Theoretical investigation of the energy resolution of an ideal hemispherical deflector analyzer and its dependence on the distance from the focal plane

T.J.M. Zouros,∗

Department of Physics, University of Crete, P.O. Box 2208, 71003 Heraklion, Crete, Greece
Institute of Electronic Structure and Laser, P.O. Box 1527, 71110 Heraklion, Crete, Greece

Abstract

In most modern hemispherical deflector analyzers (HDAs) using a position sensitive detector (PSD), due to practical geometrical constraints (fringing field correctors, grids etc.), the PSD cannot always be placed at the optimal position, i.e. the first-order focal plane following 180° deflection at h = 0. Here, the dependence of the exit radial base width Δr∗, base energy resolution R∗, and line shape L∗ on the distance h between the focal plane and the detection plane for an ideal HDA (no fringing fields) is investigated theoretically as a function of the maximum injection angle α∗ and the diameter of the entry aperture Δr0. Both exact numerical results and practical analytic formulas based on Taylor series expansions developed for any HDA show R∗ and L∗ become increasingly degraded with increasing h from their optimal values at h = 0. A detailed comparison of the resolution properties of conventional and biased paracentric HDAs is also presented. Apart from a few marginal improvements of limited utility, overall, the ideal paracentric HDA does not seem to have any distinct practical advantages over the conventional HDA. Resolution improvements recently reported for non-ideal paracentric HDAs must therefore be due to their strong fringing fields and needs to be further investigated. Our ideal HDA results provide a unique standard to evaluate the resolution performance of any HDA under realistic non-zero h-value conditions.

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1. Introduction

High resolution electron spectroscopy (as for example electron spectroscopy for chemical analysis (ESCA) [1–3] or Auger electron spectroscopy (AES) [4]) is a mature technique utilized in many different fields of physics, material science, chemistry and even biology and medicine. One of the most popular spectrometers in use today is the hemispherical deflector analyzer (HDA) also available commercially from many different high tech companies. Today’s, modern high power HDAs are equipped with state-of-the art multi-element zoom lens and position sensitive detector (PSD) [5–9] and therefore enjoy a very large collection efficiency.

In the past, when high resolution HDAs had a much lower throughput (no PSD) emphasis was primarily given to the optimization of the resolution [10] for highest étendue (the product of entrance area and solid angle) [11,12] or highest transmitted current [13,14]. The line shape was also investigated theoretically [12,15–19] using both analytic piecewise integration [12,18–20] and Monte Carlo techniques [15,21,16,22]. However, today, with the existing high throughput of modern ESCA spectrometers, high resolution has become of utmost importance. For an ideal HDA, the resolution is primarily determined by the maximum injection angle α∗ and the diameter of the entry aperture or slit (real or virtual) Δr0. First-order focusing is known to take place after deflection through 180° within the HDA and therefore the PSD should in principle be placed at this focal plane. However, in practice, due to geometrical constraints imposed primarily by field corrector schemes (grids, fringing field corrector rings, Jost apertures, see Ref. [23] for a recent...
update) the PSD must be placed at a small distance $h \sim 5–20\,\text{mm}$ from the ideal HDA focal plane at $h = 0$. While the HDA resolution formula at $h = 0$ is well known and discussed in practically all reviews dealing with electron spectroscopy (see for example Refs. [18,19,24,25]), to our knowledge, there have been no investigations of the HDA energy resolution for $h > 0$. Thus, there is no way to extrapolate the energy resolution from $h = 0$ to realistic positive $h$-values, to quantify its expected deterioration and to know its dependence on $R_0$ and $\Delta R_0$. The only $h$-dependence study known to us, reports on a related subject also of importance to PSD usage, i.e. the possible reduction of energy non-linearity in the exit radial position along a PSD for $h > 0$ [26].

Of special interest in this presentation is the investigation of the so called biased paracentric HDA [27–29], i.e. an HDA whose entry radius $R_0$ is not at the traditional mean radius $\bar{R}$ and whose value of the entry potential $V_0 \equiv \hat{V}(R_0)$ is biased (non-zero) rather than zero, as in most conventional HDAs. Such an HDA was recently shown in simulation [27] to have an improved energy resolution over that of an equal size conventional HDA and has been used with good results in the author’s laboratory for high resolution Auger projectile electron spectroscopy of ion-atom collisions [30]. The simulation [27] investigated the case of a realistic HDA with large interradial spacing between inner and outer electrode and thus included the effect of the strong fringing fields at both the entry and the exit of the HDA thought to be responsible for the resolution improvement. While the reason for this improvement is still under investigation [31,32], it is of interest to also study the energy resolution of such an HDA in the absence of strong fringing fields, i.e. for ideal fields, and compare to that of the conventional HDA.

Here, we explore theoretically the energy resolution of an ideal HDA for $h \geq 0$ and its dependence on $R_{\text{in},0}$ and $\Delta R_0$. We utilize both exact numerical and approximate analytic techniques to investigate the $h$-dependence of the exit radial base width $\Delta R_{\text{out}}$, the base energy resolution $R_{\text{in},0}$, and the response function or line shape $L_{\text{in}}$ of a generalized ideal HDA, including both conventional and paracentric [27–29] HDAs in one unified treatment.

2. Ideal hemispherical deflector analyzer

2.1. Generalized HDAs—basic definitions

The most general type of HDA utilizes an elliptical central tuning trajectory [28]. Such a trajectory enters the HDA with an incidence angle $\alpha^* = 0$, radial position $R_0$ and nominal kinetic energy $w$ (in this case also the tuning energy) and exits at radial position $R_\ast$, after a deflection through $180^\circ$ inside the HDA. All other rays enter the HDA at radial position $r_0$, incidence angle $\alpha^*$ and nominal pass energy $w$ exiting at deflection through $180^\circ$ at radial position $r_\ast$ and exiting angle $\alpha^*$. We also introduce the fractional pass energy:

$$\tau \equiv \frac{r_\ast}{w}$$

so that the central tuning trajectory will always have $\tau = 1$. Finally, we define the paracentricity parameter $\xi$:

$$\xi \equiv \frac{R}{R_0}$$

(2)

where $R = (R_1 + R_2)/2$ is the mean HDA radius. In the past [28] we have always dealt with HDAs for which $R_2 = R_\ast$ (convenient but not necessary) for which $\xi = R_2/R_0$, in this case. We shall continue assuming $R_2 = R_\ast$ also here, but will maintain both symbols for generality.

We next introduce the concept of HDA entry bias. This refers to the value of the potential $V_0 \equiv \hat{V}(R_0)$ at the central tuning ray entry radius $R_0$. Thus, we define the biasing parameter $\gamma$ so that [28]:

$$qV_0 = q\hat{V}(R_0) = (1 - \gamma)w$$

(3)

where $q$ is the particle charge (for electrons $q = -|e|$ with $e = 1.61 \times 10^{-19}\,\text{C}$) and $\hat{V}(R)$ is the potential inside the HDA [33], in this paper assumed to be ideal and given by:

$$\hat{V}(r) = \frac{k}{r} + c$$

(4)

Then, for $\gamma = 1$, $V_0 = 0$ the HDA is unbiased, while in general for $\gamma \neq 1$ the HDA is biased. The combination of $\xi$ and $\gamma$ define the particular type of HDA. Thus, conventional HDAs have $V_0 = 0$ and $R_2 = R_\ast = R$. They are therefore unbiased with $\gamma = \xi = 1$ and their central tuning trajectory is a circle. Biased paracentric HDAs with $\xi$ both larger and smaller than 1 have been reported. These, in general, will have an elliptic central tuning trajectory. Thus, for example, Belov et al. [34] describe an HDA with $R_0 > R$ ($\xi < 1$) without, however, giving specifics about the actual values of $\xi$ and $\gamma$ used. Benis et al., used an HDA with $\xi = 1.2308$ and $\gamma = 1.5$ [30] for which SIMION electron optic simulations showed improved focusing over equal size conventional HDA [27,28]. In Table 1 we summarize typical values of HDA parameters.

2.2. $h$-Dependence of the exit radius $r_\ast$

In Ref. [28] it was shown that a particle moving in the ideal $1/r$ potential $V(r)$ (see Eq. (4)) of an HDA tuned to the central tuning ray’s nominal pass energy $w$, entering at radius $r_0$ with energy $\tau$ and incidence angle $\alpha^*$, after a deflection through $180^\circ$ inside the HDA (see Fig. 1) will exit at the radius $r_\ast$ given by:

$$r_\ast = r_\ast(r_0, \alpha^*, \tau) = -r_0 + \frac{D_0}{1 + \kappa(1 - \tau \cos^2 \alpha^*)}$$

(5)

with

$$D_0 \equiv R_0 + R_\ast = (1 + \xi)R_0 \geq 2R_0$$

(6)

$$\kappa \equiv \frac{\xi}{\gamma}$$

(7)

and potential constants $k$ and $\kappa$ given by:

$$qk = \frac{wD_0}{\kappa}$$

(8)

$$qc = w\left(1 + \frac{1}{\kappa}\right)$$

(9)
Table 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_1$ (mm)</td>
<td>72.4</td>
<td>HDA inner radius</td>
</tr>
<tr>
<td>$R_2$ (mm)</td>
<td>130.8</td>
<td>HDA outer radius</td>
</tr>
<tr>
<td>$\bar{R}$ (mm)</td>
<td>101.6</td>
<td>HDA mean radius $\bar{R} = (R_1 + R_2) / 2$</td>
</tr>
<tr>
<td>$\Delta R$ (mm)</td>
<td>6</td>
<td>PSD position resolution</td>
</tr>
<tr>
<td>$d_{PSD}$ (mm)</td>
<td>40</td>
<td>PSD active diameter</td>
</tr>
<tr>
<td>$w$</td>
<td>$W/F$</td>
<td>Normalized central ray pass energy (HDA tuning energy)</td>
</tr>
<tr>
<td>$\tau$</td>
<td>$\Delta w / w$</td>
<td>Retardation factor</td>
</tr>
</tbody>
</table>

For definitions also refer to Fig. 1 and Eqs. (5)–(9)

![Schematic electron trajectories in a typical HDA spectrometer](image)
The voltages are set once by Ref. [28]:

$$qV_i$$

exiting the HDA, the charged particle is again refracted at the exit plane. For the paracentric HDA we use

$$\xi$$

and for the conventional HDA we use

$$R$$

(see Eq. (3)), difference in potentials on either side of the potential boundary will result in a change in potential such that in general u' ≠ u [28]. In deriving Eq. (5) in Ref. [28] it was assumed that the potential changes in a step-like manner in crossing the boundary. In a real HDA this potential step is, of course, more gradual.

The effect of refraction has been included in the above formulas for $$r^*_{\text{HDA}}$$ Eq. (5) as discussed in detail in Ref. [28]. On exiting the HDA, the charged particle is again refracted at the potential boundary exiting with angle $$\alpha^*$$, then it travels through the drift region, impinging on the PSD plane (at a distance h) at the axial distance $$r^*_{\text{HDA}}$$ as shown in Fig. 1, given by:

$$r^*_{\text{HDA}} = r^*_i + h \tan \alpha^*$$

(12)

Paying close attention to the sign of $$\alpha^*$$ [15] conventionally defined such that $$\alpha^* > 0$$ when the electron’s radial distance r increases at entry (see Figs. 2–4 in Ref. [28]) and using the relation between $$\alpha^*$$ and $$\alpha$$ (see Eq. (32) in Ref. [28]) we have:

$$\tan \alpha^* = \frac{r^*}{r_i} \tan \alpha$$

(13)

we can then write:

$$r^*_i = r^*_0 = \xi$$

$$\gamma \tau$$

(Fig. 2) for an ideal HDA utilizing a PSD as:

$$D = \frac{\xi}{\gamma \tau} = \frac{D_0}{\xi \tau^* (1 - \xi)}$$

(15)

where $$X = X(\tau^*) = 1 + \tau^*$$.

Our definition of the dispersion length D is seen to be dependent on the particle’s fractional pass energy, $$\tau^*_0$$, thus allowing for the inclusion of HDAs with PSD, having a large acceptance energy window around the central ray energy $$\tau^*_0 = 1$$. Then, the mean dispersion length $$\bar{D} = \frac{D(\tau^*_0 = 1)}{D(\tau^*_0 = 0)}$$ is found to be dependent on $$\tau^*_0$$ and the HDA acceptance angle, $$\alpha^*$$, it is also seen that the highest dispersion HDAs have increasingly non-linear energy dependence, of paramount importance for use with a PSD [26], particularly if the HDA voltages will be scanned for use at constant tuning energy w. Thus, while high dispersion.
analytic approximation of

The other three lines (top) mark examples of electron trajectories having

Fig. 4. Dependence of the exact exit radial base width $\Delta_{\text{exit}}$ on $h$. Open symbols refer to a conventional HDA $\gamma = 1.5$, while closed symbols refer to the equal sized ($R = 103.6$ mm) biased parametric HDA ($\gamma = 1.5$, $\xi = 1.2308$, $r_0 = 1$ and $\Delta r_0 = 0.2$ mm. For large values of $\alpha^\ast$ and small values of $h$, the parametric HDA is seen to have a smaller radial base width $\Delta_{\text{exit}}$ than the conventional HDA.

2.3. $h$-Dependence of the HDA exit radial base width $\Delta_{\text{exit}}$

The exit radial base width $\Delta_{\text{exit}}$ is the maximum total length along the dispersion direction of the trace of the electron trajectory for a monoenergetic electron of fractional pass energy $\tau_0$ due to the range of permissible input radii $r_0$ and injection angles $\alpha^\ast$, i.e.

$$R_0 - \frac{\Delta r_0}{2} \leq r_0 \leq R_0 + \frac{\Delta r_0}{2}$$

$$-\alpha^\ast_{\text{max}} \leq \alpha^\ast \leq \alpha^\ast_{\text{max}}$$

$\alpha^\ast_{\text{max}}$ and $\Delta r_0$ determine the line shape and base resolution of an ideal HDA. To reduce the tailing of the line shape due to the angular contributions, Kuyatt & Simpson [38] proposed that $\Delta_{\text{exit}} \leq \Delta r_0/2$, a condition strived for in most high resolution HDAs. Popular optimization conditions are discussed in detail and compared in Refs. [39,40]. For an HDA without a lens, $\Delta r_0$ is equal to the width of the real entry slit or aperture diameter $d_0$. However, for an HDA equipped with an injection lens, $\Delta r_0$ is the diameter of a virtual aperture given by the spot size of the lens focus. In the case of an injection lens, $\Delta r_0$ and $\alpha^\ast_{\text{max}}$ are not anymore independent, but are related via the Helmholtz–Lagrange law. In this case, as we have recently shown for $h = 0$ [41], there is an optimal choice of $\Delta r_0$ and $\alpha^\ast_{\text{max}}$ that leads to the best possible resolution of the HDA. Clearly, as long as $\Delta r_0 < d_0$, transmission is preserved. In Ref. [42] we use the results developed here to extend our optimization method [41] to the case of non-zero $h$. In this presentation, however, $\alpha^\ast_{\text{max}}$ and $\Delta r_0$ will be assumed in all generality to be independent of one another.

2.3.1. Exact calculation

For $h > 0$ special care must be exercised in computing the exit radial base width, $\Delta_{\text{exit}}$. In Fig. 1, pencils of angular divergence $\alpha^\ast$ are shown at either side of the entry aperture corresponding to the limiting cases. By inspection, we note that the minimum exit radial position $r^\ast_{\text{exit}}$ will always come from tra-
jectory 3 having \( a^* = a^*_{\text{max}} \) and \( r_0 = R_0 + \Delta r_0 / 2 \) correspond-
ing to:

\[
r^*_{\text{rmax}} = r_0^* + \left( R_0 + \frac{\Delta r_0}{2}, a^*_{\text{max}}, \tau_0, h \right)
\]

(18)

Computing the maximum radius requires more attention. For \( h = 0 \), due to first order focusing and as shown in Fig. 1 trajectory 3 (having \( a^* = 0 \)) will always give the larger radius. Thus, we always have:

\[
r^*_{\text{rmax}} = r_0^* = r_0 \left( R_0 + \frac{\Delta r_0}{2}, 0, \tau_0 \right) = -R_0 \pm \Delta r_0 \frac{D_0}{\pi}
\]

(19)

However, as seen from Fig. 1, for \( h > 0 \) trajectory 4 deriving from some negative injection angle \( a^*_{\text{min}} \) not necessarily equal to \(-a^*_{\text{max}}\) will mark the maximum radius \( r^*_{\text{rmax}} \). To find the angle \( a^*_{\text{min}} \) at which \( r^*_{\text{rmax}}(R_0 - \Delta r_0 / 2, a^*, \tau_0, h) \) is maximized the following conditions need to be fulfilled:

\[
\frac{\partial}{\partial a^*} r^*_{\text{rmax}} \left( R_0 - \frac{\Delta r_0}{2}, a^*, \tau_0, h \right) = 0
\]

(20)

\[
\frac{\partial^2}{\partial a^*^2} r^*_{\text{rmax}} \left( R_0 - \frac{\Delta r_0}{2}, a^*, \tau_0, h \right) < 0
\]

(21)

Clearly, the solution, if it exists, \( a^*_0 = a^*_\text{min}(\tau_0, h) \) will depend on the value of \( h \) and \( \tau_0 \). Then we shall always have:

\[
r^*_{\text{rmax}}(R_0 - \Delta r_0 / 2, a^*_0, \tau_0, h) \geq r_0^* \left( R_0 - \frac{\Delta r_0}{2}, 0, \tau_0, h \right)
\]

(22)

with the equality occurring at \( h = 0 \). In general \( a^*_{\text{min}}(\tau_0, h) \) is found to increase monotonically with \( h \), eventually reaching \( a^*_{\text{max}} \) at some critical distance \( h = h_0 \). Since \( a^*_0 \) is the maximum allowed injection angle, any solutions \( a^*_{\text{min}} > a^*_{\text{max}} \) are unphysical, and therefore for \( h > h_0 \), \( a^*_{\text{min}} \) must be replaced by its limit \( a^*_{\text{max}} \). Thus, \( h_0 \) must satisfy the equation,

\[
|a^*_{\text{min}}| = a^*_{\text{max}}
\]

(23)

and in general will depend on \( \Delta r_0, a^*_{\text{max}} \) and \( \tau_0 \).

The complete solution for \( a^*_{\text{min}} \) may thus be represented by the double branched function:

\[
a^*_{\text{min}} = \begin{cases} 
\text{Solution of Eq.(20)} & \text{for } 0 \leq h \leq h_0 \\
-\min_{a^*_{\text{max}}} & \text{for } h > h_0 
\end{cases}
\]

(24)

We may now evaluate \( r^*_{\text{rmin}}(R_0 - \Delta r_0 / 2, a^*, \tau_0, h) \) at \( a^* = a^*_{\text{min}} \) using Eq. (24) to obtain \( r^*_{\text{rmin}} \). This necessarily leads to the double-branched function \( r^*_{\text{rmax}} \equiv r^*_{\text{rmin}}(R_0 - \Delta r_0 / 2, a^*_{\text{min}}, \tau_0, h) \) given by:

\[
r^*_{\text{rmax}} = \begin{cases} 
\left( R_0 - \min_{a^*_{\text{max}}}, a^*_{\text{min}}, \tau_0, h \right) & \text{for } 0 \leq h \leq h_0 \text{ (or } |a^*_{\text{min}}| \leq a^*_{\text{max}}) \\
\left( R_0 - \min_{a^*_{\text{max}}}, -a^*_{\text{min}}, \tau_0, h \right) & \text{for } h \geq h_0 \text{ (or } |a^*_{\text{min}}| \geq a^*_{\text{max}}) 
\end{cases}
\]

(25)

The exit radial base width \( \Delta r^*_{\text{r}} \) is then defined as:

\[
\Delta r^*_{\text{r}} \equiv r^*_{\text{rmax}} - r^*_{\text{rmin}}
\]

(26)

In Fig. 3, we give an example for the paracentric HDA of \( r^*_{\text{rmax}}(R_0 - \Delta r_0 / 2, a^*, \tau_0, h) \) (top) and \( r^*_{\text{rmin}}(R_0 + \Delta r_0 / 2, a^*_{\text{min}}, \tau_0, h) \) (bottom) and their dependence on \( h \) for the case of \( \Delta r_0 = 2 \text{ mm}, \tau_0 = 1 \text{ and } a^*_{\text{min}} = 1^\circ \). In the case of \( r^*_{\text{rmin}}(R_0 - \Delta r_0 / 2, a^*, \tau_0, h) \), three different values of \( a^* \) including \( a^*_{\text{min}} \) are shown. The exit radial base width \( \Delta r^*_{\text{r}} \) is also marked.

Evaluation of Eq. (26) can be performed exactly. It is only necessary to solve the transcendental equation Eq. (20) for \( a^*_{\text{min}} \) numerically. Then, depending on whether \( |a^*_{\text{min}}| \) is smaller or larger than \( a^*_{\text{max}} \), the correct branch of Eq. (25) can be calculated. Therefore the value of \( h_0 \) is really superfluous to the calculation. However, since \( h \) is a physical distance, in principle directly measurable in the laboratory, while \( a^* \) is a much less accessible parameter, it is intuitively useful to also compute \( h_0 \).

In the sections to follow, we use the exact value of \( a^*_{\text{min}} \) obtained by solving Eq. (20) numerically with Mathematica [43]. However, to obtain a better understanding of the various dependencies, analytic results are also presented using Taylor series expansions of the quantities of interest to first order in \( \Delta r_0 \) and to second order in \( a^*_{\text{min}} \). These are also used in the resolution optimization presented in Ref. [42].

2.3.2. Approximate analytic calculation

A relatively simple analytic approximation to \( r^*_{\text{rmin}} \) can be obtained by using a Taylor series expansion of \( r^*_{\text{rmin}}(R_0 \pm \Delta r_0 / 2, a^*, \tau_0, h) \) to first order in \( \Delta r_0 \) and to second order in \( a^*_{\text{min}} \):

\[
r^*_{\text{rmin}}(R_0 \pm \frac{\Delta r_0}{2}, a^*, \tau_0, h) \approx r^*_{\text{rmax}} \pm h_0 \left[ G \left( 1 \pm \frac{\Delta r_0}{2R_0} \right) - 1 \right] - \Delta a^2
\]

(27)

with \( r^*_{\text{rmax}} \) given by Eq. (19) and where we have introduced the symbol:

\[
G \equiv G(\tau_0) = \frac{D_0}{(R_0X)}
\]

(28)

with the mean value given by \( G = G(\tau_0 = 1) = D_0/R_0 \). For a conventional HDA (\( \sigma = \xi = 1 \)) we also have \( G = 2/(2 - \tau_0) \) and \( G = 2 \). Setting Eq. (27) into Eq. (20) and solving for \( a^*_{\text{min}} \) we obtain the approximate analytic solution for \( a^*_{\text{min}} \). This can be represented as a double branched function in analogy to the exact solution Eq. (24):

\[
a^*_{\text{min}} \approx \begin{cases} 
-\frac{\Delta a^2}{\Delta r_0/2} & \text{for } 0 \leq h \leq h_0 \\
-\min_{a^*_{\text{max}}} & \text{for } h \geq h_0
\end{cases}
\]

(29)

\( a^*_{\text{min}} \) is indeed negative in value and also satisfies the condition for a maximum (Eq. (21)).
Using approximations Eqs. (27) and (29) to evaluate Eq. (26) we obtain the approximate analytic form of the base width $\Delta r_{b0}$:

$$\Delta r_{b0} \equiv \Delta r_{b0}(\Delta \Omega, a_{\text{max}}^*, t_0, h) \approx \Delta \Omega + h a_{\text{max}}^* \left( G \left( \frac{1 - \frac{1}{\Delta \Omega}}{1 + \frac{1}{\Delta \Omega}} \right) - 1 \right) \left( \frac{4}{G(1 + (\Delta \Omega/2R_0)) - 1} \right)^{\frac{1}{2}}$$

with an approximate value for $h_0$ given by:

$$h_0 \equiv h (\Delta \Omega, a_{\text{max}}^*, t_0) \approx \frac{4}{G(1 + (\Delta \Omega/2R_0)) - 1}$$

For $h = 0$ we obtain the well known formula for the base width $\Delta r_0^*$ of an HDA at the focal plane:

$$\Delta r_0^* = \Delta r_0 + \Delta r_{\text{cyc}}$$

All the extra $h$-terms in $\Delta r_{b0}^*$ (Eq. (30)) can be shown to be positive and therefore the situation $h > 0$ always leads to larger base widths, i.e. $\Delta r_{b0}^* \geq \Delta r_0^*$. For $h = h_0$, both branches yield the same result namely:

$$R_{b0} = \Delta r_{b0} = \frac{S + \frac{4}{G(1 + (\Delta \Omega/2R_0)) - 1} \Delta r_{\text{cyc}}^2}{\Delta \Omega + \frac{4}{G(1 + (\Delta \Omega/2R_0)) - 1} \Delta r_{\text{cyc}}^2}$$

In Figs. 4 and 5, the exact values of $\Delta r_{b0}^*$ are plotted for equal size ($R = 101.6$ mm) conventional ($R_0 = 101.6$, $\gamma = 1$) and biased paracentic ($R_0 = 82.55$, $\gamma = 1.5$) HDA with $t_0 = 1$ and entry angles $a_{\text{max}}^* = 0.1^\circ$, $1^\circ$, $5^\circ$, $10^\circ$ at 6 different values of $h = 0$, $0.5$, $1$, $1.5$, $2$, $2.5$ mm and for two different entry aperture diameters $\Delta \Omega = 2$ mm and $\Delta \Omega = 0.2$ mm. The general tendency is for $\Delta r_{b0}^*$ to increase with increasing $h$ values. This tendency becomes stronger for increasing values of $a_{\text{max}}^*$. For $a_{\text{max}}^* = 0.1^\circ$, $\Delta r_{b0}^*$ increases extremely slowly and is practically insensitive to changes in $h$. Interestingly, for small values of $h$ the paracentric HDA exhibits smaller radial base widths than those of the conventional HDA.

2.4. $h$-Dependence of the HDA base resolution $R_{b0}$

For a beam of monenergetic particles of pass energy $E_0$, the base resolution $R_{b0}$ of an energy analyzer tuned to the pass energy $E$ is defined as the ratio of the transmitted (and detected) energy width $\Delta \Omega$ (the base width) over $t_0$:

$$R_{b0} \equiv \frac{\Delta \Omega}{t_0}$$

$R_{b0}$ is a constant, dependent only on the geometrical parameters of the analyzer and independent of the pass energy $E_0$ (or equivalently $t_0$). We can convert the maximum radial base width $\Delta r_{b0}^*$ computed in Eq. (30), to an energy width using the radial distance-to-energy conversion factor, which is seen from Eq. (15) to be just $t_0/D$, where $D$ is the HDA dispersion at $t_0$. This is equivalent to the experimental energy versus position calibration of a PSD, typically performed in electron spectroscopy measurements. If we also include the width of the exit slit (or position resolution in case of a PSD) $\Delta \Theta$, we get the total base energy width $\Delta \Theta$ (or equivalently $\Delta \Omega$) [25] and therefore

$$R_{b0} = \frac{\Delta \Theta}{\Delta \Omega}$$

If we define $S$ as the “slit” term given by the sum of the width of the slits (or virtual apertures) over the dispersion:

$$S = S(t_0) = \frac{\Delta \Theta + \Delta \Theta}{\Delta \Omega}$$

then, using Eq. (26) or its approximation Eq. (30) and Eqs. (35) and (36), we finally obtain the base resolution $R_{b0} \equiv R_{b0}(\Delta \Omega, a_{\text{max}}^*, t_0, h)$ given by:

$$R_{b0} = S + \frac{4}{G(1 + (\Delta \Omega/2R_0)) - 1} \frac{\Delta \Theta^2}{\Delta \Omega^2}$$

at $h = h_0$ both branches give the same result:

$$R_{b0} = S + \frac{4}{G(1 + (\Delta \Omega/2R_0)) - 1} \frac{\Delta \Theta^2}{\Delta \Omega^2}$$

For $h = 0$, we get from the first branch the well known result for the base resolution of an HDA along the focusing plane:

$R_{b0}(t_0, h = 0) = S + \frac{4}{G(1 + (\Delta \Omega/2R_0)) - 1} \frac{\Delta \Theta^2}{\Delta \Omega^2}$

The base resolution is plotted as a function of $h$ in Figs. 6 and 7. In general, a similar $h$-dependence is observed as for $\Delta r_{b0}^*$. However, now the base resolution for a paracentric

![Fig. 5. Same as Fig. 4, but for $\Delta r_{b0} = 2$ mm.](image)
Fig. 6. Comparison of $h$-dependence of base resolution $R_B$, for a conventional (open symbols) and paracentric (closed symbols) HDA of equal size ($R = 101.6 \text{ mm}$) for $\gamma = 1$ and $\Delta r_0 = 0.2 \text{ mm}$.

(\gamma = 1.5) HDA is shown to always be larger than that of the conventional (\gamma = 1) HDA. This has to do with the fact that the dispersion length $D$ is largest for the smallest $\gamma$, as already discussed (see Eq. (15) and Fig. 2). Thus, a small $\Delta r_0$ translates into a corresponding small $R_B$, only for equal dispersion lengths.

2.5. $h$-Dependence of the HDA line shape $L_h$

As already pointed out, to limit the effect of the angular term and obtain a more symmetric line shape, Kuyatt and Simpson [38] proposed the following criterion for the ratio $\chi$ of the angular to the “slit” term:

$$\chi \equiv \frac{\alpha_{\max}^2}{S} = \frac{D\alpha_{\max}^2}{(\Delta r_1 + \Delta r_2)} \leq \frac{1}{2} \quad (40)$$

For non-zero $h$ we can extend the Kuyatt-Simpson (KS) criterion to also incorporate the $h$-dependent terms. We therefore define a new ratio $\chi_h$ given by the ratio of the sum of both angular and $h$-dependent terms over the slit term:

$$\chi_h = \frac{R_B h}{S} - 1 \quad (41)$$

which thus also becomes a double branched function. Directly from Eq. (40), it is clear that the smallest dispersion will always lead to the smallest $\chi_h$. Therefore the biased paracentric HDA with $\gamma > 1$ will always have the smallest $\chi_h$ which will also be smallest at the lowest energy $r_0$ and the smallest $h$. Thus, paracentric HDAs with $\gamma > 1$ can be expected, in principle, to provide an improved line shape. Whether this is also true for a real paracentric HDA with strong fringing fields is of course still an open question and will be explored in future publications [44,32].

Fig. 7. Same as Fig. 6, but for $\Delta r_0 = 2 \text{ mm}$.

Fig. 8. Line shapes for $h = 0 – 25 \text{ mm}$ for equal sized ($R = 101.6 \text{ mm}$) paracentric ($\xi = 1.2308$ and $\gamma = 1.5$) and conventional ($\xi = 1$) HDAs (see Table 1) at $\tau = 1$ with $\Delta r_0 = 0.2 \text{ mm}$ (top) and $\Delta r_0 = 2 \text{ mm}$ (bottom), for $\alpha_{\max} = 0.1^\circ$. Lines mark the position of the exit of the central ray with $r_0 = R_0$, $\alpha^* = 0$. 


The line shape $L_h$ gives a much more complete picture of the electron-optical characteristics of an HDA. The normalized line shape is also known as the transmission function. $L_h$ can be readily computed either by exact piecewise integration [12,18–20] or Monte Carlo techniques[15,16,21,22] assuming uniform illumination over the entire entry aperture. Here we use the second approach.

$N_e = 500,000$ monoenergetic electrons were generated with fixed energy $\tau_0$ but random $\alpha^*$ and $r_0$ values, within the ranges specified by Eqs. (16) and (17), for a specific choice of $\Delta r_0$, $\alpha_{\text{max}}^*$ and $h$ from the HDA parameters of Table 1. For each specific set of electron parameters, Eq. (12) was used together with Eq.(5) to generate the exit radii $r^*\pi h$ which were then binned using a position resolution of $\Delta r = 0.2$ mm to obtain the final distributions. These distributions then represent the response or transmission function of the HDA to a monoenergetic line. The base width of these distributions will correspond closely to the computed value of $\Delta r^*\pi h$ given by Eqs. (26) or (30).

Different line shape calculations were made for $\tau_0 = 0.9, 1.0, 1.1$ representing the 20% energy acceptance window of the HDA, with $\Delta r_0 = 0.2$ and 0.3 mm representing realistic entry size values, at $\alpha_{\text{max}}^* = 0.1^\circ, 1^\circ, 2^\circ, 5^\circ$. For $\alpha_{\text{max}}^* < 1^\circ$ and $0 \leq h \leq 25$ mm, the KS criterion is in general satisfied independent of the value of $\Delta r_0$. For larger values of the injection angle and with increasing $h, \chi_h$ increases and the KS criterion becomes less valid or eventually even violated. Due to space limitations, the generated characteristic line shapes $L_h$ of equal size (same $\bar{R}$—see Table 1) conventional ($\gamma = \xi = 1$) and paracentric ($\gamma = 1.5, \xi = 1.2308$) HDAs are compared here at different values of $h = 0–25$ mm, but only for $\tau_0 = 1$ and $\alpha_{\text{max}}^* = 0.1^\circ, 1^\circ, 2^\circ, 5^\circ$. These are shown in Figs. 8–11 for $\Delta r_0 = 0.2$ mm (top), and $\Delta r_0 = 2$ mm (bottom). The value $\alpha_{\text{max}}^* = 2^\circ$ is one of the most interesting cases since $\chi_h$ varies across 1/2, the KS limit, as $h$ increases from 0–25 mm. For values of $\alpha_{\text{max}}^* \leq 1^\circ$, $L_h$ does not changes much with $h$, basically preserving a nice symmetric trapezoidal shape for $\Delta r_0 = 2$ mm or almost triangular shape for $\Delta r_0 = 0.2$ mm with practically no difference between paracentric and conventional HDA. At larger $\alpha_{\text{max}}^*$, where the KS criterion is not satisfied, $L_h$ becomes increasing asymmetric with increasing $h$, peaking on the high energy side of $L_h$ (see Fig. 11). The paracentric HDA is found to have a broader base

![Fig. 9](image_url). Same as Fig. 8, but for $\alpha_{\text{max}}^* = 1^\circ$.

![Fig. 10](image_url). Same as Fig. 8, but for $\alpha_{\text{max}}^* = 2^\circ$. As $h$ varies from 0–25 mm, for $\Delta r_0 = 0.2$ mm the biased paracentric HDA has $\chi_h$ (Eq. (41)) vary from 0.460–5.363, while the conventional HDA has $\chi_h$ vary from 0.618–4.354. For $\Delta r_0 = 2$ mm the corresponding $\chi_h$ variations are 0.08357–0.9753 and 0.1124–0.7919, respectively.
width than the conventional HDA which, however, for $h$-values near 0 becomes slightly smaller than for the conventional HDA, as already noted. The line shape and its radial base width do not change much as the energy sweeps across the PSD with $\tau_0$ going from 0.9 to 1.1 (not shown due to space limitations). Thus, the dependence of the base resolution $R_B^h$ on the energy, is strictly a dispersion effect. The dispersion length $D$ increases with energy as already seen in Fig. 2 forcing the corresponding decrease in resolution. This is a well known effect plaguing HDAs with large PSD, the resolution on the low energy side of the PSD being substantially worse than on the high energy side.

3. Summary and conclusions

We have shown that for an ideal HDA, where no fringing fields are considered, the optimal distance to place the PSD for best energy resolution is $h = 0$, the first order focusing plane. Useful analytic formulas of exit radial width $\Delta r^e_{max}$ and base energy resolution $R_B^h$ as a function of the distance from the focal plane $h$ for given maximum injection angle $\alpha_{max}$ and entry aperture diameter $\Delta_0$ are presented. These are further illustrated by line shape calculations at various distances $h$ for specific typical values of $\alpha_{max}$ and $\Delta_0$.

In our presentation we have also made a comparison of equal size ideal conventional and paracentric HDAs. Overall, apart from a few marginal improvements of limited utility, the paracentric HDA does not seem to show any significant practical advantages over the conventional HDA. On the contrary, it has a lower dispersion length $D$ and therefore a larger base resolution. However, a smaller $D$ will satisfy the Kuyatt-Simpson criterion (see Eq. (41)) at larger $h$, thus extending the range of $h$ values over which the quality of the line shape is maintained compared to that of the equal size conventional HDA. The interesting observation that the paracentric HDA exhibits a smaller radial base width $\Delta r^e_{max}$ than the equal size conventional HDA at small $h$ values seems to apply only to angles $\alpha_{max}$ that are too large to be practical in most applications and is therefore probably of only limited interest.

Clearly, fringing field effects must be responsible for the reported improvement [27] in the resolution of the paracentric HDA over that of the conventional HDA and needs to be further investigated. Nevertheless, the analysis of the ideal case (no fringing fields) is necessary as it provides a reference for judging the importance of fringing fields, as deviations from the ideal case. The investigation of the fringing fields of realistic HDAs and their effect on the radial focusing and energy resolution is already under way using specialized electron-optics simulation software (e.g. SIMION [36,37]) and will be presented in future publications [32,44].

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