

# Kinematic Fit for the EMC Radiative Bhabha Calibration

J. M. Bauer  
University of Mississippi

## Abstract

For the radiative Bhabha calibration of BABAR's electromagnetic calorimeter, the measured energy of a photon cluster is being compared with the energy obtained via a kinematic fit involving other quantities from that event. The details of the fitting algorithm are described in this note, together with its derivation and checks that ensure that the fitting routine is working properly.

# 1 Introduction

Radiative Bhabhas can be used as one of the calibrations of the BABAR electromagnetic calorimeter (EMC). Radiative Bhabha events ( $e^-e^+ \rightarrow e^-e^+\gamma$ ) deposit photons over a large energy range everywhere in the calorimeter. If the momenta of the incoming and outgoing electrons and positrons, as well as the photon's angular position are known, the photon energy can be obtained via a kinematic fit. This fit results in an absolute measurement of the photon energy which then can be compared to the measured photon energy to obtain calibration constants.

The radiative Bhabha module is part of BABAR's Online Prompt Reconstruction (OPR) executable. Initial cuts select good electrons, positrons, and photons. Then all possible combinations of triplets (one electron, one positron, one photon) are formed. Each triplet is sent to the fitting routine to calculate its  $\chi_{\text{est}}^2$ , the "estimated  $\chi^2$ ". The triplet with the lowest  $\chi_{\text{est}}^2$  is then submitted to the full kinematic fit which returns, among other quantities, the fitted photon energy  $E_{f\gamma}$  and the error matrix of the fitted quantities. The ratio  $E_{\text{meas}}/E_{f\gamma}$  is later used to calibrate the calorimeter. Note that no information on the measured photon energy  $E_{\text{meas}}$  goes into the kinematic fit or  $\chi_{\text{est}}^2$ .

This note is the complete documentation on the algorithm for fitting the radiative Bhabha events for the purpose of calibrating the calorimeter. It describes the whole fitting procedure: the quantities for the kinematic fit and  $\chi_{\text{est}}^2$ ; the derivation and formulas for  $\chi_{\text{est}}^2$ ; the derivation and algorithm for the kinematic fit; tests to check the quality of the kinematic fit. The note details all formulas which go into the computer program so that the program can be checked directly against this document. The derivations contain more details than needed to understand the concept, but the details help to derive, check and recheck all necessary formulas. Actual results of the fitting procedure using real data are not included in this note to keep it a pure code documentation.

## 2 Defining the quantities and constraints

### 2.1 Measured quantities

From the experiment come the following measurements, which shall form the 14-dimensional vector  $\mathbf{y}$ :

$P_{ix-} \equiv y_1$	$P_{iy-} \equiv y_2$	$P_{iz-} \equiv y_3$	msrd momentum in $x$ , $y$ , and $z$ of incoming $e^-$
$P_{ix+} \equiv y_4$	$P_{iy+} \equiv y_5$	$P_{iz+} \equiv y_6$	msrd momentum in $x$ , $y$ , and $z$ of incoming $e^+$
$P_{ox-} \equiv y_7$	$P_{oy-} \equiv y_8$	$P_{oz-} \equiv y_9$	msrd momentum in $x$ , $y$ , and $z$ of outgoing $e^-$
$P_{ox+} \equiv y_{10}$	$P_{oy+} \equiv y_{11}$	$P_{oz+} \equiv y_{12}$	msrd momentum in $x$ , $y$ , and $z$ of outgoing $e^+$
$\theta_{o\gamma} \equiv y_{13}$	$\phi_{o\gamma} \equiv y_{14}$		measured $\theta$ and $\phi$ of the photon

The momenta of the incoming electron and positron and their errors are changing run-by-run. The errors of the incoming leptons are given as covariance matrices:

$$\mathbf{V}_{i-} = \begin{pmatrix} V_{ixx-} & V_{ixy-} & V_{ixz-} \\ V_{ixy-} & V_{iyy-} & V_{iyz-} \\ V_{ixz-} & V_{iyz-} & V_{izz-} \end{pmatrix} \quad \mathbf{V}_{i+} = \begin{pmatrix} V_{ixx+} & V_{ixy+} & V_{ixz+} \\ V_{ixy+} & V_{iyy+} & V_{iyz+} \\ V_{ixz+} & V_{iyz+} & V_{izz+} \end{pmatrix}$$

The errors on  $\mathbf{P}_{i-}$  and  $\mathbf{P}_{i+}$  are assumed to be independent.



## 2.2 Quantities for the kinematic fit

The kinematic fit determines the following numbers:

$f_{ix-} \equiv f_1$	$f_{iy-} \equiv f_2$	$f_{iz-} \equiv f_3$	$x, y,$ and $z$ momentum of incoming $e^-$
$f_{ix+} \equiv f_4$	$f_{iy+} \equiv f_5$	$f_{iz+} \equiv f_6$	$x, y,$ and $z$ momentum of incoming $e^+$
$f_{ox-} \equiv f_7$	$f_{oy-} \equiv f_8$	$f_{oz-} \equiv f_9$	$x, y,$ and $z$ momentum of outgoing $e^-$
$f_{ox+} \equiv f_{10}$	$f_{oy+} \equiv f_{11}$	$f_{oz+} \equiv f_{12}$	$x, y,$ and $z$ momentum of outgoing $e^+$
$\theta_{f\gamma} \equiv f_{13}$	$\phi_{f\gamma} \equiv f_{14}$	$E_{f\gamma} \equiv h_1$	$\theta$ and $\phi,$ and energy of the photon
$\lambda_1$	$\lambda_2$	$\lambda_3$	four Lagrange multipliers for momentum and
$\lambda_4$			energy conservation constraints

The variables  $f_1$  to  $f_{14}$  have corresponding measurements. The variable  $h_1$ , the photon energy, is called a ‘‘hidden variable’’. The vector  $\boldsymbol{\alpha}$  shall be defined as a 19-element composite of  $\mathbf{f}$  (14 elements),  $\mathbf{h}$  (1 element), and  $\boldsymbol{\lambda}$  (4 elements).

## 2.3 Constraints

We have four constraint equations that have to be satisfied in the kinematic fit:

$$\begin{aligned}
 p_{ix-} + p_{ix+} - p_{0x-} - p_{0x+} - E_{f\gamma} \sin \theta_{f\gamma} \cos \phi_{f\gamma} &= 0 & \text{momentum in } x \\
 p_{iy-} + p_{iy+} - p_{0y-} - p_{0y+} - E_{f\gamma} \sin \theta_{f\gamma} \sin \phi_{f\gamma} &= 0 & \text{momentum in } y \\
 p_{iz-} + p_{iz+} - p_{0z-} - p_{0z+} - E_{f\gamma} \cos \theta_{f\gamma} &= 0 & \text{momentum in } z \\
 E_{i-} + E_{i+} - E_{0-} - E_{0+} - E_{f\gamma} &= 0 & \text{energy}
 \end{aligned}$$

Here we use, *e.g.*,

$$\begin{aligned}
 E_{i-} &\equiv \sqrt{p_{ix-}^2 + p_{iy-}^2 + p_{iz-}^2 + m_e^2} \\
 &= \sqrt{f_1^2 + f_2^2 + f_3^2 + m_e^2}
 \end{aligned}$$

## 3 The estimated $\chi^2$ : $\chi_{\text{est}}^2$

This function is calculated for any given electron-positron-gamma triplet to determine which triplet should be used for the kinematic fit. At the end of this subsection, we will have a complete analytical formula for calculating  $\chi_{\text{est}}^2$ .

The formula is based on the difference between the initial and final momentum,  $\mathbf{P} \equiv \mathbf{P}_i - \mathbf{P}_o$ . The initial momentum  $\mathbf{P}_i$  is the sum of the momenta of the incoming electron and positron as defined earlier:  $\mathbf{P}_{i-}$  and  $\mathbf{P}_{i+}$ . The measured momenta of the outgoing electron, positron are given by  $\mathbf{P}_{0-}$  and  $\mathbf{P}_{0+}$ .

For the outgoing photon, we only have its angles  $\theta_{0\gamma}$  and  $\phi_{0\gamma}$ . Using the energy constraint

$$E_\gamma = E_{i-} + E_{i+} - E_{0-} - E_{0+}$$

we may substitute the unknown photon energy  $E_\gamma$  with measured values, and we obtain:

$$\mathbf{P}_{0\gamma} \equiv (E_{i-} + E_{i+} - E_{0-} - E_{0+}) \begin{pmatrix} \sin \theta_{0\gamma} \cos \phi_{0\gamma} \\ \sin \theta_{0\gamma} \sin \phi_{0\gamma} \\ \cos \theta_{0\gamma} \end{pmatrix} \equiv E_\gamma \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} \equiv E_\gamma \mathbf{n}$$

Of course,  $\mathbf{n}$  is the normal vector, the direction of the photon.

Calculating the difference to form vector  $\mathbf{P}$  is easy:

$$\mathbf{P} \equiv \begin{pmatrix} P_x \\ P_y \\ P_z \end{pmatrix} = \mathbf{P}_{i-} + \mathbf{P}_{i+} - \mathbf{P}_{o-} - \mathbf{P}_{o+} - \mathbf{P}_{o\gamma}$$

In the ideal world, this vector would be exactly zero. For its error matrix  $\mathbf{V}_p$ , we convert  $\mathbf{V}_{\text{all}}$ , the error matrix of  $\mathbf{y}$ , via a transformation matrix  $\mathbf{T}$  into  $\mathbf{V}_p$ :

$$\mathbf{V}_p = \mathbf{T}^t \mathbf{V}_{\text{all}} \mathbf{T}$$

For the transformation matrix  $\mathbf{T}$  we have to calculate expressions like  $\frac{\partial P_x}{\partial P_{ix-}}$ . We note that for  $j = x, y, z$ :

$$\frac{\partial(E_\gamma n_j)}{\partial P_{ix-}} = \frac{P_{ix-}}{P_{i-}} n_j$$

The transformation matrix is a  $3 \times 14$  matrix:

$$\mathbf{T} = \begin{pmatrix} \frac{\partial P_x}{\partial P_{ix-}} & \frac{\partial P_y}{\partial P_{ix-}} & \frac{\partial P_z}{\partial P_{ix-}} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{iy-}}{\partial P_x} & \frac{\partial P_{iy-}}{\partial P_y} & \frac{\partial P_{iy-}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{iz-}}{\partial P_x} & \frac{\partial P_{iz-}}{\partial P_y} & \frac{\partial P_{iz-}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{ix+}}{\partial P_x} & \frac{\partial P_{ix+}}{\partial P_y} & \frac{\partial P_{ix+}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{iy+}}{\partial P_x} & \frac{\partial P_{iy+}}{\partial P_y} & \frac{\partial P_{iy+}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{iz+}}{\partial P_x} & \frac{\partial P_{iz+}}{\partial P_y} & \frac{\partial P_{iz+}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{0x-}}{\partial P_x} & \frac{\partial P_{0x-}}{\partial P_y} & \frac{\partial P_{0x-}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{0y-}}{\partial P_x} & \frac{\partial P_{0y-}}{\partial P_y} & \frac{\partial P_{0y-}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{0z-}}{\partial P_x} & \frac{\partial P_{0z-}}{\partial P_y} & \frac{\partial P_{0z-}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{0x+}}{\partial P_x} & \frac{\partial P_{0x+}}{\partial P_y} & \frac{\partial P_{0x+}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{0y+}}{\partial P_x} & \frac{\partial P_{0y+}}{\partial P_y} & \frac{\partial P_{0y+}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial P_{0z+}}{\partial P_x} & \frac{\partial P_{0z+}}{\partial P_y} & \frac{\partial P_{0z+}}{\partial P_z} \\ \frac{\partial P_x}{\partial P_x} & \frac{\partial P_y}{\partial P_y} & \frac{\partial P_z}{\partial P_z} \\ \frac{\partial \theta_{0\gamma}}{\partial P_x} & \frac{\partial \theta_{0\gamma}}{\partial P_y} & \frac{\partial \theta_{0\gamma}}{\partial P_z} \\ \frac{\partial P_x}{\partial \phi_{0\gamma}} & \frac{\partial P_y}{\partial \phi_{0\gamma}} & \frac{\partial P_z}{\partial \phi_{0\gamma}} \end{pmatrix} = \begin{pmatrix} 1 - \frac{P_{ix-}}{E_{i-}} n_x & -\frac{P_{ix-}}{E_{i-}} n_y & -\frac{P_{ix-}}{E_{i-}} n_z \\ -\frac{P_{iy-}}{E_{i-}} n_x & 1 - \frac{P_{iy-}}{E_{i-}} n_y & -\frac{P_{iy-}}{E_{i-}} n_z \\ -\frac{P_{iz-}}{E_{i-}} n_x & -\frac{P_{iz-}}{E_{i-}} n_y & 1 - \frac{P_{iz-}}{E_{i-}} n_z \\ 1 - \frac{P_{ix+}}{E_{i+}} n_x & -\frac{P_{ix+}}{E_{i+}} n_y & -\frac{P_{ix+}}{E_{i+}} n_z \\ -\frac{P_{iy+}}{E_{i+}} n_x & 1 - \frac{P_{iy+}}{E_{i+}} n_y & -\frac{P_{iy+}}{E_{i+}} n_z \\ -\frac{P_{iz+}}{E_{i+}} n_x & -\frac{P_{iz+}}{E_{i+}} n_y & 1 - \frac{P_{iz+}}{E_{i+}} n_z \\ -1 + \frac{P_{0x-}}{E_{0-}} n_x & \frac{P_{0x-}}{E_{0-}} n_y & \frac{P_{0x-}}{E_{0-}} n_z \\ \frac{P_{0y-}}{E_{0-}} n_x & -1 + \frac{P_{0y-}}{E_{0-}} n_y & \frac{P_{0y-}}{E_{0-}} n_z \\ \frac{P_{0z-}}{E_{0-}} n_x & \frac{P_{0z-}}{E_{0-}} n_y & -1 + \frac{P_{0z-}}{E_{0-}} n_z \\ -1 + \frac{P_{0x+}}{E_{0+}} n_x & \frac{P_{0x+}}{E_{0+}} n_y & \frac{P_{0x+}}{E_{0+}} n_z \\ \frac{P_{0y+}}{E_{0+}} n_x & -1 + \frac{P_{0y+}}{E_{0+}} n_y & \frac{P_{0y+}}{E_{0+}} n_z \\ \frac{P_{0z+}}{E_{0+}} n_x & \frac{P_{0z+}}{E_{0+}} n_y & -1 + \frac{P_{0z+}}{E_{0+}} n_z \\ -E_\gamma \cos \theta_{0\gamma} \cos \phi_{0\gamma} & -E_\gamma \cos \theta_{0\gamma} \sin \phi_{0\gamma} & E_\gamma \sin \theta_{0\gamma} \\ E_\gamma \sin \theta_{0\gamma} \sin \phi_{0\gamma} & -E_\gamma \sin \theta_{0\gamma} \cos \phi_{0\gamma} & 0 \end{pmatrix}$$

Now we have  $\mathbf{V}_p^{-1} = \mathbf{T}^t \mathbf{V}_{\text{all}}^{-1} \mathbf{T}$ , and hence we may calculate  $\chi_{\text{est}}^2$ :

$$\chi_{\text{est}}^2 = \mathbf{P}^t \mathbf{V}_p^{-1} \mathbf{P}$$

What is the meaning of this  $\chi^2$ ? We can say that the 14 input variables are used to measure  $\mathbf{P}$ , and  $\chi_{\text{est}}^2$  tells us the deviation of the measured  $\mathbf{P}$  from the expected  $\mathbf{P}$ , which is zero.

## 4 The kinematic fit

For the derivation of the kinematic fit algorithm, we follow the description of Louis Lyons, page 151, 152 [1].

### 4.1 The $\chi^2$ -Function

The real  $\chi^2$ -function can be written down in the following way:

$$\begin{aligned} \chi^2 &= (\mathbf{f} - \mathbf{m})^t \mathbf{V}_{\text{all}}^{-1} (\mathbf{f} - \mathbf{m}) \\ &+ \lambda_1 [p_{xi-} + p_{xi+} - p_{xo-} - p_{xo+} - E_\gamma \sin \theta_\gamma \cos \phi_\gamma] \\ &+ \lambda_2 [p_{yi-} + p_{yi+} - p_{yo-} - p_{yo+} - E_\gamma \sin \theta_\gamma \sin \phi_\gamma] \\ &+ \lambda_3 [p_{zi-} + p_{zi+} - p_{zo-} - p_{zo+} - E_\gamma \cos \theta_\gamma] \\ &+ \lambda_4 [E_{i-} + E_{i+} - E_{o-} - E_{o+} - E_\gamma] \end{aligned}$$

The constraint equations are here included via Lagrange multipliers. To minimize this  $\chi^2$ , we could use a standard package like MINUIT, but standard packages are always slower than specially adapted code. Since the  $\chi^2$ -minimization is being done millions of times, it pays off to write special code for the minimization. In addition, MINUIT is not supported in BABAR's Online Prompt Reconstruction.

### 4.2 Derivation of kinematic fit algorithm

At the minimum of  $\chi^2$ , its first derivatives are to be zero. Lyons uses for this the following equations:

$$\begin{aligned} \frac{\partial \chi^2}{\partial \alpha_i} &= 0 && \text{for } i = 1 \text{ to } 14 \\ \frac{\partial \chi^2}{\partial h} &= 0 && \text{here } h = E_\gamma = \alpha_{15} \\ \frac{\partial \chi^2}{\partial \lambda_k} &= 0 && \text{here } \lambda_1 = \alpha_{16} \text{ etc.} \end{aligned}$$

The three equation sets can be written as:<sup>1</sup>

$$\begin{aligned} 2\mathbf{G}(\mathbf{f} - \mathbf{m}) + \mathbf{D}^t \boldsymbol{\lambda} &= \mathbf{0} \\ \mathbf{E}^t \boldsymbol{\lambda} &= \mathbf{0} \\ \mathbf{C} &= \mathbf{0} \end{aligned}$$

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<sup>1</sup>The factor 2 in front of  $\mathbf{V}_{\text{all}}^{-1}$  is missing in Lyons' book [1]. We could easily remove this factor from our formulas by re-defining the Lagrange multipliers in the  $\chi^2$ -function with a factor 2. This would not change the fit result or errors, as long as the subsequent calculations were carried out consistently.

where  $\mathbf{G}$  is the  $14 \times 14$  inverse error matrix of the measurements which we also call  $\mathbf{V}_{\text{all}}^{-1}$ .

$$\mathbf{D} = \begin{pmatrix} \partial C_1 / \partial \alpha_1 & \dots & \partial C_1 / \partial \alpha_{14} \\ \partial C_2 / \partial \alpha_1 & \dots & \partial C_2 / \partial \alpha_{14} \\ \partial C_3 / \partial \alpha_1 & \dots & \partial C_3 / \partial \alpha_{14} \\ \partial C_4 / \partial \alpha_1 & \dots & \partial C_4 / \partial \alpha_{14} \end{pmatrix} \quad \text{and} \quad \mathbf{E} = \begin{pmatrix} \partial C_1 / \partial \alpha_{15} \\ \partial C_2 / \partial \alpha_{15} \\ \partial C_3 / \partial \alpha_{15} \\ \partial C_4 / \partial \alpha_{15} \end{pmatrix}$$

We now expand the constraint equations  $\mathbf{C}$  around  $f_0$  and  $h_0$ , and we obtain for the four equations  $C_k$  with  $k = 1$  to 4:

$$C_k \approx C_k^{(0)} + \sum_{i=1}^{14} \frac{\partial C^{(0)}}{\partial f_i} (f_i - f_i^{(0)}) + \frac{\partial C^{(0)}}{\partial h} (h - h^{(0)}) = 0 \quad (1)$$

We may rewrite this into:

$$\sum_{i=1}^{14} \frac{\partial C^{(0)}}{\partial f_i} (f_i - m_i) + \frac{\partial C^{(0)}}{\partial h} (h - h^{(0)}) = -C_k^{(0)} + \sum_{i=1}^{14} \frac{\partial C^{(0)}}{\partial f_i} (f_i^{(0)} - m_i^{(0)})$$

Now we collect everything, use the definitions for  $\mathbf{M}$ ,  $\mathbf{Y}$ , and  $\mathbf{Z}$ ,

$$\mathbf{M} = \begin{pmatrix} 2\mathbf{G} & \mathbf{0} & \mathbf{D}^t \\ \mathbf{0} & \mathbf{0} & \mathbf{E}^t \\ \mathbf{D} & \mathbf{E} & \mathbf{0} \end{pmatrix} \quad \mathbf{Y} = \begin{pmatrix} \mathbf{f} - \mathbf{m} \\ \mathbf{h} - h_0 \\ \lambda \end{pmatrix} \quad \mathbf{Z} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ -\mathbf{R} \end{pmatrix}$$

with

$$\mathbf{R} = \mathbf{C}^{(0)} - \mathbf{D}(\mathbf{f}_0 - \mathbf{m}) = \begin{pmatrix} C_1(\mathbf{f}_0, \mathbf{h}_0) \\ C_2(\mathbf{f}_0, \mathbf{h}_0) \\ C_3(\mathbf{f}_0, \mathbf{h}_0) \\ C_4(\mathbf{f}_0, \mathbf{h}_0) \end{pmatrix} - \mathbf{D}(\mathbf{f}_0 - \mathbf{m}),$$

and we see:

$$\mathbf{M} \mathbf{Y} = \mathbf{Z}$$

This is the equation we have to solve. Since the constraint equations  $\mathbf{C} = \mathbf{0}$  contain non-linear functions like  $\sin \theta_\gamma$ , Eq. (1) is only an approximation, and we have to iterate as described in the next section.

### 4.3 Recipe for the kinematic fit algorithm

The matrix  $\mathbf{M}$  and the vector  $\mathbf{Z}$  are functions of the measurements and their error matrices as well as of the parameters  $\boldsymbol{\alpha}$ . The vector  $\mathbf{Y}$  is, as mentioned above,

$$\mathbf{Y} = \begin{pmatrix} \mathbf{f} - \mathbf{m} \\ \mathbf{h} - h_0 \\ \lambda \end{pmatrix}$$

and can be calculated with:

$$\mathbf{Y} = \mathbf{M}^{-1} \mathbf{Z}$$

Here is the iteration: Initially, we will use for the fit quantities  $\mathbf{f}_0 = \mathbf{m}$ , *i.e.* the measured quantities. For  $\mathbf{h} = h_0$ , we calculate the photon energy via simple energy conservation. These together with the measured quantities allow us to calculate  $\mathbf{M}$  and  $\mathbf{Z}$ . We multiply the inverse of  $\mathbf{M}$  with  $\mathbf{Z}$  and obtain  $\mathbf{Y}$ . This result will then give us a better set of  $\mathbf{f}$  and  $\mathbf{h}$ , which we again use to calculate  $\mathbf{M}$  and  $\mathbf{Z}$ , and then a better  $\mathbf{Y}$ . And we continue until our constraint equations are sufficiently fulfilled and the quantities  $\mathbf{f}$  and  $\mathbf{h}$  are stable.

It might happen that the iteration does not converge at the minimum, but wanders off into unphysical numbers. In that case, it would be good to have a certain boundary box around the point. If the step would make the point lie outside the box, then the program would change the step so that the point would be back inside. It might be good to implement this, although the radiative Bhabha fitting does not seem to need this part of the algorithm.

#### 4.4 Details of matrices and vectors used in the kinematic fit

We define the following variables:

$$E_i = \begin{cases} E_{i-} & \text{for } i = 1, 2, 3 \quad (p_{ix-}, p_{iy-}, p_{iz-}) \\ E_{i+} & \text{for } i = 4, 5, 6 \quad (p_{ix+}, p_{iy+}, p_{iz+}) \\ E_{0-} & \text{for } i = 7, 8, 9 \quad (p_{0x-}, p_{0y-}, p_{0z-}) \\ E_{0+} & \text{for } i = 10, 11, 12 \quad (p_{0x+}, p_{0y+}, p_{0z+}) \end{cases}$$

$$s_i = \begin{cases} 1 & \text{for } i \leq 6 \quad (p_{ix-}, p_{iy-}, p_{iz-}, p_{ix+}, p_{iy+}, p_{iz+}) \\ -1 & \text{for } i > 6 \quad (p_{0x-}, p_{0y-}, p_{0z-}, p_{0x+}, p_{0y+}, p_{0z+}) \end{cases}$$

For  $4 \times 14$  matrix  $\mathbf{D}$  we need the following expressions:

Row  $j = 1$  to 3, columns  $i = 1$  to 12:

$$\frac{\partial C_j}{\partial \alpha_i} = \begin{cases} s_i & \text{if } i = j \text{ or } i = j + 3 \text{ or } i = j + 6 \text{ or } i = j + 9 \\ 0 & \text{else} \end{cases}$$

Row  $j = 1$ , column  $i = 13$ :

$$\frac{\partial C_1}{\partial \alpha_{13}} = -E_{f\gamma} \cos \theta_{f\gamma} \cos \phi_{f\gamma} = -\alpha_{15} \cos \alpha_{13} \cos \alpha_{14}$$

Row  $j = 1$ , column  $i = 14$ :

$$\frac{\partial C_1}{\partial \alpha_{14}} = E_{f\gamma} \sin \theta_{f\gamma} \sin \phi_{f\gamma} = \alpha_{15} \sin \alpha_{13} \sin \alpha_{14}$$

Row  $j = 2$ , column  $i = 13$ :

$$\frac{\partial C_2}{\partial \alpha_{13}} = -E_{f\gamma} \cos \theta_{f\gamma} \sin \phi_{f\gamma} = -\alpha_{15} \cos \alpha_{13} \sin \alpha_{14}$$



Row  $j = 2$ , column  $i = 14$ :

$$\frac{\partial C_2}{\partial \alpha_{14}} = -E_{f\gamma} \sin \theta_{f\gamma} \cos \phi_{f\gamma} = -\alpha_{15} \sin \alpha_{13} \cos \alpha_{14}$$

Row  $j = 3$ , column  $i = 13$ :

$$\frac{\partial C_3}{\partial \alpha_{13}} = E_{f\gamma} \sin \theta_{f\gamma} = \alpha_{15} \sin \alpha_{13}$$

Row  $j = 3$ , column  $i = 14$ :

$$\frac{\partial C_3}{\partial \alpha_{14}} = 0$$

Row  $j = 4$ , columns  $i = 1$  to  $12$ :

$$\frac{\partial C_4}{\partial \alpha_i} = s_i \frac{\alpha_i}{E_i}$$

Row  $j = 4$ , column  $i = 13$  and  $14$ :

$$\frac{\partial C_4}{\partial \alpha_{13}} = \frac{\partial C_4}{\partial \alpha_{14}} = 0$$

The  $4 \times 1$  matrix  $\mathbf{E}$  is:

$$\mathbf{E} = \begin{pmatrix} -\sin \theta_{f\gamma} \cos \phi_{f\gamma} \\ -\sin \theta_{f\gamma} \sin \phi_{f\gamma} \\ -\cos \theta_{f\gamma} \\ -1 \end{pmatrix} = \begin{pmatrix} -\sin \alpha_{13} \cos \alpha_{14} \\ -\sin \alpha_{13} \sin \alpha_{14} \\ -\cos \alpha_{13} \\ -1 \end{pmatrix}$$

#### 4.5 The error matrix of the fit

The second partial derivatives of  $\chi^2$  appear in the error matrix of the fit parameters:

$$\mathbf{H} = \left( \frac{1}{2} \frac{\partial^2 \chi^2}{\partial \alpha_i \partial \alpha_j} \right)^{-1}$$

So in our case,  $\mathbf{H}$  is a  $19 \times 19$  matrix. The detailed expressions for the second derivatives of  $\chi^2$  will be given in the following section.

#### 4.6 Tests for goodness of fit

After completing the iteration on the kinematic fit, one wants to make sure that all quantities are indeed correct.

Besides the obvious tests that the constraint equations are satisfied, one can check that indeed a minimum was reached. For this, one may wiggle each final value  $\alpha_1$  to  $\alpha_{14}$  and recalculate  $\chi^2$ . In our case we have in the  $\chi^2$ -function the terms with the Lagrange multipliers. Just recalculating the  $\chi^2$  function will not lead to correct results, since the found vector  $\boldsymbol{\alpha}$  is a minimum only when

also requiring the constraints. So one has to redo the fit while forcing the selected element of  $\alpha$  to the off-minimum value.

This wiggling allows us to map out the minimum, and it also tells us whether the fit error returned for that parameter is reasonable. If we fix  $E_{f\gamma}$  to be  $\pm 1\sigma_{\gamma \text{ fit}}$  way from the real fit result, then the  $\chi^2$  should rise by 1 in either direction. When mapping out this rise, one will see the shape of a parabola. When the formulas are complicated and/or one is far away from the minimum, the parabola will be distorted.

In our case, we can indeed calculate the fit error for  $E_{f\gamma}$ , but if this would be impossible, one can find the fit error by mapping out the minimum with the above described re-fitting with fixed values. The  $\pm 1\sigma$ -error is then defined to be where  $\chi^2$  is 1 unit above the minimum. As mentioned, this function may be distorted when far away from the minimum. A complicated  $\chi^2$ -function might even distort the  $\pm 1\sigma$ -area. In this case, one can take the minimum and two points very close to it, fit a parabola through these three points, and take the sigma from that parabola as the error.

The same process also works for the hidden parameter (fitted photon energy), and we definitely have to re-fit since the fitted photon energy only appears in the constraints, where the Lagrange multipliers would influence the outcome.

Here is how we have to modify the formulas for re-fitting:

#### 4.6.1 Re-fitting with fixed $E_{f\gamma}$

We want to redo the fit with the photon energy fixed to  $E_{\text{fix}} = E_{f\gamma} + \epsilon$ . To the  $\chi^2$ -function, we add the term

$$+ X (E_{\gamma} - E_{\text{fix}})^2$$

where  $X$  is a large number compared to the original  $\chi^2$ . If we now minimize this new  $\chi^2$ -function, the additional term adds a large penalty to any deviation of  $E_{\gamma}$  from  $E_{\text{fix}}$ .

Going through the derivation again, we find the following places that have to be changed in the code:

- First partial derivative  $\frac{\partial \chi^2}{\partial \alpha_i}$  for  $i = 15$  [for  $i = k$ ] has the additional term “ $+2X(E_{\gamma} - E_{\text{fix}})$ ”.
- No change to second partial derivatives.
- Matrix  $\mathbf{M}$  has the additional term “ $+2X$ ” at (15,15). This means that the (15,15)-element of  $\mathbf{M}$  is no longer zero.
- Vector  $\mathbf{Z}$  has an additional term at position 15:

$$\mathbf{Z} = \begin{pmatrix} \mathbf{0} \\ -2X(h_0 - E_{\text{fix}}) \\ -\mathbf{R} \end{pmatrix}$$

These are all necessary changes. The iteration should converge again, but this time always result in  $E_{\gamma} = E_{\text{fix}}$  for sufficiently large  $X$ .

### 4.6.2 Re-fitting with fixed $f_k$

Let us now wiggle one of the measurement variables  $\alpha_1$  to  $\alpha_{14}$ . When fixing  $f_k$  to  $f_k = f_{k \text{ fix}}$ , we add the term

$$+ X (f_k - f_{k \text{ fix}})^2$$

to the  $\chi^2$ -function. Again,  $X$  is a large number compared to the original  $\chi^2$ . The following changes have to be made in the formulas of the algorithm:

- The first partial derivative  $\partial\chi^2/\partial\alpha_i$  gets for  $i = k$  the additional term “ $+2X(f_k - f_{k \text{ fix}})$ ”.
- Again no change to second partial derivatives.
- Matrix  $\mathbf{M}$  gets at position  $(k, k)$  the additional term “ $+2X$ ”.
- Vector  $\mathbf{Z}$  has at position  $k$  the entry “ $-2X(m_k - f_{k \text{ fix}})$ ”.

### 4.6.3 Confidence Level

If all errors of the measurements are nicely described by Gaussian distributions, and if all events are what we think they are, *i.e.*, (in our case) radiative Bhabhas, then the  $\chi^2$  values of the fits should be distributed like the  $\chi^2$ -distribution for  $n = 3$  (3 because our fit is a 3-constraint fit). Instead of looking at the  $\chi^2$  distributions directly, it is easier to map the  $\chi^2$  to a flat distribution with values between 0 and 1. This value is then called the confidence level (C.L.) of the event. If the  $\chi^2$  is really distributed as it should be, the confidence level will have a flat distribution.

So we are looking for two things in the C.L. distribution:

(1) Most of the region should have a flat distribution. If not, the errors used in the fit might be too large or too small. If the errors are underestimated, the  $\chi^2$  will be larger than expected, and the confidence level distribution will be tilted downward (when going from 0 to 1). Vice-versa, if the errors are overestimated, the C.L. distribution will be tilted upward. More information on the validity of errors might be obtained from the “pull” distributions described later.

(2) A peak at zero indicates events that do not fulfill the kinematics of radiative Bhabhas at all. They will result in very large  $\chi^2$  (=very small C.L., close to zero). These events can come from backgrounds or misidentified tracks. What can we do? We can improve our selection criteria. Or we can cut out all events belonging to that peak, taking only those events that are part of the flat distribution. A cut on the confidence level is, of course, equivalent to a cut on  $\chi^2$ .

### 4.6.4 The “Pull”

For each measured variable, one can plot the so-called “pull” [2] or “normalized stretch values” [3] [4]:

$$\text{pull } p = \frac{\text{meas} - \text{fit}}{\sqrt{\sigma_{\text{meas}} - \sigma_{\text{fit}}}}$$

The minus sign in the square root comes from the strong correlation between the measured and the fitted quantity, and “*still puzzles many users*” [2]. If all measured errors were estimated correctly

and the conditions for the fit were satisfied (*e.g.*, the event was really a radiative Bhabha event), then the pull quantity will be distributed like a Gaussian centered at 0 with  $\sigma = 1$ . If an error is for example overestimated, the pull quantity will have a more narrow distribution. In this case, the confidence level should also be affected, displaying a tilt in its distribution.

To check whether a systematic increase or decrease of one or more errors would improve the pull and/or the confidence level distributions, one can redo the whole analysis with increased or decreased errors. Perhaps one can find a set of corrections that create nice pull distributions and a nice confidence level distribution. If the errors are really not correct, one should talk with the colleagues who are responsible for the errors. However, abnormal pull quantities might not be always created by incorrect errors. Systematically shifted measurements could also cause such symptoms.

## 5 $\chi^2$ -Function — First Derivatives

For this set of equations, we will use the following notation:

$$L_i = \begin{cases} \lambda_1 & \text{for } i = 1, 4, 7, 10 \quad (p_{ix-}, p_{ix+}, p_{0x-}, p_{0x+}) \\ \lambda_2 & \text{for } i = 2, 5, 8, 11 \quad (p_{iy-}, p_{iy+}, p_{0y-}, p_{0y+}) \\ \lambda_3 & \text{for } i = 3, 6, 9, 12 \quad (p_{iz-}, p_{iz+}, p_{0z-}, p_{0z+}) \end{cases}$$

Now we calculate the first partial derivatives of the  $\chi^2$ -function, i.e., the 19 equations  $\partial\chi^2/\partial\alpha_i$ .

For  $i = 1$  to 12:

$$\frac{\partial\chi^2}{\partial\alpha_i} = 2 \sum_{j=1}^{14} \mathbf{V}_{\text{all } ij}^{-1} (f_j - m_j) + s_i L_i + s_i \lambda_4 \frac{f_i}{E_i}$$

For  $i = 13$ :

$$\begin{aligned} \frac{\partial\chi^2}{\partial\alpha_i} &= 2 \sum_{j=1}^{14} \mathbf{V}_{\text{all } ij}^{-1} (f_j - m_j) - \lambda_1 E_\gamma \cos \theta_\gamma \cos \phi_\gamma - \lambda_2 E_\gamma \cos \theta_\gamma \sin \phi_\gamma + \lambda_3 E_\gamma \sin \theta_\gamma \\ &= 2 \sum_{j=1}^{14} \mathbf{V}_{\text{all } ij}^{-1} (\alpha_j - m_j) \\ &\quad - \alpha_{16} \alpha_{15} \cos \alpha_{13} \cos \alpha_{14} - \alpha_{17} \alpha_{15} \cos \alpha_{13} \sin \alpha_{14} + \alpha_{18} \alpha_{15} \sin \alpha_{13} \end{aligned}$$

For  $i = 14$ :

$$\begin{aligned} \frac{\partial\chi^2}{\partial\alpha_i} &= 2 \sum_{j=1}^{14} \mathbf{V}_{\text{all } ij}^{-1} (f_j - m_j) + \lambda_1 E_\gamma \sin \theta_\gamma \sin \phi_\gamma - \lambda_2 E_\gamma \sin \theta_\gamma \cos \phi_\gamma \\ &= 2 \sum_{j=1}^{14} \mathbf{V}_{\text{all } ij}^{-1} (\alpha_j - m_j) + \alpha_{16} \alpha_{15} \sin \alpha_{13} \sin \alpha_{14} - \alpha_{17} \alpha_{15} \sin \alpha_{13} \cos \alpha_{14} \end{aligned}$$

For  $i = 15$ :

$$\begin{aligned} \frac{\partial\chi^2}{\partial\alpha_i} &= -\lambda_1 \sin \theta_\gamma \cos \phi_\gamma - \lambda_2 \sin \theta_\gamma \sin \phi_\gamma - \lambda_3 \cos \theta_\gamma - \lambda_4 \\ &= -\alpha_{16} \sin \alpha_{13} \cos \alpha_{14} - \alpha_{17} \sin \alpha_{13} \sin \alpha_{14} - \alpha_{18} \cos \alpha_{13} - \alpha_{19} \end{aligned}$$

For  $i = 16$ :

$$\begin{aligned}\frac{\partial \chi^2}{\partial \alpha_i} &= p_{xi-} + p_{xi+} - p_{x0-} - p_{x0+} - E_\gamma \sin \theta_\gamma \cos \phi_\gamma \\ &= \alpha_1 + \alpha_4 - \alpha_7 - \alpha_{10} - \alpha_{15} \sin \alpha_{13} \cos \alpha_{14}\end{aligned}$$

For  $i = 17$ :

$$\begin{aligned}\frac{\partial \chi^2}{\partial \alpha_i} &= p_{yi-} + p_{yi+} - p_{y0-} - p_{y0+} - E_\gamma \sin \theta_\gamma \sin \phi_\gamma \\ &= \alpha_2 + \alpha_5 - \alpha_8 - \alpha_{11} - \alpha_{15} \sin \alpha_{13} \sin \alpha_{14}\end{aligned}$$

For  $i = 18$ :

$$\begin{aligned}\frac{\partial \chi^2}{\partial \alpha_i} &= p_{zi-} + p_{zi+} - p_{z0-} - p_{z0+} - E_\gamma \cos \theta_\gamma \\ &= \alpha_3 + \alpha_6 - \alpha_9 - \alpha_{12} - \alpha_{15} \cos \alpha_{13}\end{aligned}$$

For  $i = 19$ :

$$\begin{aligned}\frac{\partial \chi^2}{\partial \alpha_i} &= E_{i-} + E_{i+} - E_{0-} - E_{0+} - E_\gamma \\ &= E_{i-} + E_{i+} - E_{0-} - E_{0+} - \alpha_{15}\end{aligned}$$

## 6 $\chi^2$ -Function — Second Derivatives

For  $i = 1$  to 12 and  $j = 1$  to 12:

$$\begin{aligned}\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= 2 \mathbf{V}_{\text{all } ij}^{-1} + s_i \lambda_4 \frac{E_i - f_i^2 / E_i}{E_i^2} = 2 \mathbf{V}_{\text{all } ij}^{-1} - s_i \alpha_{19} \frac{\alpha_i^2 - E_i^2}{E_i^3} && \text{if } i = j \\ &= 2 \mathbf{V}_{\text{all } ij}^{-1} - s_i \lambda_4 \frac{f_i f_j}{E_i^3} = 2 \mathbf{V}_{\text{all } ij}^{-1} - s_i \alpha_{19} \frac{\alpha_i \alpha_j}{E_i^3} && \text{if } E_i = E_j \text{ by definition} \\ &= 2 \mathbf{V}_{\text{all } ij}^{-1} && \text{else}\end{aligned}$$

For  $i = 1$  to 12 and  $j = 13$  to 14:

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = 2 \mathbf{V}_{\text{all } ij}^{-1}$$

For  $i = 1$  to 12 and  $j = 15$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = 0$$

For  $i = 1$  to 12 and  $j = 16$  to 18:

$$\begin{aligned}\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= s_i \quad \text{if } L_i = L_j \text{ by definition} \\ &= 0 \quad \text{else}\end{aligned}$$

For  $i = 1$  to  $12$  and  $j = 19$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = s_i \frac{f_i}{E_i} = s_i \frac{\alpha_i}{E_i}$$

For  $i = 13$  and  $j = 13$ :

$$\begin{aligned} \frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= 2 \mathbf{V}_{\text{all } ij}^{-1} + \lambda_1 E_\gamma \sin \theta_\gamma \cos \phi_\gamma + \lambda_2 E_\gamma \sin \theta_\gamma \sin \phi_\gamma + \lambda_3 E_\gamma \cos \theta_\gamma \\ &= 2 \mathbf{V}_{\text{all } ij}^{-1} + \alpha_{16} \alpha_{15} \sin \alpha_{13} \cos \alpha_{14} + \alpha_{17} \alpha_{15} \sin \alpha_{13} \sin \alpha_{14} + \alpha_{18} \alpha_{15} \cos \alpha_{13} \end{aligned}$$

For  $i = 13$  and  $j = 14$ :

$$\begin{aligned} \frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= 2 \mathbf{V}_{\text{all } ij}^{-1} + \lambda_1 E_\gamma \cos \theta_\gamma \sin \phi_\gamma - \lambda_2 E_\gamma \cos \theta_\gamma \cos \phi_\gamma \\ &= 2 \mathbf{V}_{\text{all } ij}^{-1} + \alpha_{16} \alpha_{15} \cos \alpha_{13} \sin \alpha_{14} - \alpha_{17} \alpha_{15} \cos \alpha_{13} \cos \alpha_{14} \end{aligned}$$

For  $i = 13$  and  $j = 15$ :

$$\begin{aligned} \frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= -\lambda_1 \cos \theta_\gamma \cos \phi_\gamma - \lambda_2 \cos \theta_\gamma \sin \phi_\gamma + \lambda_3 \sin \theta_\gamma \\ &= -\alpha_{16} \cos \alpha_{13} \cos \alpha_{14} - \alpha_{17} \cos \alpha_{13} \sin \alpha_{14} + \alpha_{18} \sin \alpha_{13} \end{aligned}$$

For  $i = 13$  and  $j = 16$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = -E_\gamma \cos \theta_\gamma \cos \phi_\gamma = -\alpha_{15} \cos \alpha_{13} \cos \alpha_{14}$$

For  $i = 13$  and  $j = 17$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = -E_\gamma \cos \theta_\gamma \sin \phi_\gamma = -\alpha_{15} \cos \alpha_{13} \sin \alpha_{14}$$

For  $i = 13$  and  $j = 18$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = E_\gamma \sin \theta_\gamma = \alpha_{15} \sin \alpha_{13}$$

For  $i = 13$  and  $j = 19$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = 0$$

For  $i = 14$  and  $j = 14$ :

$$\begin{aligned} \frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= 2 \mathbf{V}_{\text{all } ij}^{-1} + \lambda_1 E_\gamma \sin \theta_\gamma \cos \phi_\gamma + \lambda_2 E_\gamma \sin \theta_\gamma \sin \phi_\gamma \\ &= 2 \mathbf{V}_{\text{all } ij}^{-1} + \alpha_{16} \alpha_{15} \sin \alpha_{13} \cos \alpha_{14} + \alpha_{17} \alpha_{15} \sin \alpha_{13} \sin \alpha_{14} \end{aligned}$$

For  $i = 14$  and  $j = 15$ :

$$\begin{aligned}\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= \lambda_1 \sin \theta_\gamma \sin \phi_\gamma - \lambda_2 \sin \theta_\gamma \cos \phi_\gamma \\ &= \alpha_{16} \sin \alpha_{13} \sin \alpha_{14} - \alpha_{17} \sin \alpha_{13} \cos \alpha_{14}\end{aligned}$$

For  $i = 14$  and  $j = 16$ :

$$\begin{aligned}\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= E_\gamma \sin \theta_\gamma \sin \phi_\gamma \\ &= \alpha_{15} \sin \alpha_{13} \sin \alpha_{14}\end{aligned}$$

For  $i = 14$  and  $j = 17$ :

$$\begin{aligned}\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} &= -E_\gamma \sin \theta_\gamma \cos \phi_\gamma \\ &= -\alpha_{15} \sin \alpha_{13} \cos \alpha_{14}\end{aligned}$$

For  $i = 14$  and  $j = 18$  and  $19$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = 0$$

For  $i = 15$  and  $j = 15$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = 0$$

For  $i = 15$  and  $j = 16$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = -\sin \theta_\gamma \cos \phi_\gamma = -\sin \alpha_{13} \cos \alpha_{14}$$

For  $i = 15$  and  $j = 17$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = -\sin \theta_\gamma \sin \phi_\gamma = -\sin \alpha_{13} \sin \alpha_{14}$$

For  $i = 15$  and  $j = 18$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = -\cos \theta_\gamma = -\cos \alpha_{13}$$

For  $i = 15$  and  $j = 19$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = -1$$

For  $i = 16$  to  $19$  and  $j = 16$  to  $19$ :

$$\frac{\partial^2 \chi^2}{\partial \alpha_j \partial \alpha_i} = 0$$

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