

Fig. 1. Schematic of electrostatic parallel plate analyzer (PPMA) showing parameter definitions and reference particle trajectory.

### 2.1 Parallel Plate Mirror Analyzer (PPMA)

The PPMA is the simplest electrostatic analyzer in existence. It utilizes a uniform electric field  $\mathbf{E}$  created by placing a potential difference  $V_d$  across a pair of plane parallel plate electrodes (i.e. the well known parallel plate capacitor) as shown in Fig. 1.

Placing an entrance and exit slit in of the plates, 1st-order focusing was first reported [6, 7] to take place for an entry angle of  $45^\circ$  (Fig. 2a). When the slits are placed outside the capacitor in the field free region, 2nd order focusing was found to be attained for an entry angle of  $30^\circ$  [5, 8–10] for a particular combination of object and image distances (Fig. 2b).

Because of the simplicity of its construction and use, as well as the fact that particle trajectories in the PPMA can be described analytically it has been widely utilized in the laboratory as well as in the class room for introducing basic analyzer CPO concepts.

With the advent of 1-D and 2-D position sensitive detectors, PPAs have also been used as spectrographs in both one- and two-stage setups utilizing either

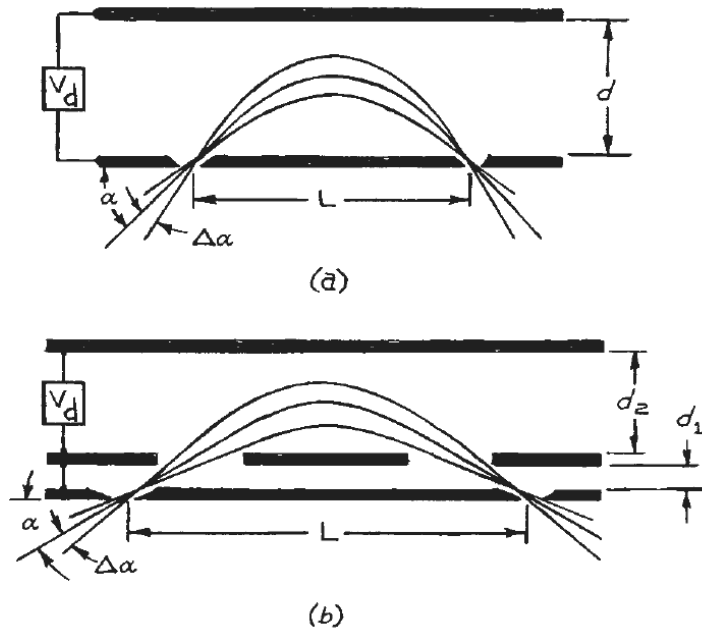


Fig. 2. Parallel plate analyzers: (a) 45° entry type, (b) 30° entry type (from Ref. [11]).

the 45° entry, but predominantly the 30° entry because of its advantageous 2nd order focusing capabilities. Never-the-less the PPMA is only a single focus device and other analyzers such as the cylindrical mirror and the spherical deflector analyzer which focus in both directions are usually preferred. We shall discuss all three analyzers in pedagogical order progressing from the simplest to the most complex and try to demonstrate the basic CPO features that make these devices attractive as analyzers and spectrographs.

Special attention will be paid to present the material in a way that can be readily implemented in a SIMION simulation. In particular, the coordinate systems in which these devices will be analyzed will be the usual SIMION coordinate system shown in Fig. .

### 2.1.1 Description of the ideal PPMA

The ideal PPMA is basically a parallel plate capacitor with a uniform and constant electric field  $\mathcal{E} = V_d/d$ , where  $V_d$  is the potential on the deflecting electrode plate, throughout the internal volume and perpendicular to the electrode plates which are separated by a distance  $d$  as shown in Fig. 1.

The electric field lies along the  $y$ -axis  $\mathbf{E} = (0, \mathcal{E}_d, 0)$  and acts in a way to deflect the particle, thus the quantity  $q\mathcal{E}_0 < 0$ . The electric field acts only in the region between the plates. Outside this region there is no electric field (and therefore No Lorentz force). In general, particles of charge  $q$ , velocity  $\vec{v}$  and energy  $E = \frac{1}{2}mv^2$  start from the source volume S at point 1 in a field free region, enter a slit or aperture in the lower plate at 2, follow a parabolic trajectory inside the PPMA and eventually exit the PPMA at 3 again into a field free region.

The trajectory equations are thus described by the Lorentz equation:

$$m\ddot{\mathbf{r}} = q\mathbf{E} \quad (4)$$

with the deflecting electrostatic field defined as:

$$\mathbf{E} = \begin{cases} 0 & y < 0, v_y > 0 \text{ (region I)} \\ (0, \mathcal{E}_d, 0) & y \geq 0, \text{ (region II)} \\ 0 & y < 0, v_y < 0 \text{ (region III)} \end{cases} \quad (5)$$

We thus have three regions of motion. In regions I and III there is no force, while in region III the force gives a constant negative acceleration (deceleration)  $a \equiv a_y = -(q/m)\mathcal{E}_d = -(q/m)V_d/d < 0$ . We note that the negative sign is appropriate since  $qV_d$  is always positive ( $V_d < 0$  for  $q < 0$  and  $V_d > 0$  for  $q > 0$ ). The trajectories in the three regions can thus be written out analytically:

In regions I and III (constant velocity  $\mathbf{v} = \mathbf{v}_i$ ):

$$x = x_i + v_{ix}t \quad v_x = v_{ix} \quad a_x = 0 \quad (6)$$

$$y = y_i + v_{iy}t \quad v_y = v_{iy} \quad a_y = 0 \quad (7)$$

$$z = z_i + v_{iz}t \quad v_z = v_{iz} \quad a_z = 0 \quad (8)$$

In region II (constant acceleration  $\mathbf{a} = (0, a, 0)$ ):

$$x = x_i + v_{ix}t \quad v_x = v_{ix} \quad a_x = 0 \quad (9)$$

$$y = y_i + v_{iy}t + \frac{1}{2}at^2 \quad v_y = v_{iy} + at \quad a_y = a \quad (10)$$

$$z = z_i + v_{iz}t \quad v_z = v_{iz} \quad a_z = 0 \quad (11)$$

We now generate the general solution of the trajectory as a function of time

for such a particle under the specific boundary conditions:

$$\mathbf{r}[t_1 = 0] = \mathbf{r}_i = (x_i, y_i, z_i) \quad (12)$$

$$\mathbf{v}[t_1 = 0] = \mathbf{v}_i = (v_{ix}, v_{iy}, v_{iz}) \quad (13)$$

$$y[t_2] = y[t_3] = 0 \quad (14)$$

where each particle leaves the source volume S at time  $t_1 = 0$ , position  $\mathbf{r}[t_1 = 0] = \mathbf{r}_i$  and velocity  $\mathbf{v}[t_1] = \mathbf{v}_i$ , enters the PPMA region II crossing the first PPMA plane at  $y = 0$  and time  $t_2$  is then deflected by the voltage  $V_d$  on the 2nd plate of the PPMA exiting region II at  $t_3$  with  $y = 0$ . Upon entering region III the particle continues its trajectory in a straight line. We can then use Eqs. 6-11 above to find  $\mathbf{r}(t)$  and  $\mathbf{v}(t)$  in each region as a function of the initial parameters:

In region I we have:

$$x_I(t) = x_i + v_{ix}t \quad v_{xI} = v_{ix} \quad a_{xI} = 0 \quad (15)$$

$$y_I(t) = y_i + v_{iy}t \quad v_{yI} = v_{iy} \quad a_{yI} = 0 \quad (16)$$

$$z_I(t) = z_i + v_{iz}t \quad v_{zI} = v_{iz} \quad a_{zI} = 0 \quad (17)$$

In region II with  $\mathbf{r}_{iII} = \mathbf{r}_I(t_2)$  and  $\mathbf{v}_{iII} = \mathbf{v}_I(t_2)$ :

$$x_{II}(t) = x_i + v_{ix}t \quad v_{xII} = v_{ix} \quad a_{xII} = 0 \quad (18)$$

$$y_{II}(t) = v_{iy}(t - t_2) + \frac{1}{2}a(t - t_2)^2 \quad v_{yII}(t) = v_{iy} + a(t - t_2) \quad a_{yII} = a \quad (19)$$

$$z_{II}(t) = z_i + v_{iz}t \quad v_{zII} = v_{iz} \quad a_{zII} = 0 \quad (20)$$

In region III with  $\mathbf{r}_{iIII} = \mathbf{r}_{II}(t_3)$  and  $\mathbf{v}_{iIII} = \mathbf{v}_{II}(t_3)$ :

$$x_{III}(t) = x_{II}(t_3) + v_{xII}(t_3)(t - t_3) \quad v_{xIII} = v_{ix} \quad a_{xIII} = 0 \quad (21)$$

$$= x_i + v_{ix}t_3 + v_{ix}(t - t_3) \quad (22)$$

$$= x_i + v_{ix}t \quad (23)$$

$$y_{III}(t) = -v_{iy}(t - t_3) \quad v_{yIII}(t) = -v_{iy} \quad a_{yIII} = 0 \quad (24)$$

$$z_{III}(t) = z_{II}(t_3) + v_{zII}(t_3)(t - t_3) \quad v_{zIII} = v_{iz} \quad a_{zIII} = 0 \quad (25)$$

$$= z_i + v_{iz}t_3 + v_{iz}(t - t_3) \quad (26)$$

$$= z_i + v_{iz}t \quad (27)$$

The times  $t_i$  ( $i = 1 - 3$ ) will be different for each particle with:

$$t_1 = 0 \quad \text{(initial condition)} \quad (28)$$

$$t_2 = -y_i/v_{iy} \quad \text{(from } y_I(t_2) = 0 \text{ in Eq. 16)} \quad (29)$$

$$t_3 = t_2 - 2v_{iy}/a = -y_i/v_{iy} - 2v_{iy}/a \quad \text{(from } y_{II}(t_3) = 0 \text{ in Eq. 19)} \quad (30)$$

$$t_{y_{max}} = t_2 - v_{iy}/a \quad \text{(from } v_{y_{II}}(t_{y_{max}}) = 0 \text{ in Eq. 19)} \quad (31)$$

$$= -y_i/v_{iy} - v_{iy}/a \quad (32)$$

$$y_{max} = y_{II}(t_{y_{max}}) \quad (33)$$

$$= v_{iy}(t_{y_{max}} - t_2) + \frac{1}{2}a(t_{y_{max}} - t_2)^2 \quad (34)$$

$$= -\frac{1}{2}v_{iy}^2/a \quad \text{y-range within PPMA} \quad (35)$$

$$x_{max} = x(t_3) - x(t_2) \quad (36)$$

$$= v_{ix}(t_3 - t_2) \quad (37)$$

$$= -2v_{iy}v_{ix}/a \quad \text{x-Range within PPMA} \quad (38)$$

The initial velocity vector  $\mathbf{v}_i$  can be expressed using SIMION's angular conventions and coordinate system (see Fig. 3) as  $\mathbf{v}_i = v_i(\cos \theta \cos \phi, \sin \theta, -\cos \theta \sin \phi)$  where  $\theta$  corresponds to the SIMION elevation angle ( $El$ ) and  $\phi$  to the SIMION azimuthal angle ( $Az$ ).

$$v_{ix} = v_i \cos \theta \cos \phi \quad (39)$$

$$v_{iy} = v_i \sin \theta \quad (40)$$

$$v_{iz} = -v_i \cos \theta \sin \phi \quad (41)$$

Introducing a reference trajectory that will be used as the principal ray and writing the initial kinetic energy in terms of an accelerating potential  $E_i = qV_i = qV_0(1 + \delta_i)$  and setting  $\theta = \theta_0 + \alpha$  and  $\phi = \phi_0 + \beta$  we have:

$$v_{ix} = \sqrt{2qV_0(1 + \delta_i)/m} \cos(\theta_0 + \alpha) \cos(\phi_0 + \beta) \quad (42)$$

$$v_{iy} = \sqrt{2qV_0(1 + \delta_i)/m} \sin(\theta_0 + \alpha) \quad (43)$$

$$v_{iz} = -\sqrt{2qV_0(1 + \delta_i)/m} \cos(\theta_0 + \alpha) \sin(\phi_0 + \beta) \quad (44)$$

where  $\delta$  is in general just the fractional kinetic energy difference from the

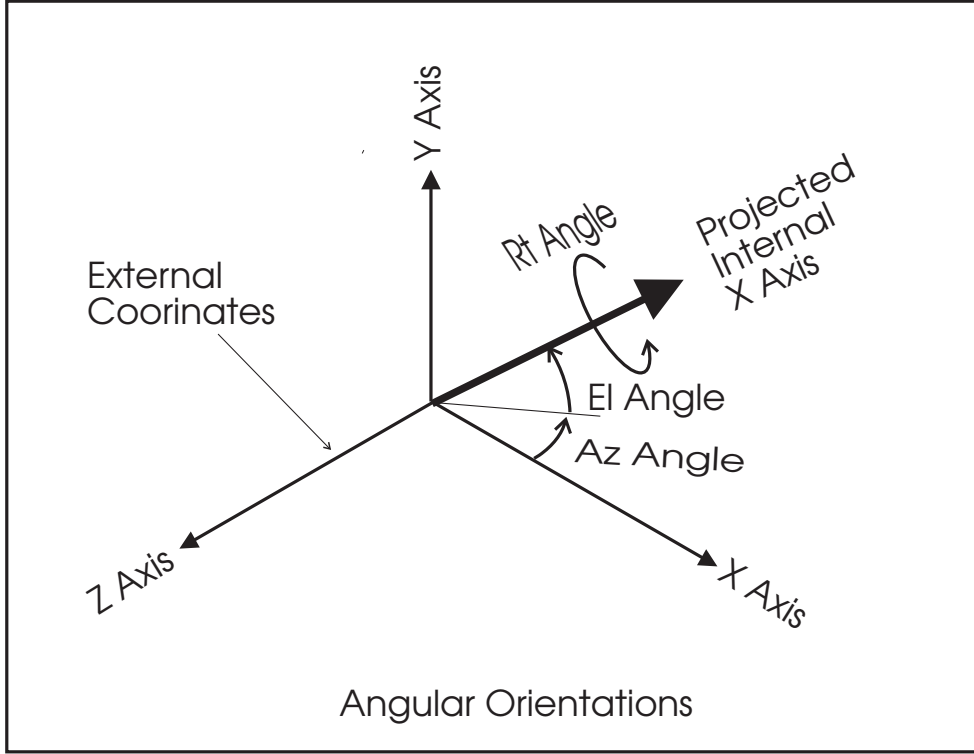


Fig. 3. SIMION's XYZ coordinate system showing angular conventions for elevation ( $El$ ) and azimuthal ( $Az$ ) angles.

reference trajectory ([12], p.34):

$$\delta \equiv \frac{\Delta E}{E_0} = \frac{E}{E_0} - 1 \quad (45)$$

and therefore

$$x_{max} = -2 \cdot 2 qV_0(1 + \delta_i) \cos(\theta_0 + \alpha) \sin(\theta_0 + \alpha) \cos(\phi_0 + \beta)/(a m) \quad (46)$$

$$= 2 d \frac{V_0}{V_d} (1 + \delta_i) \sin[2(\theta_0 + \alpha)] \cos(\phi_0 + \beta) \quad (47)$$

$$y_{max} = -qV_0(1 + \delta_i) \sin^2(\theta_0 + \alpha)/(a m) \quad (48)$$

$$= d \frac{V_0}{V_d} (1 + \delta_i) \sin^2(\theta_0 + \alpha) \quad (49)$$

which are seen to be independent of  $q$  and  $m$ .

The above notation has been motivated by the need for comparison to a reference trajectory (the principal trajectory) which now can be readily introduced such that its kinetic energy  $E_0 = \frac{1}{2}mv_0^2 = qV_0$  with  $\delta_i = 0$ ,  $\phi_0 = 0$ ,  $\mathbf{r}_{i0} = (0, h, 0)$  ( $h < 0$ ) and  $\mathbf{v}_{i0} = (v_{0x}, v_{0y}, 0)$ .

We then have for the reference trajectory:

Reference region I ( $0 \leq t \leq t_2$ ):

$$x_I(t) = v_{0x} t \quad v_{xI} = v_{0x} \quad a_{xI} = 0 \quad (50)$$

$$y_I(t) = h + v_{0y} t \quad v_{yI} = v_{0y} \quad a_{yI} = 0 \quad (51)$$

$$z_I(t) = v_{0z} t \quad v_{zI} = 0 \quad a_{zI} = 0 \quad (52)$$

Reference region II ( $t_2 \leq t \leq t_3$ ):

$$x_{II}(t) = v_{0x} t \quad v_{xII} = v_{0x} \quad a_{xII} = 0 \quad (53)$$

$$y_{II}(t) = v_{0y}(t - t_2) + \frac{1}{2}a(t - t_2)^2 \quad v_{yII}(t) = v_{0y} + a(t - t_2) \quad a_{yII} = a \quad (54)$$

$$z_{II}(t) = 0 \quad v_{zII} = 0 \quad a_{zII} = 0 \quad (55)$$

Reference region III ( $t_3 \leq t$ ):

$$x_{III}(t) = v_{0x} t \quad v_{xIII} = v_{0x} \quad a_{xIII} = 0 \quad (56)$$

$$y_{III}(t) = -v_{0y}(t - t_3) \quad v_{yIII}(t) = -v_{0y} \quad a_{yIII} = 0 \quad (57)$$

$$z_{III}(t) = 0 \quad v_{zIII} = 0 \quad a_{zIII} = 0 \quad (58)$$

For the reference trajectory  $\alpha = \beta = 0$  and we thus have:

$$v_{0x} = \sqrt{2qV_0/m} \cos \theta_0 \quad (59)$$

$$v_{0y} = \sqrt{2qV_0/m} \sin \theta_0 \quad (60)$$

$$v_{0z} = 0 \quad (61)$$

with

$$t_1 = 0 \quad (62)$$

$$t_2 = -h/v_{0y} \quad (63)$$

$$t_3 = -h/v_{0y} - 2v_{0y}/a \quad (64)$$

$$t_{max} = -h/v_{0y} - v_{0y}/a \quad (65)$$

$$y_{max} = -\frac{1}{2}v_{0y}^2/a = \frac{V_0}{V_d} \sin^2 \theta_0 d \quad (66)$$

$$x_{max} = x_{max0} = -2v_{0y} v_{0x}/a = 2 \frac{V_0}{V_d} d \sin 2\theta_0 \quad (67)$$

For a particle in region III with  $y_f$  starting at  $y_i$  we have for the total projection along the x-axis:

$$x_{III}(t_f) = x_i + v_{ix}t_f \quad (68)$$

$$y_{III}(t_f) = y_f = -v_{iy}(t_f - t_3) \quad (69)$$

$$z_{III}(t_f) = z_i + v_{iz}t_f \quad (70)$$

solving for  $t_f$  from Eq. 69 we get:

$$t_f = t_3 - \frac{y_f}{v_{iy}} = - \left[ \frac{(y_i + y_f)}{v_{iy}} + 2 \frac{v_{iy}}{a} \right] \quad (71)$$

which is indeed positive since both  $y_i$ ,  $y_f$  and  $a$  are negative.

Replacing in  $x_{III}(t_f) = x_f$  and  $z_{III}(t_f) = z_f$  and using  $a = \frac{q}{m} \mathcal{E} = -\frac{q}{m} \frac{V_d}{d}$  we obtain the exit position  $(x_f, z_f)$  and time  $t_f$  as a function of the position  $y_f$  and the voltage  $V_d$  and plate separation  $d$  of the parallel plate capacitor.

Thus, a particle of charge  $q$ , mass  $m$  which at  $t = 0$  is in the field free region at the (initial) position  $(x, y, z)_i$  with (initial) velocity  $(v_x, v_y, v_z)_i$  and kinetic energy  $E_i = q V_q = 1/2 m v_i^2$  after flying through the uniform electric field  $\mathbf{E} = (0, \mathcal{E}, 0)$  of a parallel plate capacitor with  $\mathcal{E} = -V_d/d$  will be deflected and find it self after leaving the PPMA at time  $t_f$  at the (final) position  $(x, y, z)_f$  given by:



PPMA exit positions and time in the field free region:

$$x_f(V_q, \theta, \phi) = x_i + (L_\theta - Y \cot \theta) \cos \phi \quad (72)$$

$$z_f(V_q, \theta, \phi) = z_i - (L_\theta - Y \cot \theta) \sin \phi \quad (73)$$

$$t_f(V_q, \theta) = - \sqrt{\frac{m}{2qV_q}} \left( Y \csc \theta - \frac{L_\theta}{\cos \theta} \right) \quad (74)$$

with the shorthand definitions:

$$L_\theta \equiv L_\theta(V_q) = 2d \left( \frac{V_q}{V_d} \right) \sin 2\theta \quad (75)$$

$$Y \equiv y_i + y_f \quad (76)$$

where  $m$  is the rest mass of the particle in  $eV/c^2$  (for electrons  $m = 510,998.910(13) eV/c^2$  or  $5.4857990943(23) \times 10^{-4}$  amu in SIMION) with  $c = 29.9792458$  cm/ns [13].

It is seen that  $L_\theta(V_q)$  is just the range of the trajectory  $x_{max}$  within the PPMA along the x-axis for a particle of energy  $E = qV_q$  as shown in Eq. 67.

Using excel spread sheet PPMA1.xls you can compute  $x_f, z_f$  and  $t_f$  as a function of all other parameters. Using SIMION PPMA1.iob you can simulate a PPMA and see the trajectories flown.

### 2.1.2 Energy dispersion

Using Eqs. 72-73 we may directly compute the dispersion  $D$  in each direction. From the dispersion definition Eq. 2 and noting that  $\delta E = q\delta V_q$  we then have:

$$D_x = E \frac{\partial x_f}{\partial E} = V_q \frac{\partial x_f}{\partial V_q} = L_\theta(V_q) \cos \phi \quad (77)$$

$$D_z = E \frac{\partial z_f}{\partial E} = V_q \frac{\partial z_f}{\partial V_q} = -L_\theta(V_q) \sin \phi \quad (78)$$

For  $\phi = 0$  we have maximal dispersion in the x-direction and 0 in the z-direction. Furthermore,  $D_x$  is seen to be independent of initial and final position and proportional to the particle energy  $V_q$  or  $E/q$ . It thus is inversely proportional to the charge  $q$ , but independent of the mass  $m$ .

### 2.1.3 Angular aberrations, Focusing and Trace Width

The focusing properties of the PPMA in both space and time are also readily obtained from Eqs. 72-74. We investigate focusing along the maximal dispersion direction  $\phi = 0$ .

The conditions for minimizing the trace widths (Eq. 3)  $\Delta x_f$ ,  $\Delta z_f$  and  $\Delta t_f$  given by:

$$\Delta x_{f\theta_0} = x_f(V_q, \theta = \theta_0 + \alpha, \phi = \beta) - x_f(V_q, \theta = \theta_0, \phi = 0) \quad (79)$$

$$\Delta z_{f\theta_0} = z_f(V_q, \theta = \theta_0 + \alpha, \phi = \beta) - z_f(V_q, \theta = \theta_0, \phi = 0) \quad (80)$$

$$\Delta t_{f\theta_0} = t_f(V_q, \theta = \theta_0 + \alpha, \phi = \beta) - t_f(V_q, \theta = \theta_0, \phi = 0) \quad (81)$$

establish the focusing conditions. Since  $x_f$ ,  $z_f$  and  $t_f$  are known analytically the trace widths can be computed exactly to all orders in  $\alpha$  and  $\beta$ . However, further insight is gained by expanding  $\Delta x_f$ ,  $\Delta z_f$  and  $\Delta t_f$  around  $\theta = \theta_0$ ,  $\phi = \phi_0 = 0$  up to 3rd order in  $\alpha$  and 2nd order in  $\beta$ . Then the general form of  $\Delta x_f$  will be:

$$\Delta x_f = \sum_{n=1}^{n_{max}} \sum_{m=1}^{m_{max}} A_n B_m \alpha^n \beta^m \quad (82)$$

where typically  $n_{max} = m_{max} = k + 1$  so as to include k-th order focusing. Furthermore, terms with  $n+m = k_{max} + 1$  where  $k_{max}$  is the maximum focusing order. For the 45° PPMA we have only 1st order focusing ( $k_{max} = 1$ ), while for the 30° PPMA we have 2nd order focusing ( $k_{max} = 2$ ). The expansion Eq. 82 is quite general applying to all analyzers and therefore coefficients  $A_n$  and  $B_m$  can be used to classify their aberrations and focusing properties and compare them in a universal way [14].

After some algebra (most readily obtained using the series expansion capabil-

ities of Mathematica) we obtain:

$$\Delta x_{f\theta_0} \approx -\frac{1}{6} (\beta^2 - 2) \csc \theta_0 (Y(\cos 2\theta_0 + 2) \csc^3 \theta_0 - 2L_{\theta_0} \cos 2\theta_0 \sec \theta_0) \alpha^3 \quad (83)$$

$$+ \frac{1}{2} (\beta^2 - 2) (Y \cot \theta_0 \csc^2 \theta_0 + 2L_{\theta_0}) \alpha^2 \quad (84)$$

$$- \frac{1}{2} (\beta^2 - 2) (Y \cot^2 \theta_0 + Y + 2L_{\theta_0} \cot 2\theta_0) \alpha \quad (85)$$

$$- \frac{1}{2} \beta^2 (L_{\theta_0} - Y \cot \theta_0) \quad (86)$$

$$\Delta z_{f\theta_0} \approx \frac{1}{3} \beta (4L_{\theta_0} \cot 2\theta_0 - Y(\cos 2\theta_0 + 2) \csc^4 \theta_0) \alpha^3 \quad (87)$$

$$+ \beta (Y \cot \theta_0 \csc^2 \theta_0 + 2L_{\theta_0}) \alpha^2 \quad (88)$$

$$- \beta (Y \cot^2 \theta_0 + Y + 2L_{\theta_0} \cot 2\theta_0) \alpha \quad (89)$$

$$+ \beta (Y \cot \theta_0 - L_{\theta_0}) \quad (90)$$

$$\Delta t_{f\theta_0} \approx - \frac{(-6Y \cot^3 \theta_0 - 5Y \cot \theta_0 + L_{\theta_0}) \csc \theta_0}{6\sqrt{2}\sqrt{\frac{E}{m}}} \alpha^3 \quad (91)$$

$$- \frac{(Y(2 \cot^2 \theta_0 + 1) \csc \theta_0 + L_{\theta_0} \sec \theta_0)}{2\sqrt{2}\sqrt{\frac{E}{m}}} \alpha^2 \quad (92)$$

$$+ \frac{(L_{\theta_0} + Y \cot \theta_0) \csc \theta_0}{\sqrt{2}\sqrt{\frac{E}{m}}} \alpha \quad (93)$$

There are two known solutions: i)  $\theta_0 = 45^\circ$  with  $Y = 0$ , ii)  $\theta_0 = 30^\circ$  with  $Y = -L_{\theta_0}/(2\sqrt{3})$ .

For  $\theta_0 = 45^\circ$  with  $Y = 0$  we obtain:

$$\Delta x_{f45^\circ} = -L_{45^\circ} (2\alpha^2 + \frac{1}{2}\beta^2) \quad (\text{1rst order in } \beta \text{ and } \alpha) \quad (94)$$

$$\Delta z_{f45^\circ} = -L_{45^\circ} (1 - 2\alpha^2)\beta \quad (\text{no focusing in } \beta) \quad (95)$$

$$\Delta t_{f45^\circ} = - \frac{L_{45^\circ} \sqrt{m} \alpha (\alpha^2 + 3\alpha - 6)}{6\sqrt{E}} \quad (\text{no focusing in } \alpha) \quad (96)$$

$$L_{45^\circ} = 2d \left( \frac{V_q}{V_d} \right) \quad (97)$$

For  $\theta_0 = 30^\circ$  with  $Y = -L_{30^\circ}/(2\sqrt{3})$  we obtain:

$$\Delta x_{f30^\circ} = -L_{30^\circ} \left( \frac{8}{\sqrt{3}}\alpha^3 + \frac{1}{4}(3 - 2\sqrt{3}\alpha)\beta^2 \right) \quad (\text{1rst order in } \beta \text{ and 2nd in } \alpha) \quad (98)$$

$$\Delta z_{f30^\circ} = -\frac{L_{30^\circ}}{6}(9 - 16\sqrt{3}\alpha^3)\beta \quad (\text{no focusing in } \beta) \quad (99)$$

$$\Delta t_{f30^\circ} = -\frac{L_{30^\circ}\sqrt{m}\alpha(25\alpha^2 - 5\sqrt{3}\alpha - 6)}{6\sqrt{2}\sqrt{E}} \quad (\text{no focusing in } \alpha) \quad (100)$$

$$L_{30^\circ} = \sqrt{3}d \left( \frac{V_q}{V_d} \right) \quad (101)$$

where we have used in  $L_{30^\circ}$  the fact that  $\sin(2 \cdot 30^\circ) = \sin(60^\circ) = \sqrt{3}/2$ . Thus, the PPMA is astigmatic with focusing occurring only in the x-direction and under very specific entry conditions.

### Focal plane

The focal plane (or line) is the loci of points of 1rst order focusing. The PPMA was seen to have 1rst order focusing in  $x_f$ . This is the condition obtained by setting  $\partial x_f/\partial \alpha = 0$ . From the series expansions Eq. 86 this means:

$$\frac{\partial x_f}{\partial \alpha} = (Y \cot^2 \theta_0 + Y + 2L_{\theta_0} \cot 2\theta_0) = 0 \quad (102)$$

from which we obtain the relation between  $L_{\theta_0}$  and  $Y$  for 1rst order focusing:

$$L_{\theta_0} = -\frac{1 + \cot^2 \theta_0}{2 \cot 2\theta_0} Y \quad (103)$$

which upon substituting for  $L$  in Eq. 72 gives the focal line or locus of 1rst order focusing positions  $(x_{f1}, y_{f1})$ :

$$x_{f1} = x_i - (y_i + y_{f1}) \left( \frac{(1 + \cot^2 \theta_0)}{2 \cot 2\theta_0} + \cot \theta_0 \right) \quad (104)$$

Computing the slope of the line  $dy_{f1}/dx_{f1}$  we get [8]:

$$\tan \chi = -\frac{\tan \theta_0 \cos 2\theta_0}{(1 + \cos 2\theta_0)} \quad (105)$$

For  $\theta_0 = 45^\circ$ , we find  $\chi = 0^\circ$ , while for  $\theta_0 = 30^\circ$ ,  $\chi = -\arctan(1/3\sqrt{3}) = -10.8934^\circ$ . Clearly, the surface of a position sensitive detector should lie along this line and of course any exit slit should also be on this line [12]. It is noted that the focal line might not only be inclined to the optic axis, but even curved as in the presence of 3rd or higher order chromatic aberrations [12].

### 2.1.4 Energy Resolution

According to the definition of energy resolution (Eq. 1) this can be obtained from:

$$w_1 = \Delta x_{f\theta_0}(\Delta V_q, \alpha, \beta) = x_f(V_q + \Delta V_q, \theta = \theta_0 + \alpha, \phi = \beta) - x_f(V_q, \theta_0, \phi = 0) \quad (106)$$

by solving for  $\Delta V_q$  and then forming the base resolution  $R_b = \Delta V_q/V_q = \Delta E_b/E$ . Here  $w_1$  is the entry slit width.

Following the above prescription we solve Eq. 106 for the  $\theta_0 = 45^\circ$  PPMA to obtain:

$$R_{b45^\circ} = \frac{\Delta E_b}{E} = \frac{w_1}{L_{45^\circ}} + \left(2\alpha^2 + \frac{1}{2}\beta^2\right) \quad (107)$$

Doing the same for the  $\theta_0 = 30^\circ$  PPMA to obtain:

$$R_{b30^\circ} = \frac{\Delta E_b}{E} = \frac{w_1}{L_{30^\circ}} + \left(\frac{8}{\sqrt{3}}\alpha^3 + \frac{1}{4}(3 - 2\sqrt{3}\alpha)\beta^2\right) \quad (108)$$

We note that  $L_{\theta_0}$  is the dispersion length  $D_x$  along the x-direction for  $\phi = 0$  and the part in parentheses is just the absolute value of the trace width divided by  $L_{\theta_0}$ . Adding a possible exit slit  $w_2$ , the base resolution can be written more generally as:

$$R_b = \frac{\Delta E_b}{E} = \frac{w_1 + w_2 + |\Delta x_f|}{D_x} = \frac{w_1 + w_2}{D_x} + \left| \sum_{n=1}^{n_{max}} \sum_{m=1}^{m_{max}} A_n B_m \alpha^n \beta^m \right| \quad (109)$$

where contributions are clearly separated into slit terms and angular aberration terms.

In Fig. we compare  $R_b$  for both exact and approximate values of  $\Delta x_{f\theta_0}$ .

### 2.1.5 Magnification

#### 2.1.6 PPMA deflection voltage $V_d$

The PPMA deflection voltage  $V_d$  is specified according to the active length of the PPMA along the x-direction and the energy of the analyzed particles as given by Eq. 67.

For slit spectrometers the slit separation  $x_0$  is set equal to the range  $x_{max}$  for the reference trajectory with energy  $E_0 = qV_{q0}$ , thus  $L_{\theta_0}(V_{q0}) = x_0$  with  $\phi_0 = 0^\circ$ . Thus, from Eq. 67 we have:

$$V_d = V_{q0} \left(\frac{2d}{x_0}\right) \sin 2\theta_0 \quad (110)$$

The deflector plate separation  $d$  must be sufficient to allow for the maximal height of the trajectory. According to Eq. 49 this will depend both on the choice of  $\theta_0$  and  $\alpha$  since:

$$d \geq y_{max} = \left(\frac{x_0}{2}\right) \frac{\sin^2(\theta_0 + \alpha_{max})}{\sin 2\theta_0} \quad (111)$$

Typically, we set  $d = 0.3 x_0$  which allows for an  $\alpha_{max}$ :

$$\alpha_{max} = \arcsin(\sqrt{0.3 \cdot 2 \cdot \sin 2\theta_0}) - \theta_0 \quad (112)$$

Thus, Eq. 112 for  $\theta_0 = 45^\circ$  gives  $\alpha_{max} = 5.7685^\circ$ , while for  $\theta_0 = 30^\circ$ ,  $\alpha_{max} = 16.12^\circ$  which is too large to be practical. Typically,  $\alpha_{max}$  is actually set by the entry geometry which usually is determined by the width of the entry slit  $w$  and the source distance  $y_i$  and other angle limiting apertures.

The above condition of  $d = 0.3 x_0$  is typical for many  $45^\circ$  PPMA's [15]. Setting this value in Eq. 110 we finally get:

$$V_d = 0.600000 V_{q0} \quad (45^\circ \text{ PPMA}) \quad (113)$$

$$V_d = 0.3 \cdot \sqrt{3} V_{q0} = 0.519615 V_{q0} \quad (30^\circ \text{ PPMA}) \quad (114)$$

Thus, for a maximum electron energy of  $E = 10$  keV we shall need a high voltage power supply of  $V_{max} = V_d = -0.6 \cdot 10 = -6$  kV for  $45^\circ$  entry and  $V_{max} = -5.2$  kV for  $30^\circ$  entry, respectively.

### 2.1.7 *Transmission*

### 2.1.8 *Time dispersion*

### 2.1.9 *Final design parameters for the PPMA*

### 2.1.10 *Typical experimental PPMA setups*

## 2.2 *Parallel Plate Deflector (PPD)*

## 2.3 *Cylindrical Mirror Analyzer (CMA)*

## 2.4 *Cylindrical Deflector Analyzer (CDA)*

[1] (fig. 4) for 127.2 degrees focusing