Application of a Relativistic Resonance Formula to the $e^+e^- \rightarrow \pi^+\pi^-$ Experiment*

MICHAEL PARKINSON[†]

Physics Department, Syracuse University, Syracuse, New York 13210

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The present data for the reaction $e^+e^- \rightarrow \pi^+\pi^-$ are analyzed with the aid of a general effective-range resonance formula for the ρ meson. It is concluded that (a) $m_{\rho} = 769 \pm 5$ MeV and $\Gamma_{\rho} = 109 \pm 10$ MeV provide a reasonable explanation of the present experimental points; (b) the full width at half-maximum regardless of the peak height should give an excellent estimate of the ρ width; (c) it is hard to escape $|\vec{F}_{\pi}(m_{\rho}^{2})|^{2} = m_{\rho}^{2}/\Gamma_{\rho}^{2}$; (d) the effects of final-state interactions on resonance shape ought to be investigated.

ERE we present an analysis of the pion factor as H EKE we present an analysis π^{-} experiments of measured in the $e^+e^- \rightarrow \pi^+\pi^-$ experiments of Orsav and Novosibirsk,¹ using a formula derived from a natural relativistic generalization of the Breit-Wigner formula for the ρ meson.² This relativistic resonance formula, when tested against the $\pi N \rightarrow \pi \pi N$ data, appears to be guite satisfactory,³ although we will have more to say on this subject later. For our purposes here, we need only the following expressions:

$$F_{\pi}(s) = D(0)/D(s), \quad s = (p_{+} + p_{-})^{2}$$
 (1)

$$D(s) = 1 - \frac{s - s_0}{\pi} P \int \frac{\mu(s')ds'}{(s' - s_0)^2(s' - s)} - \frac{i\mu(s)}{s - s_0}, \quad (2)$$

$$\mu(s') = \sum_{I=1}^{N} C_i^2 \rho_i(s') \theta(s'-t_i), \quad \theta(s) = 1, \quad s > 0$$

= 0, $s < 0.$ (3)

 C_i , ρ_i , and t_i are given in Table I; *i* is the channel index.

A short discussion of the derivation of (1)-(3) will be given here; for a more complete discussion, see Ref. 2.

Briefly then, for the 1^- partial wave, we write the T matrix, related to S matrix by $S=1-2i\rho T$, as T^{-1} $=K'^{-1}-i\rho$, where we have introduced the K' matrix; ρ is the matrix of relativistic phase-space factors:

$$\rho_{ij} = \rho_i(s) \delta_{ij} \theta(s - t_i).$$

As defined, K' is not analytic, because ρ contains θ functions. We assume T is analytic because all currently acceptable theories have this property. Suppose we now define $R_{ij}(s) = r_i(s)\delta_{ij}$, where

$$r_i(s) = \frac{1}{\pi} \int_{t_i}^{\infty} \frac{\rho_i(s')ds'}{s' - s - i\epsilon} + \text{possible subtractions}.$$

461 (1969).

Then $T^{-1} = K^{-1} - R$ defines an analytic K matrix which should be easier to approximate. At a resonance, T becomes pure imaginary, which means $K^{-1} \rightarrow (K_0^{-1})(s_R - s)$, with $K_0 > 0$ so that we have a pole on the second sheet. K_0 is the matrix of coupling constants to the resonance: $(K_0)_{ij} = k_i k_j$. Thus,

$$T = K_0(s_R - s - RK_0)^{-1} = K_0/[s_R - s - Tr(RK_0)],$$

or $T = K_0/\Delta(s)$ with $\Delta(s) = s_R - s - \text{Tr}(RK_0)$. In order to make Re[Tr(RK_0)] vanish as $(s-s_R)^2$ when $s \rightarrow s_R$, we subtract it twice at the mass of the resonance. This formula, like all effective-range formulas, usually has a pole on the real axis for s < 0, i.e., $\Delta(s_0) = 0$ for $s_0 < 0$. This pole must be removed to get the form factor. It can be shown that

$$\Delta(s) = (s-s_0) \left(1 - \frac{s-s_0}{\pi} \int_{-\infty}^{+\infty} \left[\sum_{i=1}^{N} C_i \rho_i(s') \theta(s'-t_i) \right] ds' \right)$$

$$(s'-s_0)^2 (s'-s-i\epsilon) ds'$$

where C_i are proportional to the k_i , and we display the zero at $s = s_0$ explicitly rather than that at $s = s_R$. Thus, $D(s) = \Delta(s)/(s-s_0)$ which leads to Eqs. (1)-(3) if we elect to normalize F(0) = 1. Observe that D corresponds to the D function in the ND^{-1} method with the left-hand cut replaced by a pole at $s = s_0$. Like the usual simple pole approximation at $s=s_R$, $D(s)\approx s_R-s-im_R\Gamma_R$ for $s \approx s_R$, but its behavior away from that point is not the same. It seems plausible that Eq. (2) ought to be better than the usual simple pole approximation, because it has more of the properties of the correct Dfunction than the latter. For example, one significant property Eq. (2) possesses is that the integral in Dgives the analytic continuation of the decay widths of the resonance into the various channels. That such an analytic continuation is needed, in general, was observed some time ago,⁴ in the calculation of the mass shift to a nuclear state due to the opening and closing of a channel as the position of the channel threshold moves. For these reasons, we will use Eq. (1) with the three channels that seem most significant $\pi\pi$, $\pi\omega$,

^{*} Work supported by the U. S. Atomic Energy Commission. † Present address: Dept. of Physics, University of Florida, Gainesville, Fla. 32601.

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⁴ J. B. Ehrman, Phys. Rev. 81, 412 (1951); R. G. Thomas, *ibid.* 88, 1109 (1952); for a modern discussion, see S. C. Frautschi, Phys. Letters 8, 141 (1964).

Channel	Particles	Masses	t Thres	u^{holds}	Coupling constants ^a	Functions ρ_i
1	ππ	$m_{\pi} = 1$	4.0	0	$C_1 \approx 0.90$	$[(s-t_1)^3/16s]^{1/2}$
2	NN(+-)	$m_N = 6.72$	180.6	0	$C_2 \approx 3.0$	$[(s-t_2)s/4]^{1/2}$
3	$\pi\omega$	$m_{\omega} = 5.61$	43.7	21.2	$C_3 \approx 0.60$	$[(s-t_3)^3(s-u_3)^3]^{1/2}/16s$

TABLE I. The relevant data for insertion into Eqs. (1)-(3). We have used the values and conventions of Ref. 2 except for a permutation of channels. The (+-) refers to the helicities of the nucleons. The integral over channel 3 has been cut off sharply at $200m_{\pi^2}$.

* These are varied in order to fit the data. The approximate values shown are those expected from other considerations: $C_1 \approx 0.90$ corresponds to a 100-125 MeV width, depending on s_0 and $D'(m_\rho^2)$, C_2 is inferred from universal ρ coupling and vector-meson dominance of the electromagnetic form factor, and C_3 comes from the $\omega \rightarrow 3\pi$ decay width. See Ref. 2 for more details.

 $\overline{N}N(+-)$, when we attempt to fit the data. These three channels were quite adequate in accounting for the ρ meson in $\pi N \rightarrow \pi \pi N$, where it was found that³

$$\Gamma_{\rho} = 152 \pm 18 \text{ MeV}$$
 and $m_{\rho} = 768 \pm 2 \text{ MeV}$. (4)

Let us now consider the $\pi\pi$ problem in the 1⁻ partial wave. In Table I, we see estimated values for the C_i . With values such as these, ReD(s) turns out to be approximately linear. We define m_{ρ}^2 and Γ_{ρ} as follows:

$$\operatorname{Re}D(m_{\rho}^{2}) = 0, \qquad (5)$$

$$m_{\rho}\Gamma_{\rho} = \frac{C_{1}^{2}\rho_{1}(m_{\rho}^{2})}{m^{2} + |s_{0}|} \frac{1}{\operatorname{Re}D'(m_{\rho}^{2})}, \quad D'(s) = \frac{\partial D}{\partial s}.$$
 (6)

Plotted against $E = \sqrt{s}$, D(0)/D(s) peaks for $E \approx m_{\rho}$ and has a full width at half-maximum approximately equal to Γ_{ρ} . These facts lead us to a quantitative test that can be applied to the $e^+e^- \rightarrow \pi^+\pi^-$ data in order to see if Eqs. (1)-(3) can reasonably explain them. For we see that

$$|F_{\pi}(m_{\rho}^{2})|^{2} = \left(\frac{D(0)}{m_{\rho}^{2} \operatorname{Re} D'(m_{\rho}^{2})}\right)^{2} \frac{m_{\rho}^{2}}{\Gamma_{\rho}^{2}}.$$
 (7)

When $\operatorname{Re}D(s)$ is approximately linear, because $D(s_0)=1$ and $\operatorname{Re}D(m_{\rho}^2)=0$, we find that

and

$$\operatorname{Re}D'(m_{\rho}^{2}) \approx 1/(m_{\rho}^{2} + |s_{0}|).$$

 $D(0)/D(s_0) \approx m_{\rho^2}/(m_{\rho^2} + |s_0|)$

We do expect D(s) to be roughly linear, and thus we expect the following relation to be true:

$$|F_{\pi}(m_{\rho}^{2})|^{2} \approx m_{\rho}^{2}/\Gamma_{\rho}^{2}.$$
(8)

Comparing Eq. (8) against experiment, we see that it is consistent at this point, but only because of the large error bars. This is particularly true of the Novosibirsk points. It will be interesting to see how Eq. (8) fares in the future as the experimental results are sharpened.

For example, it may turn out the *D* is sufficiently nonlinear so that Eq. (8) will not hold. For example, if we set $g_{\rho NN} = g_{\rho \pi \omega} = 0$, or if we take $g_{\rho \pi \omega} = 1.5$, we get sufficient nonlinearity to affect Eq. (7), quite substantially in the latter case. Neither of these examples is particularly realistic in the present scheme of things, but, nevertheless, even in these cases we find that a very good estimate of Γ_{ρ} , the ρ -meson decay width or inverse lifetime, is the full width at half-maximum in the form factor, regardless of the height of the peak. This suggests the desirability of obtaining very accurate data points around the half-maximum on each side of the peak as a way to measure the ρ width precisely and rather independently of the exact dynamics reflected, for example, in the thresholds and coupling constants which enter into Eq. (2).

APPLICATION OF EQS. (1)-(3) TO EXPERIMENTAL DATA

In Fig. 1, one sees the results of fitting Eq. (1) to the present experimental data (see the Appendix for



FIG. 1. The curve was fitted using Eqs. (1)-(3) (see Appendix for details) with four parameters, obtaining $s_0 = (380\pm8)m_{\pi}^2$, $C_1 = 1.15\pm0.01$, $C_2 = 3.0\pm0.05$, $C_3 = (0.45\pm0.20)m_{\pi}^{-1}$. The χ^2 was 25; see text for discussion.

details). It is quite reassuring to see that the $\pi\rho\omega$ and $\rho N \bar{N}$ coupling constants are consistent with the values we expect from other sources of information.⁵ Although the χ^2 obtained is not so good (5% confidence level), observe that the Novosibirsk point at 855 MeV and the Orsay point at 886 MeV are in disagreement, and alone contribute a χ^2 of 10. Furthermore, the Orsay point at 940 MeV contributes another 6. These large contributions indicate either an experimental or theoretical problem to be resolved in the future. From Eqs. (4) and (5), we obtain

$$m_{\rho} = 5.49 \pm 0.02 \ m_{\pi} = 769 \pm 3 \ \text{MeV},$$

$$\Gamma_{\rho} = 0.778 \pm 0.04 \ m_{\pi} = 109 \pm 6 \ \text{MeV}.$$
(9)

Note that the curve in Fig. 1 satisfies Eq. (7) very closely, despite the fact that D(s) deviates from linearity, as reflected in the values D(0) = 0.136and $\text{Re}D'(m_{\rho}^2) = 4.47 \times 10^{-3} m_{\pi}^{-2}$. Nevertheless, D(0)/2 $m_{\rho}^{2} \operatorname{Re}D'(m_{\rho}^{2}) = 1.01$, which shows the insensitivity of Eq. (7) to possible nonlinearity. The linear predictions for D(0) and $D'(m_0^2)$ are D(0) = 0.0732 and $\text{Re}D'(m_0^2)$ $=2.44 \times 10^{-3} m_{\pi}^{-2}$.

The above values indicate, of course, a problem, when compared with those of Eq. (4). Inasmuch as the sample of ρ 's in the $e^+e^- \rightarrow \pi^+\pi^-$ experiment are "cleaner" than those in $\pi N \rightarrow \pi \pi N$, one is inclined to take Eq. (9) more seriously.

This kind of difficulty is not new. Although the success of the hypothesis that the ρ meson is universally coupled to the isospin current has been great, we have, in fact, a list of annoying discrepancies between theory and experiment, some of which are as follows:

(1) The ρ -meson width never seems to be quite the same from experiment to experiment. This effect became so pronounced that at one point the Rosenfeld tables⁶ ceased giving a width for the ρ meson and even now merely give 125 ± 20 MeV, which would appear to be fairly safe. In the author's opinion, the probable cause for these differences is to be found in an accurate many-body calculation for those states $(\pi\pi N, \pi\pi\pi,$ $N3\pi$, $N4\pi$, etc.) where ρ mesons are seen, but rescattering effects, three-body effects, or final-state interactions are significant. One would guess that these effects broaden the peak.

(2) The nucleon isovector form factor appears to be given by something like

$1/(q^2+m_{o}^2)^2$

instead of

$1/(q^2+m_{\rho}^2)$,

the latter being what ρ -meson dominance most naturally suggests. This is even more puzzling when one discovers in Eq. (2) that the $N\bar{N}$ contribution is the most important single factor in producing the zero at $s = m_{\rho}^2$, which is to say that the $N\bar{N}$ state is the most important factor in producing the ρ meson as a resonance. As already pointed out in Ref. 2, this seems to indicate that the ρ meson is best considered an NN bound state rather than a $\pi\pi$ resonance. This is the same as saving that in a world made of nucleons, which do not bind to make pions, the ρ meson would exist as a stable particle, but that since we do have pions, it decays into them.

(3) There seems to be no ρ -meson production from ${}^{1}S_{0}$ $N\bar{N}$.⁷ This is very mysterious and is the cause, in a recent paper applying the Veneziano model to $\bar{p}n \rightarrow \pi^+\pi^-\pi^-$,⁸ for adding an *ad hoc* factor to eliminate the ρ meson. If indeed the thesis of Ref. 8 is correct, and the $\bar{p}n \rightarrow \pi^+\pi^-\pi^-$ amplitude is essentially just the $\pi^- \rightarrow \pi^+ \pi^- \pi^-$ amplitude with the initial π^- having a mass of $2m_N$, then we cannot avoid seeing ρ mesons. We do not see them; therefore, the annihilation amplitude cannot be the $\pi\pi$ scattering amplitude with one heavy π meson. Furthermore, things seem to be even much more complicated than this, because any model the author knows of says that there ought to be ρ mesons produced. There are resonance bands at an effective mass of m_{ρ} in the $\bar{p}n \rightarrow \pi^+\pi^-\pi^-$ Dalitz plot, but they are uniformly populated, which is not what one naively expects of a ρ meson. Perhaps again an adequate understanding of three-body effects would show that we have ρ mesons, but that our naive expectations are significantly altered.

These difficulties indicate at least three significant points that ought to be investigated in the world of the ρ mesons, and there are others more fundamental, e.g., the original question raised in 1960⁹ as to how the ρ meson acquires a mass if it is a Yang-Mills field. So, the ρ meson, historically the first of a new short-lived breed of meson (so short-lived, in fact, that serious questions were raised as to whether it deserved to be called a particle at all), still remains both an interesting and not very well understood member of our family of particles.

COMPARISON OF THIS ANALYSIS WITH OTHER WORK

There have been other analyses similar in nature to that undertaken here. Those of Refs. 10 and 11 are

⁵ The residues at the ρ pole are the crucial thing. We find these to be $g_{\rho NN} = 2.06 \pm 0.03$ and $g_{\rho \pi \omega} = 0.31 \pm 0.15$, compared to the expected 2.11 and 0.45. Both are in agreement with the expected values. The value 2.11 for $g_{\rho NN}$ is based on ρ dominance of the nucleon isovector form factor and ρ universality; so, the agreement here is better than we have a right to expect.

⁶ Naomi Barash-Schmidt, Angela Barbaro-Galteri, Leroy R. Price, Arthur H. Rosenfeld, Paul Söding, Charles G. Wohl, Matts Roos, and Gianni Conforto, Rev. Mod. Phys. 41, 109 (1969).

⁷ C. Baltay, P. Franzini, N. Gelfand, G. Lutjens, J. Severiens, J. Steinberger, D. Tycko, and D. Zanello, Phys. Rev. **140**, B1039 (1965); N. Gelfand, *ibid*. **169**, 1077 (1968); P. Anninos, L. Gray, P. Hagerty, T. Kalogeropoulous, S. Zenone, R. Bizzari, G. Ciapetti, M. Gaspero, I. Laasko, S. Lichtman, and G. C. Monetti, Phys. Rev. Letters **20**, 402 (1968). ⁸ C. Lovelace, Phys. Letters **28B**, 264 (1968).

⁹ J. J. Sakurai, Ann. Phys. (N. Y.) 11, 1 (1960).

contained in Eq. (1) in the following way: In Ref. 10, our Eq. (2) was used with only the $\pi\pi$ channel, and in Ref. 11, our Eq. (2) was used with only the $\pi\pi$ channel on which a cutoff was placed in addition. In Ref. 12, a great variety of formulas are presented. Their Eqs. (12b) and (13) with an interaction radius $R \approx 1/m_{o}$ ought to agree very closely with the results here. And, in fact, the curve presented here is right in the middle of the various curves they calculated. They did not, however, use $R=1/m_{\rho}$, favoring R=0 instead. Two arguments can be presented for $R \approx 1/m_{\rho}$:

(a) Nonrelativistic theory predicts $R \approx$ interaction radius $\approx 1/m_{\rho}$.

(b) The relativistic theory of Ref. 2 and here gives a phase shift close to that of the nonrelativistic formula where $R \approx 1/m_{\rho}$.

CONCLUSIONS

The analysis presented here suggests that

(a) $\Gamma_{\rho} = 109 \pm 10$ MeV, $m_{\rho} = 769 \pm 5$ MeV. The error bars are conservative estimates.

(b) A measurement of the full width at half-maximum should provide a good estimate of the ρ -meson width, regardless of the height of the peak.

(c) It is very unlikely to find anything much different from $|F_{\pi}(m_{\rho}^{2})|^{2} = m_{\rho}^{2}/\Gamma_{\rho}^{2}$.

(d) Studies of final-state interactions in $\pi N \rightarrow \pi \pi N$ and $N\bar{N} \rightarrow 3\pi$ should be undertaken in order to understand their effect on the observed resonance peaks in these interactions.

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APPENDIX

Here we present in some detail the method and functions for implementing in a numerical calculation Eqs. (1)–(3) in the text.

In Table I, we see the necessary ρ functions (phasespace functions), thresholds, masses, and approximate values of the coupling constants.

As shown in Ref. 2, we need the following functions (we take this opportunity to correct a remaining error in Ref. 2, which is the absence of an exponent of 2 on the $s-m_{\rho}^{2}$ in the fourth term of the equation for H_{3} and on the $s' - m_{\rho}^2$ under the integral sign):

$$f(s,t,u,\Lambda) = P \int_{t}^{\Lambda} \frac{ds'}{[(s'-u)(s'-t)]^{1/2}} \frac{1}{s'-s}, \quad (0 < u < t)$$
(A1)

$$f'(s,t,u,\Lambda) = \frac{1}{(s-t)(s-u)} \left[\frac{\left[(\Lambda-t)(\Lambda-u) \right]^{1/2}}{s-\Lambda} + \left(\frac{t+u}{2} - s \right) f(s,t,u,\Lambda) \right],$$
(A2)

$$H_{1}(s,t) = P \int_{t}^{\infty} \frac{(s'-t)^{2}}{[s'(s'-t)]^{1/2}} \frac{ds'}{(s'-s_{0})^{2}(s'-s)} = \frac{(s-t)^{2}}{(s-s_{0})^{2}} f(s,t,0,\infty) + \frac{(s_{0}-t)^{2}}{s_{0}-s} f'(s_{0},t,0,\infty) + \frac{(s_{0}-t)^{2}}{s_{0}-s} f'(s_{0},t,0,\infty), \quad (A3)$$

$$H_2(s,t) = P \int_t^\infty \frac{(s'-t)(s')}{[s'(s'-t)]^{1/2}} \frac{ds'}{(s'-s_0)^2(s'-s)} = \frac{(s-t)s}{(s-s_0)^2} f(s,t,0,\infty)$$

$$+\frac{\partial}{\partial s_0} \left[\frac{(s_0-t)(s_0)}{s_0-s} \right] f(s_0,t,0,\infty) + \frac{(s_0-t)(s_0)}{s_0-s} f'(s_0,t,0,\infty) , \quad (A4)$$

$$H_{3}(s,t,u,\Lambda) = P \int_{t}^{\Lambda} \frac{(s'-t)^{2}(s'-u)^{2}}{[(s'-t)(s'-u)]^{1/2}} \frac{ds'}{s'(s'-s_{0})^{2}(s'-s)} = \cosh^{-1} \left(\frac{\Lambda - \frac{1}{2}(t+u)}{\frac{1}{2}(t-u)}\right) - \frac{t^{2}u^{2}}{ss_{0}^{2}} f(0,t,u,\Lambda) + \frac{\partial}{\partial s_{0}} \left[\frac{(s_{0}-t)^{2}(s_{0}-u)^{2}}{s_{0}(s_{0}-s)}\right] f(s_{0},t,u,\Lambda) + \frac{(s_{0}-t)^{2}(s_{0}-u)^{2}}{(s_{0}-s)(s_{0})} f'(s_{0},t,u,\Lambda) + \frac{(s-t)^{2}(s-u)^{2}}{s(s-s_{0})^{2}} f(s,t,u,\Lambda)$$
(A5)

¹⁰ G. J. Gounaris and J. J. Sakurai, Phys. Rev. Letters 21, 244 (1968); G. J. Gounaris, Phys. Rev. 181, 2066 (1969).
 ¹¹ M. T. Vaughn and K. C. Wali, Phys. Rev. Letters 21, 938 (1968).
 ¹² Matts Roos and Ján Pišút, Nucl. Phys. B10, 563 (1969).

(note change in H_3 as compared to Ref. 2). We further need

$$f''(s,t,u,\Lambda) = \frac{1}{(s-t)(s-u)} \left\{ \left(\frac{t+u}{2} - s\right) f'(s,t,u,\Lambda) - f(s,t,u,\Lambda) \left[1 + \left(\frac{t+u}{2} - s\right) \left(\frac{1}{s-t} + \frac{1}{s-u}\right) \right] - \frac{\left[(\Lambda-t)(\Lambda-u) \right]^{1/2}}{s-\Lambda} \left(\frac{1}{s-t} + \frac{1}{s-u} + \frac{1}{s-\Lambda}\right) \right\}, \quad (A6)$$

where the primes of f indicate partial differentiation with respect to s.

The reason we need f'' is to be found when we consider the singular points s=0 and $s=s_0$. For these points, we do the following:

(1) Define
$$h_1(s) = (s-t)^2 f(s,t,0,\infty)$$
.

Then,

$$H_{1}(s_{0},t) = \frac{1}{2} (\partial^{2}/\partial s_{0}^{2}) h_{1}(s_{0})$$

= $f(s_{0},t,0,\infty) + (s_{0}-t) f'(s_{0},t,0,\infty)$
+ $\frac{1}{2} (s_{0}-t)^{2} f''(s_{0},t,0,\infty)$. (A7)

(2) Define
$$h_2(s) = s(s-t)f(s,t,0,\infty)$$
.

Then,

$$H_{2}(s_{0},t) = \frac{1}{2} (\partial^{2}/\partial s_{0}^{2})h_{2}(s_{0})$$

= $f(s_{0},t,0,\infty) + (2s_{0}-t)f'(s_{0},t,0,\infty)$
+ $\frac{1}{2}s_{0}(s_{0}-t)f''(s_{0},t,0,\infty)$. (A8)
(3) Define $h_{3}(s) = (s-t)^{2}(s-u)^{2}f(s,t,u,\Lambda)$.

 $H_3(0,t,u,\Lambda)$

$$= \frac{\partial}{\partial x} \left[\frac{h_3(x)}{(x-s_0)^2} \right]_{x=0} + \frac{\partial}{\partial s_0} \left(\frac{h_3(s_0)}{s_0^2} \right)$$

= $p(0,s_0) f'(0,t,u,\Lambda) + p'(0,s_0) f(0,t,u,\Lambda)$
+ $p(s_0,0) f'(s_0,t,u,\Lambda) + p'(s_0,0) f(s_0,t,u,\Lambda)$, (A9)

where

$$p(b,a) = \frac{(b-t)^2(b-u)^2}{b-a}$$
(A10)

and

$$p'(b,a) = p(b,a) \left(\frac{2}{b-t} + \frac{2}{b-u} - \frac{1}{b-a} \right).$$
(A11)

Also,

$$H_{3}(s_{0},t,u,\Lambda) = -\frac{h_{3}(0,t,u,\Lambda)}{s_{0}^{3}} + \frac{1}{2} \frac{\partial^{2}}{\partial s_{0}^{2}} \left[\frac{h_{3}(s_{0},t,u,\Lambda)}{s_{0}} \right]$$

$$= -\frac{t^{2}u^{2}f(0,t,u,\Lambda)}{s_{0}^{3}} + \frac{1}{2} \left[p(s_{0},0)f''(s_{0},t,u,\Lambda) + 2p'(s_{0},0)f'(s_{0},t,u,\Lambda) + p'''(s_{0},0)f(s_{0},t,u,\Lambda) \right], \quad (A12)$$

where

$$p^{\prime\prime}(b,a) = p(b,a) \left[\left(\frac{2}{b-t} + \frac{2}{b-u} - \frac{1}{b-a} \right)^2 + \frac{1}{(b-u)^2} - \frac{2}{(b-t)^2} - \frac{z}{(b-u)^2} \right].$$
 (A13)

 $[H_1(s,t) \text{ and } H_2(s,t) \text{ are well behaved at } s=0.]$ The need for s=0 is clear because $F_{\pi}(s)=D(0)/D(s)$. The need for $s=s_0$ is less obvious, but occurs because it is good to supply a minimizing routine with derivatives. One parameter being s_0 , we need $\partial D/\partial s_0$ and find that

$$(\partial/\partial s_0) [(s-s_0)H_i(s,t)] = H_i(s,t) - 2H_i(s_0,t),$$

so that $H_i(s_0,t)$ is required.

The formulas (A1)–(A13) were used to define the function $F_{\pi}(s)$ and its derivatives to the author's version of Davidon's variable metric¹³ which provided the results shown in Fig. 1 and discussed in the text. In Eqs. (A5), (A9), and (A12), Λ was taken as $200m_{\pi}^2$.

¹³ W. C. Davidon, Argonne National Laboratory Report No. ANL 5990, 1959 (unpublished).