DEUTSCHES ELEKTRONEN-SYNCHROTRON

DESY 94-070
April 1994



# Chaos in a Coulombic Muffin-Tin Potential

S. Brandis

*II. Institut für Theoretische Physik, Universität Hamburg*

ISSN 0418-9833

NOTKESTRASSE 85 - 22603 HAMBURG

To be sure that your preprints are promptly included in the
HIGH ENERGY PHYSICS INDEX,
send them to (if possible by air mail):

| | |
|---|---|
| **DESY**<br>**Bibliothek**<br>**Notkestraße 85**<br>**22603 Hamburg**<br>**Germany** | **DESY-IfH**<br>**Bibliothek**<br>**Platanenallee 6**<br>**15738 Zeuthen**<br>**Germany** |

DESY 94-070
April 1994

ISSN 0418-9833

# Chaos in a Coulombic Muffin-Tin Potential

S.Brandis*

II. Institut für Theoretische Physik
Universität Hamburg
Luruper Chaussee 149
22761 Hamburg

April 12, 1994

**Abstract**

We study the two-dimensional classical scattering dynamics by a Muffin-Tin potential with 3 Coulomb singularities. A complete symbolic dynamics for the periodic orbits is derived. The classical trajectories are shown to be hyperbolic everywhere in phase space and to carry no conjugate points.

*Supported by Studienstiftung des deutschen Volkes



In recent years the study of chaotic models has attracted a lot of attention [1]. However, there are only a few models, where e.g. ergodicity or complete hyperbolicity of the dynamics in phase space, two of the few well defined properties in classically chaotic systems, can be proven. These systems are usually either Euclidean billiards with nontrivial boundaries or the motion on Riemann surfaces endowed with a hyperbolic metric[1], whereas for potentials there are hardly any examples, for which these properties can be shown rigorously.

A few years ago an outstanding work by Knauf and Klein [2] has given an example of ergodicity in a potential problem using rather sophisticated mathematical tools. It treats the classical two-dimensional scattering by a rather general potential, whose main features are $n$ fixed attractive Coulomb centers and a fast decay towards infinity. For $n \geq 3$ the system exhibits all the typical characteristics of chaotic scattering. On the set of bounded orbits the motion is proven to be ergodic (with respect to a specified measure). We study here a slightly different model in order to avoid some technical difficulties and to make the physical meaning more transparent.

The potential under consideration is defined in the following way,

$$V(\vec{r}) = \begin{cases} -\sum_{i=1}^{3}\left(\frac{Z_i}{|\vec{r}-\vec{s}_i|} - \frac{Z_i}{R_i}\right) & \text{, for } |\vec{r}-\vec{s}_i| \leq R_i \\ 0 & \text{else} \end{cases} . \tag{1}$$

The vectors are two-dimensional, $\vec{s}_i$ fixed and all $Z_i$ are positive such that the potential is purely attractive. The constant terms are added for the potential to be continuous. This is a typical Muffin-Tin (MT) potential sketched by the dotted lines in Fig. 1. We shall be concerned with scattering, which takes place whenever the energy is positive, $E > 0$.

To study the solutions of the Hamiltonian system is equivalent to studying the geodesic motion on a surface with a metric defined via $(i, j = 1, 2)$

$$g^E_{ij}(\vec{r}) := (1 - \frac{V(\vec{r})}{E})\,\delta_{ij} , \tag{2}$$

changing the time to arc length [3]. The superscript expresses the explicit energy dependence of the solutions, which is a decisive difference to billiards, where the action scales with the energy. The metric is not well defined at the Coulomb centers $\vec{s}_i$, but the time a trajectory needs to hit the center is finite. The most natural thing is thus to "regularize" these points and to extend the geodesic flow to the singularities by adding a backscattering orbit whenever there is a collision with a center. By this construction one

can use important results of differential geometry. For one we can calculate the Gaussian curvature for this metric. It vanishes outside a MT and is strictly negative within,

$$K^E(\vec{r}) = -\frac{Z_i}{2E(|\vec{r}-\vec{s}_i| + \frac{Z_i}{E})^3}. \qquad (3)$$

This is a crucial property for the chaotic behaviour as we shall see later. Note that its limit, when approaching a singularity, is finite.

A characteristic of irregular scattering is the self-similar structure of singularities in quantities like the time-delay or the deflection function[4]. These are consequences of the existence of a dense set of hyperbolic periodic orbits in phase space. Therefore we will directly draw attention to these periodic geodesics.

To find the periodic orbits systematically one usually needs to have a symbolic dynamics. Here we shall present the code by which the periodic orbits (p.o.) can be represented in a symbolic way and then talk about the algorithm that finds the exact positions of the p.o. in phase space. There are two restrictions to the method applied below: 1.) The code is valid for energies $E > max(\frac{Z_i}{R_i})$ only. This is due to the fact that it requires the Kepler trajectories to be hyperbolas. 2.) The centers $\vec{s}_i$ have to be arranged on the corners of a (convex) triangle,such that the corridors, on which trajectories can move between two MT's, do not intersect.

The code is in fact fairly simple: Giving each center a number (1,2,3) a periodic orbit is uniquely represented by its history in terms of the centers it passes during one traversal. That is to say, all periodic sequences in the space of words of the letters $(1,2,3)$ without repetition and modulo cyclic permutation, represent symbolically the set of all periodic orbits. When the Kepler trajectories are hyperbolas, a repetition of numbers cannot occur, because an orbit has to touch another MT before turning around the first one a second time. We shall now sketch the idea of a geometric "proof" for this one-to-one relation:

"=>" For an orbit to be periodic it has to turn around the centers again and again. Hence given a periodic orbit, it has a well defined path through the centers and thus a single code (modulo its cyclic permutations).

"<=" Given a code one needs to show that there is only one p.o.. We shall exclude for a moment the orbits colliding with a singularity. Since the points $\vec{s}_i$ are then excluded, two orbits cannot be transformed



continuously into each other, i.e. are not homotopic, when they turn around the same center in a different orientation at least once during their traversal of the orbit. This gives rise to two possible ambiguities: (a) a topological difference, (i.e. they belong to different homotopy classes) and (b) there exists more than one orbit per homotopy class.

We can already exclude (b), since we know that the Gaussian curvature is non-positive, which allows only one geodesic per homotopy class (see e.g.[5]). To exclude (a) we split up the code into smaller parts and find three different types of pieces a periodic code can consist of:

(1): *...abc...*,

where $a, b, c \in \{1,2,3\}$ and $a \neq c$. Whether the orbit turns around $b$ clockwise or anti-clockwise (see Fig. 1), is fixed by the explicit numbers, because the Kepler orbit being a hyperbola does not allow self-crossing after one turn. Hence given a sequence like the above one in a code the orbit has a well defined orientation.

(2): *...cabab...ababc...*

in the familiar notation. On the pendulum like motion between $a$ and $b$ the angle spreads or decreases constantly because of the hyperbolas at each center. Thus it will not change the orientation in between, when it comes out the same way it went in. This is the case in (2), since the last three letters are just a cyclic permutation of the first three.

(3): *...cabab...abac....*

In this case the orientation has to change, as it comes out of the pendular motion the opposite way it went in. But as a result of the avoided self-crossing the turn around will happen exactly in the middle of the term. The pattern looks like an ancient Greek meander.

Finally, the colliding orbits have to have a mirror symmetry in the code because of their backscattering nature. In fact every code with this symmetry is a colliding one, which is then unique.

Given a one-to-one code with an appealing geometrical interpretation, we can construct each periodic orbit by an algorithm.. The p.o. consists of pieces of free motion and Kepler trajectories. We therefore obtain the scattering angle as a function of the relative angular momentum $l_i$ at the

$i-$th center of the code:

$$(\theta_{i+1}-\theta_i)_{Kep} = \begin{array}{l}\mathrm{sgn}(l_i)\,(2\,\arccos((\frac{P_i}{R_i}-1)\frac{1}{\epsilon_i})-\pi)\\ +\arcsin(\frac{l_i}{pR_i}),\end{array} \tag{4}$$

where $\theta_i$ is the direction of the momentum before the $i-$th center and $P_i$ and $\varepsilon_i$ are the parameters of the Kepler trajectory ($P_i=\frac{l_i^2}{Z_i}, \varepsilon_i^2=1+\frac{2(E-\frac{Z_i}{R_i})l_i^2}{Z_i^2}$, where the mass is set to 1). $p$ is the absolute value of the momentum of the free motion. On the other hand the relative angular momenta transform into each other by geometry

$$l_{i+1}=l_i+|\vec{s}_i-\vec{s}_{i+1}|\,p\,\sin(\alpha_{i,i+1}-\theta_{i+1}), \tag{5}$$

$\alpha_{i,i+1}$ being the angle of the vector $\vec{s}_i-\vec{s}_{i+1}$ with respect to the $x$-axis. This leads to the expression

$$(\theta_{i+1}-\theta_i)_{geo} = \begin{array}{l}\alpha_{i,i+1}-\alpha_{i-1,i}-(\arcsin(\frac{l_{i+1}-l_i}{|\vec{s}_i-\vec{s}_{i+1}|p})\\ -\arcsin(\frac{l_i-l_{i-1}}{|\vec{s}_{i-1}-\vec{s}_i|p}))\end{array}. \tag{6}$$

For periodic orbits and for each index $i$ the functions in (4) and (6) have to be equal. Thus the problem of determining p.o.'s is reduced to finding the zeros of the difference of (4) and (6) in N-dimensional angular space as a function on the N-dimensional angular momentum space, when the length of the code is N.

This has to be done numerically and works very well (tested up to the first 16617 p.o.'s, which corresponds to code length N=17). Fig. 1 shows a typical orbit. The number of periodic orbits $N(T)$ below a certain period $T$ proliferates exponentially in chaotic systems. In this case it is strongly linked to the exponential increase of the number of codewords. Especially at high energies the period becomes essentially a multiple of the free parts of the orbit, as the time spent in a MT decreases faster than the time it needs for the free motion as shown in Fig. 2. The pronounced staircase behaviour washes out as one gets to longer p.o.'s, but this is a difficult region to reach numerically.

Given a periodic orbit or any other trajectory one can calculate its stability, i.e. the linear approximation of the motion in its vicinity. Practically one needs to find an orthogonal (local) coordinate system, which splits the motion into a direction parallel and a direction transversal to the flow. This is in general not a perfectly obvious procedure. In this case a particular



problem comes about by the Coulomb singularities, such that one may easily obtain absurd results, if one is not careful enough.

The most elegant way is to return to the geodesic motion generated by $g_{ij}^E$[2, 5]. We know from differential geometry on 2-dimensional surfaces that orthogonal coordinates always exist, called geodesic coordinates. The second variation of the Lagrangian on the surface leads to the Jacobi equation for the transversal component $y$ of a vector field along the geodesic,

$$\ddot{y}+K^E(\vec{r}(\tau))\,y=0, \tag{7}$$

with the Gaussian curvature mentioned above given in terms of the arc length $\tau$ in this metric. The dot denotes the derivative with respect to $\tau$. To calculate the stability in phase space we need to extend this to the $2\times 2$ stability matrix $U(\tau)$ which is obtained as a solution of

$$\dot{U}(\tau)=\begin{pmatrix}0 & 1\\ -K^E & 0\end{pmatrix}U(\tau)\ ,\ \text{with}\ \ U(0)=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{8}$$

By the negativity of the curvature, a solution of this equation is strictly positive, which is a manifestation of the hyperbolicity of the orbits. Note as a side-remark that a solution of a differential equation of this type has a constant determinant, which reflects the Liouville Theorem on the preservation of the volume under the flow in phase space.

The stability matrix for a periodic orbit is often called monodromy matrix. In this case it is a product of those matrices that correspond to the pieces the orbit traverses. The part for a free motion reads

$$U_{free}=\begin{pmatrix}1 & t_{free}\\ 0 & 1\end{pmatrix}. \tag{9}$$

Here $t_{free}$ is the time the orbit spends between two MT's. The eigenvalues of the monodromy matrix now determine the spreading of orbits and hence the Lyapunov exponents. These are different from zero, because the solution of (8) is always positive and hence the orbits are hyperbolic.

At the end we shall sketch a proof for the fact that in this system there are no conjugate points along periodic orbits.

Let $c(\tau,u)$ be a geodesic parameterized by arc length $\tau$ and let $u$ be a variation, such that for all values of $u$ $c(\tau,u)$ is a geodesic. A Jacobi field $Y$ is a vector field along $c(\tau,u)$ generated by

$$Y(\tau):=\frac{\partial}{\partial u}c(\tau,u). \tag{10}$$

If one takes geodesic coordinates and the dual basis in tangent space, one gets for the transversal component of the Jacobi field the Jacobi equation as above. As long as $c(\tau, u)$ is differentiable with respect to $\tau$, $y(\tau)$ is differentiable as well. Since $K^E \leq 0$, the solution of the Jacobi equation is either only convex or only concave (depending on the initial condition $\dot{y}(0)$). But then it is impossible to find a non-vanishing, differentiable solution of the Jacobi equation with $y(0) = y(\tau_1) = 0\,, \tau_1 > 0$. So there are no conjugate points.

This is a slight extension of the proof found in [5] for non-smooth $c(\tau, u)$. Note that $\dot{c}(\tau, u)$ has to be continuous.

In conclusion we would like to stress that this rather old and well known analogy to differential geometry is very handy in studying potential problems in general, especially for the calculation of the stability exponents.

The properties of this system are particularly suitable for studying the quantum analog in terms of semiclassical methods, which is our ultimate interest. A forthcoming paper will give a more detailed and also a numerical description of the classical dynamics and the quantum mechanics [6].

I would like to thank Prof. F. Steiner for many fruitful and encouraging discussions.

## References

[1] E.g. M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, New York, 1990); *Chaos and Quantum Physics*, edited by M.-J. Giannoni, A. Voros, J. Zinn-Justin (North Holland, Amsterdam, 1991) and references therein

[2] A. Knauf and M.Klein, *Classical Planar Scattering by Coulombic Potentials*, Lecture Notes in Physics **13**, (Springer, Heidelberg, 1992)

[3] R. Abraham and J.E. Marsden, *Foundations of Classical Mechanics* (Reading, Benjamin, 1978)

[4] For a recent review see E. Ott and T.Tel in CHAOS **3**(4)(1993), special issue on scattering theory

[5] S. Gallot, D. Hulin, J. Lafontaine, *Riemannian Geometry*, Universitext (Springer, Berlin, 1990)

[6] S. Brandis, in preparation



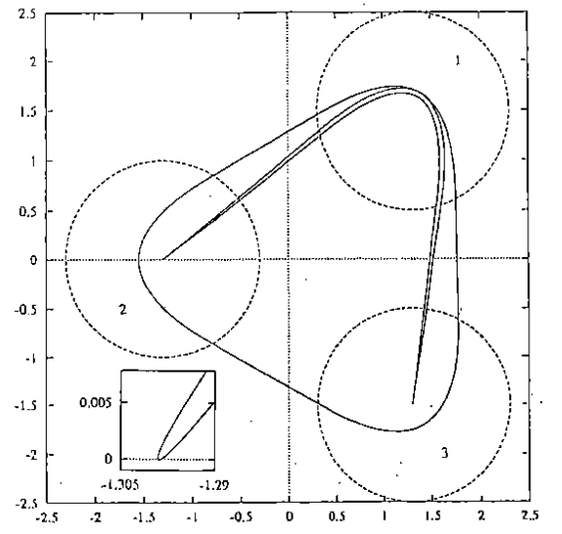


Figure 1: The periodic orbit corresponding to the codeword (1231213) in a potential, where all Muffin-Tins are of same strength $Z_i = 8$ and placed on an equilateral triangle. The dashed lines encircle the regions of non-vanishing potential. The inset is a blow-up of nucleus number 2 to show that the orbit does not collide.

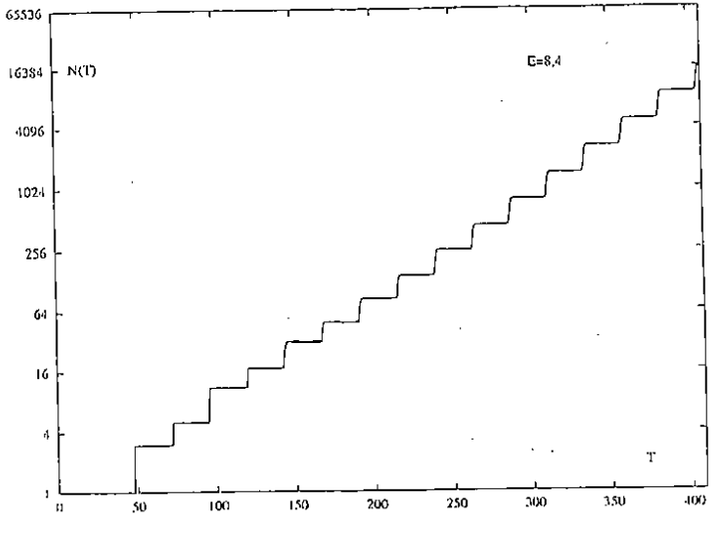


Figure 2: $N(T)$ at $E = 8.4$ for the configuration shown in Fig. 1