found by integrating along the periodic orbit the $n \times n$ differential equations given by

$$\frac{d\mathbf{J}_{||}(\xi(\tau))}{d\tau} = \mathbf{A}_{||}(\xi(\tau))\mathbf{J}_{||}(\xi(\tau)),$$

whereas the stability perpendicular to the plane are found by integrating

$$\frac{d\mathbf{J}_{\perp}(\xi(\tau))}{d\tau} = \mathbf{A}_{\perp}(\xi(\tau))\mathbf{J}_{\perp}(\xi(\tau)).$$

Just to recall, here we have put

$$\mathbf{A}_{||}(\xi) = \mathbf{w}\frac{\partial^2 K_{co}(Q_1, Q_4, P_1, P_4)}{\partial(Q_1, Q_4, P_1, P_4)^2}|_{\xi}$$

and

$$\mathbf{A}_{\perp}(\xi) = \mathbf{w}\frac{\partial^2 K(Q_1, Q_2, Q_3, Q_4, P_1, P_2, P_3, P_4)}{\partial(Q_2, Q_3, P_2, P_3)^2}|_{\xi}.$$

According to [1] the action is found as $2T_p$ where T_p is the period of the orbit. Recalling the time transformation and scaling we end up with the relation $S_p(E) = 2T_p/\sqrt{E}$ and

$$T_p = \oint Q_1(\tau)^2 Q_2(\tau)^2 d\tau.$$

Here one introduces the effective energy $z = z(E) = \frac{1}{\sqrt{E}}$, thus $S_p(z) = z2T_p \equiv zS_p$. At last, α_p is simply twice the code length.

3.6.3 How to find zeroes of $\zeta_+^{-1}(z)$.

The general theory tells us that roots of $\zeta_+^{-1}(z)$ should be found in values $z \in \mathbb{R}_+$ being (effective) eigenenergies of the quantum mechanical helium atom. From standard tables on quantum spectra (reprinted in [4]) for the chosen values of k and m, one finds the spectrum

$$\begin{aligned} E_{eff} = \frac{1}{\sqrt{E}} &= \{0.587, 1.134, 1.302, 1.682, 1.885, 2.231, 2.456, \\ &\quad 2.575, 2.780, 3.020, 3.159, 3.329, 3.580, 3.733, \\ &\quad 3.883, 4.138, 4.301, 4.411, 4.686, 4.865\}. \end{aligned}$$

These values should be taken as a guideline where to search for zeroes. We will accept zeroes located slightly above or under the real axis, in fact it turns out that all roots are found with small imaginary parts in the interval $[-0.02, 0.02]$. By standard software (like IDL) a contour plot can be made of $|\zeta_+^{-1}(z)|$ for $z \in [0.5, 5] + i[-0.02, 0.02]$ and from here a qualitative view of positions of zeroes can be obtained. At last any Newton-Raphson search starting in the neighborhood of the roots should converge without any complications.

4 Results from numerical work.

In this section I will shortly comment on the results of my numerical work.

4.1 Periodic orbits.

A few short trajectories were found by an ordinary Newton routine as described in ch. 6 [1]. However, longer orbits were not possible to obtain with this method. Multiple shooting was implemented, tested successfully on the Rössler system (all orbits up to length 10 were found) but a revised implementation taking into account the symmetries of the Helium atom was never accomplished.

4.2 The quantities $\lambda_p, S_p, \sigma_p, \alpha_p$.

Unfortunately, I did not succeed in finding the periodic orbits, and thus I could not proceed with the calculation of stability eigenvalues and action. In order to finish the rest of the calculation I have taken the data from [1]. These are shown in Table 3.

p	$\frac{S_p^{fd}}{2\pi}$	λ_p^{fd}	σ_p^{fd}	α_p^{fd}
0	1.829	0.6012	0.5393	2
01	3.61825	1.8622	1.0918	4
011	5.32615	3.4287	1.6402	6
001	5.39451	1.8603	1.6117	6
0111	6.96673	4.4378	2.1710	8
0011	7.04133	2.3417	2.1327	8
0001	7.25849	3.1124	2.1705	8
01111	8.56618	5.1100	2.6919	10
00111	8.64306	2.7207	2.6478	10
01011	8.93700	5.1563	2.7292	10
00011	8.94620	4.5932	2.7173	10
00101	9.02689	4.1765	2.7140	10
00001	9.07179	3.3424	2.6989	10
01111	10.13872	5.604	3.2073	12
001111	10.21673	3.0324	3.1594	12
010111	10.57067	6.1393	3.2591	12
000111	10.57628	5.6766	3.2495	12
010011	10.70699	5.3252	3.2520	12
001011	10.70699	5.3252	3.2520	12
000011	10.74303	4.3317	3.2332	12
000101	10.87855	5.0002	3.2626	12
000001	10.91015	4.2408	3.2467	12

Table 3: Action $S_p^{fd}/2\pi$, Lyapunov exponent and winding number $\lambda_p^{fd}, \sigma_p^{fd}$ and topological index α_p^{fd} as calculated in the fundamental domain along the periodic orbits with symbolic dynamics p. These data are taken from [1].

4.3 Zeroes of $\zeta_+^{-1}(z)$.

To locate the roots I made a zoom-in contour plot on the domain of interest, that is z values with real part between 0.5 and 5 and imaginary parts between -0.03 and 0.03. The plots are shown on page 30. The innermost circles among the contours denotes points at which the zeta function has a value less than 0.01. The triangles on the real axis denotes the expected zeroes (taken from [1]). From here it can qualitatively be inferred that out of 20 expected roots, 20 are approximately found; of these about 5 are less acceptable. 14 false zeroes are found.

For an exact determination of the roots I used a built in routine in IDL based on something called an optimal M method. The expected zeroes together with the ones I found are listed below.

Expected	0.584	1.134	1.308	1.684	1.883	2.243	2.456
Found	0.5852	1.1479	1.3065	1.6836	1.8845	2.2453	2.4580
Expected	2.574	2.783	3.025	3.154	3.343	3.586	3.733
Found	2.5777	2.7760	3.0272	3.1591	3.3414	3.5880	3.7360
Expected	3.903	4.140	4.305	4.429	4.689	4.865	
Found	3.9083	4.1430	4.3055	4.4216	4.6967	4.8641	

As can be seen in most cases the values coincide within three digits of significance. Not bad, but taking into consideration that I have reused exactly the same values of λ_p, σ_p, S_p and α_p, I had expected to find exactly the same roots. Even though the original roots were found by another method than the one I have used, one should not expect general deviations in the results.

5 Concluding remarks.

One part of this report was devoted to find periodic orbits of Helium, calculate stabilities, action etc. and finally find the roots of the dynamical zeta function. Only a fraction of this was achieved. From tests on the Rössler system I know that my routines including fourth order Runge-Kutta integration, ordinary Newton-Raphson search and multiple shooting work as they are intended to. The difference between Rössler and collinear Helium is the degree of symmetry. In fact, no symmetries exist for Rössler whereas the symmetry group for the collinear Helium consists of eight symmetries (cf. section 3.2.1). Only by a proper use of these symmetries, efficiency in the numerical routines can be obtained, in specific, any search for periodic orbits should be restricted to the fundamental domain. These modifications in implementation turned out to be quite time consuming, and hence I never succeeded. Nevertheless, I think with some more time devoted to the numerical work, an exhausting search could have been accomplished with the multiple shooting method. The last part of the numerical work, namely finding the roots of the zeta function, was fully accomplished.

For the theoretical part, I have accomplished what I set out to do. I have made a (more or less) complete line of reasoning from the Hamiltonian of the system, through symmetry (section 2.1 and 3.2) and coordinate transformations (section 2.2), to a practicable reduction of the zeta function (section3.2.6). A number of results about symmetry in the flow (section 2.1.1 and 2.1.2) and in the stability matrices (section 2.1.3), about conservation under smooth coordinate transformations of stability eigenvalues (section 2.2.2) and topological index (section 2.2.3), have been analytically derived. In the specific case of Helium I found the symmetry group (section 3.2.1), introduced the fundamental domain modulo this symmetry group (section 3.2.2), justified that all important quantities equally well could be obtained by integration in this domain (section 3.2.3-3.2.5) and finally I arrived at a reduced expression for the zeta function which respects all symmetries in the system (section 3.2.6). Besides this I arrived at explicit expressions for everything needed in order to numerically implement and find periodic orbits and zeroes of the zeta function (section 3.6)

A Technical details about the implementation.

All code regarding determination of cycles was implemented in C++. A routine for matrix inversion was taken from Numerical Recipes [6], a general fourth order Runge-Kutta routine was adopted for all integrations. Besides the implementation of the multiple shooting method, a general Newton search routine was implemented. With this I succeeded to find short orbits (accuracy $\approx 10^{-5}$) but because no symmetry was exploited in this, for longer orbits the method turned out to be intractable.

All code regarding determination of zeroes of the zeta function was implemented in IDL. The zeta function (absolute value) was explored on a 18000×200 grid for $z \in [0.5, 5] \times [-0.03, 0.03]$. From here a detailed contour plot was obtained. Exact roots was found at all places indicated on the contour plot by a built-in routine in IDL.

B Contour plot of the zeta function.

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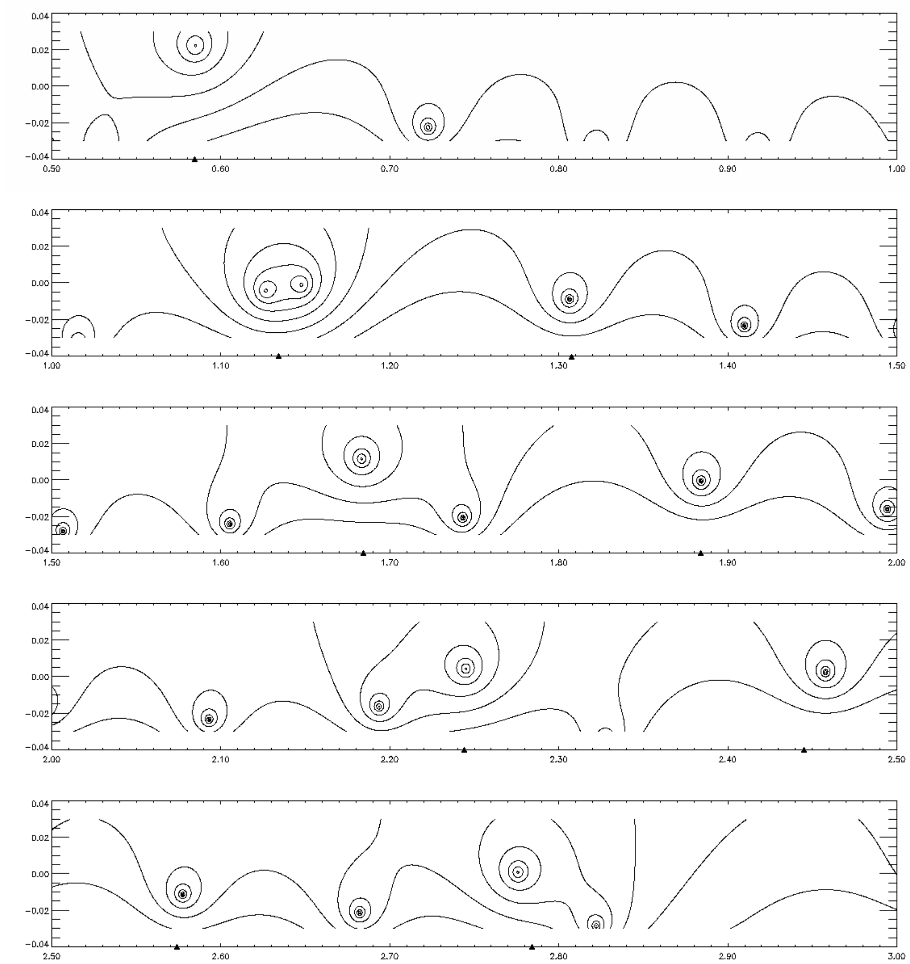

Figure 4: (Continued next page) Above is shown a contour plot of the absolute values of the dynamical zeta function $\zeta^{-1}(z)$ with complex variable z close to the real axis in the interval of interest, $0.5 < Re(z) < 5$. Levels of contours are $0.01, 0.05, 0.1, 0.2, 0.4, 0.8, 1.6, 3.2$. The small inner circles on the plots correspond in most cases to absolute values less than 0.01.

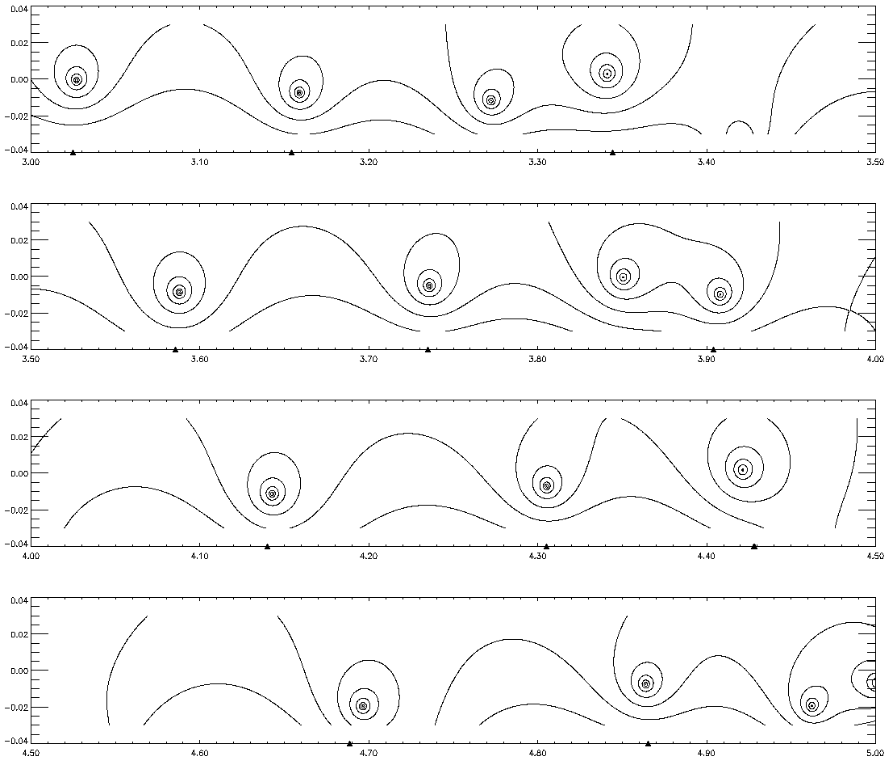

Figure 5: Continuation of figure 4.