Use of Iteration Procedures to Generate Scattering Approximations*

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Our subject is the class of iteration procedures which can be written as a functional $F(\psi)$ used, via the rule $\psi_{n+1}=F(\psi_n)$, to generate a sequence $\psi_0, \psi_1, \psi_2, \cdots$ desired to converge quickly to the wave function of a quantum-mechanical system. Given such a functional $F_1(\psi)$, we seek methods of manipulating it to obtain an improvement $F_2(\psi)$; the starting point is the functional which generates the Born expansion. Four such methods are developed which, if applied serially, are capable of generating many likely iteration procedures. Only simple potential scattering is considered, but our methods seem to promise extension to cases much more complex. In these methods a central role is played by matrix elements J and T which measure the behavior of a functional for small and large distances from the scattering center. The resulting $F(\psi)$ are highly nonlinear; the ψ_n they generate are rational functions of the coupling constant with coefficients given by various combinations of J- and T-matrix elements. Numerical results for the first two orders of approximations are presented for square-well and exponential potentials. One of the procedures $F(\psi)$ gives the Fredholm determinantal expansion, and in a form more easily calculated than the expressions usually employed; this expansion is shown to be unitary, and a relation is obtained connecting the Fredholm determinant and a dispersion integral of the T matrix off the energy shell. Another of the improvements generates the inverse T-matrix expansion; this is shown to converge for coupling constant less than the smallest value which puts the phase shift at $\pm 180°$. In all of the above, the iteration sequence was started with ψ_0 being the free-wave solution corresponding to the scattering energy: An important advantage of iteration procedures is that, in contrast with the perturbation expansion, they are not pinned to this choice of ψ_0. We go on to select as input the free-wave solution of a different energy which better represents the average wavelength in the scattering region. The above iteration procedures then become much more powerful. When applied to the square-well potential, they yield the exact solution on the first iteration.

I. INTRODUCTION

LET ψ_∞ be the scattering wave function of energy E for a quantum system with Hamiltonian H:

$$H\psi_\infty = E\psi_\infty . \tag{1.1}$$

Probably the most generally applied method for solving for ψ_∞ is the Born perturbation expansion,[1] whereby the Hamiltonian is split into two parts:

$$H = H_0 + V \equiv H_0 + \lambda V_0 \tag{1.2}$$

and ψ_∞ is obtained as a power series in the coupling constant λ. The method, which requires a knowledge of the unperturbed eigenfunctions ϕ,

$$H_0\phi = E\phi , \tag{1.3}$$

yields

$$\psi_\infty = \phi + K\phi + K^2L + K^3\phi + \cdots , \tag{1.4}$$

with[2]

$$K = (E - H_0 + i\epsilon)^{-1}V . \tag{1.5}$$

This procedure fails whenever $|\lambda|$ is large enough to support a resonance, and is thus inapplicable to a very large domain of problems. There have been various attempts at extending the Born expansion, either through rearrangements of the series (1.4), or by modifying the split (1.2), or both.[3–7]

The present work explores a different approach for obtaining the scattering solution ψ_∞. We seek a single-valued functional[2] $F(\psi)$ having the property

$$\psi_\infty = F(\psi_\infty) , \tag{1.6}$$

which will be used, via the rule

$$\psi_{n+1} = F(\psi_n) , \tag{1.7}$$

to generate a sequence $\psi_0, \psi_1, \psi_2, \cdots$. One hopes that this sequence will quickly converge; Eq. (1.6) implies that if this sequence converges at all, it must converge to the exact solution ψ_∞ of Eq. (1.1).

An example of such a procedure is furnished by the Born expansion itself[8] with the iteration functional of Eq. (1.6) taken to be[9]

$$B(\psi) = \phi + K\psi . \tag{1.8}$$

For the choice

$$\psi_0 = \phi , \tag{1.9}$$

one finds

$$\begin{aligned} \psi_1 &= \phi + K\phi , \\ \psi_2 &= \phi + K\phi + K^2\phi , \\ &\cdots \\ \psi_n &= \phi + K\phi + \cdots + K^n\phi . \end{aligned} \tag{1.10}$$

* The main results of this paper were reported at the Washington, D. C. meeting of the American Physical Society, April, 1966, and sketched in a problem note in Report of NRL Progress (March, 1966), pp. 42–44 (unpublished).

[1] M. Born, Z. Physik **38**, 803 (1929). See, for example, Refs. 12 to 16.

[2] Our notation will be that $\psi_\infty(x)$ and $\phi(x)$ are the exact and unperturbed wave functions, as defined by Eqs. (1.1) and (1.3). $\psi(x)$ shall represent an arbitrary continuous function of the configuration space variables $x=(x_1,x_2,\cdots,x_p)$. The K of Eq. (1.5) is an integral operator: $K\psi(x) \equiv \int K(x,x')\psi(x')dx'$.

[3] G. A. Baker, Advan. Theoret. Phys. **1**, 1 (1965).

[4] M. Rotenberg, Ann. Phys. (N.Y.) **21**, 579 (1963).

[5] S. Weinberg, J. Math. Phys. **5**, 743 (1964).

[6] S. Weinberg, Phys. Rev. **131**, 440 (1963); M. Scadron and S. Weinberg, *ibid.* **133**, B1589 (1964).

[7] M. Wellner, Phys. Rev. **132**, 1848 (1963).

[8] I. Manning, Phys. Rev. **139**, B495 (1965).

[9] With the choice (1.8), Eq. (1.7) is just the Lippmann-Schwinger equation $\psi_\infty = \phi + K\psi_\infty$.

Our starting point will be this functional $B(\psi)$; we seek methods of operating on it to obtain an improved procedure $F(\psi)$. While the present work deals only with simple potential scattering, we shall restrict ourselves to improvements which, it seems to me, promise extensions to the more complex cases of actual physical interest.

The idea of using iteration procedures to generate functional approximations is of course not new.[10,11] Much of the work done in this field is unfamiliar to physicists, perhaps because the results, while possessing mathematical elegance, have been of limited utility for quantum mechanics. In the present work we give up the condition that the outcome be susceptible to mathematical analysis and, instead, take an approach guided by physical considerations. Our main result will be the observation that, working within the framework of iteration procedures, a pedestrian approach can lead to substantial improvements on the Born expansion.

II. J AND T MEASURE

In our methods a central role is played by matrix elements J and T which measure the behavior of a wave function at asymptotically small and large distances from the scattering center. To fix ideas, consider the case of simple potential scattering with ϕ an eigenfunction of energy and angular momentum. One then has for the operator K of Eq. (1.5)[12–16]

$$K(\mathbf{r},\mathbf{r}')=-i\pi\phi^*(\mathbf{r}_<)\chi(\mathbf{r}_>)V(\mathbf{r}') \tag{2.1}$$

$$=-i\pi\phi(\mathbf{r}_<)\chi'^*(\mathbf{r}_>)V(\mathbf{r}'), \tag{2.2}$$

where $\mathbf{r}_<$ and $\mathbf{r}_>$ are the $\mathbf{r},\mathbf{r}'$ of (respectively) lesser and greater magnitudes, ϕ is the unperturbed solution of Eq. (1.3), and[17]

$$\phi(\mathbf{r})=(2p/\pi)^{1/2}j_l(pr)Y_{lm}(\hat{r}), \tag{2.3}$$

$$\chi(\mathbf{r})=(2p/\pi)^{1/2}h_l^{(1)}(pr)Y_{lm}(\hat{r}), \tag{2.4}$$

$$\chi'(\mathbf{r})=(2p/\pi)^{1/2}h_l^{(2)}(pr)Y_{lm}(\hat{r}). \tag{2.5}$$

Given a wave function ψ, we define its T measure[18] to be

$$\{\psi\}_T\equiv\lim_{r\to\infty}\psi/\chi, \tag{2.6}$$

where r is the separation of collision products and χ is a fixed function—given by Eq. (2.4) in our case—chosen so that for the exact solution

$$\{\psi_\infty-\phi\}_T=-i\pi T_\infty, \tag{2.7}$$

where T_∞ is the (exact) scattering T matrix.[19] From Eqs. (2.1) to (2.4), one finds

$$\{K\psi\}_T=-i\pi T(\psi), \tag{2.8}$$

where $T(\psi)$ is the usual T matrix of scattering theory[20]:

$$T(\psi)\equiv(\phi,V\psi). \tag{2.9}$$

We introduce the J measure $\{\psi\}_J$ of a wave function ψ to discuss its behavior at the scattering center;

$$\{\psi\}_J\equiv\lim_{r\to0}\psi/\phi. \tag{2.10}$$

One finds

$$\{K\psi\}_J=-i\pi J(\psi), \tag{2.11}$$

where J is the matrix element

$$J(\psi)\equiv(\chi',V\psi), \tag{2.12}$$

χ' being given by Eq. (2.5).

Note the parallelism of the two asymptotic measures. The function χ in the definition of $\{\psi\}_T$ is closely related to the adjoint of the function χ' in the definition of $J(\psi)$; the ϕ in the definition of $\{\psi\}_J$ is the same as that appearing in the definition[21] of $T(\psi)$.

Given a sequence of wave functions $\psi_0, \psi_1, \psi_2, \cdots$ (which we hope will converge to ψ_∞), we define a corresponding sequence $T_1, T_2, T_3, \cdots$ of approximations to T_∞:

$$T_n\equiv-i\pi\{\psi_n-\phi\}_T. \tag{2.13}$$

Thus, for the Born expansion (1.10),

$$(T_n)_{\text{Born}}=T(\phi)+T(K\phi)+\cdots+T(K^{n-1}\phi).$$

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[10] See, for example, H. A. Antosiewicz and W. C. Rheinboldt, in *Survey of Numerical Analysis*, edited by J. Todd (McGraw-Hill Book Co., New York, 1962), Chap. 14.

[11] H. Buckner, Duke Math. J. **15**, 197 (1948).

[12] M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964).

[13] K. Gottfried, *Quantum Mechanics* (W. A. Benjamin, Inc., New York, 1966).

[14] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1965).

[15] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill Book Co., New York, 1966).

[16] T. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1962).

[17] We use units such that $\hbar=m=1$. The spherical Bessel functions j_l, $h_l^{(1)}$, and $h_l^{(2)}$ are as defined, for example, in P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Co., New York, 1952).

[18] "Measure" is a misnomer for the complex number $\{\psi\}$; it does not have the properties of the length $\|\psi\|$ of functional analysis. However, in dealing with iteration functionals $F(\psi)$ we will be using $\{\psi\}$ in a way similar to that which $\|\psi\|$ is ordinarily employed.

[19] See Refs. 12–16. For scattering from a spherically symmetric potential, $T_\infty=-\pi^{-1}\sin\delta\exp(i\delta)$, where δ is the phase shift.

[20] In terms of the notation above, $T_\infty=T(\psi_\infty)$.

[21] For completeness we give a connection between $J(\psi)$ and the off-diagonal (i.e., off the energy shell) T matrix. Inserting a complete set of states into the expression $\{K\psi\}=\lim K\psi/\phi$, one finds $\{K\psi\}=\sum_{E'}\{\phi_{E'}\}_J(E-E'+i\epsilon)^{-1}(\phi_{E'},V\psi)$, where $\phi_{E'}$ is the unperturbed solution of energy E', and E is the scattering energy. For our case this can be written as

$$\{K\psi\}_J=\int_0^\infty dE'\,(E'/E)^{(2l+1)/4}(E'-E+i\epsilon)^{-1}T_{E'}(\psi).$$

When combined with Eq. (A1.13) and the Lippmann-Schwinger equation, this provides a connection between the Fredholm determinant D_∞ and the off-diagonal T matrix: $\{\psi_\infty\}_J=D_\infty^{-1}=1+\{K\psi_\infty\}_J$, with the term $\{K\psi_\infty\}_J$ given by the above integral.

III. IMPROVEMENT BY J AND T CLAMPING

1. J-Controlled Iteration Procedure

Given a wave function ψ, define a corresponding altered function

$$\psi_A = c\psi(x), \tag{3.1}$$

where c is a number depending on ψ but not x: $c=c(\psi)$. We start with the Born functional $B(\psi)$ of Eq. (1.8) and consider as a candidate for an improved procedure the functional

$$F(\psi)\equiv B(\psi_A). \tag{3.2}$$

This amounts to a modification of the rule $\psi_{n+1}=B(\psi_n)$: Before using ψ_n as input, we are first scaling it by the constant $c(\psi_n)$; the resulting output is $F(\psi_n)$. Our approach is to choose the scaling constant to make ψ_A look to $B(\psi)$ as much as possible like the exact solution ψ_∞; in fact, we would like to mimic the Lippmann-Schwinger equation: $\psi_A=B(\psi_A)$. We cannot satisfy this equation at every point x but we can at a single point, for example, the scattering center;

$$\{\psi_A\}_J=\{B(\psi_A)\}_J. \tag{3.3}$$

That is to say, this improvement technique rescales the input in such a way that output and input are forced (clamped) to equal each other at the scattering center.

Equations (3.1), (3.2), and (3.3) give

$$F(\psi)=\phi+\frac{1}{\{\psi\}_J-\{K\psi\}J}K\psi. \tag{3.4}$$

We shall refer to this result [improving $B(\psi)$ by J clamping] as the J-controlled iteration procedure. For $\psi_0=\phi$, one finds

$$\begin{aligned}\psi_1&=\phi+\frac{K\phi}{1-\{K\phi\}_J},\\ \psi_2&=\phi+\frac{K\phi-\{K\phi\}_JK\phi+K^2\phi}{1-\{K\phi\}_J+\{K\phi\}^2_J-\{K^2\phi\}J}.\end{aligned} \tag{3.5}$$

On applying the definitions of Sec. II one obtains[22] as approximations to T_∞

$$\begin{aligned}T_1&=\frac{T(\phi)}{1+i\pi J(\phi)},\\ T_2&=\frac{T(\phi)+i\pi J(\phi)T(\phi)+T(K\phi)}{1+i\pi J(\phi)-\pi^2J^2(\phi)+i\pi J(K\phi)}.\end{aligned} \tag{3.6}$$

These are typical of the results we shall find for all our improvements. Instead of the polynomial in the coupling constant λ generated by the Born expansion (1.10) for ψ_n, we have a rational function in λ, the numerator of which is a rearrangement of the Born series, the denominator a c number. The coefficients in the rational function T_n will in general be various combinations of J- and T-matrix elements.

Also typical of the results we shall find, $F(\psi)$ is highly nonlinear and does not seem to be easily susceptible to

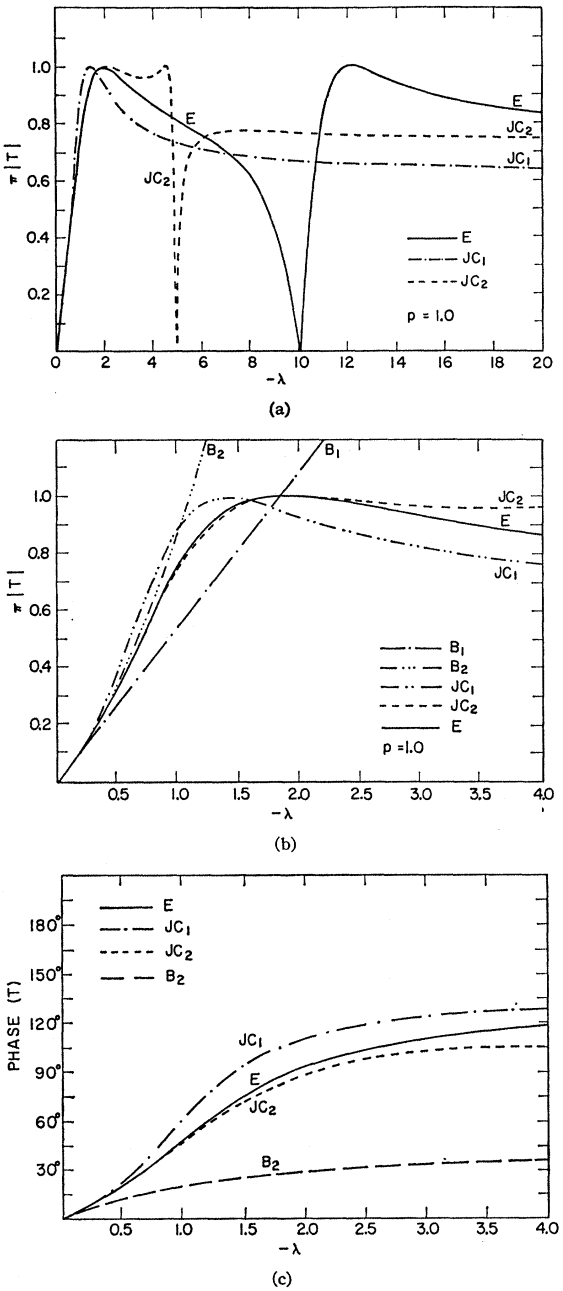


FIG. 1(a) Magnitudes of the first- and second-order J-controlled approximations, Eq. (3.6), for an attractive square-well potential, Eq. (3.7), and unit momentum. Key: E=exact (T_∞); JC_1, JC_2=(T_1 and T_2) for the J-controlled procedure, Eq. (3.6). (b) An expansion of Fig. 1(a) with additions. B_1, B_2=Born expansion, Eq. (2.14). (c) The curves, corresponding to Fig. 1(b), for the phase of the T matrix.

[22] Following a similar approach, W. F. Ford [Phys. Rev. **157**, 1226 (1967)] obtains and applies the plane-wave analog of the expression (3.6) for T_1, both diagonal and off diagonal.

analysis; it appears that the approximations generated will have to be investigated by acutally applying them to specific cases and building up a body of experience. Figures 1(a)–1(c) depict the approximations (3.6) for the case of S-wave scattering from an attractive square well of unit radius:

$$V(r)=\lambda<0, \quad r\leq 1$$
$$=0, \quad r>1. \tag{3.7}$$

While the present work does not, in general, attempt to analyze the improvements $F(\psi)$, the J-controlled procedure (3.4) is further examined in Appendix I. There it is shown that, for $\psi_0=\phi$, the ψ_n generated is just the result of truncating the Fredholm determinantal expansion.[23–26]

Now, for nonpathological cases, the determinantal expansion is known to converge at all energies for all values of the coupling constant,[6,13–16] so our very first example establishes the main point of this paper. A pedestrian approach can yield substantial improvements on the Born expansion. The J-controlled procedure provides a new formulation of the determinantal method, the expressions of which are easier to calculate than those usually employed.[23–26]

But the result (3.4) does much more: it casts the determinantal method as an *iteration procedure*. So far we have been considering only the case where the approximation sequence is started with $\psi_0=\phi$, the known exact eigenfunction of H_0. In contrast with the power-series method, iteration procedures are not pinned to this choice of ψ_0: Any likely guess can be used as input in the hope that it will start a quickly cconverging sequence, and we shall see in Sec. V that only when this freedom is exploited do iteration procedures achieve their full utility. For example, the J-controlled procedure (3.4) will be used to obtain a generalization of the determinantal method which appears to far surpass it in power.

2. T-Controlled Iteration Procedure

Here we proceed in much the same way as the previous section. Again, an improvement $F(\psi)$ is sought via Eq. (3.2). However, instead of Eq. (3.1), use

$$\psi_A=(1-c)\phi+c\psi, \tag{3.8}$$

where c is as before a number depending on ψ but not on x; $c=c(\psi)$. The exact solution is of the form

$$\psi_\infty=\phi+\omega, \tag{3.9}$$

where the term ω tends to zero at asymptotically large distances from the scattering center; the approximations (3.5) and (1.10) are also of this form. The input ψ_A of Eq. (3.8) is now also constrained to this form by scaling (by the constant c) only the second term ω. Also, in contrast with the previous section, we clamp the iteration procedure at asymptotically large distances from the scattering center;

$$\{\psi_A-\phi\}_T=\{B(\psi_A)-\phi\}_T. \tag{3.10}$$

Equations (3.2) and (3.8) give the improvement

$$F(\psi)=\phi+K\phi+\frac{\{K\phi\}_T}{\{\psi-\phi\}_T-\{K(\psi-\phi)\}_T}K(\psi-\phi). \tag{3.11}$$

We shall refer to this functional as the T-controlled iteration procedure; it is the result of improving the Born procedure $B(\psi)$ by our method of T clamping. Since the choice $\psi_0=\phi$ leads to an undefined result, this method obliges us to start with a first-order approximation. Starting with the first-order Born approximation $\psi_1=\phi+K\phi$, one finds

$$\psi_2=\phi+K\phi+\frac{\{K\phi\}_T}{\{K\phi\}_T-\{K^2\phi\}_T}K^2\phi. \tag{3.12}$$

The corresponding approximation to the T matrix is

$$T_2=\frac{T^2(\phi)}{T(\phi)-T(K\phi)}, \tag{3.13}$$

which is depicted in Fig. 2 for the square well of Eq. (3.7).

Appendix II shows that the sequence $T_2,T_3,T_4,\cdots$ is essentially the power-series expansion for the inverse T matrix.[27] This sequence converges whenever

$$|\lambda|<|\lambda_T|, \tag{3.14}$$

where λ_T is the smallest (real) value of the coupling constant λ which sets the phase shift δ to $\pm 180°$. This is to be compared with the Born series which converges only for

$$|\lambda|<|\lambda_B|, \tag{3.15}$$

where $\delta=\pm 90°$ at $\lambda=\lambda_B$. So the T-controlled procedure (started with $\psi_0=\phi+K\phi$) converges over a domain approximately twice as large as that of the Born expansion.

IV. IMPROVEMENT BY VARIATION OF PARAMETER

1. General Method for Improving Iteration Procedures

The following[28] is modeled on a method for improving iteration procedures for numbers[29] rather than functions. Suppose one has two iteration procedures $G(\psi)$ and

[23] R. Jost and A. Pais, Phys. Rev. **82**, 840 (1951).
[24] J. Schwinger, Phys. Rev. **94**, 1372 (1954).
[25] B. S. DeWitt, Phys. Rev. **103**, 1565 (1956).
[26] M. Baker, Ann. Phys. (N. Y.) **4**, 271 (1958).

[27] The inverse T matrix has been investigated by P. T. Mathews and A. Salam, Nuovo Cimento **13**, 381 (1959); G. Feldman, P. T. Mathews ,and A. Salam, *ibid.* **16**, 549 (1960); Bjorken and Goldberg, Ref. 30; and K. Wilson, as quoted in Ref. 30.
[28] Section IV can be skipped without loss of continuity.
[29] I. Manning, Proc. Cambridge Phil Soc. **63**, 22 (1967).

$H(\psi)$ for the same ψ_∞;

$$\psi_\infty = G(\psi_\infty) = H(\psi_\infty). \tag{4.1}$$

Then, for any finite quantity μ, the functional

$$F(\psi) \equiv \mu G(\psi) + (1-\mu) H(\psi) \tag{4.2}$$

also satisfies Eq. (1.6) and is therefore a possible iteration procedure. A criterion for the "goodness" of an iteration procedure $F(\psi)$ is that, for a given variation $\delta\psi$, the quantity

$$\delta F \equiv F(\psi+\delta\psi) - F(\psi) \tag{4.3}$$

should be small.[8,10] Equation (4.2) yields

$$\delta F = [\mu(\delta G - \delta H) + \delta H] + (G-H)\delta\mu. \tag{4.4}$$

Our approach here is to choose μ such that δF is likely to be smaller than δG or δH. It requires of G and H only that they be continuous and satisfy Eq. (4.1); neither procedure need necessarily converge. Given a nontrivial functional G, there exist many functionals H which may be used to explore the method; for example, $H(\psi)=\psi$, ψ^2/G, G^2/ψ, and so on.

In keeping with the spirit of this paper, we make two simplifications which will allow the outcome to be tractable for our applications. Since these (severe) assumptions cannot be mathematically justified, they can be defended, if at all, only by the utility of the results. First, instead of δF we shall work with the measure $\{\delta F\}$ in the hope that, if the latter is small, then so is the former. Secondly, we restrict the family of variations $\delta\psi$: Given a function $\psi(x)$, define an extension $\Psi(x,c)$ of it, depending on a constant c, such that

$$\psi(x) = \Psi(x,c)\,|_{c=1}. \tag{4.5}$$

The variations we shall deal with are defined by

$$\delta\psi \equiv \frac{\partial}{\partial c}\psi(x,c)\,|_{c=1}\delta c \equiv \psi'\delta c. \tag{4.6}$$

In terms of this notation, Eq. (4.3) gives

$$\delta F \equiv \frac{\partial}{\partial c}F(\psi)\,|_{c=1}\delta c \equiv F'\psi'\delta c. \tag{4.7}$$

Having made these two drastic assumptions, it is easy to carry out the analog of Ref. 29. Set the measure of the bracketed term in Eq. (4.4) to zero, thus fixing μ;

$$\mu(\psi) = -\frac{\{H'(\psi)\}}{\{G'(\psi)\}-\{H'(\psi)\}}. \tag{4.8}$$

$\{\delta F\}$ will then be small whenever the second term of Eq. (4.4) is small; (for μ finite) this is certainly true for $\psi=\psi_\infty$ where, by Eq. (4.1), the second term is zero. In addition to the two drastic assumptions, we are hoping that the above $\mu(\psi)$ is slowly varying, so that the second term of Eq. (4.4) will remain small over the domain (of ψ) of interest. Having determined μ, the candidate for improvement $F(\psi)$ is given by Eq. (4.2).

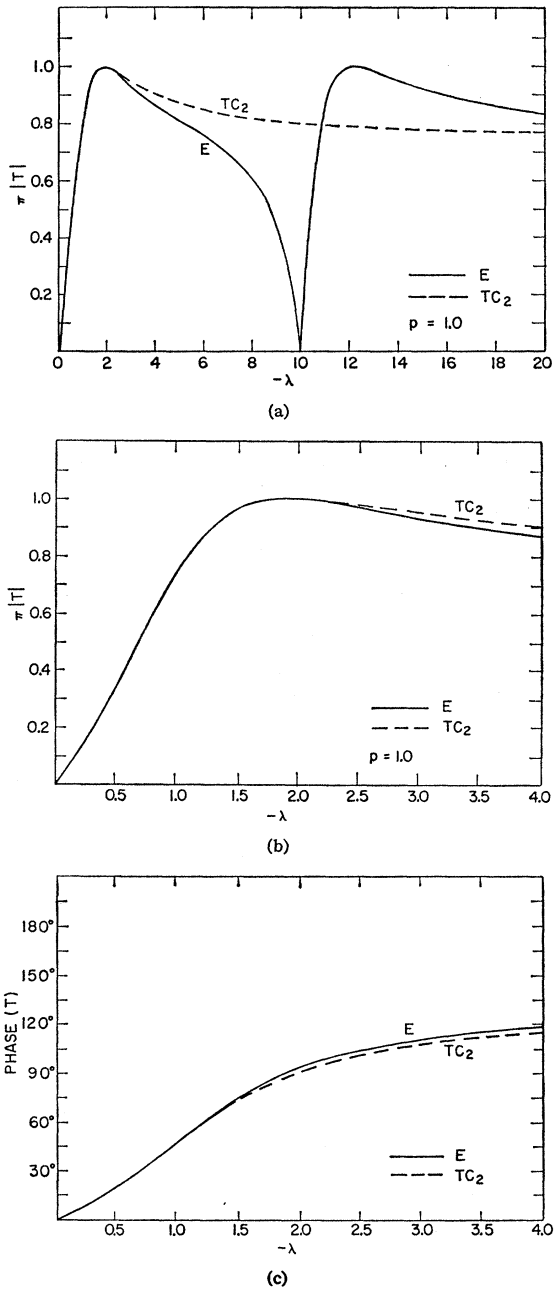
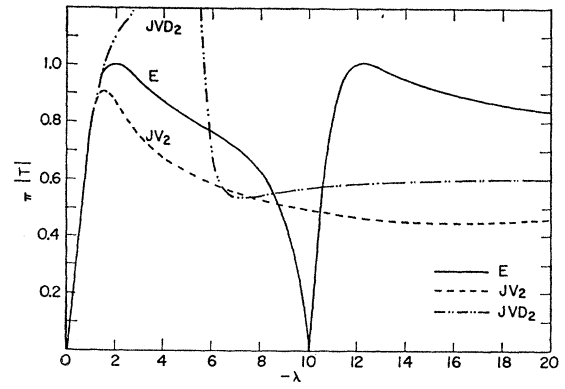


FIG. 2. The T-controlled approximation, Eq. (3.13) (curve TC_2), plotted (a) as in Fig. 1(a), (b) as in Fig. 1(b), and (c) as in Fig. 1(c).

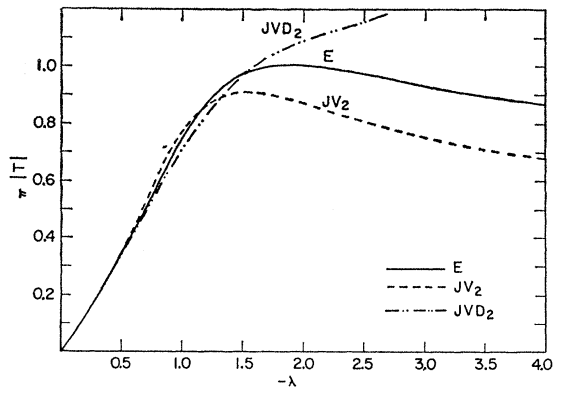
2. Improvement of Born Expansion by J Variation

As a first illustration, define the extension $\Psi(x,c)$ of Eq. (4.3) to be

$$\Psi(x,c) = c\psi(x). \tag{4.9}$$



(a)



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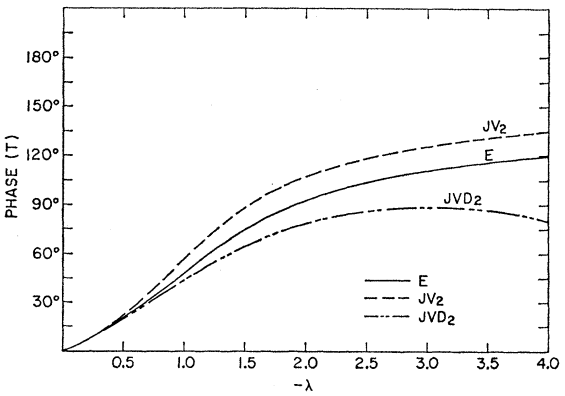

(c)

FIG. 3. Improvement by J variation plotted (a) as in Fig. 1(a), (b) as in Fig. 1(b), and (c) as in Fig. 1(c). JV_2=Eq. (4.10) started with $\psi_1=\phi+K\phi$; JVD_2=two iterations, using Eq. (4.10) started with $\psi_0=\phi$. The JVD_2 curve rises to a maximum of about 5.8 in Fig. 3(a).

We shall refer to the family $\delta\psi$ so generated as J variation. Choosing $G(\psi)$ to be the Born functional $B(\psi)$ [Eq. (1.8)],

$$H(\psi)=\psi, \tag{4.10}$$

and the measure to be J measure, one finds from Eqs. (4.2) and (4.7)

$$F(\psi)=\phi-\frac{\{K\psi\}_J}{\{\psi\}_J-\{K\psi\}_J}(\psi-\phi)+\frac{\{\psi\}_J}{\{\psi\}_J-\{K\psi\}_J}K\psi. \tag{4.11}$$

For $\psi_0=\phi$, ψ_1 is identical with that of the J-controlled procedure, Eq. (3.4); the other ψ_n are different. The resulting T_2 is depicted in Figs. 3 for the square well of Eq. (3.7).

3. Improvement of Born Expansion by T Variation

Here we choose for Eq. (4.3) the extension (3.8);

$$\psi(x,c)\equiv(1-c)\phi(x)+c\psi(x) \tag{4.12}$$

and designate the measure to be T measure. Proceeding as in the previous section (IV 2), one finds

$$F(\psi)=\phi-\frac{\{K(\psi-\phi)\}_T}{\{\psi-\phi\}_T-\{K(\psi-\phi)\}_T}(\psi-\phi)+\frac{\{\psi-\phi\}}{\{\psi-\phi\}_T-\{K(\psi-\phi)\}_T}K\psi. \tag{4.13}$$

For $\psi_1=\phi+K\phi$, ψ_2 is identical to that given by the T-controlled iteration procedure (3.10); the other ψ_n are different.

V. OFF-DIAGONAL PROCEDURES

As mentioned in Sec. III 1, a major advantage of iteration procedures is that they are not restricted to the choice $\psi_0=\phi$; any appealing guess can be used as input, in the hopes that the ensuing sequence ψ_1, ψ_2, $\psi_3,\cdots$ will rapidly converge. Here we consider the choice

$$\psi_0=\phi_{E'}, \tag{5.1}$$

the eigenfunction of H_0 corresponding to energy E' different from the scattering energy E. We aim to choose E' such that the input better represents the average wavelength of ψ_∞ in the scattering region. That is to say, we wish to adjust E' so that, to the iteration procedure $F(\psi)$, the input ψ_0 looks as much as possible like ψ_∞. Mimicking Eq. (1.1), we would like to have

$$(E-H)\phi_{E'}=0, \tag{5.2}$$

which, of course, is impossible, Nor can one set the expectation value of $(E-H)$ to zero, since the wave function $\phi_{E'}$ is not normalizable. Even if we could, it would not be the most desirable choice since all our iteration procedures $F(\psi)$ employ the scattering operator K of Eq. (1.5), which weights the value $\psi(x)$ by $V(x)$. In configuration space, those parts of $\psi(x)$ are most important where $V(x)$ is large. We therefore select E' such

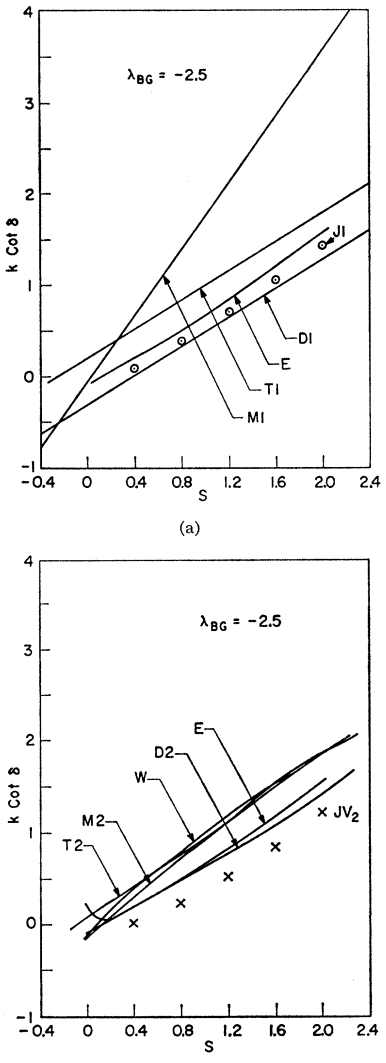

FIG. 4. (a) Effective-range plot, $p\cot\delta$ as a function of $s=p^2$ for the attractive exponential potential of Eq. (5.7). This is Fig. 7 of the paper by Bjorken and Goldberg, Ref. 30, to which we have added points depicting an approximation of the present work. On account of the difference in units, λ_{BG} is twice our coupling constant λ. Key: E=exact, $M1$=first-order Mandelstam, $T1$=first-order expansion of $\tan\delta$ in powers of λ (not discussed in the present work), $D1$=first-order determinantal [which coincides with our diagonal J-controlled approximation, Eq. (3.6)]. The added points $J1$ are our off-diagonal J-controlled approximation to first order, the result of starting the procedure of Eq. (3.13) with $\psi_0=\phi_{E'}$, of Eq. (5.4). (b) Second-order approximations for the attractive exponential potential of Fig. 4(a). W is the second-order expansion of $\cot\delta$ in powers of λ [and coincides with our diagonal T-controlled approximation Eq. (3.13)]. See the caption of Fig. 4(a) for a key to the other curves. This is Fig. 8 of the paper by Bjorken and Goldberg. The added points JV_2 are the improvement by J-variation Eq. (4.10), off-diagonal, started with ψ_1 of Eqs. (5.5) and (5.4). To the scale of this figure, other approximations of the present work nearly coincide with the (exact) E curve; they are depicted in Table I.

that the expectation value of $(E-H)$ weighted by V vanishes;

$$\langle\phi_{E'}|(E-H)V|\phi_{E'}\rangle=0, \tag{5.3}$$

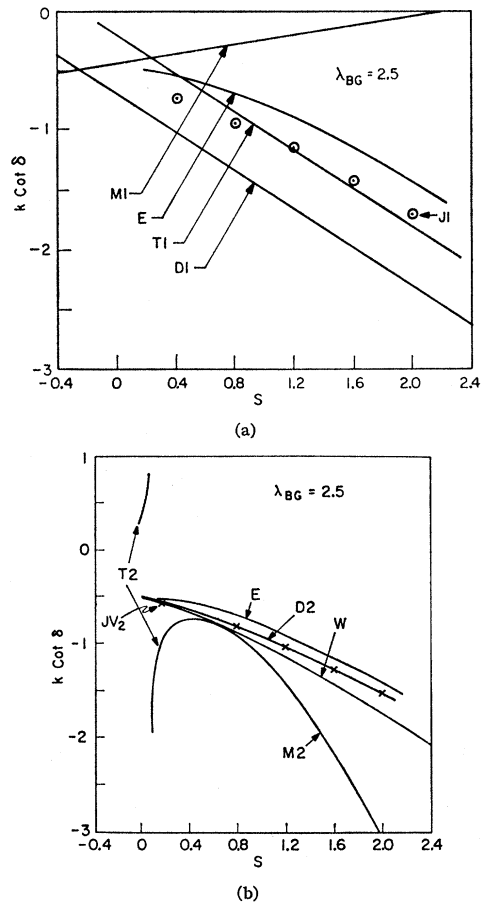

FIG. 5. (a) First-order approximations for a repulsive exponential potential. See the caption of Fig. 4(a). This is Fig. 5 of the paper by Bjorken and Goldberg with the E curve shifted to correct a small plotting error, and with the added points $J1$ of the present work. (b) Second-order approximations for a repulsive exponential potential. See the captions of Figs. 4(a) and 4(b). This is Fig. 6 of the paper by Bjorken and Goldberg with the E curve shifted to correct a small plotting error, and with the added points JV_2 of the present work. To the scale of this figure, other approximations of the present work nearly coincide with the (exact) E curve; they are depicted in Table II.

which gives a transcendental equation for E';

$$E'=E-\frac{\langle\phi_{E'}|V^2|\phi_{E'}\rangle}{\langle\phi_{E'}|V|\phi_{E'}\rangle}. \tag{5.4}$$

Some of our improvements required that the form (3.9) be preserved; in such cases start the sequence with

$$\psi_1=\phi+K\phi_{E'} \tag{5.5}$$

instead of the ψ_0 of Eq. (5.1).

With Eqs. (5.1) or (5.5) as input, all of the iteration procedures again yield approximations of the general form discussed in Sec. III 1, with the coefficients in the rational function in λ now involving mixtures of J- and T-matrix elements, both diagonal (in energy E) and off diagonal.[22] (The emergence of these off-diagonal ele-

TABLE. I. Approximations which nearly coincide with the exact curve of Fig. 4(b). This table depicts the errors in $p\cot\delta$; error = (approx)-(exact). The curve $D2$ of Fig. 4(b) is included for comparison. $JC2$ is the off-diagonal J-controlled approximation obtained from Eqs. (3.4) and (5.4); $TC2$ is the off-diagonal T-controlled approximation, Eq. (5.6).

Approx \ s	0.4	0.8	1.2	1.6	2.0
$D2$	1.0×10^{-2}	-4.0×10^{-2}	-6.6×10^{-2}	-8.4×10^{-2}	-9.7×10^{-2}
$JC2$	2.3×10^{-2}	1.2×10^{-2}	5.1×10^{-3}	-4.3×10^{-5}	-4.2×10^{-3}
$TC2$	-1.2×10^{-2}	-4.5×10^{-3}	-1.4×10^{-3}	-5.9×10^{-4}	-9.3×10^{-4}

TABLE. II. Approximations which nearly coincide with the exact curve of Fig. 5(b). (See the caption of Table I.)

Approx \ s	0.4	0.8	1.2	1.6	2.0
$D2$	-8.7×10^{-2}	-1.1×10^{-1}	-1.1×10^{-1}	-1.1×10^{-1}	-1.0×10^{-1}
$JC2$	-6.0×10^{-2}	-6.6×10^{-2}	-6.5×10^{-2}	-6.1×10^{-2}	-5.7×10^{-2}
$TC2$	-3.4×10^{-3}	-7.9×10^{-4}	-6.4×10^{-3}	1.1×10^{-2}	1.5×10^{-2}

ments prompted the title of this section.) For example, the T-controlled procedure (3.11) gives

$$T_2=\frac{T(\phi_E)T(\phi_{E'})}{T(\phi_{E'})-T(K\phi_{E'})}. \tag{5.6}$$

With the square-well potential (3.7) and any of our improvements, the above off-diagonal inputs *generate the exact solution ψ_∞ at the first iteration* for all scattering energies and all values of the coupling constant.

To differentiate between the various off-diagonal approximations it is therefore necessary to calculate a different example; the exponential potential

$$V(r)=\lambda e^{-r} \tag{5.7}$$

was selected, since comparisons with other approximations already exist in the work of Bjorken and Goldberg.[30] Results are depicted in Figs. 4 and 5, and in Tables I and II.

VI. CONCLUSION

The four improvement methods described in this paper were applied only to improving the Born expansion $B(\psi)$. They are, however, applicable to a much wider class of iteration procedures and, by applying these methods serially, many approximations can be generated, each of which is a candidate for improvement over the Born expansion. For example, one might use improvement by T variation (see Sec. IV 3) with $G(\psi)$ the J-controlled procedure (3.4) and $H(\psi)=\psi$, $B(\psi)$, the T-controlled procedure (3.11), or some other procedure. It is clear that iteration procedures are a rich source of possible improvements.

When expanding a function in a power series, one must select an expansion point for which all the derivatives are known. Correspondingly, the Born expansion requires that the Hamiltonian be split in such a way that, in Eq. (1.2), the eigenfunction ϕ be exactly known; the sequence yielding the Born expansion is correspondingly started with $\psi_0=\phi$. In contrast with usual perturbation theory, iteration procedures are not pinned to this choice of input; Sec. V suggests that this advantage of these procedures is of even greater importance than their richness.

[30] J. D. Bjorken and A. Goldberg, Nuovo Cimento **16**, 539 (1960).

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APPENDIX I: SOME PROPERTIES OF J-CONTROLLED PROCEDURE

One easily proves by induction that, for $\psi_0=\psi$, the iteration procedure (3.4) yields

$$\psi_N=\phi+N_N/D_N, \tag{A1.1}$$

with

$$N_N=\sum_{n=1}^{N} B_n\phi \tag{A1.2}$$

and

$$D_N=\sum_{n=0}^{N} d_n. \tag{A1.3}$$

The operators B_n and the c numbers d_n satisfy the recursion relations

$$B_{n+1}=d_nK+KB_n \tag{A1.4}$$

and

$$d_n=-\{B_n\phi\}_J, \tag{A1.5}$$

as well as the conditions $d_0=1$ and $B_1=K$.

Reference 31 shows that the ψ_N above is the truncation of the Fredholm determinantal expansion for ψ_∞.

The above ψ_N is also unitary, that is to say, Eq. (2.13) gives an asymptotic behavior [from Eq. (2.13)] of the form

$$T_N=-\pi^{-1}(\cot\delta_N-i)^{-1}, \tag{A1.6}$$

thus ensuring that it satisfy the relation[12–16]

$$T_N^*-T_N=2\pi i|T_N|^2. \tag{A1.7}$$

To see this, consider the exact solution

$$\psi_\infty=\phi+N_\infty/D_\infty, \tag{A1.8}$$

the T matrix of which is

$$T_\infty=A_\infty/D_\infty, \tag{A1.9}$$

with

$$A_\infty=i\pi^{-1}\{N_\infty\}_T. \tag{A1.10}$$

Being unitary, T_∞ satisfies Eq. (A1.6);

$$\text{Im}\, T_\infty^{-1}=\pi. \tag{A1.11}$$

Now, for real potentials, the phase of T_∞ equals that of $\{\psi_\infty\}_J$ since they both equal the (constant) phase of $u(r)$ in

$$\psi_\infty=[u(r)/r]Y_{lm}(\hat{r}). \tag{A1.12}$$

Upon using the condition[31]

$$\{\psi_\infty\}_J=D_\infty^{-1}, \tag{A1.13}$$

we therefore have in Eq. (A1.9) that

$$\text{Im}\, A_\infty=0. \tag{A1.14}$$

Combining (A1.9), (A1.11), and (A1.14),

$$\text{Im}\, D_\infty=\pi A_\infty. \tag{A1.15}$$

The key point of the proof is that N_∞(and hence A_∞) and D_∞ are entire functions[6,12–16] of λ, so that Eqs. (A1.14) and (A1.15) can be expanded in a power series, and they remain valid if the power series is truncated at the Nth term;

$$\begin{aligned}&\text{Im}\, A_N=0,\\ &\text{Im}\, D_N=\pi A_N.\end{aligned} \tag{A1.16}$$

These in turn imply, by

$$T_N=A_N/D_N, \tag{A1.17}$$

that

$$\text{Im}\, T_N^{-1}=\pi, \tag{A1.18}$$

which completes the proof.

[31] I. Manning, J. Math. Phys. **5**, 1223 (1964). Note the change in notation: D_n of that work equals B_{n+1} of Appendix I.

APPENDIX II: SOME PROPERTIES OF T-CONTROLLED PROCEDURE

It is easy to prove by induction that, for the choice $\psi_0=\phi+K\phi$, the iteration procedure (3.11) yields

$$\psi_N=\phi+N_N/D_N, \tag{A2.1}$$

with

$$N_N=\sum_{n=2}^{N}B_n\phi \tag{A2.2}$$

and

$$D_N=\sum_{n=0}^{N-1}d_n, \tag{A2.3}$$

and the operators B_n and c numbers d_n satisfy the recursion relations

$$B_{n+1}=d_{n-1}K+KB_n \tag{A2.4}$$

and

$$d_{n-1}=-\{B_n\phi\}_T/\{K\phi\}_T, \tag{A2.5}$$

as well as the conditions $d_0=1$ and $B_2=K^2$.

Applying the definition (2.13) for T_N gives

$$\begin{aligned}-i\pi T_N&=\Big(\sum_{n=0}^{N-1}\{K\phi\}_T d_n+\sum_{n=2}^{N}\{B_n\phi\}_T\Big)D_N^{-1}\\ &=\{K\phi\}_T/D_N,\end{aligned} \tag{A2.6}$$

where we have used the condition (A2.5). Since D_N is a simple polynomial in the coupling constant λ, we find that $T(\phi)/T_N$ is the truncation of the power-series expansion of $T(\phi)/T_\infty$.[27]

The diagonal procedure therefore converges for

$$|\lambda|<|\lambda_T|, \tag{A2.7}$$

where λ_T is the smallest pole of $T(\phi)/T_\infty$, and hence the smallest zero of T_∞. It is easy to see that λ_T is real, so that at $\lambda=\lambda_T$ the (physical) scattering phase shift is $\delta=\pm 180°$: For, in Eq. (A1.9), T_∞ has a zero only when A_∞ does. The demonstration follows by noting that A_∞ is real [Eq. (A1.14)], and applying the Schwartz reflection principle

$$A_\infty(\lambda^*)=A_\infty^*(\lambda) \tag{A2.8}$$

to demonstrate that

$$\lambda_T^*=\lambda_T. \tag{A2.9}$$

The approximation T_N is also unitary. Multiplying Eq. (A1.11) by $T(\phi)$, expanding in a power series, and truncating at the Nth term, we have

$$\text{Im}\,(T(\phi)/T_N)=\pi T(\phi), \tag{A2.10}$$

so T_N satisfies Eq. (A1.18).