Low-energy scattering by nonspherically symmetric targets

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A number of studies have been made over the years of the near-threshold behavior of phase shifts for the scattering of electrons by spherically symmetric atomic targets, allowing for the important effect of long-range polarization forces. For targets that are not spherically symmetric, the theory must be extended to account for a superposition of asymptotic power-law potentials, including an inverse-cube potential for targets with a permanent quadrupole moment, which couple the various channels. Such an extension is described here. A degenerate perturbation theory, extended to arbitrarily high orders through the introduction of continued-fraction representations, is developed for the construction of the asymptotic states. Results of illustrative numerical calculations are reported. The asymptotic solutions, along with a variational principle for the reaction matrix, provide the basis for a modified effective-range theory. A minimum principle, valid at threshold, is available for the calculation of scattering length and effective range matrices. [S1050-2947(99)04402-9]

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I. INTRODUCTION

The effective long-range interaction between an electron and an atomic system may be represented as a superposition of inverse power-law potentials and this leads to modifications [1] of the energy dependence of low-energy scattering parameters found for short-range potentials [2]. For targets that lack spherical symmetry, the effective potential will, in general, have an angular dependence [3]. Some progress has been made in determining the threshold behavior of the (angle-dependent) scattering amplitude in such cases [4]. An alternative approach, based on a reduction of the Schrödinger equation to a set of coupled radial equations, appears to provide certain advantages (as noted in Ref. [4]) and is adopted here. For definiteness, and to focus on the essential features of the problem, a very specific model is considered. Two channels are involved, with identical threshold energies, and with orbital quantum numbers l_1 and $l_2=l_1+2$. The 2×2 potential matrix is assumed to have the asymptotic form $V \sim V^L$ for $r\to\infty$, where, for a neutral target,

$$-\frac{2m}{\hbar^2}V^L=\begin{pmatrix} r^{-4}\beta_4^{(1)^2} & r^{-3}\beta_3+r^{-4}\beta_4'^2 \\ r^{-3}\beta_3+r^{-4}\beta_4'^2 & r^{-4}\beta_4^{(2)^2}\end{pmatrix}, \qquad (1.1)$$

with real-valued parameters β_3, β_4', $\beta_4^{(1)}$, and $\beta_4^{(2)}$. It is not difficult to extend the theory to include components of the potential falling off as r^{-n}, with $n>4$.

A key element in any analysis of scattering in the presence of long-range interactions is the introduction of sufficiently accurate asymptotic solutions of the wave equation. A perturbation theory for single-channel scattering by a superposition of power-law potentials has been developed by Cavagnero [5]. The method can be extended in a number of ways [6]. An application to multichannel scattering in the absence of the off-diagonal r^{-4} component (that is, with $\beta_4'=0$) is straightforward and this provides the starting point for a derivation of a modified effective range theory for this class of scattering systems [7]. Somewhat surprisingly, inclusion of the $r^{-4}\beta_4'^2$ component in Eq. (1.1) leads to the appearance of a degeneracy. As described below in Sec II A, this requires a modification of the original method of Ref. [5] for its removal, involving the diagonalization of an effective Hamiltonian in a manner similar to that employed in standard degenerate perturbation theory, although here the eigenvalue problem is a nonlinear one. A more elaborate version of the perturbation theory for the asymptotic states is developed in Sec. II B, involving partial summations of the series expansion expressed in terms of continued fractions. A diagrammatic aid to the calculation of the level shifts that arise in this formulation is described; the method is illustrated with numerical evaluations of polarization eigenphases and mixing parameters in second order. The remarkable formal similarity of this procedure with that arising in the theory of electronic and atomic interactions with a radiation field [8,9] is demonstrated. With only the inverse-cube potential present, the continued-fraction representation can be developed in greater detail, as shown in the Appendix. A similar treatment, accompanied by a numerical illustration, is presented there for the diagonal r^{-4} potential.

The low-energy behavior of the regular and irregular solutions of the wave equation in the presence of the potential V^L determines the form of the threshold singularities of the scattering matrix, as described in Sec. III. Here one sees how the standard Wigner threshold law [2], developed in the context of nuclear reaction theory, is modified. A description of the scattering formalism appropriate to this system, along with a demonstration of unitarity, is included in this discussion.

With threshold singularities removed, a modified reaction matrix may be defined that varies slowly with energy. The introduction, in Sec. III C, of a variational principle for the modified reaction matrix not only confirms this smooth energy dependence near threshold but provides a means for finding accurate approximations for the parameters—the scattering length and effective range matrices—that appear in the effective range expansion of the reaction matrix. It is observed that for diagonal elements of the scattering length matrix the variational principle is, in fact, a minimum prin-

ciple, a property offering clear calculational advantages. Results reported here are summarized in Sec. IV.

II. ASYMPTOTIC STATES

A. Almost-degenerate perturbation theory

The radial Schrödinger equation considered here takes the form of two coupled equations with the matrix form $L\Psi=0$, where, in atomic units,

$$L_{ji}=-\frac{1}{2}\left[\frac{d^2}{dr^2}+k^2-l_j(l_j+1)/r^2\right]\delta_{ji}+V_{ji}, \quad i,j=1,2, \tag{2.1}$$

with $l_2=l_1+2$; the energy is $k^2/2$. We look for asymptotic solutions in which the (real, symmetric) matrix V is replaced by the long-range component V^L shown in Eq. (1.1). Starting with the regular solution, we define $z=kr$ and write $f_{ji}(z)=C_i(\pi z/2)^{1/2}m_{ji}(z)$, where C_i is a normalization factor to be determined. The matrix m is then seen to satisfy

$$\left[z^2\frac{d^2}{dz^2}+z\frac{d}{dz}+z^2-\left(l_j+\frac{1}{2}\right)^2\right]m_{ji}(z) = -\left(\frac{\Delta_3}{z}+\frac{\Delta_4}{z^2}\right)m_{j\bar{i}}(z)-\frac{D_j}{z^2}m_{ji}(z). \tag{2.2}$$

Here we have defined the dimensionless parameters $\Delta_3=\beta_3 k$, $\Delta_4=(\beta_4' k)^2$, and $D_j=(\beta_4^{(j)}k)^2$, and have let the symbol $\bar{j}$ take the value 2 for $j=1$ and 1 for $j=2$. We seek an approximate solution in the form of a perturbation expansion

$$m_{ji}=\sum_{n=0}^{\infty} m_{ji}^{(n)}; \tag{2.3}$$

with Δ_3 treated as a parameter of first order and Δ_4 and D_j as quantities of second order, the nth term in the expansion is of order n. The lowest-order solution is assumed to be proportional to the regular Bessel function; we have

$$m_{ji}^{(0)}(z)=a_{ji}J_{\eta_{ji}+1/2}(z), \tag{2.4a}$$

where

$$\eta_{ji}=l_j-(2/\pi)\delta_i, \tag{2.4b}$$

with the phase δ_i and the matrix a_{ji} to be determined. [An identical procedure is followed in the construction of the irregular solution of Eq. (2.2), but with the regular Bessel function $J_\nu(z)$ replaced everywhere by the Neumann function $N_\nu(z)$.] Substituting the first-order approximation $m_{ji}\cong m_{ji}^{(0)}+m_{ji}^{(1)}$ into Eq. (2.2), we find, with the aid of the recurrence relation $z^{-1}J_{\eta+1/2}(z)=(2\eta+1)^{-1}[J_{\eta+3/2}(z)+J_{\eta-1/2}(z)]$, that

$$m_{ji}^{(1)}(z)=[\alpha_{ji}^{(1)}J_{\eta_{ji}^{-}+3/2}(z)+\beta_{ji}^{(1)}J_{\eta_{ji}^{-}-1/2}(z)], \tag{2.5a}$$

with

$$\alpha_{ji}^{(1)}=a_{j\bar{i}}\Delta_3(2\eta_{ji}^{-}+1)^{-1}[(l_j+\tfrac{1}{2})^2-(\eta_{ji}^{-}+\tfrac{3}{2})^2]^{-1},$$

$$\beta_{ji}^{(1)}=a_{j\bar{i}}\Delta_3(2\eta_{ji}^{-}+1)^{-1}[(l_j+\tfrac{1}{2})^2-(\eta_{ji}^{-}-\tfrac{1}{2})^2]^{-1}. \tag{2.5b}$$

At this stage, in the absence of singularities, we would have $a_{ji}=\delta_{ji}$ and $\delta_i=0$. However, a straightforward extension of this iteration procedure to second order would lead to near-singularity difficulties owing to the appearance of small denominators of the form $(l_1+\frac{1}{2})^2-(\eta_{2i}-\frac{3}{2})^2$ and $(l_2+\frac{1}{2})^2-(\eta_{1i}+\frac{5}{2})^2$. To surmount this problem, we isolate the potentially troublesome terms arising in the iteration procedure by making use of the relations $J_{\eta_{1i}+5/2}=J_{\eta_{2i}+1/2}$ and $J_{\eta_{2i}-3/2}=J_{\eta_{1i}+1/2}$ and equating to zero the coefficients of the terms proportional to $J_{\eta_{1i}+1/2}$ and $J_{\eta_{2i}+1/2}$. In this way we arrive at coupled equations of the form

$$[(\eta_{ji}+\tfrac{1}{2})^2-(l_j+\tfrac{1}{2})^2]a_{ji}+\sum_{j'=1}^{2}\Gamma_{jj'}a_{j'i}=0. \tag{2.6}$$

In a given order, the effective potential matrix Γ, free of near-singularities, may be determined; one then searches for two distinct values, δ_1 and δ_2, of the phase parameter allowing for a solution of Eq. (2.6) and providing values for the ratios a_{2i}/a_{1i}. The matrix a_{ji} is then fixed by the normalization condition $a_{1i}^2+a_{2i}^2=1$. The results of this type of calculation will now be described in second order, where only two solutions are possible. To choose the appropriate solutions in higher orders, one requires that they merge smoothly with the second-order solutions in the limit of small coupling parameters.

The off-diagonal elements of the second-order Γ matrix are found to be

$$\Gamma_{21}=\Delta_4(2\eta_{1i}+1)^{-1}(2\eta_{1i}+3)^{-1} \tag{2.7a}$$

and

$$\Gamma_{12}=\Delta_4(2\eta_{2i}+1)^{-1}(2\eta_{2i}-1)^{-1}. \tag{2.7b}$$

It will be convenient to have available a diagrammatic representation of the terms appearing in the perturbation expansion; once a set of rules are specified higher-order terms may be written down quite readily. To make use of familiar concepts we may envision (somewhat formally) an infinite set of ''states'' associated with channel 1, labeled as $(1,m)$, where $m=0,\pm1,\pm2,...$, and similarly for states $(2,m)$ belonging to channel 2. Then Γ_{21} may be thought of as the amplitude for a transition between states (1,0) and (2,0), with Γ_{12} representing the reverse transition. The diagrams associated with Eqs. (2.7a) and (2.7b) appear in Figs. 1(a) and 1(b), respectively. They represent the effect of the off-diagonal $\Delta_4 z^{-2}$ interaction in Eq. (2.2). Each factor z^{-1} contributes a factor $[2(\eta_{ji}+m)+1]^{-1}$, where the indices j and m correspond to the state from which the interaction originates, as indicated by the position of the filled circle in the diagrams.

The (second-order) matrix element Γ_{11} (playing the role of a level-shift interaction) is generated by the combination of the diagonal $D_1 z^{-2}$ term in Eq. (2.2) and the off-diagonal $\Delta_3 z^{-1}$ taken in second order. The explicit form is

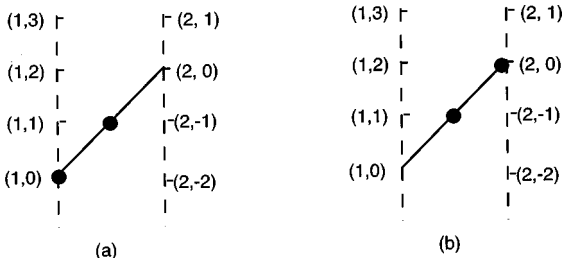

FIG. 1. Off-diagonal elements of the level-shift matrix in second order, given in Eqs. (2.7a) and (2.7b), are represented in diagrams (a) and (b), respectively.

$$\Gamma_{11}=D_1(2\eta_{1i}+1)^{-1}[(2\eta_{1i}+3)^{-1}+(2\eta_{1i}-1)^{-1}]$$
$$+\Delta_3^2(2\eta_{1i}+1)^{-1}\{[(l_2+\tfrac{1}{2})^2$$
$$-(\eta_{2i}-\tfrac{1}{2})^2]^{-1}(2\eta_{2i}-1)^{-1}$$
$$+[(l_2+\tfrac{1}{2})^2-(\eta_{2i}-\tfrac{5}{2})^2]^{-1}(2\eta_{2i}-5)^{-1}\}. \quad (2.8)$$

The two diagrams associated with the $D_1 z^{-2}$ interaction are shown in Figs. 2(a) and 2(b). The iterated $\Delta_3 z^{-1}$ interaction leads to a sum of two terms corresponding to the diagrams in Figs. 2(c) and 2(d). Figure 2(c), for example, is interpreted (in conformity with the language of ''states'' and ''transitions'' adopted here) as a sequence consisting of a transition $(1,0)\rightarrow(2,-1)$, followed by propagation in state $(2,-1)$—this is represented diagrammatically as an open circle—and then the reverse transition back to the reference state (1,0). In Fig. 2(d) the first transition is $(1,0)\rightarrow(2,-3)$, followed by propagation in state $(2,-3)$ and then a transition back to the reference state. In general, a ''propagator'' in state (j,m) is represented as $[(l_j+\frac{1}{2})^2-(\eta_{ji}+m+\frac{1}{2})^2]^{-1}$, with $(l_j+\frac{1}{2})^2$ playing the role of the total energy in channel j, while the term $(\eta_{ji}+m+\frac{1}{2})^2$ may be thought of as the ''kinetic energy'' in state (j,m). (This analogy with nonrelativistic scattering theory, while it may appear forced, can be developed much further in a useful way, as will be shown below in Sec. II B in connection with a discussion of diagram summation methods.) The expression for Γ_{22}, as well as for each matrix element in higher orders, may be written down directly following the diagrammatic rules just described. Similar rules apply to the construction of the functions $m_{ji}^{(n)}(z)$ appearing in the expansion shown in Eq. (2.3), as will be discussed further below.

The (normalized) matrix a in second order is orthogonal, a property that may be understood in terms of the unitarity

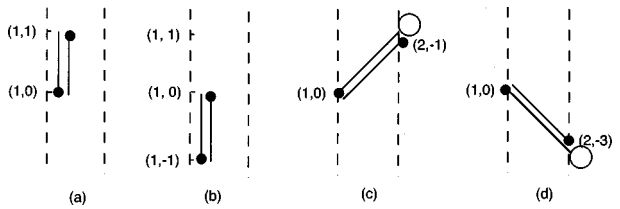

FIG. 2. Diagrams representing a diagonal element of the level-shift matrix in second order, as given in Eq. (2.8). The first two terms in that equation are represented in (a) and (b) and the second two terms are represented in (c) and (d). Interactions and propagators may be read off from the positions of the filled and open circles in the diagrams using rules given in the text.

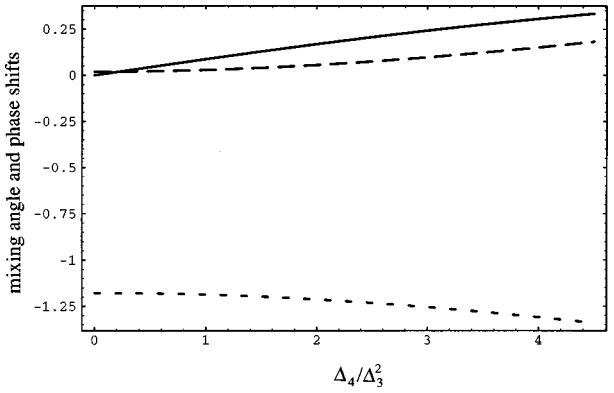

FIG. 3. Plots of the mixing angle ε (solid curve) and scaled polarization phases δ_1/Δ_3^2 (short-dashed curve) and δ_2/Δ_3^2 (long-dashed curve) as functions of Δ_4/Δ_3^2 for $l_1=0$, with strength parameters D_1, D_2, and Δ_3^2 all taken to be equal. The notation is that of Sec. II of the text.

condition for scattering in the field of the long-range potential as discussed below in Sec. III. It may, therefore, be represented as

$$a=\begin{pmatrix}\cos\varepsilon & \sin\varepsilon\\ -\sin\varepsilon & \cos\varepsilon\end{pmatrix}. \quad (2.9)$$

The mixing angle ε vanishes in the limit $\Delta_4=0$ [10]. As a numerical illustration, the mixing angle is plotted as the solid curve in Fig. 3 for $l_1=0$ over a range of values of the ratio Δ_4/Δ_3^2 with $D_1=D_2=\Delta_3^2$. We have also calculated, for the same choices of strength parameters, the phases δ_i defined earlier in Eq. (2.4b). The short- and long-dashed curves represent δ_1/Δ_3^2 and δ_2/Δ_3^2, respectively [11].

Terms in the perturbative expansion of the wave function may be constructed most easily using diagrammatic rules of the type just described; with near-singularities having been accounted for, transitions to states (1,0) and (2,0) are to be omitted in the determination of the functions $m_{ji}^{(n)}$. Thus in second order we have, for example,

$$m_{2i}^{(2)}=\alpha_{2i}^{(2)}J_{\eta_{2i}+5/2}(z)+\beta_{2i}^{(2)}J_{\eta_{2i}-3/2}(z)+\gamma_{2i}^{(2)}J_{\eta_{2i}-7/2}(z). \quad (2.10)$$

The coefficient $\alpha_{2i}^{(2)}$ is represented by the two diagrams in Fig. 4, from which its explicit form may be read off as

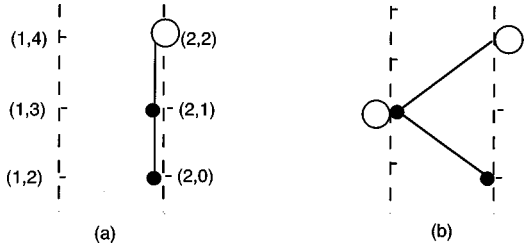

FIG. 4. The first and second terms in the expansion coefficient given in Eq. (2.11) are represented in diagrams (a) and (b), respectively.

$$\alpha_{2i}^{(2)}=a_{2i}(2\eta_{2i}+1)^{-1}\{D_2(2\eta_{2i}+3)^{-1}+\Delta_3^2[(l_1+\tfrac{1}{2})^2-(\eta_{1i}+\tfrac{7}{2})^2](2\eta_{1i}+7)^{-1}\}[(l_2+\tfrac{1}{2})^2-(\eta_{2i}+\tfrac{5}{2})^2]^{-1}. \tag{2.11}$$

Note that in constructing the diagrams for $m_{ji}^{(n)}$ we draw all possible sequences, of order n, of potential lines followed by propagator circles starting at one of the reference states and ending at a state (j,m), with $m\neq 0$. In the diagrams associated with Eq. (2.10), for example, the initial and terminal states are $(2,0)\rightarrow(2,2)$ for $\alpha_{2i}^{(2)}$, $(1,0)\rightarrow(2,-2)$ *and* $(2,0)\rightarrow(2,-2)$ for $\beta_{2i}^{(2)}$, and $(1,0)\rightarrow(2,-4)$ for $\gamma_{2i}^{(2)}$. Perturbation contributions of arbitrary order may be determined straightforwardly with the aid of these rules. As mentioned above, approximations to the irregular solution of Eq. (2.2) are obtained by the replacement of $J_\nu(z)$ with $N_\nu(z)$.

B. Level-shift reformulation

It is undoubtedly possible to arrive at the diagram summation procedure, now to be obtained, without setting up an analogy with the Green's-function formalism of scattering theory but doing so appears to be a helpful device. Thus we set up an abstract dynamical system in parallel with the one of actual interest and that enables us to make use of powerful operator methods. This is a heuristic procedure; all results obtained in this manner may be verified by reference to the original problem.

Consider a Hamiltonian matrix $h=h_0+u$ operating in a space of states $|j,m\rangle$ with the connection $|2,m\rangle=|1,m+2\rangle$. We set

$$u=\begin{pmatrix} D_1v^2 & \Delta_3v+\Delta_4v^2 \\ \Delta_3v+\Delta_4v^2 & D_2v^2 \end{pmatrix}, \tag{2.12}$$

with

$$v|j,m\rangle=[2(\eta_{ji}+m)+1]^{-1}[|j,m+1\rangle+|j,m-1\rangle] \tag{2.13}$$

and

$$h_0|j,m\rangle=(\eta_{ji}+m+\tfrac{1}{2})^2|j,m\rangle. \tag{2.14}$$

We seek a solution of the Schrödinger equation $(h-\lambda)|\psi_i\rangle=0$, where

$$\lambda=\begin{pmatrix} (l_1+\frac{1}{2})^2 & 0 \\ 0 & (l_2+\frac{1}{2})^2 \end{pmatrix} \tag{2.15}$$

and $\eta_{ji}=l_j-(2/\pi)\delta_i$, with the δ_i to be determined. Projection operators p and $q=1-p$ are introduced such that $p=p_{10}+p_{20}$ where, with the introduction of some notation that will also be useful later on,

$$p_{jm}\begin{pmatrix} |1m'\rangle \\ |2m'\rangle \end{pmatrix}=|\Phi_{jm}\rangle\delta_{mm'} \tag{2.16}$$

and

$$|\Phi_{1m}\rangle=\begin{pmatrix} |1,m\rangle \\ 0 \end{pmatrix},\quad |\Phi_{2m}\rangle=\begin{pmatrix} 0 \\ |2,m\rangle \end{pmatrix}. \tag{2.17}$$

We write $|\psi_i\rangle=(p+q)|\psi_i\rangle$ and set

$$p|\psi_i\rangle=\begin{pmatrix} a_{1i}|1,0\rangle \\ a_{2i}|2,0\rangle \end{pmatrix}. \tag{2.18}$$

A perturbation expansion based on this dynamics may be shown to reproduce that developed in Sec. II A for the original system. To introduce partial summation methods, we make use of standard projection-operator techniques [12] starting with the definition of the resolvent $g=[q(\lambda-h)q]^{-1}$, in terms of which we have the representations

$$q|\psi_i\rangle=gh|p\psi_i\rangle \tag{2.19a}$$

and

$$p(h_0-\lambda)|p\psi_i\rangle+p[u+ugu]|p\psi_i\rangle=0. \tag{2.19b}$$

A level-shift matrix Γ may now be defined by the relation

$$p_{j'0}[u+ugu]|\Phi_{j0}\rangle=|\Phi_{j'0}\rangle\Gamma_{j'j}. \tag{2.20}$$

Now, with the substitutions $|2,-2\rangle=|1,0\rangle$ and $|1,2\rangle=|2,0\rangle$, we may rewrite Eq. (2.19b) as a set of coupled equations for the coefficients a_{1i} and a_{2i}; they are precisely of the form shown in Eq. (2.6).

The matrix Γ may be determined perturbatively, thereby reproducing the results of Sec. II A, by introducing, into Eq. (2.20) the expansion

$$g=g_0+g_0ug_0+g_0ug_0ug_0+\cdots, \tag{2.21}$$

where $g_0=[q(\lambda-h_0)q]^{-1}$. We now describe a rearrangement of this series leading to a continued-fraction representation of the resolvent g [13]. Thus we define a modified resolvent from which a particular state $|j_a,m_a\rangle\equiv|a\rangle$ has been removed (in addition to the states $|1,0\rangle$ and $|2,0\rangle$ projected out of g). More precisely, let $p_a\equiv p_{j_am_a}$ be the projector onto the vector $|\Phi_{j_am_a}\rangle\equiv|\Phi_a\rangle$, and define $q_a=q-p_a$. Then, with $g_a=[q_a(\lambda-h)q_a]^{-1}$, we have the partitioning identity [14]

$$g=g_a+(1+g_au)p_agp_a(1+ug_a), \tag{2.22a}$$

where

$$p_agp_a=[p_a(\lambda-h_0-u-ug_au)p_a]^{-1}. \tag{2.22b}$$

We may write

$$p_ag_ap_a=p_a(d_a^a)^{-1} \tag{2.23a}$$

with

$$d_a^a=(l_{j_a}+\tfrac{1}{2})^2-(\eta_{j_ai}+m_a+\tfrac{1}{2})^2-\Gamma_{aa}^a. \tag{2.23b}$$

The superscript on Γ indicates that the state Φ_a has been projected out; this modified level-shift matrix is determined by the relation

$$p_a(u+ug_au)|\Phi_a\rangle=|\Phi_a\rangle\Gamma_{aa}^a. \tag{2.24}$$

The process of state removal may be continued. Thus, in Eq. (2.24) we may write $g_a=g_a\Sigma_bp_b$, where p_b projects onto states Φ_b differing from Φ_a, Φ_{10}, and Φ_{20}. Then, with

the aid of the partitioning identity (2.22) now applied to g_a, we obtain (in an obvious extension of the notation already introduced) the relation

$$g_a p_b = (1+g_{ab}u)p_b(d_b^{ab})^{-1} \tag{2.25a}$$

with

$$d_b^{ab} = (l_{j_b}+\tfrac{1}{2})^2 - (\eta_{j_b i}+m_b+\tfrac{1}{2})^2 - \Gamma_{bb}^{ab}; \tag{2.25b}$$

here, the modified level shift is defined by

$$p_b(u+ug_{ab}u)|\Phi_b\rangle = |\Phi_b\rangle\Gamma_{bb}^{ab}. \tag{2.25c}$$

This continued-fraction structure effectively includes perturbation terms of arbitrarily high order at each stage. Moreover, a state may give rise to a small denominator [in Eq. (2.23b), for example], but it no longer appears in later stages of the subtraction procedure and this can improve convergence properties. A numerical example illustrating these remarks is given in the Appendix.

The same continued-fraction expansion for the resolvent g may be combined with the representation (2.19a) to provide a successive approximation procedure for constructing the (regular and irregular) asymptotic wave functions. It is possible to put this series expansion in more explicit form. This is done in the Appendix for special cases in which the off-diagonal r^{-4} potential is absent, but we shall not do so here for the general case. A similar expansion was described earlier [9], though in connection with a different class of systems—the interaction of an electron or atom with a radiation field—and those results may be taken over quite easily to apply to the problem at hand.

III. NEAR-THRESHOLD SCATTERING

A. Formulation

It will be convenient in this formal discussion to work with regular and irregular asymptotic solutions having a different (and simpler) long-distance behavior from those introduced in Sec. II. The two sets of solutions are closely related in a manner described below. The regular solution considered here has the asymptotic form

$$f_{ji}^L(r) \sim \sin(kr - l_j\pi/2)\,\delta_{ji} + K_{ji}^L \cos(kr - l_j\pi/2), \tag{3.1}$$

where the reaction matrix K^L is real and symmetric. Letting x represent the orthogonal matrix that diagonalizes K^L, we have

$$K^L x = x \tan\delta^L. \tag{3.2}$$

The diagonal elements δ_i^L differ from the phases δ_i defined in Sec. II; we return to this point below. Now using Eq. (3.2) we find that the function $\phi_{ji} \equiv (f^L x)_{ji} \cos_i^L (2/k)^{1/2}$ behaves, for $r\to\infty$, as

$$\phi_{ji}(r) \sim x_{ji} \sin(kr - l_j\pi/2 + \delta_i^L)(2/k)^{1/2}. \tag{3.3}$$

In a similar way we may define an irregular solution with the asymptotic form

$$\xi_{ji}(r) \sim x_{ji} \cos(kr - l_j\pi/2 + \delta_i^L)(2/k)^{1/2}. \tag{3.4}$$

A scattering matrix S^0 may be defined by consideration of a scattering solution, valid throughout space, and expressed in terms of undistorted incoming and outgoing waves as

$$\Psi_{ji}^0(r) \sim (2/k)^{1/2}[e^{-i(kr - l_j\pi/2)} - e^{i(kr - l_j\pi/2)} S_{ji}^0] \tag{3.5}$$

for $r\to\infty$. Alternatively, in terms of the distorted waves,

$$I_{ji}(r) = \xi_{ji}(r) - i\varphi_{ji}(r), \quad O_{ji}(r) = \xi_{ji}(r) + i\varphi_{ji}(r), \tag{3.6}$$

we have the related solution behaving as

$$\Psi_{ji}(r) \sim I_{ji}(r) - \sum_{j'=1}^{2} O_{jj'} S_{j'i}. \tag{3.7}$$

The relation between the two solutions is readily seen to be $\Psi^0 = \Psi B$, where

$$B^T = x \exp(i\delta^L), \tag{3.8}$$

the superscript T denoting transpose. The relation between the two scattering matrices is

$$S^0 = B^T S B. \tag{3.9a}$$

Since x is orthogonal and the δ_i^L are real, it follows that B is unitary. Then the unitarity property satisfied by S^0 is seen to be passed on to the modified scattering matrix S. In terms of transition matrices, conventionally defined by the relations $S^0 = 1 + 2iT^0$ and $S = 1 + 2iT$, we find the unitarity relation $T - T^\dagger = 2iTT^\dagger$ and the connection

$$T^0 = x e^{i\delta^L} \sin\delta^L x^T + B^T T B. \tag{3.9b}$$

To work with standing waves we introduce a reaction matrix K through the relation $T^{-1} = K^{-1} - i$. The unitarity of T implies that K is Hermitian; it is in fact real and symmetric (as may be confirmed directly with the aid of the variational principle derived in Sec. III C). Noting that the function $(i/2)\Psi$ behaves asymptotically as $\phi T^{-1} + O$, we may define $U = (i/2)\Psi K$ with asymptotic form

$$U \sim \phi + \xi K. \tag{3.10}$$

To have available an approximation procedure for the construction of the solutions φ and ξ we may relate them to the regular and irregular solutions introduced in Sec. II: this is accomplished by comparison of asymptotic forms. Thus we write

$$f_{ji}(r) \sim (2/k)^{1/2}[c_{ji} \sin(kr - l_j\pi/2 + \delta_j) + d_{ji} \cos(kr - l_j\pi/2 + \delta_i)] \tag{3.11a}$$

for $r\to\infty$, where, up to an overall normalization yet to be fixed, the coefficient matrices c and d are determined by the methods described earlier in Sec. II. Rewriting Eq. (3.11a) as

$$f_{ji}(r) \sim (2/k)^{1/2}[\overline{c}_{ji} \sin(kr - l_j\pi/2) + \overline{d}_{ji} \cos(kr - l_j\pi/2)] \tag{3.11b}$$

with

$$\bar{c}_{ji}=c_{ji}\cos\delta_i-d_{ji}\sin\delta_i\,,\quad \bar{d}_{ji}=c_{ji}\sin\delta_i+d_{ji}\cos\delta_i\,, \tag{3.11c}$$

we may, by comparison with the asymptotic form shown in Eq. (3.3), conclude that the functions f and ϕ are identical and that

$$\bar{c}_{ji}=x_{ji}\cos\delta_i^L\,,\quad \bar{d}_{ji}=x_{ji}\sin\delta_i^L\,. \tag{3.12}$$

In a similar way we may identify the irregular asymptotic solution defined in Sec. II with $-\xi$. Another useful relation found from this comparison of solutions is $K^L=\bar{d}(\bar{c})^{-1}$. Thus in addition to ϕ and ξ, we may determine K^L, and by diagonalization x and δ^L by application of the perturbation procedure outlined in Sec. II. Moreover, when the relation shown in Eq. (3.8) is compared with Eqs. (3.12) we may conclude that $B^T=\bar{c}+i\bar{d}$. From the real and imaginary parts of the unitarity relation $BB^\dagger=1$ we find that

$$c^Tc+d^Td=1, \tag{3.13}$$

which supplies the required normalization condition to be combined with the perturbation procedure; in addition, the symmetry property $c^Td=d^Tc$ is uncovered. We note finally that the normalization condition implied by Eq. (3.13), taken in second order and evaluated at threshold, leads to the result that the matrix a is orthogonal in second order [15], as remarked earlier in connection with Eq. (2.9).

B. Threshold behavior

The threshold behavior of the asymptotic solutions may be inferred from the small argument limits of the Bessel functions from which they are composed. The regular solution ϕ, having been identified with the function f studied earlier, is expressed as

$$\phi_{ji}=[C_i(k/2)^{1/2}](\pi r)^{1/2}m_{ji}\,. \tag{3.14}$$

From the normalization condition placed on this function we may conclude that the factor $[C_i(k/2)^{1/2}]$ is finite at threshold. Then the threshold behavior of ϕ_{ji} may be deduced from that of m_{ji}, with the latter determined from an examination of the structure of the perturbation expansion. One finds in this way that the function

$$\bar{\phi}_{ji}(r)=k^{-(\eta_{1i}+1/2)}\phi_{ji}(r) \tag{3.15}$$

is finite and nonvanishing at threshold and may be expanded in powers of k^2. A very similar analysis shows that the reduced irregular solution, defined as

$$\bar{\xi}_{ji}(r)=k^{(\eta_{2i}+1/2)}\xi_{ji}(r) \tag{3.16}$$

is finite and nonvanishing at threshold. One understands the appearance of orbital quantum number l_1 in the threshold factor in Eq. (3.15) and l_2 in Eq. (3.16) by recalling that the angular momentum states are coupled; the threshold behavior of the regular and irregular solutions are determined by the lowest and highest partial waves, respectively, that are present asymptotically.

Having determined how threshold singularities are to be isolated, we may define a reduced wave function $\bar{U}_{ji}=k^{-(\eta_{1i}+1/2)}U_{ji}$ with asymptotic form

$$\bar{U}_{ji}(r)\sim\bar{\phi}_{ji}(r)+\sum_{i'}\bar{\xi}_{ji'}(r)\bar{K}_{i'i}\,. \tag{3.17}$$

The smooth threshold behavior of the asymptotic solutions appearing in Eq. (3.17) implies that the matrix

$$\bar{K}_{i'i}=k^{-(\eta_{2i'}+1/2)}K_{i'i}k^{-(\eta_{1i}+1/2)} \tag{3.18}$$

is free of threshold singularities. This central property will be confirmed below with the aid of a variational argument. The threshold behavior of the T matrix may now be deduced from the relation $T^{-1}=K^{-1}-i$ given earlier. If, for notational simplicity, we define the diagonal matrix η_j with diagonal elements η_{j1} and η_{j2}, we obtain the representation

$$T=k^{\eta_2+1/2}[\bar{K}^{-1}-ik^{\eta_1+\eta_2+1}]^{-1}k^{\eta_1+1/2}, \tag{3.19}$$

which, by virtue of the relation shown in Eq. (2.4b) with δ_i of order k^2, contains the logarithmic contributions to the energy dependence at threshold that is characteristic of scattering with long-range potentials.

C. Variational principle

A variational principle for the reaction matrix $\bar{K}$ defined in Eq. (3.18) may be derived by extending the procedure described in Ref. [7] to account for the asymptotic coupling of channels. The derivation begins with the introduction of a trial function $\bar{U}_{ji,t}(r)$, vanishing at the origin and satisfying the asymptotic form (3.17) with $\bar{K}$ replaced by a trial matrix $\bar{K}_t$. The matrix

$$\sum_{j,j'}\int_0^\infty[\bar{U}_{j'i'}(L_{j'j}\bar{U}_{ji,t})-(L_{jj'}\bar{U}_{j't'})\bar{U}_{ji,t}]dr$$

is evaluated in two ways, first through the use of the Schrödinger equation $L\bar{U}=0$ and then by integration by parts taking into account the boundary conditions and making use of the Wronskian relation

$$\frac{1}{2}\sum_j\left[\frac{d\bar{\phi}_{ji'}}{dr}\bar{\xi}_{jj''}-\bar{\phi}_{ji'}\frac{d\bar{\xi}_{jj''}}{dr}\right]=\delta_{i'j''}\,. \tag{3.20}$$

This leads to the identity

$$\bar{K}_{i'i}=\bar{K}_{i'i,t}-\sum_{j,j'}\int_0^\infty\bar{U}_{j'i'}L_{j'j}\bar{U}_{ji,t}dr. \tag{3.21}$$

Actually, it is the matrix element $\bar{K}_{ii'}$ that originally appears on the left-hand side, but this matrix is symmetric (as may be verified by performing the above calculation with the trial function replaced by the exact solution). It will be convenient to express the trial function for all r as

$$\bar{U}_{ji,t}(r)=y_{s,ji}(r)+\sum_{j'}y_{c,jj'}(r)\bar{K}_{j'i,t}\,, \tag{3.22}$$

where $y_s \sim \overline{\phi}$ and $y_c \sim \overline{\xi}$ asymptotically. A trial function $\overline{U}_\tau$ is defined as in Eq. (3.22) but with $\overline{K}_t$ replaced by $\overline{K}_\tau$. A variational principle is obtained by replacing the exact wave function in the identity (3.21) with $\overline{U}_\tau$. The trial matrices $\overline{K}_t$ and $\overline{K}_\tau$ may be determined by requiring that the variational expression be stationary with respect to variations in these parameters. To simplify the form of the resultant expression we introduce some notation, starting with the definition $w = Ly_s$. A scalar product is now defined permitting the abbreviation

$$(a_j, b_i) \equiv \sum_{j'} \int_0^\infty a_{j'j} b_{j'i} dr. \tag{3.23}$$

With this notation we define the matrix

$$X_{j'j} = (y_{c,j'}, Ly_{c,j}). \tag{3.24}$$

After some algebra the variational approximation $\overline{K}_v$ may be seen to take the form

$$\overline{K}_{i'i,v} = -(y_{s,i'}, w_i) + \sum_{j,j'} (w_{i'}, y_{c,j'})(X^{-1})_{j'j}(y_{c,j}, w_i). \tag{3.25}$$

With threshold singularities removed, the trial functions y_c and y_s may be connected smoothly, from their prescribed forms at great distances from the origin, to ''inside'' functions that vanish at the origin. In line with the conventional effective range approximation, the inside functions may be chosen to be independent of energy near threshold. The error in the trial functions thereby incurred will be of first order in the energy and this leads to an error in $\overline{K}_v$ of second order. Then, with the effective range approximation expressed in the standard manner as

$$(\overline{K})^{-1} \cong -A^{-1} + \tfrac{1}{2} r_0 k^2, \tag{3.26}$$

variational estimates of the scattering length and effective range matrices are available.

At zero energy the variational principle becomes a minimum principle for diagonal elements of the scattering length matrix. A particularly useful version of the minimum principle is based on the addition to the right-hand side of Eq. (3.22) a superposition of normalizable basis functions with linear parameters determined variationally. That is, we write the zero-energy trial function as

$$\overline{U}_{ji,t}(r) = y_{s,ji}(r) + \sum_{j'=1}^{p} y_{c,jj'}(r) b_{j'i,t} \tag{3.27}$$

with the parameters $b_{ji,t}$ determined variationally. For $j' = 1,2$ the trial functions $y_{c,jj'}$ are the (normalizable) zero-energy limits of the functions introduced above, while for $j' = 3,4,...,p$ they are chosen from a normalizable basis set. A similar form is taken for the trial function $\overline{U}_{ji,\tau}$. The variational expression for one of the elements A_{ii} of the scattering length matrix, involving p basis functions, then takes the form

$$A_{ii,v}^{(p)} = (y_{s,i'}, w_i) - \sum_{j,j'=1}^{p} (w_{i'}, y_{c,j'})(X^{-1})_{j'j}(y_{c,j}, w_i). \tag{3.28}$$

If there are no bound states, $A_{ii}^{(0)}$ provides an upper bound on the exact matrix element A_{ii} and as the number of basis functions is increased, each successive term decreases the value of the approximation obtained at the previous stage. More generally, suppose that N bound states exist. One examines the sequence of scattering length approximations $A_{ii}^{(p)}$, $p = 0,1,...,n$, where $n \geqslant N$. After one verifies N upward jumps along this sequence, the variational method is ensured to give an upper bound on A_{ii}. The details of the derivation of this result differ only slightly from those given earlier [16], in connection with the problem of scattering by a tensor force of short range [17], and will not be repeated here.

IV. SUMMARY

A modified version of effective range theory has been developed that is applicable to the study of low-energy scattering of an electron by an atomic target with a ground-state wave function that is not spherically symmetric. For simplicity, only the inverse-cube and inverse-fourth-power contributions to the long-range effective electron-target interaction has been retained. A two-channel model was adopted, with channel thresholds taken to be identical, corresponding to the degeneracy of the two target states differing only in spin projection. Exact analytic asymptotic solutions of the wave equation are not available for potentials of this type. A general method for developing approximate solutions that describe fairly accurately the nature of the threshold singularities was described in Sec. II with additional details given in the Appendix. The method is based on perturbation theory, enhanced through the introduction of diagram summation techniques. A distorted-wave theory was presented in Sec. III, based on the availability of these asymptotic wave functions. This analysis leads to the representation of a modified scattering amplitude given in Eq. (3.19), in which the kinematical factors singular at threshold are displayed. This leaves a reaction matrix, denoted there as $\overline{K}$, that varies smoothly with energy and may, therefore, be parametrized in the standard manner of effective range theory. A variational procedure was presented in Sec. III C for estimating the scattering length and effective range matrices.

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APPENDIX

The continued-fraction structure of the modified perturbation theory presented in Sec. II becomes more transparent in the absence of the off-diagonal r^{-4} potential. Here we examine two special cases, each of interest in its own right, for which the perturbation expansion can be developed in more explicit form.

Consider first the case where only the β_3/r^3 contribution appears in the long-range potential shown in Eq. (1.1). The Γ

matrix is then diagonal, the mixing angle in Eq. (2.9) vanishes, and Eq. (2.6) decouples. Assuming that the system is in channel 1 in the limit of vanishing β_3, we need only consider a single level-shift element corresponding to the virtual transitions $(1,0)\rightarrow(2,-1)\rightarrow(1,0)$ and $(1,0)\rightarrow(2,-3)\rightarrow(1,0)$. To simplify notation we denote the states $(1,m)$ as (m) for m even and states $(2,m)$ as $(m+2)$ for m odd. The matrix element Γ_{11} of interest is denoted as Γ_0. Dropping the subscript i in Eq. (2.4b) we write that equation for $j=1$ as $\eta=l_1-(2/\pi)\delta$, so that η_1 has become η and $\eta_2=\eta+2$. Then η is determined from the relation

$$(\eta+\tfrac{1}{2})^2-(l_1+\tfrac{1}{2})^2+\Gamma_0=0. \tag{A1}$$

Writing $\Gamma_0=\Gamma_{0+}+\Gamma_{0-}$, we have

$$\Gamma_{0+}=v_{01}(1/d_{1+})v_{10}, \tag{A2}$$

with $v_{10}=\Delta_3(2\eta+1)^{-1}$ and $v_{01}=\Delta_3(2\eta+3)^{-1}$. The subscript $+$ on d_1 is inserted to emphasize that since the states (0) and (1) are removed, and there are no interactions in this model causing transitions $(1)\rightarrow(m)$ for $m<0$, only those states with $m>0$ appear as intermediate states. The propagator is now expressed in the form

$$d_{1+}=(l_2+\tfrac{1}{2})^2-(\eta+\tfrac{3}{2})^2-\Gamma_{1+}. \tag{A3}$$

Here we have

$$\Gamma_{1+}=v_{12}(1/d_{2+})v_{21}, \tag{A4}$$

with $v_{21}=\Delta_3(2\eta+3)^{-1}$ and $v_{12}=\Delta_3(2\eta+5)^{-1}$. This ascending sequence may be continued in an obvious way; in general, we have $v_{m'm}=\Delta_3[2(\eta+m)+1]^{-1}$ with $m'=m\pm1$. The descending sequence is developed similarly, with

$$\Gamma_{0-}=v_{0(-1)}(1/d_{(-1)-})v_{(-1)0}. \tag{A5}$$

We have

$$d_{(-1)-}=(l_2+\tfrac{1}{2})^2-(\eta-\tfrac{1}{2})^2-\Gamma_{(-1)-} \tag{A6}$$

and

$$\Gamma_{(-1)-}=v_{(-1)(-2)}(1/d_{(-2)-})v_{(-2)(-1)}. \tag{A7}$$

The wave function satisfies Eq. (2.2) with $\Delta_4=D_j=0$. In the absence of any perturbation, the system is in state (0) with wave function $J_{\eta+1/2}(z)$. The perturbation expansion shown in Eq. (2.3) is rewritten as $m_j=\Sigma_{n=0}^{\infty}m_j^{(n)}$ with subscript j retained as a channel index. For $j=1$ the nth-order contribution, with $n=2,4,...$, is

$$m_1^{(n)}(z)=\alpha_n J_{\eta+n+1/2}(z)+\alpha_{-n}J_{\eta-n+1/2}(z), \tag{A8}$$

where

$$\alpha_n=(1/d_{n+})v_{nn-1}\cdots v_{21}(1/d_{1+})v_{10} \tag{A9a}$$

and

$$\alpha_{-n}=(1/d_{(-n)-})v_{-n(-n+1)}\cdots v_{-2(-1)}(1/d_{(-1)-})v_{(-1)0}. \tag{A9b}$$

This has the form of the lowest nonvanishing order of perturbation theory, but with modified propagators; these propagators are represented by continued fractions, as indicated above. The wave function in channel 2 is given by a similar expansion, but with the nonvanishing orders of the perturbation expansion taking on the values $n=1,3,...$.

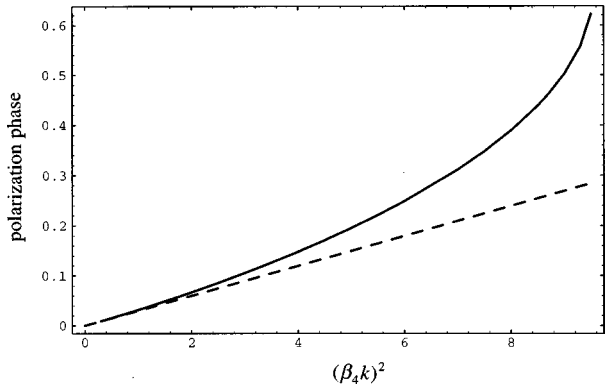

FIG. 5. Plot of the polarization phase for d-wave scattering in an inverse fourth-power potential as a function of the strength parameter $(\beta_4 k)^2$ obtained using the continued-fraction formulation (solid curve) in an approximation carried to the third level (as defined in the text). The dashed curve represents the lowest-order approximation, given (for all l) in Eq. (A16).

We now consider the single-channel scattering problem with the long-range potential taken to be β_4^2/r^4. We may, therefore, drop the channel label and write the appropriate version of Eq. (2.6) as $(\eta+\frac{1}{2})^2-(l+\frac{1}{2})^2+\Gamma=0$, where

$$\Gamma=\Gamma_{0+}+\Gamma_{0-}. \tag{A10}$$

With the interactions now given by $u_{m'm}=(\beta_4 k)[2(\eta+m)+1]^{-1}$, $m'=m\pm1$, we have

$$\Gamma_{0+}=u_{01}u_{10}+u_{01}u_{12}(1/d_{2+})u_{21}u_{10}, \tag{A11}$$

with

$$d_{2+}=(l+\tfrac{1}{2})^2-(\eta+\tfrac{5}{2})^2-\Gamma_{2+} \tag{A12}$$

and

$$\Gamma_{2+}=u_{23}u_{32}+u_{23}u_{34}(1/d_{4+})u_{43}u_{32}. \tag{A13}$$

The structure of this ascending sequence should now be clear. The descending sequence has the form

$$\Gamma_{0-}=u_{0(-1)}u_{(-1)0}+u_{0(-1)}u_{-1(-2)}\times(1/d_{(-2)-})u_{-2(-1)}u_{(-1)0} \tag{A14}$$

with

$$d_{(-2)-}=(l+\tfrac{1}{2})^2-(\eta-\tfrac{3}{2})^2-\Gamma_{(-2)-}, \tag{A15}$$

and so forth. The sequences are terminated, in practice, by setting $\Gamma_{2n+}=\Gamma_{2n-}=0$; we may say that such an approximation is carried to the nth ''level.'' The solid curve in Fig. 5 represents the results of a third-level calculation of the polarization phase δ for $l=2$ as a function of $(\beta_4 k)^2$. Results at levels two and four differ only slightly. Instabilities,

signaling the onset of complex phases [11] in the calculation, appear for $(\beta_4 k)^2 > 9.5$. The precise numerical calculation done by Holzwarth [11] gives the onset of the instability at $(\beta_4 k)^2 = 10.5$. The level-one calculation gives no better than 10% accuracy for $(\beta_4 k)^2 > 4$ and fails for $(\beta_4 k)^2 > 6$. For comparison, a plot of the polarization phase in lowest order, namely,

$$\delta \cong \frac{\pi(\beta_4 k)^2}{(2l+3)(2l+1)(2l-1)}, \tag{A16}$$

is given (for $l=2$) by the dashed curve.

The wave function is expanded as $m(z) = \Sigma_{n=0}^{\infty} m^{(n)}(z)$. We have, for $n = 2,4, \ldots,$

$$m^{(n)} = \gamma_n J_{\eta+n+1/2} + \gamma_{-n} J_{\eta-n+1/2}, \tag{A17}$$

with

$$\gamma_n = (1/d_{n+}) u_{n(n-1)} u_{n-1(n-2)} \cdots u_{43} u_{32} (1/d_{2+}) u_{21} u_{10} \tag{A18a}$$

and

$$\gamma_{-n} = (1/d_{(-n)-}) u_{-n(-n+1)} u_{-n+1(-n+2)} \cdots u_{-4(-3)} u_{-3(-2)} \times (1/d_{(-2)-}) u_{-2(-1)} u_{-10}. \tag{A18b}$$

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