

Numerical Solution of Fixed-Source Field Theories*

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A modification of the Tamm-Dancoff method for fixed-source meson theories is set up for automatic computation. The Chew (1954) model of pion-nucleon interactions is calculated with up to six virtual mesons. Bound-state parameters and scattering phase shifts are obtained, accurate to about 1%, at a cost of about 3 min of computer time each.

INTRODUCTION

THE virtue of a quantized field theory for elementary particle interactions is that it provides (what is postulated to be) a complete dynamical description for the system. However, it has been possible up to now to carry out calculations with these theories only in the weak coupling limit (perturbation theory); and for the realm of "strong interaction physics" this is clearly inapplicable. Over the years there have been many approximate calculations made, but none, it appears, have been successful enough that one could say the theory has been "solved." We have set out on our quest for effective nonperturbative calculational techniques with the following ideas in mind: that we shall construct not one approximation, but a sequence of approximations, the successive evaluations of which will give a series of well-converging numerical answers to all physical questions; and that we shall make the fullest use of modern computing machines in this effort. This second point does not imply a surrender to the brute force of mechanical tools—for, as the reader may readily see, such an attack will fail grossly—but rather a blending of modest analytical and numerical techniques.

Realizing that a computer deals only with discrete and finite quantities, one can make the following list of continuous or unbounded quantities which are known to occur in quantum field theory:

- (1) indefinite number of dependent variables (number of particles);
- (2) continuum of independent variables (space-time) associated with each dependent variable;
- (3) divergences at large spacial distances (associated with the vacuum state);
- (4) divergences at large momenta (due to the point interactions).

We are not able to handle all of these problems. In the present paper we study only fixed-source models in which difficulty number 3 does not arise and number 4 is removed by the use of a cutoff; thus our present interest is with problems number 1 and 2. (Problem number 2 is also faced in its simplest form since we will have only one spatial dimension to deal with

here.) Within covariant perturbation theory there have been devised means of handling all of these problems, and so many practicing field theorists would never consider numbers 1, 2, 3 as problems at all, and number 4 as solved by the renormalization technique. However, once we give up the expansion in coupling constant, all these questions must be considered anew.

THE APPROXIMATION SCHEME

Let us now start with the Hamiltonian for a quantized field linearly coupled to a fixed source.

$$\mathcal{H} = \int d\mathbf{k} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \omega_{\mathbf{k}} + g \int d\mathbf{k} (a_{\mathbf{k}} v_{\mathbf{k}} + a_{\mathbf{k}}^\dagger v_{\mathbf{k}}^\dagger). \quad (1)$$

The function $v_{\mathbf{k}}$ may contain a cutoff, as well as further details of the coupling such as spin operators, etc. We wish only to describe the general approach now; the specifics of a particular problem will be given later.

We can give the Fock space representation for the state vector built up from the bare vacuum state $|0\rangle$.

$$\begin{aligned} \Psi = & F_0 |0\rangle + \int d\mathbf{k} F_1(\mathbf{k}) a_{\mathbf{k}}^\dagger |0\rangle \\ & + \int \int d\mathbf{k} d\mathbf{k}' F_2(\mathbf{k}, \mathbf{k}') a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}^\dagger |0\rangle + \dots \quad (2) \end{aligned}$$

Then substituting (2) into the variational principle for the energy (of a discrete state) we get the following infinite set of coupled integral equations for the N -particle amplitudes F_N containing the energy eigenvalue E :

$$(\sum \omega - E) F_N + g v^\dagger F_{N-1} + g \int v F_{N+1} = 0. \quad (3)$$

$$N = 0, 1, 2, \dots$$

(For simplicity we have not put in the k variables in the functions F_N , v , ω or in the integral.)

Now since one does not expect to be able to solve the infinite system (3) some approximation must be made. By expanding F_N and E in power series in the coupling constant g one gets the well-known results of perturbation theory; but since those formulas become increas-

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ingly more complicated to evaluate in partice as one proceeds to higher orders, this method is useful only for sufficiently small numerical values of g .

The Tamm-Dancoff method¹ (of order N_0) consists of putting to zero all the amplitudes F_N for $N > N_0$; one then has a finite system of equations [the $(N_0+1) \times (N_0+1)$ truncation of (3)] to solve. When this scheme has been applied in the past, one has usually gone only to the lowest significant order because the labor needed to solve several coupled integral equations in several variables has seemed to be beyond the available resources. (Numerical integration in one dimension is commonplace, and in two dimensions is not rare; but for three and more dimensions almost nothing has been done, even with the great capacity of modern computing machines.)

Another interesting approximation scheme is that invented by Tomonaga,² which may be characterized by the replacement

$$F_N(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_N) \rightarrow u(\mathbf{k}_1)u(\mathbf{k}_2) \dots u(\mathbf{k}_N). \quad (4)$$

The description of what is allowed here is that any number of mesons is allowed but they all go into one space state (mode) described by the function u . One then easily solves (3) to find the best function u , and the results obtained include, as special cases, the well-known strong-coupling ($g \rightarrow \infty$) solution, as well as the lowest order perturbation-theory ($g \rightarrow 0$) result. No one, however, has described a systematic method for improving this approximation.

The approximation scheme we shall study in this paper may be looked upon as both an extension of the Tomonaga method and an effective reduction of the Tamm-Dancoff equations to manageable form. We start by selecting some convenient complete set of functions in the (momentum) space variables, $u_n(\mathbf{k})$, and introduce the expansions

$$F_1(\mathbf{k}) = \sum_n C_n^{(1)} u_n(\mathbf{k}), \\ F_2(\mathbf{k}, \mathbf{k}') = \sum_{nn'} C_{nn'}^{(2)} u_n(\mathbf{k}) u_{n'}(\mathbf{k}'), \quad \text{etc.} \quad (5)$$

As the expansion (2) reduces the single abstract equation,

$$H\Psi = E\Psi,$$

to the singly infinite set of equations (3) for the functions F_N , the expansions (5) now reduce these equations to a multiply infinite set of linear algebraic equations for the numbers $C_{nn' \dots}^{(N)}$. Now in order to solve this we must truncate to a finite system of equations. The plan is to set up a sequence of successively larger sets of these equations, solve for the eigenvectors and eigenvalues of the finite matrices we thus get as approximations to the infinite matrix of the Hamiltonian, and so arrive at a sequence of approximation values for various

quantities of interest. The crucial question is, "Will these results converge sufficiently rapidly so that we obtain a good approximation to the true answer before our computing facilities are exhausted?"

For any particular problem this question of convergence rate will be answered with certainty only by trying the program, but we can attempt a few general guesses. The ordering of the numbers C proceeds naturally in two directions: the total meson number N ; and the mode (space state) indices n, n', \dots . We can select special model problems to study the convergence in these two directions separately.

First consider neutral scalar theory, i.e., take the Hamiltonian (1) literally with $v_{\mathbf{k}}$ depending only on the magnitude of \mathbf{k} . The different momenta are uncoupled and we have only to solve the famous problem of a displaced harmonic oscillator:

$$\mathcal{H}C = \omega a^\dagger a + (g/(2\omega)^{1/2})(a + a^\dagger). \quad (6)$$

The exact solution for the ground state can be compared with the "Tamm-Dancoff" expansion,

$$\Psi = C^{(0)}|0\rangle + C^{(1)}|1\rangle + C^{(2)}|2\rangle + \dots, \\ |N\rangle = ((a^\dagger)^N/(N!)^{1/2})|0\rangle, \quad (7)$$

and we easily find the N -meson probability³:

$$|C^{(N)}|^2 = (\epsilon^N/N!)e^{-\epsilon}; \quad \epsilon = g^2/2\omega^3. \quad (8)$$

We would thus expect the variational calculation with a truncated (at N) expansion (7) to converge well when N exceeds the parameter ϵ , which can be interpreted as the mean number of excitations present in the exact solution. Thus for very strong coupling problems we may expect much difficulty; however, for the pion-nucleon problem the effective value of ϵ is less than 2, and so we are encouraged to proceed.

The second useful simple example is the Lee model.⁴ Here the operators $v_{\mathbf{k}}$ are so constructed that the lowest order Tamm-Dancoff equations are exact, and so we can here test our method for solving the integral equations by expansion in the mode functions u_n . This test can be carried out explicitly only after we have specified the functions u_n to be used, and it will be very important to see that we get a very rapid convergence to the solution of this simple problem as we employ the successively larger sets

$$u_0, \\ u_0, u_1, \\ u_0, u_1, u_2, \text{ etc.} \quad (9)$$

The number of states we can have, putting N mesons into n modes, is

$$(N+n-1)/(N-1)n!;$$

and this number can grow painfully fast if the maximum

¹ I. Tamm, J. Phys. (USSR) 9, 449 (1945); S. M. Dancoff, Phys. Rev. 78, 382 (1950).

² S. Tomonaga, Progr. Theoret. Phys. (Kyoto) 2, 6 (1947).

³ This sort of formula may be found in Ref. 2.

⁴ T. D. Lee, Phys. Rev. 95, 1329 (1954).

number of modes n is not kept small. We shall typically work with something like 1% accuracy from about 3 modes.

We shall now set up the general problem in terms of creation and annihilation operators for the modes. The original operators obey

$$[a_i(\mathbf{k}), a_j^\dagger(\mathbf{k}')] = \delta_{ij} \delta(\mathbf{k} - \mathbf{k}'), \quad (10)$$

where the i, j subscripts refer to possible internal degrees of freedom, such as isospin. The three-dimensional momentum variables \mathbf{k} will be described by a complete orthonormal set of functions u_{nlm} ; and we define

$$A_{nlmi} = \int d\mathbf{k} u_{nlm}^*(\mathbf{k}) a_i(\mathbf{k}) \quad (11)$$

or

$$a_i(\mathbf{k}) = \sum_{nlm} u_{nlm}(\mathbf{k}) A_{nlmi}.$$

This preserves the canonical commutation relations,

$$[A_{nlmi}, A_{n'l'm'}^\dagger] = \delta_{ij} \delta_{nn'} \delta_{ll'} \delta_{mm'}. \quad (12)$$

The free field part of the Hamiltonian is now

$$\mathcal{H}_0 = \sum_{lm} \sum_{nn'} \omega_{nn'}^{(l)} A_{n'lmi}^\dagger A_{nlmi}, \quad (13)$$

where

$$\omega_{nn'}^{(l)} = \int_0^\infty k^2 dk f_{nl}(k) \omega(k) f_{n'l}^*(k) \quad (14)$$

and we have taken a separation in spherical polar coordinates

$$u_{nlm}(\mathbf{k}) = Y_{lm}(\theta, \varphi) f_{nl}(k), \quad (15)$$

and

$$\omega(k) = (k^2 + \mu^2)^{1/2}. \quad (16)$$

We are using units of $\hbar = c = 1$, and the meson rest mass μ , taken as the unit of energy, will frequently be set equal to 1. The interaction term in the Hamiltonian, for a given partial wave lm and internal component i , will be taken as

$$\mathcal{H}_1^{lmi} = \frac{g}{(2\pi)^{3/2}} \int \frac{d\mathbf{k}}{(2\omega(k))^{1/2}} \theta(k) \left[\frac{4\pi}{2l+1} \right]^{1/2} k^l \times [Y_{lm}^*(\theta, \varphi) a_i(\mathbf{k}) + Y_{lm}(\theta, \varphi) a_i^\dagger(\mathbf{k})] \quad (17)$$

$$= (g/2\pi) \sum_n (G_n^{(l)} A_{nlmi} + G_n^{*(l)} A_{nlmi}^\dagger), \quad (18)$$

where

$$G_n^{(l)} = \int_0^\infty \frac{k^2 dk f_{nl}(k)}{(2l+1)^{1/2}} \frac{k^l \theta(k)}{(\omega(k))^{1/2}}. \quad (19)$$

Next we fix the cutoff function θ to be a step function

$$\theta(k) = 1, \quad k < K \\ = 0, \quad k > K \quad (20)$$

and we must now choose suitable functions $f_{nl}(k)$. It

was decided to focus on the variable ω rather than k and so we introduce the normalized variable x :

$$x = ((\omega - 1)/(\Omega - 1)), \quad \Omega = (K^2 + 1)^{1/2}; \quad 0 \leq x \leq 1. \quad (21)$$

Now the volume of integration is

$$\int_0^K k^2 dk = \int_1^\Omega k \omega d\omega, \quad (22)$$

and we also want the boundary condition

$$f_{nl}(k) \xrightarrow[k \rightarrow 0]{} \text{const } k^l \quad (23)$$

so we construct f_{nl} as follows:

$$f_{nl}(k) = \frac{1}{k^{1/2} \omega^{1/2}} (\omega - 1)^{l/2 + 1/4} (\Omega - 1)^{-(l/2 - 3/4)} \tilde{f}_{nl}(x) \quad (24)$$

having made use of $(\omega - 1)^{1/2} \xrightarrow[k \rightarrow 0]{} \text{const } k$. The orthonormality integral is now

$$\int_0^K k^2 dk f_{nl}(k) f_{n'l}(k) = \int_0^1 dx x^{l+1/2} \tilde{f}_{nl}(x) \tilde{f}_{n'l}(x) = \delta_{nn'} \quad (25)$$

and so we use Jacobi polynomials⁵ for \tilde{f}_{nl} .

$$\tilde{f}_{nl}(x) = \frac{(-1)^n (2n + l + \frac{3}{2})^{1/2}}{n! x^{l+1/2}} \frac{d^n}{dx^n} [x^{n+l+1/2} (1-x)^n]. \quad (26)$$

The resulting formulas for $\omega_{nn'}^{(l)}$ and $G_n^{(l)}$ are given in the Appendix. There is of course nothing unique about the above choice of mode functions; any complete set will do. That these "decorated" Jacobi polynomials worked quite well can be judged by the Lee model test mentioned above. Shown in Table I are the variationally computed sequence of eigenvalues E , obtained as approximations to the solution of the integral equation,

$$E = -\frac{g^2}{4\pi^2} \int_0^K \frac{k^2 dk}{\omega(\omega - E)}, \quad (27)$$

by restricting the mesons to 1, 2, 3, 4, 5, 6 of the space modes given above. In the table the single asterisks indicate, for each value of g and K , the point at which we could stop with less than 1% error, and the double asterisk shows the 1/10⁴ accuracy level. It is interesting to note that the poorest convergence occurs for the small g values (where perturbation theory could be used); and we may expect that for the problems of interest 2 or 3 or 4 of our mode functions will suffice.

The next model problem we looked at was the charged

⁵ See, for example, W. Magnus and F. Oberhettinger, *Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1954), p. 83.

TABLE I. Variational approximations to the self energy in the degenerate $l=0$ Lee model, using from one to six of the mode functions (24), (26) to describe the momentum distribution of the meson. The single asterisks indicate, for each value of g and K , the point at which we could stop with less than 1% error, and the double asterisk shows the $1/10^4$ accuracy level.

| $g^2/4\pi^2 \backslash K$ | 1 | 10 | 100 | 1000 |
|---------------------------|-------------|------------|-----------|----------|
| 0.01 | -0.00212992 | -0.0743468 | -0.801928 | -8.05233 |
| | * | | | |
| | -0.00214220 | -0.0817942 | -0.901345 | -9.05686 |
| | ** | | | |
| | -0.00214229 | -0.0832270 | -0.929253 | -9.34282 |
| | * | | | |
| | -0.00214229 | -0.0835536 | -0.939764 | -9.45290 |
| * | | | | |
| -0.00214229 | -0.0836327 | -0.944337 | -9.50222 | |
| -0.00214229 | -0.0836524 | -0.946495 | -9.52630 | |
| | | ** | | |
| 1.0 | -0.185727 | -4.44618 | -46.0896 | -461.421 |
| | * | | * | * |
| | -0.186410 | -4.50431 | -46.5534 | -465.740 |
| | ** | | | |
| | -0.186414 | -4.50542 | -46.55 | -465.747 |
| | ** | | | |
| | -0.186414 | -4.50543 | -46.5581 | -465.840 |
| ** | | | | |
| -0.186414 | -4.50543 | -46.5608 | -465.894 | |
| ** | | | | |
| -0.186414 | -4.50543 | -46.5618 | -465.917 | |
| 100.0 | -4.57456 | -66.3986 | -671.034 | -6705.85 |
| | ** | * | * | * |
| | -4.57467 | -66.5117 | -674.272 | -6742.87 |
| | -4.57467 | -66.5190 | -674.664 | -6747.92 |
| | ** | ** | ** | ** |
| | -4.57467 | -66.5194 | -674.720 | -6748.81 |
| | ** | | | |
| -4.57467 | -66.5195 | -674.732 | -6749.05 | |
| -4.57467 | -66.5195 | -674.735 | -6749.13 | |

scalar theory. Here we had to handle the expansions both in number of mesons and in modes. At this point the computer programming becomes quite interesting. One has many states, characterized by sets of occupation numbers, and the matrix elements of the Hamiltonian have the well-known selection rules which leave only a very few scattered nonzero contributions. All this must be arranged efficiently, both regarding time and storage space, so that one will be able to accommodate the larger problems to come. The charged scalar theory gave no trouble and so we proceeded to the semiphysical problem of the pion-nucleon interaction in the Chew model⁶ of a fixed nucleon and $\sigma \cdot \mathbf{k} \tau \cdot \phi$ coupling.

THE STATIC MODEL FOR π -N INTERACTIONS

The meson field has three internal charge states ($i=0, \pm 1$), and is coupled only in the $l=1$ orbit ($m=0, \pm 1$). The interaction Hamiltonian is now written

$$\mathcal{H}_I = \frac{g}{2\pi} \sum_{m,i=-1}^{+1} \sum_{n=0}^{\infty} G_n^{(i)} [\sigma_m \tau_i A_{nlmi} + \text{H.c.}], \quad (28)$$

⁶ For a thorough discussion and original references see S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson Company, Evanston Illinois, 1961), pp. 372 f.

where σ_m, τ_i are the 2×2 matrices for the spin and isospin of the nucleon.

$$\begin{aligned} \sigma_0, \tau_0: & \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}, \\ \sigma_{+1}, \tau_{+1}: & \begin{pmatrix} 0 & +2 \\ 0 & 0 \end{pmatrix}, \\ \sigma_{-1}, \tau_{-1}: & \begin{pmatrix} 0 & 0 \\ +2 & 0 \end{pmatrix}. \end{aligned} \quad (29)$$

In writing down basis vectors for this system we must specify one of four states for the nucleon, and one of nine states for each mode (n) of the mesons. This leads to an enormous proliferation in the listing of the states compared to what we had in the simpler models discussed above; but of course there are symmetries in the problem which should allow us to greatly reduce the basis needed. The total angular momentum $\mathbf{J} = \mathbf{L} + 1/2\boldsymbol{\sigma}$ and total isospin $\mathbf{T} = \mathbf{t} + 1/2\boldsymbol{\tau}$ are the well-known constants of the motion; but for more than 2 or 3 mesons it becomes a terribly messy job to construct all the possible eigenfunctions of J^2 and T^2 . We satisfied ourselves with merely selecting from all possible states (in the m, i representation) only those with the desired eigenvalues for J_0 and T_0 ; this is a trivial counting operation. Then in the process of constructing the eigenvector of the Hamiltonian matrix at any step of our approximation scheme we will get automatically an eigenfunction of J^2 and T^2 . In this way we reduced the size of the basis by about an order of magnitude, but if we could start with only correct T^2 and J^2 eigenfunctions then we could reduce the basis by still another order of magnitude. We did enforce one other simple symmetry: the exchange of spin and isospin labels, and this saved us almost a factor of two in basis size.

Aside from the sometimes tricky innovations of the spin counting problem the programming for this problem was the same as for the earlier charged scalar case. In Table II are shown the resulting values for the nucleon self-energy (lowest $J=T=\frac{1}{2}$ state) obtained with several sets of limited meson number and modes available. The parameters used for this data,

$$g^2/4\pi^2 = 0.15, \quad K = 5.6 \mu, \quad (30)$$

are close to those which have been used in the past with this model to give some fair fit of the experimental scattering data.

There is of course no physical significance to be attached to the self energy of a fixed particle, but the eigenfunctions Ψ which also come out of the computations will be used shortly. The thing to note from the data presented in Table II is that the approximation scheme does appear to converge well. The final extrapolated value of E is thought to be in error by less than one part in a thousand. This result should be judged in

TABLE II. Results of the nucleon self-energy calculations with increasing set of basis functions. The parameter values are given in (30).

| New occupations allowed $n=01234$ | Total number of states | $-E/\mu$ |
|---|---------------------------|--------------------|
| 0 | 1 | 0 |
| 1 | 4 | 8.312261 |
| 01 | 7 | 8.334930 |
| 001 | 10 | 8.335515 |
| 0001 | 13 | 8.335525 |
| 00001 | 16 | 8.335525 |
| 2 | 25 | 11.076151 |
| 11 | 40 | 11.099030 |
| 101 | 55 | 11.099317 |
| 1001 | 70 | 11.099326 |
| 10001 | 85 | 11.099326 |
| 02 | 94 | 11.099330 |
| 3 | 115 | 12.181440 |
| 21 | 166 | 12.196376 |
| 201 | 217 | 12.196669 |
| 2001 | 268 | 12.196676 |
| 12 | 319 | 12.196860 |
| 4 | 364 | 12.669309 |
| 31 | 499 | 12.678588 |
| 301 | 634 | 12.678972 |
| 5 | 721 | 12.874209 |
| 41 | 1030 | 12.879702 |
| 6 | 1189 | 12.951715 |
| extrapolate \longrightarrow | | 12.992 \pm 0.008 |

relation to its cost, which was in terms of a few minutes computing time (for production, not including exploration) on an IBM 7090.

With the eigenvector for the one-nucleon state we can compute some interesting quantities. From the "vertex renormalization constant" Z , defined by

$$Z = (\Psi, \sigma_0 \tau_0 \Psi) / (\Psi, \Psi), \quad (31)$$

we get the "renormalized coupling constant"

$$f_r^2 / 4\pi = Z^2 (g^2 / 4\pi); \quad (32)$$

and our numerical results are (for the stated values of g and K)

$$Z = 0.393, \quad f_r^2 / 4\pi = 0.0726 \quad (33)$$

with an uncertainty of about 1%.

We can also compute the probabilities P_N for finding N mesons in the eigenstate Ψ . (P_0 is also called the "wave function renormalization constant" Z_2 .) For our best eigenfunction, with at most six mesons, we find the probabilities

$$20\%, 34\%, 25\%, 13\%, 5\%, 2\%, 1\% \\ \text{for } N=0, \dots, 6.$$

The average value of N is 1.6; and this distribution is rather well described by the simple formula (8).

One could proceed to calculate other quantities, such as electromagnetic form factors, but the static model is probably far from the truth of things and we did not bother further. Our main objective was to see if we could solve a "strong interaction" problem without recourse

to unverifiable approximations, and in this we believe we have succeeded.

Our pride in this achievement was somewhat shaken by our belated discovery of the work of Halpern *et al.*⁷ These authors had succeeded in getting good results for the one-nucleon state in this model by using Halpern's "method of moments."⁸ That method is a variational calculation in which the basis elements of the trial state vector are gotten by successive multiplication by the complete Hamiltonian operator upon some simple initial vector. They obtained results nearly as accurate as ours by going up to five-meson states; they had to solve a matrix of dimension only 5 (compared to our dimensions of more than one thousand) but their matrix elements were quite a lot more complicated to compute. For this particular problem we probably should admit that their method was simpler than ours, but we believe our general approach is more flexible and may be applied to other problems where the special exigencies of the method of moments do not apply.

After completing the bound state problem, we turned to a meson-nucleon scattering calculation. The Kohn variational principle⁹ provides the simplest extension of the Rayleigh-Ritz method for discrete states to the continuum. We set up the problem of elastic π - N scattering in the $J = T = \frac{3}{2}$ state as follows. Starting with an approximate (normalized) wave function Ψ_0 and eigenvalue E_0 for the nucleon (calculated above) we construct a trial wave function,

$$\Psi_t = [A_{k111}^{+(0)} + \tan \delta_t A_{k111}^{+(1)}] \Psi_0 + \chi, \quad (34)$$

to describe the scattering state at an energy

$$E = E_0 + \omega = E_0 + (k^2 + 1)^{1/2}. \quad (35)$$

Here

$$A_{k111}^{+(0)} = \int d\mathbf{k}' Y_{1m}(\theta', \varphi') \delta(k'^2 - k^2) a_i^\dagger(\mathbf{k}') \quad (36)$$

and

$$A_{k111}^{+(1)} = \frac{P}{\pi} \int d\mathbf{k}' Y_{1m}(\theta', \varphi') \frac{H_k(k')}{k'^2 - k^2} a_i^\dagger(\mathbf{k}') \quad (37)$$

with

$$H_k(k) = 1. \quad (38)$$

The variational expression is then

$$\lambda = 2\lambda_t + (4\pi\omega^2/k^4) (\Psi_t, (E - H)\Psi_t), \quad (39)$$

where

$$\lambda_t = \omega \tan \delta_t / k^3 \quad (40a)$$

is taken as one of the parameters to be varied and

$$\lambda = \omega \tan \delta / k^3 \quad (40b)$$

is the stationary result containing the phase shift δ .

⁷ F. R. Halpern, L. Sartori, K. Nishimura, and R. Spitzer, *Ann. Phys. (N. Y.)* **7**, 154 (1959).

⁸ F. R. Halpern, *Phys. Rev.* **107**, 1145 (1957).

⁹ W. Kohn, *Phys. Rev.* **84**, 495 (1951). This method has been used together with the Tomonaga approximation by T. D. Lee and R. Christian, *Phys. Rev.* **94**, 1760 (1954) and also R. J. Riddell, Jr. and B. D. Fried, *ibid.* **94**, 1736 (1954).

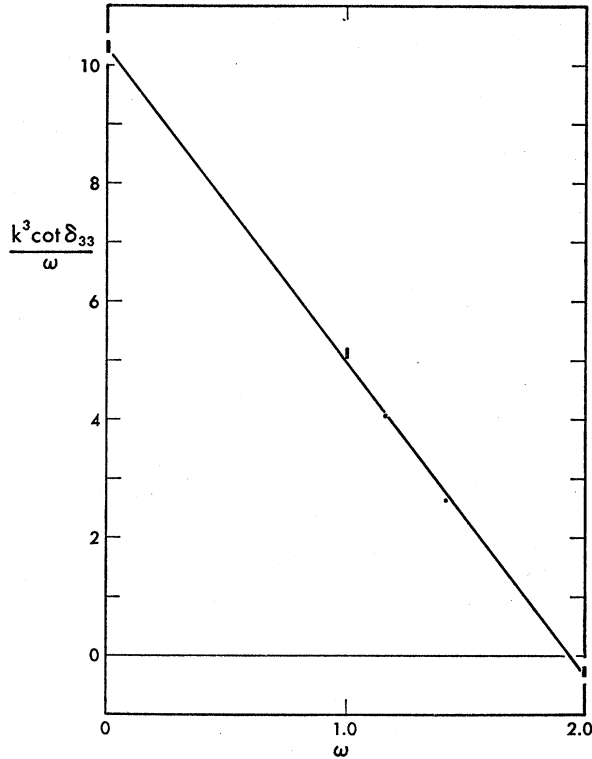


FIG. 1. Results of our elastic π - N scattering calculations at four energies for the $J = T = \frac{3}{2}$ state. The parameters used were $K = 5.6 \mu$ and $g^2/4\pi^2 = 0.15$. The renormalized coupling constant was calculated to be $f_r^2/4\pi = 0.0726$ and the point $3\pi/f_r^2$ is shown on the $\omega = 0$ axis. The vertical height on the points indicates our estimated inaccuracy in the computed value.

Most of the variation is taken up in the function χ which is constructed in the same manner as was Ψ_0 , except that it has quantum numbers $J_0 = T_0 = \frac{3}{2}$.

Our previous experience with variational calculations in atomic structure problems was reproduced here: the scattering problem, as compared to the bound-state required rather more algebraic and programming preparation, and the numerical results did not converge as fast. Nevertheless the work was successful in that we did obtain phase shifts accurate to about one percent with several minutes of computer time. At four values of the energy we obtained the following results: $k=0$, $\lambda=0.195(4)$; $k=0.6$, $\lambda=0.246(2)$; $k=1.0$, $\lambda=0.379(2)$; $k=1.732$, $\lambda=-4.1(1)$; where the numbers in parentheses indicate our estimate of the uncertainty in the last figure given. These values are displayed in Fig. 1, the famous plot of $k^3 \cot \delta / \omega$ versus ω . A straight line intersecting the $\omega = 0$ axis at $3\pi/f_r^2$ has been drawn to represent the form of the result predicted by the famous effective-range formula of the Chew-Low¹⁰ treatment of this model. The fit of this straight line to our accurate values is very good.

¹⁰ See Ref. 6.

CONCLUSIONS

We have been pleased to find that, within the confines of the fixed source model, the field theory of strong interactions is amenable to direct and accurate numerical resolution. This result will encourage us to seek for effective nonperturbation-theory attacks on more realistic models of the elementary particles.

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APPENDIX

We give here some of the details of the numerical work. First the integrals of the kinetic-energy matrix (14) are easily found:

$$\begin{aligned} \omega_{nn'}^{(l)} &= \int_0^1 dx x^{l+1/2} \tilde{f}_{nl}(x) \tilde{f}_{n'l}(x) [1 + (\Omega - 1)x] \\ &= \delta_{nn'} + (\Omega - 1) [x_{nn}^{(l)} \delta_{n,n'} + x_{n,n+1}^{(l)} \delta_{n+1,n'} \\ &\quad + x_{n-1,n}^{(l)} \delta_{n-1,n'}], \end{aligned} \quad (41)$$

where

$$x_{nn}^{(l)} = -\frac{1}{2} + \frac{1}{2} \frac{(l + \frac{1}{2})^2}{(2n + l + \frac{1}{2})(2n + l + \frac{5}{2})} \quad (42a)$$

$$x_{n,n+1}^{(l)} = \frac{(n+1)(n+l+\frac{3}{2})}{(2n+l+\frac{5}{2})[(2n+l+\frac{3}{2})(2n+l+\frac{7}{2})]^{1/2}}. \quad (42b)$$

Next the integrals for the interaction term are

$$\begin{aligned} G_n^{(l)} &= \frac{(\Omega - 1)^{l+1}}{(2l+1)^{1/2}} \int_0^1 dx x^{l+1/2} \tilde{f}_{nl}(x) \left(x + \frac{2}{\Omega - 1} \right)^{(l/2)+(1/4)} \\ &= \frac{(\Omega - 1)^{l+1}}{(2l+1)^{1/2}} (2n+l+\frac{3}{2})^{1/2} \\ &\quad \times \sum_{m=0}^n \frac{(-1)^{m+n} (n+l+m+\frac{1}{2})!}{m!(n-m)!(l+m+\frac{1}{2})!} S_{m+1}^{(l)}, \end{aligned} \quad (43)$$

where

$$S_N^{(l)} = \int_0^1 dx x^{N+l-1/2} \left(x + \frac{2}{\Omega - 1} \right)^{(l/2)+(1/4)} \quad (44)$$

can be calculated by the recursive scheme

$$\begin{aligned} S_N^{(l)} &= \frac{1}{(N + \frac{3}{2}l + \frac{3}{4})} \\ &\quad \times \left[\left(\frac{\Omega + 1}{\Omega - 1} \right)^{(l/2)+(5/4)} - \frac{2}{\Omega - 1} (N + l - \frac{1}{2}) S_{N-1}^{(l)} \right]. \end{aligned} \quad (45)$$

There is actually much numerical cancellation here, but double precision arithmetic is a simple cure. We now need only the first member of this family $S_1^{(l)}$, and this we compute from infinite series.

$$S_1^{(l)} = Z^{-(l/2)-(1/4)} \sum_{m=0}^{\infty} \frac{(m-\frac{1}{2}l-5/4)!(l+\frac{1}{2})!}{(-l/2-5/4)!(m+l+\frac{3}{2})!} Z^m, \quad (46)$$

where

$$Z = (\Omega - 1)/(\Omega + 1)$$

converges well if Ω is not too large. Alternatively we can use

$$S_1^{(l)} = \sum_{m=0}^{\infty} \frac{(m-\frac{1}{2}l-5/4)!(-1)^m}{m!(-\frac{1}{2}l-5/4)!(-m+\frac{3}{2}l+7/4)!} \left(\frac{2}{\Omega-1}\right)^m + \left(\frac{2}{\Omega-1}\right)^{(3l/2)+(7/4)} C_l, \quad (47)$$

with

$$C_l = -\frac{\Gamma(\frac{1}{2}l+5/4)\Gamma(l+\frac{3}{2})}{\Gamma(\frac{3}{2}l+11/4)}. \quad (48)$$

Thus the only input needed by the computer is the gamma function of argument one fourth.¹¹ (We actually let the computer generate this value also from an infinite series; our Ref. 11 is given for the historically minded reader.)

For the scattering problem we made the choice

$$H_k(k') = \frac{\omega + \omega' f_{0l}(k')}{2\omega f_{0l}(k)}; \quad (49)$$

¹¹ The standard source table of $\log(x!)$ to 20 decimal places was computed by K. F. Gauss (1777-1855); see his *Werke* (Göttingen, 1876), Vol. 3, pp. 161-162.

and the several sets of integrals needed were evaluated by methods of recursion formulas and infinite series, as done above.

After these integrals were tabulated, the matrix of $(E-H)$ was constructed and the remaining task was the numerical solution of a very large—but sparse—system of simultaneous linear equations for the eigenvector at some given value of E .

The following method worked very well for our equations of the form

$$A \cdot x = b. \quad (50)$$

(A is an $N \times N$ matrix, b is a given N -vector, and x is the N -vector to be found.) Take a small submatrix a of A and compute its inverse a^{-1} by a direct numerical method such as Gaussian elimination. For a of dimension 50×50 this takes about a second, while for the largest matrix A of dimension 1188 it would have required perhaps an hour. We then construct an approximation to the inverse of A (call it \bar{A}) by adjoining to a^{-1} the diagonal matrix composed of the inverses of the diagonal elements of the remainder $A-a$. We then iterate the solution

$$x^{(i+1)} = x^{(i)} + \bar{A} \cdot (b - A \cdot x^{(i)}) \quad (51)$$

starting with

$$x^{(0)} = a^{-1} \cdot b. \quad (52)$$

The reason that this very economical procedure converged well is that the submatrix a , being made up of contributions from the “important” states of the whole basis, gave a roughly good approximation to the complete problem; the remainder $A-a$ gave relatively small contributions. Thus the iteration (51) did not have to move the vector x very far in the N -dimensional vector space.