

# Dynamics in Paul Traps

Les Houches, January 2012

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Confinement with only DC electric fields?

No,  $\vec{\nabla} \cdot \vec{E} = 0 \Rightarrow$  <sup>ion</sup> charge will follow field line + escape.  
(Earnshaw's theorem)

- Penning traps solve this problem by using DC  $\vec{B}$  also.
- Paul traps solve problem by using AC  $\vec{E}$  also.

Incomplete Lists:

## When to Use Penning Traps

- Large #s
- When you need large  $B$  anyway

~~(e.g. Stern-Gerlach, Hall effect, etc.)~~

~~(e.g. g-2 or mass ratio experiments)~~

(Caveat: See Bollinger, Itano, Wineland, etc.  
NIST experiments for  $B$ -insensitive  
precision measurements ~~at~~ at  
 $B \neq 0$ . Still, not as many  
digits as rf ion clocks.)

## When to Use Paul Traps

- For trap-independent  $B$ -tuning.  $B \neq 0$  or  $B = 0$  both OK.
- Best precision ~~is~~ when  $B \approx 0$   
(ion clocks better than 17 digits right now)

Reasons: a) No  $B$  instability  
b) No  $E$  instability  
(to leading order),  
b/c  $\vec{E}(t) = 0$  at center

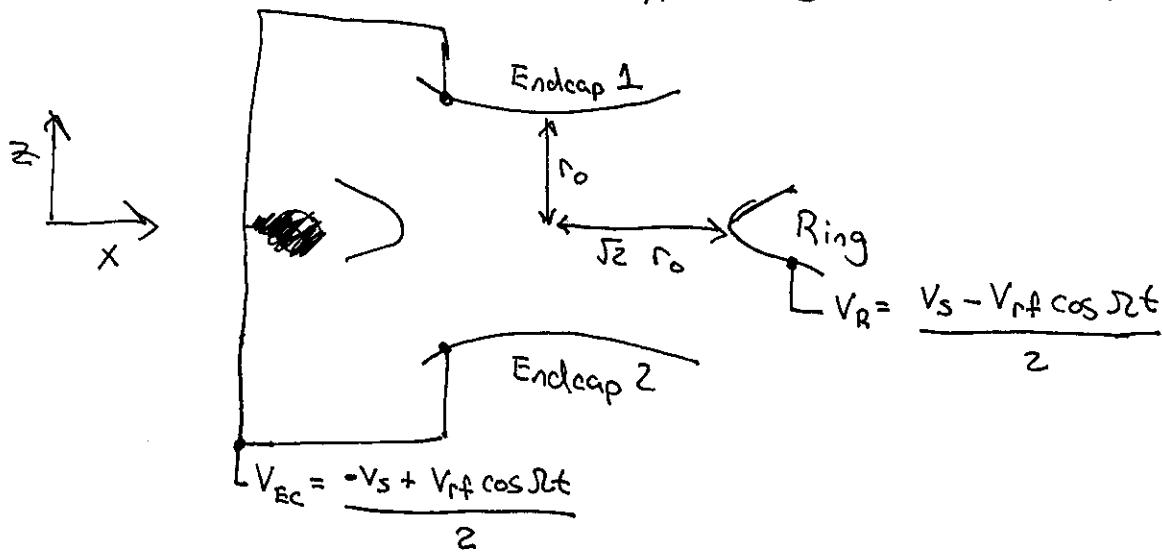
- For 1D string of ions, e.g. QIP  
(quantum information processing)

\* A good general reference: Ion Traps (book), by Pradip Ghosh

Two typical geometries:

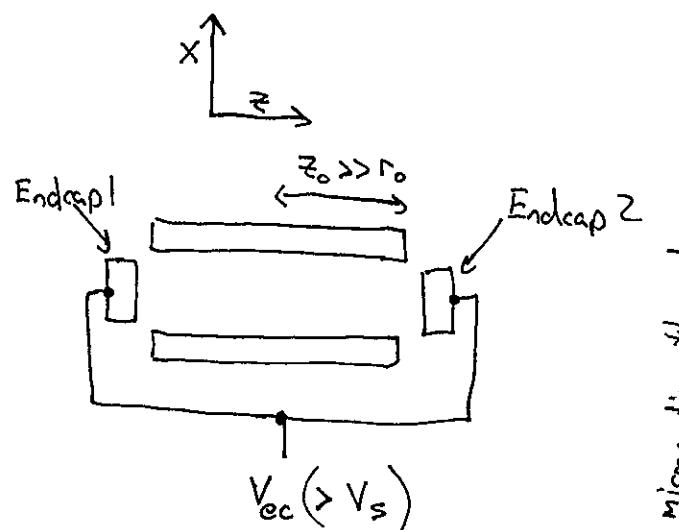
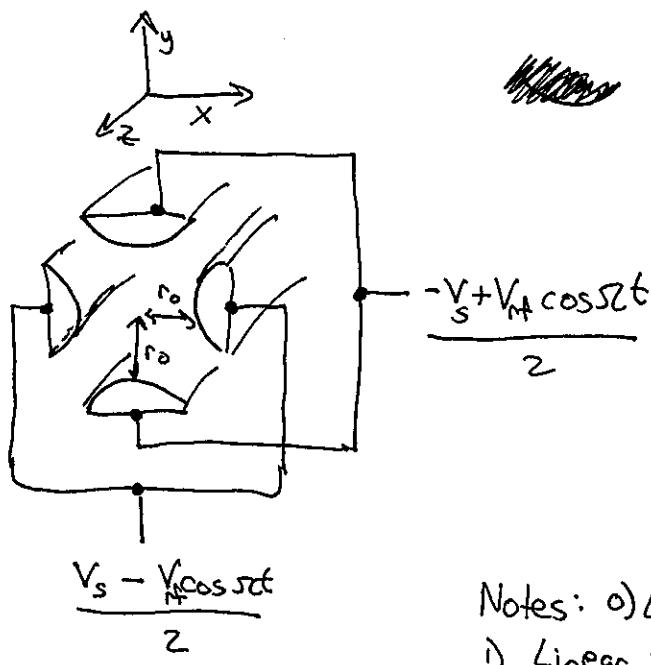
### Quadrupole Paul Trap

Electrodes are hyperboloids of revolution



Without rf, ~~ions~~ would want to move away from ring + hit endcap. RF changes the story.

### Linear Paul Trap (i.e. Linear RF Trap)



- Notes:
- 0) Linear traps are nice because of field-free axis.
  - 1) Linear trap has 6 electrodes, ~~quadrupole~~ has 3. They are not topologically equivalent.
  - 2) In practice, electrode shapes ~~are~~ often not hyperboloids.

$$\phi = \left(\frac{\phi_0}{2r_0^2}\right)(\lambda x^2 + \sigma y^2 + \gamma z^2) \quad \text{where } \phi_0(t) \text{ is an externally applied potential}$$

$$\nabla^2 \phi = 0$$

$$\Rightarrow \left(\frac{\phi_0}{2r_0^2}\right)(2\lambda + 2\sigma + 2\gamma) = 0$$

$$\Rightarrow \lambda + \sigma + \gamma = 0$$

For quadrupole trap,  
 $\lambda = \sigma = \frac{\gamma}{2}$

## How Does the Paul Trap Work?

Three answers, of improving predictive value: (We will consider quadrupole trap geometry)

A Confused ion model

B Adiabatic / small micromotion approximation.

C Mathieu equation solutions.

### A Confused ion model



Ion falls toward ring

Ion falls toward endcap

So, the ion gets "confused." It falls one way, then the other & cannot escape the trap.

Problems with the model:

~~WKB~~

- ① The model only predicts motion at the rf frequency  $\omega_r$ . That's wrong.
- ② The ~~model~~ has no force toward the center of the trap. This is wrong.
- ③ The model does not predict any instabilities where amplitude grows for certain  $\Omega_m$ . This is wrong.

So, the Confused Ion model is really pretty bad.

### B Adiabatic / Small Micromotion Approximation

We will see that this model has only partial predictive power, but it gets some important features right, and it is honest about its limitations.

How does the ion respond to a pure rf drive ( $V_s = 0$ )?

$$\vec{E}(t) = E_0 \cos \omega t \hat{\alpha}, \text{ where } \hat{\alpha} \text{ is some direction}$$

$$m \ddot{\vec{r}}_f = \vec{F}(t) \Rightarrow \ddot{\vec{r}}_f = \frac{QE_0 \cos \omega t}{m} \hat{\alpha} \quad \cancel{\vec{r}_f = \frac{QE_0}{m\omega^2} \sin \omega t}$$

"f" for fast - we'll see why later

$r_f \equiv r_f(t)$ , but we drop the "(t)", since it is understood

$$\Rightarrow \vec{r}_f = -\frac{QE_0}{m\omega^2} \cos \omega t + c_1 t + c_2 \quad \begin{matrix} \nearrow \text{we will take care} \\ \nearrow \text{of these terms later.} \end{matrix}$$

Let's postulate that

(5)

$$\vec{r}(t) = \vec{r}_s(t) + \vec{r}_f(t)$$

↓ slow      "      ↓  
$$-\frac{QE_0(z_s)}{m\omega^2} \cos \omega t$$

Note: we use the slow component position to get the fast v amplitude component

Two approximations:

①  $r_f(t) \ll r_s(t)$  (small "micromotion")

②  $r_s$  evolution is slow compared with  $T = \frac{2\pi}{\omega}$  (adiabatic approximation)

$\vec{E}$  is ~~the~~ local field experienced by the ion ( $\vec{E} \approx \vec{E}(t)$ , again dropping "(t)")

Consider an ion moving along the  $\hat{z}$  axis: ( $x=y=0$ )

$$\vec{E} = E_0 \cos \omega t \hat{z}$$

$$\vec{E} = \vec{E}(z_s) + \underbrace{\Delta z \frac{\partial}{\partial z} \vec{E}(z_s)}_{\text{where } \Delta z = z_f = -\frac{QE_0(z_s) \cos \omega t}{m\omega^2}} + \dots,$$

where  $\Delta z = z_f = -\frac{QE_0(z_s) \cos \omega t}{m\omega^2} - \frac{QE_0(z_s) \cos \omega t}{m\omega^2}$

$$= -\frac{Q \cos \omega t}{m\omega^2} E_0(z_s) \frac{\partial}{\partial z} E_0(z_s) \cos \omega t$$

$$= -\frac{Q \cos^2 \omega t}{2m\omega^2} \frac{\partial^2}{\partial z^2} E_0(z_s) \approx -\frac{Q}{4m\omega^2} \frac{\partial^2}{\partial z^2} E_0(z_s)$$

The small micromotion approximation allows us to drop higher order terms. The adiabatic approximation lets us time average over the fast motion, if we are only interested in dynamics of  $r_s$ .

$$\Rightarrow \vec{E} = E_0(z_s) \cos \omega t \hat{z} + -\frac{Q}{4m\omega^2} \frac{\partial^2}{\partial z^2} E_0(z_s)$$

But also

$$\vec{E} = \cancel{\frac{m \ddot{r}_f}{Q}} + \frac{m \ddot{r}_s}{Q}$$

Identifying the fast + slow terms with each other,  
for the slow one we have

$$\frac{m}{Q} \ddot{z}_s = -\frac{Q}{4\pi\epsilon_0^2} \frac{\partial}{\partial z} E_0^2(z_s)$$

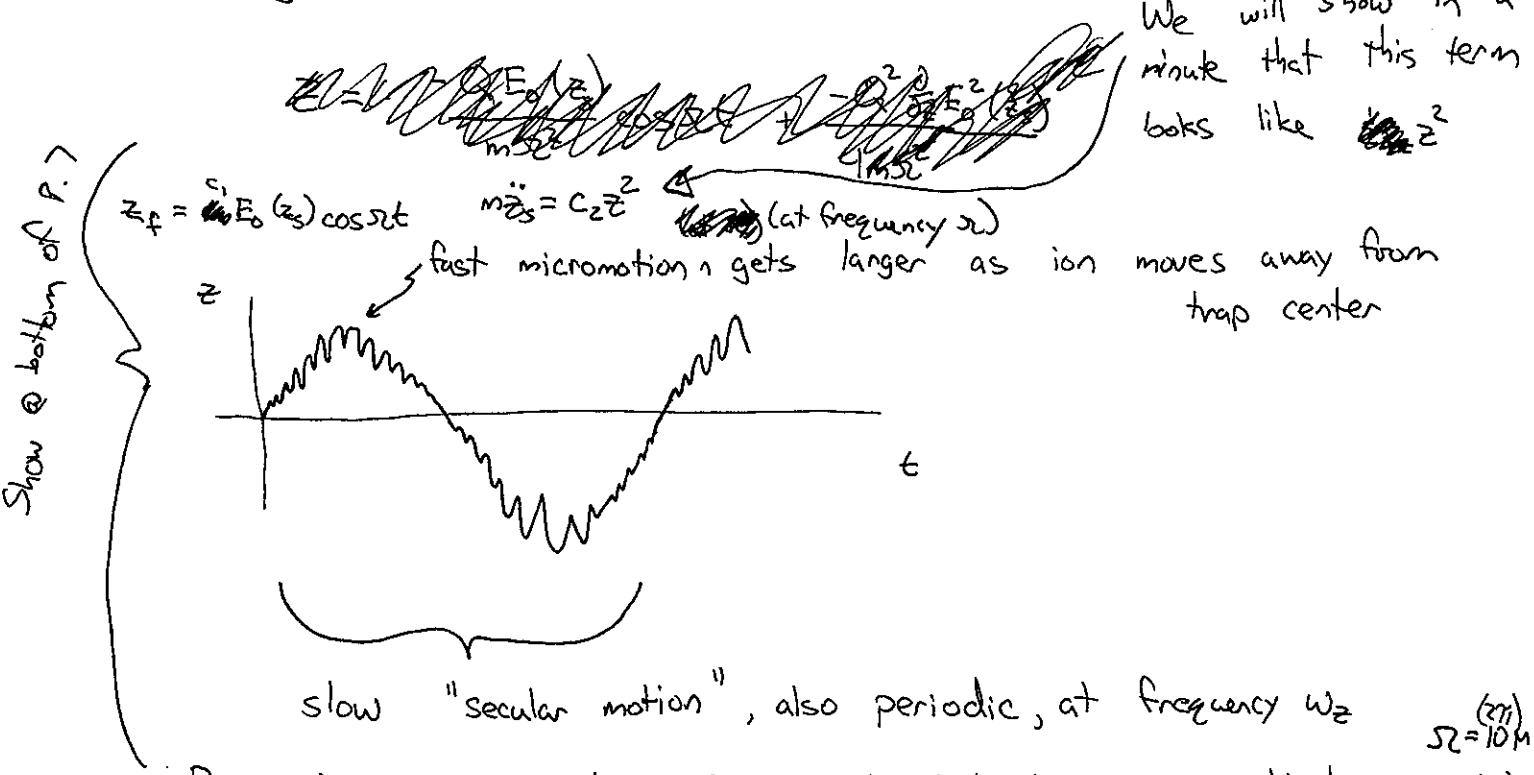
or  $m \ddot{z}_s = \cancel{-\frac{Q}{4\pi\epsilon_0^2}} \frac{\partial}{\partial z} V^*$

where the pseudopotential  $\cancel{V}$  is given by

$$V^* = \frac{Q^2 E_0^2}{4\pi\epsilon_0^2} . \text{ Same story for } \hat{x} \text{ & } \hat{y} \text{ directions.}$$

As far as the slow motion is concerned, the ion is convinced it is trapped in a pseudopotential. If  $E_0$  increases with  $r$ , then we have a trap. Remember:  $E_0$  is the amplitude of the rf oscillating field.

Putting both terms together again, we have



Parameters vary, but in small clock traps, you might have  $\omega_z = (2\pi) / 1 \text{ ms}$

That was only with the rf pseudopotential  
Now, we need to switch back on the  
static potential.  $V_{\text{eff}}$  describes the slow motion.

$$V_{\text{eff}}(\vec{r}) = \frac{Q^2 E_0^2(r)}{4m\omega^2} + Q\phi_s(r)$$

For quadrupole trap,

$$\phi(\vec{r}, t) = \cancel{\text{something}} \quad (V_{\text{rf}} + V_s \text{ are the voltages})$$

$$(V_{\text{rf}} \cos \omega t + V_s) \frac{x^2 + y^2 - 2z^2}{2r_0^2}$$

$$\Rightarrow \vec{E}_0 = -\vec{\nabla} V_{\text{rf}} \frac{x^2 + y^2 - 2z^2}{2r_0^2} = \left( \frac{-V_{\text{rf}}}{r_0^2} \right) (x\hat{x} + y\hat{y} - 2z\hat{z})$$

$$\Rightarrow E_0^2 = \left( \frac{V_{\text{rf}}^2}{r_0^4} \right) (x^2 + y^2 + 4z^2)$$

$$\Rightarrow V_{\text{eff}}(\vec{r}) = \left( \frac{Q^2 V_{\text{rf}}^2}{4m\omega^2 r_0^4} \right) (x^2 + y^2 + 4z^2) + \left( \frac{QV_s}{2r_0^2} \right) (x^2 + y^2 - 2z^2)$$

Using substitutions:

$$q_x = \frac{-2QV_{\text{rf}}}{m\omega^2 r_0^2} \quad q_z = \frac{4QV_{\text{rf}}}{m\omega^2 r_0^2}$$

$$\alpha_x = \frac{4QV_s}{m\omega^2 r_0^2} \quad \alpha_z = \frac{-8QV_s}{m\omega^2 r_0^2}$$

Harmonic oscillator:

$$V = \frac{1}{2}kx^2, \quad \omega = \sqrt{\frac{k}{m}}$$

~~Harmonic oscillator~~

$$\omega_x = \omega_y = \sqrt{\frac{\omega^2}{2} + \frac{q_x^2}{2}}$$

$$\omega_z = \sqrt{\frac{\omega^2}{2} + \frac{q_z^2}{2}}$$

\* Show plot here.

So, the adiabatic/small micromotion model is pretty good. It shows us that an ~~trap~~ electrode configuration with  $E_0^2$  increasing with  $r$  can act as a trap. And, it shows us how to calculate secular frequencies. But, it doesn't tell us about stability. (We assumed that  $r_f \ll r_s$ , but that is not always the case. For some parameter regimes, micromotion grows in time, rather than staying stable + small).

### C Mathieu Equation Solutions

Using those substitutions again, we have equations for the ion in the pseudopotential:

$$\frac{\partial^2 x}{\partial \gamma^2} + (\alpha_x - 2q_x \cos(2\gamma))x = 0, \text{ where } \gamma = \omega t / 2, \text{ a rescaled time}$$

That would be a harmonic oscillator equation, if it weren't for the  $\cos(2\gamma)$  term.

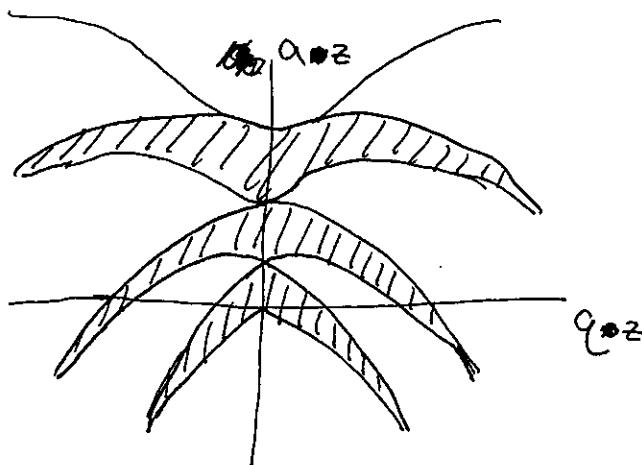
Also

$$\frac{\partial^2 y}{\partial \gamma^2} + (\alpha_y - 2q_y \cos(2\gamma))y = 0$$

$$\frac{\partial^2 z}{\partial \gamma^2} + (\alpha_z - 2q_z \cos(2\gamma))z = 0$$

The solutions to Mathieu's equations are well known! 9

In the  $a_{x,z}$  plane, there are regions of stability & instability.



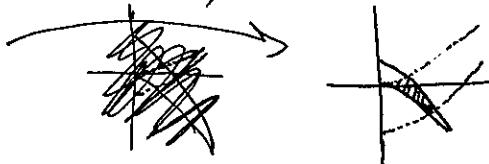
Hatched regions are stable, un-hatched regions are unstable.

Now, for the quadrupole trap

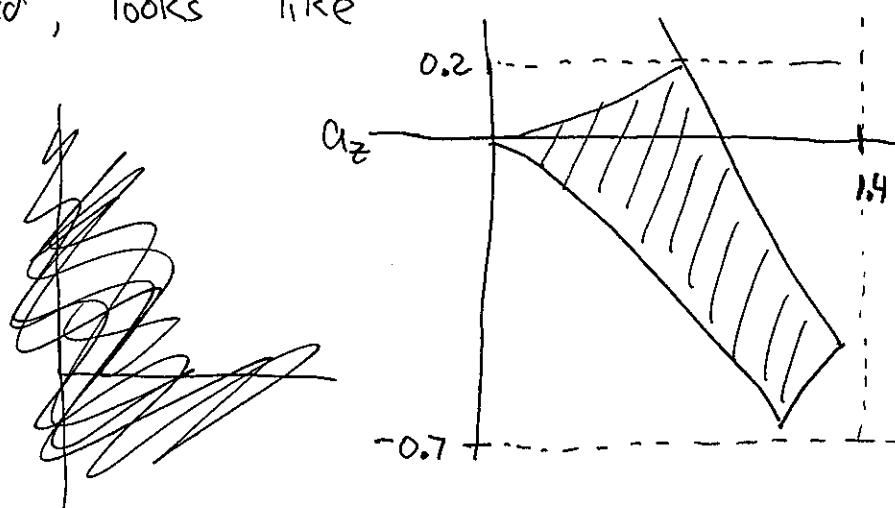
$$q_z = -2q_x$$

$$a_z = -2a_x$$

So, the ~~x~~-stability plot can be plotted on the  ~~$a_x, a_z$~~  plane. Both dimensions must be stable for overall stability! The  $x$ -stability regions will be flipped & ~~expanded~~.



The first stability region, in which traps are usually operated, looks like



So, finally we have the answer to our last question. We know when the trap is stable.

(Certain combinations of  $\frac{Q}{m}, \omega, V_{rf}, V_s$ , work,  
and others do not.)

- You can recover the adiabatic/small micromotion solution by expanding Mathieu solutions, but I won't do it here.
- We can use instabilities to tune  $V_s$  or  $V_{rf}$  & eject unwanted species.

### Beyond the Single Particle Equations.

- The 1-particle equations above are usually good for a lot.
- They describe particles in a pseudopotential with superimposed micromotion (which grows ~~weakly~~ as you move off center).
- However inter-ion Coulomb repulsion makes the ~~multiple~~ particle equations non-linear.

#### Consequences:

- a) Micromotion energy couples into secular motion. The rf drive heats ~~a~~ a cloud ~~or~~ or crystal of  $\approx 1$  ion.  
the secular motion
- b) Watch out for the resonances Martina mentioned yesterday.  $l\omega_x + m\omega_y + n\omega_z = N\omega$ . Trap is unstable for large ~~numbers~~ at these points.