PHYSICAL REVIEW VOLUME 185, NUMBER 1 5 SEPTEMBER 1969

Tables of Coefficients to Determine the Long-Range Contributions to Low-Energy Electron-Atom Scattering*†

R. Oppenheim Berger, H. B. Snodgrass,‡ and Larry Spruch

Physics Department, Washington Square, New York University, New York, New York

(Received 24 July 1968; revised manuscript received 7 March 1969)

The difficulty in the extrapolation or interpolation in energy of the phase shifts deduced from electron-atom scattering data stems from the presence of an effective one-body long-range potential $U(r)$. $U(r)$ has its origin in the static and dynamic polarizabilities of the atom, assumed to have a spherically symmetric ground state, and gives rise to an unusual and rapidly varying energy dependence.

The usual effective-range theory is inapplicable, but a modified effective-range theory (MERT) exists in which the effect of $U(r)$ is taken into account exactly for arbitrarily strong (but specified) $U(r)$. The applicability of MERT has previously been limited to $U(r)$ sufficiently weak for the Born approximation to be adequate (because of the unavailability of numerical values for the long-range functions necessary for the analysis). We here tabulate these functions for the case in which $U(r) \rightarrow -\frac{1}{2}\alpha_1 e^2/r^4$, where α_1 is the atomic electric dipole polarizability. The functions have been tabulated in terms of dimensionless parameters over a range of values of angular momentum L, α_1, and wave number k such that the entire elastic region for almost all atoms can be covered. The only interpolation necessary is that over k. A study of the e^-H and e^+H $L=0$ phase shifts provides an illustration of the application of the tables.

1. INTRODUCTION

In the presence of the effective long-range potentials which have their origin in the static and dynamic polarizability of the atom, the phase shifts in the low-energy scattering of electrons or positrons by spherically symmetric atoms or ions can vary very rapidly with energy. It is therefore difficult to extrapolate or interpolate experimental data in a study of phase shifts as functions of the energy unless one explicitly extracts long-range contributions.

More precisely, it is known that the usual effective-range theory is not applicable in the presence of long-range forces,[1] and a modified effective-range theory (MERT) exists[1,2] for which the contributions of the long-range interactions can be extracted for the long-range interactions assumed to be known. The emphasis of the modified theory was on the contribution which varies as a_1/r^4, where a_1 is the electric dipole polarizability and r is the electron-atom separation, but the treatment is reasonably general.[3] With the long-range interaction effects extracted, the residual contribution, that due to short-range forces, is a relatively slowly varying function of the energy, and it becomes much easier to extrapolate and interpolate experimentally determined partial cross sections.

The original formulation[1,2] was completely general, but explicit (approximate) forms for the extraction of long-range effects were given only for the case for which long-range effects are small. These forms have been used in a number of detailed analyses[4,5] and have served as checks and guidelines in any number of other calculations. The approximate forms are convenient, but for large values of a_1, low energies, and low angular momenta, they can be quite inaccurate. A precise formulation of the numerical problem of extracting all long-range effects was given not only for neutral-atom targets[6] but for ionic targets.[7] To use this formulation, one must know three sets of functions, $\rho(k)$, $\tilde{C}(k)$, and $\tilde{h}(k)$, where ρ is the phase shift due to the long-range interaction alone, and $\tilde{C}$ and $\tilde{h}$ are analogs of the function C and h which occur in effective-range theory for the basic long-range problem, Coulomb scattering. Tables which determine ρ, $\tilde{C}$, and $\tilde{h}$ have now been prepared for the neutral-atom case for the long-range interaction of the form $-\frac{1}{2}\alpha_1 e^2/r^4$, as functions of the energy, of α_1, and of the orbital angular momentum. As a matter of practice, though not of principle, the point at which the long-range interaction is truncated, to avoid a singularity at the origin, is a matter of some importance and will be elaborated upon.

The essential result of I is that the introduction of the functions[8] $\rho(k)$, $\tilde{C}(k)$, and $\tilde{h}(k)$, defined completely in terms of a one-body long-range potential scattering problem, enables us to construct a function

$$\tilde{F}(k^2) \equiv \tilde{C}^2(k) k^{2L+1} \cot\delta(k) + \tilde{h}(k) \qquad (1.1)$$

which is analytic in k^2. Here $\delta(k)$ is defined by

$$\delta(k)=\eta(k)-\rho(k), \tag{1.2}$$

where $\eta(k)$ is the actual phase shift for the scattering process under consideration. The analysis will be useful for cases for which the expansion[9]

$$\tilde{F}(k^2)=-(1/\tilde{A})+\tfrac{1}{2}\tilde{r}_0k^2+\tilde{P}r_0^3k^4+\cdots \tag{1.3}$$

is rapidly convergent. The essential content of the present paper is the presentation of extensive tables which, with the help of a simple scaling procedure, determine the long-range functions for essentially all elastic electron or positron scattering problems for neutral spherically symmetric atoms with electric dipole polarizability a_1 for which $1\lesssim a_1/a_0^3\lesssim 10^3$. We will also illustrate the use of the tables for extrapolation and interpolation of data by an analysis of the low-energy elastic scattering of electrons and positrons by hydrogen atoms.

The formal analysis can be given in quite general terms, but numerical results can only be obtained for concrete assumptions about the long-range effective interaction $U(r)$. To begin, we assume that the asymptotic form of $U(r)$ is given by

$$U(r)\rightarrow -\tfrac{1}{2}\alpha_1e^2/r^4\ , \tag{1.4}$$

with corrections which fall off faster than any power of $1/r$. [The term in $1/r^6$, which has its origins in nonadiabatic terms[10] (whose numerical coefficient is known exactly for hydrogen and approximately for a number of other atoms) and in the adiabatic electric quadrupole polarizability can often be adequately taken into account in the Born approximation.] Though not a matter of principle [except for $L=0$ for which $U(r)$ cannot be extended into the origin], the details of the modification of $U(r)$ to avoid a singularity at the origin are in practice a matter of great importance. In the calculation here, as ultimately in I, we use a simple truncation with

$$U(r)=0,\ \ r<d;\ \ U(r)=-\tfrac{1}{2}\alpha_1e^2/r^4,\ \ r\geq d. \tag{1.5}$$

The choice of d will be discussed in considerable detail later. For the moment, we restrict ourselves to two remarks about the choice of d. First, we have some feeling for the distance at which the effective interaction is closely approximated by the $1/r^4$ interaction, and we therefore know "physically" what a reasonable choice for d is. Nevertheless, it will not be necessary to predetermine d. One can simply try a number of values of d and see which gives the best results. Second, we note that the "peculiarities" associated with long-range interactions, such as the fact that $k^{2L+1}\cot\eta$ is *not* an analytic function of k^2, have their origin in effects from arbitrarily great distances. It follows that, formally, we will have extracted out long-range "peculiarities" even if we choose d to be extremely large. A very large d is nevertheless not usually a good choice unless α_1 is very small, for the range of convergence of $\tilde{F}(k^2)$ may well decrease with increasing d, with the coefficients in the expansion very large, since we have a situation in which the "short-range" interaction V extends out to the large distance d.

In the usual effective-range theory, one obtains useful results if the analog $F(k^2)$ of the $\tilde{F}(k^2)$ of Eq. (1.3) is rapidly convergent *or*, by inverting the analog of Eq. (1.3), if $1/F(k^2)$ is rapidly convergent. In the present modified effective-range theory we have not two possibilities but two continua of possibilities; useful results are obtained if, for any d, $\tilde{F}(k^2)$ or $1/\tilde{F}(k^2)$ is rapidly convergent.

2. NUMERICAL EVALUATION OF THE LONG-RANGE FUNCTIONS

The true scattering problem is formally defined by the equivalent one-body Schrödinger equation

$$\left(-\frac{d^2}{dr^2}+\frac{L(L+1)}{r^2}+\frac{2m}{\hbar^2}\left[U(r)+V\right]-k^2\right)\psi=0, \tag{2.1}$$

where the entire complexity of the problem is buried in the energy-dependent nonlocal interaction V. The decomposition into U and V is not unique, except asymptotically. (V is known only in a formal sense, but by definition V is a short-range interaction.) The long-range functions can be determined[6] from a knowledge of the regular and irregular solutions, $f(k,r)$ and $g(k,r)$, respectively, of Eq. (2.1) with V omitted. It will be useful to repeat the definitions given in I. To begin, f is uniquely defined by the boundary conditions

$$f(k,0)=0;$$

$$f(k,r)\rightarrow\sin(kr-\tfrac{1}{2}L\pi+\rho),\quad r\rightarrow\infty; \tag{2.2a}$$

$\rho(k)$ is simultaneously determined. Then $g(k,r)$ is uniquely determined by the boundary condition

$$g(k,r)\rightarrow\cos(kr-\tfrac{1}{2}L\pi+\rho),\quad r\rightarrow\infty.$$

With $U(r)=0$ for $r<d$, we define $\tilde{C}(k)$ by the relationship

$$f(k,r)=\tilde{C}(k)krj_L(kr),\quad r<d \tag{2.2b}$$

and $\tilde{E}(k)$ by

$$g(k,r) = -\frac{krn_L(kr)}{\tilde{C}(k)} + \tilde{E}(k)krj_L(kr), \quad r<d. \tag{2.3}$$

Finally $\tilde{h}(k)$ is defined by

$$\tilde{h}(k) = k^{2L+1}\tilde{C}(k)\tilde{E}(k) - \lim_{k\to 0}\,[k^{2L+1}\tilde{C}(k)\tilde{E}(k)]\,. \tag{2.4}$$

Specializing now to the case where $U(r)$ is given by Eq. (1.5), let us set $x = kr$ and introduce β through

$$\beta^2 = \alpha_1 me^2/\hbar^2 = \alpha_1/a_0\,. \tag{2.5}$$

Then we have the dimensionless form

$$\left(-\frac{d^2}{dx^2} + \frac{L(L+1)}{x^2} - \frac{(\beta k)^2}{x^4}\,S(x-kd) - 1\right) \times (f,g) = 0\,, \tag{2.6}$$

where S is the unit step function. This shows that the dimensionless long-range functions depend only on two dimensionless quantities which are most conveniently taken to be βk and β/d. The functions will be determined for a series of values of βk and β/d. In an application β will be specified and d will be chosen to have a value roughly that to be expected on physical grounds and such that β/d is one of the values for which the functions are tabulated. (One should also do the calculation for neighboring values of d to verify that the results are effectively independent of d, since a proper value of d is one which lies in a range for which the extrapolated quantities do not depend on it. This is the ultimate criterion governing the choice for d, an equivalent criterion; namely that of the straightness of the extrapolation curve is considered in Sec. 4 below. If experimental values of η are known for specified values of k, the values of the long-range functions at the corresponding values of βk can be obtained by interpolating the tabulated values or directly from Figs. 1 to 4.

The functions $\rho(k)$ and $\tilde{C}(k)$ are determined by integrating $f(k,r)$ from d to a large radius R with slope and value at d determined from the function

$$f(k,r)/\tilde{C}(k) = krj_L(kr)\,.$$

The contribution due to the region from R to ∞ is estimated in the Born approximation, and convergence is tested by comparing results obtained

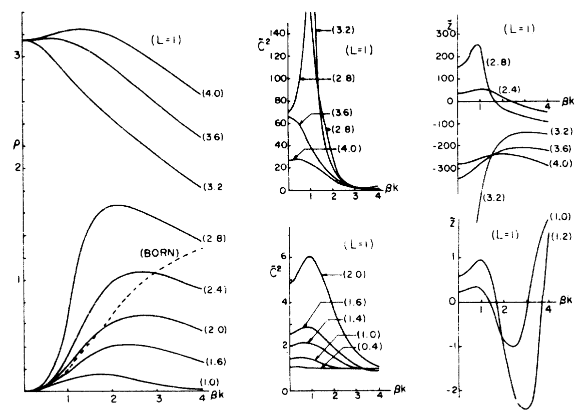

FIG. 2. Plots of ρ, $\tilde{C}^2$, and $\tilde{Z}$ as functions of βk, for various values of β/d (the values in parentheses), for $L=1$. The Born approximation for ρ, the dashed line, is for the choice $d=0$.

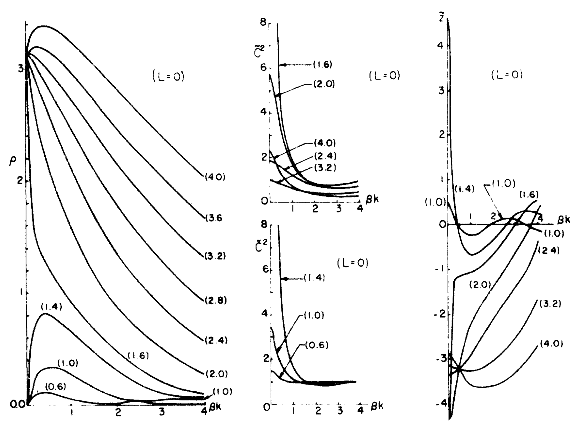

FIG. 1. Plots of ρ, $\tilde{C}^2$, and $\tilde{Z}$ as functions of βk, for various values of β/d (the values in parentheses), for $L=0$.

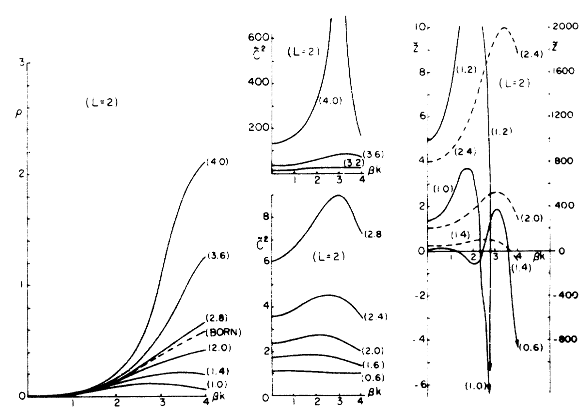

FIG. 3. Same caption as for Fig. 2, but for $L=2$ rather than $L=1$.

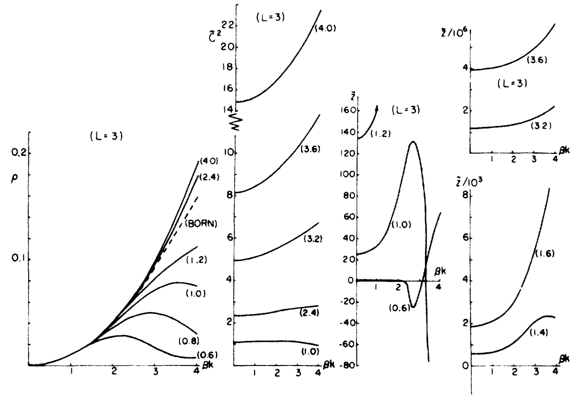

FIG. 4. Same caption as for Fig. 2, but for $L=3$ rather than $L=1$.

for several values of R. (The details may be found in the Ph. D. dissertation referred to in the footnote denoted by †.) $\tilde{E}(k)$ is then obtained by integrating $g(k, r)$ inward from R, using the values for ρ and $\tilde{C}$ corrected for the contribution from R to ∞, with the convergence of $\tilde{E}$ tested by examining its dependence on R. Checks on the results are made by comparison with the Born-approximation results for small values of β/d. (Appendix A contains a discussion of the Born approximation and of its expansion in powers of β^2 to give an alternate derivation of the MERT expansion[1,2] in β^2.) It is also found that ρ is monotonic in the potential, increasing as d is decreased or as β is increased, as it should. The ability to reproduce the known results for $e^{\pm}$ scattering by atomic hydrogen, as discussed in Sec. 4, provides still another check.

By means of convergence and mesh-size studies the results obtained can be estimated to be accurate to at least 0.01% over the range of βk, β/d, and L considered.

For long-range forces, most of the quantities that appear in the usual effective-range theory that are appropriate to short-range forces do not even exist.[1,2] In particular, if $U(r)$ vanishes as $1/r^4$, all of the effective ranges r_0, and all of the scattering lengths A but that associated with $L=0$, are infinite. It will be of interest, for $L=0$, to find the connection between A and $\tilde{A}$. Note that A represents the zero-energy asymptotic relative amplitude of irregular and regular free solutions while $\tilde{A}$ represents the zero-energy asymptotic relative amplitude of irregular and regular solutions associated with the $1/r^4$ potential.

We note first that $\tilde{h}(0)=0$ and, excluding the possibility of a zero-energy bound state, that $\tilde{C}(0)\neq\infty$. Furthermore, we have

$$\eta \to -kA (\mathrm{mod}\, \pi) \text{ for } k\to 0$$

by definition. We define a scattering length A' associated with $U(r)$ as given by Eq. (1.5), so that we have

$$\rho \to -kA' (\mathrm{mod}\, \pi) \text{ for } k \to 0 \ .$$

Finally, on letting k approach zero in Eqs. (1.1), (1.2), and (1.3), we obtain the relationship

$$A=A'+\tilde{C}^2(0)\tilde{A} \, . \tag{2.7}$$

3. TABLES OF THE LONG-RANGE FUNCTIONS

The numerical results are presented in Tables I–IV and Figs. 1–4. The computations were performed on the New York University CDC-6600. For purposes of interpolation, the values are given to more figures than might otherwise appear to be necessary. Rather than tabulating ρ, $\tilde{C}$, and $\tilde{h}$, we give ρ, $\tilde{C}^2$, and $\tilde{Z}$, where

$$\tilde{Z}(k)\equiv(\beta k)^{2L+1}\tilde{E}(k)\tilde{C}(k) \, , \tag{3.1}$$

since the latter functions are more closely related to the functions which appear in Eq. (1.1). [The $\tilde{Z}(k)$ defined by Eq. (3.1) differs by a factor of $(\beta/a_0)^{2L+1}$ from the $\tilde{Z}(k)$ defined in the thesis referred to in the reference denoted by †.] Furthermore, $\tilde{Z}(k)$ is dimensionless whereas $\tilde{h}(k)$ is not. If we absorb $\tilde{Z}(0)/\beta^{2L+1}$ into the definition of the constant term in the expansion in powers of k^2, which is a slight computational saving, we have, replacing $\tilde{F}(k^2)$ by $\tilde{F}'(k^2)$,

$$\tilde{F}'(k^2)\equiv\tilde{C}^2(k)k^{2L+1}\cot\delta(k)+\frac{\tilde{Z}(k)}{\beta^{2L+1}}$$

$$=-(1/\tilde{A}')+\tfrac{1}{2}\tilde{r}_0k^2+\tilde{P}\tilde{r}_0^{\,3}k^4+\cdots, \tag{3.2}$$

$$\text{where } -(1/\tilde{A}')\equiv-(1/\tilde{A})+\tilde{Z}(0)/\beta^{2L+1}. \tag{3.3}$$

If $\eta(k)$ is known for a given L for a number of values of k, the quantities $\tilde{A}'$ and $\tilde{r}_0$ and perhaps $\tilde{P}$ can be determined. This in turn determines $\eta(k)$ down to $k=0$.

Note that in the tables we do not utilize any absolute definitions of ρ, that is, we ignore multiples of π, restricting ρ to lie between $-\frac{1}{2}\pi$ and $+\frac{1}{2}\pi$.

A. Scope of the Tables

Very small values of d can be expected to lead to poor convergence of (3.2), for since the true

TABLE I. ρ, $\tilde{C}^2$, and $\tilde{Z}$ as functions of βk and β/d for $L=0$.

βk \ β/d	0.4	00.6	0.8	1.0	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4.0
0.01	0.0041	0.0067	0.0102	0.0155	0.0256	0.0577	−0.3308	−0.0219	−0.0093	−0.0037	0.0005	0.0048	0.0115
	1.1780	1.4670	2.0584	3.4217	7.6028	34.440	1055.8	5.7709	1.8382	1.1258	1.0028	1.2424	2.3359
	0.0227	0.0839	0.2293	0.5566	1.3695	4.3743	−32.3264	−4.1844	−3.3160	−3.1556	−3.1416	−3.1068	−2.8434
0.05	0.0184	0.0313	0.0484	0.0743	0.1235	0.2737	1.0757	−0.1109	−0.0479	−0.0201	0.0004	0.0219	0.0546
	1.1675	1.4503	2.0283	3.3525	7.3437	30.928	312.10	5.7130	1.8264	1.1176	0.9939	1.2283	2.2965
	0.0207	0.0799	0.2213	0.5383	1.3100	3.8833	−10.0464	−4.1675	−3.3160	−3.1570	−3.1438	−3.1108	−2.8547
0.1	0.0319	0.0568	0.0897	0.1391	0.2308	0.4842	−1.3683	−0.2226	−0.0990	−0.0441	−0.0038	0.0383	0.1014
	1.1459	1.4132	1.9582	3.1852	6.7136	23.807	98.485	5.5690	1.8024	1.1009	0.9748	1.1963	2.2023
	0.0157	0.0693	0.1996	0.4881	1.1530	2.8537	−3.6876	−4.1140	−3.3147	−3.1603	−3.1496	−3.1218	−2.8861
0.2	0.0461	0.0913	0.1505	0.2368	0.3857	0.7149	1.5493	−0.4400	−0.2062	−0.1004	−0.0233	0.0557	0.1703
	1.0955	1.3189	1.7733	2.7452	5.1916	12.959	27.148	5.1120	1.7412	1.0597	0.9262	1.1114	1.9484
	0.0027	0.0384	0.1344	0.3414	0.7447	1.2223	−1.6318	−3.9138	−3.3044	−3.1691	−3.1674	−3.1567	−2.9825
0.3	0.0484	0.1080	0.1862	0.2965	0.4731	0.8019	1.4250	−0.6417	−0.3165	−0.1642	−0.0542	0.0561	0.2097
	1.0510	1.2256	1.5866	2.3194	3.9367	7.7292	12.741	4.5325	1.6716	1.0168	0.8752	1.0213	1.6885
	−0.0080	0.0060	0.0632	0.1881	0.3859	0.3943	−1.2622	−3.6371	−3.2807	−3.1766	−3.1879	−3.1986	−3.0922
0.4	0.0435	0.1121	0.2030	0.3280	0.5156	0.8257	1.3303	−0.8234	−0.4268	−0.2327	−0.0931	0.0438	0.2263
	1.0182	1.1454	1.4258	1.9717	3.0556	5.1431	7.5474	3.9354	1.5977	0.9758	0.8271	0.9375	1.4618
	−0.0137	−0.0204	0.0005	0.0580	0.1230	−0.0348	−1.1524	−3.3409	−3.2436	−3.1803	−3.2076	−3.2404	−3.1951
0.5	0.0353	0.1077	0.2066	0.3398	0.5303	0.8198	1.2495	−0.9849	−0.5356	−0.3039	−0.1378	0.0219	0.2263
	0.9974	1.0839	1.2960	1.7035	2.4525	3.7214	5.0930	3.3861	1.5217	0.9375	0.7837	0.8635	1.2751
	−0.0141	−0.0383	−0.0486	−0.0432	−0.0613	−0.2798	−1.1119	−3.0628	−3.1945	−3.1789	−3.2243	−3.2786	−3.2844
0.6	0.0263	0.0980	0.2010	0.3384	0.5277	0.7988	1.1772	−1.1281	−0.6417	−0.3765	−0.1864	−0.0071	0.2142
	0.9868	1.0373	1.1942	1.4997	2.0335	2.8644	3.7359	2.9118	1.4452	0.9020	0.7451	0.7996	1.1241
	−0.0103	−0.0475	−0.0834	−0.1177	−0.1890	−0.4298	−1.0937	−2.8190	−3.1358	−3.1721	−3.2371	−3.3117	−3.3592

TABLE I. (*continued*)

βk \ β/d	0.4	0.6	0.8	1.0	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4.0
0.8	0.0120	0.0720	0.1741	0.3122	0.4942	0.7357	1.0488	−1.3693	−0.8432	−0.5231	−0.2913	−0.0791	0.1668
	0.9862	0.9825	1.0566	1.2274	1.5173	1.9307	2.3567	2.1914	1.2965	0.8383	0.6805	0.6976	0.9033
	0.0020	−0.0435	−0.1152	−0.2036	−0.3353	−0.5861	−1.0715	−2.4390	−2.9988	−3.1423	−3.2496	−3.3611	−3.4703
1.0	0.0059	0.0462	0.1383	0.2704	0.4426	0.6621	0.9349	−1.5656	−1.0288	−0.6680	−0.4016	−0.1627	0.1008
	0.9970	0.9648	0.9809	1.0684	1.2318	1.4520	1.7017	1.7103	1.1600	0.7826	0.6295	0.6219	0.7549
	0.0093	−0.0206	−0.1082	−0.2285	−0.3922	−0.6430	−1.0427	−2.1693	−2.8490	−3.0927	−3.2447	−3.3892	−3.5415
1.5	0.0088	0.0134	0.0582	0.1564	0.2979	0.4772	0.6923	1.2032	−1.4258	−1.0100	−0.6811	−0.3923	−0.0982
	1.0035	0.9934	0.9409	0.9142	0.9303	0.9809	1.0454	1.0825	0.8944	0.6702	0.5401	0.5021	0.5457
	−0.0051	0.0312	−0.0057	−0.1377	−0.3317	−0.5827	−0.9026	−1.7283	−2.4716	−2.9008	−3.1635	−3.3814	−3.6039
2.0	0.0049	0.0172	0.0239	0.0729	0.1737	0.3168	0.4943	0.9259	1.3953	−1.3154	−0.9503	−0.6273	−0.3112
	0.9971	1.0135	0.9884	0.9201	0.8660	0.8405	0.8354	0.8226	0.7289	0.5887	0.4830	0.4351	0.4421
	0.0012	0.0027	0.0733	0.0347	−0.1268	−0.3672	−0.6642	−1.3825	−2.1064	−2.6392	−2.9993	−3.2845	−3.5580
2.5	0.0038	0.0188	0.0271	0.0373	0.0906	0.1928	0.3351	0.7045	1.1331	1.5568	−1.2018	−0.8556	−0.5226
	1.0018	0.9993	1.0231	0.9823	0.9007	0.8280	0.7771	0.7115	0.6344	0.5331	0.4452	0.3946	0.3838
	0.0017	−0.0226	0.0345	0.1414	0.1047	−0.0761	−0.3459	−1.0204	−1.7310	−2.3245	−2.7655	−3.1148	−3.4349
3.0	0.0039	0.0111	0.0350	0.0390	0.0536	0.1111	0.2145	0.5237	0.9115	1.3193	−1.4337	−1.0731	−0.7274
	0.9992	0.9936	1.0138	1.0312	0.9750	0.8822	0.7964	0.6768	0.5878	0.4994	0.4214	0.3698	0.3488
	−0.0033	0.0042	−0.0414	0.0969	0.2406	0.2081	0.0146	−0.6113	−1.3209	−1.9594	−2.4691	−2.8803	−3.2472
3.5	0.0022	0.0076	0.0304	0.0514	0.0535	0.0729	0.1344	0.3780	0.7234	1.1095	1.4951	−1.2785	−0.9238
	1.0000	1.0017	0.9929	1.0334	1.0376	0.9669	0.8645	0.6917	0.5760	0.4845	0.4089	0.3557	0.3278
	0.0035	0.0160	−0.0448	−0.0318	0.1955	0.3753	0.3478	−0.1562	−0.8616	−1.5402	−2.1121	−2.5843	−3.0000
4.0	0.0023	0.0092	0.0194	0.0538	0.0685	0.0705	0.0950	0.2663	0.5643	0.9241	1.3005	−1.4713	−1.1112
	1.0005	1.0035	0.9889	1.0069	1.0541	1.0422	0.9580	0.7455	0.5928	0.4867	0.4069	0.3501	0.3164
	−0.0025	−0.0071	0.0101	−0.1043	0.0173	0.3353	0.5490	0.3166	−0.3491	−1.0621	−1.6936	−2.2274	−2.6951

TABLE II. ρ, $\tilde{C}^2$, and $\tilde{Z}$ as functions of βk and β/d for $L=1$.

βk \ β/d	0.4	0.6	0.8	1.0	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4.0
0.01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	1.0551	1.1292	1.2438	1.4125	1.6579	2.0186	2.5625	4.8385	12.626	69.874	3008.5	66.218	27.952
	0.0020	0.0161	0.0698	0.2212	0.5775	1.3256	2.7853	10.476	36.722	157.81	−1646.3	−343.96	−280.37
0.05	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.0006	0.0003	0.0005	0.0005
	1.0564	1.1308	1.2459	1.4150	1.6611	2.0229	2.5684	4.8514	12.668	70.224	2963.5	66.223	27.987
	0.0021	0.0163	0.0703	0.2222	0.5793	1.3288	2.7907	10.492	36.774	158.12	−1632.8	−343.69	−280.27
0.1	0.0018	0.0019	0.0019	0.0020	0.0020	0.0021	0.0021	0.0021	0.0022	0.0024	0.0002	0.0019	0.0020
	1.0584	1.1339	1.2501	1.4206	1.6685	2.0328	2.5823	4.8835	12.776	71.205	2825.1	66.126	28.047
	0.0023	0.0168	0.0717	0.2251	0.5849	1.3388	2.8077	10.540	36.937	159.13	−1592.3	−342.83	−279.94
0.2	0.0062	0.0070	0.0074	0.0078	0.0080	0.0082	0.0084	0.0088	0.0094	0.0110	−0.0052	0.0065	0.0076
	1.0609	1.1402	1.2601	1.4350	1.6888	2.0615	2.6240	4.9856	13.143	73.864	2351.5	65.388	28.133
	0.0028	0.0190	0.0773	0.2369	0.6072	1.3784	2.8756	10.736	37.591	163.19	−1449.4	−339.47	−278.63
0.3	0.0117	0.0143	0.0157	0.0167	0.0175	0.0182	0.0188	0.0201	0.0222	0.0279	−0.0216	0.0126	0.0161
	1.0593	1.1435	1.2686	1.4496	1.7114	2.0956	2.6760	5.1242	13.681	80.874	1789.6	63.799	28.089
	0.0033	0.0221	0.0860	0.2559	0.6437	1.4437	2.9881	11.064	38.693	170.24	−1263.3	−334.11	−276.52
0.4	0.0170	0.0227	0.0260	0.0283	0.0301	0.0317	0.0332	0.0365	0.0415	0.0562	−0.0487	0.0188	0.0267
	1.0533	1.1422	1.2730	1.4610	1.7320	2.1298	2.7317	5.2870	14.368	89.574	1291.3	61.363	27.855
	0.0033	0.0252	0.0965	0.2805	0.6924	1.5324	3.1426	11.519	40.249	180.57	−1073.8	−327.11	−273.71
0.5	0.0212	0.0312	0.0374	0.0419	0.0454	0.0485	0.0514	0.0579	0.0681	0.0994	−0.0839	0.0238	0.0388
	1.0438	1.1357	1.2719	1.4669	1.7476	2.1599	2.7854	5.4627	15.182	101.46	909.72	58.197	27.402
	0.0020	0.0267	0.1067	0.3077	0.7496	1.6398	3.3331	12.094	42.248	194.45	−903.11	−318.90	−270.32
0.6	0.0236	0.0391	0.0492	0.0567	0.0627	0.0680	0.0731	0.0845	0.1028	0.1625	−0.1242	0.0267	0.0514
	1.0323	1.1245	1.2647	1.4660	1.7559	2.1824	2.8316	5.6393	16.093	117.05	638.26	54.486	26.724
	−0.0005	0.0253	0.1137	0.3337	0.8100	1.7587	3.5500	12.768	44.645	211.75	−758.71	−309.94	−266.54

TABLE II. *(continued)*

βk \ β/d	0.4	0.6	0.8	1.0	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4.0
0.8	0.0229	0.0506	0.0713	0.0873	0.1007	0.1129	0.1249	0.1524	0.1988	0.3720	−0.2110	0.0237	0.0753
	1.0099	1 0920	1.2333	1.4416	1.7445	2.1934	2.8834	5.9393	17.989	157.73	323.48	46.239	24.761
	−0.0078	0.0094	0.1073	0.3623	0.9107	1.9884	4.0006	14.269	50.124	248.29	−545.08	−291.33	−258.53
1.0	0.0171	0.0547	0.0878	0.1152	0.1390	0.1612	0.1835	0.2364	0.3303	0.7130	−0.2988	0.0070	0.0933
	0.9956	1.0547	1.1858	1.3904	1.6942	2.1501	2.8586	6.0716	19.383	184.26	174.97	38.047	22.226
	−0.0109	−0.0232	0.0599	0.3283	0.9300	2.1196	4.3352	15.583	54.723	240.89	−406.98	−273.72	−251.06
1.5	0.0048	0.0384	0.0952	0.1534	0.2092	0.2645	0.3223	0.4654	0.7247	1.4770	−0.5055	−0.0874	0.0952
	0.9982	0.9898	1.0570	1.2081	1.4573	1.8469	2.4640	5.2868	16.260	69.639	50.252	22.094	15.470
	0.0173	−0.0822	−0.2056	−0.1257	0.3398	1.4528	3.6414	14.549	44.864	22.573	−235.98	−239.78	−239.71
2.0	0.0063	0.0157	0.0677	0.1429	0.2248	0.3104	0.4017	0.6249	0.9834	−1.4870	−0.6929	−0.2291	0.0353
	1.0025	0.9862	0.9814	1.0525	1.2099	1.4749	1.8975	3.7005	8.9941	20.643	19.784	12.899	10.255
	−0.0139	0.0507	−0.3391	−0.8044	−0.9959	−0.6712	0.4469	6.4127	14.659	−36.974	−172.01	−220.04	−239.28
2.5	0.0043	0.0104	0.0354	0.1047	0.1972	0.3010	0.4142	0.6836	1.0657	−1.5070	−0.8660	−0.3896	−0.0674
	0.9980	1.0048	0.9700	0.9697	1.0414	1.1949	1.4509	2.4738	4.8425	8.6563	9.6362	7.8951	6.8730
	−0.0017	0.1357	0.0155	−1.0065	−2.2213	−3.2201	−3.8201	−3.9371	−9.2242	−54.536	−148.22	−211.14	−246.12
3.0	0.0029	0.0140	0.0191	0.0635	0.1488	0.2574	0.3807	0.6716	1.0515	1.5541	1.0284	−0.5544	−0.1944
	1.0010	1.0057	0.9933	0.9511	0.9546	1.0237	1.1655	1.7396	2.9062	4.5801	5.4469	5.1110	4.7567
	0.0244	−0.1059	0.5491	−0.2616	−2.4180	−4.9876	−7.5969	−13.410	−26.339	−67.169	−142.44	−210.31	−257.51
3.5	0.0032	0.0121	0.0199	0.0361	0.0991	0.1994	0.3227	0.6195	0.9906	1.4506	1.1824	−0.7168	−0.3333
	0.9998	0.9968	1.0129	0.9729	0.9302	0.9357	0.9992	1.3180	1.9488	2.8221	3.4351	3.4935	3.4150
	−0.0431	−0.1704	0.4158	1.1127	−1.0502	−5.0073	−9.7225	−20.991	−39.617	−79.249	−145.74	−215.44	−272.04
4.0	0.0016	0.0070	0.0246	0.0278	0.0615	0.1417	0.2557	0.5466	0.9070	1.3379	−1.3296	−0.8744	−0.4772
	0.9998	0.9973	1.0103	1.0053	0.9478	0.9071	0.9131	1.0738	1.4330	1.9366	2.3567	2.5096	2.5409
	0.0463	0.1772	−0.4486	1.8618	1.6032	−2.7095	−9.2802	−26.001	−50.056	−90.900	−153.76	−224.77	−288.92

TABLE III. ρ, $\tilde{C}^2$, and $\tilde{Z}$ as functions of βk and β/d for $L=2$.

βk \ β/d	0.6	0.8	1.0	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4.0
0.01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	1.0750	1.1379	1.2250	1.3421	1.4973	1.7029	2.3445	3.5514	6.0571	12.129	31.160	131.76
	0.0365	0.2775	1.3458	4.9239	14.857	38.993	200.83	798.95	2.7101(3)	8.4240(3)	2.5890(4)	9.0922(4)
0.1	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003
	1.0761	1.1392	1.2265	1.3438	1.4994	1.7053	2.3482	3.5574	6.0680	12.153	31.230	132.14
	0.0370	0.2796	1.3522	4.9404	14.894	39.068	201.09	799.73	2.7122(3)	8.4299(3)	2.5908(4)	9.1005(4)
0.3	0.0027	0.0027	0.0027	0.0027	0.0027	0.0027	0.0027	0.0027	0.0027	0.0027	0.0027	0.0027
	1.0803	1.1453	1.2340	1.3530	1.5104	1.7188	2.3691	3.5925	6.1347	12.304	31.688	134.75
	0.0414	0.2975	1.4067	5.0783	15.201	39.693	203.23	806.03	2.7295(3)	8.4777(3)	2.6056(4)	9.1679(4)
0.5	0.0073	0.0074	0.0075	0.0075	0.0076	0.0076	0.0076	0.0076	0.0076	0.0076	0.0076	0.0076
	1.0853	1.1526	1.2440	1.3657	1.5265	1.7390	2.4018	3.6495	6.2459	12.563	32.502	139.65
	0.0527	0.3398	1.5295	5.3795	15.859	41.011	207.68	819.01	2.7650(3)	8.5754(3)	2.6359(4)	9.3067(4)
1.0	0.0249	0.0281	0.0295	0.0302	0.0307	0.0309	0.0313	0.0315	0.0317	0.0319	0.0322	0.0328
	1.0789	1.1595	1.2632	1.3974	1.5720	1.8012	2.5138	3.8590	6.6797	13.632	36.085	163.56
	0.1069	0.3047	2.2947	7.1843	19.648	48.369	231.41	906.49	2.9466(3)	9.0729(3)	2.7911(4)	1.0036(5)
1.5	0.0367	0.0524	0.0607	0.0654	0.0684	0.0704	0.0730	0.0747	0.0763	0.0780	0.0804	0.0864
	1.0410	1.1314	1.2509	1.4029	1.5977	1.8511	2.6361	4.1268	7.2994	15.318	42.403	214.52
	−0.0575	0.7980	3.6149	10.856	27.667	63.950	280.35	1.0219(3)	3.3050(3)	1.0051(4)	3.1009(4)	1.1597(5)
2.0	0.0314	0.0657	0.0893	0.1047	0.1151	0.1225	0.1328	0.1402	0.1469	0.1547	0.1668	0.2007
	1.0009	1.0731	1.1956	1.3601	1.5736	1.8518	2.7182	4.3873	8.0327	17.641	52.693	327.52
	−0.6420	−0.4823	3.3439	14.125	38.207	87.445	360.87	1.2489(3)	3.9095(3)	1.1722(4)	3.6509(4)	1.4767(5)
2.5	0.0169	0.0606	0.1033	0.1360	0.1603	0.1789	0.2064	0.2278	0.2485	0.2740	0.3180	0.4736
	0.9882	1.0153	1.1145	1.2721	1.4886	1.7784	2.7021	4.5339	8.6946	20.355	68.092	597.39
	−0.1962	−3.7864	−2.6175	9.6236	41.271	106.96	460.17	1.5611(3)	4.7823(3)	1.4226(4)	4.5232(4)	2.0561(5)

TABLE III. (continued)

βk \ β/d	0.6	0.8	1.0	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4.0
3.0	0.0088	0.0428	0.0983	0.1500	0.1928	0.2281	0.2840	0.3311	0.3798	0.4443	0.5686	1.1084
	0.9982	0.9832	1.0380	1.1650	1.3609	1.6368	2.5538	4.4458	8.9453	22.439	84.756	901.17
	1.8898	−5.0535	−14.870	−10.796	20.168	96.440	528.75	1.8700(3)	5.7474(3)	1.7102(4)	5.4817(4)	1.9363(5)
3.5	0.0098	0.0245	0.0786	0.1443	0.2058	0.2603	0.3528	0.4363	0.5275	0.6552	0.9137	−1.3518
	1.0056	0.9816	0.9871	1.0682	1.2240	1.4614	2.2934	4.0759	8.4555	22.061	85.225	457.85
	0.6877	2.0351	−24.657	−46.265	−36.768	28.136	489.89	1.9939(3)	6.3227(3)	1.8614(4)	5.3729(4)	2.1597(4)
4.0	0.0108	0.0154	0.0538	0.1232	0.1988	0.2711	0.4023	0.5271	0.6679	0.8675	1.2471	−1.0575
	1.0010	0.9970	0.9681	0.9990	1.1051	1.2903	1.9837	3.5080	7.2589	18.529	61.732	167.70
	−4.3069	14.094	−15.744	−80.152	−123.53	−108.43	279.74	1.7493(3)	5.9698(3)	1.6850(4)	3.6131(4)	−3.2290(4)

TABLE IV. ρ, $\bar{C}^2$, and $\bar{Z}$ as functions of βk and β/d for $L=3$.

βk \ β/d	0.6	0.8	1.0	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4.0
0.01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	1.0529	1.0962	1.1549	1.2314	1.3291	1.4528	1.8057	2.3745	3.3239	4.9979	8.1821	14.904
	0.2543	3.4123	25.668	134.02	544.38	1.8412(3)	1.4302(4)	7.7896(4)	3.3412(5)	1.2124(6)	3.9111(6)	1.1665(7)
0.1	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
	1.0533	1.0967	1.1554	1.2320	1.3298	1.4536	1.8067	2.3759	3.3260	5.0011	8.1877	14.9148
	0.2561	3.4260	25.734	134.26	545.10	1.8431(3)	1.4312(4)	7.7933(4)	3.3424(5)	1.2128(6)	3.9120(6)	1.1667(7)
0.3	0.0009	0.0009	0.0009	0.0009	0.0009	0.0009	0.0009	0.0009	0.0009	0.0009	0.0009	0.0009
	1.0553	1.0991	1.1583	1.2353	1.3336	1.4580	1.8127	2.3843	3.3385	5.0212	8.2227	14.983
	0.2715	3.5399	26.279	136.24	551.01	1.8585(3)	1.4390(4)	7.8235(4)	3.3522(5)	1.2156(6)	3.9198(6)	1.1688(7)
0.5	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025
	1.0579	1.1026	1.1624	1.2402	1.3394	1.4648	1.8222	2.3980	3.3592	5.0548	8.2821	15.100
	0.3069	3.7857	27.422	140.32	563.12	1.8898(3)	1.4547(4)	7.8843(4)	3.3720(5)	1.2214(6)	3.9355(6)	1.1729(7)

TABLE IV. *(continued)*

βk \ β/d	0.6	0.8	1.0	1.2	1.4	1.6	2.0	2.4	2.8	3.2	3.6	4.0
1.0	0.0098	0.0100	0.0100	0.0101	0.0101	0.0101	0.0101	0.0101	0.0101	0.0101	0.0101	0.0101
	1.0622	1.1111	1.1746	1.2558	1.3586	1.4880	1.8560	2.4482	3.4374	5.1844	8.5159	15.573
	0.5855	5.3588	33.952	162.22	625.73	2.0482(3)	1.5322(4)	8.1795(4)	3.4673(5)	1.2490(6)	4.0102(6)	1.1926(7)
1.5	0.0202	0.0220	0.0225	0.0228	0.0228	0.0229	0.0229	0.0229	0.0229	0.0229	0.0229	0.0229
	1.0553	1.1131	1.1832	1.2704	1.3789	1.5146	1.8982	2.5145	3.5443	5.3670	8.8541	16.275
	1.2743	9.8235	50.377	211.65	756.65	2.3625(3)	1.6767(4)	8.7123(4)	3.6361(5)	1.2973(6)	4.1401(6)	1.2269(7)
2.0	0.0276	0.0361	0.0391	0.0403	0.0408	0.0411	0.0413	0.0414	0.0414	0.0414	0.0415	0.0415
	1.0331	1.1006	1.1812	1.2773	1.3943	1.5386	1.9429	2.5902	3.6727	5.5942	9.2882	17.203
	−0.0504	17.061	84.677	312.68	1.0083(3)	2.9322(3)	1.9175(4)	9.5576(4)	3.8962(5)	1.3704(6)	4.3345(6)	1.2778(7)
2.5	0.0260	0.0473	0.057	0.0614	0.0635	0.0645	0.0655	0.0659	0.0661	0.0662	0.0663	0.0664
	1.0061	1.0715	1.162	1.2695	1.3977	1.5532	1.9836	2.6688	3.8158	5.8604	9.8165	18.372
	−9.4132	10.622	127.93	483.49	1.4505(3)	3.9134(3)	2.3050(4)	1.0844(5)	4.2778(5)	1.4751(6)	4.6093(6)	1.3492(7)
3.0	0.0169	0.0500	0.0717	0.0832	0.0891	0.0924	0.0956	0.0969	0.0977	0.0981	0.0985	0.0989
	0.9919	1.0336	1.1247	1.2419	1.3822	1.5509	2.0121	2.7419	3.9653	6.1582	10.438	19.812
	−13.057	−49.620	106.96	664.95	2.0897(3)	5.4410(3)	2.9067(4)	1.2765(5)	4.8272(5)	1.6220(6)	4.9884(6)	1.4470(7)
3.5	0.0088	0.0427	0.0785	0.1014	0.1148	0.1228	0.1309	0.1346	0.1367	0.1382	0.1393	0.1404
	0.9951	1.0[illegible]3	1.0764	1.1947	1.3438	1.5249	2.0187	2.7979	4.1082	6.4749	11.149	21.556
	30.1387	−164.11	−134.03	608.36	2.6833(3)	7.3904(3)	3.7794(4)	1.5548(5)	5.6059(5)	1.8259(6)	5.5067(6)	1.5797(7)
4.0	0.0072	0.0297	0.0749	0.1118	0.1365	0.1524	0.1699	0.1786	0.1837	0.1873	0.1904	0.1932
	1.0031	0.9858	1.0293	1.1350	1.2841	1.4723	1.9941	2.8227	4.2256	6.7879	11.928	23.630
	63.582	−171.14	−701.75	−147.72	2.5295(3)	8.9918(3)	4.8996(4)	1.9367(5)	6.6798(5)	2.1046(6)	6.2097(6)	1.7594(7)

effective interaction does not have a $1/r^4$ component for small r, the choice of a $U(r)$ which does have the $1/r^4$ component for small r leads to a V which has a strong compensating $1/r^4$ component for small r. The effects of V will then be to give a rather rapid energy dependence to $\delta(k)$. We have therefore chosen our maximum value of β/d to be 4.0, so that d can be as small as $\sim \frac{1}{2}a_0$ for a small polarizability such as $\alpha_1/a_0^3 = \frac{9}{2}$ (that of hydrogen), and as large as $5a_0$ for a large polarizability of $\alpha_1/a_0^3 \approx 400$. (The best choice of d can be expected to increase with β, for a highly polarizable system will not generate a simple $1/r^4$ dependence except for large r.) On the other hand, the smallest value of β/d, for which the functions are tabulated, has been determined by the criterion that the Born approximation be accurate to better than 1% for $L=0$ and $L=1$ and to better than 3% for $L \geq 2$, for almost the entire range of βk, and never be much worse than that. For smaller values of β/d than those used here, the functions can rather easily be obtained numerically by evaluating the Born integrals of Appendix A. For values of kd sufficiently small such that the expansions of j_L and n_L are valid, one may directly use the expansions provided in Appendix A. In this domain, however, the original MERT expansion[1,2] in β^2 is valid.

The range of βk over which the functions are tabulated has been chosen to be $0 \leq \beta k \leq 4.0$, with intervals chosen for convenience in interpolation. The maximum value of βk includes the entire elastic region for almost all atomic species. Large values of β correspond generally to atoms with low-lying excited states, and we are concerned with elastic scattering. This leads to a reduction of the variation, from atom to atom, of the maximum value of βk required, and makes advantageous the choice of βk as one of the two dimensionless parameters in terms of which the data are presented.

If we use Eq. (3.2) rather than its inverse, we must [because of the presence of $\cot\delta(k)$] choose d such that $\eta(k) \neq \rho(k) \pmod{\pi}$ within the range of interest in k.[11] It follows that $\eta(k)$ and $\rho(k)$ must have, very roughly, the same k dependence within this range of interest. We see here again that the choice of d must bear some relation to the physical situation, lest V be so strongly attractive or repulsive that $\eta(k) - \rho(k)$ varies by π or more over the range of interest in k. We can go further, for, in the case of electron scattering, V will be attractive, at least for small r, and we therefore expect η to be greater than ρ, or δ to be positive. By the same argument, we expect δ to be negative for positron scattering. These expectations on the phase shifts lead to expectations on the most appropriate values of d. In any case, the values of β/d for which the functions have been tabulated are spaced so that one may examine the expansion for several cutoff distances d.

As L increases, the Born approximation becomes increasingly valid for ρ and $\tilde{C}$ but not for $\tilde{E}$ nor for $\tilde{Z}$. The Born approximation is nevertheless valid for large L in the sense that the functions ρ, $\tilde{C}$, and $\tilde{Z}$ that appear (explicitly or implicitly) in Eq. (3.2) can be replaced by their Born approximations, because for large L, the effect of $\tilde{Z}$ becomes negligible. That is, though $\tilde{Z}$ itself is increasing, and is not adequately given by the Born approximation, $\tilde{Z}$ does not increase as rapidly as the $\cot\delta$ term and can be neglected. The rapid rise in $\cot\delta$ follows from the fact that δ vanishes as k^{2L+1}. [δ is *not* simply the phase shift associated with a short-range potential, but the phase shift associated with a short-range potential in the presence of a long-range potential which we have assumed vanishes as $1/r^4$. That δ nevertheless vanishes as k^{2L+1} follows from Eq. (3.2) and the fact that $\tilde{C}$ and $\tilde{Z}$ approach constants as $k \to 0$.]

It was found for $L=3$ that for the entire range of β/d considered, ρ was independent of d to within 5% or else ρ was adequately given by the Born integral

$$\tan\rho \approx -\beta^2 k \int_d^\infty [j_L^2(kr)/r^2]\, dr.$$

(By the Born approximation we will mean the same integral but with limits 0 to ∞.) We took this to imply that for $L \geq 4$, η may be safely regarded as being equal to ρ, and thus in turn equal to the Born integral and to the Born approximation to within a few percent. In other words, short-range effects become negligible for $L \geq 4$ in the range of β/d considered and the Born approximation[2]

$$\tan\rho \approx \tfrac{1}{8}\pi(\beta k)^2 (L+\tfrac{3}{2})(L+\tfrac{1}{2})(L-\tfrac{1}{2}) \qquad (3.4)$$

should be adequate. It must be emphasized that we can tolerate a reasonable error in the use of (3.4) since contributions from $L \geq 4$ are already small compared with contributions from smaller values of L. We therefore terminated our tabulations with $L=3$.

B. General Description of Results

The general properties of the long-range functions are much more easily deduced from the figures than from the tables. The monotonicity of ρ for fixed k as a function of β/d, commented on earlier, is readily apparent. Note that for $L=0$, one bound state is introduced for some value of β/d between 1.4 and 1.6; the curves for $\rho(k)$ for $\beta/d = 3.6$ and 4.0 exhibit a Ramsauer-Townsend–like behavior.

For $L=1$ a bound state is introduced for some value of β/d between 2.8 and 3.2. For $L>0$, we have also plotted the first term in the Born expansion for ρ, given in Eq. (3.4). (Note incidentally that ρ is the only long-range function for which the Born approximation has a limit as $d \to 0$.)

One must of course be careful in the use of the tables or figures in regions in which the long-range functions vary rapidly, and in particular in regions of a singularity. We concentrate on the $L=0$ case because it is the most important and also the simplest to treat. We note that $\tilde{C}(0)=\infty$ for values of β and d for which $\rho(0)$ is an odd multiple of $\frac{1}{2}\pi$, i.e., for which $U(r)$ supports a bound state of zero energy. To understand this, we note that for $L=0$ and k very small, we have, from Eq. (2.2b),

$$f(k,r) \approx \tilde{C}(k)kr, \quad r<d, \tag{3.5}$$

while for r large but fixed, i.e., $r\to\infty$, $k\to 0$, $kr\to 0$, Eq. (2.2a) gives

$$f(k,r) \to \pm 1\ , \tag{3.6}$$

since $\rho(0)=\frac{1}{2}\pi(\text{mod}\ \pi)$ for a zero-energy bound state. Since $f(k,r)$ must be of the form of a function of r multiplied by a function of k for k sufficiently small, it follows from (3.5) and (3.6) that $\tilde{C}(k)k$ approaches a constant, that is, that $\tilde{C}(k)$ diverges as $1/k$ for the $L=0$, $E=0$ bound state.

Concerning the function $\tilde{Z}$, one notes that especially for large L and small values of β/d its behavior becomes quite wild as βk becomes appreciable. However, fortunately, it is exactly in this region that its magnitude relative to that of $\tilde{C}^2 k^{2L+1}\cot\delta$ becomes negligible, as discussed earlier.

4. AN ILLUSTRATIVE EXAMPLE

Although there is every reason to believe that accurate experimental data will be abundantly forthcoming in the near future, there seems, apart possibly from some rare-gas cases, to be very little accurate data now available on low-energy differential cross sections for electron scattering by neutral spherically symmetric atoms. We will therefore use the theoretically determined data for the $L=0$ phase shifts for $e^{\pm}$ scattering by hydrogen atoms at energies from zero up to the threshold for excitation for e^-H and up to the threshold for pick up for e^+H. A number of reliable calculations exist; the very best is probably the variational calculation of Schwartz.[12]

The effects of long-range forces are significant but not dramatic for hydrogen, for $\alpha_1/a_0^3=\frac{9}{2}$ represents a rather small polarizability. The effects have in fact been treated adequately[4] by the explicit approximations which include effects through terms of order β^2. The present study should be illuminating nevertheless, largely because it very clearly exhibits the influence of the choice of d on the analysis, and the accuracy of the variational calculation[12] enables one to study small effects.

There are three separate problems: singlet e^-H, triplet e^-H, and e^+H scattering. The corresponding phase shifts will be denoted by η_s^-, η_t^-, and η^+, respectively. The values of ρ and of the three phase shifts of Schwartz are plotted in Fig. 5. Using the known values of η for each case, and the calculated long-range functions (which are the same for all three cases), we plot $\tilde{F}'(k^2)$, the left-hand side of Eq. (3.2), as a function of $(ka_0)^2$ for a number of values of d.[13] The most desirable choice of d, which may or may not be possible, is one for which the curve obtained is effectively a straight line, i.e., for which we obtain good convergence using only the first two terms on the (far) right-hand side of Eq. (3.2). It would of course be perfectly possible to obtain useful predictions, given enough data, if we could match the curve to a parabola or higher-order polynomial in k^2.

A. Singlet e^-H $L=0$ Scattering

A plot of the left-hand side of (3.2) versus $(ka_0)^2$ for various values of d is given in Fig. 6. Even for $d=\infty$ [for which $\rho=\tilde{h}=0$, $\delta=\eta$, $\tilde{C}=1$, and we return to the usual (unmodified) effective-range theory], we obtain essentially a straight line except in the immediate neighborhood of $k=0$, where

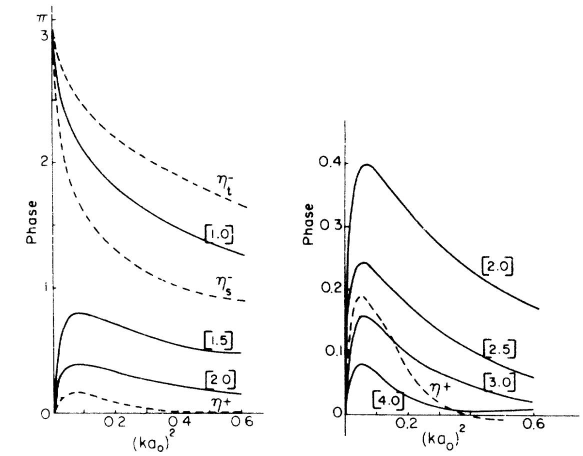

FIG. 5. The dashed curves represent plots of the three phase shifts η^+(e^+H scattering), η_s^-(e^-H singlet scattering), and η_t^- (e^-H triplet scattering), as functions of $(ka_0)^2$. The solid curves represent plots of the long-range phase shift ρ as a function of $(ka_0)^2$ for various choices of the cutoff distance d (the values in square brackets); ρ is the same for all three cases.

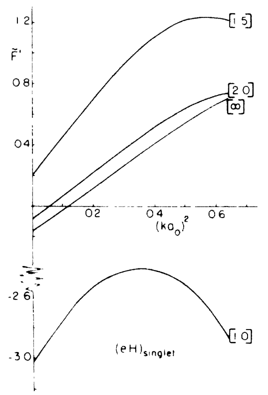

FIG. 6. Plot of the analytic function $\bar{F}'(k^2)$, defined by Eq. (3.2), as a function of $(ka_0)^2$, for various choices of d (the values in square brackets), for electron-hydrogen singlet scattering.

an expanded curve shows a slight curvature. (This effect will be more clearly exhibited in the triplet case to be treated next.) Even for d as large as $10a_0$, we obtain an effectively straight line which reproduces Schwartz's results to within the accuracy of those results, i.e., we adequately account for the long-range polarization effects. For smaller values of d, $d \approx 2.5a_0$, the curve remains straight for small ka_0, but begins to curve over for larger values of ka_0. The curving over becomes more pronounced as d is reduced still further. We are here seeing the effect described in Sec. 1, in which we are decomposing $V+U$ in such a way that U is overly attractive and therefore, to compensate, V is overly repulsive for small r. V therefore generates a rapidly varying energy dependence.

Note that the better choices of d are those for which $\eta > \rho$, in agreement with the expectation that V is basically attractive.

B. Triplet e^-H $L = 0$ Scattering

This case is more interesting from our point of view since long-range effects are more significant, the curvature near $k=0$ in the curve $k\cot\eta$ (which corresponds to $d=\infty$) being much more pronounced. (See Fig. 7.) The curve is not now so straight for d as large as $10a_0$, but we get an excellent straight line for all values of d in the range $1.5 \lesssim d/a_0 \lesssim 6$. Thus we were given data at only 3 points, the third point to check consistency, at say $ka_0 = 0.4$, 0.5, and 0.6, we could predict $\eta(k)$ clear down to $ka_0 = 0$. Once again the curves for small d begin to curve over for large $(ka_0)^2$ though it is not as clear as on Fig. 6 since we do not in Fig. 7 include as large values of $(ka_0)^2$. However, since $\eta_t^- > \eta_s^-$ and since the curvature becomes transparent for ρ approximating η, it will not happen in the triplet case until smaller values of d are chosen than those for which it happened in the singlet case.

The fact that the choice $d = 10a_0$ does not lead to a straight line is an example of the situation discussed earlier in which long-range effects have been formally extracted but for which a simple expansion will not work. The curve for large d really does have a straight-line behavior for extremely small $(ka_0)^2$. The curvature as $(ka_0)^2$ becomes a little larger results from V, and the straight-line behavior for larger values of $(ka_0)^2$ is the usual behavior for a short-range potential when the effective-range approximation is adequate. The two straight-line segments of the curve for large d thus have different origins, and the linear extrapolation of the short-range (large k) segment leads to incorrect predictions for $\eta(k)$ for small k.

C. e^+H $L = 0$ Scattering

This is a more revealing case than the previous two since η becomes negative. The expansion of $k\cot\eta$ will of course not converge beyond the point at which η passes through zero. Indeed the $k\cot\eta$ curve shown in Fig. 8 is not well approximated by a straight line for any reasonable range of values of $(ka_0)^2$. Referring to Fig. 5 we note that the curve for η crosses any curve for ρ for which $d \geqslant 3a_0$ at a value of $(ka_0)^2$ smaller than the value at which η assumes the value zero. It follows that for $d \geqslant 3a_0$ the region of convergence of the function $\bar{F}'(k^2)$ is even smaller than the region of convergence of $k\cot\eta$. It seems reasonable to choose d such that $\eta < \rho$, since $\bar{F}'(k^2)$ will then have an increased range of convergence. Furthermore, we expect V to be repulsive, at least for small r, and this also leads us to expect a good choice of d to be one for which $\eta < \rho$. Indeed we see from Fig. 8 that for $d = a_0$, for which ρ is

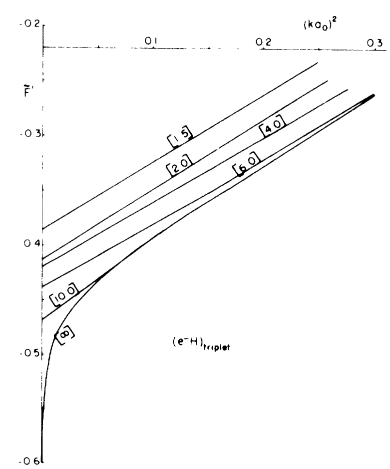

FIG. 7. Same caption as for Fig. 6, but for e^-H triplet rather than e^-H singlet scattering.

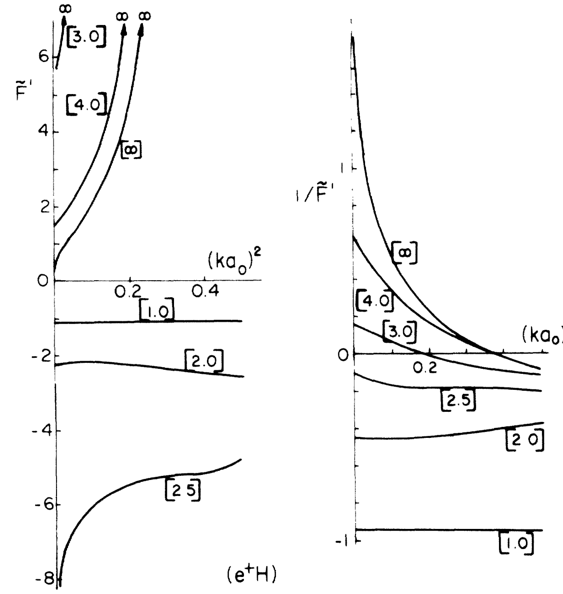

FIG. 8. Same caption as for Fig. 6, but for e^+H scattering rather than e^-H singlet scattering.

substantially bigger than η, a fairly good straight line is obtained.

In this example, it seems that there is not too much advantage to plotting $1/\tilde{F}'(k^2)$ rather than $\tilde{F}'(k^2)$, though one does at least convert the singular curves to nonsingular curves.

5. DISCUSSION

The approximate forms of MERT, expansions in powers of k and of $\ln k$, are valid for k "sufficiently small," or, to be a little less imprecise, for $1/k$ large compared with any of the characteristic lengths for the scattering problem, including β, d, and the scattering length. The severe limitation on k thereby introduced for large values of β is eliminated by the present approach; βk can be arbitrarily large. Note too that the expansion of $\tilde{F}(k^2)$ involves a smaller number of terms to a given power of k than does the expansion of $\tan\eta$.

APPENDIX A

In this appendix we give a derivation of MERT in closed form, good to order β^2, which is somewhat simpler than previous derivations in that it does not require a knowledge of the properties of Mathieu functions nor of the theory of asymptotic expansions. Furthermore, for $L > 0$ our result is a slight improvement over the original result in that it gives explicitly an additional term in the expansion in k.

From Eq. (1.1), we have the exact relation

$$\tan\eta = \frac{(\tilde{F}-\tilde{h})\tan\rho + \tilde{C}^2 k^{2L+1}}{(\tilde{F}-\tilde{h}) - \tilde{C}^2 k^{2L+1}\tan\rho} . \qquad \text{(A1)}$$

The long-range functions can be obtained directly from the integral equations given in the Appendix of I. Using Eq. (1.5), we have

$$\sin\rho = (\beta^2/k)\int r^{-4}\bar{j}\, f(k,r)\,dr , \qquad \text{(A2a)}$$

$$\tilde{C} = \cos\rho - (\beta^2/k)\int r^{-4}\bar{n} f(k,r)\,dr, \qquad \text{(A2b)}$$

$$\tilde{E} = \sin\rho - (\beta^2/k)\int r^{-4}\bar{n} g(k,r)\,dr , \qquad \text{(A2c)}$$

where all the integrals are from d to ∞ and where $\bar{j} \equiv krj_L(kr)$ and $\bar{n} \equiv krn_L(kr)$. Introducing the symbol

$$I(G,H) = \int_{kd}^{\infty}[G_L(x)H_L(x)/x^2]\,dx , \qquad \text{(A3)}$$

where G and H are arbitrary, we find in the Born approximation, that is, dropping terms of order β^4,

$$\tan\rho \approx (\beta k)^2 I(j,j) , \qquad \text{(A4a)}$$

$$\tilde{C} \approx 1 - (\beta k)^2 I(j,n), \qquad \text{(A4b)}$$

$$\tilde{E} \approx -\sin\rho + (\beta k)^2 I(n,n) . \qquad \text{(A4c)}$$

The integrals I are all finite, with an integrand $q(x)$ which has a known expansion for $0 \leqslant x \leqslant x_0$ for some x_0. We denote the closed form by $q(x)$, and its expansion by $q_+(x) + q_-(x)$, where $q_-(x)$ and $q_+(x)$ are the partial sums over negative and positive powers of x, respectively. Writing

$$I = \int_0^{x_0}[q(x) - q_-(x)]\,dx - \int_0^{kd} q_+(x)\,dx + \int_{kd}^{x_0} q_-(x)\,dx + \int_{x_0}^{\infty} q(x)\,dx , \qquad \text{(A5)}$$

and using the expansion of the integrals in Eqs. (A4), we obtain

$$\tan\rho = (\beta k)^2\left(\pi b(L) - \frac{(kd)^{2L-1}}{(2L-1)B(+L)} + O(k^{2L+1})\right) + O(\beta^4) , \qquad \text{(A6a)}$$

$$\tilde{C} = 1 + (\beta/d)^2/2(2L+1) - 2b(L)(\beta k)^2\ln(kd) + O(k^2,\beta^4) , \qquad \text{(A6b)}$$

$$\tilde{E} = -\tan\rho + (\beta k)^2\left(\frac{B(-L)(kd)^{-2L-3}}{2L+3} + D(L)(kd)^{-2L-1} + O(k^{-2L+1})\right) + O(\beta)^4 , \qquad \text{(A6c)}$$

where

$$b(L) \equiv [(2L+3)(2L+1)(2L-1)]^{-1}, \qquad (A7a)$$

$$B(\pm L) \equiv [(2L \pm 1)!!]^2, \qquad (A7b)$$

$$D(L) = (2L-3)!!(2L-1)!!/(2L+1), \qquad (A7c)$$

$$(2n-1)!! = (2^n/\pi^{1/2})\Gamma(n+\tfrac{1}{2})$$

and, in particular, $(-1)!! = 1$ and $(-3)!! = -1$. After some straightforward algebra, one finds, using the Kronecker δ function δ_{L0},

$$\tilde{h} = D(L)(\beta k)^2/d^{2L+1} + \delta_{L0}[-(\beta k)^2 d^{-1} + 0(k^3)] + 0(\beta^4, k^4). \qquad (A8)$$

To complete the analysis, we expand the denominator of Eq. (A1) and find

$$\tan\eta = \tan\rho + (k^{2L+1}\tilde{C}^2/\tilde{F}) \times [1 + (\tilde{h} + k^{2L+1}\tan\rho)/\tilde{F}] + 0(\beta^4), \qquad (A9)$$

a relationship valid to all orders in k. Making use of Eqs. (A6) and expanding in powers of k, we obtain

$$\tan\eta = \pi b(L)(\beta k)^2 - k^{2L+1}\left[\frac{d^{2L-1}\beta^2}{(2L-1)B(+L)} + \tilde{A}\left(1 + \frac{(\beta/d)^2}{2L+1}\right)\right] + O[k^{2L+3}\ln(kd)], \quad \text{for } L > 0, \qquad (A10)$$

and $\tan\eta = -kA^* - \frac{1}{3}\pi(\beta k)^2 - \frac{4}{3}(\beta k)^2\tilde{A}k\ln(kd) + O(k^2)$, for $L = 0$, (A11)

where A^*, defined by

$$A^* \equiv \tilde{A}[1 + (\beta/d)^2] - (\beta^2/d), \qquad (A12)$$

differs from A by terms of order β^4. We can rewrite Eq. (A11) as

$$k\cot\eta = -1/A - \pi\beta^2 k/3A^2 + 4\beta^2 k^2 \ln(kd)/3A + O(k^2\beta^4). \qquad (A13)$$

The above approach can obviously be readily adapted to yield similar formulas for any long-range interaction. Note that the cutoff parameter d appears explicitly in the formulas just derived. To understand this, recall that we have assumed a range of k such that $kd \ll 1$.

---

*The work reported in this article was sponsored by the U. S. Office of Naval Research and the Advanced Research Projects Agency under Contract Nos. Nonr-285(49) and NRO12-109.

†Portions of this article represent a part of the work submitted by R. Oppenheim Berger in partial fulfillment of the requirements of the degree of Doctor of Philosophy at New York University, granted in February, 1965.

‡ Present address: Physics Department, University of California, Berkeley, Calif.

[1]L. Spruch, T. F. O'Malley, and L. Rosenberg, Phys. Rev. Letters 5, 375 (1960).

[2]T. F. O'Malley, L. Spruch, and L. Rosenberg, J. Math. Phys. 2, 491 (1961).

[3]For a more mathematical approach, see B. R. Levy and J. B. Keller, J. Math. Phys. 4, 54 (1963).

[4]T. F. O'Malley, L. Spruch, and L. Rosenberg, Phys. Rev. 125, 1300 (1962).

[5]T. F. O'Malley, Phys. Rev. 130, 1020 (1963).

[6]R. Oppenheim Berger, T. F. O'Malley, and L. Spruch, Phys. Rev. 137, A1068 (1965). This paper will be referred to as I.

[7]R. Oppenheim Berger and L. Spruch, Phys. Rev. 138, B1106 (1965).

[8]We use the argument k for simplicity. The functions also depend upon L, α_1, and the details of the modification of $U(r)$ for small r.

[9]The quantities $\tilde{A}$, $\tilde{r}_0$, ..., on the right-hand side of Eq. (1.3) were unfortunately written without tildes in I. To distinguish between the usual scattering length A, the usual effective range r_0, ..., which appear in the usual effective-range theory appropriate to short-range forces, and the quantities appropriate to long-range forces, we insert tildes on the latter quantities.

[10]A. Dalgarno and R. McCarroll, Proc. Roy. Soc. (London) A237, 383 (1956); M. H. Mittleman and K. M. Watson, Phys. Rev. 113, 198 (1959); M. H. Mittleman, Ann. Phys. (N. Y.) 14, 94 (1961); C. Kleinman, Y. Hahn, and L. Spruch, Phys. Rev. 165, 53 (1968).

[11]An absolute definition of $\rho(k)$ is a simple matter since it is the phase shift associated with potential scattering. The absolute definition of η, arising as it does in scattering by a compound system, is a much more delicate matter. [See Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. 134, B397 (1964).] An absolute definition is not necessary for present purposes, but since we are concerned here with η as a function of k, and not as a function of the strength of a potential, it will simplify the discussion if we define $\eta(k)$ to be continuous in k.

[12]C. Schwartz, Phys. Rev. 124, 1468 (1961).

[13]The work presented in this section was done before the tables were prepared. We simply chose a number of values of d (the long-range functions were then evaluated at these values of d) rather than choosing d to give specified values of β/d. Apart from this trivial point, the study presented in this section is identical in form to a study based on direct use of the tables.