8.311 Recitation Notes

Eric R. Anschuetz

MIT Center for Theoretical Physics,

77 Massachusetts Avenue,

Cambridge,

MA 02142,

USA[*]

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I. INTRODUCTION

Today I am going to talk about what is the most relevant application of quadrupoles in my field (quantum information): quadrupole ion traps!

II. EARNSHAW'S THEOREM

Consider the problem of trapping a charged particle with charge q at position $\boldsymbol{r}$ with static fields. For this to be true, the Laplacian of the potential energy landscape at $\boldsymbol{r}$ must be zero. However, we calculate that:

$$\begin{aligned}\nabla^2 U(\boldsymbol{r}) &= q\nabla^2\phi(\boldsymbol{r}) \\ &= -\frac{q\rho(\boldsymbol{r})}{\epsilon_0} \\ &= 0.\end{aligned} \tag{1}$$

Thus, U is not concave in some direction and therefore $\boldsymbol{r}$ is not a stable equilibrium point for the point charge.

Though this is true for each electric potential configuration ϕ, it is not true that a particle may be confined on average, by changing the fields rapidly.

[*] eans@mit.edu

III. THE QUADRUPOLE POTENTIAL

For a quadrupole moment $\boldsymbol{Q}(t)$, the general potential is of the form:

$$\phi(\boldsymbol{r}, t) = \frac{1}{8\pi\epsilon_0 r^3} \sum_{i,j} Q_{ij}(t)\, \hat{n}_i \hat{n}_j, \tag{2}$$

where $\boldsymbol{Q}(t)$ is the quadrupole moment

$$Q_{ij} = \int \mathrm{d}^3 r\, \rho(\boldsymbol{r}, t) \left(3 r_i r_j - r^2 \delta_{ij}\right). \tag{3}$$

If we assume our quadrupole configuration is azimuthally symmetric, we know the most general $\frac{1}{2r^2} \sum_{i,j} Q_{ij} \hat{n}_i \hat{n}_j$ is of the form:

$$\frac{1}{2r^2} \sum_{i,j} Q_{ij}(t)\, \hat{n}_i \hat{n}_j = \frac{q_0}{\rho_0^2} \left(\lambda(t)\, \rho^2 + \gamma(t)\, z^2\right) \tag{4}$$

for some q_0, $\lambda(t)$, and $\gamma(t)$. Defining $q_0 \lambda(t)$ to be such that at $(\rho = \rho_0, z = 0, t)$, the potential is $\phi_0(t)$, we have that:

$$\phi(\rho, z, t) = \frac{\phi_0(t)}{\rho_0^2} \left(\rho^2 + q_0 \gamma(t)\, z^2\right). \tag{5}$$

Finally, as $\nabla^2 \phi(\mathbf{0}, t) = 0$, we have that:

$$\begin{aligned} &4 + 2 q_0 \gamma(t) = 0 \\ \implies\ & q_0 \gamma(t) = -2. \end{aligned} \tag{6}$$

Therefore,

$$\phi(\rho, z, t) = \frac{\phi_0(t)}{\rho_0^2} \left(\rho^2 - 2 z^2\right). \tag{7}$$

For this configuration to be static, the electrodes must be as given in Fig. 1.

IV. CONFINEMENT

From Eq. (7), we have that the force on a particle of charge q and mass m at $\boldsymbol{r}$ is:

$$\begin{aligned} \boldsymbol{F}(\rho, z, t) &= -q \boldsymbol{\nabla} \phi(\rho, z, t) \\ &= \frac{2 q \phi_0(t)}{\rho_0^2} \left(2\boldsymbol{z} - \boldsymbol{\rho}\right). \end{aligned} \tag{8}$$

Using Newton's second law and taking:

$$\phi_0(t) = V \cos(\mathit{\Omega} t), \tag{9}$$

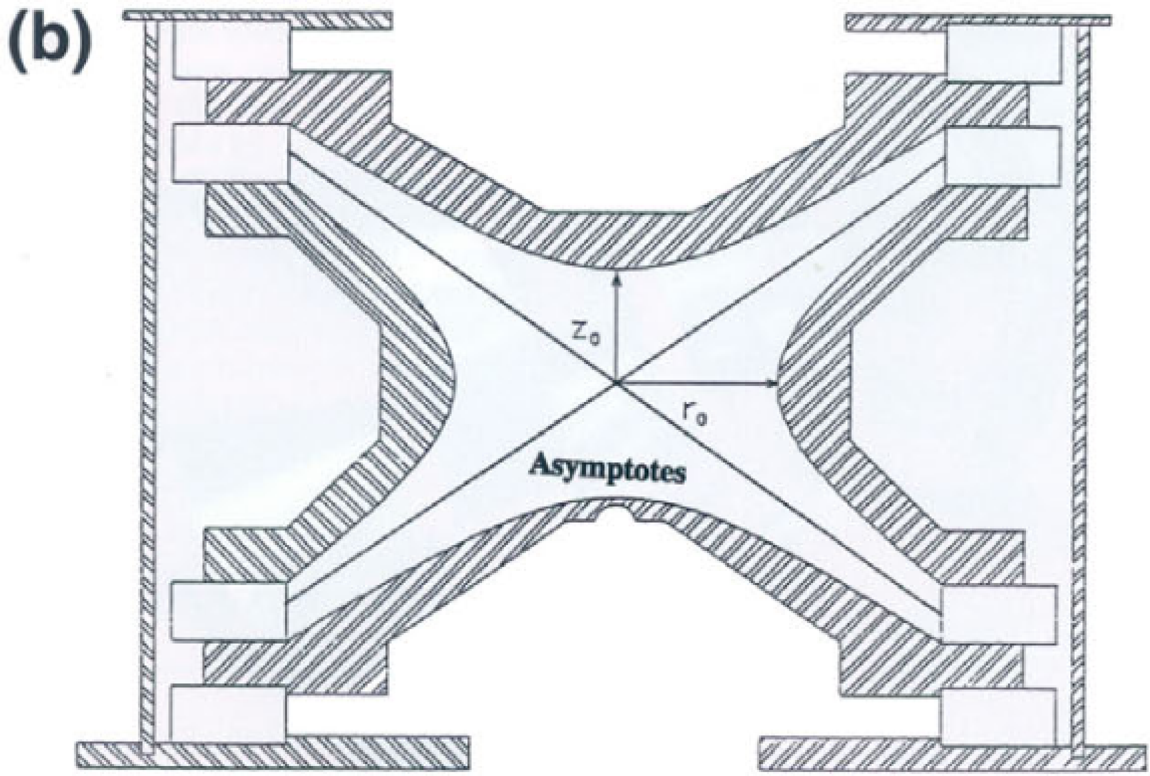

FIG. 1 A schematic of a quadrupole ion trap. Here, $z_0 = \frac{r_0}{\sqrt{2}}$. Figure from (March, 1997).

we therefore have that:

$$m\ddot{\boldsymbol{r}}(t) = \frac{2qV}{\rho_0^2}\cos(\varOmega t)\left(2\boldsymbol{z}(t) - \boldsymbol{\rho}(t)\right). \tag{10}$$

Solutions of differential equations of this form are called *Mathieu functions*; thus, the movement of the charged ion is governed by a Mathieu function. It turns out that these functions are bounded only for specific ranges of the parameters, and thus whether or not the ions are trapped are governed by the relative magnitudes of the parameters m, q, V, ρ_0, and $\varOmega$.

REFERENCES

March, R. E. (1997), J. Mass Spectrom. **32** (4), 351.