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Relativistic quantum-defect theory. General formulation

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A relativistic multichannel quantum-defect theory is formulated in the same way as in the nonrelativistic theory of Seaton. The solutions to the radial Dirac-Coulomb equations are reviewed in complex values of energy. The simple-model problem with finite-range potentials is used to clarify the scattering matrix and the reactance K matrix. The close-coupling approximation is discussed for real atomic systems.

I. INTRODUCTION

Quantum-defect theory (QDT) is concerned with an electron moving in a positive atomic field. In relativistic single-channel QDT of Johnson and Cheng,[1] the effective quantum number ν of a discrete state is related to its energy ϵ by

$$\nu=\alpha Z\epsilon/(m^2-\epsilon^2)^{1/2}\,, \tag{1.1}$$

where Z is the ionic charge and α is the fine-structure constant. In particular, we have ν_{Coul} for pure Coulomb field of a nuclear charge Z. The quantum defect μ for this discrete state is defined as

$$\mu=\nu_{\text{Coul}}-\nu\ . \tag{1.2}$$

In the asymptotic region with $r\to\infty$, the wave function of the electron in continuum state is characterized by the phase shift δ and in discrete state by the quantum defect μ. Since the wave function changes smoothly across the ionization threshold, a relation exists between the phase shift δ and the quantum defect μ.

A relativistic multichannel QDT has been formulated by Lee and Johnson,[2] which is an extension of relativistic single-channel QDT of Johnson and Cheng[1] and includes the relativistic random-phase approximation for calculating dynamical parameters. Our work is an alternative method of analysis and gives a more complete account of the general theory, following nonrelativistic multichannel QDT of Seaton.[3,4]

Natural units are used throughout. In the Appendix, some formulas in atomic units are described.

II. COULOMB FUNCTIONS

In this section, after summarizing Coulomb functions as mentioned by Johnson and Cheng,[1] we introduce traveling wave functions φ^+ and φ^- and then express analytic functions f and g in terms of φ^+ and φ^-. The single-particle Dirac wave function $\psi(\vec{r})$ is defined as

$$\psi(\vec{r})=\begin{bmatrix} P(r)\chi_{\kappa m} \\ iQ(r)\chi_{-\kappa m}\end{bmatrix}\,, \tag{2.1}$$

where $P(r)$ and $Q(r)$ are the large and small components of radial function, respectively, and $\chi_{\kappa m}$ is a spin-orbit eigenfunction. The definition of $\psi(\vec{r})$ here is different from that of Johnson and Cheng[1] in that here i is connected with $Q(r)$. The Dirac-Coulomb radial equations are

$$\frac{dP}{dr}+\frac{\kappa}{r}P-\left[m+\epsilon+\frac{\alpha Z}{r}\right]Q=0\,, \tag{2.2}$$

$$\frac{dQ}{dr}-\frac{\kappa}{r}Q-\left[m-\epsilon-\frac{\alpha Z}{r}\right]P=0\,. \tag{2.3}$$

Defining

$$k=|\kappa|\,,\quad \gamma=[k^2-(\alpha Z)^2]^{1/2}\,,$$

$$\lambda=(m^2-\epsilon^2)^{1/2},\quad z=2\lambda r\,,$$

$$\nu=\alpha Z\epsilon/\lambda,\quad \nu'=\alpha Zm/\lambda\,,$$

and using the solution

$$y=\binom{P}{Q}=(m\pm\epsilon)^{1/2}z^{\gamma}\exp(-z/2)(Q_1\pm Q_2)\,, \tag{2.4}$$

we can reduce Eqs. (2.2) and (2.3) to

$$zQ_1''+(2\gamma+1-z)Q_1'-(\gamma+1-\nu)Q_1=0\,, \tag{2.5}$$

$$zQ_2''+(2\gamma+1-z)Q_2'-(\gamma-\nu)Q_2=0\,, \tag{2.6}$$

where the prime means the derivative with respect to z. Solutions to Eq. (2.5) or (2.6) are confluent hypergeometric functions. For more details, the reader may refer to Berestetskii, Lifshitz, and Pitaevskii.[5] Coulomb functions are

$$y_1=(m\pm\epsilon)^{1/2}z^{\gamma}\exp(-z/2)[a\,{}_1F_1(a+1,b,z)\pm(-\kappa+\nu')_1F_1(a,b,z)]\ , \tag{2.7}$$

$$y_2=(m\pm\epsilon)^{1/2}z^{-\gamma}\exp(-z/2)[(1+a-b)_1F_1(2+a-b,2-b,z)\pm(-\kappa+\nu')_1F_1(1+a-b,2-b,z)]\ , \tag{2.8}$$

$$y_5=(m\pm\epsilon)^{1/2}z^{\gamma}\exp(-z/2)(-\kappa+\nu')[(\kappa+\nu')U(a+1,b,z)\pm U(a,b,z)]\ , \tag{2.9}$$

$$y_7=(m\pm\epsilon)^{1/2}z^{\gamma}\exp(z/2)[-U(b-a-1,b,-z)\pm(-\kappa+\nu')U(b-a,b,-z)]\ , \tag{2.10}$$

$$y_R=y_1/c_1\ , \tag{2.11}$$

$$y_I=y_2/c_2\ , \tag{2.12}$$

where $a=\gamma-\nu$, $b=2\gamma+1$,

$$c_1=[(m+\epsilon)]^{1/2}(\lambda)^{\gamma}(-\kappa+\gamma+\nu'-\nu)\times\Gamma(2\gamma+1)\ , \tag{2.13}$$

and

$$c_2=[(m+\epsilon)]^{1/2}(\lambda)^{-\gamma}(-\kappa-\gamma+\nu'-\nu)\times\Gamma(-2\gamma+1)\ . \tag{2.14}$$

It should be noted that the sign of the small component is the opposite of that defined in Johnson and Cheng.[1] The coefficient a_0 in Eq. (A1) of Ref. 1 is set to $2^{\gamma}/\Gamma(2\gamma+1)$. The functions y_R and y_I are analytic in ϵ and γ. Two points should be emphasized:

(a) If the energy ϵ is taken as complex, so is λ. For the case when ϵ is real and $\epsilon>m$, Coulomb functions are obtained from Eqs. (2.7)–(2.12) by the replacements

$$(m-\epsilon)^{1/2}\to-i(\epsilon-m)^{1/2},\quad \lambda\to-ip\ ,$$

$$p=(\epsilon^2-m^2)^{1/2},\quad z=-2ipr,\quad \nu\to i\eta\ ,$$

$$\eta=\alpha Z\epsilon/p,\quad \nu\to i\eta',\quad \eta'=\alpha Zm/p\ .$$

(b) $U(a,b,z)$ is a many-valued function. The asymptotic form is

$$U(a,b,z)=z^{-a}[1+O(1/|z|)]\ ,\qquad |\arg(z)|<3\pi/2 \tag{2.15}$$

so that y_5 and y_7 have asymptotic forms

$$y_5=(m\pm\epsilon)^{1/2}z^{\nu}\exp(-z/2)(\pm1)\times(-\kappa+\nu')[1+O(1/|z|)],\qquad |\arg(z)|<3\pi/2 \tag{2.16}$$

$$y_7=(m\pm\epsilon)^{1/2}z^{-\nu}\exp(z/2)\times e^{Di\pi(a-b)}[1+O(1/|z|)],\qquad |\arg(z)|<3\pi/2\ . \tag{2.17}$$

Here we follow the sign convention of Slater[6]

$$D=\begin{cases}1 & \text{if } \arg(z)>0\\ -1 & \text{otherwise}\end{cases}$$

and, in particular, $-z=e^{-Di\pi}z$. This sign convention is applied and related only to the variable z in the confluent hypergeometric function.

A. Functions φ^+ and φ^-

We define

$$\varphi^+=-\Gamma(b)\exp(Di\pi a)y_5/N_1\ , \tag{2.18}$$

$$\varphi^-=a\Gamma(b)\exp[Di\pi(a-b)]y_7/N_1\ , \tag{2.19}$$

where

$$N_1=[i\lambda(\kappa-\nu')(\gamma-\nu)]^{1/2}\Gamma(b)\times\exp(Di\pi a/2)\ . \tag{2.20}$$

For $|\arg(z)|<3\pi/2$, these functions have asymptotic forms:

$$\varphi^+\sim[(\gamma-\nu)/(\kappa-\nu')]^{-1/2}z^{\nu}e^{-z/2}\exp(Di\pi a/2)\begin{bmatrix}[(m+\epsilon)/(i\lambda)]^{1/2}\\ -[(m-\epsilon)/(i\lambda)]^{1/2}\end{bmatrix}, \tag{2.21}$$

$$\varphi^-\sim[(\gamma-\nu)/(\kappa-\nu')]^{1/2}z^{-\nu}e^{z/2}\exp(-Di\pi a/2)\begin{bmatrix}[(m+\epsilon)/(i\lambda)]^{1/2}\\ [(m-\epsilon)/(i\lambda)]^{1/2}\end{bmatrix}. \tag{2.22}$$

In particular, when ϵ is real and $\epsilon > m$, we have

$$N_1=[p(\kappa-i\eta')(\gamma-i\eta)]^{1/2}\Gamma(b)\times\exp(-i\pi\gamma/2-\pi\eta/2)\ , \tag{2.23}$$

$$\varphi^+\sim\exp[i(pr+\eta\ \ln 2pr-\pi\gamma/2+\xi)]\times\begin{bmatrix}[(m+\epsilon)/p]^{1/2}\\ i[(\epsilon-m)/p]^{1/2}\end{bmatrix}, \tag{2.24}$$

$$\varphi^-\sim\exp[-i(pr+\eta\ \ln 2pr-\pi\gamma/2+\xi)]\times\begin{bmatrix}[(m+\epsilon)/p]^{1/2}\\ -i[(\epsilon-m)/p]^{1/2}\end{bmatrix}, \tag{2.25}$$

where

$$\exp(-2i\xi)=(\gamma-i\eta)/(\kappa-i\eta')\ . \tag{2.26}$$

B. Relations among Coulomb functions φ^+ and φ^-

The expressions for y_1 and y_2 in terms of y_5 and y_7 are

$$y_1=[\Gamma(b)e^{Di\pi a}/\Gamma(b-a)]y_5+[\Gamma(b)e^{Di\pi(a-b)}/\Gamma(a)]y_7\ , \tag{2.27}$$

$$y_2=[-\Gamma(2-b)e^{Di\pi(a-b)}/\Gamma(1-a)]y_5+[\Gamma(2-b)e^{Di\pi(a-b)}/\Gamma(1+a-b)]y_7\ . \tag{2.28}$$

Using Eqs. (2.18) and (2.19), we have

$$y_1=N_1[\varphi^-/\Gamma(1+a)-\varphi^+/\Gamma(b-a)]\ , \tag{2.29}$$

$$y_2=N_1[d_1\varphi^-/\Gamma(1+a)-d_2\varphi^+/\Gamma(b-a)]\ , \tag{2.30}$$

where

$$d_1=\Gamma(2-b)\Gamma(b-a)\sin\pi(b-a)/[\Gamma(b)\Gamma(1-a)\sin\pi a]\ , \tag{2.31}$$

$$d_2=-\Gamma(2-b)\Gamma(b-a)\exp(-Di\pi b)/[\Gamma(b)\Gamma(1-a)]\ . \tag{2.32}$$

The identity $\Gamma(z)\Gamma(1-z)=\pi\csc\pi z$ is used here and hereafter. In turn, we obtain

$$y_R=(N_1/c_1)[\varphi^-/\Gamma(1+\gamma-\nu)-\varphi^+/\Gamma(1+\gamma+\nu)]\ , \tag{2.33}$$

$$y_I=(N_1/c_1)[\varphi^-A\sin\pi b(\cot\pi b-\cot\pi a)/\Gamma(1+\gamma-\nu)-\varphi^+A\sin\pi b(\cot\pi b-Di)/\Gamma(1+\gamma+\nu)]\ , \tag{2.34}$$

where

$$A(\nu,\gamma)=-(c_1/c_2)\Gamma(2-b)\Gamma(b-a)/[\Gamma(b)\Gamma(1-a)]=-(\alpha Z\epsilon)^{2\gamma}R(\nu,\nu')a(\nu,\gamma) \tag{2.35}$$

and where

$$R(\nu,\nu')=\frac{\nu}{(\nu-\gamma)}\frac{(-\kappa+\gamma+\nu'-\nu)}{(-\kappa-\gamma+\nu'-\nu)}\ , \tag{2.36a}$$

$$a(\nu,\gamma)=\frac{\Gamma(1+\gamma+\nu)}{\nu^{2\gamma+1}\Gamma(\nu-\gamma)}\ . \tag{2.36b}$$

$a(\nu,\gamma)$ is usually a complex function and can be represented by

$$a(\nu,\gamma)=a_r(\nu,\gamma)+ia_i(\nu,\gamma)\ . \tag{2.36c}$$

C. Analytic functions f and g

If we regard γ as an independent variable and define

$$f(\epsilon,\gamma;r)=y_R(\epsilon,\gamma;r) \tag{2.37}$$

then

$$f(\epsilon,-\gamma;r)=y_I(\epsilon,\gamma;r)\ . \tag{2.38}$$

The Wronskian of y_R and y_I is

$$W(y_R,y_I)=(2\epsilon+2\alpha Z/r)[\sin\pi(2\gamma+1)]/(\pi\alpha Z)\ . \tag{2.39}$$

The functions y_R and y_I are no longer independent when $\gamma=\gamma_c$=positive integer or half integer. Specifically, we have

$$y_I(\epsilon,\gamma_c;r)=(-1)^{2\gamma_c+1}A(\nu,\gamma_c)y_R(\epsilon,\gamma_c;r)\ . \tag{2.40}$$

As in the nonrelativistic case,[3] we consider a second irregular solution

$$\bar{g}(\epsilon,\gamma;r)=[A(\nu,\gamma)\cos\pi(2\gamma+1)y_R(\epsilon,\gamma;r)-y_I(\epsilon,\gamma;r)]/\sin\pi(2\gamma+1) \tag{2.41}$$

which becomes at $\gamma=\gamma_c$

$$\bar{g}(\epsilon,\gamma_c;r)=(2\pi)^{-1}\left[A(\nu,\gamma)\frac{\partial}{\partial\gamma}y_R(\epsilon,\gamma;r)+(-1)^{2\gamma+2}\frac{\partial}{\partial\gamma}y_I(\epsilon,\gamma;r)+y_R(\epsilon,\gamma;r)\frac{\partial}{\partial\gamma}A(\nu,\gamma)\right]_{\gamma=\gamma_c} . \tag{2.42}$$

The term involving $(\partial/\partial\gamma)A(\nu,\gamma)$ is not an analytic function of ϵ. Following Eq. (2.46) in Greene, Fano, and Strinati,[7] we construct an analytic solution of ϵ as

$$g(\epsilon,\gamma;r)=\bar{g}(\epsilon,\gamma;r)-G(\nu,\gamma)y_R(\epsilon,\gamma;r) , \tag{2.43}$$

where

$$G(\nu,\gamma)=[A(\nu,\gamma)\cos\pi(2\gamma+1)-\cos^2 2\pi(\gamma-\bar{\gamma}_c)A(\nu,\bar{\gamma}_c)\cos\pi(2\bar{\gamma}_c+1)]/\sin\pi(2\gamma+1) . \tag{2.44}$$

The value $\bar{\gamma}_c$ is the γ_c which is closest to γ. Using Eqs. (2.33) and (2.34) we obtain

$$g(\epsilon,\gamma;r)=(N_1/c_1)[\varphi^-(-G+A\cot\pi a)/\Gamma(1+\gamma-\nu)-\varphi^+(-G+DiA)/\Gamma(1+\gamma+\nu)] . \tag{2.45}$$

When ϵ is real, $z=2\lambda r$ and $\arg(z)=0$ for $\epsilon<m$, and $z=-2ipr$ and $\arg(z)=-\pi/2$ for $\epsilon>m$. By sign convention $D=-1$, and thus

$$f=(N_1/c_1)[\varphi^-/\Gamma(1+\gamma-\nu)-\varphi^+/\Gamma(1+\gamma+\nu)] , \tag{2.46}$$

$$g=(N_1/c_1)[\varphi^-(\mathcal{G}+CB)/\Gamma(1+\gamma-\nu)-\varphi^+(\mathcal{G}+iB)/\Gamma(1+\gamma+\nu)] , \tag{2.47}$$

where, for $\epsilon<m$

$$B=B_<=(\alpha Z\epsilon)^{2\gamma}R(\nu,\nu')a(\nu,\gamma) , \tag{2.48}$$

$$\mathcal{G}=\mathcal{G}_<=B_<\cot\pi b+\cos^2 2\pi(\gamma-\bar{\gamma}_c)A(\nu,\bar{\gamma}_c)\cos\pi(2\bar{\gamma}_c+1)/\sin\pi(2\gamma+1) , \tag{2.49}$$

$$C=-\cot\pi a , \tag{2.50}$$

and for $\epsilon>m$

$$B=B_>=(\alpha Z\epsilon)^{2\gamma}R(i\eta,i\eta')\bar{a}(\eta,\gamma) , \tag{2.51}$$

$$\mathcal{G}=\mathcal{G}_>=B_>(\cot\pi b+\csc\pi b\, e^{-2\pi\eta})+\cos^2 2\pi(\gamma-\bar{\gamma}_c)A(i\eta,\bar{\gamma}_c)\cos\pi(2\bar{\gamma}_c+1)/\sin\pi(2\gamma+1) , \tag{2.52}$$

$$C=-i , \tag{2.53}$$

and where

$$\bar{a}(\eta,\gamma)=|\Gamma(1+\gamma+i\eta)|^2 e^{\pi\eta}/(2\pi\eta^{2\gamma+1}) . \tag{2.54}$$

III. DESCRIPTIONS OF ATOMIC SYSTEM AND CLOSE-COUPLING EQUATIONS

We consider an atomic system consisting of a nucleus of charge $Z_{\rm nuc}$ together with $N+1$ electrons. We are interested in bound states and in states with one electron in the continuum. We define such states as

$$\mathcal{A}[\Psi,\psi]^{J,M}=\mathcal{A}\sum C(J_a jJ;M_a mM)\,|J_aM_a\rangle\,|jm\rangle=(N+1)^{1/2}\sum_i(-1)^{N+1-i}[\Psi(r^{-i}),\psi(r_i)]^{J,M} , \tag{3.1}$$

where $\Psi=|J_aM_a\rangle$ is a wave function for the N-electron system, and $\psi=|jm\rangle$ is a single-particle wave function. The number of coupled channels is the total number of allowed states $\mathcal{A}(\Psi,\psi)^{J,M}$ appropriate for the total angular momentum J. Substituting $\Theta=\sum\mathcal{A}(\Psi,\psi)^{J,M}$ in $H_{N+1}\Theta=E\Theta$, where

$$H_{N+1}=\sum_{i=1}^{N+1}(\vec{\alpha}\cdot\vec{\rm p}_i+\beta m-\alpha Z_{\rm nuc}/r_i)+\sum_{i<j}1/r_{ij} , \tag{3.2}$$

we obtain the close-coupling equations as

$$\frac{dP_i}{dr}+\frac{\kappa_i}{r}P_i-\left[m+\epsilon_i+\frac{\alpha Z}{r}\right]Q_i+\sum_j(V_{ij}+W_{ij})Q_j=0 , \tag{3.3}$$

$$\frac{dQ_i}{dr}-\frac{\kappa_i}{r}Q_i-\left[m-\epsilon_i-\frac{\alpha Z}{r}\right]P_i-\sum_j(V_{ij}+W_{ij})P_j=0 , \tag{3.4}$$

where $Z = Z_{\text{nuc}}$, V_{ij} is the direct potential, and W_{ij} is the exchange kernel. The total energy is

$$E = E_i + \epsilon_i \ , \tag{3.5}$$

E_i being the energy for the channel i in the N-electron system.

The direct potential is defined by

$$V_{ij}(r_{N+1}) = \text{Ang}\left\langle [\Psi_i, \psi_i(r_{N+1})] \left| \sum_{k=1}^{N} 1/r_{k,N+1} \right| [\Psi_j, \psi_j(r_{N+1})] \right\rangle \ , \tag{3.6}$$

where the symbol Ang means that only the radial integral of the electron with coordinate r_{N+1} is left out. We may choose a radius r_0 such that when $r > r_0$, the exchange can be neglected. Since $r_{N+1} > r_k$ for $k = 1, \ldots, N$ when $r > r_0$, we expand

$$\sum_{k=1}^{N} 1/r_{k,N+1} = \sum_{\lambda=0}^{\infty} (r_{N+1})^{-\lambda-1} \sum_{k=1}^{N} r_k^{\lambda} P_{\lambda}(\cos\theta_{k,N+1}) \ . \tag{3.7}$$

The close-coupling equations may be written as

$$\frac{d}{dr}P_i + \frac{\kappa_i}{r}P_i - \left[m + \epsilon_i + \frac{\alpha Z}{r} \right] Q_i + \sum_{j=1}^{n} \sum_{\lambda=1}^{l} a_{ij}^{\lambda} r^{-\lambda-1} Q_j = 0 \ , \quad i = 1, \ldots, n \tag{3.8}$$

$$\frac{d}{dr}Q_i - \frac{\kappa_i}{r}Q_i - \left[m - \epsilon_i - \frac{\alpha Z}{r} \right] P_i + \sum_{j=1}^{n} \sum_{\lambda=1}^{l} a_{ij}^{\lambda} r^{-\lambda-1} P_j = 0 \ , \quad r > r_0 \tag{3.9}$$

where $Z = Z_{\text{nuc}} - N$, n is the number of channels, and the coefficients

$$a_{ij}^{\lambda} = \text{Ang}\left\langle [\Psi_i, \psi_i(r_{N+1})] \left| \sum_{k=1}^{N} r_k^{\lambda} P_{\lambda}(\cos\theta_{k,N+1}) \right| [\Psi_j, \psi_j(r_{N+1})] \right\rangle \ , \tag{3.10}$$

where the maximum value of λ denoted by l depends on the channels i and j.

The asymptotic solutions of the close-coupling equations have not been obtained numerically. In the relativistic R-matrix method[8,9] or in-out method,[10] Eqs. (3.8) and (3.9) were reduced to their counterparts in nonrelativistic theory. We may write the close-coupling equations in a simple matrix form as

$$(D_+ + W_+ + \epsilon_+)F = 0 \ , \tag{3.11}$$

where D_+ and ϵ_+ are diagonal matrices and W_+ and F are nondiagonal matrices. Each element of matrices D_+, W_+, and ϵ_+ is a 2×2 matrix defined as

$$(D_+)_{ij} = \begin{bmatrix} \delta_{ij}\dfrac{d}{dr} & 0 \\ 0 & \delta_{ij}\dfrac{d}{dr} \end{bmatrix} , \tag{3.12}$$

$$(W_+)_{ij} = \begin{bmatrix} \delta_{ij}\kappa_i/r & -\delta_{ij}(m + \alpha Z/r) + U_{ij} \\ -\delta_{ij}(m - \alpha Z/r) - U_{ij} & -\delta_{ij}\kappa_i/r \end{bmatrix} , \tag{3.13}$$

$$(\epsilon_+)_{ij} = \begin{bmatrix} 0 & -\delta_{ij}\epsilon_i \\ \delta_{ij}\epsilon_i & 0 \end{bmatrix} , \tag{3.14}$$

where, for $r < r_0$, $U_{ij}(r)$ may include direct and exchange potentials and, for $r > r_0$,

$$U_{ij}(r) = \sum_{\lambda=1}^{l} a_{ij}^{\lambda} r^{-\lambda-1} \ , \tag{3.15}$$

and each element of F is a 2×1 column $\binom{P}{Q}$.

The potentials $U_{ij}(r)$ are not of finite range. For finite r, the solutions cannot be expressed as linear combinations of Coulomb functions. In Sec. IV we shall consider a simple-model problem with finite-range potentials.

IV. SOLUTIONS OF THE COUPLED EQUATIONS

A. Simple-model problem

The simple model is the same as in the nonrelativistic theory of Seaton.[4] We define three regions $0 \le r_0 \le r_1 < \infty$ such that (i) in the region $0 \le r \le r_0$, $rU_{ii}(r)$ and $r^{-q_{ij}}U_{ij}(r)$ are analytic functions, where $q_{ij} \ge |\gamma_i - \gamma_j|$ and $i \ne j$; (ii) in the region $r_0 \le r \le r_1$, all the elements $U_{ij}(r)$ are piecewise continuous; (iii) in the region $r > r_1$, all the elements

$$U_{ij}(r) = 0 \ . \tag{4.1}$$

We shall assume that the $U_{ij}(r)$ are real and symmetric. For this simple-model problem, we obtain coupled differential equations of the form (3.11). With N_t equations of the type (3.11), we have N_t linearly independent sets of solutions.

The solutions $F(E;r)$ have the boundary conditions at the origin as $F(E;r) \to 0$, for $r \to 0$. Specifically, we take

$$\lim_{r\to 0}[r^{-\gamma_i}F_{ij}(E;r)] = \begin{bmatrix} \delta_{ij} \\ \delta_{ij}\alpha Z/(\kappa_i - \gamma_i) \end{bmatrix} \ . \tag{4.2}$$

Each suffix $j = 1, \ldots, N_t$ specifies a particular set of solutions. For all finite r, the solutions $F(E;r)$ will be analytic functions of E, following the proof given by Ham[11] in the nonrelativistic theory. Because of condition (iii), we have

$$F(E;r) = f(\epsilon,\kappa;r)I + g(\epsilon,\kappa;r)J \ , \quad r > r_1 \tag{4.3}$$

where $f(\epsilon,\kappa;r)$ and $g(\epsilon,\kappa;r)$ are diagonal matrices with diagonal elements $f(\epsilon_i,\kappa_i;r)$ and $g(\epsilon_i,\kappa_i;r)$, respectively, and I and J are nondiagonal matrices. Since f, g, and $F(E;r)$ are analytic functions of E for all finite values of r, $I(E)$ and $J(E)$ will also be analytic functions of E.

Substituting expressions (2.46) and (2.45) for f and g into Eq. (4.3), we obtain

$$F(E;r) = \varphi^- \frac{N_1}{c_1\Gamma(1+\gamma-\nu)}[I + (-G + A\cot\pi a)J] - \varphi^+ \frac{N_1}{c_1\Gamma(1+\gamma+\nu)}[I + (-G + DiA)J] \ , \quad r > r_1 \ . \tag{4.4}$$

Multiplying both sides by $[I + (-G + A\cot\pi a)J]^{-1}c_1\Gamma(1+\gamma-\nu)/N_1$, we have

$$F(S;r) = F(E;r)[I + (-G + A\cot\pi a)J]^{-1}c_1\Gamma(1+\gamma-\nu)/N_1, \quad r > r_1 \tag{4.5}$$

where

$$F(S;r) = \varphi^- - \varphi^+ S \ , r > r_1 \tag{4.6}$$

and where

$$S = \frac{N_1}{c_1\Gamma(1+\gamma+\nu)}[I + (-G + DiA)J][I + (-G + A\cot\pi a)J]^{-1}\frac{c_1\Gamma(1+\gamma-\nu)}{N_1} \ . \tag{4.7}$$

This scattering matrix S is valid for $|\arg(z)| < 3\pi/2$, where $z = 2\lambda r$.

B. Scattering matrix for ϵ real

When ϵ is real, we obtain

$$S = \frac{N_1}{c_1\Gamma(1+\gamma+\nu)}[I + (\mathcal{G} + iB)J][I + (\mathcal{G} + CB)J]^{-1}\frac{c_1\Gamma(1+\gamma-\nu)}{N_1} \ . \tag{4.8}$$

The matrix U is real and symmetric. We may take $F(E;r)$ to be real and I and J to be real. We define F^T as the transpose of F and take the following integral with the upper limit $r_2 > r_1$:

$$\int_0^{r_2}\{F^T(D_+ + W_+ + \epsilon_+)F - [(D_+ + W_+ + \epsilon_+)F]^T F\}dr = 0 \ . \tag{4.9}$$

Since the terms with W_+ and ϵ_+ cancel out, we find that

$$I^T J = J^T I \ , \tag{4.10}$$

and from this we have

$$(IJ^{-1})^T = (J^{-1})^T J^T I J^{-1} = IJ^{-1} \tag{4.11}$$

so that IJ^{-1} is symmetric. Thus we may write the scattering matrix in a more symmetric form

$$S=\frac{N_1}{c_1\Gamma(1+\gamma+\nu)}B^{1/2}[1+iB^{1/2}(IJ^{-1}+\mathcal{G})^{-1}B^{1/2}][1+CB^{1/2}(IJ^{-1}+\mathcal{G})^{-1}B^{1/2}]^{-1}B^{-1/2}\frac{c_1\Gamma(1+\gamma-\nu)}{N_1} . \tag{4.12}$$

Defining

$$K=B^{1/2}(IJ^{-1}+\mathcal{G})^{-1}B^{1/2} \tag{4.13}$$

we express S in terms of K as

$$S=u(1+iK)(1+CK)^{-1}v , \tag{4.14}$$

where, for $\epsilon<m$,

$$u=[i(\gamma-\nu)]^{1/2}\exp(-i\pi a/2)M , \tag{4.15}$$

$$v=\frac{2\pi[i(\gamma-\nu)]^{1/2}\exp(-i\pi a/2)M}{[1-\exp(-2\pi ia)]} , \tag{4.16}$$

and, for $\epsilon>m$,

$$u=\exp(i\omega) , \tag{4.17}$$

$$v=\exp(i\omega) , \tag{4.18}$$

and where

$$M=[\Gamma(1+\gamma+\nu)\Gamma(1-\gamma+\nu)]^{-1/2} , \tag{4.19}$$

$$\omega=\arg\Gamma(1+\gamma-i\eta) . \tag{4.20}$$

Here the identity $\Gamma(z^*)=[\Gamma(z)]^*$ is used, where the asterisk stands for the complex conjugate. It should be noted that the indices of diagonal matrix elements in Eqs. (4.15)–(4.20) are omitted.

In the one-channel case, since $\varphi^-\to\exp(\lambda r)$ when $\epsilon<m$, we require the coefficient of φ^- in Eq. (4.4) to vanish, i.e.,

$$I+[\mathcal{G}_<-\cot(\pi a)B_<]J=0 . \tag{4.21}$$

Letting $\beta(\epsilon)=-J/I$ we obtain

$$\beta(\epsilon)=1/[\mathcal{G}_<-\cot(\pi a)B_<] . \tag{4.22}$$

Defining the quantum defect $\mu=a+n-k$, where n is the principal quantum number, we have $\cot\pi a=\cot\pi\mu$. Generalizing to the many-channel problem we define

$$\tan\pi\mu=B_<^{1/2}(IJ^{-1}+\mathcal{G}_<)^{-1}B_<^{1/2} . \tag{4.23}$$

When all channels are closed, $\tan\pi\mu=K$.

C. Functions s and c for ϵ real

Using Eq. (4.14) and multiplying both sides of Eq. (4.6) by $-v^{-1}(1+CK)/(2i)$, we obtain

$$F(K;r)=F(S;r)[-v^{-1}(1+CK)/(2i)] , \quad r>r_1 \tag{4.24}$$

where

$$F(K;r)=s+cK \tag{4.25}$$

and where

$$s=(\varphi^+u-\varphi^-v^{-1})/(2i) , \tag{4.26}$$

$$c=(\varphi^+u+i\varphi^-v^{-1}C)/2 . \tag{4.27}$$

The functions $F(K;r)$ for $r>r_1$ are also solutions of coupled equations. Using Eqs. (2.46) and (2.47) we obtain

$$s=(\alpha Z/2)^{1/2}B^{1/2}f , \tag{4.28}$$

$$c=-(\alpha Z/2)^{1/2}B^{-1/2}(g-\mathcal{G}f) . \tag{4.29}$$

For $\epsilon>m$, using Eqs. (4.17) and (4.18)

$$s=(\varphi^+e^{i\omega}-\varphi^-e^{-i\omega})/(2i) , \tag{4.30}$$

$$c=(\varphi^+e^{i\omega}+\varphi^-e^{-i\omega})/2 . \tag{4.31}$$

Their asymptotic forms are

$$s\sim\begin{vmatrix}[(m+\epsilon)/p]^{1/2}\sin\theta\\ [(\epsilon-m)/p]^{1/2}\cos\theta\end{vmatrix} , \tag{4.32}$$

$$c\sim\begin{vmatrix}[(m+\epsilon)/p]^{1/2}\cos\theta\\ -[(\epsilon-m)/p]^{1/2}\sin\theta\end{vmatrix} , \tag{4.33}$$

where

$$\theta=pr+\eta\ln 2pr-\pi\gamma/2+\xi+\arg\Gamma(1+\gamma-i\eta) .$$

For $\epsilon<m$, using Eqs. (4.15), (4.16), (2.18), and (2.19),

$$s=e^{-i\pi a}y^--\sin(\pi a)y^+ , \tag{4.34}$$

$$c=\exp[-i\pi(a-\tfrac{1}{2})]y^-+\cos(\pi a)y^+ , \tag{4.35}$$

where

$$y^-=2^{-1}[\lambda(\nu'-\kappa)\Gamma(1+\gamma+\nu)\Gamma(1-\gamma+\nu)]^{-1/2}y_5 , \tag{4.36}$$

$$y^+=-(2\pi)^{-1}\{\Gamma(1+\gamma+\nu)\Gamma(1-\gamma+\nu)/[\lambda(\nu'-\kappa)]\}^{1/2}\exp[-i\pi(a-b)]y_7 . \tag{4.37}$$

The pair s and c are equivalent to the pair f and g in Eqs. (25a) and (25b) of Johnson and Cheng[1] and in Eq. (3) of Lee and Johnson.[2]

D. All channels open

When all channels are open ($\epsilon_i > m$ for all i)

$$S = e^{i\omega}(1+iK)(1-iK)^{-1}e^{i\omega} . \tag{4.38}$$

A phase matrix δ may be defined by

$$K = \tan\delta . \tag{4.39}$$

In the open channel case, we have

$$\tan\delta = B_{>}^{1/2}(IJ^{-1}+\mathcal{G}_{>})^{-1}B_{>}^{1/2} . \tag{4.40}$$

Substituting in the expressions for $B_{>}$ and $\mathcal{G}_{>}$ from Eqs. (2.51) and (2.52) and again defining $\beta(\epsilon) = -J/I$, we obtain

$$\beta(\epsilon) = (\mathcal{G}_{>} - B_{>}^{1/2}\cot\delta\, B_{>}^{1/2})^{-1} . \tag{4.41}$$

In general, using Eqs. (4.23) and (4.40) and the condition that $\alpha_r(\nu,\gamma)$ goes to $\alpha_r(i\eta,\gamma)$ continuously across the threshold, i.e., $\alpha_r(\nu,\gamma)$ goes to $\bar{\alpha}(\eta,\gamma)(1+\cos\pi b\, e^{-2\pi\eta})$, we find that the connection between the phase shift and quantum defect is

$$\cot\delta = (1+\cos\pi b\, e^{-2\pi\eta})^{1/2} \times \cot\pi\mu(1+\cos\pi b\, e^{-2\pi\eta})^{1/2} + \sin\pi b\, e^{-2\pi\eta} . \tag{4.42}$$

This matrix relation generalizes Eq. (4) of Johnson and Cheng.[1]

E. All channels closed

When all channels are closed ($\epsilon_i < m$ for all i) we put

$$Y(r) = F(S;r)S^{-1}V = \varphi^{-}S^{-1}V - \varphi^{+}V \quad \text{for } r > r_1 \tag{4.43}$$

where V is a column vector. For closed channels, φ^{-} increases exponentially in the asymptotic region. For $Y(r)$ to represent a bound state we must, therefore, have

$$S^{-1}V = 0 . \tag{4.44}$$

Using Eq. (4.14) with $C = -\cot\pi a$, the above equation may be written

$$v^{-1}\cot\pi a\,(\tan\pi a - K)(1+iK)^{-1}u^{-1}V = 0 . \tag{4.45}$$

Putting

$$X = (1+iK)^{-1}u^{-1}V \tag{4.46}$$

Eq. (4.45) will be satisfied if

$$(\tan\pi a - K)X = 0 , \tag{4.47}$$

which requires that

$$|\tan\pi a - K| = 0 . \tag{4.48}$$

For the one-channel case we have $K = \tan\pi\mu$ and the solution of Eq. (4.48) is $a = \mu - n + k$.

The bound state has an asymptotic form

$$Y = -\varphi^{+}V \quad \text{for } r > r_1 . \tag{4.49}$$

We may express Y in terms of the real function Y_5 as

$$Y = MY_5N_5 \quad \text{for } r > r_1 \tag{4.50}$$

where Y_5 is a diagonal matrix with diagonal elements of y_5. Using expression (2.18) and

$$V = u(1+iK)X , \tag{4.51}$$

we obtain

$$N_5 = [\lambda(-\nu'+\kappa)\cos^2\pi a]^{-1/2}X . \tag{4.52}$$

Let us define a diagonal matrix

$$\tau = B_{<}^{-1}\tan\pi a . \tag{4.53}$$

Using Eq. (4.47) we obtain

$$[\tau - (IJ^{-1}+\mathcal{G}_{<})^{-1}]B_{<}^{1/2}X = 0 . \tag{4.54}$$

The condition (4.48) is equivalent to

$$|\tau - (IJ^{-1}+\mathcal{G}_{<})^{-1}| = 0 . \tag{4.55}$$

F. Some channels open and some closed

When some channels are open and some closed, we write F as a partitioned matrix

$$F = \begin{bmatrix} F_{oo} & F_{oc} \\ F_{co} & F_{cc} \end{bmatrix} , \tag{4.56}$$

where o and c indicate "open" and "closed." The energy parameters ϵ_i are put in a decreasing order and

$$\begin{aligned} &\epsilon_i \geq m \quad \text{for } i \leq N_o \\ &\epsilon_i < m \quad \text{for } i > N_o \end{aligned} \tag{4.57}$$

where N_o is the number of open channels.

We further define

$$F_o = \begin{bmatrix} F_{oo} \\ F_{co} \end{bmatrix} \tag{4.58}$$

and require that

$$F_{co} \to 0 \quad \text{for } r \to \infty . \tag{4.59}$$

At this stage, we introduce two matrices $\mathcal{X}$ and $\mathcal{S}$ as those defined by Seaton,[12]

$$\mathcal{X}=(i-K)(i+K)^{-1}, \tag{4.60}$$

$$\mathcal{S}=(i-K)(T+K)^{-1}, \tag{4.61}$$

where $T=C^{-1}$. From Eq. (4.14) we have

$$S=-iu\mathcal{S}Tv . \tag{4.62}$$

The matrix $\mathcal{X}$ is defined in solutions $F(\mathcal{X};r)$ to coupled equations as

$$F(\mathcal{X};r)=\varphi_{-}-\varphi_{+}\mathcal{X}, \quad r>r_1 \tag{4.63}$$

where

$$\varphi_{+}=c+is, \tag{4.64}$$

$$\varphi_{-}=c-is . \tag{4.65}$$

Eliminating K between Eqs. (4.60) and (4.61), we obtain

$$\mathcal{S}[(T+i)+(T-i)\mathcal{X}]=2i\mathcal{X} . \tag{4.66}$$

In turn, we have

$$\mathcal{S}_{co}=\mathcal{X}_{co}-\mathcal{X}_{cc}[\mathcal{X}_{cc}-\exp(2\pi ia)]^{-1}\mathcal{X}_{co}, \tag{4.67}$$

$$\mathcal{S}_{oo}=\mathcal{X}_{oo}-\mathcal{X}_{oc}[\mathcal{X}_{cc}-\exp(2\pi ia)]^{-1}\mathcal{X}_{co} . \tag{4.68}$$

From Eq. (4.61) we obtain

$$\mathcal{S}_{oo}=(i-K'_{oo})(i+K'_{oo})^{-1}, \tag{4.69}$$

where

$$K'_{oo}=K_{oo}-K_{oc}(K_{cc}-\tan\pi a)^{-1}K_{co} . \tag{4.70}$$

In atomic physics computations, we are interested in solutions satisfying the condition (4.59) and having the forms as

$$F_{oo}(K';r)=s_o+c_oK', \quad r>r_1 \tag{4.71}$$

$$F_{oo}(\mathcal{S}';r)=\varphi_{-,o}-\varphi_{+,o}\mathcal{S}', \quad r>r_1 \tag{4.72}$$

where K' and $\mathcal{S}'$ are usually defined as the reactance and scattering matrices and have dimensions (N_o,N_o). We express $F_o(K')$ in terms of $F(K)$ as

$$F_o(K')=F(K)\begin{bmatrix}1_{oo}\\ D_{co}\end{bmatrix} . \tag{4.73}$$

This gives

$$F_{oo}(K')=F_{oo}(K)+F_{oc}(K)D_{co}, \tag{4.74}$$

$$F_{co}(K')=F_{co}(K)+F_{cc}(K)D_{co} . \tag{4.75}$$

From Eq. (4.25), for $r>r_1$,

$$F_{co}(K')=c_cK_{co}+(s_c+c_cK_{cc})D_{co} . \tag{4.76}$$

Using Eqs. (4.34) and (4.35) this gives

$$F_{co}(K')=y^{-}e^{-i\pi a}[iK_{co}+(1+iK_{cc})D_{co}]+y^{+}\{\cos(\pi a)K_{co}-[\sin(\pi a)-\cos(\pi a)K_{cc}]D_{co}\} . \tag{4.77}$$

The coefficient of y^{+} should vanish in order to satisfy the condition (4.59), we obtain

$$D_{co}=-(K_{cc}-\tan\pi a)^{-1}K_{co} \tag{4.78}$$

and

$$F_{co}=-y^{-}(K_{cc}\cos\pi a-\sin\pi a)^{-1}K_{co} . \tag{4.79}$$

From Eq. (4.74),

$$F_{oo}(K')=s_o+c_o(K_{oo}+K_{oc}D_{co}) . \tag{4.80}$$

Using Eq. (4.71), we obtain

$$K'=K_{oo}-K_{oc}(K_{cc}-\tan\pi a)^{-1}K_{co} . \tag{4.81}$$

K' is the same as K'_{oo} in Eq. (4.70).

Similarly, we express $F_o(\mathcal{S}')$ in terms of $F(\mathcal{X})$ as

$$F_o(\mathcal{S}')=F(\mathcal{X})\begin{bmatrix}1_{oo}\\ E_{co}\end{bmatrix} \tag{4.82}$$

and choosing E_{co} to eliminate the exponentially increasing functions, using Eqs. (4.64) and (4.65), we obtain

$$E_{co}=-[\mathcal{X}_{cc}-\exp(2\pi ia)]^{-1}\mathcal{X}_{co}, \tag{4.83}$$

$$F_{co}=2iy^{-}e^{i\pi a}[\mathcal{X}_{cc}-\exp(2\pi ia)]^{-1}\mathcal{X}_{co}, \tag{4.84}$$

and

$$\mathcal{S}'=\mathcal{X}_{oo}-\mathcal{X}_{oc}[\mathcal{X}_{cc}-\exp(2\pi ia)]^{-1}\mathcal{X}_{co} . \tag{4.85}$$

$\mathcal{S}'$ is the same as $\mathcal{S}_{oo}$ in Eq. (4.68).

G. Normalization

If the matrix F has elements $y=\binom{P}{Q}$, we define a function matrix $\tilde{F}$ with elements $\tilde{y}=(\underline{Q}_{\,P})$. Similarly, we define $\tilde{\varphi}^{-}$ and $\tilde{\varphi}^{+}$ for φ^{-} and φ^{+}, respectively. Furthermore, we define two diagonal matrices D_{-} and ϵ_{-} and a nondiagonal matrix W_{-} with elements as

$$(D_{-})_{ij}=\begin{bmatrix}0 & \delta_{ij}\dfrac{d}{dr}\\ -\delta_{ij}\dfrac{d}{dr} & 0\end{bmatrix}, \tag{4.86}$$

$$(W_-)_{ij}=\begin{bmatrix}-\delta_{ij}(m-\alpha Z/r)-U_{ij} & -\delta_{ij}\kappa_i/r\\ -\delta_{ij}\kappa_i/r & \epsilon_{ij}(m+\alpha Z/r)-U_{ij}\end{bmatrix}, \quad (4.87)$$

$$(\epsilon_-)_{ij}=\begin{bmatrix}\delta_{ij}\epsilon_i & 0\\ 0 & \delta_{ij}\epsilon_i\end{bmatrix}. \quad (4.88)$$

If F is an eigenfunction for total energy E and F' for energy E', then

$$(D_-+W_-+\epsilon_-)F=0\ , \quad (4.89)$$

$$(D_-+W_-+\epsilon'_-)F'=0\ , \quad (4.90)$$

where, by Eq. (3.5),

$$\epsilon'_i-\epsilon_i=E'-E \quad (4.91)$$

is independent of channel index i; thus, we shall suppress the subscript i.

Defining $F^\dagger$ as the Hermitian conjugate of F, we have

$$\int_0^{r_2}\{F^\dagger(D_-+W_-+\epsilon'_-)F' -[(D_-+W_-+\epsilon_-)F]^\dagger F'\}dr=0\ . \quad (4.92)$$

Since F and F' are both zero at the origin and the terms with W_- cancel out, we obtain

$$(\epsilon-\epsilon')\int_0^{r_2}F^\dagger F'dr=[F^\dagger\widetilde{F}']_{r=r_2}\ , \quad (4.93)$$

where $\epsilon-\epsilon'$ is just a number. For a large value of r_2, we may take $F=F(S)$ and $F'=F'(S)$ and, therefore,

$$(\epsilon-\epsilon')\int_0^\infty F^\dagger F'dr =\lim_{r\to\infty}(\varphi^- -\varphi^+S)^\dagger(\widetilde{\varphi}^- -\widetilde{\varphi}^+S)'\ . \quad (4.94)$$

We consider first the case when all channels are open. Putting $\epsilon'=\epsilon$ and using Eqs. (2.24) and (2.25) in the limit $r\to\infty$, we have $(\varphi^+)^\dagger\widetilde{\varphi}^- =(\varphi^-)^\dagger\widetilde{\varphi}^+=0$, $(\varphi^-)^\dagger\widetilde{\varphi}^-=-2i$, $(\varphi^+)^\dagger\widetilde{\varphi}^+=2i$, thus

$$S^\dagger S=1\ . \quad (4.95)$$

For $\epsilon'\neq\epsilon$, we obtain

$$\int_0^\infty F^\dagger F'dr=4\pi\delta(\epsilon-\epsilon')\ . \quad (4.96)$$

If some channels are open and some closed, Eq. (4.96) remains valid for matrix elements associated with open channels. Explicitly, we have

$$\int_o^\infty F_o^\dagger F'_o dr=4\pi\delta(\epsilon_o-\epsilon'_o)\ , \quad (4.97)$$

where F_o is defined as in Eq. (4.58), and ϵ_o is a diagonal matrix with dimensions (N_o,N_o).

When all channels are closed, we take an eigenfunction

$$Y=FS^{-1}V \text{ with } S^{-1}V=0\ , \quad (4.98)$$

and assume

$$Y'=(FS^{-1}V)'\ , \quad (4.99)$$

where

$$V'=u'(1+i\tan\pi a')X' \quad (4.100)$$

such that Y' are solutions of Eq. (4.90) for energies which are not eigenvalues and vectors V' and X' are not yet defined. We may take $X'=X$.

From Eq. (4.94), we have

$$(\epsilon'-\epsilon)\int_0^\infty Y^\dagger Y'dr =\lim_{r\to\infty}(\varphi^+V)^\dagger(\widetilde{\varphi}^-S^{-1}-\widetilde{\varphi}^+)'V'\ . \quad (4.101)$$

Since φ^+ vanishes at infinity, the norm of Y is

$$\text{Norm}(Y) =\int_0^\infty Y^\dagger Y\,dr =\lim_{r\to\infty}\lim_{\epsilon'\to\epsilon}V^\dagger(\varphi^+)^\dagger(\widetilde{\varphi}^-S^{-1}V)'/(\epsilon'-\epsilon)\ , \quad (4.102)$$

where $(\varphi^-)'\to\varphi^-$, when $\epsilon'\to\epsilon$. Using Eqs. (2.21) and (2.22),

$$(\varphi^+)^\dagger\widetilde{\varphi}^-=2\exp(i\pi a)\ , \quad (4.103)$$

and hence

$$\text{Norm}(Y)=\lim_{\epsilon'\to\epsilon}V^\dagger 2\exp(i\pi a)(S^{-1}V)'/(\epsilon'-\epsilon)\ . \quad (4.104)$$

Using Eq. (4.45) with $X'=X$, we have

$$(S^{-1}V)'=[v^{-1}\cot\pi a(\tan\pi a-K)]'X\ . \quad (4.105)$$

Since $K=\tan\pi\mu$, we obtain, to first order in $\epsilon'-\epsilon$,

$$(S^{-1}V)'=v^{-1}\cot\pi a(\epsilon'-\epsilon) \times\left[\frac{\partial}{\partial\epsilon}(\tan\pi a-\tan\pi\mu)'\right]_{\epsilon'=\epsilon}X\ . \quad (4.106)$$

From $a=\gamma-\nu$, we have

$$\left[\frac{\partial}{\partial\epsilon}(\tan\pi a-\tan\pi\mu)'\right]_{\epsilon'=\epsilon} =-\pi\alpha Zm^2\zeta(\nu)/(\lambda^3\cos^2\pi a)\ , \quad (4.107)$$

where

$$\zeta(\nu)=(1+d\mu/d\nu)\ . \tag{4.108}$$

The normalization integral becomes

$$\mathrm{Norm}(Y)=V^{\dagger}2\exp(i\pi a)v^{-1}\cot\pi a \times\left[-\frac{\pi\alpha Z m^2}{\lambda^3}\right]\frac{\zeta(\nu)}{\cos^2\pi a}X\ . \tag{4.109}$$

Using Eqs. (4.51) and (4.52) to express $V^{\dagger}$ and X in terms of N_5, we find that $Y=MY_5N_5$ will be normalized to

$$\mathrm{Norm}(Y)=1 \tag{4.110}$$

provided that

$$N_5^{\dagger}(M^*/M)[2(\nu'-\kappa)(\nu')^2\zeta(\nu)/(\alpha Z)]N_5=1\ . \tag{4.111}$$

For the one-channel case, this is equivalent to Eq. (69) of Johnson and Cheng.[1]

V. DISCUSSION OF THE CLOSE-COUPLING APPROXIMATION

There are two differences between the close-coupling approximation and the simple model, i.e., (i) the exchange integral operators W_{ij} in the internal region and (ii) the long-range potentials in the external region. With fixed boundary conditions of Eq. (4.2) the solutions to the close-coupling equations (3.3) and (3.4) may cause the exchange integral to diverge, if the exponential increase of these solutions is faster than the exponential decrease of the functions $y(\epsilon,\kappa;r)$ used to construct the core state Ψ. In practical computation, we may cut off the exponential decreasing tail by setting the values within 10^{-6} to zero, and impose the orthogonality condition $(y(\epsilon,\kappa;r)\,|\,F_{ij})=0$ for the component F_{ij} having the same κ.

In the presence of long-range potentials, the equalities for $r>r_1$ in the simple-model problem are replaced by asymptotic formulas valid in the limit $r\to\infty$. To solve Eqs. (3.3) and (3.4) in the asymptotic region is to obtain the K matrix.

For all channels open, the matrix K is obtained by computing solutions with asymptotic form

$$F(K;r)\sim s+cK\ . \tag{5.1}$$

For some channels closed, the matrix K is obtained from solutions $F_{ij}(K;r)$ with asymptotic forms, for $j=1$ to N_o,

$$F_{ij}(K;r)\sim\begin{cases} s_i\delta_{ij}+c_iK_{ij}\ , & i<N_o \quad (5.2)\\ 0\ , & i>N_o \quad (5.3)\end{cases}$$

where N_o is the number of open channels.

In nonrelativistic theory, the asymptotic solutions for a two-channel example are described in detail by Seaton.[4] In relativistic cases, the procedures will remain the same.

In the close-coupling eigenchannel analysis,[2] the K matrix is diagonalized by a unitary transformation matrix U as

$$U^{\dagger}KU=\tan\pi\mu\ , \tag{5.4}$$

where $\tan\pi\mu$ is a diagonal matrix. A function matrix $F(\mu;r)$ is introduced as

$$F(\mu;r)=F(K;r)U\cos\pi\mu\ . \tag{5.5}$$

Using Eq. (4.25) we obtain

$$F(\mu;r)\sim sU\cos\pi\mu+cU\sin\pi\mu\ . \tag{5.6}$$

This relation serves as the starting point for the eigenchannel analysis.

APPENDIX

When we write equations in atomic units, we usually shift the energy scale such that the origin $\epsilon=0$ is at the threshold and write c explicitly. For the Dirac-Coulomb equation, we have

$$(c\vec{\alpha}\cdot\vec{p}+\beta'c^2-Z/r)\psi(\vec{r})=\epsilon\psi(\vec{r})\ , \tag{A1}$$

where $\beta'=\beta-1$. We can write equations related to radial functions in atomic units using the following replacements:

$$\alpha\to 1/c,\quad m\to c,\quad \epsilon\to c+\epsilon/c\ ,$$

$$m+\epsilon\to 2c+\epsilon/c,\quad m-\epsilon\to -\epsilon/c\ ,$$

and

$$\gamma=[k^2-(\alpha Z)^2]^{1/2}\to\gamma=[k^2-(Z/c)^2]^{1/2}\ ,$$

$$\lambda=(m^2-\epsilon^2)^{1/2}\to\lambda=[-2\epsilon-(\epsilon/c)^2]^{1/2}\ ,$$

$$p=(\epsilon^2-m^2)^{1/2}\to p=[2\epsilon+(\epsilon/c)^2]^{1/2}\ ,$$

$$\nu=\alpha Z\epsilon/\lambda\to\nu=(1/c)Z(c+\epsilon/c)/\lambda\ ,$$

$$\nu'=\alpha Zm/\lambda\to\nu'=Z/\lambda\ ,$$

$$\eta=\alpha Z\epsilon/p\to\eta=(1/c)Z(c+\epsilon/c)/p\ ,$$

$$\eta'=\alpha Zm/p\to\eta'=Z/p\ .$$

For example, the radial Dirac-Coulomb equations become

$$\frac{dP}{dr}+\frac{\kappa}{r}P-\left[2c+\frac{\epsilon}{c}+\frac{Z}{cr}\right]Q=0\ , \tag{A2}$$

$$\frac{dQ}{dr}-\frac{\kappa}{r}Q+\left[\frac{\epsilon}{c}+\frac{Z}{cr}\right]P=0\ . \tag{A3}$$

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