MATHIEU’S EQUATIONS AND THE IDEAL RF-PAUL TRAP

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Abstract. Of great use to physics is the ion trap. Though there are various models in use, we focus here on Paul style models. To do so, we need understand Mathieu’s equations and their corresponding solutions in enough detail to grasp the function of the Paul ion trap. In this report, we explore the behavior of Mathieu’s equation and their solution for the Paul ion trap.

1. The basic theoretical foundation of the Paul trap

To confine an ion, we should require a force such that \( F = -kr \). What would this entail for an electrical potential? Since the electric field is proportional to the force, and is equal to the divergence of the potential, we should require

\[
\Phi \propto (\alpha x^2 + \beta y^2 + \gamma z^2)
\]

That is, we require an electric quadrupole field, say,

\[
\Phi = \Phi_0 \frac{2r_0^2}{2r_0^2} (\alpha x^2 + \beta y^2 + \gamma z^2)
\]  \tag{1.1}

Equation 1.1 must obey that condition imposed on all potentials where there is no free charge distribution, namely that

\[
\nabla^2 \Phi = 0 \rightarrow \alpha + \beta + \gamma = 0
\]

We can satisfy this in more than one way. The two of import are that associated with the linear Paul Trap, whose initial manifestations were not as a trap but as a focusing tunnel of sorts, but which can be turned into a ‘race track’ ion trap,

\[
\alpha = 1 = -\gamma, \quad \beta = 0 \rightarrow \Phi = \Phi_0 \frac{x^2 - z^2}{2r_0^2}
\]  \tag{1.2}

and that associated with the “Ionenkäfig”, the chamber rf Paul ion trap

\[
\alpha = 1 = \beta, \quad \beta = 0 \rightarrow \Phi = \Phi_0 \frac{r^2 - 2z^2}{r_0^2 + 2z_0^2}, \quad \text{at } 2z_0^2 = r_0^2
\]  \tag{1.3}

![Figure 1.1. The linear rf Paul trap (a) and the chamber rf Paul trap (b). This Figure from [1]](1)
Such potentials can be provided via hyperbolic electrodes. We can perform a successive over relaxation of a cross section of these electrodes and find that indeed a two-dimensional stable equilibrium is created at the center (though this is unstable in the third dimension, z) when we satisfy the above conditions (Figure 1.2, also see our report on the SOR method).

![Hyperbolic Electrodes via SOR, N=1000, n=1318, Tolerance=0.0001](image1)

**Figure 1.2.** SOR calculation for hyperbolic electrodes. The outer box is held at ground, the horizontal electrodes held at V and the vertical ones held at -V. The grid was 1000 by 1000, our tolerance was 0.0001.

In both cases, we have a repulsive force in the z direction which must be avoided. This can be done via the clever mechanism of rotating the field so that the focusing and defocusing is applied alternatively in each direction. If done at the right set of frequencies, the ion will maintain a stable orbit near the center of the ion trap.

A way to visualize this is with W. Paul’s mechanical analog [1, 2]. Paul made an equivalent potential as that described above by carving an hyperbolic saddle surface out of plexiglass. Placing a ball on top of this surface would result in the ball falling off of it, of course. But if the surface is rotated at a proper rate, the ball will stay on the surface (Figure 1.3).

![The mechanical analog to the rf Paul trap](image2)
The applied potential is thus
\[(1.4) \quad \Phi_0 = U + V \cos \omega t\]
If the particle has a charge \(e\) and mass \(m\), then its equation of motion are
\[\ddot{x} + \frac{e}{mr_0^2} (U + V \cos \omega t)x = 0 \quad (1.5) \quad \ddot{z} - \frac{e}{mr_0^2} (U + V \cos \omega t)z = 0\]
Since cosine is an even function, we can generalize this to
\[(1.6) \quad \ddot{y} + (a - 2q \cos(2 \tau)) \eta = 0, \quad a = \frac{4eU}{mr_0^2 \omega^2}, \quad q = -\frac{2eV}{mr_0^2 \omega^2}, \quad \tau = \frac{\omega t}{2}\]
For the \(z\) equation, \(a \rightarrow -a\). The solution to this equation is simple enough though not trivial, and we give an informal derivation below.

2. Mathieu’s Equation, Solution, and Stability

2.1. Basics and Floquet’s Theorem. Our derivation below can be found in greater detail and better form in many references [3, 4, 5], and our derivation follows the spirit of these. An equation such as Mathieu’s equation,
\[
(2.0) \quad \ddot{y} + (a - 2q \cos(2 \tau)) \eta = 0
\]
is of a class of differential equations of the type [7],
\[
(2.1) \quad L[y] = y'' + p(t)y' + q(t)y = 0
\]
Any two fundamental solutions to this equation, \(y_1(t), y_2(t)\), will satisfy the set of boundary value equations,
\[
\begin{align*}
c_1 y_1(t_0) + c_2 y_2(t_0) &= y_0 \quad (2.2) \quad \text{Y} c = y \\
c_1 y_1'(t_0) + c_2 y_2'(t_0) &= y_0'
\end{align*}
\]
We thus require that the determinant of \(Y\) (called the Wronskian) is not equal to zero,
\[(2.3) \quad W(Y) = \text{det}(Y) = \begin{vmatrix} y_1(t_0) & y_2(t_0) \\ y_1'(t_0) & y_2'(t_0) \end{vmatrix} \neq 0\]
The set of even/odd solutions:
\[
\begin{align*}
y_1 : & \quad y(t_0) = 1, \quad y'(t_0) = 0 \\
y_2 : & \quad y(t_0) = 0, \quad y'(t_0) = 1
\end{align*}
\]
\[\text{W}(Y) = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} = 1\]
Are thus fundamental sets of solutions. We may follow Floquet’s theorem [3], which tells us that Mathieu’s equation has at least one solution \(\exists \eta\)
\[(2.4) \quad y(z) : (y(z + \pi) = \sigma y(z)) \quad \text{Floquet’s Theorem}\]
The proof of this is outlined as follows. Since Mathieu’s equations will have an even \((w_1(\eta))\) and odd \((w_2(\eta))\) solution pair, these two functions may define any other solution, e.g., consider
\[
\begin{align*}
w_1(\eta + \pi) &= \alpha w_1(\eta) + \beta w_2(\eta) & \Rightarrow & & w_1'(\eta + \pi) &= \alpha w_1'(\eta) + \beta w_2'(\eta) \quad \exists \\
w_1(0) &= w_2'(0) = 0 & \Rightarrow & & w_1'(0) &= \alpha, \quad w_1'(\pi) = \beta \quad \exists \\
w_1(\eta + \pi) &= w_1(\pi)w_1(\eta) + w_1'(\pi)w_2(\eta), \text{ as well,} & & w_2(\eta + \pi) &= w_2(\pi)w_1(\eta) + w_2'(\pi)w_2(\eta)
\end{align*}
\]
Let
\[
A = \begin{pmatrix} w_1(\pi) & w_1'(\pi) \\ w_2(\pi) & w_2'(\pi) \end{pmatrix}, \quad w(\eta) = \begin{pmatrix} w_1(\eta) \\ w_2(\eta) \end{pmatrix} \quad \Rightarrow & & Aw(\eta) &= w(\eta + \pi)
\]
According to Floquet’s theorem, we thus require,
\[
|A - \sigma I| = 0
\]
an eigenvalue equation which can be satisfied with the proper value of $\sigma$. We consider further that Mathieu’s equation has a solution of the form $e^{i\mu} \phi(\eta)$

$$\sigma = e^{i\mu}, \quad \phi(\eta) = e^{-i\mu} y(\eta) \ni \phi(\eta + \pi) = e^{-i(\pi+\pi)} y(\eta + \pi) = e^{-i\mu} y(\eta) = \phi(\eta)$$

2.2. Hill’s Method solution. With Floquent’s theorem we assume a series solution, due to G. W. Hill,

$$(2.5)\quad w = e^{i\mu} \phi(\eta) = e^{i\eta} \sum_{r=-\infty}^{\infty} c_{2r} e^{2iri\eta} = \sum_{r=-\infty}^{\infty} c_{2r} e^{(\mu+2iri)\eta}$$

When we put this into Mathieu’s equation,

$$\sum_{r=-\infty}^{\infty} c_{2r} \left( (\mu + 2ir)^2 + a - 2q \frac{e^{2i\eta} + e^{-2i\eta}}{2} e^{(\mu+2i)\eta} \right) = 0$$

matching terms in power of $r$, we get the equation

$$(2.6)\quad -qc_{2r-2} + (\mu + 2ir)^2 + a c_{2r} - qc_{2r+2} = 0$$

Multiplying through by $-1 = i^2$, and then dividing by the middle term,

$$(2.7)\quad q \frac{c_{2r-2} + c_{2r}}{(2r - \mu)^2 - a} + q \frac{c_{2r} + c_{2r+2}}{(2r - \mu)^2 - a} = 0$$

We now define

$$\gamma_{2r} = \frac{q}{(2r - \mu)^2 - a}$$

That these coefficients, $c_i$, have non-trivial solutions requires the infinite determinant $\Delta$ to vanish for noninfinite $r$:

$$(2.8)\Delta(i\mu) = \begin{vmatrix} \cdots & \gamma_{-2} & 1 & \gamma_{-2} & \gamma_0 \\ \gamma_{-2} & 1 & \gamma_0 \\ \gamma_{0} & 1 & \gamma_2 \\ \gamma_{2} & 1 & \cdots \end{vmatrix} = 0$$

But of course, this is not a simple object to understand and solve. We can approach this problem from a rather clever angle introduced by E. T. Whittaker.

Consider the function

$$\lambda = \frac{1}{\cos \pi i\mu - \cos \pi \sqrt{a}}$$

Like our determinant, $\lambda$ has a simple pole at $a = (2r - i\mu)^2$, so that the function

$$\zeta = \Delta(i\mu) - \kappa \lambda$$

has no singularities if $\kappa$ is chosen properly and is bound at infinity, where $\Delta(i\mu) = 1$ since the $\gamma$ functions all vanish and the diagonal term is all that remains, and $\lambda = 0$ since $\cosh(x)$ limits to zero as $x$ tends towards infinity.

$$\lambda = \Delta(i\mu) - \kappa \lambda \rightarrow 1 - 0$$

By Liouville’s theorem (of complex calculus), since this limits to a constant, it is a constant always, so we have

$$\kappa = \frac{\Delta(i\mu) - 1}{\lambda}$$

Next we consider the $\mu = 0$ case and find,

$$\kappa = (\Delta(0) - 1)(1 - \cos \pi \sqrt{a}) \rightarrow \frac{\Delta(i\mu) - 1}{\lambda} = (\Delta(0) - 1)(1 - \cos \pi \sqrt{a})$$

Next we suppose that $\mu$ is chosen to satisfy our requirement that the determinant vanish. We thus have

$$\cos \pi i\mu - \cos \pi \sqrt{a} = (1 - \Delta(0))(1 - \cos \pi \sqrt{a}) \rightarrow i\mu = \frac{1}{\pi} \cos^{-1} \left( 1 - \Delta(0)(1 - \cos \pi \sqrt{a}) \right)$$
Recall that our solution took the form,
\[ w = e^{\mu\phi(\eta)} \]
This solution will be unbounded unless \( \mu \in \mathbb{Z} \), in which case we have
\[
\mu = \frac{1}{\pi} \cos^{-1} \left( 1 - \Delta(0)(1 - \cosh \pi \sqrt{a}) \right)
\]
We can easily encode this result, say,
\[
\text{if}(a>0)\{ \text{mu}=\text{acos} \left( 1 - (d[100])*(1-\cos(\pi*\text{sqrt}(a))) / (\pi) \right) \};
\]
\[
\text{if}(a<0)\{ \text{mu}=\text{acos} \left( 1 - (d[100])*(1-\cosh(\pi*\text{sqrt}(\text{fabs}(a)))) / (\pi) \right) \};
\]
\[
\text{if}(\text{mu} != \text{mu})\{\text{mu}=0.000000;\} //\text{If mu=nan then make it zero}
\]
But first we must calculate \( \Delta(0) \). This task has been made exceedingly simple by the recent work of J. E. Sträng [5] who has found an efficient recursion formula.

2.3. Sträng’s recursion formula for \( \Delta(0) \). First we note that by the symmetry of \( \Delta(0) \), \( \gamma_{-n} = \gamma_n \). Following Sträng, we define

\[
A_i = \begin{pmatrix}
1 & \gamma_{2i} & 0 \\
\gamma_{2(i-1)} & 1 & \gamma_{2(i-1)} \\
0 & \gamma_{2(i-2)} & 1 \\
& & & \ddots & \ddots & \ddots \\
& & & \ddots & \ddots & \ddots \\
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& & & & & \ddots & \ddots & \ddots \\
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\end{pmatrix}
\]

We have \( \Delta_i = \text{det}(A_i) \supseteq \Delta(0) = \lim_{i \to \infty} \Delta_i \). We can decompose \( A_i \) in terms of \( A_{i-1} \),

\[
A_i = \begin{pmatrix}
1 & \gamma_{2i} \\
\gamma_{2(i-1)} & 1 & \ddots \\
& & \ddots & \ddots & \ddots \\
& & & \ddots & \ddots & \ddots \\
& & & & \ddots & \ddots & \ddots \\
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& & & & & & & & & & & & & & & & \ddots & \ddots & \ddots \\
\end{pmatrix}
\]

A Laplace decomposition yields

\[
\text{det}(A_i) = \begin{vmatrix}
A_{i-1} & \gamma_{2i} \\
\gamma_{2(i-1)} & 1 \\
& & \ddots & \ddots & \ddots \\
& & & \ddots & \ddots & \ddots \\
& & & & \ddots & \ddots & \ddots \\
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& & & & & & & & & & & & & & & & \ddots & \ddots & \ddots \\
\end{vmatrix}
\]

Here \( rA_{i-1} \) represents \( A_{i-1} \) with its leftmost column chopped off. Again, following Sträng we define \( LA \) as the matrix \( A \) with its rightmost column removed, \( uA \) the matrix \( A \) with its lowest row removed, \( LA \) the matrix \( A \) with its upper most row removed. Ultimately, \( uldr(A_{i-1}) = A_{i-2} \), and given the symmetry involved, \( \text{det}(rd(A_{i-1})) = \text{det}(ul(A_{i-1})) \). Following this procedure we find

\[
\Delta_i = \Delta_{i-1} - 2\gamma_{2i}\gamma_{2(i-1)}\text{det}(rd(A_{2(i-1)})) + (\gamma_{2i}\gamma_{2(i-1)})^2\Delta_{i-2}
\]

We also note, similarly using Laplacian decomposition,
\[
\Omega_i = \text{det}(ul(A_i)) = \text{det}(rd(A_i)) \quad \Rightarrow \quad \Omega_i = \text{det}(A_{i-1}) - \gamma_{2i}\gamma_{2(i-1)}\Omega_{i-2}
\]
so that
\[
\frac{\Delta_{i-1} - \Omega_i}{\gamma_2(\gamma_2(i-1))} = \Omega_{i-1} = \det(rd(A_{i-1}))
\]
and
\[
\Delta_i = \Delta_{i-1} + 2(\Omega_i - \Delta_{i-1}) + (\gamma_2(\gamma_2(i-1)))^2 \Delta_{i-2}
\]
\[
\Delta_i + \Delta_{i-1} - (\gamma_2(\gamma_2(i-1)))^2 \Delta_{i-2} = \Omega_i \Rightarrow \frac{\Delta_{i-1} + \Delta_{i-2} - (\gamma_2(i-1)\gamma_{i-2})^2 \Delta_{i-3}}{2} = \Omega_{i-1}
\]
Plugging this into Equation 2.13,
\[
\Delta_i = (1 - \gamma_2(\gamma_2(i-1))) \Delta_{i-1} + (\gamma_2(\gamma_2(i-1)))^2 \Delta_{i-2} + \gamma_2(\gamma_2(i-1))(\gamma_2(i-1)\gamma_2(i-2))^2 \Delta_{i-3}
\]
Define \(\alpha_{2i} = \gamma_2(\gamma_2(i-1))\) and \(1 - \alpha_{2i} = \beta_{2i}\) and find,
\[
(2.14) \quad \Delta_i = \beta_{2i} \Delta_{i-1} - \alpha_{2i} \beta_{2i} \Delta_{i-2} + \alpha_{2i} \beta_{2i}/2(\gamma_2(i-1)\gamma_{i-2}^2) \Delta_{i-3}
\]
We can recursively solve for \(\Delta(0) = \lim_{i \to \infty} \Delta_i\) to as much accuracy as necessary, though the program presented below found convergence to a fair tolerance quickly. We first must “seed” the recursion with the first three \(\Delta_i\). This can be done by hand, though we have deferred to the kindness of our computer algebraic program Maple instead.

Maple finds:

```maple
with(linalg):
C:=matrix([[1,e6,0,0,0,0,0],[e4,1,e4,0,0,0,0],[0,e2,1,e2,0,0,0],[0,0,0,e0,1,e0,0,0],[0,0,0,0,e2,1,e2,0],[0,0,0,0,0,e4,1,e4],[0,0,0,0,0,0,e6,1]]):
dc:=det(C);
dc := -2*e2^2*e0*e4^2*e6+e2^2*e4^2-2*e4^2*e2*e0*e6^2+2*e2*e4^2*e6+e4^2*e6^2+2*e2^2*e0+4*e2*e0*e6*e4-2*e2*e4-2*e6*e4-2*e2*e0+1
A:= matrix([[1,e4,0,0,0,0],[e2,1,e2,0,0,0],[0,e0,1,e0,0,0],[0,0,0,e2,1,e2,0],[0,0,0,0,e4,1,e4],[0,0,0,0,0,e6,1]]):
da:=det(A);
da := 1-2*e2*e4-2*e2*e0+2*e2^2*e4^2+2*e2*e4^2*e6+4*e2*e4^2*e6*e4-2*e2*e4^2+2*e2*e0+1
B:=matrix([[1,e2,0],[e0,1,e0],[0,e2,1]]):
db:=det(B);
db := 1-2*e2*e0
```

Our program seeks to find all stable values of \(\mu\), i.e. those that satisfy Equation 2.9 as real values (i.e. all iso-\(\mu\) for which \(\mu\) is exclusively imaginary.

Our code finds all such iso-\(\mu\) by looping through the a and q axis. If our \(\mu\) formula returns “nan” which is the C language’s way of saying not a real number, then we set the value of \(\mu\) to zero, though of course it is only the imaginary part of \(\mu\) which is actually zero. We perform a contour plot on our data output and find the elegant avian like image of the stability region of Mathieu’s equation (Figure 2.1).

For the quadropole field, the rf linear Paul trap, we have the following stability regime (Figure 2.2). The original stability diagram is simply reflected about the x-axis as \(a \to -a\) between the two.

For the chamber rf Paul trap, we recall that for the z direction we must allow for \((a, q) \to (2a, 2q)\) (Equation 1.3), and so the lowest region of stability (and the largest region at that) has a slightly different look (Figure 2.4).
Figure 2.1. Stability diagram for Mathieu’s general equation

Figure 2.2. Stability diagram for linear rf Paul trap; stable regions are those in which the two stability diagrams intersect.

Figure 2.3. Stability diagram for linear rf Paul trap, closer view of lowest region of mutual stability (intersection).

3. C Program for calculating the stability regions of Mathieu’s equation

Many thanks to Christian Schneider for spotting typos here!
Figure 2.4. Stability diagram for rf Paul trap, lowest region of stability (intersection of isobars).

```c
#include<stdio.h>
#include<math.h>

int main()
{
    FILE *fp; // Prepare to print to file
    fp=fopen("mat.dat","w");
    int m,i,j;
    float e[200],d[101],alpha,beta,alpha1,mu,a,q;
    float pi=3.141592653589;
    a=0.5;
    q=0;
    for(q=-10;q<10;q+=0.02){ //Loop over the desired
        for(a=-5;a<10;a+=0.07){ //a-q region
            for(m=0;m<=248;m+=2){ //The first seed determinants, from Maple worksheet
                e[m]=q/((m*m*1.0)-a);
            }
            d[1]=1-2*e[2]*e[0];
            d[0]=1;
            for(m=4; m<100; m++) //Here goes Strang's interation method
                alpha=e[2*m]*e[2*(m-1)];
        }
    }
    return 0;
}
```
beta=1-alpha;
alpha1=e[2*(m-1)]*e[2*(m-2)];
d[m]=beta*d[m-1] - alpha*beta*d[m-2] + alpha*alpha1*alpha1*d[m-3];

//Find mu, make sepearate case for -a situation
if(a>=0){ mu=acos( 1 - (d[100])*(1-cos(pi*sqrt(a)))) / (pi);}
if(a<0){ mu=acos( 1 - (d[100])*(1-cosh(pi*sqrt(fabs(a))))) / (pi);}
if (mu != mu){mu=0.000000;} //If mu=nan then make it zero

fprintf(fp,"%f %f %f 
", q, a, mu);fprintf(fp,"\n");

As a final note, we wish to add the code used for gnuplot. One run was to outline the edge of the $\mu = 0$ isobar, since gnuplot does not plot contour this (starts with 0.05). The second run does the overall contouring as seen in the above figures.

For the border outline:

```
set data style lines
set contour base
set cntrparam levels discrete 0.001
set nosurface
set view 0,0
splot 'so2.txt'
```

For the inner contours:

```
set data style lines
set cntrparam levels 20
set contour
set nosurface
set view 0,0
splot 'so2.txt'
```

4. Activation of the equation for the ideal rf Paul trap

Now that we have demonstrated the fundamentals of Mathieu’s equation, we can apply it more directly to the ideal rf Paul. Here we follow the outline from [8].

4.1. Kapitza’s Secular Approximation. We neglect the DC potential $U$ for now and assume the equations of motion are of the form, for the rf Paul Ideal chamber trap:

$$
\ddot{r} + \frac{2e}{m(r_0^2 + 2z_0^2)}(V\cos\omega t)r = 0
$$

$$
\ddot{z} - \frac{4e}{m(r_0^2 + 2z_0^2)}(V\cos\omega t)z = 0
$$

(4.1)

Define $d_0 = r_0^2 + 2z_0^2$. Assume that the $r$ and $z$ motion can be partitioned into large-amp slow “secular” motion $r$ and $z$, and small-amp high frequency micromotion $r_\mu$, $z_\mu$ at the frequency of the applied potential $\omega$. Then our equations become
\[
\ddot{r} + \dot{r}_\mu = -\frac{2e}{md_0^2}(V \cos \omega t)(r + r_\mu)
\]
\[
\ddot{z} + \dot{z}_\mu = \frac{4e}{md_0^2}(V \cos \omega t)(z + z_\mu)
\]

(4.2)

\[
(r_\mu \ll r, \ \dot{r}_\mu \gg \ddot{r}) \rightarrow r_\mu \approx + \left( \frac{2eV}{md_0^2} \right) r \cos \omega t
\]

\[
(z_\mu \ll z, \ \dot{z}_\mu \gg \ddot{z}) \rightarrow z_\mu \approx - \left( \frac{4eV}{md_0^2} \right) z \cos \omega t
\]

\[
\ddot{r} \approx - \left( \frac{4eV}{md_0^2} \cos \omega t - \frac{4e^2V^2}{m^2d_0^4} \cos^2 \omega t \right) r,
\]

\[
\ddot{z} \approx \left( \frac{8eV}{md_0^2} \cos \omega t - \frac{16e^2V^2}{m^2d_0^4} \cos^2 \omega t \right) z
\]

\[
\ddot{r} \approx \left( \frac{2e^2V^2}{m^2d_0^2\omega^2} \right) r \rightarrow r \approx - \cos \left( \frac{\sqrt{2}eV}{md_0^2\omega} t \right) = \cos \omega_r t
\]

\[
\ddot{z} \approx - \left( \frac{8e^2V^2}{m^2d_0^2\omega^2} \right) z \rightarrow z \approx \cos \left( \frac{2\sqrt{2}eV}{md_0^2\omega} t \right) = \cos \omega_z t
\]

Evidently, \( \omega_r = \omega_z / 2 \). We can thus write,
\[
r_{\text{tot}} \approx - \cos(\omega_z t/2) \left( 1 - \frac{2eV}{md_0^2\omega^2} \cos \omega t \right)
\]
\[
z_{\text{tot}} \approx \cos(\omega_z t) \left( 1 - \frac{4eV}{md_0^2\omega^2} \cos \omega t \right)
\]

The results of these approximations are graphically displayed in Figures 4.1 and 4.2 created with the following C code:

```c
float w=53;
float wz=4;
float r,z;
float t=0.0;
while(t<1000){
    r=-cos(wz*t/2)*(1-0.3*cos(w*t));
    z=cos(wz*t)*(1-0.6*cos(w*t));
    t+=0.01;
}
```

**Figure 4.1.** Secular approximation time series
4.2. A solution with Mathieu’s Equation. For a more formal analysis refer to [6]. Starting with the equation,

$$\frac{d^2z}{d\eta^2} + (a_z - 2q_z \cos(2\eta)) z = 0, \quad \eta = \frac{\omega t}{2}, \quad a_z = \frac{-16eU}{md_0^2\omega^2}, \quad q_z = \frac{-8eV}{md_0^2\omega^2}$$

We apply Floquet’s theorem and the subsequent corollary to suppose solutions of the form,

$$u_1(\eta) = e^{\mu \eta} \phi_1(\eta), \quad u_2(\eta) = e^{-\mu \eta} \phi_2(\eta)$$

The conditions for stability require that $\mu$ be purely imaginary. It is typical to write $\mu = \alpha + i\beta$, and so we can take a fourier expansion of the $\phi_i$, and recalling that the original equation contains $\cos(2\eta)$, we assume a general solution,

$$z(\eta) = A \sum_{n=-\infty}^{\infty} C_{2n} e^{i(2n+\beta)\eta} + B \sum_{n=-\infty}^{\infty} C_{2n} e^{-i(2n+\beta)\eta}$$

As before, we can find a useful recursion relation. Define:

$$D_{2n} = \frac{a_z - (2n + \beta)^2}{q_z} \quad \rightarrow \quad D_{2n} C_{2n} - C_{2n-2} - C_{2n+2} = 0$$

When $n = 0$ we have

$$D_0 = \frac{a_z - \beta^2}{q_z} = \frac{C_{-2}}{C_0} + \frac{C_2}{C_0}$$

With this recursion relationship we may solve for $\beta$ with increasing levels of accuracy, for example,

$$C_{2n} = \frac{C_{2n-2}}{D_{2n}} + \frac{C_{2n+2}}{D_{2n}}$$

$$= \frac{C_{2n-4}}{D_{2n-2}} + \frac{C_{2n-2}}{D_{2n-2}} + \frac{C_{2n}}{D_{2n+2}} + \frac{C_{2n+2}}{D_{2n+2}}$$

As a first approximation, we set $C_{\pm4} = 0$ and obtain

$$D_0 = \frac{1}{D_2} + \frac{1}{D_2}$$

$$\frac{a - \beta^2}{q} = q \left( \frac{1}{a - (-2 + \beta)^2} + \frac{1}{a - (2 + \beta)^2} \right)$$
When we assume $4 \gg \beta^2$, $\beta$, $a$ we obtain the approximation,

$$\beta = \sqrt{a + \frac{q^2}{2}}$$

If we take $U = 0 \gg a = 0$ then we find we have recovered the approximation of the previous section,

$$\omega_z = \frac{2\sqrt{2eV}}{md_0^2\omega}$$

From such references as [8] we know that the next approximation is

$$\beta = \sqrt{\frac{a + q^2 \left(\frac{3}{8} + \frac{3}{8} \right) + \frac{a^2}{128}}{1 - q^2 \left(\frac{5}{8} + \frac{5a}{16}\right)}}$$

The motion will have frequencies of $(2n + \beta)$, of which the lowest and second to the lowest correspond roughly with the secular approximation secular and micromotion. We could carry this process on ad infinitum ad nauseum. This is but one method to solve for $\beta$. The other method is the numerical method we used to find the stable points of the iso-$\mu$. A third method is to use the more technical solutions to the Mathieu equation developed by the mathematicians. We will close this report with a brief review of one such solution.

5. TECHNICAL DETAILS

This form of the solution can be found in many references ([4] for example). We need consider the case in which our bound periodic solution to the Mathieu equation is of integral order (integer $\times \pi$) and fractional order $\nu\pi$ where $\nu$ is real but may be rational or irrational.

5.1. Integral order. We write the Mathieu equation as

$$\frac{d^2y}{dz^2} + (a - 2q \cos(2z))y = 0$$

And consider the case when $q = 0$ and write $a = m^2$ and have solutions $\pm \cos mz$, $\pm \sin mz$. We then suppose that the case when $q$ is nonzero can be taken into account as a series based on this initial solution. Let

$$(5.1) \quad a = 1 + \sum_{i=1}^{\infty} \alpha_i q^i$$

Then we suppose that

$$(5.2) \quad y = \cos z + \sum_{i=1}^{\infty} q^i c_i(z)$$

We determine the nature of the $c_i$ functions as follows. Plugging our solution into the Mathieu equation, we get

$$y'' = -\cos z + \sum_{i=1}^{\infty} q^i c_i''(z)$$

$$ay = \cos z + \sum_{i=1}^{\infty} q^i \left( c_i + \alpha_i \cos z + \sum_{k=1}^{i-1} \alpha_k c_{i-k} \right)$$
Using the identity

\[ 2 \cos\left(\frac{1}{2}(A + B)\right) \cos\left(\frac{1}{2}(A - B)\right) = \frac{e^{A + e^{-A}} + e^{-A - B}}{2} \]

\[ = \cos A + \cos B \]

\[-(2q \cos z) y = -q(\cos(z) + \cos(3z) - 2 \cos(2z) \sum_{i=1}^{\infty} q^{i+1} c_1) \]

Coefficients are matched:

- \( q^0 \) \[ \cos z = \cos z = 0 \]
- \( q^1 \) \[ c''_1 + c_1 - \cos(3z) + (\alpha_1 - 1) \cos z = 0 \]
- \( q^2 \) \[ c''_2 + C_2 + \alpha_1 c_1 - 2c_1 \cos 2z + \alpha_2 \cos z = 0 \]

The particular solution corresponding to \((\alpha_1 - 1) \cos z\) is \(\frac{1}{2}(1 - \alpha_1) \sin z\) which is not bounded, thus we require that \(\alpha_1 = 1\) such that

\[ c''_1 + c_1 = \cos 3z \]

\[ w'' + w = A \cos mz \rightarrow w = \frac{A \cos mz}{(m^2 - 1)} \]

\[ c_1 = -\frac{1}{8} \cos 3z \]

The arguments presented before imply that

\[ \alpha_2 = -\frac{1}{8} \Rightarrow c''_2 + c_2 = \frac{1}{8} \cos 3z - \frac{1}{8} \cos 5z \]

\[ \Rightarrow c_2 = -\frac{1}{64} \cos 3z + \frac{1}{192} \cos 5z \]

Following [4], we write

\[ \alpha_3 = -\frac{1}{64}, c_3 = -\frac{1}{152} \left( \frac{\cos 3z}{3} - \frac{4 \cos 5z}{9} + \frac{\cos 7z}{18} \right) \]

and so we find the \(c\) functions can be represented by “cosine-elliptic” function,

\[ cc_1(z, q) = \cos z - \frac{1}{8} q \cos 3z + \frac{1}{64} q^2 \left( -\cos 3z + \frac{\cos 5z}{3} \right) - \]

\[ \frac{q^3}{512} \left( \frac{\cos 3z}{3} - \frac{4 \cos 5z}{9} + \frac{\cos 7z}{18} \right) + O(q^4) \]

(5.3)

(5.4)

\[ a = 1 + q - \frac{q^2}{8} - \frac{q^3}{64} + O(q^4) \]

5.2. Fractional order. Now we suppose solutions of the form

\[ cc_\nu(z, q) = \cos \nu z + \sum_{r=1}^{\infty} q^r c_r(z) \]

(5.5)

\[ a = v^2 + \sum_{r=1}^{\infty} \alpha_r q^r \]

(5.6)
Quoting again our references [4, 3], the above procedure may be applied to find, \[ ce_\nu(z, q) = \cos \nu z - \frac{q}{4} \left( \frac{\cos(\nu + 2)z}{\nu + 1} - \frac{\cos(\nu - 2)z}{\nu - 1} \right) \]
\[ + \frac{q^2}{32} \left( \frac{\cos(\nu + 4)z}{(\nu + 1)(\nu + 2)} + \frac{\cos(\nu - 4)z}{(\nu - 1)(\nu - 2)} \right) + O(q^3) \]
(5.7)

(5.8) \[ a = v^2 + \frac{q^2}{2(\nu^2 - 1)} + \frac{(5\nu^2 + 7)q^4}{32(\nu^2 - 1)^3(\nu^3 - 4)} + \frac{(9\nu^4 + 58\nu^3 + 29)q^6}{64(\nu^2 - 1)^5(\nu^2 - 4)(\nu^2 - 9)} + \cdots \]
The latter can be rewritten,

(5.9) \[ v^2 = a - \frac{q^2}{2(\nu^2 - 1)} - \frac{(5\nu^2 + 7)q^4}{32(\nu^2 - 1)^3(\nu^3 - 4)} - \frac{(9\nu^4 + 58\nu^3 + 29)q^6}{64(\nu^2 - 1)^5(\nu^2 - 4)(\nu^2 - 9)} - \cdots \]

A first approximation is \( v^2 = a \). Putting this into the \( q^2 \) coefficient gives a second approximation,

\[ v^2 = a - \frac{q^2}{2(a - 1)} \]

And repeating the process gives

\[ v^2 = a - \frac{a - 1}{2(a - 1)^2 - q^2} - \frac{5a - 7}{32(a - 1)^3(a - 4)}q^4 + O(q^6) \]

Finally we note that \( v^2 = (m + \beta)^2 \) (the integral and fractional component), we have the approximation

(5.10) \[ \beta \approx \left( a - \frac{a - 1}{2(a - 1)^2 - q^2} - \frac{5a - 7}{32(a - 1)^3(a - 4)}q^4 \right)^{1/2} - m \]

The cosine functions have sine equivalents which we have not included for the sake of brevity. These formulations are not uncommon in the literature, though for obvious reasons the previous derivations were presented in fuller context as they seem to be the preferred method of dealing with the Mathieu equation. But alas, after presenting so many ways of looking at Mathieu’s equation, like Pandora’s box, last out is hope.

6. Mathieu & Maple, forever

Maple ‘help’ tells us about a number of Mathieu related functions in her tool box, including:

The Mathieu functions MathieuC(a, q, x) and MathieuS(a, q, x) are solutions of the Mathieu differential equation.

MathieuC and MathieuS are even and odd functions of x, respectively.

MathieuFloquet(a, q, x) is a Floquet solution of Mathieu’s equation.
where \( \nu = \text{MathieuExponent}(a, q) \) is the characteristic exponent and \( P(x) \) is a \( \pi \) periodic function.

We present a few plots to demonstrate the usefulness of these functions below. This report has treated, in some detail, the mathematics behind the ideal rf Paul trap. Of course, the actual realization of the trap differs in many important ways from its ideal, but we may approach these realizations, in their many forms, with a fundamental understanding of their operational basis.
Figure 6.1. On the left, the ion is trapped with secular and micromotion; on the right, unbound orbit, the ion is lost forever.

Figure 6.2. A bound orbit, different formal solution \( ce \), and a few of its components

Figure 6.3. The components of the \( ce \) function
Figure 6.4. Fascinating behavior of $\mu$ as $q$ is varied, a transition from bound to unbound behavior.

**References**


