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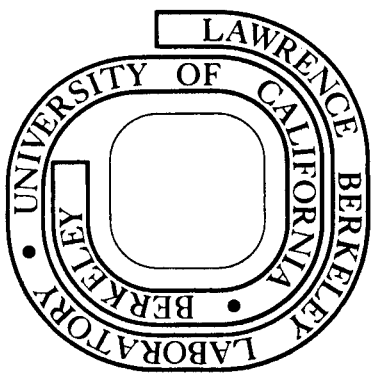

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AMALGAMATION OF MESON-NUCLEON SCATTERING DATA

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Abstract

We present a series of numerical and statistical techniques for interpolating and combining ("amalgamating") data from meson-nucleon scattering experiments. These techniques have been extensively applied to πp elastic and charge-exchange differential cross section and polarization data in the resonance region. The amalgamation is done by fitting a momentum and angle dependent interpolating surface to the data over a moderately narrow momentum range, typically ~150 MeV/c, using the interpolating surface to shift data in a narrower central momentum region into fixed angular bins at a predetermined central momentum, and then statistically combining the data in each bin. The fitting procedure takes into account normalization errors, momentum calibration errors, momentum resolution, electromagnetic corrections, threshold structure, and inconsistencies among the data. The full covariance matrix of the amalgamated data is calculated, including contributions of statistical error, systematic error, and interpolation error. Techniques are presented for extracting from the covariance matrix information on the collective statistical fluctuations which correlate the errors of the amalgamated data. These fluctuations are described in terms of "correlation vectors" which facilitate the use of the amalgamated data as input for resonance region phenomenology.

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I. Introduction

The best modern measurements of two-body meson-nucleon scattering in the resonance region have such high statistical precision that it is important to take systematic errors carefully into account when the data are used. Some sources of systematic error, such as normalization error and beam momentum calibration error, are routinely monitored and documented by experimentalists, but are not always taken into account by data analysts. Other sources of systematic error arise from unknown experimental biases, and show up only as discrepancies between the results of overlapping measurements, or as discontinuities between nearby measurements. Data analysis itself can introduce systematic biases not present in the original data, e.g., by the common practice of binning together several measurements made at slightly different angles and/or momenta.

This paper describes techniques designed to deal with these problems and to produce "amalgamated" differential cross-section and polarization data in an accurate and economically usable form. The purpose is twofold: first, to resolve many questions about systematic errors and discrepant data at an early stage of analysis which is essentially model independent, and second, to summarize the content of an original data set which may contain hundreds of data extending over a band of momenta by a fixed-momentum dataset which will be smaller and more manageable when used in subsequent stages of analysis. The second purpose is similar to that of a more commonly employed procedure, which is to replace the actual data by a set of "Legendre coefficients" or a similar set of parameters. We believe our approach is superior, because the amalgamated data are a more direct and faithful representation of all the features of the original data. The statistical correlations between the amalgamated data are also smaller

and are more easily handled in a subsequent analysis than are the correlations between expansion coefficients.

The general procedure begins by fitting the available data of a given type in a narrow momentum range with a momentum and angle dependent "interpolating surface". The momentum range is chosen to be narrow enough so that the interpolating surface can be taken to be quadratic in the laboratory momentum. In practice, this fit often involves many parameters and many constraints. We have developed a fast and accurate fitting procedure using a two-variable orthogonal polynomial technique tailored to the comparatively simple structure of the relevant χ^2-function. Systematic errors and systematic discrepancies between different measurements are taken into account during the fit of the interpolating surface. Once the surface is determined, data in a narrower central momentum range (in practice, about one-third as wide as the full range of the fit) where the surface is particularly well determined are shifted along the surface to the nearest of a set of closely spaced preselected angles at a preselected central momentum. The shifted data in each angular "bin" are then statistically combined ("amalgamated").

The amalgamated data are correlated through their common dependence on the interpolating surface and on the systematic errors of the original input data. The covariance matrix of the amalgamated data can be calculated directly from the errors of the input data using the two-variable orthogonal polynomials mentioned above. We have found that the correlation properties of the amalgamated data can be accurately represented in terms of collective fluctuations characterized by "correlation vectors". The use of these correlation vectors simplifies the χ^2-function that one would use

in a fit to the amalgamated data, and they can also be used to correct the data for the effect of collective fluctuations.

The techniques described here have been developed in the course of an extensive πN partial wave analysis[1], and have so far only been applied to πp elastic and charge-exchange cross-section and polarization data[2]. In most of the following description we use somewhat more general language appropriate to any elastic or two-body inelastic meson-nucleon cross-section and polarization data. The generality of the description is somewhat illusory, however, because our methods are designed for situations in which there is a large amount of high precision data, and this is presently true of only a few meson-nucleon reactions. In principle, the technique could also be extended to deal with other types of data such as spin-rotation parameter measurements in meson-nucleon scattering or measurements with the various combinations of polarized targets and polarized beams possible in photoproduction or pp scattering, but we will not consider such possibilities here.

II. Parametrization of the Interpolating Surface

The purpose of the interpolating surface is to accurately approximate the true physical values of the measured quantities for which we are amalgamating data. We emphasize that this surface is only an intermediate tool, and is not to be thought of as the final result. Before considering its full energy and angular dependence, let us discuss the angular dependence of the interpolating surface at fixed energy. The differential cross section at fixed energy, I, is a sum of squares of real and imaginary parts of invariant amplitudes all of which are functions of x (=cosθ) analytic throughout the cut x-plane except for singularities along the real axis. The polarization itself is a quotient, but the polarized cross section, IP, is a bilinear form in the real and imaginary parts of the invariant amplitudes multiplied by an overall kinematic factor of sinθ. It is the quantities I and IP/sinθ for which we actually form interpolating surfaces in the fitting procedure described in the following sections, and their fixed energy behavior can thus be represented by analytic functions of x with singularities at the same locations as those of the invariant amplitudes. Specifically, an interpolating surface for meson-nucleon scattering at fixed energy has right- and left-hand cuts starting at the t- and u-channel thresholds and may have poles and dipoles corresponding to baryon exchange (the same analyticity domain as that of the invariant amplitude Re B). For an elastic reaction, I and IP/sinθ also have a singularity at x=1 corresponding to Coulomb scattering, but we omit this from the interpolating surface. Coulomb corrections are taken into account separately and are discussed in the following section and in Appendix A.

The parametrization we use to represent the angular dependence is a

polynomial in the angular variable z of Cutkosky and Deo[3]. This variable is defined in terms of two points on the real axis of the x-plane denoted as x_+ and $-x_-$ which lie to the right and left, respectively, of the physical region ($x_\pm > 1$). The variable z is then defined by the requirement that it map the x-plane cut along (x_+,∞) and $(-\infty,-x_-)$ onto the interior of a unifocal ellipse with the cuts mapped onto the periphery, the interval $(-x_-,x_+)$ mapped onto the real axis, and the points $x=\pm 1$ mapped onto $z=\pm 1$. This mapping stretches the physical region in the forward and backward peaks while compressing it in the wide-angle region, thus tending to produce flatter structure in z than in x and to thereby reduce the number of terms required in a polynomial expansion for a good fit to the data. As discussed in Ref. 3, the most rapidly convergent polynomial expansion of a scattering amplitude is a sum of explicit pole terms and a polynomial in z with x_+ and $-x_-$ located at the tips of the physical t- and u-channel cuts. We adopt here a simpler and more flexible version of the parametrization in which we omit pole terms and treat x_+ and $-x_-$ as phenomenological parameters representing "effective" cut positions at which the strengths of the right- and left-hand singularities (including poles) first become appreciable. The reason for omitting explicit pole contributions is twofold, first because it is more complicated to include pole contributions in observables than in amplitudes[4], and second because the fitting problem we are dealing with here, unlike the problem of determining an amplitude from data, has no continuum ambiguity and the constraining effect of the known residue of a baryon-exchange pole is consequently less important. The reason for not requiring the strict optimal convergence prescription for x_+ and x_- is that it may happen that

the main features of the angular dependence of the data are controlled by singularities which are stronger and more distant than those which determine truly asymptotic convergence rates. In πN scattering, for example, the right-hand cut begins at $t=4m_\pi^2$, and is weak there, while the nearest t-channel resonance exchange poles lie on unphysical sheets at $t=(m_\rho \pm i\Gamma_\rho/2)^2$. We have found in practice that acceptable fits can be obtained with values of x_+ corresponding to intermediate values of $t\approx(m_\rho-\Gamma_\rho)^2$. For the left-hand cut, on the other hand, the strong nucleon exchange in π^+p elastic and π^-p charge-exchange scattering must be taken into account by using a value of x_- corresponding to $u=m_N^2$, while for π^-p elastic scattering we can use $u\approx(m_\Delta-\Gamma_\Delta)^2$. A typical example of the mapping for π^+p scattering at 2 GeV/c is shown in Fig. 1.

We have made several tests which verify that the prescription for $x_\pm$ is well matched to the characteristics of the data. In particular, in tests in which we used $x_\pm=\infty$ (in which case $z=x$, so that our expansion is equivalent to the usual one) our fits were generally less satisfactory and also required more terms. Choosing x_+ to correspond to $t=4m_\pi^2$ also tended to give less satisfactory results.

The energy dependence of the surface is handled more simply because we always fit data over a rather narrow range. The energy range is always chosen to be sufficiently narrow so that quadratic interpolation is sufficient, and the surface is taken to be of quadratic (or lower) degree in the laboratory momentum q. We introduce the normalized variable,

$$y = \frac{q-\bar{q}}{q_0} \qquad \text{(II.1)}$$

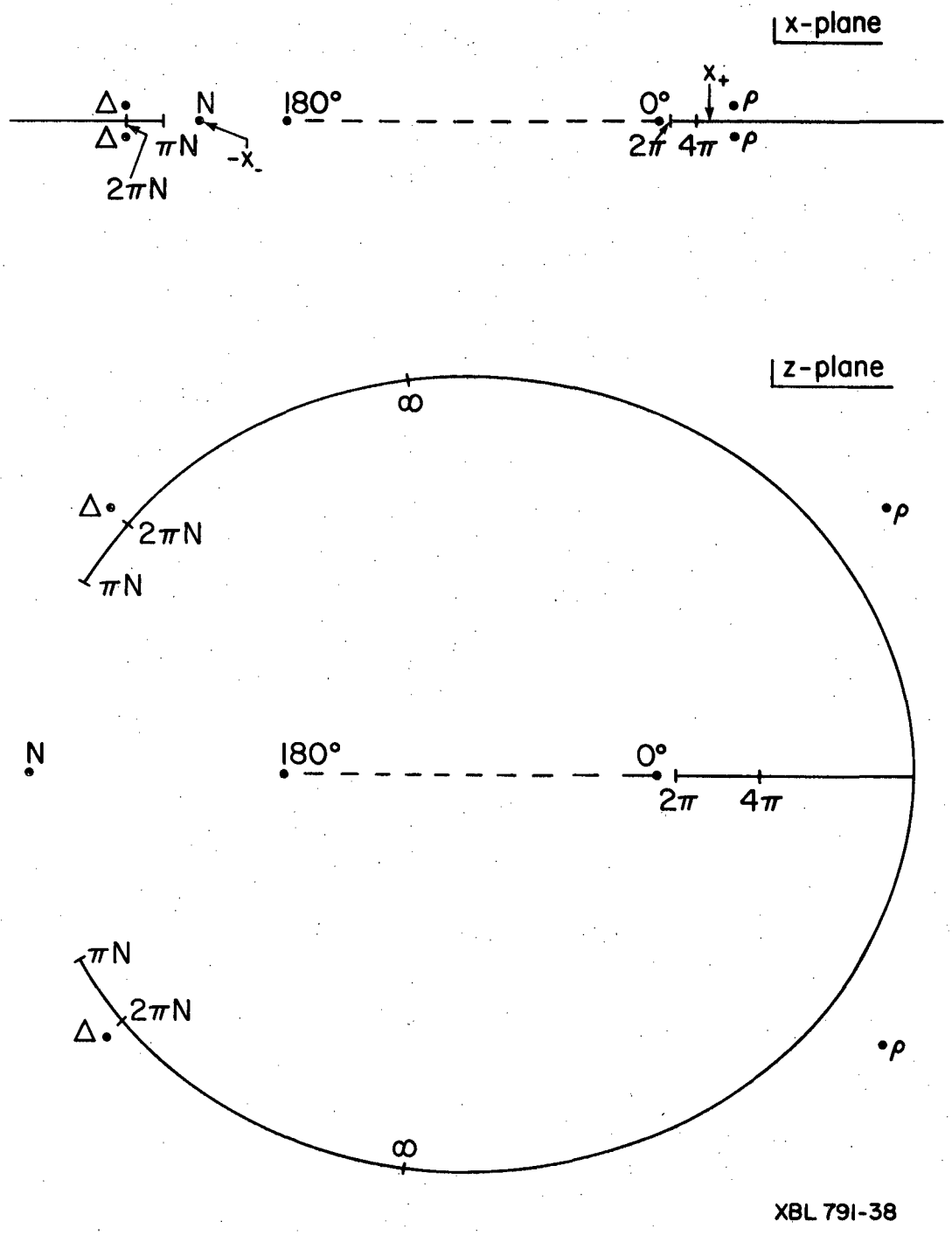

Fig. 1. Conformal mapping of the x-plane onto the z-plane for $\pi^+ p$ scattering at 2 GeV/c. Nearby pole and branch-point singularities in the t- and u-channels are shown, and the "effective" branch points, $\pm x_\pm$, are indicated. The distortion of the physical region is shown by a dashed line which is drawn with equal intervals of 0.1 in the x-plane, and with the corresponding mapped intervals in the z-plane.

where $\bar{q}$ is a weighted average beam momentum for all of the input data. The parameter q_o is chosen to match the amount of momentum dependent curvature of the surface required by the data; for πp scattering q_o is usually about 300 MeV/c. The surface can now be represented in the form,

$$f(z,y) = \sum_{k=0}^{K} y^k f_k(z) \qquad \text{(II.2)}$$

where $f_k(z)$ is a polynomial in z. In principle the relation between z and x is energy dependent, but we neglect this small effect within the momentum range of a single amalgamation, and use a fixed function z(x) appropriate to the central momentum. In the following discussion we allow K to be either 0,1, or 2, although K=2 is by far the most common case encountered in practice. The higher order coefficients of the polynomials f_k are constrained to be of comparable magnitude by the "truncation function" of Eq. (III.8). Thus, for K=2, q_o is the momentum range over which the surface develops a large amount of angle-dependent curvature.

Threshold singularities are not introduced into the interpolating surface itself, but are handled in a manner similar to the Coulomb corrections. This is discussed in the following section and in Appendix B. The only threshold that has been treated in detail so far is the ηn threshold at 687 MeV/c, but it should also be possible to include the ωn threshold at 1092 MeV/c.

III. Definition of the X^2-function

The interpolating surface is fit to experimental data by minimizing the function,

$$\mathrm{X}^2 = \chi^2 + \Phi \qquad \text{(III.1)}$$

where χ^2 contains the constraints imposed by the data, and Φ is a "truncation function" (TF)[5] which imposes a smooth truncation on the number of parameters used in the fit. In this section we give detailed definitions of χ^2 and Φ.

The available world data of a particular type in a narrow momentum range typically consists of several "blocks" of data from different experiments covering various regions of scattering angle at different momenta. We denote each data block by a Greek subscript, and denote the i^{th} datum of block ε as $D_{\varepsilon i}$. The inverse square statistical error of $D_{\varepsilon i}$ is called $w_{\varepsilon i}$, and the value of the interpolating surface $f(z_{\varepsilon i}, y_{\varepsilon})$ at datum εi is designated by $f_{\varepsilon i}$. (For the moment we ignore the finite momentum spread of the beam. See Eq. (IV.2) for a more precise definition of $f_{\varepsilon i}$.) Each data block has an overall normalization error and a corresponding fitted scale factor. For later convenience, we chose to construct χ^2 using the reciprocal of the normalization scale factor, λ_{ε}, rather than the scale factor itself. Thus the renormalized datum εi is $D_{\varepsilon i}/\lambda_{\varepsilon}$. As long as the normalization error is small compared to unity the error in λ_{ε} is the same as the original normalization error. Each data block also has a measured beam momentum p_{ε} with a calibration error, and a corresponding fitted beam momentum q_{ε}. Note that the definition of $f_{\varepsilon i}$ given above uses the fitted momentum q_{ε}. Non-analytic effects (Coulomb scattering and/or

threshold effects) which are not allowed for in the interpolating surface, are taken into account by calculating an explicit correction term for each datum, $c_{\varepsilon i}$, which includes these effects. The calculation of the correction terms is described in Appendices A and B. They are to be subtracted from the renormalized input data before these are compared with the interpolating surface in the χ^2-function. Finally, as discussed in the previous section, when dealing with polarization data we multiply by a factor $s_{\varepsilon i}$, equal to the corresponding cross-section interpolating surface divided by $\sin\theta_{\varepsilon i}$, and evaluated at the fitted momentum q_ε. The χ^2-function constructed in this manner is,

$$\chi^2 = \sum_{\epsilon i} \frac{\lambda_\epsilon^2 W_{\epsilon i}}{S_{\epsilon i}^2}\left[f_{\epsilon i} - S_{\epsilon i}\left(\frac{D_{\epsilon i}}{\lambda_\epsilon} - C_{\epsilon i}\right)\right]^2 \qquad \text{(III.2)}$$

$$+ \sum_{\epsilon\eta} W^1_{\epsilon\eta}(\lambda_\epsilon - 1)(\lambda_\eta - 1) + \sum_{\epsilon\eta} W^2_{\epsilon\eta}(\beta_\epsilon - \beta_\epsilon)(\beta_\eta - \beta_\eta)$$

where $s_{\varepsilon i}=1$ for cross-section data. The matrices $w^1_{\varepsilon\eta}$ and $w^2_{\varepsilon\eta}$ are the inverse covariance matrices of the normalizations and beam momenta, respectively, with correlations taken into account by appropriate off-diagonal elements.

A simpler, approximate χ^2-function obtained from Eq.(III.2) is much more convenient for actual computations. Let,

$$d_{\epsilon i} = D_{\epsilon i} - C_{\epsilon i} \qquad \text{(III.3)}$$

then the sum over individual data points in χ^2 can be rewritten as,

$$\sum_{\epsilon i}\left[\frac{W_{\epsilon i}}{S_{\epsilon i}^2}\left(\lambda_\epsilon f_{\epsilon i}-S_{\epsilon i}d_{\epsilon i}\right)^2+\frac{2W_{\epsilon i}C_{\epsilon i}(\lambda_\epsilon-1)}{S_{\epsilon i}}\left(\lambda_\epsilon f_{\epsilon i}-S_{\epsilon i}d_{\epsilon i}\right)+W_{\epsilon i}C_{\epsilon i}^2(\lambda_\epsilon-1)^2\right] \tag{III.4}$$

which has the form of an expansion in quantities of order,

$$\theta_{\epsilon i}\equiv\frac{|C_{\epsilon i}|\cdot(\text{normalization error})_{\epsilon i}}{(\text{statistical error})_{\epsilon i}} \tag{III.5}$$

There is some arbitrariness in the correction terms, in that we can include in them any analytic contributions we like (as long as these contributions vary slowly enough to be well represented by the interpolating surface), in addition to the specifically non-analytic effects that they are intended to represent. This freedom can be used to keep $|c_{\epsilon i}|$ small, and it is fairly easy to arrange that the quantity,

$$|C_{\epsilon i}|/(\text{statistical error})_{\epsilon i} \tag{III.6}$$

is typically of order unity where non-analytic effects are important and much smaller elsewhere. Thus for well normalized data $\theta_{\epsilon i}$ is small, and the second and third sums in Eq.(III.4) will be small compared to the first. Furthermore, the summand in the second sum fluctuates in sign so we expect a further reduction by a factor or order (total number of data)$^{1/2}$ compared to the first sum. The weakest point in this line of reasoning occurs for elastic differential cross-section data at very small angles,

where the Coulomb correction terms can in principle become arbitrarily large. However, it is difficult to make a measurement far into the Coulomb region without encountering backgrounds which also make the statistical error grow. In explicit checks we have found that even for the most forward available πp data $\theta_{\varepsilon i}$ seldom exceeds 0.3. Occasional data points for which $\theta_{\varepsilon i}>0.3$ can be handled by artificially increasing the statistical error to keep $\theta_{\varepsilon i}$ small. Thus, in the remainder of this paper we will use the χ^2-function,

$$\chi^2=\sum_{\epsilon i}\frac{W_{\epsilon i}}{S_{\epsilon i}^2}\left(\lambda_\epsilon f_{\epsilon i}-S_{\epsilon i}\,d_{\epsilon i}\right)^2 \qquad \text{(III.7)}$$
$$+\sum_{\epsilon\eta}W'_{\epsilon\eta}(\lambda_\epsilon-1)(\lambda_\eta-1)+\sum_{\epsilon\eta}W^2_{\epsilon\eta}(q_\epsilon-p_\epsilon)(q_\eta-p_\eta)$$

The advantage of this form over Eq.(III.2) is that the correction terms can now simply be subtracted from the data before fitting, as in Eq.(III.3), and do not enter explicitly into the χ^2-function itself.

The free parameters to be determined by fitting are the coefficients of the polynomials $f_k(z)$, the scale parameters λ_ε, and the momenta q_ε. The polynomials $f_k(z)$ typically have appreciable coefficients up to order 8 or higher, so that there is no well defined sharp cutoff point for the number of polynomial coefficients retained. We therefore use the TF Φ to impose a smooth truncation on the higher powers of z. This is done by minimizing $\chi^2+\Phi$, rather than χ^2 alone, where

$$\Phi=\frac{2\Omega}{\pi}\sum_{k=0}^{K}\oint\left|\frac{dz}{\sqrt{1-z^2}}\right|\left|f_k(z)\right|^2 \qquad \text{(III.8)}$$

with the line integral being taken around the unifocal ellipse onto which the t- and u-channel cuts are mapped by the Cutkosky-Deo mapping. The lengths of the semi-axes of the ellipse are typically between 2 and 6 (depending on the momentum) so the higher powers of z are magnified with respect to the lower powers on the boundary of the ellipse, and the addition of Φ to χ^2 cuts off these higher powers smoothly. The region in which the cutoff becomes effective is controlled by adjusting the constant Ω. The ellipse shrinks with increasing energy so that Φ naturally allows the number of effectively free parameters to increase with increasing energy even if Ω is held fixed. The particular weight function used in the integral is chosen because Chebyshev polynomials are orthogonal with respect to this weight and this facilitates computation of Φ as discussed in the following section.

In our applications to πp scattering we found that a single value of $10^{-7}(\text{mb/ster})^{-2}$ for Ω gave generally satisfactory results for both cross sections and polarizations throughout the resonance region. This value was arrived at in the usual way, by decreasing Ω until χ^2 per degree of freedom stopped improving. In a few cases where the data were particularly sparse and the interpolating surface was poorly constrained, we used values as large as $10^{-6}(\text{mb/ster})^{-2}$. There are also some data sets with pronounced structure where Ω can be decreased further before χ^2 per degree of freedom stops improving. Although we are aware that some of this structure may turn out to be spurious, we have usually attempted to accomodate it by choosing a conservatively small value of Ω, sometimes as small as $10^{-8}(\text{mb/ster})^{-2}$.

IV. Construction of Orthogonal Polynomials

As a preliminary to the discussion of the full minimization of X^2, we consider here the problem of minimizing X^2 with fixed values of the normalization and momentum parameters. This is a linear least squares problem which can be solved analytically. We represent the fitted surface as

$$f(z,y) = \sum_{m=0}^{M} a_m T_m(z,y) \qquad \text{(IV.1)}$$

where the functions $T_m(z,y)$ are polynomials in z and y and the M+1 parameters a_m are variable coefficients to be determined by minimizing X^2. It is useful for numerous aspects of the amalgamation procedure to attack the problem of determining the coefficients a_m by first chosing the polynomials T_m to diagonalize the a_m-sector of the second-derivative matrix of X^2. All of the difficulties of the fixed λ_ε and q_ε minimization problem are then contained in the construction of polynomials T_m which satisfy an appropriate orthogonality condition (Eq.(IV.10) below), and once these polynomials are constructed the determination of the coefficients is trivial. This section is devoted to the formulation of the orthogonality condition and to the construction of the polynomials which satisfy it.

The terms in X^2 which are bilinear in the coefficients are those containing $f_{\varepsilon i}^2$ and those coming from Φ. The quantity $f_{\varepsilon i}$ is the average of the fitted surface over the spectrum of the ε^{th} beam. If the beam resolution function is $B_\varepsilon(q)$ we have[6],

$$f_{\epsilon i} = \langle f(z_{\epsilon i}, y) \rangle_\epsilon = \int dq\, B_\epsilon(q) f(z_{\epsilon i}, y) \Big/ \int dq\, B_\epsilon(q) \qquad \text{(IV.2)}$$

Since f(z,y) is at most quadratic in y, $f_{\epsilon i}$ can be evaluated completely in terms of the average momentum $\langle q \rangle_\epsilon$, which we take to be the fitted momentum q_ϵ, and the mean squared deviation $\langle (q-\langle q \rangle_\epsilon)^2 \rangle \equiv b_\epsilon^2$. Using the decomposition of Eq.(IV.1) we have,

$$f_{\epsilon i} = \sum_{m=0}^{M} a_m T_{m\epsilon i} \tag{IV.3}$$

where

$$T_{m\epsilon i} = T_m(z_{\epsilon i}, Y_\epsilon) + \frac{1}{2}\rho_\epsilon^2 \frac{\partial^2 T_m(z_{\epsilon i}, Y_\epsilon)}{\partial Y_\epsilon^2}$$

$$\rho_\epsilon = b_\epsilon / q_0 \,, \quad Y_\epsilon = (q_\epsilon - \bar{q})/q_0 \tag{IV.4}$$

The TF has been designed to take advantage of the orthogonality property of Chebyshev polynomials on unifocal ellipses. For any ellipse with focii at z=±1 we have,

$$\oint \left| \frac{dz}{\sqrt{z^2-1}} \right| P_\ell(z) P_{\ell'}(z) = \frac{\pi N_\ell}{2} \delta_{\ell\ell'}$$

$$N_\ell = 2\delta_{\ell 0} + R^{2\ell} + R^{-2\ell} \tag{IV.5}$$

where R is the sum of the semi-axes of the ellipse[7]. To use this relation we represent the polynomials T_m as,

$$T_m(z,Y) = \sum_{\ell=0}^{L} \sum_{k=0}^{K} D_{\ell k}^m P_\ell(z) Y^k \tag{IV.6}$$

where (L+1)(K+1)=M+1. Comparing with Eq.(II.2) we find

$$f_k(z) = \sum_{m=0}^{M} \sum_{l=0}^{L} a_m D^m_{lk} P_l(z) \qquad \text{(IV.7)}$$

Thus the TF can be expressed as,

$$\Phi = \sum_{m=0}^{M} \sum_{n=0}^{M} \tau_{mn} a_m a_n \qquad \text{(IV.8)}$$

where the "truncation matrix" τ is,

$$\tau_{mn} = \sum_{l=0}^{L} \sum_{k=0}^{K} \omega_{lk} D^m_{lk} D^n_{lk} \qquad \text{(IV.9)}$$

$$\omega_{lk} = \Omega N_l$$

We now have all the notation necessary to write down the coefficient sector of the second derivative matrix of X^2 and the orthogonality condition to be imposed on the T_m. This is,

$$\frac{1}{2} \frac{\partial^2 X^2}{\partial a_m \partial a_n} = \sum_{\epsilon i} \omega_{\epsilon i} T_{m\epsilon i} T_{n\epsilon i} + \sum_{lk} \omega_{lk} D^m_{lk} D^n_{lk} = \delta_{mn}$$

$$\omega_{\epsilon i} = W_{\epsilon i} \lambda^2_\epsilon / S^2_{\epsilon i} \qquad \text{(IV.10)}$$

When this condition is satisfied the values of the coefficients which minimize X^2 are easily found to be,

$$\bar{a}_m = \sum_{\epsilon i} \alpha_{\epsilon i} T_{m\epsilon i}$$

$$\alpha_{\epsilon i} = W_{\epsilon i} \lambda_\epsilon d_{\epsilon i} / S_{\epsilon i} \qquad \text{(IV.11)}$$

The actual construction of the orthogonal polynomials can be carried out by a recursion method which is a generalization of the familiar recursion relation $Q_n=(A_n x+B_n)Q_{n-1}+C_n Q_{n-2}$ for orthogonal polynomials Q_n in a real variable x. The lowest order polynomial is chosen to be a constant,

$$T_0(z,y)=D^0_{00}=\left(\sum_{\epsilon i}\omega_{\epsilon i}+\omega_{00}\right)^{-1/2} \qquad \text{(IV.12)}$$

Higher order polynomials are generated by expressing them as a linear combination of all lower order polynomials, plus a linearly independent "leading term", L_m.

$$T_m(z,y)=C_{mm}L_m(z,y)+\sum_{n=0}^{m-1}C_{mn}T_n(z,y)\ ,\ m>0 \qquad \text{(IV.13)}$$

For the first K polynomials with m>0 we define L_m to introduce higher powers of y. For m>K we consecutively introduce higher powers of z in groups of K+1 linearly independent terms. Specifically,

$$L_m(z,y)=\begin{cases} yT_{m-1}(z,y)\ , & 0<m\le K \\ zT_{\tilde{m}}(z,y)\ , & m>K \end{cases} \qquad \text{(IV.14)}$$

where $\tilde{m}=m-(K+1)$. For example, if K=2 new powers of z and y are introduced in the following order: 1, y, y^2, z, zy, zy^2, z^2, z^2y, z^2y^2, z^3,... From Eqs.(IV.13) and (IV.14) we immediately find that

$$D^m_{\ell k}=0 \quad \text{if} \quad m<(K+1)\ell+k \qquad \text{(IV.15)}$$

Note that unlike the familiar real-variable recursion relation, we cannot truncate the lower side of the sum in (IV.13) at some small value of m-n. This is because the TF is a scalar-product type of integral over complex values of z, and as a result L_m will in general not be orthogonal to any of the polynomials T_n with n<m.

We must now solve for the coefficients C_{mn} by imposing the orthogonality relation (IV.10) on the representation (IV.13). For the first sum in the orthogonality relation we need the representation corresponding to (IV.13) for the "evaluated" polynomials $T_{m\epsilon i}$. This is,

$$T_{m\epsilon i} = C_{mm} L_{m\epsilon i} + \sum_{n=0}^{m-1} C_{mn} T_{n\epsilon i}, \quad m>0 \tag{IV.16}$$

where

$$\begin{aligned} L_{1\epsilon i} &= Y_\epsilon T_{0\epsilon i}, \quad K>0 \\ L_{2\epsilon i} &= Y_\epsilon T_{1\epsilon i} + C_{11} \rho_\epsilon^2 T_{0\epsilon i}, \quad K=2 \\ L_{m\epsilon i} &= Z_{\epsilon i} T_{\tilde{m}\epsilon i}, \quad m>K \end{aligned} \tag{IV.17}$$

For the second sum we will need the analog of Eq. (IV.13) for the coefficients $D^m_{\ell k}$. Making a decomposition similar to Eq.(IV.6) for the $L_m(z,y)$,

$$L_m(z,y) = \sum_{\ell=0}^{L} \sum_{k=0}^{K} \Delta^m_{\ell k} P_\ell(z) y^k, \quad m>0 \tag{IV.18}$$

we obtain

$$D^m_{\ell k} = C_{mm}\,\Delta^m_{\ell k} + \sum_{n=0}^{m-1} C_{mn}\,D^n_{\ell k}\ ,\ m>0 \qquad \text{(IV.19)}$$

The coefficients $\Delta^m_{\ell k}$ vanish when $(K+1)\ell+k>m$, and by using the definition (IV.17) of the L_m and the relation

$$z\,P_\ell(z) = \tfrac{1}{2}\left(P_{\ell+1}(z) + P_{\ell-1}(z)\right),\ \ell \geq 1 \qquad \text{(IV.20)}$$

we can express all the Δ-coefficients with $(K+1)\ell+k\leq m$ in terms of D-coefficients corresponding to lower values of m. These relations are given below, where we use integers λ and κ defined by the decomposition $m=(K+1)\lambda+\kappa$ with $\lambda\geq 0$ and $0\leq\kappa\leq K$.

$$\left.\begin{aligned}\Delta^m_{00} &= 0\\ \Delta^m_{0k} &= D^{m-1}_{0,k-1}\ ,\ k\geq 1\end{aligned}\right\}\ \lambda=0$$

$$\left.\begin{aligned}\Delta^m_{0k} &= 0\\ \Delta^m_{1k} &= D^{\tilde m}_{0k}\end{aligned}\right\}\ \lambda=1$$

$$\left.\begin{aligned}\Delta^m_{0k} &= \tfrac{1}{2}D^{\tilde m}_{1k}\ ,\ k\leq K\\ \Delta^m_{0k} &= 0\ ,\ k>K\\ \Delta^m_{1k} &= D^{\tilde m}_{0k}\\ \Delta^m_{2k} &= \tfrac{1}{2}D^{\tilde m}_{1k}\end{aligned}\right\}\ \lambda=2 \qquad \text{(IV.21)}$$

$$\left.\begin{aligned}\Delta^m_{0k} &= \tfrac{1}{2}D^{\tilde m}_{1k}\\ \Delta^m_{1k} &= D^{\tilde m}_{0k} + \tfrac{1}{2}D^{\tilde m}_{2k}\ ,\ k\leq K\\ \Delta^m_{1k} &= D^{\tilde m}_{0k}\ ,\ k>K\\ \Delta^m_{\ell k} &= \tfrac{1}{2}D^{\tilde m}_{\ell-1,k}\ ,\ \ell\geq 2\end{aligned}\right\}\ \lambda=3$$

$$
\left.
\begin{aligned}
\Delta^m_{0k} &= \tfrac{1}{2} D^{\tilde{m}}_{1k} \\
\Delta^m_{1k} &= D^{\tilde{m}}_{0k} + \tfrac{1}{2} D^{\tilde{m}}_{2k} \\
\Delta^m_{\ell k} &= \tfrac{1}{2}\left(D^{\tilde{m}}_{\ell-1,k} + D^{\tilde{m}}_{\ell+1,k}\right) && ,\ 2 \le \ell \le \lambda-3 \\
\Delta^m_{\lambda-2,k} &= \tfrac{1}{2}\left(D^{\tilde{m}}_{\lambda-3,k} + D^{\tilde{m}}_{\lambda-1,k}\right) && ,\ k \le K \\
\Delta^m_{\lambda-2,k} &= \tfrac{1}{2} D^{\tilde{m}}_{\lambda-3,k} && ,\ k > K \\
\Delta^m_{\ell k} &= \tfrac{1}{2} D^{\tilde{m}}_{\ell-1,k_2} && ,\ \ell \ge \lambda-1
\end{aligned}
\right\} \lambda \ge 4
$$

The procedure for solving the recursion relations is now straightforward. Suppose that we have determined all the quantities $C_{nn'}$, $T_{n\epsilon i}$, and $D^n_{\ell k}$ for $n<m$, $n'<m$. The next stage of the process is to substitute Eqs. (IV.16) and (IV.19) into (IV.10), and impose orthogonality between $T_m(z,y)$ and all $T_n(z,y)$ with $n<m$. This gives,

$$
\frac{C_{mn}}{C_{mm}} = -\sum_{\epsilon i} \omega_{\epsilon i} L_{m\epsilon i} T_{n\epsilon i} - \sum_{\ell k} \omega_{\ell k} \Delta^m_{\ell k} D^n_{\ell k} \quad , n<m \tag{IV.22}
$$

which, with the help of (IV.17) and (IV.21), expresses the ratios C_{mn}/C_{mm} in terms of previously calculated quantities. Imposing the normalization condition expressed by Eq. (IV.10) with m=n we obtain

$$
C_{mm} = \left[\sum_{\epsilon i} \omega_{\epsilon i} (L_{m\epsilon i})^2 + \sum_{\ell k} \omega_{\ell k} (\Delta^m_{\ell k})^2 - \sum_{n=0}^{m-1} \left(\frac{C_{mn}}{C_{mm}} \right)^2 \right]^{-1/2} \tag{IV.23}
$$

which is also in terms of previously calculated quantities. $T_{m\epsilon i}$ and $D^m_{\ell k}$ can now be calculated from Eqs. (IV.16) and (IV.19), and one can proceed to index m+1. The polynomials $T_m(z,y)$ themselves can either be calculated recursively using the coefficients C_{mn}, or directly using the coefficients $D^m_{\ell k}$.

V. Effects of Individual Coefficients and Constraints

In the previous section we solved the problem of minimizing X^2 when the normalization and momentum parameters are fixed. We now show that the orthogonal polynomial formalism developed there allows us to make quite specific statements about the effect of individual coefficients and constraints on the resulting value of X^2 at minimum. The part of X^2 which involves the coefficients directly is

$$X_a^2 = \sum_{\epsilon i} \frac{W_{\epsilon i}}{S_{\epsilon i}^2}\left(\lambda_\epsilon f_{\epsilon i} - S_{\epsilon i} d_{\epsilon i}\right)^2 + \Phi \qquad \text{(V.1)}$$

and we can use the results of the previous section (particularly Eqs. (IV.3) and (IV.8)-(IV.11)) to rewrite this as

$$X_a^2 = \sum_{\epsilon i} W_{\epsilon i} d_{\epsilon i}^2 - 2\sum_m \bar{a}_m a_m + \sum_m a_m^2 \qquad \text{(V.2)}$$

The effect of an individual coefficient a_m on the minimum value of X_a^2 is now clear. The minimum value is,

$$X_{a,min}^2 = \sum_{\epsilon i} W_{\epsilon i} d_{\epsilon i}^2 - \sum_m \bar{a}_m^2 \qquad \text{(V.3)}$$

and the result of omitting the m^{th} term from the sum (IV.1) is to increase $X_{a,min}^2$ by $\bar{a}_m^2$ without changing the values of the remaining coefficients.

To describe the effects of individual constraints we rewrite X_a^2 as

$$X_a^2 = \sum_{\epsilon i} \chi_{\epsilon i}^2 + \sum_{\ell k} \phi_{\ell k}^2 \tag{V.4}$$

where

$$\chi_{\epsilon i}^2 = \frac{w_{\epsilon i}}{S_{\epsilon i}^2}\left(\lambda_\epsilon f_{\epsilon i} - S_{\epsilon i} d_{\epsilon i}\right)^2$$

$$\phi_{\ell k}^2 = \omega_{\ell k}\left(\sum_m a_m D_{\ell k}^m\right)^2 \tag{V.5}$$

and consider the effect of omitting one of the constraining terms, i.e., setting one of the $w_{\epsilon i}$ or $\omega_{\ell k}$ to zero. The resulting decrease in $X^2_{a,\min}$ can then be calculated by reminimizing and will generally be greater than the corresponding value of $\chi^2_{\epsilon i}$ or $\phi^2_{\ell k}$ at the original minimum.

Suppose we omit the constraint corresponding to datum ηj, and denote quantities in which this datum is omitted by primes. Then,

$$X_a'^2 = X_a^2 - \chi_{\eta j}^2$$

$$= \sum_{\epsilon i}{}' w_{\epsilon i} d_{\epsilon i}^2 - 2\sum_m b_m a_m + \sum_{mn} S_{mn} a_m a_n \tag{V.6}$$

where

$$b_m = \bar{a}_m - \alpha_{\eta j} T_{m\eta j}$$

$$S_{mn} = \delta_{mn} - \omega_{\eta j} T_{m\eta j} T_{n\eta j} \tag{V.7}$$

Minimizing $X_a'^2$ we obtain

$$\bar{a}'_m = (S^{-1}b)_m$$

$$\chi'^2_{a,min} = \sum_{\epsilon i}{}' w_{\epsilon i} d^2_{\epsilon i} - b^T S^{-1} b \tag{V.8}$$

where we have converted to matrix notation. The inverse of S is,

$$S^{-1}_{mn} = \delta_{mn} + \left(\frac{\omega_{\eta j}}{1-\Lambda_{\eta j}}\right) T_{m\eta j}\, T_{n\eta j} \tag{V.9}$$

where

$$\Lambda_{\eta j} = \omega_{\eta j} \sum_m T^2_{m\eta j} \tag{V.10}$$

It is easily verified that the fitted value of the surface corresponding to datum ηj,

$$\bar{f}_{\eta j} = \sum_m \bar{a}_m T_{m\eta j} \tag{V.11}$$

is changed by an amount

$$\bar{f}'_{\eta j} - \bar{f}_{\eta j} = \left(\frac{\Lambda_{\eta j}}{1-\Lambda_{\eta j}}\right)\left(\bar{f}_{\eta j} - \frac{S_{\eta i}\, d_{\eta j}}{\lambda_\eta}\right) \tag{V.12}$$

by the reminimization and that the decrease in the minimum value of χ^2_a is

$$\chi^2_{a,min} - \chi'^2_{a,min} = \bar{\chi}^2_{\eta j} / (1-\Lambda_{\eta j}) \tag{V.13}$$

where $\bar{\chi}^2_{\eta j}$ is the value of $\chi^2_{\eta j}$ at the original minimum.

If we omit the TF constraint corresponding to $\omega_{\ell k}$ a similar calculation gives equations analogous to (V.12) and (V.13).

$$\sum_m (\bar{a}'_m - \bar{a}_m) D^m_{\ell k} = \left(\frac{\Lambda_{\ell k}}{1-\Lambda_{\ell k}}\right)\left(\sum_m \bar{a}_m D^m_{\ell k}\right) \tag{V.14}$$

$$X^2_{a,min} - X'^2_{a,min} = \bar{\Phi}^2_{\ell k}/(1-\Lambda_{\ell k}) \tag{V.15}$$

where

$$\Lambda_{\ell k} = \omega_{\ell k} \sum_m (D^m_{\ell k})^2 \tag{V.16}$$

It is clear from Eqs. (V.12)-(V.15) that the quantity $\Lambda_{\epsilon i}$ (or $\Lambda_{\ell k}$) is a measure of the "pull" of constraint ϵi (or ℓk) on the fitted parameters $\bar{a}_m$ and on the value of $X^2_{a,min}$. The sense in which this is true can be made more precise by noting that the orthogonality relation implies that,

$$\sum_{\epsilon i} \Lambda_{\epsilon i} + \sum_{\ell k} \Lambda_{\ell k} = M+1 \tag{V.17}$$

Thus it is natural to identify $\Lambda_{\epsilon i}$ (or $\Lambda_{\ell k}$) with the effective number of parameters used in fitting constraint ϵi (or ℓk). Eq.(V.17) can be rewritten in terms of the truncation matrix defined in Eqs.(IV.9) as,

$$\sum_{\epsilon i} \Lambda_{\epsilon i} = (M+1) - T_r\ \tau \tag{V.18}$$

We identify (M+1)-Tr τ as the number of parameters used in fitting the surface to the data, and Tr τ as the number of parameters held fixed by the TF constraint. The quantities $\Lambda_{\varepsilon i}$ and $\Lambda_{\ell k}$ are found to be quite useful in practice for understanding how individual data points and data blocks influence a particular fit and for identifying the position and range of the smooth cut-off imposed by the TF.

VI. Iterative Minimization Scheme

We now consider the problem of minimizing the full X^2-function (Eqs.(III.1), (III.7), and (IV.8)) with respect to all of the free parameters, including λ_ε and q_ε as well as the polynomial coefficients. We have found that this problem can be efficiently handled by an iterative procedure in which minimization at fixed values of λ_ε and q_ε as described above is alternated with full minimization of a quadratic approximation to X^2.

Suppose that we have found a set of orthogonal polynomials, $T_m(z,y)$, satisfying (IV.10) and a set of polynomial coefficients, a_m°, satisfying (IV.11) for particular fixed values, $\lambda_\varepsilon^\circ$ and q_ε°, of the normalization and momentum parameters. We now set,

$$\begin{aligned} a_m &= a_m^\circ + \delta a_m \\ \lambda_\epsilon &= \lambda_\epsilon^\circ + \delta\lambda_\epsilon \\ q_\epsilon &= q_\epsilon^\circ + \delta q_\epsilon \end{aligned} \qquad \text{(VI.1)}$$

and expand X^2 to second order in δa_m, $\delta\lambda_\varepsilon$, and δq_ε. Define parameter and derivative vectors,

$$\delta_1^T = (\delta a_0, \delta a_1, \cdots, \delta a_M)$$

$$\delta_2^T = (\delta\lambda_1, \delta\lambda_2, \cdots, \delta q_1, \delta q_2, \cdots) \qquad \text{(VI.2)}$$

$$d_2^T = -\frac{1}{2}\left(\left.\frac{\partial X^2}{\partial\lambda_1}\right|_0, \left.\frac{\partial X^2}{\partial\lambda_2}\right|_0, \cdots, \left.\frac{\partial X^2}{\partial q_1}\right|_0, \left.\frac{\partial X^2}{\partial q_2}\right|_0, \cdots\right)$$

and second-derivative matrices,

$$(D_{12})_{mn} = \frac{1}{2}\left.\frac{\partial^2 X^2}{\partial a_m \partial(\delta_2)_n}\right|_o$$

$$(D_{22})_{mn} = \frac{1}{2}\left.\frac{\partial^2 X^2}{\partial(\delta_2)_m \partial(\delta_2)_n}\right|_o \qquad \text{(VI.3)}$$

Using $\partial X^2/\partial a_m|_o = 0$ and $\frac{1}{2}\partial^2 X^2/\partial a_m \partial a_n|_o = \delta_{mn}$, the second order expansion of X^2 now becomes,

$$X^2 = X_o^2 - 2\alpha^T\delta + \delta^T D\,\delta + \mathcal{O}(\delta^3) \qquad \text{(VI.4)}$$

where

$$\alpha = \begin{pmatrix} 0 \\ \alpha_2 \end{pmatrix}, \quad \delta = \begin{pmatrix} \delta_1 \\ \delta_2 \end{pmatrix}, \quad D = \begin{pmatrix} I_{11} & D_{12} \\ D_{12}^T & D_{22} \end{pmatrix} \qquad \text{(VI.5)}$$

Minimization with respect to δ gives,

$$\delta = D^{-1}\alpha \qquad \text{(VI.6)}$$

and we can take advantage of the special form of d and D to find that

$$\delta_2 = (D_{22} - D_{12}^T D_{12})^{-1}\alpha_2 \qquad \text{(VI.7)}$$

$$\delta_1 = -D_{12}\,\delta_2 \qquad \text{(VI.8)}$$

For reference we give below explicit expressions for the derivatives that appear in d and D. Primes on $f_{\varepsilon i}$ and $s_{\varepsilon i}$ denote differentiation with

respect to q_ε.

$$\frac{1}{2}\frac{\partial X^2}{\partial \lambda_\epsilon} = \sum_i \frac{W_{\epsilon i} f_{\epsilon i}}{S_{\epsilon i}^2}\left(\lambda_\epsilon f_{\epsilon i} - S_{\epsilon i} d_{\epsilon i}\right) + \sum_\eta W'_{\epsilon\eta}(\lambda_\eta - 1)$$

$$\frac{1}{2}\frac{\partial X^2}{\partial q_\epsilon} = \sum_i \frac{W_{\epsilon i}\lambda_\epsilon}{S_{\epsilon i}^2}\left(f'_{\epsilon i} - \frac{f_{\epsilon i} S'_{\epsilon i}}{S_{\epsilon i}}\right)\left(\lambda_\epsilon f_{\epsilon i} - S_{\epsilon i} d_{\epsilon i}\right)$$
$$+ \sum_\eta W^2_{\epsilon\eta}(q_\eta - \beta_\eta)$$

$$\frac{1}{2}\frac{\partial^2 X^2}{\partial a_m \partial \lambda_\epsilon} = \sum_i \frac{W_{\epsilon i} T_{m\epsilon i}}{S_{\epsilon i}^2}\left(2\lambda_\epsilon f_{\epsilon i} - S_{\epsilon i} d_{\epsilon i}\right) \qquad \text{(VI.9)}$$

$$\frac{1}{2}\frac{\partial^2 X^2}{\partial a_m \partial q_\epsilon} = \sum_i \frac{W_{\epsilon i}\lambda_\epsilon}{S_{\epsilon i}^2}\left[\lambda_\epsilon f_{\epsilon i}\left(T'_{m\epsilon i} - \frac{2 S'_{\epsilon i} T_{m\epsilon i}}{S_{\epsilon i}}\right)\right.$$
$$\left. - S_{\epsilon i} d_{\epsilon i}\left(T'_{m\epsilon i} - \frac{S'_{\epsilon i} T_{m\epsilon i}}{S_{\epsilon i}}\right) + \lambda_\epsilon f'_{\epsilon i} T_{m\epsilon i}\right]$$

$$\frac{1}{2}\frac{\partial^2 X^2}{\partial \lambda_\eta \partial \lambda_\epsilon} = \delta_{\epsilon\eta}\left(\sum_i \frac{W_{\epsilon i} f_{\epsilon i}^2}{S_{\epsilon i}^2}\right) + W'_{\epsilon\eta}$$

$$\frac{1}{2}\frac{\partial^2 X^2}{\partial \lambda_\eta \partial q_\epsilon} = \delta_{\epsilon\eta}\left[\sum_i \frac{W_{\epsilon i}}{S_{\epsilon i}^2}\left(f'_{\epsilon i} - \frac{f_{\epsilon i} S'_{\epsilon i}}{S_{\epsilon i}}\right)\left(2\lambda_\epsilon f_{\epsilon i} - S_{\epsilon i} d_{\epsilon i}\right)\right]$$

$$\frac{1}{2}\frac{\partial^2 X^2}{\partial q_\eta \partial q_\epsilon} = \delta_{\epsilon\eta}\left\{\sum_i \frac{W_{\epsilon i}\lambda_\epsilon}{S_{\epsilon i}^2}\left[\left(\lambda_\epsilon f_{\epsilon i} - S_{\epsilon i} d_{\epsilon i}\right)\left(f''_{\epsilon i} - \frac{2 f'_{\epsilon i} S'_{\epsilon i} + f_{\epsilon i} S''_{\epsilon i}}{S_{\epsilon i}} + \frac{2 f_{\epsilon i}(S'_{\epsilon i})^2}{S_{\epsilon i}^2}\right) + \lambda_\epsilon\left(f'_{\epsilon i} - \frac{f_{\epsilon i} S'_{\epsilon i}}{S_{\epsilon i}}\right)^2\right]\right\} + W_{\epsilon\eta}^2$$

For most purposes terms proportional to $\lambda_\varepsilon f_{\varepsilon i} - s_{\varepsilon i} d_{\varepsilon i}$ are sufficiently small to be safely neglected in the above expressions for the second derivatives. This has no effect on the final minimum, which occurs at $d_2=0$, and does not degrade the convergence rate of the iterative procedure significantly. In particular, it is never necessary to compute the second derivatives $f''_{\varepsilon i}$ and $s''_{\varepsilon i}$ because they are contained in a term proportional to $\lambda_\varepsilon f_{\varepsilon i} - s_{\varepsilon i} d_{\varepsilon i}$.

Our basic iteration scheme is to find a set of polynomials and coefficients at fixed values of λ_ε and q_ε, then shift λ_ε and q_ε according to Eq.(VI.7), find new polynomials and coefficients, etc. However, it is well known that the type of multi-dimensional Newton-Raphson approximation which led to Eq.(VI.7) can have serious instability problems, and we must modify this scheme somewhat to avoid these difficulties. At the outset of a minimization we start from initial values of $\lambda_\varepsilon=1$ and $q_\varepsilon=p_\varepsilon$, and hold q_ε fixed, iterating with the a_m and λ_ε parameters only, until a stable solution is found. The q_ε variables are then released and the full iterative procedure is followed. The initial minimization at fixed q_ε is necessary because the momentum derivatives of X^2 are poorly known during the initial iterative steps, and large, unstable, highly correlated shifts of the normalization and momentum variables away from their input values can

occur if the full iterative scheme is applied at the outset. After each calculation of δ it is useful to check that the adjusted parameters actually give a decrease in X^2. This is done by evaluating X^2 approximately to fourth order in δ, and comparing the result with the previous value. If it is found that X^2 has actually increased, we replace δ by $\beta\delta$ where the scale factor β is chosen to minimize X^2. The fourth order evaluation of X^2 results in a cubic equation for β which can be solved analytically. Sometimes X^2 will appear to decrease when δ is chosen, but because the approximate fourth order evaluation is insufficiently accurate, it will be found that X^2 has actually increased when an exact evaluation is made with new polynomials and coefficients in the next iterative step. In this case we multiply δ by a factor of 0.3 and try again. Failures requiring the scale factor β or the factor of 0.3 are often associated with unstable behavior of the interpolating surface rather than λ_ε and q_ε, because the latter are directly constrained by $w^1_{\varepsilon\eta}$ and $w^2_{\varepsilon\eta}$. We can therefore often correct this behavior and move closer to the minimum by temporarily holding the interpolating surface fixed as we shift λ_ε and q_ε, i.e., by replacing Eqs.(VI.8) and (VI.7) with $\delta_1=0$ and $\delta_2=D_{22}^{-1}d_2$. This replacement is also useful in the initial iteration when λ_ε first departs from unity, and in the first step in which q_ε is allowed to depart from p_ε. With these safequards against instability the iterative procedure usually converges in somewhat less than 40 full steps, i.e., somewhat less than 40 re-evaluations of the polynomials and their coefficients.

VII. Error adjustment

The chi-squared confidence levels of fits obtained as described in the previous sections are often very small. This is due to unknown experimental biases and errors in some of the data, and these effects will propagate into the amalgamated data unless they are explicitly removed. The nature of the problem can be clearly seen in histograms of the data point and data block confidence level distributions calculated on the assumption of Gaussian errors. Examples are shown in Fig. 1 of Ref. 2. Instead of being flat, the distributions are peaked at low confidence levels. These peaks are nearly always present though their heights and widths vary with momentum. The data block confidence level distribution is usually even more sharply peaked than that of the data points, indicating a fairly even scattering of bad data among the different blocks.

We deal with this problem by doing the X^2 minimization in two passes. After the first pass error bars of data in the low confidence level peak are stretched as described below, and the data is then refit. After the second fit the stretching is done again, but at this stage the low confidence level peak has essentially disappeared so the effect is minor. The stretching algorithm is defined in terms of

$$\tilde{\chi}^2_{\epsilon i} = N_d \, \overline{\chi}^2_{\epsilon i} / N_f \qquad \text{(VII.1)}$$

where N_d is the number of data points (including normalizations and momenta) and

$$N_f = N_d + T_r \, \tau - (M+1) - N_s \qquad \text{(VII.2)}$$

is the effective number of degrees of freedom (N_s is the number of normalization and momentum parameters contributing to χ^2). The quantities $\tilde{\chi}^2_{\varepsilon i}$, and similarly defined quantities for the normalizations and momenta, are expected to be distributed approximately in a chi-squared distribution for one degree of freedom if the errors are truly Gaussian. The error $e_{\varepsilon i}$ of datum εi is stretched according to the algorithm,

$$e_{\epsilon i} \text{ unchanged if } \tilde{\chi}^2_{\epsilon i} < \delta_0^2$$

$$e_{\epsilon i} \rightarrow e_{\epsilon i}\left[1+(\delta_1-1)\left(\frac{\sqrt{\tilde{\chi}^2_{\epsilon i}}-\delta_0}{\delta_1-\delta_0}\right)^2\right] \text{ if } \tilde{\chi}^2_{\epsilon i} > \delta_0^2 \qquad \text{(VII.3)}$$

and a similar procedure is applied to the normalization and momentum covariance matrices. Thus stretching begins when $\tilde{\chi}^2_{\varepsilon i}$ exceeds δ_0^2, and becomes extreme when $\tilde{\chi}^2_{\varepsilon i}$ exceeds δ_1^2; δ_0 and δ_1 are chosen to lie near the edge and the middle of the low confidence level peak, respectively. Typical values are $\delta_0=2$ and $\delta_1=3$. About 10% of the errors are usually adjusted by this algorithm, and only about half of these are stretched by a factor of more than 1.5.

Provision is also made for simultaneous stretching of all the error bars in data blocks that remain poorly fit after the above procedure is carried out, but this is seldom necessary and the overall stretching factor is seldom larger than about 1.2.

VIII. Interpolation, Error Propagation, and Amalgamation

The covariance matrix of the shifted data is obtained by calculating their response to fluctuations in the input data. These fluctuations are represented in terms of a statistical model of input data in which the data actually used are considered to be a single sample point in a space of Gaussian random variables whose mean values are the true physical values of the measured quantities. The X^2-function corresponding to a general sample point in this space, in the same approximation as that of Eq.(III.7), is

$$X_g^2 = \sum_{\epsilon i} \frac{\tilde{W}_{\epsilon i}}{S_{\epsilon i}^2}\left(\lambda_\epsilon f_{\epsilon i} - s_{\epsilon i} D_{\epsilon i}\right)^2$$
$$+ \sum_{\epsilon\eta} \tilde{W}'_{\epsilon\eta}(\lambda_\epsilon - \Lambda_\epsilon)(\lambda_\eta - \Lambda_\eta) + \sum_{\epsilon\eta} \tilde{W}^2_{\epsilon\eta}(q_\epsilon - P_\epsilon)(q_\eta - P_\eta)$$
$$+ \sum_{mn} \tau_{mn}(a_m - A_m)(a_n - A_n) \qquad \text{(VIII.1)}$$

The general sample point is here represented by the quantities

$$\begin{aligned} D_{\epsilon i} &= D^0_{\epsilon i} + \delta D_{\epsilon i} \\ \Lambda_\epsilon &= \Lambda^0_\epsilon + \delta\Lambda_\epsilon \\ P_\epsilon &= P^0_\epsilon + \delta P_\epsilon \\ A_m &= A^0_m + \delta A_m \end{aligned} \qquad \text{(VIII.2)}$$

which have the particular values $d_{\varepsilon i}$, 1, p_ε, and 0, respectively, in the actual fit. (The $D_{\varepsilon i}$ in Eq.(VIII.2) should not be confused with the $D_{\varepsilon i}$ in Eqs.(III.2) and (III.3).) The quantities with superscript 0 in (VIII.2) represent the mean values of the random variables which are assumed to be equal to the true physical values of the relevant quantities. The inverse

covariance matrices of $D_{\varepsilon i}$, Λ_ε, P_ε, and A_m are taken to be $\tilde{w}_{\varepsilon i}$ (diagonal), $\tilde{w}^1_{\varepsilon\eta}$, $\tilde{w}^2_{\varepsilon\eta}$, and τ_{mn}, respectively, where the matrices $\tilde{w}$, $\tilde{w}^1$, and $\tilde{w}^2$ are the original matrices w, w^1, and w^2 as modified by error bar stretching, and τ is the truncation matrix defined in Eqs.(IV.9). Inclusion of the quantities A_m with covariance matrix τ^{-1} in the space of random variables allows for fluctuations of the appropriate scale in the a priori values of the coefficients.

The error propagation calculation does not take into account the effect of fluctuations in the input cross section data on the shifted polarization data through the factor $s_{\varepsilon i}$. We neglect this effect because the cross section data are generally considerably more precise than the polarization data. Tests have been made to check that the effect is in fact negligible. We also neglect fluctuations in the adjusted inverse covariance matrices $\tilde{w}$, $\tilde{w}^1$, and $\tilde{w}^2$, and in the truncation matrix, τ.

Our goal is now to calculate the covariance matrix of the fitted parameters that is implied by this prescription for the statistical nature of the input data. We denote the variable parameters as,

$$\begin{aligned} a_m &= a_m^0 + \delta a_m \\ \lambda_\epsilon &= \lambda_\epsilon^0 + \delta\lambda_\epsilon \\ g_\epsilon &= g_\epsilon^0 + \delta g_\epsilon \end{aligned} \qquad \text{(VIII.3)}$$

where the quantities with superscript zero are the values taken at the minimum of X^2_g for the case of mean value input data. In the following we also use polynomials which satisfy an orthogonality condition appropriate to the case of mean value input data,

$$\sum_{\epsilon i} \tilde{\omega}_{\epsilon i} T^{o}_{m\epsilon i} T^{o}_{n\epsilon i} + \tau_{mn} = \delta_{mn} \qquad \text{(VIII.4)}$$

where $\tilde{\omega}_{\varepsilon i}=\tilde{w}_{\varepsilon i}(\lambda^{o}_{\varepsilon})^2/(s^{o}_{\varepsilon i})^2$ and $T^{o}_{m\epsilon i}$ is the quantity in Eq.(IV.4) evaluated at $y_{\varepsilon}=y^{o}_{\varepsilon}=(q^{o}_{\varepsilon}-\bar{q})/q_{o}$. The conditions for a minimum of X^2_g satisfied by a^{o}_{m}, $\lambda^{o}_{\varepsilon}$, and q^{o}_{ε} are

$$a^{o}_{m} = \sum_{\epsilon i} \frac{\tilde{W}_{\epsilon i}\lambda^{o}_{\epsilon} D^{o}_{\epsilon i}}{S^{o}_{\epsilon i}} T^{o}_{m\epsilon i} + \sum_{n} \tau_{mn} A^{o}_{n} \qquad \text{(VIII.5)}$$

$$\sum_{i} \frac{\tilde{W}_{\epsilon i} f^{o}_{\epsilon i}}{(S^{o}_{\epsilon i})^2}\left(\lambda^{o}_{\epsilon} f^{o}_{\epsilon i} - S^{o}_{\epsilon i} D^{o}_{\epsilon i}\right) + \sum_{\eta} \tilde{W}'_{\epsilon\eta}(\lambda^{o}_{\eta} - \Lambda^{o}_{\eta}) = 0$$

$$\sum_{i} \frac{\tilde{W}_{\epsilon i}\lambda^{o}_{\epsilon}}{(S^{o}_{\epsilon i})^2}\left((f'_{\epsilon i})^{o} - \frac{f^{o}_{\epsilon i}(S'_{\epsilon i})^{o}}{S^{o}_{\epsilon i}}\right)\left(\lambda^{o}_{\epsilon} f^{o}_{\epsilon i} - S^{o}_{\epsilon i} D^{o}_{\epsilon i}\right) + \sum_{\eta} \tilde{W}^{2}_{\epsilon\eta}(q^{o}_{\eta} - P^{o}_{\eta}) = 0$$

Using these definitions and minimum conditions we now expand X^2_g to second order about its mean value minimum, i.e., to second order in the quantities $\delta D_{\varepsilon i}$, $\delta\Lambda_{\varepsilon}$, δP_{ε}, δA_{m}, δa_{m}, $\delta\lambda_{\varepsilon}$, and δq_{ε}. To simplify the notation we also define the following quantities (where r and s take the values 1 and 2),

$$F_{1\epsilon i} = f^{o}_{\epsilon i} \quad , \quad F_{2\epsilon i} = \lambda^{o}_{\epsilon}\left((f'_{\epsilon i})^{o} - \frac{f^{o}_{\epsilon i}(S'_{\epsilon i})^{o}}{S^{o}_{\epsilon i}}\right)$$

$$\Omega_{r\epsilon,s\eta} = \delta_{rs}\tilde{W}^{r}_{\epsilon\eta} + \delta_{\epsilon\eta}\sum_{i} \frac{\tilde{W}_{\epsilon i} F_{r\epsilon i} F_{s\epsilon i}}{(S^{o}_{\epsilon i})^2}$$

$$\beta_{m,r\epsilon} = \sum_{i} \frac{\tilde{W}_{\epsilon i}\lambda^{o}_{\epsilon}}{(S^{o}_{\epsilon i})^2} T^{o}_{m\epsilon i} F_{r\epsilon i} \qquad \text{(VIII.6)}$$

$$\delta h_{1\epsilon} = \delta\lambda_\epsilon \,, \quad \delta h_{2\epsilon} = \delta g_\epsilon$$

$$\delta H_{1\epsilon} = \delta\Lambda_\epsilon \,, \quad \delta H_{2\epsilon} = \delta P_\epsilon$$

$$\delta G_{r\epsilon} = \sum_\eta \tilde{W}^r_{\epsilon\eta}\, \delta H_{r\eta} + \sum_i \frac{\tilde{W}_{\epsilon i}}{S^\circ_{\epsilon i}} F_{r\epsilon i}\, \delta D_{\epsilon i}$$

$$\delta K_m = \sum_n \tau_{mn}\, \delta A_n + \sum_{\epsilon i} \frac{\tilde{W}_{\epsilon i}\, \lambda^\circ_\epsilon}{S^\circ_{\epsilon i}} T^\circ_{m\epsilon i}\, \delta D_{\epsilon i}$$

The result of the second order expansion is then,

$$\begin{aligned} \chi^2_g &= (\chi^2_g)^\circ + 2\,\Xi + \sum_{\epsilon i} \tilde{W}_{\epsilon i} (\delta D_{\epsilon i})^2 \\ &+ \sum_{r\epsilon\eta} \tilde{W}^r_{\epsilon\eta}\, \delta H_{r\epsilon}\, \delta H_{r\eta} + \sum_{mn} \tau_{mn}\, \delta A_m\, \delta A_n \\ &- 2 \sum_m \delta a_m\, \delta K_m - 2 \sum_{r\epsilon} \delta h_{r\epsilon}\, \delta G_{r\epsilon} \qquad \text{(VIII.7)} \\ &+ \sum_m (\delta a_m)^2 + 2 \sum_{mr\epsilon} \beta_{m,r\epsilon}\, \delta a_m\, \delta h_{r\epsilon} \\ &+ \sum_{r\epsilon,s\eta} \Omega_{r\epsilon,s\eta}\, \delta h_{r\epsilon}\, \delta h_{s\eta} \end{aligned}$$

where

$$\begin{aligned} \Xi &= -\sum_{\epsilon\eta} \tilde{W}^1_{\epsilon\eta} (\lambda^\circ_\eta - \Lambda^\circ_\eta)\, \delta\Lambda_\epsilon - \sum_{\epsilon\eta} \tilde{W}^2_{\epsilon\eta} (g^\circ_\eta - P^\circ_\eta)\, \delta P_\epsilon \\ &- \sum_{mn} \tau_{mn} (a^\circ_n - A^\circ_n)\, \delta A_m + \sum_{\epsilon i} \frac{\tilde{W}_{\epsilon i}}{(S^\circ_{\epsilon i})^2} \left(\lambda^\circ_\epsilon f^\circ_{\epsilon i} - S^\circ_{\epsilon i} D^\circ_{\epsilon i} \right) \\ &\Big\{ - S^\circ_{\epsilon i}\, \delta D_{\epsilon i} + \sum_m T^\circ_{m\epsilon i}\, \delta a_m\, \delta\lambda_\epsilon \qquad \text{(VIII.8)} \end{aligned}$$

$$+\lambda_\epsilon^0 \sum_m \left[(T'_{m\epsilon i})^0 - \frac{T^0_{m\epsilon i}(S'_{\epsilon i})^0}{S^0_{\epsilon i}} \right] \delta a_m \, \delta q_\epsilon + \frac{F_{2\epsilon i}}{\lambda^0_\epsilon} \delta q_\epsilon \, \delta \lambda_\epsilon$$

$$+\tfrac{1}{2}\lambda^0_\epsilon \left[(f''_{\epsilon i})^0 - \frac{2(f'_{\epsilon i})^0 (S'_{\epsilon i})^0 + f_{\epsilon i} S_{\epsilon i}}{S^0_{\epsilon i}} + \frac{2 f^0_{\epsilon i} (S'^0_{\epsilon i})^2}{(S^0_{\epsilon i})^2} \right] (\delta q_\epsilon)^2 \Bigg\}$$

All terms in Ξ contain factors proportional to the deviation of the mean value input data from the corresponding fitted quantities. Assuming that the parametrization has been appropriately chosen, we expect these factors to be first-order in magnitude and to fluctuate in sign. This results in a suppression of the linear terms in Ξ relative to the second-order part of X^2_g which is positive definite, and a further suppression of the quadratic terms in Ξ which will actually be of third-order magnitude. On this basis we neglect Ξ in the following calculations.

Out next step is to obtain the fitted values of δa_m, $\delta\lambda_\epsilon$, and δq_ϵ in terms of $\delta D_{\epsilon i}$, $\delta\Lambda_\epsilon$, δP_ϵ, and δA_m. Minimizing the expression (VIII.7) for X^2_g (with Ξ neglected) gives the following relations,

$$\delta \bar{a}_m = \delta K_m - \sum_{r\epsilon} \beta_{m,r\epsilon} \, \delta \bar{h}_{r\epsilon}$$

$$\sum_{s\eta} \Omega_{r\epsilon,s\eta} \, \delta \bar{h}_{s\eta} = \delta G_{r\epsilon} - \sum_m \beta_{m,r\epsilon} \, \delta \bar{a}_m \qquad \text{(VIII.9)}$$

where the barred quantities indicate values at minimum. Converting to matrix notation these equations become,

$$\delta \bar{a} = \delta K - \beta \, \delta \bar{h}$$
$$\Omega \, \delta \bar{h} = \delta G - \beta^T \delta \bar{a} \qquad \text{(VIII.10)}$$

The solution is,

$$\delta\bar{a} = A^{-1}\delta\tilde{K}$$
$$\delta\bar{h} = B^{-1}\delta\tilde{G} \qquad \text{(VIII.11)}$$

where

$$\delta\tilde{K} = \delta K - \beta\Omega^{-1}\delta G$$
$$\delta\tilde{G} = \delta G - \beta^T\delta K \qquad \text{(VIII.12)}$$

$$A = 1 - \beta\Omega^{-1}\beta^T$$
$$B = \Omega - \beta^T\beta$$

For later use we note the relation,

$$A^{-1} = 1 + \beta B^{-1}\beta^T \qquad \text{(VIII.13)}$$

which may be obtained as follows:

$$A^{-1} = A^{-1}(A + \beta\Omega^{-1}\beta^T) = 1 + A^{-1}(\beta\Omega^{-1}B)B^{-1}\beta^T$$
$$= 1 + A^{-1}(A\beta)B^{-1}\beta^T = 1 + \beta B^{-1}\beta^T \qquad \text{(VIII.14)}$$

We can now use relations (VIII.11) to express the fluctuations in the shifted data in terms of the fluctuations in the input data. A shifted datum, $D_{b\varepsilon i}$, which is originally the i^{th} data point of data block ε and is shifted to central bin b at the central momentum q_c is defined

to be,

$$D_{b\epsilon i} = \frac{\bar{f}_b}{s_b} + r_{b\epsilon i}\left(\frac{D_{\epsilon i}}{\bar{\lambda}_\epsilon} - \frac{\bar{f}_{\epsilon i}}{\bar{s}_{\epsilon i}}\right) + c_b \qquad \text{(VIII.15)}$$

where s_b and c_b are defined similarly to $s_{\epsilon i}$ and $c_{\epsilon i}$, $r_{b\epsilon i}$ is unity for cross-section data and is $(\sin\theta_b)/(\sin\theta_{\epsilon i})$ for polarization data, and

$$\begin{aligned}
\bar{f}_b &= \sum_m \bar{a}_m T_{mb} \\
\bar{f}_{\epsilon i} &= \sum_m \bar{a}_m \bar{T}_{m\epsilon i} \\
T_{mb} &= T_m(z_b, Y_c) \\
\bar{T}_{m\epsilon i} &= T_m(z_{\epsilon i}, \bar{Y}_\epsilon) + \tfrac{1}{2}\rho_\epsilon^2 \frac{\partial^2 T_m(z_{\epsilon i}, Y_\epsilon)}{\partial Y_\epsilon^2}
\end{aligned} \qquad \text{(VIII.16)}$$

Thus renormalized cross-section data are shifted parallel to the fitted surface while the deviations of renormalized polarization data from the fitted polarization are modulated by $\sin\theta$. To exhibit the fluctuating part of the shifted datum we rewrite it as,

$$D_{b\epsilon i} = D^o_{b\epsilon i} + \Delta_{b\epsilon i} \qquad \text{(VIII.17)}$$

where

$$D^o_{b\epsilon i} = \frac{f^o_b}{s_b} + r_{b\epsilon i}\left(\frac{D^o_{\epsilon i}}{\lambda^o_\epsilon} - \frac{f^o_{\epsilon i}}{s^o_{\epsilon i}}\right) + c_b \qquad \text{(VIII.18)}$$

$$f^o_b = \sum_m a^o_m T_{mb}$$

Expanding $D_{b\epsilon i}-D^{o}_{b\epsilon i}$ we find that the fluctuating part of $D_{b\epsilon i}$ is, to first order,

$$\Delta_{b\epsilon i} = \frac{\Gamma_{b\epsilon i}}{\lambda^{o}_{\epsilon}}\left(\delta D_{\epsilon i} - \frac{D^{o}_{\epsilon i}}{\lambda^{o}_{\epsilon}}\delta\bar{\lambda}_{\epsilon} - \frac{F_{2\epsilon i}}{S^{o}_{\epsilon i}}\delta\bar{q}_{\epsilon}\right) + \sum_{m}\left(\frac{T_{mb}}{S_{b}} - \frac{\Gamma_{b\epsilon i}T^{o}_{m\epsilon i}}{S^{o}_{\epsilon i}}\right)\delta\bar{a}_{m} \qquad \text{(VIII.19)}$$

Following the same argument that we used to neglect Ξ, we expect that the approximation

$$\frac{D^{o}_{\epsilon i}}{\lambda^{o}_{\epsilon}} \approx \frac{f^{o}_{\epsilon i}}{S^{o}_{\epsilon i}}$$

is accurate to first order. We can therefore replace $D^{o}_{\epsilon i}/\lambda^{o}_{\epsilon}$ in (VIII.19) and obtain,

$$\Delta_{b\epsilon i} = \Gamma_{b\epsilon i}\left[\frac{\delta D_{\epsilon i}}{\lambda^{o}_{\epsilon}} - \frac{1}{\lambda^{o}_{\epsilon}S^{o}_{\epsilon i}}\sum_{r}F_{r\epsilon i}\delta\bar{h}_{r\epsilon} - \frac{1}{S^{o}_{\epsilon i}}\sum_{m}\tau^{m}_{b\epsilon i}\delta\bar{a}_{m}\right] \qquad \text{(VIII.20)}$$

where

$$\tau^{m}_{b\epsilon i} = T^{o}_{m\epsilon i} - \left(\frac{S^{o}_{\epsilon i}}{\Gamma_{b\epsilon i}S_{b}}\right)T_{mb} \qquad \text{(VIII.21)}$$

Equations (VIII.20) and (VIII.11) express $\Delta_{b\epsilon i}$ as a linear function of the fluctuations in the input data which have the prescribed covariances,

$$\langle \delta D_{\epsilon i}\, \delta D_{\eta j}\rangle = \delta_{\epsilon i,\eta j}/\tilde{W}_{\epsilon i}$$
$$\langle \delta H_{r\epsilon}\, \delta H_{s\eta}\rangle = \delta_{rs}\,(\tilde{W}^{r})^{-1}_{\epsilon\eta} \qquad \text{(VIII.22)}$$
$$\langle \delta A_m\, \delta A_n\rangle = \tau^{-1}_{mn}$$

Using these we can calculate the covariance of two shifted data,

$$V_{b\epsilon i,d\eta j} \equiv \langle \Delta_{b\epsilon i}\, \Delta_{d\eta j}\rangle \qquad \text{(VIII.23)}$$

The following are useful intermediate steps in the calculation,

$$\langle \delta D_{\epsilon i}\, \delta K_n\rangle = \lambda^{o}_{\epsilon}\, T^{o}_{n\epsilon i}/S^{o}_{\epsilon i}$$
$$\langle \delta D_{\epsilon i}\, \delta G_{s\eta}\rangle = \delta_{\epsilon\eta}\, F_{s\epsilon i}/S^{o}_{\epsilon i}$$
$$\langle \delta K_m\, \delta K_n\rangle = \delta_{mn} \qquad \text{(VIII.24)}$$
$$\langle \delta G_{r\epsilon}\, \delta G_{s\eta}\rangle = \Omega_{r\epsilon,s\eta}$$
$$\langle \delta K_m\, \delta G_{s\eta}\rangle = \beta_{m,s\eta}$$

$$\langle \delta D_{\epsilon i}\, \delta \tilde{K}_n\rangle = \frac{1}{S^{o}_{\epsilon i}}\left[\lambda^{o}_{\epsilon}\, T^{o}_{n\epsilon i} - \sum_{r}(\beta\Omega^{-1})_{n,r\epsilon}\, F_{r\epsilon i}\right]$$
$$\langle \delta D_{\epsilon i}\, \delta \tilde{G}_{s\eta}\rangle = \frac{1}{S^{o}_{\epsilon i}}\left[\delta_{\epsilon\eta}\, F_{s\epsilon i} - \lambda^{o}_{\epsilon}\sum_{m}\beta_{m,s\eta}\, T^{o}_{m\epsilon i}\right]$$
$$\langle \delta \tilde{K}_m\, \delta \tilde{K}_n\rangle = A_{mn} \qquad \text{(VIII.25)}$$
$$\langle \delta \tilde{G}_{r\epsilon}\, \delta \tilde{G}_{s\eta}\rangle = B_{r\epsilon,s\eta}$$
$$\langle \delta \tilde{K}_m\, \delta \tilde{G}_{s\eta}\rangle = -(\beta\Omega^{-1}B)_{m,s\eta}$$

$$\langle \delta D_{\epsilon i}\, \delta \bar{a}_n \rangle = \frac{1}{S^o_{\epsilon i}} \left[\lambda^o_\epsilon \sum_m A^{-1}_{nm} T^o_{m\epsilon i} - \sum_r (\beta B^{-1})_{n,r\epsilon} F_{r\epsilon i} \right]$$

$$\langle \delta D_{\epsilon i}\, \delta \bar{h}_{s\eta} \rangle = \frac{1}{S^o_{\epsilon i}} \left[\sum_r B^{-1}_{s\eta, r\epsilon} F_{r\epsilon i} - \lambda^o_\epsilon \sum_m (\beta B^{-1})_{m,s\eta} T^o_{m\epsilon i} \right]$$

$$\langle \delta \bar{a}_m\, \delta \bar{a}_n \rangle = A^{-1}_{mn} \qquad \text{(VIII.26)}$$

$$\langle \delta \bar{h}_{r\epsilon}\, \delta \bar{h}_{s\eta} \rangle = B^{-1}_{r\epsilon, s\eta}$$

$$\langle \delta \bar{a}_m\, \delta \bar{h}_{s\eta} \rangle = -(\beta B^{-1})_{m,s\eta}$$

The last three entries of Eqs.(VIII.26) make up the covariance matrix of the fitted parameters. We denote this matrix as a whole as,

$$U \equiv \begin{pmatrix} A^{-1} & -(\beta B^{-1}) \\ -(\beta B^{-1})^T & B^{-1} \end{pmatrix} \qquad \text{(VIII.27)}$$

U is proportional to the inverse second derivative matrix of X^2_g with terms contained in Ξ neglected. To make an explicit comparison with the second derivatives displayed in Eqs.(VI.9), we introduce a superscript 0 on the matrices D_{12}, D_{22}, and D which denotes (1) evaluation at the mean value minimum, (2) neglect of terms proportional to $\lambda^o_\varepsilon f^o_{\varepsilon i} - s^o_{\varepsilon i} D^o_{\varepsilon i}$, and (3) replacement of all input weight matrices by their stretched versions, i.e., $w_{\varepsilon i} \to \tilde{w}_{\varepsilon i}$, etc. Then it is easily verified that,

$$D^o_{12} = \beta$$

$$D^o_{22} = \Omega \qquad \text{(VIII.28)}$$

$$(D^o)^{-1} = U$$

The covariance matrix of the shifted data can now be obtained

directly from Eqs. (VIII.20) and (VIII.26). The result is,

$$V_{b\epsilon i, d\eta j} = \delta_{\epsilon i,\eta j}\, r^2_{b\epsilon i} / \tilde{W}_{\epsilon i} (\lambda^0_\epsilon)^2$$
$$- \frac{r_{b\epsilon i}\, r_{d\eta j}}{S^0_{\epsilon i}\, S^0_{\eta j}} \left\{ \sum_{nm} U_{nm} \left[T^0_{n\epsilon i}\, T^0_{m\eta j} - \frac{S^0_{\epsilon i}\, S^0_{\eta j}\, T_{nb}\, T_{md}}{S_b\, S_d\, r_{b\epsilon i}\, r_{d\eta j}} \right] \right.$$
$$+ \frac{1}{\lambda^0_\eta} \sum_{nr} U_{n,r\eta}\, T^0_{n\epsilon i}\, F_{r\eta j} + \frac{1}{\lambda^0_\epsilon} \sum_{nr} U_{n,r\epsilon}\, T^0_{n\eta j}\, F_{r\epsilon i}$$
$$\left. + \frac{1}{\lambda^0_\epsilon\, \lambda^0_\eta} \sum_{rs} U_{r\epsilon, s\eta}\, F_{r\epsilon i}\, F_{s\eta j} \right\} \qquad \text{(VIII.29)}$$

Although the formal derivation of (VIII.29) has been facilitated by expanding about a point corresponding to the true physical values of the relevant quantities, it is of course impossible to use these values in a numerical evaluation of V. In practice we make the replacements $a^0_m \to \bar{a}_m$, $\lambda^0_\varepsilon \to \bar{\lambda}_\varepsilon$, $q^0_\varepsilon \to \bar{q}_\varepsilon$, $T^0_{n\varepsilon i} \to \bar{T}_{n\varepsilon i}$ where the barred quantities are the values at minimum for the particular fit under consideration. These replacements are no less accurate than the various other first-order approximations involved in the derivation of (VIII.29).

The first term of V is primarily due to the errors of the original data while the remaining terms represent errors of interpolation, renormalization, and momentum shifting. These latter errors are generally somewhat smaller than, but comparable to, those of the original data.

The final step of our procedure is the construction of the amalgamated data and their covariance matrix. The amalgamated datum in bin b is a linear combination of the shifted data in that bin,

$$D_b = \sum_{\epsilon i}^{b} \gamma_{b\epsilon i} D_{b\epsilon i} \qquad \text{(VIII.30)}$$

with normalized coefficients,

$$\sum_{\epsilon i}^{b} \gamma_{b\epsilon i} = 1 \qquad \text{(VIII.31)}$$

The covariance matrix of the amalgamated data is,

$$C_{bd} = \sum_{\epsilon i}^{b} \sum_{\eta j}^{d} \gamma_{b\epsilon i} \gamma_{d\eta j} V_{b\epsilon i, d\eta j} \qquad \text{(VIII.32)}$$

We choose the coefficients $\gamma_{b\epsilon i}$ to minimize the variance of D_b subject to the normalization constraint (VIII.31), i.e., we require

$$\frac{\partial}{\partial \gamma_{b\epsilon i}} \left(C_{bb} - \mu \sum_{\epsilon i}^{b} \gamma_{b\epsilon i} \right) = 0 \qquad \text{(VIII.33)}$$

where μ is a Lagrange multiplier. This yields,

$$\gamma_{b\epsilon i} = \sum_{\eta j}^{b} w^{b}_{\epsilon i, \eta j} \Big/ \sum_{\delta k, \eta j}^{b} w^{b}_{\delta k, \eta j} \qquad \text{(VIII.34)}$$

where w^b is the inverse of the submatrix of V pertaining to bin b.

IX. Correlation Vectors

The amalgamated data, D_b, obtained in Sec. VIII are intended to be useful as precise input data for fitting programs, such as partial wave analysis programs. They are more complicated than "raw" experimental data, however, because they have highly correlated errors as expressed by their covariance matrix, C_{bd}. The correlations arise through the mutual dependence of the amalgamated data on the interpolating surface and on the systematic errors of the original input data. Most of the error correlation corresponds to collective fluctuations with rather smooth angular variation, although more complicated correlations also occur. Although the matrix C_{bd} contains complete information on the error correlations, including their collective aspects, this information is not expressed in a particularly transparent way. In this section we show how to extract from C_{bd} a simple, quantitative description of the collective fluctuations. One result of this will be the ability to perform a fit to the amalgamated data with a χ^2-function which involves only single sums over the data points, rather than a double sum over all the matrix elements of C_{bd}. A more important result will be the ability to extract from a particular fit, fitted amplitudes for the collective fluctuations. These amplitudes can be used to perform collective adjustments to the data, in a direct generalization of the common procedure of renormalizing data using a fitted scale factor.

Before embarking on a general discussion of fluctuation-affected data, we will consider a particular simple example by way of introduction. The example is a set of data, $\tilde{D}_b$, with independent "statistical" errors, $\pm e_b$, for each data point, and an overall normalization error of $\pm n$.

More precisely, we represent $\tilde{D}_b$ by a statistical model in which

$$\tilde{D}_b = \lambda d_b \tag{IX.1}$$

where the random variables λ and d_b have means 1 and $\bar{d}_b$, respectively, and have the following covariance matrix:

$$\begin{aligned} \langle (\delta\lambda)^2 \rangle &= n^2 \\ \langle \delta d_b \, \delta d_c \rangle &= \delta_{bc} \, e_b^2 \\ \langle \delta\lambda \, \delta d_b \rangle &= 0 \end{aligned} \tag{IX.2}$$

where

$$\begin{aligned} \delta\lambda &\equiv \lambda - 1 \\ \delta d_b &\equiv d_b - \bar{d}_b \end{aligned} \tag{IX.3}$$

Expanding $\tilde{D}_b$ to first order in $\delta\lambda$ and δd_b we obtain,

$$\begin{aligned} \tilde{D}_b &= \bar{d}_b + \delta\tilde{D}_b \\ \delta\tilde{D}_b &= \delta d_b + \bar{d}_b \, \delta\lambda \end{aligned} \tag{IX.4}$$

The covariance matrix of the normalization-error-affected data is,

$$\tilde{C}_{bc} = \langle \delta\tilde{D}_b \, \delta\tilde{D}_c \rangle = \delta_{bc} \, e_b^2 + n^2 \bar{d}_b \, \bar{d}_c \tag{IX.5}$$

Now suppose that we wish to approximate the covariance matrix, C_{bd}, of some actual amalgamated data, D_b, by a parametrization of the type obtained in Eq.(IX.5). We need to choose values for $\bar{d}_b$, e_b, and n.

There is no unique way to do this, but after testing several approaches we have settled on the following method. For $\bar{d}_b$ we use the fitted value corresponding to bin b,

$$\bar{d}_b = \bar{f}_b / s_b \tag{IX.6}$$

The error e_b is chosen by requiring that the diagonal elements of C and $\tilde{C}$ be equal. This gives e_b in terms of n,

$$e_b^2 = C_{bb} - n^2 \bar{d}_b^2 \tag{IX.7}$$

Finally, to determine n itself we define the residual correlation matrix,

$$\delta\rho_{bc} = \frac{C_{bc} - \tilde{C}_{bc}}{\sqrt{C_{bb} C_{cc}}} \tag{IX.8}$$

and the sum of squares of its off-diagonal elements,

$$\Gamma = \sum_{b<c} (\delta\rho_{bc})^2 \tag{IX.9}$$

n is chosen to minimize Γ, giving

$$n^2 = \left(\sum_{b<c} \frac{C_{bc} \bar{d}_b \bar{d}_c}{C_{bb} C_{cc}} \right) \left(\sum_{b<c} \frac{\bar{d}_b^2 \bar{d}_c^2}{C_{bb} C_{cc}} \right)^{-1} \tag{IX.10}$$

Note that nothing in Eqs.(IX.7) and (IX.10) guarantees that $e_b^2 > 0$ and $n^2 > 0$. This depends on whether the amalgamated data really do have the statistical character of normalization-error-affected data so that the parametrization embodied in $\tilde{C}$ is adequate to provide a good approximation to C.

Once we have determined an approximate error matrix we may consider using it in a fit to the amalgamated data. We would then do the fit by minimizing the approximate χ^2-function,

$$\tilde{\chi}^2 = \sum_{bc} \tilde{C}_{bc}^{-1} (F_b - D_b)(F_c - D_c) \qquad \text{(IX.11)}$$

where F_b is the value of the fitting function at bin b. The inverse of $\tilde{C}$ is,

$$\tilde{C}_{bc}^{-1} = \frac{\delta_{bc}}{e_b^2} - \beta^2 n^2 \frac{\bar{d}_b \bar{d}_c}{e_b^2 e_c^2} \qquad \text{(IX.12)}$$

where

$$\beta^2 = \left(1 + n^2 \sum_b \frac{\bar{d}_b^2}{e_b^2}\right)^{-1} \qquad \text{(IX.13)}$$

So $\tilde{\chi}^2$ reduces to,

$$\tilde{\chi}^2 = \sum_b \left(\frac{F_b - D_b}{e_b}\right)^2 - \left(\frac{\Xi}{\beta}\right)^2 \qquad \text{(IX.14)}$$

where

$$\Xi = \beta^2 \sum_b \frac{n \bar{d}_b}{e_b^2} (D_b - F_b) \qquad \text{(IX.15)}$$

Thus $\tilde{\chi}^2$ has the property of involving only single sums over the data points.

It is of interest to consider the rather peculiar looking χ^2-function of Eq.(IX.14) further, and to interpret it in terms of our statistical

model of normalization-error-affected data. Returning to the model, suppose we have a set of data, $\tilde{D}_b$, and the associated covariance matrix, $\tilde{C}_{bc}$, which we want to fit with some fitting function, F_b. Let us try to devise a way to fit the "normalized" variables, d_b, and the normalization variable, λ, simultaneously, even though we only have data on the combination λd_b. The obvious procedure is to represent the normalized variables by,

$$\tilde{D}_b/\lambda \approx \tilde{D}_b - \bar{d}_b \delta\lambda \qquad \text{(IX.16)}$$

and to introduce an auxiliary normalization parameter to represent λ. For later convenience we will actually use a normalization parameter, ξ, which represents $\delta\lambda/n$. Since the "normalized" variables have independent errors $\pm e_b$ and $\delta\lambda/n$ has unit error we are led to guess that the following χ^2-function is appropriate.

$$\tilde{\Psi}^2 = \sum_b \left(\frac{F_b - \tilde{D}_b + n\bar{d}_b\xi}{e_b} \right)^2 + \xi^2$$
$$= \sum_b \left(\frac{F_b - \tilde{D}_b}{e_b} \right)^2 - \frac{2\xi\tilde{\tilde{\Xi}}}{\beta^2} + \frac{\xi^2}{\beta^2} \qquad \text{(IX.17)}$$

where

$$\tilde{\tilde{\Xi}} = \beta^2 \sum_b \frac{n\bar{d}_b}{e_b^2} (\tilde{D}_b - F_b) \qquad \text{(IX.18)}$$

Minimizing $\tilde{\Psi}^2$ with respect to ξ gives,

$$\xi_{min} = \tilde{\Xi}$$

$$\tilde{\Psi}^2_{min} = \sum_b \left(\frac{F_b - \tilde{D}_b}{e_b}\right)^2 - \left(\frac{\tilde{\Xi}}{\beta}\right)^2 \qquad \text{(IX.19)}$$

This shows two things. First, our guessed χ^2-function, $\tilde{\Psi}^2$, is indeed correct because, once ξ is eliminated, $\tilde{\Psi}^2_{min}$ is identical in form to $\tilde{\chi}^2$ which was explicitly constructed from the correct error matrix for the model data. Second, when the fit is completed and F_b has been determined by minimizing $\tilde{\Psi}^2_{min}$, we are able to construct explicitly the fitted value of λ, which is $1+n\tilde{\Xi}$. We can then return to the original data and construct renormalized data,

$$(\tilde{D}_b)_{rnr} \equiv \tilde{D}_b/(1+n\tilde{\Xi}) \approx \tilde{D}_b - n d_b \tilde{\Xi} \qquad \text{(IX.20)}$$

in which the effect of normalization fluctuation has been suppressed. In an application to actual amalgamated data with C approximated by $\tilde{C}$ we interpret

$$(D_b)_{rnr} \equiv D_b/(1+n\Xi) \approx D_b - n d_b \Xi \qquad \text{(IX.21)}$$

as renormalized data. The renormalization procedure is especially useful in a highly constrained fit with $\tilde{\chi}^2$ entering as one contribution to a total χ^2-function which includes contributions from many other data besides D_b. To the extent that the normalization of F_b is overconstrained by the other data, the fitted value of Ξ in such a case may provide a particularly accurate measure of the normalization of D_b.

The above formalism is not only illustrative, but actually provides

a useful first approximation to the description of the correlated error structure of amalgamated data. In most cases a significant amount of correlation does arise from uncertainties in overall normalization. However, this parametrization employs only one free parameter, n^2, to describe all the off-diagonal elements of C, and it is not sufficiently precise for general use. We next develop a more flexible parametrization which allows the detailed structure of the specific fluctuations affecting a particular dataset to be extracted from its covariance matrix.

Consider a statistical model of fluctuation-affected data, $\tilde{D}_b$, specified in terms of random variables d_b and ζ_n as

$$\tilde{D}_b = d_b + \sum_{n=1}^{N} \zeta_n K_b^n = \bar{d}_b + \delta\tilde{D}_b \qquad \text{(IX.22)}$$

where

$$\begin{aligned} d_b &= \bar{d}_b + \delta d_b \\ \overline{\zeta_n} &= 0 \\ \langle \delta d_b \delta d_c \rangle &= \delta_{bc} e_b^2 \\ \langle \zeta_n \zeta_m \rangle &= \delta_{nm} \\ \langle \delta d_b \zeta_n \rangle &= 0 \end{aligned} \qquad \text{(IX.23)}$$

The "correlation vectors" K^n describe the profiles of N statistically independent fluctuations whose amplitudes are given by the random variables ζ_n. We will require that the correlation vectors be linearly independent, and will impose this condition by requiring them to satisfy the following orthogonality relation:

$$\sum_b \frac{K_b^n K_b^m}{e_b^2} = 0 \quad \text{if} \quad n \neq m \qquad \text{(IX.24)}$$

The particular form of the orthogonality relation is chosen for later convenience. The choice involves no significant loss of generality because, in practice, the orthogonality conditions always represent a small number of relations between a large number of free parameters. The covariance matrix of the fluctuation-affected data is,

$$\tilde{C}_{bc} = \langle \delta\tilde{D}_b \, \delta\tilde{D}_c \rangle = \delta_{bc} e_b^2 + \sum_{n=1}^{N} K_b^n K_c^n \qquad \text{(IX.25)}$$

If we now wish to approximate an actual covariance matrix using this parametrization we must choose values for a large number of free parameters (the diagonal errors e_b and the elements of N orthogonal correlation vectors). We have found that a practical way to do this is to require equality of the diagonal elements of C and $\tilde{C}$, and to minimize Γ, defined as in Eq.(IX.9), by varying the correlation vectors one at a time. This constrained minimization procedure is described in Appendix C. An indication of the accuracy of the approximation of C by $\tilde{C}$ is given by the final value of $2\Gamma/N_o(N_o-1)$ where N_o is the number of occupied bins. This is the mean square value of $\delta\rho_{bc}$ and it should be small compared to unity. However, it is important to realize that although we have found minimization of Γ to be a particularly stable and simple way to fit C with the parametrization embodied in $\tilde{C}$, the final value of Γ itself is a rather arbitrary measure of the accuracy of this approximation.

Other quantitative measures are given below, and these are also used in assessing the accuracy of approximation. In our applications we have obtained adequate accuracy with one or two correlation vectors. The best accuracy is usually attained by choosing N=2, but the addition of a second vector does not always lead to significant improvement so we sometimes choose N=1. Occasionally it even happens that no improvement is possible over the simple normalization-error parametrization, so we use N=1 with K^1 given by Eq.(C.16).

The approximate χ^2-function for a fit to the amalgamated data with the approximated error matrix is of the same form as Eq.(IX.11), but with

$$\tilde{C}_{bc}^{-1} = \frac{\delta_{bc}}{e_b^2} - \frac{1}{e_b^2 e_c^2} \sum_n \beta_n^2 K_b^n K_c^n \qquad \text{(IX.26)}$$

where

$$\beta_n^2 = \left[1 + \sum_b \left(\frac{K_b^n}{e_b}\right)^2\right]^{-1} \qquad \text{(IX.27)}$$

So $\tilde{\chi}^2$ reduces to,

$$\tilde{\chi}^2 = \sum_b \left(\frac{F_b - D_b}{e_b}\right)^2 - \sum_n \left(\frac{\Xi_n}{\beta_n}\right)^2 \qquad \text{(IX.28)}$$

where

$$\Xi_n = \beta_n^2 \sum_b \frac{K_b^n}{e_b^2} (D_b - F_b) \qquad \text{(IX.29)}$$

The particularly simple form of $\tilde{C}^{-1}$ is a result of our choice of the

orthogonality relation for the correlation vecotrs. We interpret $\tilde{\chi}^2$ by returning to the statistical model of Eqs.(IX.22) and (IX.23). To fit the random variables d_b and ζ_n simultaneously, using only data on the combination given by $\tilde{D}_b$, we introduce auxiliary parameters ξ_n to represent the fluctuation amplitudes ζ_n, and construct the quantities

$$\tilde{D}_b - \sum_n \xi_n K_b^n \tag{IX.30}$$

to represent the "unfluctuated" variables d_b. We are thus led to the χ^2-function,

$$\tilde{\Psi}^2 = \sum_b \left(\frac{F_b - \tilde{D}_b + \sum_n \xi_n K_b^n}{e_b} \right)^2 + \sum_n \xi_n^2$$
$$= \sum_b \left(\frac{F_b - \tilde{D}_b}{e_b} \right)^2 - 2 \sum_n \frac{\xi_n \tilde{\tilde{\Xi}}_n}{\beta_n^2} + \sum_n \frac{\xi_n^2}{\beta_n^2} \tag{IX.31}$$

where

$$\tilde{\tilde{\Xi}}_n = \beta_n^2 \sum_b \frac{K_b^n}{e_b^2} (\tilde{D}_b - F_b) \tag{IX.32}$$

Minimization with respect to ξ_n gives,

$$\xi_{n,min} = \tilde{\tilde{\Xi}}_n$$
$$\tilde{\Psi}^2_{min} = \sum_b \left(\frac{F_b - \tilde{D}_b}{e_b} \right)^2 - \sum_n \left(\frac{\tilde{\tilde{\Xi}}_n}{\beta_n} \right)^2 \tag{IX.33}$$

As with Eqs.(IX.19) these results vindicate our choice of $\tilde{\Psi}^2$, and provide us with explicit formulas for the fitted values of the fluctuation

amplitudes. In an application to amalgamated data with C approximated by $\tilde{C}$ we interpret

$$(D_b)_{adj} \equiv D_b - \sum_n \Xi_n K_b^n \qquad \text{(IX.34)}$$

as adjusted data in which the effects of fluctuations have been suppressed. The adjusted data will be particularly accurate when F_b, and hence Ξ_n, are overconstrained by other data besides D_b. The collective fluctuation amplitudes, Ξ_n, represent primarily the effects of the normalization and momentum calibration uncertainties of the original data. The fitted normalizations and momenta of different data sets are correlated, but they are not completely determined. Uncertainties in the interpolating surface also contribute to the collective fluctuations.

We close this section by considering measures of the accuracy of approximation of C by $\tilde{C}$ other then the rms value of $\delta\rho_{bc}$. Consider the χ^2-function for a set of amalgamated data D_b with respect to their own mean values, $\bar{D}_b$.

$$\chi^2 = \sum_{bc} C^{-1}_{bc} (D_b - \bar{D}_b)(D_c - \bar{D}_c) \qquad \text{(IX.35)}$$

Now since

$$\langle (D_b - \bar{D}_b)(D_c - \bar{D}_c) \rangle = C_{bc} \qquad \text{(IX.36)}$$

by definition, we have

$$\langle \chi^2 \rangle = Tr\, C^{-1} C = N_0 \qquad \text{(IX.37)}$$

Using the relation (valid for Gaussian statistics),

$$\langle (D_b - \bar{D}_b)(D_c - \bar{D}_c)(D_d - \bar{D}_d)(D_e - \bar{D}_e) \rangle = C_{bc} C_{de} + C_{bd} C_{ce} + C_{be} C_{cd} \tag{IX.38}$$

we find similarly that,

$$\langle (\chi^2)^2 \rangle = N_o^2 + 2 N_o \tag{IX.39}$$

Thus we reproduce the well-known results that the mean and central variance of χ^2 are N_o and $2N_o$, respectively. To judge the accuracy of $\tilde{C}$ for practical applications we calculate the mean and central variance of

$$\tilde{\chi}^2 = \sum_{bc} \tilde{C}^{-1}_{bc} (D_b - \bar{D}_b)(D_c - \bar{D}_c) \tag{IX.40}$$

for comparison with the ideal values of N_o and $2N_o$. Using Eqs.(IX.36) and (IX.38) one finds that,

$$\langle \tilde{\chi}^2 \rangle = \mathrm{Tr}\, \tilde{C}^{-1} C$$
$$\langle (\tilde{\chi}^2)^2 \rangle - \langle \tilde{\chi}^2 \rangle^2 = 2\, \mathrm{Tr}\, \tilde{C}^{-1} C\, \tilde{C}^{-1} C \tag{IX.41}$$

It is important to monitor these two quantities in practice, because it is quite possible to achieve a small value of $2\Gamma/N_o(N_o-1)$ accompanied by bad values of the mean and central variance. This can usually be corrected by stopping the minimization of Γ somewhat short of an absolute minimum. Typical values of these quantities that we obtain in applications with N=2 are less than 0.1 for the rms value of $\delta\rho_{bc}$, order unity for the bias $\mathrm{Tr}\, \tilde{C}^{-1} C - N_o$, and 2.0 N_o to 2.4 N_o for the central variance.

X. Conclusions

We have presented techniques for amalgamating data from two-body meson-nucleon scattering experiments. The techniques take account of statistical experimental errors, known systematic experimental errors, unknown experimental biases which appear as inconsistencies between overlapping or neighboring data sets, and errors of interpolation. The resulting amalgamated data are highly correlated. We are able to parametrize the correlations in terms of collective fluctuations using one or two correlation vectors.

The techniques described herein have been applied to a collection of all existing $\pi^{\pm}p$ elastic and $\pi^{-}p$ charge-exchange differential cross section and polarization data between 349 and 2055 MeV/c. We have produced amalgamated data for these reactions at 35 momenta from 429 to 1995 MeV/c, in angular bins of 3^{o} spacing. Some of these results are described in Ref. 2. We believe that these data will be particularly useful for partial wave analysis and other resonance-region phenomenology. A description of our own partial wave analysis using these data is given in Ref. 1. The data will shortly be made available to interested users. The computer program developed for this project runs on the LBL CDC-7600, and could be modified for use with data on various two-body reactions. The program will also be supplied to interested users. Inquiries should be directed to one of the authors.

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5. The truncation function is referred to as a "convergence test function" in Refs. 3 and 4 and in many other publications. We prefer the new terminology as being more descriptive.

6. In principle the integration in Eq.(IV.2) should be done at fixed laboratory angle rather than fixed center-of-mass angle. For πN scattering in the resonance region this distinction is insignificant for typical momentum bites ($\pm$2% or better) and angular resolutions ($\pm$0.01 or worse in cosθ). A more significant question is how to extract the rms width of the beam, b_ε, from a quoted momentum bite. The momentum bite is usually only vaguely defined in publications. As a rule we interpret it as refering to the half-width at half-maximum, and multiply by a factor of 0.60 to estimate b_ε. This is the correct factor for a trapezoidal momentum distribution with flat-top to base ratio of 0.6. For comparison, the correct factors are 0.58 and 0.66 for flat-top to base ratios of 1.0 and 0.3, respectively.

7. To avoid any possible confusion, we note that P_ℓ is used in this paper to designate the ℓ^{th} Chebyshev polynomial. The notation T_m is reserved for the two-variable polynomials in z and y.

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Appendix A. Electromagnetic Corrections

The electromagnetic (EM) part of the correction $c_{\varepsilon i}$ (defined in Sec.III) for an elastic differential cross section datum consists of pure Coulomb scattering and Coulomb-nuclear interference contributions. That is, if we write the scattering amplitudes as sums of EM and nuclear parts,

$$\begin{aligned} f &= f_{EM} + f_N \\ g &= g_{EM} + g_N \end{aligned} \tag{A.1}$$

the corresponding correction term is

$$|f_{EM}|^2 + |g_{EM}|^2 + 2\,\mathrm{Re}(f_{EM} f_N^*) + 2\,\mathrm{Re}(g_{EM} g_N^*) \tag{A.2}$$

We use the amplitudes of Tromberg et al.[8] for f_{EM} and g_{EM}, calculated in the manner described in Sec.II-C of the following paper[1].

General expressions for the nuclear amplitudes are given in Eqs.(II.32) of the following paper, but in applications to πp data amalgamation we have modified these somewhat. First, rather than multiplying each partial wave by the appropriate Coulomb phase factor, we multiply by an average overall phase factor, $e^{2i\sigma_3}$, where σ_3 is the non-relativistic Coulomb phase shift for F waves. We have verified that σ_3 is a reasonable average of Σ_{JS} (see Ref.1) for D, F, G, and H waves in the relevant energy range. S and P waves are omitted from the average because the Coulomb phase shift is small compared to typical statistical errors in the phases of these waves. Second, because we are most interested in accurately reproducing the single photon exchange pole contribution, we renormalize the real part of $e^{-2i\sigma_3} f_N$ to enforce agreement with forward dispersion

relation determinations of the real part at 0°. We also ignore the energy dependence of the empirical partial waves used in constructing f_N and g_N, and use fixed values obtained by linear interpolation to the central momentum q_c. This is necessary because of the erratic energy dependence of empirical partial wave amplitudes. The error introduced in the EM corrections at momenta different from q_c by this choice of amplitudes is a smooth function of momentum which is compensated by the interpolating surface. The parametrization of f_N and g_N is thus,

$$f_N(\theta) = e^{2i\sigma_3}\left[\mathrm{Re}\, f_D(0^{\circ})\,\mathrm{Re}\, f_P(\theta)/\mathrm{Re}\, f_P(0^{\circ}) + i\,\mathrm{Im}\, f_P(\theta)\right]$$

$$g_N(\theta) = e^{2i\sigma_3} g_P(\theta) \qquad \text{(A.3)}$$

where $\mathrm{Re}\, f_D(0^{\circ})$ is the dispersion relation calculation for the forward real part evaluated at p_ε, and f_P, g_P are the standard partial wave sums for f_N, g_N evaluated at q_c without Coulomb phase factors. The identification of $\mathrm{Re}\, f_D(0^{\circ})$ with the "Coulomb-phase-free" version of f_N is discussed in Sec. II-D of the following paper. In our applications to πp scattering we have used the dispersion relation predictions of Engelmann and Hendrick[9], and the partial wave amplitudes of Ayed[10].

EM corrections, and the threshold corrections discussed in Appendix B, have been applied to differential cross section data only. These corrections are unimportant for polarization data because of their lower statistical precision. Since the corrections are made before fitting they must be made at the measured momenta, p_ε, rather than the fitted momenta, q_ε. This is acceptable for EM corrections which show little energy variation over ranges corresponding to typical momentum calibration errors. This

point is more delicate for threshold corrections, and is discussed further in Appendix B.

With EM effects removed in the manner described, the interpolating surface at 0° represents the forward nuclear differential cross section. We have included in our cross-section data sets (both elastic and charge-exchange) predictions (with errors) for this quantity obtained by using the total cross sections and the optical theorem, along with the dispersion-theory predictions for the real parts of the amplitudes as calculated by Engelmann and Hendrick[9]. These predictions help to determine the shape of the interpolating surface near the forward direction, and also help to determine the normalization parameters of the other data sets. However, we do not include these 0° predictions in forming the amalgamated data by the method described in Sec. VIII.

Appendix B. Corrections for Threshold Structure

We begin with a review of the effect of an inelastic threshold on a communicating open channel. Consider the S-matrix for N two-body channels with definite values of all conserved quantum numbers J, P, etc. We examine the behavior of S when the first N-1 channels are open, and the N^{th} is an S-wave channel near threshold. Let q be the cm momentum in the N^{th} channel so that $S_{MN} \propto \sqrt{q}$ (M<N) and $S_{NN}-1 \propto q$ near q=0. The general form of S to lowest non-trivial order in q is,

$$S = \begin{pmatrix} S_0 + S_1 q & i\sqrt{2}\, B \sqrt{q} \\ i\sqrt{2}\, B^T \sqrt{q} & 1 + A q \end{pmatrix} \tag{B.1}$$

where S_o and S_1 are symmetric (N-1)x(N-1) matrices, B is an (N-1)-component vector, and A is a scalar. We require that S be unitary above threshold (q>0), and that $S_o+S_1 q$ be unitary below threshold ($q=i|q|$). After some algebra one finds that this leads to the following relations among the parameters of S,

$$\begin{aligned} S_o S_o^\dagger &= 1 \\ S_1 &= -B B^T \\ A &= -B^\dagger B \\ B &= \sqrt{S_o}\, B_o, \quad \mathrm{Im}\, B_o = 0 \end{aligned} \tag{B.2}$$

In particular this implies that for M<N,

$$\begin{aligned} S_{MN} &= i\sqrt{2}\, B_M \sqrt{q} \\ S_{MM} &= (S_o)_{MM} - B_M^2 q \end{aligned} \tag{B.3}$$

Eliminating B_M we obtain

$$S_{MM} = (S_o)_{MM} + \tfrac{1}{2}(S_{MN})^2 \qquad \text{(B.4)}$$

which is the basic relation between an opening production channel and the corresponding elastic channel. The term $\frac{1}{2}(S_{MN})^2$ produces a square-root cusp in S_{MM} because $q \propto (s-s_{th})^{\frac{1}{2}}$. For N=2 the S-matrix reduces to

$$S = \begin{pmatrix} e^{2i\delta}(1-B_o^2 q) & i\sqrt{2}\,B_o e^{i\delta}\sqrt{q} \\ i\sqrt{2}\,B_o e^{i\delta} q & 1-B_o^2 q \end{pmatrix} \qquad \text{(B.5)}$$

Eq.(B.5) displays the simple relation between the elastic phase shift at threshold and the phase of the production amplitude which is characteristic of the two-channel case.

We now specialize to $\pi^- p$ scattering near the ηn threshold at 1488 MeV (687 MeV/c), and let S be the IJP=$\frac{1}{2}\frac{1}{2}-$ S-matrix. It is assumed that the above description in terms of N two-body channels is adequate for our purposes, although multi-body channels account for nearly all of the inelasticity at this threshold. The production cross section near threshold is,

$$\sigma_{\pi^- p \to \eta n} = \frac{2}{3}\frac{\pi}{q_\pi^2}\left|S_{\pi N,\eta N}\right|^2 = \sigma_\eta' q_\eta \qquad \text{(B.6)}$$

where q_π and q_η are the cm momenta in the $\pi^- p$ and ηn channels, respectively, and

$$\sigma_\eta' \equiv \left.\frac{d\sigma_{\pi^- p \to \eta n}}{dq_\eta}\right|_{th} = \frac{4\pi}{3q_{\pi,th}^2}\left|B_{\pi N}\right|^2 \qquad \text{(B.7)}$$

This determines $|B_{\pi N}|$ in terms of the slope of the production cross-section at threshold. The measured value of σ_η' is 21.2±1.8 μb/(MeV/c).[11] Using (B.3) and (B.7) we find that the elastic T-matrix element near threshold is,

$$T \equiv \frac{S_{\pi N,\pi N} - 1}{2i} = T_{th} + \frac{3i}{8\pi} q^2_{\pi,th} \sigma_\eta' e^{2i\alpha} q_\eta \tag{B.8}$$

where α is the phase of $B_{\pi N}$. Bhandari and Chao[12] have determined α to be $41^\circ \pm 6^\circ$ by fitting the backward $\pi^- p$ elastic differential cross section data of Debenham et al.[13]. The πN S_{11} amplitude is fairly elastic near the ηn threshold ($\eta \sim 0.9$), so it is not surprising that α is consistent with the threshold value of the elastic phase shift, $\delta \sim 39^\circ$.

Consider now the problem of amalgamating $\pi^- p$ elastic or charge-exchange differential cross section data in a range of lab momenta, $p_2 > p_{lab} > p_1$, which includes 687 MeV/c. We will construct correction terms, contributions to $c_{\varepsilon i}$, which represent the interference between the cusp term in Eq.(B.8), and the regular part of the f amplitude at threshold. As discussed in Sec. III, we are free to modify Eq.(B.8) by adding analytic terms which can be fit by the interpolating surface, e.g., we can add a quadratic polynomial in p_{lab}. This freedom can be used to control the magnitude of the correction terms away from the immediate vicinity of threshold. Thus we parametrize T as,

$$T = T_o + T_c - T_Q \tag{B.9}$$

where T_C contains the cusp contribution, T_Q is a quadratic approximation to T_C, and T_o is a constant to be determined. It is convenient to

introduce a new variable,

$$x = \frac{2p_{lab} - p_2 - p_1}{p_2 - p_1} \tag{B.10}$$

which varies from -1 to 1 as p_{lab} varies from p_1 to p_2. We choose T_C to be proportional to $\sqrt{x-x_{th}}$, and to be normalized to agree with the square-root singularity in Eq.(B.8). This gives,

$$T_c = iDe^{2i\alpha}\sqrt{x - x_{th}} \tag{B.11}$$

where the square root is positive for $x_{th}<x<1$ and positive imaginary for $-1<x<x_{th}$. The constant D is,

$$D = \frac{3}{8\pi} g^2_{\pi,th}\,\sigma_\gamma' \left(\frac{p_2 - p_1}{2}\right)^{1/2} \left(\frac{dq^2_\gamma}{dp_{lab}}\right)^{1/2}_{th}$$

$$\left(\frac{dq^2_\gamma}{dp_{lab}}\right)_{th} = \frac{2m_p m_n m_\gamma V_{lab,th}}{(m_n + m_\gamma)^2} \tag{B.12}$$

For T_Q we construct a quadratic function of x which approximates $\sqrt{x-x_{th}}$ in the range $|x|<1$,

$$h(x) = \sum_{\ell=0}^{2} h_\ell P_\ell(x) \tag{B.13}$$

where P_ℓ is the ℓ^{th} Legendre polynomial and

$$h_\ell = \frac{2\ell+1}{2}\int_{-1}^{1} dx\,\sqrt{x - x_{th}}\;P_\ell(x) \tag{B.14}$$

Note that h_ℓ is in general complex. T_Q is now given by,

$$T_Q = iDe^{2i\alpha}h(x) \tag{B.15}$$

The constant T_o is determined by linear interpolation of the cusp-free quantity $T-(T_C-T_Q)$ to threshold, using the empirical S_{11} partial wave amplitudes of Ref. 10 for T.

Correction terms are now constructed from the f amplitude,

$$f = f_o + \frac{K}{q_\pi}(T_c - T_Q) \tag{B.16}$$

where f_o is the partial wave sum for f with the S_{11} amplitude replaced by the quantity T_o constructed above, and with the other partial waves evaluated at threshold by simple linear interpolation. K is the isospin factor for the reaction under consideration; 2/3 for $\pi^-p\to\pi^-p$ and $-\sqrt{2}/3$ for $\pi^-p\to\pi^o n$. The correction term is,

$$\frac{2K}{q_\pi}\mathrm{Re}\left[f_o^*(T_c - T_Q)\right] \tag{B.17}$$

This must be evaluated at $(\cos\theta)_{\varepsilon i}$ and integrated over the momentum spectrum of data block ε before being added to $c_{\varepsilon i}$. The momentum averaging is particularly important when p_ε is close to 687 MeV/c. If the spectral shape is a polynomial in p_{lab}, and we neglect the weak momentum dependence of f_o/q_π, the integral can be done exactly by Gaussian integration in the variable $|\sqrt{x-x_{th}}|$ over appropriate sub-ranges. For most π^-p data we have used a rectangular momentum spectrum for this integration. For the data of Debenham et al.[13,14] we use a triangular shape appropriate to the

conditions of that experiment.

We finally consider the problems associated with making the above corrections at the measured momenta, p_ε, rather than the fitted momenta, q_ε. This is not really justified for threshold effects, and a better procedure would be to adjust the correction terms iteratively as the q_ε are being determined so that they end up being evaluated at the fitted momenta. In our present applications, however, we have followed the simpler procedure for two reasons. First, much of the existing $\pi^- p$ data near 687 MeV/c are taken at too widely spaced momenta and/or are insufficiently precise for cusp effects to be clearly present. The complication of evaluating $c_{\varepsilon i}$ at q_ε rather than p_ε is unwarranted for these data. Second, the data of Debenham et al., which does display prominent cusp effects, has a momentum spectrum with a 1.2% full width at half maximum, and a momentum calibration error of ±0.1%. Thus the difference between p_ε and q_ε is completely washed out by the momentum bite integration. Similar, though less extreme, mismatches between momentum bite and calibration error are present in the other existing high precision data sets near the ηn threshold.

Appendix C. Determination of the Correlation Vectors

We consider the problem posed in Sec. IX of approximating a given covariance matrix C_{bc} by the parametrization given in Eq.(IX.25) subject to the orthogonality constraint of Eq.(IX.24). Our approach will be to require equality of the diagonal elements of C and $\tilde{C}$, and to minimize Γ, defined as in Eq.(IX.9), by varying the correlation vectors one at a time. To describe the procedure we introduce the following notation,

$$\begin{aligned} d_b &= C_{bb}/e_b^2 \\ V_b^n &= K_b^n/\sqrt{C_{bb}} \\ \tilde{\rho}_{bc} &= \tilde{C}_{bc}/\sqrt{C_{bb}C_{cc}} = \delta_{bc}/d_b + \sum_n V_b^n V_c^n \\ \rho_{bc} &= C_{bc}/\sqrt{C_{bb}C_{cc}} \\ \delta\rho_{bc} &= \rho_{bc} - \tilde{\rho}_{bc} \end{aligned} \tag{C.1}$$

Now suppose we want to iterate vector 1, holding the rest fixed. We introduce the matrix a,

$$a_{bc} = \rho_{bc} - \sum_{n>1} V_b^n V_c^n = \frac{\delta_{bc}}{d_b} + V_b^1 V_c^1 + \delta\rho_{bc} \tag{C.2}$$

which has known matrix elements given by ρ_{bc} and the fixed vectors. It is also useful to simplify the orthogonality conditions by replacing the vector elements v_b^1 with new independent variables,

$$x_b = d_b V_b^1 = \frac{V_b^1}{a_{bb} - (V_b^1)^2} \tag{C.3}$$

where the latter equality follows from the requirement that $\delta\rho_{bb}=0$. The problem is now to vary x_b so as to minimize

$$\Gamma = \sum_{b<c} (\delta\rho_{bc})^2 = \sum_{b<c} \left(a_{bc} - V_b' V_c' \right)^2 \qquad \text{(C.4)}$$

where

$$V_b' = \frac{1}{2X_b} \left(\sqrt{1 + 4 a_{bb} X_b^2} - 1 \right) \qquad \text{(C.5)}$$

subject to the constraints

$$\sum_b X_b V_b^n = 0 \quad \text{for} \quad n > 1 \qquad \text{(C.6)}$$

We do this by an iterative Newton-Raphson minimization of the quantity

$$\Omega = \Gamma + 2 \sum_{n>1} \kappa_n (x^+ V^n) \qquad \text{(C.7)}$$

where the κ_n are Lagrange multipliers and we are using vector notation for the sum over bins. Denote the derivative vector and second-derivative matrix of Γ at $x_b = x_b^o$ by

$$\alpha_b = -\frac{1}{2} \left. \frac{\partial \Gamma}{\partial X_b} \right|_o$$

$$\beta_{bc} = \frac{1}{2} \left. \frac{\partial^2 \Gamma}{\partial X_b \partial X_c} \right|_o \qquad \text{(C.8)}$$

and expand Ω to second order about x_b^o,

$$\Omega = \Omega_o - 2 \left(\alpha^+ - \sum_{n>1} \kappa_n (V^n)^+ \right) \delta x + (\delta x)^+ \beta (\delta x) \qquad \text{(C.9)}$$

where

$$\delta x = x - x_o \tag{C.10}$$

Minimization of Ω determines the increment in x to be,

$$\delta x = \beta^{-1}\left(\alpha - \sum_{n>1} \kappa_n V^n\right) \tag{C.11}$$

The starting vector x^o is assumed to satisfy the orthogonality conditions, so the Lagrange multipliers are determined by requiring that

$$(V^n)^\dagger(\delta x) = (V^n)^\dagger \beta^{-1}\alpha - \sum_{m>1} Q_{nm}\kappa_m = 0 \tag{C.12}$$

where

$$Q_{nm} = (V^n)^\dagger \beta^{-1} V^m \tag{C.13}$$

Thus,

$$\kappa_n = \sum_{m>1} \hat{Q}^{-1}_{nm} (V^m)^\dagger \beta^{-1}\alpha \tag{C.14}$$

where $\hat{Q}$ is the submatrix of Q obtained by deleting the first row and column. The step from x^o to x results in a decrease in Γ given by,

$$\Gamma - \Gamma^o = \alpha^\dagger \beta^{-1}\alpha - \sum_{nm} Q_{nm}\kappa_n\kappa_m \tag{C.15}$$

In applications of the correlation vector parametrization we have obtained adequate accuracy by always choosing N=1 or N=2. In either case

we begin with a single correlation vector appropriate to normalization fluctuations,

$$K_b^1 = n\bar{f}_b / S_b \tag{C.16}$$

where n^2 is given by Eq.(IX.10), and then vary K_b^1 to minimize Γ. If N=2 it is important to construct a fairly good guess for the second vector before beginning the Newton-Raphson iteration. To describe this, let a be defined as in Eq.(C.2), except that v^2 is now the variable vector with v^1 held fixed. We calculate the quantities,

$$\begin{aligned} S_{bc} &= \sum_d a_{bd} a_{dc} (1-\delta_{bd})(1-\delta_{cd}) \\ &= V_b^2 V_c^2 \sum_d (V_d^2)^2 (1-\delta_{bd})(1-\delta_{cd}) + \mathcal{O}(\delta\rho) \end{aligned} \tag{C.17}$$

$$\begin{aligned} t_b &= \sum_c a_{bc} S_{bc} (1-\delta_{bc}) \\ &= (V_b^2)^2 \sum_{cd} (V_c^2 V_d^2)^2 (1-\delta_{bc})(1-\delta_{cd})(1-\delta_{db}) + \mathcal{O}(\delta\rho) \end{aligned}$$

and our initial guess for v^2 is,

$$V_b^2 = S_{bB} - \left(\sum_c \frac{S_{cB} V_c^1}{a_{cc}}\right)\left(\sum_c \frac{(V_c^1)^2}{a_{cc}}\right)^{-1} V_c^1 \tag{C.18}$$

where B is the value of b for which t_b is a maximum. The second term in Eq.(C.18) approximately orthogonalizes v^2 to v^1. Now we go through an iteration in which we alternatively scale v^2 by the factor

$$\left(\sum_{b<c} a_{bc} V_b^2 V_c^2\right)^{1/2} \left(\sum_{b<c} (V_b^2 V_c^2)^2\right)^{-1/2} \tag{C.19}$$

which minimizes Γ, and then replace v^2 by $v^2-\alpha v^1$ where

$$\alpha = \left(\sum_b d_b V_b^1 V_b^2\right)\left(\sum_b d_b (V_b^1)^2 + 2\sum_b (d_b V_b^1 V_b^2)^2\right)^{-1} \tag{C.20}$$

is chosen to orthogonalize v^1 and v^2 to first order. During this iteration limits must be imposed on the size of each element of v^2 to ensure that $a_{bb} > (v_b^2)^2$. The process converges when α becomes vanishingly small, and the full minimization procedure with all elements of v^2 varying independently can then begin. Alternative variation of v^1 and v^2 is continued until convergence is achieved. Instabilities of the Newton-Raphson method sometimes occur, but they can usually be avoided by temporarily switching to a simple steepest descent minimization.

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