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Powder X-ray Diffraction Method

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8. Effects of Instrumental Aberrations

8.1 Equatorial aberration

It has been known that a flat-specimen can effectively but not strictly satisfy the Rowland (focusing) condition in a commonly used powder diffraction measurement system with Bragg-Brentano geometry, and the slight deviation from the focusing condition certainly causes detectable shifts and deformation of observed powder diffraction peak profile. The effect was formerly called "flat-specimen aberration," (Cheary & Coelho, 1992; Ida & Kimura, 1999) but the effect of the divergence of the beam along the equatorial direction is also affected by the finite size of the detector, when a one-dimensional (linear) position sensitive detector (LPSD) is used. (Cheary & Coelho, 1994; Słowik & Zięba, 2001).

8.1.1 Flat-specimen aberration for point detector

Flat-specimen aberration function is given by

$$\omega_{\mathrm{FS}}(\Delta 2\Theta;\Theta) = \begin{cases} \dfrac{1}{\Phi^2 \cot\Theta}\left(-\dfrac{2\Delta 2\theta}{\Phi^2\cot\Theta}\right)^{-1/2} & \left[-\dfrac{\Phi^2\cot\Theta}{2} < \Delta 2\Theta < 0\right] \\ 0 & \left[\text{elsewhere}\right] \end{cases}, \quad (8.1.1.1)$$

where Φ is the effective equatorial divergence angle of the incident beam, and it coincides with the divergence slit open angle Φ_{DS}, when the irradiated area on the sample face does not exceed the sample width.

The critical apparent diffraction angle $2\Theta_{\mathrm{c}}$ defined by the lowest goniometer angle where the spill out of the irradiated does not occur is given by

$$2\Theta_{\mathrm{c}} = 2\arcsin\frac{[1-(W/2R)^2]\tan\Phi_{\mathrm{DS}}}{W/R} \approx 2\arcsin\frac{R\Phi_{\mathrm{DS}}}{W} \quad (8.1.1.2)$$

for the goniometer radius of R and sample width of W (Appendix 8.1.A).

When the apparent diffraction angle 2Θ is lower than the critical angle $2\Theta_c$, the effective divergence angle Φ_{eff} should be determined by R and W (Appendix 8.1.B),

$$\Phi = \min(\Phi_{DS}, \Phi_{eff}) \tag{8.1.1.3}$$

$$\Phi_{eff} = \arctan \frac{(W/R)\sin\Theta}{1-(W/2R)^2} . \tag{8.1.1.4}$$

Spill out of the incident beam occurs for $2\Theta < 2\Theta_c$, and the observed intensities should be multiplied by

$$\frac{\Phi_{eff}}{\Phi_{DS}} = \frac{1}{\Phi_{DS}} \arctan \frac{(W/R)\sin\Theta}{1-(W/2R)^2} , \tag{8.1.1.5}$$

to those of "constant irradiated volume" condition for the angles $2\Theta_c \leq 2\Theta$ in symmetric reflection mode.

If $W \ll R$ and $\Phi_{DS} \sim 0$ are assumed, the critical angle $2\Theta_c$ can be approximated by

$$2\Theta_c \approx 2 \arcsin \frac{R\Phi_{DS}}{W} , \tag{8.1.1.6}$$

and

$$\Phi_{eff} \approx \frac{W\sin\Theta}{R} , \tag{8.1.1.7}$$

and the intensity correction factor is then given by

$$\frac{\Phi_{eff}}{\Phi_{DS}} \approx \frac{W\sin\Theta}{R\Phi_{DS}}. \tag{8.1.1.8}$$

The values of the critical angle are estimated at $2\Theta_c = 18.75^\circ$ by eq. (8.1.1.5) and $2\Theta_c = 18.83^\circ$ by eq. (8.1.1.8) for a standard condition of a powder diffraction measurement system Rigaku MiniFlex 600-C with a SSXD (Rigaku DteX/Ultra2), $\Phi = 1.25^\circ$, $R = 150$ mm, $W = 20$ mm.

The normalized formula of the equatorial aberration function can be expressed by

$$\omega_{FS}(z) = \frac{1}{\Phi} \int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}} \delta\left(z + \frac{2\phi^2}{\tan\Theta}\right) d\phi . \tag{8.1.1.9}$$

The first- to fourth-order cumulants $\kappa_1, \kappa_2, \kappa_3$ and κ_4 of the flat-specimen aberration function are given by (Appendix 8.1.C)

$$\kappa_1 = -\frac{\Phi^2}{6\tan\Theta}. \tag{8.1.1.10}$$

$$\kappa_2 = \frac{\Phi^4}{45\tan^2\Theta}. \tag{8.1.1.11}$$

$$\kappa_3 = -\frac{2\Phi^6}{945\tan^3\Theta} \tag{8.1.1.12}$$

$$\kappa_4 = -\frac{2\Phi^8}{4725\tan^4\Theta} . \tag{8.1.1.13}$$

The negative signal about the 4th order cumulant of the function indicates that the function has more collapsed profile than the Gaussian (normal distribution) function.

8.1.2 Equatorial aberration for continuous-scan integration of silicon strip X-ray detector

Formulas of equatorial aberration for linear position sensitive detector (LPSD) have already been reported (Cheary & Coelho, 1994; Słowik & Zięba, 2001), but an explicit formula of the aberration function for data collected by continuous scan integration of silicon strip X-ray detector (SSXD), called RTMS (real-time multiple strip technology) by Panalytical or TDI (time delay integration) by Rigaku, has not been reported.

The exact and approximate formulas of the equatorial aberration function for the continuous scan integration of SSXD are derived and compared in this section. The restriction $2\Theta_c < 2\Theta$ is assumed here (Appendix 8.1.D).

8.1.2.1 Exact formula of equatorial aberration

The instrumental parameters for the equatorial aberration are illustrated in Fig. 8.1.2.1. $R = \overline{XG} = \overline{GC}$ is the goniometer radius, Φ is the equatorial divergence angle, and 2Ψ is the view angle of the SSXD, given by $2\Psi = 2\arctan(L/R)$ for the the effective detector length $2L$.

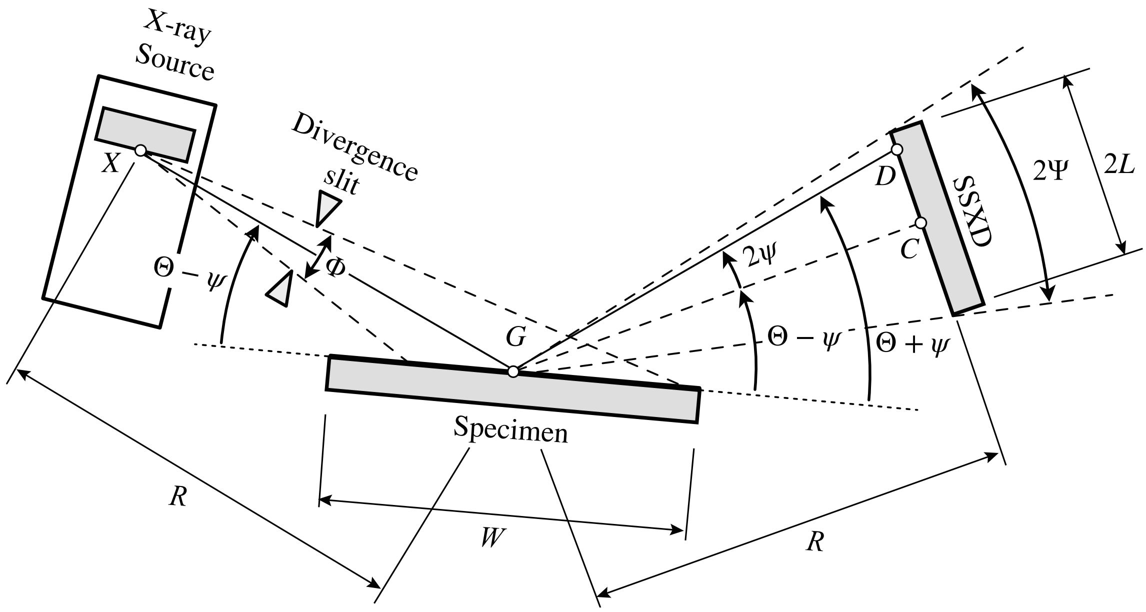

Fig. 8.1.2.1 Instrumental parameters for equatorial aberration of continuous scan integration measurement with SSXD. R: goniometer radius, Φ: divergence slit open angle and 2Ψ: view angle of SSXD. It is assumed that the intensity detected by the off-center detector strip D with the offset angle 2ψ is assigned to 2Θ, when the apparent incident and center-strip glancing angles are $\Theta - \psi$.

It is assumed that the X-ray beam is generated at the focal point (X), and the center strip (C) of SSXD is symmetrically rotated about the goniometer axis (G) to (X) as shown in Fig. 8.1.2.1. It is assumed that the intensity detected by a off-center detector strip D with the offset angle of 2ψ is assigned to the apparent diffraction angle 2Θ, when the apparent incident glancing angle is $\Theta - \psi$, and the apparent reflected glancing angle for the center strip C is also given by $\Theta - \psi$.

Figure 8.1.2.2 illustrates the case that the diffraction at the off-center position P on the specimen face is detected by the off-center strip D with the offset angle 2ψ. The equatorial deviation angle is given by ϕ. The true diffraction angle, which is identical to the supplementary angle of $\angle XPD$, is given by 2θ. The apparent diffraction angle 2Θ is assumed to be assigned to the supplementary angle of $\angle XGD$.

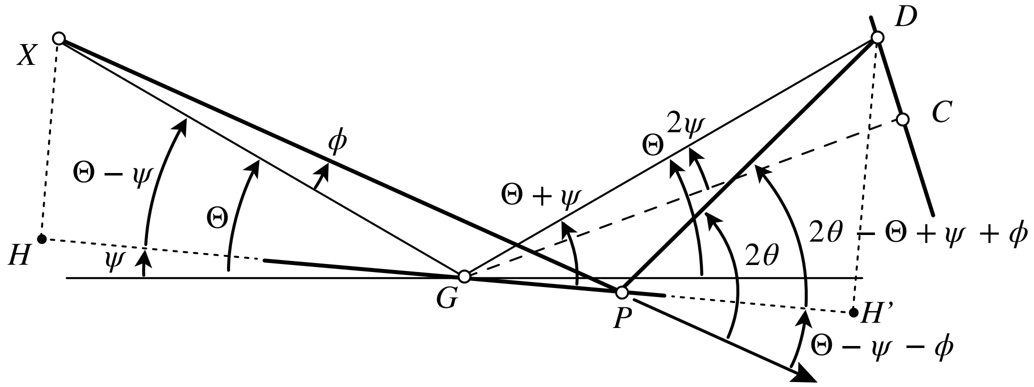

Fig. 8.1.2.2 Relations of the apparent diffraction angle 2Θ and true diffraction angle 2θ, equatorial deviation angle ϕ, and off-center strip offset angle 2ψ.

Our current interest is to derive the formula of the difference between the apparent diffraction angle 2Θ and the true diffraction angle 2θ, $\Delta 2\Theta \equiv 2\Theta - 2\theta$. If the formula is expressed by a function of 2Θ, ϕ and ψ, that is,

$$\Delta 2\Theta = f(2\Theta, \phi, \psi), \tag{8.1.2.1}$$

the explicit instrumental function for the equatorial aberration $\omega_{\mathrm{E}}(\Delta 2\Theta; 2\Theta, \Phi, \Psi)$ is given by

$$\omega_{\mathrm{E}}(\Delta 2\Theta; 2\Theta, \Phi, \Psi) = \int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}} \int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}} \delta\left(\Delta 2\Theta - f(\Theta, \phi, \psi)\right) g(\phi) h(\psi)\, \mathrm{d}\phi\, \mathrm{d}\psi, \tag{8.1.2.2}$$

where $\delta(x)$ is Dirac delta function, $g(\phi)$ is the intensity distribution function about the equatorial deviation angle ϕ, and $h(\psi)$ is the density distribution function about the offset angle ψ. Uniform distribution functions,

$$g(\phi) = \begin{cases} \dfrac{1}{\Phi} & \left[-\dfrac{\Phi}{2} < \phi < \dfrac{\Phi}{2}\right] \\ 0 & [\text{otherwise}] \end{cases}, \tag{8.1.2.3}$$

$$h(\psi) = \begin{cases} \dfrac{1}{\Psi} & \left[-\dfrac{\Psi}{2} < \psi < \dfrac{\Psi}{2}\right] \\ 0 & [\text{otherwise}] \end{cases}, \tag{8.1.2.4}$$

are assumed here, for simplicity, but it will not be difficult to incorporate corrections about (a) non-spherical and (b) oblique-incidence (Ida, 2016), if necessary.

Following relations can be found in Fig. 8.1.2.2,

$$\begin{aligned} \overline{GP} = \overline{PH} - \overline{GH} &= \frac{\overline{XH}}{\tan(\Theta-\psi-\phi)} - \overline{XG}\cos(\Theta-\psi) \\ &= \frac{\overline{XG}\sin(\Theta-\psi)}{\tan(\Theta-\psi-\phi)} - \overline{XG}\cos(\Theta-\psi) \\ &= R\left[\frac{\sin(\Theta-\psi)}{\tan(\Theta-\psi-\phi)} - \cos(\Theta-\psi)\right] \end{aligned} \tag{8.1.2.5}$$

$$\overline{GP} = \overline{GH'} - \overline{PH'} = \overline{GD}\cos(\Theta+\psi) - \frac{\overline{DH'}}{\tan(2\theta-\Theta+\psi+\phi)}$$
$$= \overline{GD}\cos(\Theta+\psi) - \frac{\overline{GD}\sin(\Theta+\psi)}{\tan(2\theta-\Theta+\psi+\phi)}$$
$$= \frac{R}{\cos 2\psi}\left[\cos(\Theta+\psi) - \frac{\sin(\Theta+\psi)}{\tan(2\theta-\Theta+\psi+\phi)}\right]. \quad (8.1.2.6)$$

Then the following relations about Θ, θ, ψ and ϕ can be derived,

$$\frac{\sin(\Theta-\psi)}{\tan(\Theta-\psi-\phi)} - \cos(\Theta-\psi) = \frac{1}{\cos 2\psi}\left[\cos(\Theta+\psi) - \frac{\sin(\Theta+\psi)}{\tan(2\theta-\Theta+\psi+\phi)}\right]. \quad (8.1.2.7)$$

Solution of eq. (8.1.2.7) about 2θ,

$$2\theta = \Theta - \psi - \phi + \arctan\frac{\sin(\Theta+\psi)}{g(\Theta,\phi,\psi)}, \quad (8.1.2.8)$$

$$g(\Theta,\phi,\psi) = \cos(\Theta-\psi)\,\cos 2\psi + \cos(\Theta+\psi) - \frac{\sin(\Theta-\psi)\,\cos 2\psi}{\tan(\Theta-\psi-\phi)}, \quad (8.1.2.9)$$

gives an exact expression about $\Delta 2\Theta \equiv 2\Theta - 2\theta$,

$$\Delta 2\Theta = \Theta + \psi + \phi - \arctan\frac{\sin(\Theta+\psi)}{g(\Theta,\phi,\psi)} \quad (8.1.2.10)$$

Dependence of the deviation angle $\Delta 2\Theta \equiv 2\Theta - 2\theta$ on ϕ and ψ is shown in Fig. 8.1.2.3.

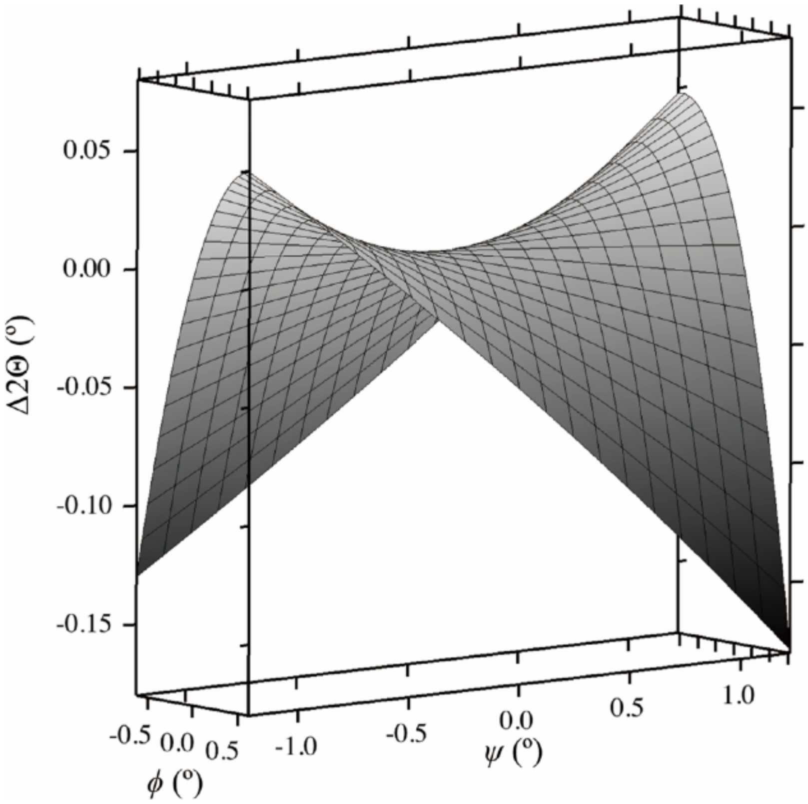

Fig. 8.1.2.3 Three dimensional view of the deviation angle $\Delta 2\Theta \equiv 2\Theta - 2\theta$ depending on equatorial deviation angle ϕ and half offset angle ψ, for the case $\Phi = 1.25°$ and $2\Psi = 4.89°$ and $2\Theta = 30°$.

The exact equatorial aberration function should then formally be given by

$$\omega_{\mathrm{E}}(\Delta 2\Theta; \Theta, \Phi, \Psi) = \frac{1}{\Phi\Psi} \int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}} \int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}} \delta \left(\Delta 2\Theta - \Theta - \psi - \phi + \arctan \frac{\sin(\Theta + \psi)}{g(\Theta, \phi, \psi)} \right) \mathrm{d}\psi \, \mathrm{d}\phi \tag{8.1.2.11}$$

It is not difficult to derive a numerical solution about the exact equatorial aberration function.

(1) Calculate $N \times N$ values of $\Delta 2\Theta_{ij}$ ($N = 1001$ for example) for

$$\phi_i = -\frac{\Phi}{2} + \frac{i-1}{N-1}\Phi \qquad (i = 1, \cdots N)$$

$$\psi_j = -\frac{\Psi}{2} + \frac{j-1}{M-1}\Psi \qquad \left(j = 1, \cdots N\right)$$

(2) Make an N-bin histogram of $\Delta 2\Theta_{ij}$. When the minimum and maximum values of $\Delta 2\Theta_{ij}$ is given by $\Delta 2\Theta_{\mathrm{min}}$ and $\Delta 2\Theta_{\mathrm{max}}$, the width of a bin w may be determined by

$$w = \frac{\Delta 2\Theta_{\mathrm{max}} - \Delta 2\Theta_{\mathrm{min}}}{N-1}.$$

And let k-th bin covers the range

$$\Delta 2\Theta_{\mathrm{min}} + (k - 1.5)w \le \Delta 2\Theta_{ij} < \Delta 2\Theta_{\mathrm{min}} + (k - 0.5)w \, .$$

Then the value $\Delta 2\Theta_{\mathrm{min}}$ will be covered by the 1st bin, because the range is given by

$$\Delta 2\Theta_{\mathrm{min}} - 0.5w \le \Delta 2\Theta_{ij} < \Delta 2\Theta_{\mathrm{min}} + 0.5w,$$

for $k = 1$, and the value $\Delta 2\Theta_{\mathrm{max}}$ will be covered by the N-th bin, because

$$\Delta 2\Theta_{\mathrm{max}} - 0.5w \le \Delta 2\Theta_{ij} < \Delta 2\Theta_{\mathrm{max}} + 0.5w,$$

for $k = N$.

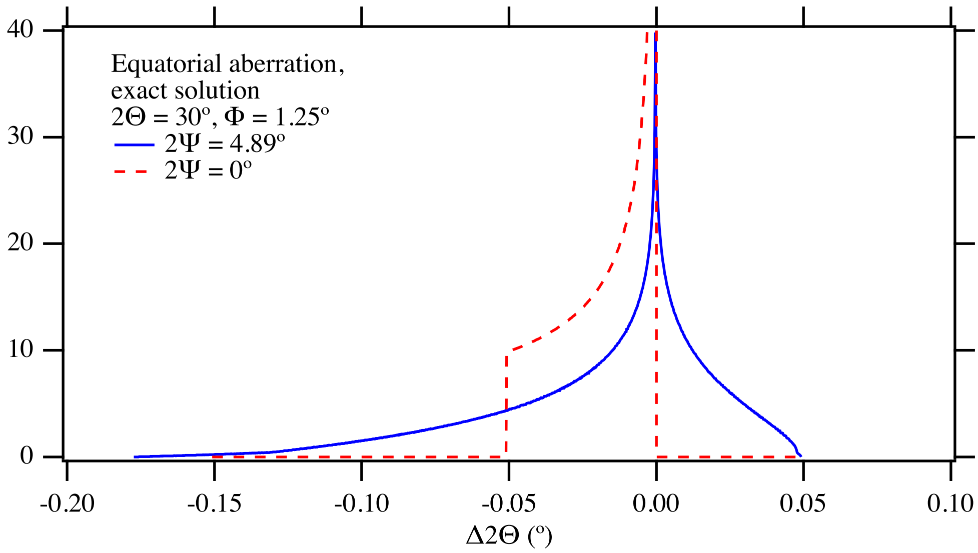

Fig. 8.1.2.4 Exact equatorial aberration function as a 1001-bin histogram, for the case $\Phi = 1.25°$ and $2\Psi = 4.89°$ and $2\Theta = 30°$.

Figure 8.1.2.4 shows a numerical solution of the exact equatorial aberration function as a 1001-bin histogram calculated by the above procedures.

8.1.2.2 Approximate formula of equatorial aberration

According to an approximate formula proposed by Słowik & Zięba (2001), the following formula for the deviation angle $\Delta 2\Theta \equiv 2\Theta - 2\theta$ can be derived,

$$\Delta 2\Theta \equiv 2\Theta - 2\theta \approx -\frac{2\phi(\phi+\psi)}{\tan\Theta} \; . \tag{8.1.2.12}$$

The formula can straightly be derived by second-order expansion of the exact formula (Appendix 8.1.E). The approximate dependence of the deviation angle $\Delta 2\Theta \equiv 2\Theta - 2\theta$ on ϕ and ψ is shown in Fig. 8.1.2.5. As compared with the exact dependence shown in Fig. 8.1.2.3, it is found that the main feature of the exact dependence is well simulated by the approximation, but small difference is detectable.

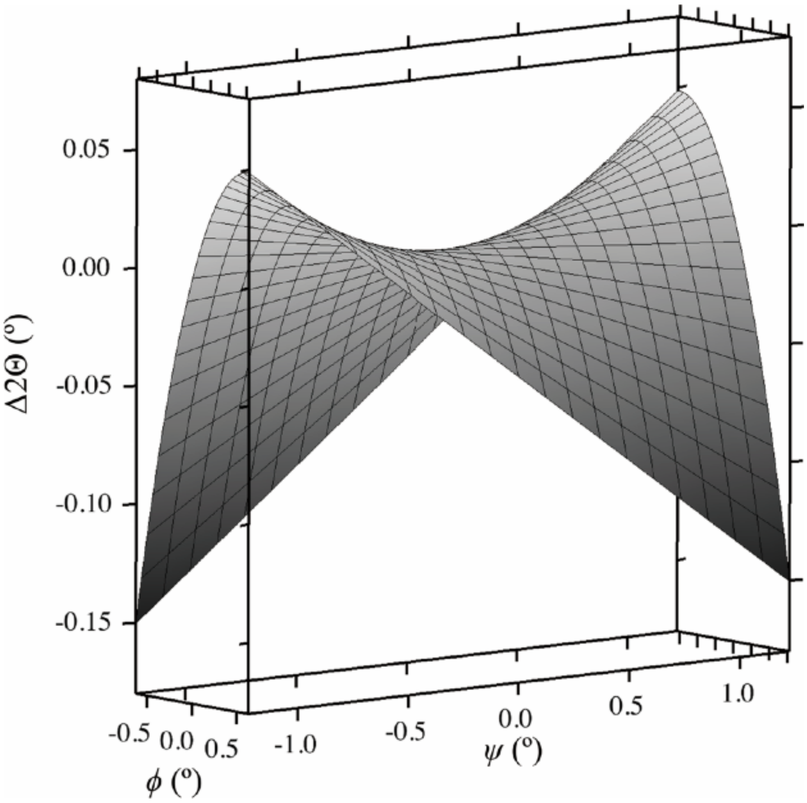

Fig. 8.1.2.5 Three dimensional view of the approximate dependence of the deviation angle $\Delta 2\Theta \equiv 2\Theta - 2\theta$ on equatorial deviation angle ϕ and half offset angle ψ, for the case $\Phi = 1.25°$ and $2\Psi = 4.89°$ and $2\Theta = 30°$.

The approximate equatorial aberration function is given by

$$\omega_{\mathrm{E}}(\Delta 2\Theta; \Theta, \Phi, \Psi) = \frac{1}{\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}} \delta\left(\Delta 2\Theta + \frac{2\phi\,(\phi+\psi)}{\tan\Theta}\right) \mathrm{d}\psi\,\mathrm{d}\phi \; . \tag{8.1.2.13}$$

Analytical expressions of the first- to fourth-order cumulants $\kappa_1, \kappa_2, \kappa_3$ and κ_4 of the approximate aberration function can be derived (Appendix 8.1.F).

$$\kappa_1 = \langle \Delta 2\Theta \rangle = -\frac{\Phi^2}{6\tan\Theta} \; , \tag{8.1.2.14}$$

$$\kappa_2 = \frac{\Phi^2}{\tan^2\Theta}\left(\frac{\Phi^2}{45} + \frac{\Psi^2}{36}\right), \tag{8.1.2.15}$$

$$\kappa_3 = -\frac{\Phi^4}{\tan^3\Theta}\left(\frac{2\Phi^2}{945} + \frac{\Psi^2}{90}\right), \tag{8.1.2.16}$$

$$\kappa_4 = -\frac{\Phi^4}{\tan^4\Theta}\left(\frac{2\Phi^4}{4725} - \frac{2\Phi^2\Psi^2}{945} - \frac{\Psi^4}{5400}\right) \tag{8.1.2.17}$$

An explicit expression about the approximate equatorial aberration function is given by (Appendix 8.1.G)

$$\omega_{\mathrm{E}}(\Delta 2\Theta; \Theta, \Phi, \Psi) = \begin{cases} \dfrac{2\tan\Theta}{\Phi\Psi} \ln \dfrac{\phi_{\mathrm{U}}}{\phi_{\mathrm{L}}} & [\Delta 2\Theta_{\mathrm{min}} < \Delta 2\Theta < \Delta 2\Theta_{\mathrm{max}}] \\ 0 & [\text{otherwise}] \end{cases}, \tag{8.1.2.18}$$

where

$$\Delta 2\Theta_{\mathrm{min}} = -\frac{\Phi^2 + \Phi\Psi}{2\tan\Theta}, \tag{8.1.2.19}$$

$$\Delta 2\Theta_{\mathrm{max}} = \begin{cases} \dfrac{\Phi^2}{8\tan\Theta} & [\Psi \le 2\Phi] \\ \dfrac{-\Phi^2 + \Phi\Psi}{2\tan\Theta} & [2\Phi < \Psi] \end{cases}, \tag{8.1.2.20}$$

$$\phi_{\mathrm{L}} = \max\left\{-\frac{\Psi}{4} + \sqrt{D}, \frac{\Psi}{4} - \sqrt{D}\right\}, \tag{8.1.2.21}$$

$$\phi_{\mathrm{U}} = \min\left\{\frac{\Phi}{2}, \frac{\Psi}{4} + \sqrt{D}\right\}, \tag{8.1.2.22}$$

$$D = \frac{\Psi^2}{16} - \frac{\Delta 2\Theta \tan\Theta}{2}. \tag{8.1.2.23}$$

The functions $\max\{a, b\}$ and $\min\{a, b\}$ in eqs. (8.1.2.21) & (8.1.2.22) return the larger and smaller values of a and b, respectively.

The instrumental function calculated by the explicit formula given by eqs. (8.1.2.18)–(8.1.2.23) for the values $2\Theta = 30°$, $\Phi = 1.25°$ and $2\Psi = 4.89°$ is shown in Fig. 8.1.2.6.

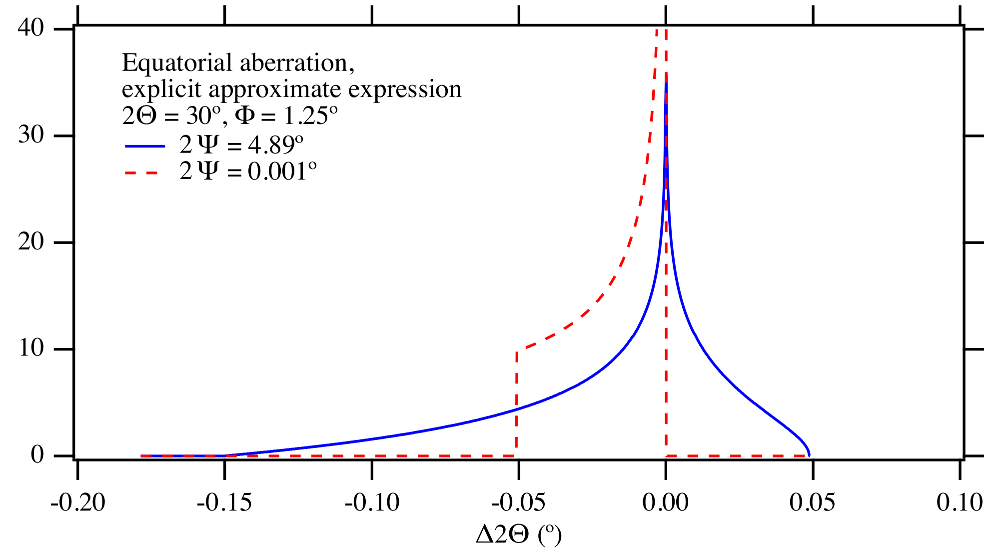

Fig. 8.1.2.6 Approximate equatorial aberration function calculated by an explicit expressions, for the case $\Phi = 1.25°$ and $2\Psi = 4.89°$, 0.01° and $2\Theta = 30°$.

8.1.2.3 Scale transform about approximate equatorial aberration

The following scale transform is applied,

$$\chi = \begin{cases} \ln \dfrac{\sec\Theta}{\sec\Theta_c} & [2\Theta_c \le 2\Theta] \\ \ln \dfrac{\tan\Theta}{\tan\Theta_c} & [2\Theta < 2\Theta_c] \end{cases}, \tag{8.1.2.24}$$

for deconvolutional treatment.

From the following relations,

$$d\chi = \left\{ \begin{array}{ll} \tan\Theta \, d\Theta & [2\Theta_c \le 2\Theta] \\ \dfrac{d\Theta}{\sin\Theta\cos\Theta} & [2\Theta < 2\Theta_c] \end{array} \right\} = \begin{cases} \dfrac{\tan\Theta \, d2\Theta}{2} & [2\Theta_c \le 2\Theta] \\ \dfrac{d2\Theta}{\sin 2\Theta} & [2\Theta < 2\Theta_c] \end{cases}, \tag{8.1.2.25}$$

$$w_E(\chi; \Theta, \Phi, \Psi)\, d\chi = \omega_E(\Delta 2\Theta; \Theta, \Phi, \Psi)\, d2\Theta , \tag{8.1.2.26}$$

the approximate equatorial aberration function on the transformed scale χ is given by

$$w_E(\chi; \Theta, \Phi, \Psi) = \frac{d2\Theta}{d\chi} \omega_E(\Delta 2\Theta; \Theta, \Phi, \Psi) = \frac{2}{\tan\Theta} \omega_E\left(\frac{2\chi}{\tan\Theta}; \Theta, \Phi, \Psi\right)$$
$$= \begin{cases} \dfrac{2}{\Phi\Psi} \ln \dfrac{\phi_U}{\phi_L} & [\chi_{min} < \chi < \chi_{max}] \\ 0 & [\text{elsewhere}] \end{cases} \tag{8.1.2.27}$$

$$\chi_{min} = \frac{\tan\Theta}{2} \Delta 2\Theta_{min} = -\frac{\Phi\Psi + \Phi^2}{4} \tag{8.1.2.28}$$

$$\chi_{\max} = \frac{\tan\Theta}{2}\Delta 2\Theta_{\max} = \begin{cases} \dfrac{\Phi\Psi - \Phi^2}{4} & [2\Phi < \Psi] \\ \dfrac{\Psi^2}{16} & [\Psi \leq 2\Phi] \end{cases} \tag{8.1.2.29}$$

$$\phi_{\mathrm{L}} = \max\left\{\frac{\Psi}{4} - \sqrt{\frac{\Psi^2}{16} - \chi}, -\frac{\Psi}{4} + \sqrt{\frac{\Psi^2}{16} - \chi}\right\} \tag{8.1.2.30}$$

$$\phi_{\mathrm{U}} = \min\left\{\frac{\Phi}{2}, \frac{\Psi}{4} + \sqrt{\frac{\Psi^2}{16} - \chi}\right\} \tag{8.1.2.31}$$

When the same scale transformation is applied to the flat-specimen aberration function:

$$\omega_{\mathrm{FS}}(\Delta 2\Theta; \Phi) = \begin{cases} \dfrac{\tan\Theta}{\Phi^2}\left(-\dfrac{2\Delta 2\Theta \tan\Theta}{\Phi^2}\right)^{-1/2} & \left[-\dfrac{\Phi^2}{2\tan\Theta} < \Delta 2\Theta < 0\right] \\ 0 & [\text{elsewhere}] \end{cases}, \tag{8.1.2.32}$$

an expression of the aberration function on the transformed scale is given by

$$w_{\mathrm{FS}}(\chi; \Phi) = \begin{cases} \dfrac{2}{\Phi^2}\left(-\dfrac{4\chi}{\Phi^2}\right)^{-1/2} & \left[-\dfrac{\Phi^2}{2\tan\Theta} < \dfrac{2\chi}{\tan\Theta} < 0\right] \\ 0 & [\text{elsewhere}] \end{cases}$$

$$= \begin{cases} \dfrac{2}{\Phi^2}\left(-\dfrac{4\chi}{\Phi^2}\right)^{-1/2} & \left[-\dfrac{\Phi^2}{4} < \chi < 0\right] \\ 0 & [\text{elsewhere}] \end{cases} \tag{8.1.2.33}$$

Appendix 8.1.A Critical diffraction angle $2\Theta_c$

As the condition $\Phi_{\mathrm{eff}} < \Phi_{\mathrm{DS}}$ is expressed by

$$\arctan\frac{(W/R)\sin\Theta}{1-(W/2R)^2} < \Phi_{\mathrm{DS}} \Leftrightarrow \frac{(W/R)\sin\Theta}{1-(W/2R)^2} < \tan\Phi_{\mathrm{DS}}$$

$$\Leftrightarrow \sin\Theta < \frac{[1-(W/2R)^2]\tan\Phi_{\mathrm{DS}}}{W/R}$$

$$\Leftrightarrow 2\Theta < 2\arcsin\frac{[1-(W/2R)^2]\tan\Phi_{\mathrm{DS}}}{W/R}.$$

Then the critical angle is given by

$$2\Theta_c = 2\arcsin\frac{[1-(W/2R)^2]\tan\Phi_{\mathrm{DS}}}{W/R}.$$

Appendix 8.1.B Effective equatorial divergence angle Φ_{eff} for lower diffraction angles

Effective equatorial divergence angle for goniometer radius R and specimen width W is given by

$$\Phi_{\text{eff}} = \arctan \frac{\sin\Theta}{\cos\Theta - W/2R} - \arctan \frac{\sin\Theta}{\cos\Theta + W/2R} = \arctan \frac{\dfrac{\sin\Theta}{\cos\Theta - W/2R} - \dfrac{\sin\Theta}{\cos\Theta + W/2R}}{1 + \dfrac{\sin^2\Theta}{\cos^2\Theta - W^2/4R^2}}$$

$$= \arctan \frac{\sin\Theta(\cos\Theta + W/2R) - \sin\Theta(\cos\Theta - W/2R)}{1 - W^2/4R^2} = \arctan \frac{(W/R)\sin\Theta}{1-(W/2R)^2}$$

Appendix 8.1.C Cumulants of flat-specimen aberration function

The first-order cumulant κ_1 of the flat-specimen aberration function

$$\omega_{\mathrm{F}}(\Delta 2\Theta;\Theta) = \begin{cases} \dfrac{1}{\Phi^2\cot\Theta}\left(-\dfrac{2\Delta 2\theta}{\Phi^2\cot\Theta}\right)^{-1/2} & \left[-\dfrac{\Phi^2\cot\Theta}{2} < \Delta 2\Theta < 0\right] \\ 0 & [\text{elsewhere}] \end{cases},$$

$$\Leftrightarrow \quad \omega_{\mathrm{F}}(z) = \frac{1}{\Phi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}} \delta\left(z + \frac{2\phi^2}{\tan\Theta}\right)\mathrm{d}\phi \tag{8.1.C.1}$$

is given by

$$\kappa_1 = \int_{-\infty}^{\infty} z\,\omega_{\mathrm{F}}(z)\,\mathrm{d}z = \frac{1}{\Phi}\int_{-\infty}^{\infty}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}} z\,\delta\left(z + \frac{2\phi^2}{\tan\Theta}\right)\mathrm{d}\phi\,\mathrm{d}z$$

$$= \frac{1}{\Phi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(-\frac{2\phi^2}{\tan\Theta}\right)\mathrm{d}\phi = -\frac{4}{\Phi\tan\Theta}\int_0^{\frac{\Phi}{2}}\phi^2\mathrm{d}\phi = -\frac{4}{\Phi\tan\Theta}\left[\frac{\phi^3}{3}\right]_0^{\frac{\Phi}{2}}$$

$$= -\frac{\Phi^2}{6\tan\Theta}. \tag{8.1.C.2}$$

The second-order cumulant is given by

$$\kappa_2 = \int_{-\infty}^{\infty} z^2\omega_{\mathrm{E}}(z)\,\mathrm{d}z - \kappa_1^2 = \frac{1}{\Phi}\int_{-\infty}^{\infty}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}} z^2\,\delta\left(z + \frac{2\phi^2}{\tan\Theta}\right)\mathrm{d}\phi\,\mathrm{d}z - \kappa_1^2$$

$$= \frac{1}{\Phi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(-\frac{2\phi^2}{\tan\Theta}\right)^2\mathrm{d}\phi - \kappa_1^2 = \frac{8}{\Phi\tan^2\Theta}\int_0^{\frac{\Phi}{2}}\phi^4\mathrm{d}\phi - \kappa_1^2$$

$$= \frac{8}{\Phi\tan^2\Theta}\left[\frac{\phi^5}{5}\right]^{\frac{\Phi}{2}} - \kappa_1^2 = \frac{\Phi^4}{20\tan^2\Theta} - \kappa_1^2 = \frac{\Phi^4}{20\tan^2\Theta} - \frac{\Phi^4}{36\tan^2\Theta}$$

$$= \frac{\Phi^4}{45\tan^2\Theta}. \tag{8.1.C.3}$$

The third-order cumulant κ_3 is given by

$$\kappa_3 = \langle z^3\rangle - 3\langle z^2\rangle\langle z\rangle + 2\langle z\rangle^3 = \langle z^3\rangle - 3\left(\langle z^2\rangle - \langle z\rangle^2\right)\langle z\rangle - \langle z\rangle^3$$

$$= \langle z^3\rangle - 3\kappa_2\kappa_1 - \kappa_1^3$$

$$= \frac{1}{\Phi}\int_{-\infty}^{\infty}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}} z^3\,\delta\left(z + \frac{2\phi^2}{\tan\Theta}\right)\mathrm{d}\phi\,\mathrm{d}z - 3\kappa_2\kappa_1 - \kappa_1^3$$

$$= \frac{1}{\Phi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(-\frac{2\phi^2}{\tan\Theta}\right)^3\mathrm{d}\phi - 3\left(\frac{\Phi^4}{45\tan^2\Theta}\right)\left(-\frac{\Phi^2}{6\tan\Theta}\right) - \left(-\frac{\Phi^2}{6\tan\Theta}\right)^3$$

$$= -\frac{16}{\Phi \tan^3\Theta}\int_0^{\frac{\Phi}{2}} \phi^6 \mathrm{d}\phi + \frac{\Phi^6}{90\tan^3\Theta} + \frac{\Phi^6}{216\tan^3\Theta}$$

$$= -\frac{\Phi^6}{56\tan^3\Theta} + \frac{17\Phi^6}{1080\tan^3\Theta}$$

$$= -\frac{2\Phi^6}{945\tan^3\Theta} \tag{8.1.C.4}$$

And the fourth-order cumulant κ_4 is given by

$$\kappa_4 = \langle z^4\rangle - 4\langle z^3\rangle\langle z\rangle - 3\langle z^2\rangle^2 + 12\langle z^2\rangle\langle z\rangle^2 - 6\langle z\rangle^4$$

$$= \langle z^4\rangle - 4\left(\langle z^3\rangle - 3\langle z^2\rangle\langle z\rangle + 2\langle z\rangle^3\right)\langle z\rangle - 12\langle z^2\rangle\langle z\rangle^2 + 8\langle z\rangle^4$$

$$-3\langle z^2\rangle^2 + 12\langle z^2\rangle\langle z\rangle^2 - 6\langle z\rangle^4$$

$$= \langle z^4\rangle - 4\kappa_3\langle z\rangle - 3\langle z^2\rangle^2 + 2\langle z\rangle^4$$

$$= \frac{1}{\Phi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(-\frac{2\phi^2}{\tan\Theta}\right)^4 \mathrm{d}\phi - 4\left(-\frac{2\Phi^6}{945\tan^3\Theta}\right)\left(-\frac{\Phi^2}{6\tan\Theta}\right) - 3\left(\frac{\Phi^4}{20\tan^2\Theta}\right)^2$$

$$+2\left(-\frac{\Phi^2}{6\tan\Theta}\right)^4$$

$$= \frac{32}{\Phi\tan^4\Theta}\int_0^{\frac{\Phi_F}{2}} \phi^8 \mathrm{d}\phi - \frac{4\Phi^8}{81\times 5\times 7\tan^4\Theta} - \frac{3\Phi^8}{16\times 25\tan^4\Theta} + \frac{\Phi^8}{8\times 81\tan^4\Theta}$$

$$= \frac{32}{\Phi\tan^4\Theta}\left[\frac{\phi^9}{9}\right]_0^{\frac{\Phi}{2}} + \frac{3\Phi^8}{8\times 81\times 5\times 7\tan^4\Theta} - \frac{3\Phi^8}{16\times 25\tan^4\Theta}$$

$$= \frac{\Phi^8}{16\times 9\tan^4\Theta} + \frac{\Phi^8}{8\times 27\times 5\times 7\tan^4\Theta} - \frac{3\Phi^8}{16\times 25\tan^4\Theta}$$

$$= \frac{107\Phi^8}{16\times 27\times 5\times 7\tan^4\Theta} - \frac{3\Phi^8}{16\times 25\tan^4\Theta} = -\frac{32\Phi^8}{16\times 27\times 25\times 7\tan^4\Theta}$$

$$= -\frac{2\Phi^8}{27\times 25\times 7\tan^4\Theta} = -\frac{2\Phi^8}{4725\tan^4\Theta}\,. \tag{8.1.C.5}$$

Appendix 8.1.D Restriction $2\Theta_c < 2\Theta$ for equatorial aberration function

Possible application of a deconvolutional method to equatorial aberration is examined. Let the critical angle $2\Theta_c$ be

$$2\Theta_c = 2\arcsin\frac{R\Phi}{W}\,, \tag{8.1.D.1}$$

and the effective divergence angle for $2\Theta < 2\Theta_c$ will be expressed by

$$\Phi_{\mathrm{eff}} = \begin{cases} \dfrac{W\sin\Theta}{R} & [2\Theta < 2\Theta_c] \\ \Phi & [2\Theta_c \le 2\Theta] \end{cases}\,, \tag{8.1.D.2}$$

and the cumulants for the approximate aberration functions are given by

$$\kappa_1 = -\frac{\Phi_{\mathrm{eff}}^2}{6\tan\Theta} = -\frac{W^2\sin^2\Theta}{6R^2\tan\Theta} = -\frac{W^2\sin\Theta\cos\Theta}{6R^2} = -\frac{W^2\sin 2\Theta}{12R^2} \tag{8.1.D.3}$$

$$\kappa_2 = \frac{\Phi_{\mathrm{eff}}^2}{\tan^2\Theta}\left(\frac{\Phi_{\mathrm{eff}}^2}{45} + \frac{\Psi^2}{144}\right) = \frac{W^2\sin^2\Theta}{R^2\tan^2\Theta}\left(\frac{W^2\sin^2\Theta}{45R^2} + \frac{\Psi^2}{144}\right) \tag{8.1.D.4}$$

$$\kappa_3 = -\frac{\Phi_{\text{eff}}^4}{\tan^3\Theta}\left(\frac{2\Phi_{\text{eff}}^2}{945} + \frac{\Psi^2}{360}\right) = -\frac{W^4\sin^4\Theta}{R^4\tan^3\Theta}\left(\frac{2W^2\sin^2\Theta}{945R^2} + \frac{\Psi^2}{360}\right)$$

$$= -\frac{2W^6\sin^3\Theta\cos^3\Theta}{945R^6} - \frac{W^4\Psi^2\sin\Theta\cos^3\Theta}{360R^4} \tag{8.1.D.5}$$

$$\kappa_4 = -\frac{\Phi_{\text{eff}}^4}{\tan^4\Theta}\left(\frac{\Phi_{\text{eff}}^4}{4725} - \frac{\Phi_{\text{eff}}^2\Psi^2}{1890} - \frac{\Psi^4}{86400}\right). \tag{8.1.D.6}$$

It is not easy to find appropriate formula for scale transformation.

It may be possible to reproduce the 1st and 3rd cumulants by using a relation

$$\left(a\sin\Theta + b\right)^3\cos^3\Theta + \left(a\sin\Theta - b\right)^3\cos^3\Theta = 2a^3\sin^3\Theta\cos^3\Theta + 6ab^2\sin\Theta\cos^3\Theta\,, \tag{8.1.D.7}$$

if the following relations are assumed,

$$2a^3 = -\frac{2W^6}{945R^6} \tag{8.1.D.8}$$

$$6ab^2 = -\frac{W^4\Psi^2}{360R^4} \tag{8.1.D.9}$$

$$a = -\frac{W^2}{\sqrt[3]{945}R^2} = -\frac{W^2}{3\sqrt[3]{35}R^2} \tag{8.1.D.10}$$

$$b^2 = -\frac{W^4\Psi^2}{360R^4}\times\frac{1}{6a} = \frac{W^4\Psi^2}{360R^4}\times\frac{3\sqrt[3]{35}R^2}{6W^2} = \frac{\sqrt[3]{35}W^2\Psi^2}{720R^2}$$

$$\Rightarrow b = \pm\frac{\sqrt[6]{35}W\Psi}{6\sqrt{20}R} \tag{8.1.D.11}$$

$$\int\frac{\sec\Theta\,\mathrm{d}2\Theta}{\left(a\sin\Theta + b\right)} = \frac{2}{a}\int\frac{\sec\Theta\,\mathrm{d}\Theta}{\left(\sin\Theta + b/a\right)} \tag{8.1.D.12}$$

$$\frac{b}{a} = \pm\frac{\sqrt[6]{35}W\Psi}{6\sqrt{20}R}\times\left(-\frac{3\sqrt[3]{35}R^2}{W^2}\right) = \mp\frac{\sqrt[6]{35^3}R\Psi}{2\sqrt{20}W} = \mp\frac{\sqrt{35}R\Psi}{2\sqrt{20}W} \tag{8.1.D.13}$$

$$\int\frac{\sec\Theta\,\mathrm{d}\Theta}{\left(\sin\Theta + c\right)} = \frac{\ln\left|c + \sin\Theta\right|}{1 - c^2} - \frac{\ln\left(1 + \sin\Theta\right)}{2 - 2c} - \frac{\ln\left(1 - \sin\Theta\right)}{2 + 2c}$$

$$= \frac{\ln\left(c + \sin\Theta\right)^2 - (1 + c)\ln\left(1 + \sin\Theta\right) - (1 - c)\ln\left(1 - \sin\Theta\right)}{2 - 2c^2} \tag{8.1.D.14}$$

$$\frac{\mathrm{d}}{\mathrm{d}\Theta}\left[\frac{1}{2 - 2c^2}\ln\frac{\left(c + \sin\Theta\right)^2}{\left(1 + \sin\Theta\right)^{1+c}\left(1 - \sin\Theta\right)^{1-c}}\right]$$

$$= \frac{1}{2 - 2c^2}\left[\frac{2\cos\Theta}{c + \sin\Theta} - \frac{(1 + c)\cos\Theta}{1 + \sin\Theta} + \frac{(1 - c)\cos\Theta}{1 - \sin\Theta}\right]$$

$$= \frac{\cos\Theta}{2 - 2c^2}$$

$$\times\frac{2 - 2\sin^2\Theta - (1 + c)\left(c + \sin\Theta\right)\left(1 - \sin\Theta\right) + (1 - c)\left(c + \sin\Theta\right)\left(1 + \sin\Theta\right)}{\left(c + \sin\Theta\right)\left(1 + \sin\Theta\right)\left(1 - \sin\Theta\right)}$$

$$= \frac{\cos\Theta}{2 - 2c^2}\times\frac{2 - 2\sin^2\Theta - \left(c + \sin\Theta\right)\left[(1 + c)\left(1 - \sin\Theta\right) - (1 - c)\left(1 + \sin\Theta\right)\right]}{\left(c + \sin\Theta\right)\cos^2\Theta}$$

$$= \frac{1}{2 - 2c^2}\times\frac{2 - 2\sin^2\Theta - \left(c + \sin\Theta\right)\left(2c - 2\sin\Theta\right)}{\left(c + \sin\Theta\right)\cos\Theta}$$

$$= \frac{1}{1-c^2} \times \frac{1-\sin^2\Theta - \left(c+\sin\Theta\right)\left(c-\sin\Theta\right)}{\left(c+\sin\Theta\right)\cos\Theta}$$

$$= \frac{1}{1-c^2} \times \frac{1-\sin^2\Theta - c^2 + \sin^2\Theta}{\left(c+\sin\Theta\right)\cos\Theta}$$

$$= \frac{1}{1-c^2} \times \frac{1-c^2}{\left(c+\sin\Theta\right)\cos\Theta}$$

$$= \frac{1}{\left(c+\sin\Theta\right)\cos\Theta} \,. \tag{8.1.D.15}$$

But it is still unclear that the above relation can be utilized, at this moment.

The restriction $2\Theta_c \le 2\Theta$ is applied here, and the scale transform $(2\Theta, Y) \to (\chi, \eta)$ should be given by

$$\chi = 2\ln\frac{\sec\Theta}{\sec\Theta_c} \tag{8.1.D.16}$$

$$\frac{d\chi}{d2\Theta} = \tan\Theta \Rightarrow \frac{d\chi}{\tan\Theta} = d2\Theta \tag{8.1.D.17}$$

$$\eta = YC(2\Theta)\tan\Theta \tag{8.1.D.18}$$

Appendix 8.1.E Derivation of approximate formula of equatorial aberration function

As shown in eq. (8.1.2.9) & eq. (8.1.2.10), an exact expression about the deviation angle $\Delta 2\Theta \equiv 2\Theta - 2\theta$ is given by

$$\Delta 2\Theta \equiv 2\Theta - 2\theta = \Theta + \psi + \phi - \arctan\frac{\sin(\Theta+\psi)}{g} \tag{8.1.E.1}$$

$$g = \cos(\Theta-\psi)\cos 2\psi + \cos(\Theta+\psi) - \frac{\sin(\Theta-\psi)\cos 2\psi}{\tan(\Theta-\psi-\phi)}, \tag{8.1.E.2}$$

$$g_0 = 2\cos\Theta - \frac{\sin\Theta}{\tan\Theta} = \cos\Theta \,. \tag{8.1.E.3}$$

One of the partial derivatives $\partial\Delta 2\Theta/\partial\phi$ is given by

$$\frac{\partial\Delta 2\Theta}{\partial\phi} = 1 - \left[1+\frac{\sin^2(\Theta+\psi)}{g^2}\right]^{-1}\left[-\frac{\sin(\Theta+\psi)}{g^2}\right]\frac{\partial g}{\partial\phi} = 1 + \frac{\sin(\Theta+\psi)}{g^2+\sin^2(\Theta+\psi)}\frac{\partial g}{\partial\phi}\,, \tag{8.1.E.4}$$

where

$$\frac{\partial g}{\partial\phi} = -\frac{\sin(\Theta-\psi)\cos 2\psi}{\sin^2(\Theta-\psi-\phi)}\,. \tag{8.1.E.5}$$

The values of $\partial g/\partial\phi$ and $\partial\Delta 2\Theta/\partial\phi$ for $\phi = 0$ and $\psi = 0$ are expressed by $\left(\partial g/\partial\phi\right)_0$ $\left(\partial\Delta 2\Theta/\partial\phi\right)_0$, and they are given by

$$\left(\frac{\partial g}{\partial\phi}\right)_0 = -\frac{1}{\sin\Theta}\,, \tag{8.1.E.6}$$

$$\left(\frac{\partial\Delta 2\Theta}{\partial\phi}\right)_0 = 1 + \frac{\sin\Theta}{g_0^2+\sin^2\Theta}\left(\frac{\partial g}{\partial\phi}\right)_0 = 1 + \frac{\sin\Theta}{\cos^2\Theta+\sin^2\Theta}\times\left(-\frac{1}{\sin\Theta}\right) = 0\,. \tag{8.1.E.7}$$

Another partial derivative $\partial\Delta 2\Theta/\partial\phi$ is given by

$$\frac{\partial\Delta 2\Theta}{\partial\psi} = 1 - \left[1+\frac{\sin^2(\Theta+\psi)}{g^2}\right]^{-1}\left[\frac{\cos(\Theta+\psi)}{g} - \frac{\sin(\Theta+\psi)}{g^2}\frac{\partial g}{\partial\psi}\right]$$

$$= 1 - \frac{\cos(\Theta+\psi)g - \sin(\Theta+\psi)\left(\partial g/\partial\psi\right)}{g^2+\sin^2(\Theta+\psi)}\,, \tag{8.1.E.8}$$

where

$$\frac{\partial g}{\partial \psi} = \sin(\Theta - \psi)\,\cos 2\psi - 2\cos(\Theta - \psi)\,\sin 2\psi - \sin(\Theta + \psi)$$

$$-\frac{-\cos(\Theta - \psi)\,\cos 2\psi - 2\sin(\Theta - \psi)\,\sin 2\psi}{\tan(\Theta - \psi - \phi)} - \frac{\sin(\Theta - \psi)\,\cos 2\psi}{\sin^2(\Theta - \psi - \phi)} \,. \tag{8.1.E.9}$$

The values of $\partial g/\partial \psi$ and $\partial \Delta 2\Theta/\partial \psi$ for $\phi = 0$ and $\psi = 0$, expressed by $\left(\partial g/\partial \psi\right)_0$ and $\left(\partial \Delta 2\Theta/\partial \psi\right)_0$, are given by

$$\left(\frac{\partial g}{\partial \psi}\right)_0 = \frac{\cos\Theta}{\tan\Theta} - \frac{1}{\sin\Theta} = \frac{\cos^2\Theta - 1}{\sin\Theta} = -\sin\Theta \,, \tag{8.1.E.10}$$

$$\left(\frac{\partial \Delta 2\Theta}{\partial \psi}\right)_0 = 1 - \frac{\cos\Theta\, g_0 - \sin\Theta\left(\partial g/\partial \psi\right)_0}{g_0^2 + \sin^2\Theta} = 1 - \frac{\cos^2\Theta - \sin\Theta \times \left(-\sin\Theta\right)}{\cos^2\Theta + \sin^2\Theta} = 1 - 1 = 0 \tag{8.1.E.11}$$

One of the second-order partial derivatives $\partial^2 \Delta 2\Theta/\partial \phi^2$ is given by

$$\frac{\partial^2 \Delta 2\Theta}{\partial \phi^2} = \frac{\partial}{\partial \phi}\left[1 + \frac{\sin(\Theta + \psi)}{g^2 + \sin^2(\Theta + \psi)}\frac{\partial g}{\partial \phi}\right] = -\frac{2\sin(\Theta + \psi)\, g}{\left[g^2 + \sin^2(\Theta + \psi)\right]^2}\left(\frac{\partial g}{\partial \phi}\right)^2 + \frac{\sin(\Theta + \psi)}{g^2 + \sin^2(\Theta + \psi)}\frac{\partial^2 g}{\partial \phi^2} \tag{8.1.E.12}$$

where

$$\frac{\partial^2 g}{\partial \phi^2} = -\frac{\partial}{\partial \phi}\frac{\sin(\Theta - \psi)\,\cos 2\psi}{\sin^2(\Theta - \psi - \phi)} = -\frac{2\sin(\Theta - \psi)\,\cos 2\psi\,\cos(\Theta - \psi - \phi)}{\sin^3(\Theta - \psi - \phi)} \,. \tag{8.1.E.12}$$

The values of $\partial^2 g/\partial \phi^2$ and $\partial^2 \Delta 2\Theta/\partial \phi^2$ for $\phi = 0$ and $\psi = 0$, expressed by $\left(\partial^2 g/\partial \phi^2\right)_0$ and $\left(\partial^2 \Delta 2\Theta/\partial \phi^2\right)_0$, are given by

$$\left(\frac{\partial^2 g}{\partial \phi^2}\right)_0 = -\frac{2\cos\Theta}{\sin^2\Theta} \,, \tag{8.1.E.13}$$

$$\left(\frac{\partial^2 \Delta 2\Theta}{\partial \phi^2}\right)_0 = -2\sin\Theta\,\cos\Theta\left(-\frac{1}{\sin\Theta}\right)^2 + \sin\Theta\left(-\frac{2\cos\Theta}{\sin^2\Theta}\right) = -\frac{4}{\tan\Theta} \,. \tag{8.1.E.14}$$

Another second-order derivative $\partial^2 \Delta 2\Theta/\partial \psi \partial \phi$ is given by

$$\frac{\partial^2 \Delta 2\Theta}{\partial \psi \partial \phi} = \frac{\partial}{\partial \psi}\left[1 + \frac{\sin(\Theta + \psi)}{g^2 + \sin^2(\Theta + \psi)}\frac{\partial g}{\partial \phi}\right]$$

$$= \frac{\cos(\Theta + \psi)}{g^2 + \sin^2(\Theta + \psi)}\frac{\partial g}{\partial \phi} - \frac{\sin(\Theta + \psi)}{\left[g^2 + \sin^2(\Theta + \psi)\right]^2}\left[2g\frac{\partial g}{\partial \psi} + 2\sin(\Theta + \psi)\,\cos(\Theta + \psi)\right]\frac{\partial g}{\partial \phi}$$

$$+\frac{\sin(\Theta + \psi)}{g^2 + \sin^2(\Theta + \psi)}\frac{\partial^2 g}{\partial \psi \partial \phi} \,, \tag{8.1.E.15}$$

where

$$\frac{\partial^2 g}{\partial \psi \partial \phi} = -\frac{\partial}{\partial \psi}\frac{\sin(\Theta - \psi)\,\cos 2\psi}{\sin^2(\Theta - \psi - \phi)}$$

$$= \frac{\cos(\Theta - \psi)\,\cos 2\psi + 2\sin(\Theta - \psi)\,\sin 2\psi}{\sin^2(\Theta - \psi - \phi)} - \frac{2\sin(\Theta - \psi)\,\cos 2\psi\,\cos(\Theta - \psi - \phi)}{\sin^3(\Theta - \psi - \phi)} \,. \tag{8.1.E.16}$$

The values of $\partial^2 g/\partial \phi \partial \psi$ and $\partial^2 \Delta 2\Theta/\partial \phi \partial \psi$ for $\phi = 0$ and $\psi = 0$, expressed by $\left(\partial^2 g/\partial \phi \partial \psi\right)_0$ and $\left(\partial^2 \Delta 2\Theta/\partial \phi \partial \psi\right)_0$, are given by

$$\left(\frac{\partial^2 g}{\partial \psi \partial \phi}\right)_0 = \frac{\cos\Theta}{\sin^2\Theta} - \frac{2\cos\Theta}{\sin^2\Theta} = -\frac{\cos\Theta}{\sin^2\Theta} \tag{8.1.E.17}$$

$$\left(\frac{\partial^2\Delta 2\Theta}{\partial\psi\partial\phi}\right)_0 = \cos\Theta\left(-\frac{1}{\sin\Theta}\right) - \sin\Theta\left[2\cos\Theta\left(-\sin\Theta\right) + 2\sin\Theta\,\cos\Theta\right]\left(-\frac{1}{\sin\Theta}\right)$$
$$+\sin\Theta\left(-\frac{\cos\Theta}{\sin^2\Theta}\right)$$
$$= -\frac{2}{\tan\Theta}\,. \tag{8.1.E.18}$$

Finally, $\partial^2\Delta 2\Theta/\partial\psi^2$ is given by

$$\frac{\partial^2\Delta 2\Theta}{\partial\psi^2} = \frac{\partial}{\partial\psi}\left[1 - \frac{\cos(\Theta+\psi)g - \sin(\Theta+\psi)\big(\partial g/\partial\psi\big)}{g^2 + \sin^2(\Theta+\psi)}\right]$$
$$= -\frac{-\sin(\Theta+\psi)g + \cos(\Theta+\psi)\big(\partial g/\partial\psi\big) - \cos(\Theta+\psi)\big(\partial g/\partial\psi\big) - \sin(\Theta+\psi)\Big(\partial^2 g/\partial\psi^2\Big)}{g^2 + \sin^2(\Theta+\psi)}$$
$$+\frac{\cos(\Theta+\psi)g - \sin(\Theta+\psi)\big(\partial g/\partial\psi\big)}{\left[g^2 + \sin^2(\Theta+\psi)\right]^2}\left[2g\frac{\partial g}{\partial\psi} + 2\sin(\Theta+\psi)\,\cos(\Theta+\psi)\right]$$
$$= -\frac{-\sin(\Theta+\psi)g - \sin(\Theta+\psi)\Big(\partial^2 g/\partial\psi^2\Big)}{g^2 + \sin^2(\Theta+\psi)}$$
$$+\frac{\cos(\Theta+\psi)g - \sin(\Theta+\psi)\big(\partial g/\partial\psi\big)}{\left[g^2 + \sin^2(\Theta+\psi)\right]^2}\left[2g\frac{\partial g}{\partial\psi} + 2\sin(\Theta+\psi)\,\cos(\Theta+\psi)\right]\,, \tag{8.1.E.19}$$

where

$$\frac{\partial^2 g}{\partial\psi^2} = \frac{\partial}{\partial\psi}\Big[\sin(\Theta-\psi)\,\cos 2\psi - 2\cos(\Theta-\psi)\,\sin 2\psi - \sin(\Theta+\psi)$$
$$-\frac{-\cos(\Theta-\psi)\,\cos 2\psi - 2\sin(\Theta-\psi)\,\sin 2\psi}{\tan(\Theta-\psi-\phi)} - \frac{\sin(\Theta-\psi)\,\cos 2\psi}{\sin^2(\Theta-\psi-\phi)}\Big]$$
$$= \frac{\partial}{\partial\psi}\Big[-\sin(\psi-\Theta)\,\cos 2\psi - 2\cos(\psi-\Theta)\,\sin 2\psi - \sin(\psi+\Theta)$$
$$-\frac{\cos(\psi-\Theta)\,\cos 2\psi - 2\sin(\psi-\Theta)\,\sin 2\psi}{\tan(\psi+\phi-\Theta)} + \frac{\sin(\psi-\Theta)\,\cos 2\psi}{\sin^2(\psi+\phi-\Theta)}\Big]$$
$$= -\cos(\psi-\Theta)\,\cos 2\psi + 2\sin(\psi-\Theta)\,\sin 2\psi$$
$$+2\sin(\psi-\Theta)\,\sin 2\psi - 4\cos(\psi-\Theta)\,\cos 2\psi$$
$$-\cos(\psi+\Theta)$$
$$-\frac{-\sin(\psi-\Theta)\,\cos 2\psi - 2\cos(\psi-\Theta)\,\sin 2\psi - 2\cos(\psi-\Theta)\,\sin 2\psi - 4\sin(\psi-\Theta)\,\cos 2\psi}{\tan(\psi+\phi-\Theta)}$$
$$+\frac{\cos(\psi-\Theta)\,\cos 2\psi - 2\sin(\psi-\Theta)\,\sin 2\psi}{\sin^2(\psi+\phi-\Theta)}$$
$$+\frac{\cos(\psi-\Theta)\,\cos 2\psi - 2\sin(\psi-\Theta)\,\sin 2\psi}{\sin^2(\psi+\phi-\Theta)} - \frac{2\sin(\psi-\Theta)\,\cos 2\psi\,\cos(\psi+\phi-\Theta)}{\sin^3(\psi+\phi-\Theta)}$$
$$= -5\cos(\psi-\Theta)\,\cos 2\psi + 4\sin(\psi-\Theta)\,\sin 2\psi - \cos(\psi+\Theta)$$
$$+\frac{5\sin(\psi-\Theta)\,\cos 2\psi + 4\cos(\psi-\Theta)\,\sin 2\psi}{\tan(\psi+\phi-\Theta)} + \frac{\cos(\psi-\Theta)\,\cos 2\psi - 2\sin(\psi-\Theta)\,\sin 2\psi}{\sin^2(\psi+\phi-\Theta)}$$
$$+\frac{\cos(\psi-\Theta)\,\cos 2\psi - 2\sin(\psi-\Theta)\,\sin 2\psi}{\sin^2(\psi+\phi-\Theta)} - \frac{2\sin(\psi-\Theta)\,\cos 2\psi\,\cos(\psi+\phi-\Theta)}{\sin^3(\psi+\phi-\Theta)}$$
$$= -5\cos(\psi-\Theta)\,\cos 2\psi + 4\sin(\psi-\Theta)\,\sin 2\psi - \cos(\psi+\Theta)$$

$$+\frac{5\sin(\psi-\Theta)\cos 2\psi+4\cos(\psi-\Theta)\sin 2\psi}{\tan(\psi+\phi-\Theta)}+\frac{2\cos(\psi-\Theta)\cos 2\psi-4\sin(\psi-\Theta)\sin 2\psi}{\sin^2(\psi+\phi-\Theta)}$$
$$-\frac{2\sin(\psi-\Theta)\cos 2\psi\ \cos(\psi+\phi-\Theta)}{\sin^3(\psi+\phi-\Theta)} \tag{8.1.E.12}$$

The values of $\partial^2 g/\partial\psi^2$ and $\partial^2\Delta 2\Theta/\partial\psi^2$ for $\phi=0$ and $\psi=0$, expressed by $\left(\partial^2 g/\partial\psi^2\right)_0$ and $\left(\partial^2\Delta 2\Theta/\partial\psi^2\right)_0$, are given by

$$\left(\frac{\partial^2 g}{\partial\psi^2}\right)_0=-6\cos\Theta+\frac{5\sin\Theta}{\tan\Theta}+\frac{2\cos\Theta}{\sin^2\Theta}-\frac{2\sin\Theta\cos\Theta}{\sin^3\Theta}$$
$$=-6\cos\Theta+5\cos\Theta+\frac{2\cos\Theta}{\sin^2\Theta}-\frac{2\cos\Theta}{\sin^2\Theta}=-\cos\Theta \tag{8.1.E.13}$$

$$\left(\frac{\partial^2\Delta 2\Theta}{\partial\psi^2}\right)_0=-\frac{-\sin\Theta\, g_0-\sin\Theta\left(\partial^2 g/\partial\psi^2\right)_0}{g_0^2+\sin^2\Theta}$$
$$+\frac{\cos\Theta\, g_0-\sin\Theta\left(\partial g/\partial\psi\right)_0}{\left(g_0^2+\sin^2\Theta\right)^2}\left[2g_0\left(\frac{\partial g}{\partial\psi}\right)_0+2\sin\Theta\cos\Theta\right]$$
$$=-\frac{-\sin\Theta\cos\Theta-\sin\Theta\,(-\cos\Theta)}{\cos^2\Theta+\sin^2\Theta}$$
$$+\frac{-\cos^2\Theta-\sin\Theta\,(-\sin\Theta)}{\left(\cos^2\Theta+\sin^2\Theta\right)^2}\left[2\cos\Theta\,(-\sin\Theta)+2\sin\Theta\cos\Theta\right]$$
$$=0\,. \tag{8.1.E.14}$$

In summary, following relations have been found,

$$(\Delta 2\Theta)_0=0,\left(\frac{\partial\Delta 2\Theta}{\partial\phi}\right)_0=0,\left(\frac{\partial\Delta 2\Theta}{\partial\psi}\right)_0=0,$$
$$\left(\frac{\partial^2\Delta 2\Theta}{\partial\phi^2}\right)_0=-\frac{4}{\tan\Theta},\left(\frac{\partial^2\Delta 2\Theta}{\partial\phi\,\partial\psi}\right)_0=-\frac{2}{\tan\Theta},\left(\frac{\partial^2\Delta 2\Theta}{\partial\psi^2}\right)_0=0 \tag{8.1.E.15}$$

The dependence of the deviation angle $\Delta 2\Theta$ on ϕ and ψ is approximated by

$$\Delta 2\Theta\approx(\Delta 2\Theta)_0+\left(\frac{\partial\Delta 2\Theta}{\partial\phi}\right)_0\phi+\left(\frac{\partial\Delta 2\Theta}{\partial\psi}\right)_0\psi$$
$$+\left(\frac{\partial^2\Delta 2\Theta}{\partial\phi^2}\right)_0\frac{\phi^2}{2}+\left(\frac{\partial^2\Delta 2\Theta}{\partial\phi\,\partial\phi}\right)_0\phi\psi+\left(\frac{\partial^2\Delta 2\Theta}{\partial\psi^2}\right)_0\frac{\psi^2}{2}$$
$$=-\frac{2(\phi^2+\phi\psi)}{\tan\theta} \tag{8.1.E.16}$$

Appendix 8.1.F Cumulants of approximate equatorial aberration functions

The 1st order cumulant κ_1 of the approximate equatorial aberration function is given by

$$\kappa_1=\int_{-\infty}^{\infty}z\,w_{\mathrm{E}}(z)\,\mathrm{d}z=\frac{1}{\Phi\Psi}\int_{-\infty}^{\infty}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}z\,\delta\left(z+\frac{2\phi^2+2\phi\psi}{\tan\Theta}\right)\mathrm{d}\psi\,\mathrm{d}\phi\,\mathrm{d}z$$
$$=\frac{1}{\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}\left(-\frac{2\phi^2+2\phi\psi}{\tan\Theta}\right)\mathrm{d}\psi\,\mathrm{d}\phi=-\frac{4}{\Phi\Psi\tan\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{0}^{\frac{\Psi}{2}}\phi^2\mathrm{d}\psi\,\mathrm{d}\phi$$

$$= -\frac{4}{\Phi\Psi\tan\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left[\phi^2\psi\right]_0^{\frac{\Psi}{2}}\mathrm{d}\phi = -\frac{2}{\Phi\tan\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\phi^2\mathrm{d}\phi = -\frac{4}{\Phi\tan\Theta}\int_0^{\frac{\Phi}{2}}\phi^2\mathrm{d}\phi$$

$$= -\frac{4}{\Phi\tan\Theta}\left[\frac{\phi^3}{3}\right]_0^{\frac{\Phi}{2}} = -\frac{4}{\Phi\tan\Theta}\left(\frac{\Phi^3}{24}\right) = -\frac{\Phi^2}{6\tan\Theta} \tag{8.1.F.1}$$

The average of squared variable $\langle z^2\rangle$ is given by

$$\langle z^2\rangle = \int_{-\infty}^{\infty} z^2\omega_{\mathrm{E}}(z)\,\mathrm{d}z = \frac{1}{\Phi\Psi}\int_{-\infty}^{\infty}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}} z^2\,\delta\left(z+\frac{2\phi^2+2\phi\psi}{\tan\Theta}\right)\mathrm{d}\psi\,\mathrm{d}\phi\,\mathrm{d}z$$

$$= \frac{1}{\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}\left(-\frac{2\phi^2+2\phi\psi}{\tan\Theta}\right)^2\mathrm{d}\psi\,\mathrm{d}\phi = \frac{4}{\Phi\Psi\tan^2\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}\left(\phi^4+2\phi^3\psi+\phi^2\psi^2\right)\mathrm{d}\psi\,\mathrm{d}\phi$$

$$= \frac{8}{\Phi\Psi\tan^2\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left[\phi^4\psi+\frac{\phi^2\psi^3}{3}\right]_0^{\frac{\Psi}{2}}\mathrm{d}\phi = \frac{8}{\Phi\Psi\tan^2\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(\frac{\phi^4\Psi}{2}+\frac{\phi^2\Psi^3}{24}\right)\mathrm{d}\phi$$

$$= \frac{1}{\Phi\tan^2\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(4\phi^4+\frac{\phi^2\Psi^2}{3}\right)\mathrm{d}\phi = \frac{2}{\Phi\tan^2\Theta}\int_0^{\frac{\Phi}{2}}\left(4\phi^4+\frac{\phi^2\Psi^2}{3}\right)\mathrm{d}\phi$$

$$= \frac{2}{\Phi\tan^2\Theta}\left[\frac{4\phi^5}{5}+\frac{\phi^3\Psi^2}{9}\right]_0^{\frac{\Phi}{2}} = \frac{2}{\Phi\tan^2\Theta}\left(\frac{\Phi^5}{40}+\frac{\Phi^3\Psi^2}{72}\right) = \frac{1}{\tan^2\Theta}\left(\frac{\Phi^4}{20}+\frac{\Phi^2\Psi^2}{36}\right) \tag{8.1.F.2}$$

Then the second order cumulant κ_2 is given by

$$\kappa_2 = \int_{-\infty}^{\infty} z^2\omega_{\mathrm{E}}(z)\,\mathrm{d}z - \left[\int_{-\infty}^{\infty} z\,\omega_{\mathrm{E}}(z)\,\mathrm{d}z\right]^2 = \frac{1}{\tan^2\Theta}\left(\frac{\Phi^4}{20}+\frac{\Phi^2\Psi^2}{36}\right) - \frac{\Phi^4}{36\tan^2\Theta}$$

$$= \frac{1}{\tan^2\Theta}\left[\frac{(9-5)\,\Phi^4}{4\times5\times9}+\frac{\Phi^2\Psi^2}{36}\right] = \frac{1}{\tan^2\Theta}\left(\frac{\Phi^4}{45}+\frac{\Phi^2\Psi^2}{36}\right). \tag{8.1.F.3}$$

The average of cubic variable $\langle z^3\rangle$ is given by

$$\langle z^3\rangle = \int_{-\infty}^{\infty} z^3 w_{\mathrm{E}}(z)\,\mathrm{d}z = \frac{1}{\Phi\Psi}\int_{-\infty}^{\infty}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}} z^3\,\delta\left(z+\frac{2\phi^2+2\phi\psi}{\tan\Theta}\right)\mathrm{d}\psi\,\mathrm{d}\phi\,\mathrm{d}z$$

$$= \frac{1}{\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}\left(-\frac{2\phi^2+2\phi\psi}{\tan\Theta}\right)^3\mathrm{d}\psi\,\mathrm{d}\phi$$

$$= -\frac{8}{\Phi\Psi\tan^3\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}\left(\phi^6+3\phi^5\psi+3\phi^4\psi^2+\phi^3\psi^3\right)\mathrm{d}\psi\,\mathrm{d}\phi$$

$$= -\frac{16}{\Phi\Psi\tan^3\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left[\phi^6\psi+\phi^4\psi^3\right]_0^{\frac{\Psi}{2}}\mathrm{d}\phi = -\frac{16}{\Phi\Psi\tan^3\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(\frac{\phi^6\Psi}{2}+\frac{\phi^4\Psi^3}{8}\right)\mathrm{d}\phi$$

$$= -\frac{1}{\Phi\tan^3\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(8\phi^6+2\phi^4\Psi^2\right)\mathrm{d}\phi = -\frac{1}{\Phi\tan^3\Theta}\int_0^{\frac{\Phi}{2}}\left(16\phi^6+4\phi^4\Psi^2\right)\mathrm{d}\phi$$

$$= -\frac{1}{\Phi\tan^3\Theta}\left[\frac{16\phi^7}{7}+\frac{4\phi^5\Psi^2}{5}\right]_0^{\frac{\Phi}{2}}$$

$$= -\frac{1}{\Phi\tan^3\Theta}\left(\frac{\Phi^7}{7\times 8}+\frac{\Phi^5\Psi^2}{5\times 8}\right) = -\frac{1}{\tan^3\Theta}\left(\frac{\Phi^6}{56}+\frac{\Phi^4\Psi^2}{40}\right) \tag{8.1.F.4}$$

The 3rd order cumulant κ_3 is given by

$$\kappa_3 = \int_{-\infty}^{\infty} z^3 w_{\mathrm{E}}(z)\,\mathrm{d}z - 3\left[\int_{-\infty}^{\infty} z^2 w_{\mathrm{E}}(z)\,\mathrm{d}z\right]\left[\int_{-\infty}^{\infty} z\,w_{\mathrm{E}}(z)\,\mathrm{d}z\right] + 2\left[\int_{-\infty}^{\infty} z\,w_{\mathrm{E}}(z)\,\mathrm{d}z\right]^3$$

$$= -\frac{1}{\tan^3\Theta}\left(\frac{\Phi^6}{56}+\frac{\Phi^4\Psi^2}{40}\right) - 3\left[\frac{1}{\tan^2\Theta}\left(\frac{\Phi^4}{20}+\frac{\Phi^2\Psi^2}{36}\right)\right]\left(-\frac{\Phi^2}{6\tan\Theta}\right)$$

$$+2\left(-\frac{\Phi^2}{6\tan\Theta}\right)^3$$

$$= -\frac{1}{\tan^3\Theta}\left(\frac{\Phi^6}{56}+\frac{\Phi^4\Psi^2}{40}-\frac{\Phi^6}{40}-\frac{\Phi^4\Psi^2}{72}+\frac{\Phi^6}{108}\right)$$

$$= -\frac{1}{\tan^3\Theta}\left(\frac{\Phi^6}{8\times 7}+\frac{\Phi^4\Psi^2}{8\times 5}-\frac{\Phi^6}{8\times 5}-\frac{\Phi^4\Psi^2}{8\times 9}+\frac{\Phi^6}{4\times 27}\right)$$

$$= -\frac{1}{\tan^3\Theta}\left[\frac{(135-189+70)\Phi^6}{8\times 27\times 5\times 7}+\frac{(9-5)\Phi^4\Psi^2}{8\times 9\times 5}\right]$$

$$= -\frac{1}{\tan^3\Theta}\left(\frac{2\Phi^6}{27\times 5\times 7}+\frac{\Phi^4\Psi^2}{2\times 9\times 5}\right) = -\frac{1}{\tan^3\Theta}\left(\frac{2\Phi^6}{945}+\frac{\Phi^4\Psi^2}{90}\right). \tag{8.1.F.5}$$

The average of the fourth power of the variable $\langle z^4\rangle$ is given by

$$\langle z^4\rangle = \int_{-\infty}^{\infty} z^4 \omega_{\mathrm{E}}(z)\,\mathrm{d}z = \frac{1}{\Phi\Psi}\int_{-\infty}^{\infty}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}} z^4\,\delta\left(z+\frac{2\phi^2+2\phi\psi}{\tan\Theta}\right)\mathrm{d}\psi\,\mathrm{d}\phi\,\mathrm{d}z$$

$$= \frac{1}{\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}\left(-\frac{2\phi^2+2\phi\psi}{\tan\Theta}\right)^4\mathrm{d}\psi\,\mathrm{d}\phi$$

$$= \frac{16}{\Phi\Psi\tan^4\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}\left(\phi^8+4\phi^7\psi+6\phi^6\psi^2+4\phi^5\psi^3+\phi^4\psi^4\right)\mathrm{d}\psi\,\mathrm{d}\phi$$

$$= \frac{32}{\Phi\Psi\tan^4\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left[\phi^8\psi+2\phi^6\psi^3+\frac{\phi^4\psi^5}{5}\right]_0^{\frac{\Psi}{2}}\mathrm{d}\phi = \frac{32}{\Phi\Psi\tan^4\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(\frac{\phi^8\Psi}{2}+\frac{\phi^6\Psi^3}{4}+\frac{\phi^4\Psi^3}{160}\right)\mathrm{d}\phi$$

$$= \frac{1}{\Phi\tan^4\Theta}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\left(16\phi^8+8\phi^6\Psi^2+\frac{\phi^4\Psi^4}{5}\right)\mathrm{d}\phi = \frac{2}{\Phi\tan^4\Theta}\left[\frac{16\phi^9}{9}+\frac{8\phi^7\Psi^2}{7}+\frac{\phi^5\Psi^4}{25}\right]_0^{\frac{\Phi}{2}}$$

$$= \frac{1}{\Phi\tan^4\Theta}\left(\frac{\Phi^9}{16\times 9}+\frac{\Phi^7\Psi^2}{8\times 7}+\frac{\Phi^5\Psi^4}{16\times 25}\right) = \frac{\Phi^4}{\tan^4\Theta}\left(\frac{\Phi^4}{16\times 9}+\frac{\Phi^2\Psi^2}{8\times 7}+\frac{\Psi^4}{16\times 25}\right), \tag{8.1.F.6}$$

And the 4th order cumulant is given by

$$\kappa_4 = \langle z^4\rangle - 4\langle z^3\rangle\langle z\rangle - 3\langle z^2\rangle^2 + 12\langle z^2\rangle\langle z\rangle^2 - 6\langle z\rangle^4$$

$$= \frac{\Phi^4}{\tan^4\Theta}\left(\frac{\Phi^4}{16\times 9}+\frac{\Phi^2\Psi^2}{8\times 7}+\frac{\Psi^4}{16\times 25}\right) - 4\left[-\frac{1}{\tan^3\Theta}\left(\frac{\Phi^6}{56}+\frac{\Phi^4\Psi^2}{40}\right)\right]\left(-\frac{\Phi^2}{6\tan\Theta}\right)$$

$$-3\left[\frac{1}{\tan^2\Theta}\left(\frac{\Phi^4}{20}+\frac{\Phi^2\Psi^2}{36}\right)\right]^2+12\left[\frac{1}{\tan^2\Theta}\left(\frac{\Phi^4}{20}+\frac{\Phi^2\Psi^2}{36}\right)\right]\left(-\frac{\Phi^2}{6\tan\Theta}\right)^2-6\left(-\frac{\Phi^2}{6\tan\Theta}\right)^4$$

$$=\frac{\Phi^4}{\tan^4\Theta}\left(\frac{\Phi^4}{16\times 9}+\frac{\Phi^2\Psi^2}{8\times 7}+\frac{\Psi^4}{16\times 25}\right)+\frac{\Phi^4}{\tan^4\Theta}\left(-\frac{\Phi^4}{4\times 3\times 7}-\frac{\Phi^2\Psi^2}{4\times 3\times 5}\right)$$

$$-\frac{3\Phi^4}{\tan^4\Theta}\left(\frac{\Phi^2}{4\times 5}+\frac{\Psi^2}{4\times 9}\right)^2+\frac{\Phi^4}{\tan^2\Theta}\left(\frac{\Phi^4}{4\times 3\times 5}+\frac{\Phi^2\Psi^2}{4\times 27}\right)-\frac{\Phi^8}{8\times 27\tan^4\Theta}$$

$$=\frac{\Phi^4}{\tan^4\Theta}\left(\frac{\Phi^4}{16\times 9}+\frac{\Phi^2\Psi^2}{8\times 7}+\frac{\Psi^4}{16\times 25}\right)+\frac{\Phi^4}{\tan^4\Theta}\left(-\frac{\Phi^4}{4\times 3\times 7}-\frac{\Phi^2\Psi^2}{4\times 3\times 5}\right)$$

$$-\frac{\Phi^4}{\tan^4\Theta}\left(\frac{3\Phi^2}{16\times 25}+\frac{\Phi^2\Psi^2}{8\times 3\times 5}+\frac{\Psi^4}{16\times 27}\right)+\frac{\Phi^4}{\tan^2\Theta}\left(\frac{\Phi^4}{4\times 3\times 5}+\frac{\Phi^2\Psi^2}{4\times 27}\right)-\frac{\Phi^8}{8\times 27\tan^4\Theta}$$

$$=\frac{\Phi^8}{16\times 9\tan^4\Theta}+\frac{\Phi^6\Psi^2}{8\times 7\tan^4\Theta}+\frac{\Phi^4\Psi^4}{16\times 25\tan^4\Theta}-\frac{\Phi^8}{4\times 3\times 7\tan^4\Theta}-\frac{\Phi^6\Psi^2}{4\times 3\times 5\tan^4\Theta}-\frac{3\Phi^8}{16\times 25\tan^4\Theta}$$

$$-\frac{\Phi^6\Psi^2}{8\times 3\times 5\tan^4\Theta}-\frac{\Phi^4\Psi^4}{16\times 27\tan^4\Theta}+\frac{\Phi^8}{4\times 3\times 5\tan^4\Theta}+\frac{\Phi^6\Psi^2}{4\times 27\tan^4\Theta}-\frac{\Phi^8}{8\times 27\tan^4\Theta}$$

$$=\frac{\Phi^8}{16\times 9\tan^4\Theta}-\frac{\Phi^8}{4\times 3\times 7\tan^4\Theta}-\frac{3\Phi^8}{16\times 25\tan^4\Theta}+\frac{\Phi^8}{4\times 3\times 5\tan^4\Theta}-\frac{\Phi^8}{8\times 27\tan^4\Theta}$$

$$+\frac{\Phi^6\Psi^2}{8\times 7\tan^4\Theta}-\frac{\Phi^6\Psi^2}{4\times 3\times 5\tan^4\Theta}-\frac{\Phi^6\Psi^2}{8\times 3\times 5\tan^4\Theta}+\frac{\Phi^6\Psi^2}{4\times 27\tan^4\Theta}$$

$$+\frac{\Phi^4\Psi^4}{16\times 25\tan^4\Theta}-\frac{\Phi^4\Psi^4}{16\times 27\tan^4\Theta}$$

$$=\frac{\Phi^8\left(3\times 25\times 7-4\times 9\times 25-81\times 7+4\times 9\times 5\times 7-2\times 25\times 7\right)}{16\times 27\times 25\times 7\tan^4\Theta}$$

$$+\frac{\Phi^6\Psi^2\left(27\times 5-2\times 9\times 7-9\times 7+2\times 5\times 7\right)}{8\times 27\times 5\times 7\tan^4\Theta}+\frac{\Phi^4\Psi^4\left(27-25\right)}{16\times 27\times 25\tan^4\Theta}$$

$$=-\frac{32\Phi^8}{16\times 81\times 25\times 7\tan^4\Theta}+\frac{16\Phi^6\Psi^2}{8\times 27\times 5\times 7\tan^4\Theta}+\frac{2\Phi^4\Psi^4}{16\times 27\times 25\tan^4\Theta}$$

$$=-\frac{2\Phi^8}{27\times 25\times 7\tan^4\Theta}+\frac{2\Phi^6\Psi^2}{27\times 5\times 7\tan^4\Theta}+\frac{\Phi^4\Psi^4}{8\times 27\times 25\tan^4\Theta}$$

$$=-\frac{1}{\tan^4\Theta}\left(\frac{2\Phi^8}{4725}-\frac{2\Phi^6\Psi^2}{945}-\frac{\Phi^4\Psi^4}{5400}\right) \tag{8.1.F.7}$$

Appendix 8.1.G Explicit formula of approximate equatorial aberration function

The approximate equatorial aberration function is given by

$$w_{\mathrm{E}}(z;\Theta,\phi,\psi)=\frac{2}{\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{-\frac{\Psi}{2}}^{\frac{\Psi}{2}}\delta\left(z+\frac{2\phi\left(\phi+\psi\right)}{\tan\Theta}\right)\mathrm{d}\psi\,\mathrm{d}\phi \tag{8.1.G.1}$$

Substitution of the variable ψ by y :

$$z+\frac{2\phi\left(\phi+\psi\right)}{\tan\Theta}\equiv y$$

$$2\phi\left(\phi+\psi\right)=\left(y-z\right)\tan\Theta\Rightarrow\psi=\frac{\left(y-z\right)\tan\Theta}{2\phi}-\phi\Rightarrow\mathrm{d}\psi=\frac{\mathrm{d}y\,\tan\Theta}{2\phi}$$

$$\psi \quad : \quad -\frac{\Psi}{2} \quad \rightarrow \quad \frac{\Psi}{2}$$

$$y \quad : \quad z + \frac{2\phi\left(\phi - \Psi/2\right)}{\tan\Theta} \quad \rightarrow \quad z + \frac{2\phi\left(\phi + \Psi/2\right)}{\tan\Theta}$$

is applied to eq. (8.1.G.1), which gives

$$\omega_{\rm E}(z;\Theta,\Phi,\Psi) = \frac{1}{\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\int_{z+\frac{2\phi\left(\phi-\frac{\Psi}{2}\right)}{\tan\Theta}}^{z+\frac{2\phi\left(\phi+\frac{\Psi}{2}\right)}{\tan\Theta}} \delta\left(y\right)\frac{\tan\Theta\,{\rm d}y}{2\phi}{\rm d}\phi$$

$$= \frac{1}{\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\frac{\tan\Theta}{2\phi}\int_{z+\frac{2\phi\left(\phi-\frac{\Psi}{2}\right)}{\tan\Theta}}^{z+\frac{2\phi\left(\phi+\frac{\Psi}{2}\right)}{\tan\Theta}} \delta\left(y\right){\rm d}y\,{\rm d}\phi\,. \tag{8.1.G.2}$$

Since

$$\int_a^b \delta(x){\rm d}x = \begin{cases} 1 & \left[a \le 0 \le b\right] \\ -1 & \left[b \le 0 \le a\right], \\ 0 & \left[\text{otherwise}\right] \end{cases} \tag{8.1.G.3}$$

the aberration function is rewritten as

$$\omega_{\rm E}(z;\Theta,\Phi,\Psi) = \frac{\tan\Theta}{2\Phi\Psi}\int_{-\frac{\Phi}{2}}^{\frac{\Phi}{2}}\frac{1}{\phi}\left\{\begin{array}{ll} 1 & \left[z+\dfrac{2\phi\left(\phi-\Psi/2\right)}{\tan\Theta} < 0 < z+\dfrac{2\phi\left(\phi+\Psi/2\right)}{\tan\Theta}\right] \\ -1 & \left[z+\dfrac{2\phi\left(\phi+\Psi/2\right)}{\tan\Theta} < 0 < z+\dfrac{2\phi\left(\phi-\Psi/2\right)}{\tan\Theta}\right] \\ 0 & \left[\text{otherwise}\right] \end{array}\right\}{\rm d}\phi\,. \tag{8.1.G.4}$$

The effective integral range about ϕ is illustrated in Fig. 8.1.G.1. From the symmetry, the above equation is rewritten as

$$\omega_{\rm E}(z;\Theta,\Phi,\Psi) = \frac{\tan\Theta}{\Phi\Psi}\int_{0}^{\frac{\Phi}{2}}\frac{1}{\phi}\left\{\begin{array}{ll} 1 & \left[z+\dfrac{2\phi\left(\phi-\Psi/2\right)}{\tan\Theta} < 0 < z+\dfrac{2\phi\left(\phi+\Psi/2\right)}{\tan\Theta}\right] \\ 0 & \left[\text{otherwise}\right] \end{array}\right\}{\rm d}\phi\,. \tag{8.1.G.5}$$

In the above equation, the inequality:

$$z+\frac{2\phi\left(\phi-\Psi/2\right)}{\tan\Theta} < 0 < z+\frac{2\phi\left(\phi+\Psi/2\right)}{\tan\Theta} \tag{8.1.G.6}$$

can be rewritten as

$$\frac{z\tan\Theta}{2}+\phi\left(\phi-\frac{\Psi}{2}\right) < 0 < \frac{z\tan\Theta}{2}+\phi\left(\phi+\frac{\Psi}{2}\right)$$

$$\Leftrightarrow \left(\phi-\frac{\Psi}{4}\right)^2-\frac{\Psi^2}{16}+\frac{z\tan\Theta}{2} < 0 < \left(\phi+\frac{\Psi}{4}\right)^2-\frac{\Psi^2}{16}+\frac{z\tan\Theta}{2}$$

$$\Leftrightarrow \begin{cases} \left(\phi-\dfrac{\Psi}{4}\right)^2-\dfrac{\Psi^2}{16}+\dfrac{z\tan\Theta}{2} < 0 \\ 0 < \left(\phi+\dfrac{\Psi}{4}\right)^2-\dfrac{\Psi^2}{16}+\dfrac{z\tan\Theta}{2} \end{cases}. \tag{8.1.G.7}$$

The discriminant D is given by

$$D = \frac{\Psi^2}{16} - \frac{z \tan\Theta}{2}. \tag{8.1.G.8}$$

If $D < 0$, there is no valid integral range, so the value of the instrumental function should be zero.

The maximum value of z, $z_{\max}$, for the range where the instrumental function has non-zero values, is determined by the crossing point of the parabola:

$$\left(\phi - \frac{\Psi}{4}\right)^2 - \frac{\Psi^2}{16} + \frac{z_{\max} \tan\Theta}{2} = 0 \tag{8.1.G.9}$$

and the vertical line: $\phi = \Phi/2$, and the following relation is derived,

$$\left(\frac{\Phi}{2} - \frac{\Psi}{4}\right)^2 - \frac{\Psi^2}{16} + \frac{z_{\max} \tan\Theta}{2} = 0 \Rightarrow \frac{\Phi^2}{4} - \frac{\Phi\Psi}{4} + \frac{z_{\max} \tan\Theta}{2} = 0$$

$$\Rightarrow z_{\max} = \frac{\Phi\Psi - \Phi^2}{2 \tan\Theta} \tag{8.1.G.10}$$

for the case $2\Phi < \Psi$, which means the upper limit $\phi = \Phi/2$ is smaller than the axial position $\phi = \Psi/4$.

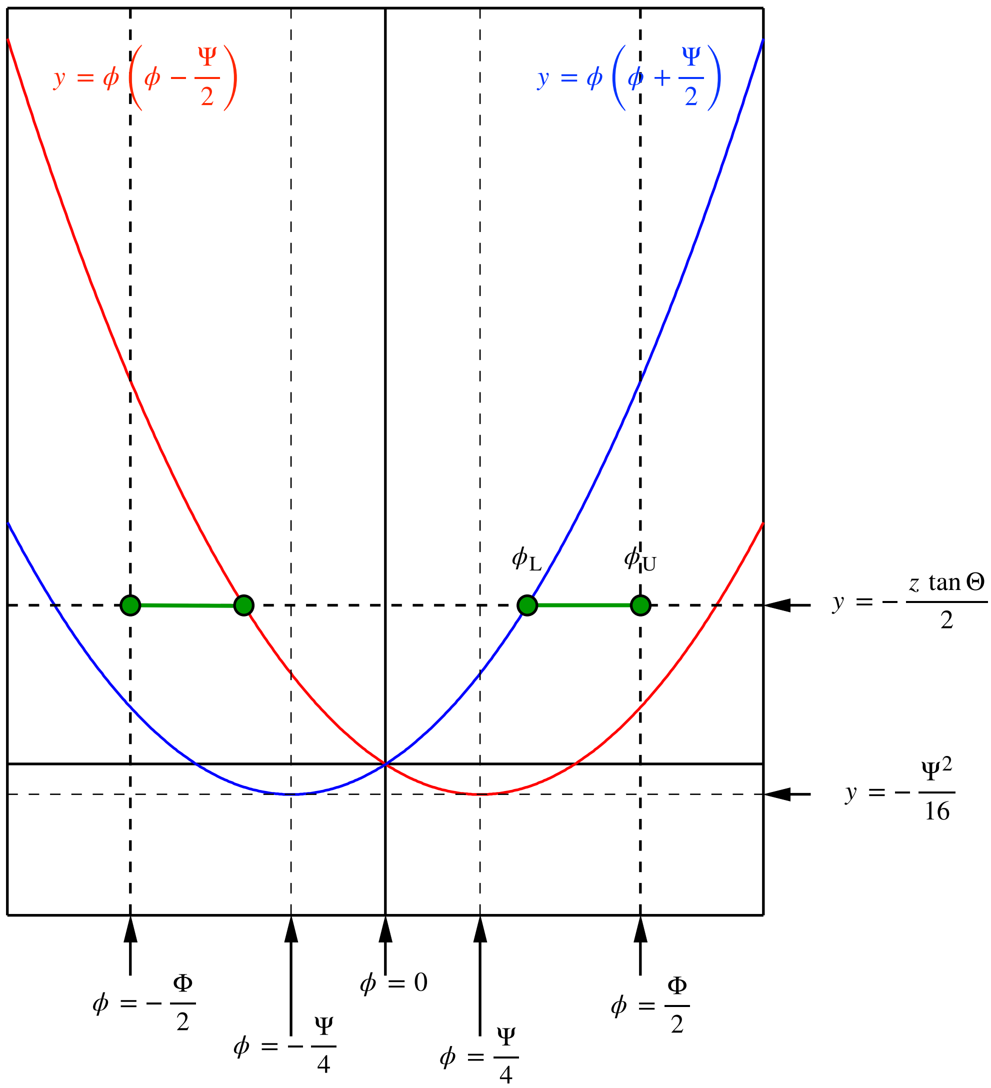

Fig. 8.1.G.1 Valid integral range about ϕ in eq. (8.1.G.4).

The value of $z_{\max}$ should be determined by the bottom of the parabola:

$$\left(\phi - \frac{\Psi}{4}\right)^2 - \frac{\Psi^2}{16} + \frac{z_{\max}\tan\Theta}{2} = 0, \tag{8.1.G.11}$$

which is identical to the crossing point of the parabola with $\phi = \Psi/4$, and

$$-\frac{\Psi^2}{16} + \frac{z_{\max}\tan\Theta}{2} = 0 \Rightarrow z_{\max} = \frac{\Psi^2}{8\tan\Theta}\,, \tag{8.1.G.12}$$

for $\Psi \leq 2\Phi$.

The minimum value of z, $z_{\min}$, for the range where the instrumental function has non-zero values, is always determined by the crossing point of the parabola:

$$\left(\phi + \frac{\Psi}{4}\right)^2 - \frac{\Psi^2}{16} + \frac{z_{\min}\tan\Theta}{2} = 0 \tag{8.1.G.13}$$

and the vertical line $\phi = \Phi/2$, then

$$\left(\frac{\Phi}{2} + \frac{\Psi}{4}\right)^2 - \frac{\Psi^2}{16} + \frac{z_{\min}\tan\Theta}{2} = 0 \Rightarrow \frac{\Phi^2}{4} + \frac{\Phi\Psi}{4} + \frac{z_{\min}\tan\Theta}{2} = 0$$

$$\Rightarrow z_{\min} = -\frac{\Phi\Psi + \Phi^2}{2\tan\Theta} \tag{8.1.G.14}$$

Equation (8.1.G.4) is simply expressed by

$$\omega_{\mathrm{E}}(z;\Theta,\Phi,\Psi) = \frac{\tan\Theta}{\Phi\Psi}\int_{\phi_{\mathrm{L}}}^{\phi_{\mathrm{U}}}\frac{\mathrm{d}\phi}{\phi} = \frac{\tan\Theta}{\Phi\Psi}\left[\ln\phi\right]_{\phi_{\mathrm{L}}}^{\phi_{\mathrm{U}}} = \frac{\tan\Theta}{\Phi\Psi}\ln\frac{\phi_{\mathrm{U}}}{\phi_{\mathrm{L}}}\,, \tag{8.1.G.15}$$

where ϕ_{L} and ϕ_{U} are the lower and upper bound of the valid integral range.

The lower bound ϕ_{L} is given by

$$\left(\phi_{\mathrm{L}} - \frac{\Psi}{4}\right)^2 - \frac{\Psi^2}{16} + \frac{z\tan\Theta}{2} = 0 \Rightarrow \phi_{\mathrm{L}} = \frac{\Psi}{4} - \sqrt{\frac{\Psi^2}{16} - \frac{z\tan\Theta}{2}}\,, \tag{8.1.G.16}$$

for $0 < z < z_{\max}$, and

$$\left(\phi_{\mathrm{L}} + \frac{\Psi}{4}\right)^2 - \frac{\Psi^2}{16} + \frac{z\tan\Theta}{2} = 0 \Rightarrow \phi_{\mathrm{L}} = -\frac{\Psi}{4} + \sqrt{\frac{\Psi^2}{16} - \frac{z\tan\Theta}{2}} \tag{8.1.G.17}$$

for $z_{\min} < z < 0$. The above two expressions can be replaced by the following expression:

$$\phi_{\mathrm{L}} = \max\left\{\frac{\Psi}{4} - \sqrt{\frac{\Psi^2}{16} - \frac{z\tan\Theta}{2}}, -\frac{\Psi}{4} + \sqrt{\frac{\Psi^2}{16} - \frac{z\tan\Theta}{2}}\right\}. \tag{8.1.G.18}$$

The upper bound ϕ_{U} is given by

$$\left(\phi_{\mathrm{H}} - \frac{\Psi}{4}\right)^2 - \frac{\Psi^2}{16} + \frac{z\tan\Theta}{2} = 0 \Rightarrow \phi_{\mathrm{U}} = \frac{\Psi}{4} + \sqrt{\frac{\Psi^2}{16} - \frac{z\tan\Theta}{2}}, \tag{8.1.G.19}$$

or

$$\phi_{\mathrm{U}} = \frac{\Phi}{2}\,, \tag{8.1.G.20}$$

and the following expression:

$$\phi_{\mathrm{U}} = \min\left\{\frac{\Phi}{2}, \frac{\Psi}{4} + \sqrt{\frac{\Psi^2}{16} - \frac{z\tan\Theta}{2}}\right\} \tag{8.1.G.21}$$

can be applied.

Reference 8.1

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