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Fredholm Method. I. A Numerical Procedure for Elastic Scattering

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The Fredholm expansion of the determinant whose phase gives the elastic-scattering phase shift is "summed" by use of numerical quadrature, reducing the calculation of the phase shift to evaluation of a single finite-dimensional determinant. The method is essentially exact and is applicable, without modification, to nonlocal potentials. Results for the low-energy static and static-exchange scattering of electrons from hydrogen atoms are presented as a simple illustration of the method.

I. INTRODUCTION

The theory developed by Fredholm[1] for the solution of certain types of linear integral equations was first applied to problems in quantum scattering theory by Jost and Pais[2] in a discussion of the convergence of the Born series. They show that the Fredholm method allows the expansion of the partial-wave scattering amplitude as the ratio of two series, each of which converges absolutely for all values of the coupling parameter λ. The fact that these series converge absolutely makes them of great formal importance; however, Jost and Pais mention the fact that the method does not seem to lend itself to numerical computation, as the series may converge very slowly, except in special cases.

A remark by Schwinger[3] and subsequent development by Baker[4] rekindled interest in the Fredholm method: It may be shown that the phase of the partial-wave Fredholm determinant is directly related to the potential-scattering phase shift; as this result

depends only on density-of-states arguments[5] and the use of free-particle wave functions, it is independent of ordinary Schrödinger dynamics. This latter fact suggested that the method might be useful in high-energy physics where the dynamics are largely unknown, but phenomenological potentials might be found. Newton[6] and Blankenbecler[7] have extended these potential-scattering results by giving prescriptions whereby the whole multichannel S matrix may be constructed from the Fredholm determinant. Sugar and Blankenbecler[8] have applied the method to many-particle scattering and suggested methods of attacking the three-body problem.

Numerical applications of the Fredholm method have been limited; attempts to obtain numerical results by effectively keeping only a few terms in the expansion of the Fredholm determinant have been, at best, semiquantitative.[9] For some potentials, keeping only one or two powers of λ in the expansion seems to give good results at high

energies[10]; for other potentials these same low-order approximations become worse as the energy increases.[11]

The idea that the S matrix can be extracted from a determinant is very attractive; if a workable computational method could be developed, one would avoid numerical solution of large sets of coupled integrodifferential equations. The many-channel problem without exchange is well in hand[12]; however, there are still considerable numerical difficulties involved in solving large systems of coupled equations containing exchange terms. More specifically, in the case of electron-atom scattering, optical potentials may be constructed for elastic or inelastic processes using many-body perturbation theory as proposed by Bell and Squires.[13, 14] Optical potentials of this type allow formal reduction of many-particle scattering problems to multichannel potential-scattering problems. The price paid for this apparent simplification is that the optical potential is energy dependent, nonlocal, and rather cumbersome. It would be very convenient if scattering information could be *constructed* from the optical potential via the Fredholm determinant, rather than obtained by the more usual procedure of *solving* the wave equation and then constructing the S-matrix elements. In their work on the elastic scattering of electrons from atoms, Pu and Chang,[15] and Kelly[16] have avoided solving the Schrödinger equation by making use of the distorted-wave Born approximation and thereby extracting scattering information directly from the optical potential. The distorted-wave Born approximation is certainly appropriate if static and static-exchange effects dominate the scattering; however, one would like a more detailed description near resonances or thresholds, certainly in the case of inelastic or rearrangement collisions.

It is the purpose of this paper to give a convenient and arbitrarily accurate numerical procedure whereby elastic scattering information may be extracted directly from the potential via the construction of the Fredholm determinant. The prescription is given, after a short review of the formalism, in Sec. II. In Sec. III an alternate derivation based on the Lippmann-Schwinger equation is presented. Section IV presents numerical results for s-, p-, and d-wave scattering of electrons from hydrogen atoms in the static approximation, and triplet s-wave scattering in the static-exchange approximation. Section V contains a brief summary and a conclusion.

II. CALCULATION OF THE FREDHOLM DETERMINANT

The principal result of the Fredholm method as

developed by Schwinger[3] and Baker[4] is that, for scattering from a fixed potential V, the "reference"[4] determinant[17] $D(z)$ contains all the scattering information:

$$D(z) = \det\left[(z - H)/(z - H^0)\right] = \det\left[1 - \lambda G^0(z)V\right] , \tag{2.1}$$

where λV is the potential and $G^0(z) = (z - H^0)^{-1}$ is the free-particle Green's function. We note in passing that the operator $\lambda G^0(E + i\epsilon)V$ is the kernel of the Lippmann-Schwinger equation

$$\psi^+ = \phi + \lambda G^0(E + i\epsilon)V\psi^+ \tag{2.2}$$

and that $D(E + i\epsilon)$ is, in fact, the Fredholm determinant for this equation. In the case that V is spherically symmetric, $D(z)$ may be factored as

$$D(z) = \prod_l D_l(z) = \prod_l \det[1 - \lambda G_l^0(z)V] , \tag{2.3}$$

where the l's refer to the different partial waves. Focusing attention on one partial wave, the key result is that the phase of $D_l(E + i\epsilon)$ is the negative of the partial-wave scattering phase shift $\delta_l(E)$:

$$D_l(E + i\epsilon) = \left|D_l(E + i\epsilon)\right| e^{-i\delta_l(E)} . \tag{2.4}$$

Knowledge of $D_l(z)$ thus allows determination of the S-matrix elements

$$S_l(E) = e^{2i\delta_l(E)} = D_l(E - i\epsilon)/D_l(E + i\epsilon) , \tag{2.5a}$$

the K-matrix elements

$$K_l(E) = \tan\delta_l(E) = \pi A_l(E)/d_l(E) , \tag{2.5b}$$

or the partial-wave scattering amplitudes

$$f_l(E) = e^{i\delta_l(E)} \sin\delta_l(E) = \pi A_l(E)/D_l(E + i\epsilon) , \tag{2.5c}$$

where $A_l(E) = -\pi^{-1}\mathrm{Im}[D_l(E + i\epsilon)]$ and $d_l(E) = \mathrm{Re}[D_l(E + i\epsilon)]$. In the sequel we will use the K-matrix formalism to avoid complex arithmetic; we will also drop the subscript l, with the understanding that we are considering one partial wave at a time.

The determinant $D(z)$ may be determined using the operator identity[4]

$$\det D(z) = \exp \mathrm{tr} \ln D(z) , \tag{2.6}$$

which gives the expansion[17]

$$D(z) = 1 - \lambda \int_0^\infty \frac{dE_1 V_{11}}{z - E_1} + \frac{\lambda^2}{2!} \int_0^\infty \int_0^\infty \frac{dE_1}{z - E_1}$$

$$\frac{dE_2}{z-E_2} \begin{vmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{vmatrix} + \cdots$$

$$+ \frac{(-\lambda)^n}{n!} \int_0^\infty \cdots \int_0^\infty \frac{dE_1 \cdots dE_n}{(z-E_1)\cdots(z-E_n)}$$

$$\times \begin{vmatrix} V_{11} & V_{12} \cdots & V_{1n} \\ \vdots & \cdots & \vdots \\ V_{n1} & & V_{nn} \end{vmatrix} + \cdots \quad , \tag{2.7}$$

where the matrix elements are defined as[17]:

$$V_{ij} = \langle i | V | j \rangle \equiv 2/\pi (k_i k_j)^{1/2} \int_0^\infty dr\, r^2 j_l(k_i r) V(r) j_l(k_j r) \quad , \tag{2.8a}$$

with $k_i = (2E_i)^{1/2}$ and $|i\rangle \equiv \left(\frac{2k_i}{\pi}\right)^{1/2} j_l(k_i r)$. (2.8b)

This expansion of $D(z)$ is useful in discussions of potential scattering as the series converges absolutely for all λ, subject only to the rather weak conditions that[4, 17, 18]

$$\lim [r^2 V(r)] = 0, \quad \text{as } r \to 0$$

$$\lim [r V(r)] = 0, \quad \text{as } r \to \infty \quad . \tag{2.9}$$

From a computational view, the expansion (2.7) is attractive in that the absolute convergence tells us that if we take enough terms things are bound to improve, sooner or later; this is in marked contrast to the Born expansion, which often has a small radius of convergence. However, absolute convergence tells us nothing about the rate of convergence, and, as mentioned in the Introduction, low-order approximations (first or second order in λ) do not always give satisfactory results. The difficulties associated with the term by term calculation of higher-order terms in the expansion (2.7) are self-evident. Thus, it would be very convenient to have a method which could be used to calculate the sum of the series (2.7) directly to any necessary order. This is easily achieved by returning to the original derivation of the Fredholm method.

Fredholm's original derivation[19] of the solutions of the class of linear integral equations of the form

$$\phi(x) = f(x) + \lambda \int_a^b \phi(x') K(x', x) dx' \quad , \tag{2.10}$$

where $x \epsilon (a, b)$ and f and K are known functions, is based on approximating the integral by a trapezoidal-rule numerical quadrature and then solving the resulting set of simultaneous linear algebraic equations using Cramer's rule. The Cramer's rule determinants are then expanded (Laplace expansion) and rearranged in power series in λ. The individual terms in the expansion can be interpreted as trapezoidal-rule approximations to actual multiple integrals. Fredholm replaced these sums by the corresponding integrals giving a formal series solution to the integral equation in terms of expansions of determinants which are equivalent to use of the identity of Eq. (2.6). This procedure motivated the observations of the following paragraphs.

Comparison of the expansion (2.7) with the definition of the K-matrix elements in Eq. (2.5c) reveals that, for $k_0 = (2E)^{1/2}$:

$$A(E) = A(k_0) = -V_{00} + \cdots + \frac{(-1)^{n+1}(2)^n}{n!} P \int_0^\infty \frac{k_1 \cdots k_n dk_1 \cdots dk_n}{(k_0^2 - k_1^2)\cdots(k_0^2 - k_n^2)} \begin{vmatrix} V_{00} & \cdots & V_{0n} \\ \vdots & & \vdots \\ V_{n0} & \cdots & V_{nn} \end{vmatrix} + \cdots \quad , \tag{2.11}$$

and $d(E) = d(k_0) = 1 + \cdots + \frac{(-1)^n(2)^n}{n!} P \int_0^\infty \frac{k_1 \cdots k_n dk_1 \cdots dk_n}{(k_0^2 - k_1^2)\cdots(k_0^2 - k_n^2)} \begin{vmatrix} V_{11} & \cdots & V_{1n} \\ \vdots & & \vdots \\ V_{n1} & \cdots & V_{nn} \end{vmatrix} + \cdots \quad . \tag{2.12}$

To evaluate the integrals in these series we must use numerical integration techniques. The principal-value integrations

$$P \int k\, dk\, f(k)/(k_0^2 - k^2) \tag{2.13a}$$

are replaced by sums of the form

$$\sum_{i=1}^N \frac{k_i f(k_i) \omega_i}{k_0^2 - k_i^2} \quad , \tag{2.13b}$$

where the k_i are the numerical quadrature points and the ω_i are the associated weights. In the neighborhood of the singularity of the integrand, the quadrature points must be placed symmetrically.

If an N-point numerical quadrature is used for each integration, it may be verified by direct expansion that

$$A(k_0) \equiv \det \underline{A} = \begin{vmatrix} -\langle 0|V|0\rangle & \Big| & -\dfrac{2\langle 0|V|1\rangle\omega_1 k_1}{k_0^2-k_1^2} & \cdots & -\dfrac{2\langle 0|V|N\rangle\omega_N k_N}{k_0^2-k_N^2} \\ \hline \vdots & \Big| & & & \\ -\langle N|V|0\rangle & \Big| & & \underline{d} & \\ & \Big| & & & \end{vmatrix} \quad , \tag{2.14}$$

where

$$d(k_0) \equiv \det \underline{d} = \begin{vmatrix} 1-\dfrac{2\langle 1|V|1\rangle\omega_1 k_1}{k_0^2-k_1^2} & -\dfrac{2\langle 1|V|2\rangle\omega_2 k_2}{k_0^2-k_2^2} & \cdots & -\dfrac{2\langle 1|V|N\rangle\omega_N k_N}{k_0^2-k_N^2} \\ -\dfrac{2\langle 2|V|1\rangle\omega_1 k_1}{k_0^2-k_1^2} & 1-\dfrac{2\langle 2|V|2\rangle\omega_2 k_2}{k_0^2-k_2^2} & \cdots & -\dfrac{2\langle 2|V|N\rangle\omega_N k_N}{k_0^2-k_N^2} \\ \vdots & & & \vdots \\ -\dfrac{2\langle N|V|1\rangle\omega_1 k_1}{k_0^2-k_1^2} & \cdots & & 1-\dfrac{2\langle N|V|N\rangle\omega_N k_N}{k_0^2-k_N^2} \end{vmatrix} . \tag{2.15}$$

Making use of the elementary properties of determinants we can rewrite $d(k_0)$ and $A(k_0)$ in the more symmetric forms

$$d(k_0) = \prod_{i=1}^{N} [2/(k_0^2-k_i^2)] \det \underline{d}' \quad , \tag{2.16a}$$

$$A(k_0) = \prod_{i=1}^{N} [2/(k_0^2-k_i^2)] \det \underline{A}' \quad , \tag{2.16b}$$

where the matrix elements of $\underline{d}'$ are given by

$$d'_{ij} = [\tfrac{1}{2}(k_0^2-k_i^2)]\delta_{ij} - \tilde{V}_{ij} \tag{2.17}$$

and

$$\underline{A}'(k_0) = \begin{pmatrix} & & & \Big| & -\tilde{V}_{10} \\ & \underline{d}' & & \Big| & \vdots \\ & & & \Big| & -\tilde{V}_{N0} \\ \hline -\tilde{V}_{01} & \cdots & -\tilde{V}_{0N} & \Big| & -\tilde{V}_{00} \end{pmatrix} \tag{2.18}$$

with

$$\tilde{V}_{ij} = (k_i\omega_i)^{1/2} V_{ij}(k_j\omega_j)^{1/2}, \quad i,j=0,\ldots,N,$$

and $\omega_0 = 1/k_0$. $\tag{2.19}$

We now note that

$$\tan\delta(k_0) = \pi A'(k_0)/d'(k_0) \quad . \tag{2.20}$$

Equation (2.20) is the principal result of this section. The determinants $A'(k_0)$ and $d'(k_0)$, as opposed to $A(k_0)$ and $d(k_0)$ themselves, have no singular matrix elements, and, in fact, appear to be very well conditioned. We also note that, although the manipulations of this section are simple, an enormous computational simplification has been achieved: Calculation of the value of an $N \times N$ determinant takes the order of N^3 multiplications[20]; on the other hand the direct, term by term calculations of the series (2.11) or (2.12) would involve the order of $N!$ multiplications, as these series expansions are essentially nothing but the direct expansions of the determinants, which, by definition, contain $N!$ terms.

In preparation for an alternate derivation of Equation (2.20), we note that a Laplace expansion of $A'(k_0)$ based on the last row gives

$$\tan\delta(k_0)/\pi = -\tilde{V}_{00} + \sum_{i=1}^{N} c'_i \tilde{V}_{0i} \quad , \tag{2.21}$$

where the c'_i are the solutions of

$$\sum_{i=1}^{N} c_i' \left[\left(\frac{k_0^2 - k_i^2}{2} \right) \delta_{ij} - \tilde{V}_{ij} \right] = - \tilde{V}_{j0}, \quad j = 1 \dots N \; ; \tag{2.22}$$

or, rewriting this equation in terms of the matrix elements $\langle i|V|j\rangle$, we obtain

$$\tan\delta(k_0)/\pi = - \langle 0|V|0\rangle + \sum_{i=1}^{N} c_i \langle 0|V|i\rangle \;, \tag{2.21'}$$

where the c_i are the solutions of

$$\sum_{i=1}^{N} c_i \left[\left(\frac{k_0^2 - k_i^2}{2k_i\omega_i} \right) \delta_{ij} - \langle i|V|j\rangle \right] = - \langle j|V|0\rangle,$$
$$j = 1 \dots N \tag{2.22'}$$

where $c_i' = c_i/(\omega_i k_i)^{1/2}$.

The fact that $\tan\delta(k_0)$ may be expressed in terms of the principal value solution of the Lippmann-Schwinger equation, $\psi_l(k_0 r)$, as

$$\tan\delta_l(k_0) = - 2k_0 \int_0^\infty r^2 dr\, j_l(k_0 r) V(r) \psi_l(k_0 r)$$
$$= - \pi\langle 0|V|\psi\rangle$$

suggests that

$$|\psi\rangle = |0\rangle - \sum_{i=1}^{N} c_i|i\rangle \tag{2.23}$$

and that Eq. (2.22) is the appropriate form of the Lippmann-Schwinger equation to employ with a continuum basis set which has been made discrete by use of numerical quadrature. In Sec. III we will see that this is indeed the case.

III. ALTERNATE DERIVATION OF THE FREDHOLM RESULTS BASED ON THE LIPPMANN-SCHWINGER EQUATIONS

Although the principal results of the Fredholm method as applied to potential scattering can be shown to follow from considerations more general than Schrödinger dynamics, it is of interest to re-derive the result of Eq. (2.20) directly from the Lippmann-Schwinger equation.

For elastic scattering at an energy $E = \frac{1}{2}k_0^2$, the principal-value Lippmann-Schwinger equation is

$$|\psi\rangle = |k_0\rangle + (k_0^2/2 - H_0 - V)^{-1}V|k_0\rangle, \tag{3.1}$$

where the kets are those of Eq. (2.8b).
We now expand $|\psi\rangle$ as

$$|\psi\rangle = |k_0\rangle - P\int_0^\infty c(k, k_0)|k\rangle dk \;, \tag{3.2}$$

where $P\int_0^\infty$ is $\lim \int_0^{k_0-\epsilon} + \int_{k_0+\epsilon}^\infty$, as $\epsilon \to 0$

and the $c(k, k_0)$ are expansion coefficients which may be determined by requiring that $|\psi\rangle$ satisfy Eq. (3.1). Direct substitution and use of the normalization $\langle k|k'\rangle = \delta(k-k')/k$ gives the integral equation

$$c(k, k_0)[(k_0^2 - k^2)/2k] = - \langle k|V|k_0\rangle$$
$$+ P\int_0^\infty c(k', k_0)\langle k|V|k'\rangle dk' \tag{3.3}$$

for the $c(k, k_0)$.

Noting that

$$\frac{\tan\delta_l(k_0)}{\pi} = - \langle k_0|V|k_0\rangle$$
$$+ P\int_0^\infty c(k', k_0)\langle k_0|V|k'\rangle dk' \tag{3.4}$$

gives, by comparison with Eq. (3.3), the result

$$\frac{\tan\delta_l(k_0)}{\pi} = \lim \frac{c(k, k_0)(k_0^2 - k^2)}{2k} \;, \quad \text{as } k \to k_0. \tag{3.5}$$

We may thus set

$$c(k, k_0) = 2\omega(k, k_0)k/(k_0^2 - k^2) \;,$$

where $\omega(k_0, k_0) = \tan\delta_l(k_0)/\pi$.

In this form it is not difficult to check that the wave function $|\psi\rangle$ has the asymptotic form

$$|\psi\rangle \sim j_l(k_0 r) + \pi\omega(k_0, k_0)\eta_l(k_0 r) \tag{3.6}$$

as is required for consistency.

Approximating the integrals in Eqs. (2.2)–(2.4) by numerical quadrature with weights ω_i and defining $c(k_i)\omega_i \equiv c_i$, we immediately regain Eqs. (2.22), (2.22'), (2.23) of Sec. II, which are equivalent to the result of Eq. (2.20).

IV. COMPUTATIONAL METHOD AND RESULTS

In this section we present the numerical results obtained for the low-energy scattering of electrons from the hydrogen atom in the static and static-exchange approximations. In the static case the matrix elements V_{ij}^{static} are given by Eq. (2.8a), where

$$V(r) = - e^{-2r}[1 + (1/r)] \;; \tag{4.1a}$$

in the static-exchange (s.e.) case, for triplet scattering,

$$V_{ij}^{s,e.} = V_{ij}^{static} - (2/\pi)(k_ik_j)^{1/2} \int_0^\infty dr\, r^2 j_l(k_ir)$$

$$\times \phi_{1s}(r) \left[(1/r) \int_0^r dr'\, r'^2 j_l(k_jr')\phi_{1s}(r') \right.$$

$$\left. + \int_r^\infty dr'\, r' j_l(k_jr')\phi_{1s}(r') \right] , \qquad (4.1b)$$

where $\phi_{1s}(r)$ is the normalized ground-state wave function for the hydrogen atom. Preliminary numerical work revealed that, for these potentials, highly accurate values of the determinants $A'(k_0)$ and $d'(k_0)$ could be obtained by the straightforward use of Gaussian elimination without either scaling or pivoting. This is not surprising when one notes that the matrices $\underline{A}'$ and $\underline{d}'$ are dominated by large diagonal elements, and that the matrix elements decrease fairly rapidly as one moves away from the diagonal. Use of Gaussian elimination obviates the necessity of separate calculation of the determinants $A'(k_0)$ and $d'(k_0)$. In the Gaussian method, [21] if $\underline{N}^d$ is the (lower triangular) matrix which triangularizes $\underline{d}'$, the fact that $\underline{A}'$ is simply a bordered form of $\underline{d}'$ implies that the matrix which triangularizes $\underline{A}'$ is of the form

$$\underline{N}^A = \begin{pmatrix} & & & & 0 \\ & & \underline{N}^d & & 0 \\ & & & & \vdots \\ & & & & \vdots \\ & & & & 0 \\ \hline N_{N+1}^A \cdots N_{N+1}^A & & & 1 \end{pmatrix}, \qquad (4.2)$$

where N is the number of quadrature points. Application of $\underline{N}^A$ to $\underline{A}'$ results in a triangular matrix $\underline{N}^A\underline{A}'$ with diagonal elements a'_{ii}, $i=1,\ldots,N+1$, where the first N of these diagonal elements are identical with the diagonal elements of the triangular matrix $\underline{N}^d\underline{d}'$. We then have

$$\frac{\tan\delta_l(k_0)}{\pi} = \frac{A'(k_0)}{d'(k_0)} = \prod_{i=1}^{N+1} a'_{ii} / \prod_{i=1}^{N} a'_{ii} = a'_{N+1,N+1},$$
$$(4.3)$$

where use has been made of the fact that the matrices $\underline{N}^A$ and $\underline{N}^d$ both have unit determinants. In all the calculations reported here, $\underline{A}'$ was set up as in Eq. (2.18), triangularized by Gaussian elimination; and the tangent of $\delta(k_0)$ constructed from $a'_{N+1,N+1}$.

Table I shows how the static and static-exchange phase shifts for s waves converge with the number of numerical quadrature points; for comparison the results of the first and second Fredholm [i.e., expansion of $A(k_0)$ and $d(k_0)$ keeping terms of order λ and λ^2, respectively] approximations, as calculated by Moiseiwitsch and O'Brien, [9] are shown for the same energy. Table II gives the s-, p-, and d-wave static phase shifts and the s-wave triplet phase shifts for several energies. The numerical work was carried out with an eye to achieving an accuracy of four places past the decimal point. Comparison with the work of John, [22] and Kelly[16a] revealed that the only phase which did not meet this

TABLE I. Values of the s-wave static and (triplet) static-exchange phase shifts as a function of the number of numerical quadrature points. For comparison, results obtained by use of the first and second Fredholm[a] approximation are given. The exact phase shifts are 0.9055 and 1.3905, respectively, for $k=1$ a.u.

Static phase shifts $l=0$, $k=1$ (a.u.)				Triplet static-exchange phase shifts $l=0$, $k=1$ (a.u.)	
Numerical quadrature method[b]		First Fredholm[a]	Second Fredholm[a]	Numerical quadrature method[c]	
No. of quadrature points[c]	Phase shift			No. of quadrature points[c]	Phase shift
16	0.6970	−1.512	0.658	16	1.1834
24	0.9005			24	1.3971
32	0.9055			32	1.3905
40	0.9055			40	1.3905

[a]Moiseiwitsch and O'Brien, Ref. 9.

[b]The numerical quadrature used was of the Legendre-Gauss form as described in Handbook of Mathematical Functions, edited by A. Abramowitz and I. A. Stegun (U.S. Department of Commerce, Nat'l. Bur. Stds., Washington, D.C., 1964), Appl. Math. Ser. 55, Chap. 25.

[c]The 16-point quadrature was carried out using an 8-point Legendre-Gauss quadrature in each of the intervals $k=0-1$ and 1–2 a.u. The succeeding results add eight more points in each of the intervals 2–10 , 10–60, and 60–500 a.u.

TABLE II. s- p-, and d-wave static and s-wave (triplet) static-exchange phase shifts for a range of energies. In each case, 48 Legendre-Gauss quadrature points were used.

Energy	Static			Triplet static-exchange
	δ_0	δ_1	δ_2	δ_0
$k = 0.2$	0.9725	0.0021	0.00002	2.679
$k = 0.4$	1.057	0.0146	0.0005	2.257
$k = 0.6$	1.021	0.0405	0.0029	1.901
$k = 0.8$	0.9634	0.0751	0.0087	1.614
$k = 1.0$	0.9055	0.1115	0.0178	1.391

requirement was that for the static s-wave phase shift at $k = 0.2$ a.u., where John reports a phase shift of 0.9726 rad.

Before leaving this section it seems worthwhile to mention that the values of k in the 48-point numerical quadrature used in calculating the results of Table II would be quite insufficient to give accurate values of the integrals in the first and second Fredholm approximations; this is simply because the diagonal matrix elements $\langle k |V| k \rangle$ do not decrease very rapidly, so that, for example, values of k of the order of 10^7 a.u. are needed to obtain the value of the integral

$$P \int_0^\infty dk \, k \langle k |V| k \rangle / (1.0 - k^2) \qquad (4.4)$$

to four or five significant figures. Thus, it appears that, for the potentials in question, a large amount of cancellation occurs between the various terms in the Fredholm expansion. Physically one expects cancellation of this type to occur: It is reasonable to expect that virtual processes occurring with energies 13 orders of magnitude larger than those of interest will not play a significant role in the actual determination of phase shifts. Computationally,

it is a great advantage to be able to sum the whole Fredholm series as a function of the cutoff energy (momentum) rather than looking at the convergence properties of individual integrals in the series, which may be quite different from those of the sum.

V. SUMMARY AND CONCLUSIONS

It has been shown that the Fredholm expansion of the determinant whose phase gives the elastic scattering phase shift may be "summed" by use of numerical quadrature, and, thus, the evaluation of the whole series reduced to the numerical evaluation of a single determinant. That such a summation can be carried out directly is guaranteed by the absolute convergence of the expansion – this is in marked contrast to the usual series summations of many-body perturbation theory where a (possibly) divergent series is formally rearranged and summed, and then reexpanded in the hope of obtaining a rapidly convergent, or, at least, a useful asymptotic result.

The method gives essentially exact numerical results when applied to the simple problems of static and static-exchange scattering of electrons from the hydrogen atom. The important numerical advantage of the method is that exchange potentials add no complication. This should make the method particularly useful for accurate calculations of electron-atom scattering cross sections when used in conjunction with the optical potential of Bell and Squires. The numerical method presented here can be immediately extended to multichannel scattering by the functional techniques of Blankenbecler or the Jost function formalism of Newton: It is of course in the many-channel problem with exchange that the real utility of direct calculation of scattering information without explicit calculation of the intermediate wave functions will be found.

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[17]For a simple discussion of the derivation of this equation, see K. Gottfried, Quantum Mechanics (W. A. Benjamin, Inc., New York, 1966), Vol. I, p. 380.

[18]Potentials not satisfying these conditions may be treated using a distorted-wave basis for computation of the determinants, essentially factoring out badly behaved parts of the potential.

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