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Boundary-Condition Constraints for the Shell Model: A Method for Nuclear Structure and Nuclear Reactions

W. TOBOCMAN* AND M. A. NAGARAJAN†
Physics Department, Case Institute of Technology, Cleveland, Ohio
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It is proposed that the asymptotic boundary conditions be used as constraints for shell-model calculations. Two formalisms which permit this to be done are presented. In one formalism the boundary conditions are introduced as constraints in a variational principle. In the other formalism Green's theorem is used to make the dependence on the boundary conditions explicit. The use of boundary-condition constraints permits the use of the shell-model method for scattering and reactions as well as for nuclear-structure calculations. It is suggested that the constrained-shell-model method will improve the representation of the nuclear surface and will provide the basis for a truly unified treatment of nuclear reactions. In such a unified treatment compound-nucleus resonances, direct-reaction transitions, and optical-model scattering will be generated from a single, fairly fundamental model.

I. INTRODUCTION

PERHAPS the most powerful method presently available for studying the nuclear many-body problem is the shell model or individual-particle model.[1] In this model the wave function is approximated by a finite linear combination of Slater determinants of given single-particle wave functions. The coefficients of this expansion are determined by diagonalizing the Hamiltonian in that portion of Hilbert space spanned by these Slater determinants. This model has been very successful in describing what might be called "volume properties" of nuclear bound states. These properties include excitation energies and electromagnetic and beta-decay transition rates. Phenomena that involve primarily the nuclear surface are not so well described by the shell model. Such phenomena are alpha decay and direct reactions. This shortcoming of the shell model is to be expected because the shell-model wave function does not have the correct asymptotic behavior.

In this paper we suggest a modification of the usual shell-model approach that should provide a better description of the nuclear surface. We propose that the shell-model approximate wave function be used only for the "inside region" or "compound-nucleus region" of configuration space where all the nucleons making up the system are relatively close to each other. In the "outside region" or "channel region" of configuration space the wave function is to be approximated by a sum of terms corresponding to all the various two-body channels that can be formed by the system. Each such term describes two noninteracting subnuclei whose relative-motion wave function is determined by the asymptotic boundary conditions and the energetics of the situation. The basic idea is that we force the inside-region shell-model wave function to have radial logarithmic derivatives at the boundaries separating the inside and outside regions that will assure smooth connection with the outside-region wave function.

Our objective, then, is to apply the shell model to calculate the nuclear wave function in the inside region. This wave function is required to satisfy certain boundary conditions on the boundary of the inside region. We will present two different formalisms that enable us to achieve our objective. In the first formalism we use the boundary conditions as constraints in a variational principle for the wave function. In the second formalism we use Green's theorem to relate the wave function in the inside region to its value and slope at the boundary.

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[1] J. P. Elliott and A. M. Lane, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 39, p. 241; A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic Press Inc., New York, 1963).

Achieving an improved treatment of the nuclear-bound-state problem is not the only application that can be found for our method. By using asymptotic boundary conditions appropriate for scattering instead of those appropriate for the bound-state problem we get a shell-model-type treatment for nuclear scattering and nuclear reactions. It would appear that our method may provide a practical basis for nuclear-reaction calculations in which compound-nucleus resonances, direct-interaction transitions, and optical-potential scattering can result in a natural way from a single model.

In Sec. II the boundary conditions to be used as constraints are formulated. In Sec. III the boundary conditions are used as constraints in a variational principle for the bound-state problem. An alternative derivation, based on Green's theorem, is presented in Sec. IV. The Green's-theorem-method results apply to the scattering case as well as the bound-state case. In Sec. V the Green's theorem method results are cast into a more symmetrical form and shown to be equivalent to the constrained-variation-method results.

II. THE ASYMPTOTIC BOUNDARY CONDITIONS

Suppose we have a system consisting of A nucleons in interaction. The energy is assumed to be low enough so that there are no three-or-more-body channels open. Then there exists a length R such that at points more distant than R from the center of mass of the system, the wave function of the system is well approximated by a sum over channels of the form

$$\Psi^{JM}\approx\sum_\alpha \Phi_\alpha{}^{JM}(\xi_\alpha,\Omega_\alpha)\chi_\alpha(r_\alpha), \tag{1}$$

where

$$\Phi_\alpha{}^{JM}(\xi_\alpha,\Omega_\alpha) = \sum_{M_\alpha m_\alpha M_{1\alpha} M_{2\alpha}} (J_\alpha l_\alpha M_\alpha m_\alpha | JM)(J_{1\alpha} J_{2\alpha} M_{1\alpha} M_{2\alpha} | J_\alpha M_\alpha) \times Y_{l_\alpha}{}^{m_\alpha}(\Omega_\alpha)\mathcal{A}\Phi_{1\alpha}{}^{J_{1\alpha}M_{1\alpha}}(\xi_{1\alpha})\Phi_{2\alpha}{}^{J_{2\alpha}M_{2\alpha}}(\xi_{2\alpha}), \tag{2}$$

$\Phi_{1\alpha}{}^{J_{1\alpha}M_{1\alpha}}(\xi_{1\alpha})$ = the internal-motion wave function of a bound state of $A_{1\alpha}$ nucleons having angular momentum $\hbar J_{1\alpha}$ with projection $\hbar M_{1\alpha}$;

$$A=A_{1\alpha}+A_{2\alpha}=A_{1\beta}+A_{2\beta}=\cdots.$$

$\mathcal{A}$ is the antisymmetrization operator;

$\mathbf{r}_\alpha=(r_\alpha,\Omega_\alpha)$ = the displacement of the center of mass of nucleus 1α from that of nucleus 2α.

The asymptotic boundary conditions satisfied by Ψ^{JM} are specified by giving the values of the logarithmic derivatives of the χ_α,

$$\mathfrak{L}_\alpha=[r_\alpha(d/dr_\alpha)\ln r_\alpha\chi_\alpha]_{R_\alpha}, \tag{3}$$

at the channel radii $R_\alpha>R$. For scattering cases the logarithmic derivative $\mathfrak{L}_\omega$ for the incident channel is excluded from the boundary condition specification.

Let $\mathcal{S}$ be a closed $(3A-1)$-dimensional hypersurface in our $3A$-dimensional configuration space which encloses the origin. This hypersurface will be chosen so that it is normal to each channel coordinate $\mathbf{r}_\alpha$ and so that the intersection with $\mathbf{r}_\alpha$ occurs at $r_\alpha=R_\alpha$. Thus the boundary conditions we are discussing are boundary conditions on the surface $\mathcal{S}$. Let $\mathcal{R}$ be the hypervolume enclosed by $\mathcal{S}$.

If ψ^{JM} is a given approximation to the true wave function Ψ^{JM}, then the requirement that ψ^{JM} satisfy the correct boundary conditions is the requirement that $\lambda_\alpha=\mathfrak{L}_\alpha$ where[2]

$$\lambda_\alpha=[r_\alpha(d/dr_\alpha)\ln r_\alpha(\Phi_\alpha{}^{JM}|\psi^{JM})]_{R_\alpha}. \tag{4}$$

It is assumed that R is large enough so that on hypersurface $\mathcal{S}$ the overlap of the different $\Phi_\alpha{}^{JM}$'s is negligible. For convenience we introduce the quantities

$$\gamma_\alpha=(\hbar^2R_\alpha/2m_\alpha)^{1/2}(\Phi_\alpha{}^{JM}|\psi^{JM})_{R_\alpha}, \tag{5}$$

$$\zeta_\alpha{}^{JM}=(\hbar^2R_\alpha/2m_\alpha)^{1/2}\Phi_\alpha{}^{JM}(\xi_\alpha,\Omega_\alpha)^* \times(\mathfrak{L}_\alpha+r_\alpha(d/dr_\alpha))(\delta(r_\alpha-R_\alpha)/R_\alpha{}^2), \tag{6}$$

$$\xi_\alpha{}^{JM}=(\hbar^2R_\alpha/2m_\alpha)^{1/2}\Phi_\alpha{}^{JM}(\xi_\alpha,\Omega_\alpha)^* \times(\lambda_\alpha+r_\alpha(d/dr_\alpha))(\delta(r_\alpha-R_\alpha)/R_\alpha{}^2), \tag{7}$$

where m_α is the reduced mass in channel α and γ_α will be called the reduced width for channel α. The boundary condition constraint can now be written

$$0=\langle\zeta_\alpha{}^{JM*}|\psi^{JM}\rangle=\gamma_\alpha(\mathfrak{L}_\alpha-\lambda_\alpha). \tag{8}$$

The superscript JM will be dropped henceforth.

For the bound-state case the logarithmic derivatives $\mathfrak{L}_\alpha$ are taken to equal those of the tails of two-body bound-state wave functions in channels α with separation energies $\epsilon_\alpha=E_{1\alpha}+E_{2\alpha}-E$. Here $E_{1\alpha}$ is the energy of nucleus 1α. For the scattering case the logarithmic derivatives $\mathfrak{L}_\alpha$ (excepting the one for the incident channel $\mathfrak{L}_\omega$) are chosen to have values appropriate to purely outgoing radial wave functions in the individual channels α with relative kinetic energies $-\epsilon_\alpha$.

III. THE VARIATIONAL METHOD FOR BOUND STATES

We seek a solution of the Schrödinger equation

$$(E-H)\psi=0 \tag{9}$$

which is regular in the inside or compound-nucleus region of configuration space: $r_\alpha<R_\alpha$ for all channels α. This solution is required to have radial logarithmic derivatives equal to $\mathfrak{L}_\alpha$ at the channel entrances $r_\alpha=R_\alpha$. This set of constraints is made manifest in the requirement $\langle\zeta_\alpha{}^*|\psi\rangle=0$ for all α.

The variational principle appropriate to our problem

[2] We will use the convention that in matrix elements involving $\Phi_\alpha{}^{JM}$ round brackets denote integration over all coordinates except r_α; pointed brackets denote integration over all coordinates.

is

$$0=\delta\{\langle\psi|H-E|\psi\rangle+2\sum D_\alpha\langle\psi|\zeta_\alpha\rangle\}, \quad (10)$$

where we have used the fact that ψ is real. The D_α are Lagrange multipliers associated with our boundary condition constraints. The Euler-Lagrange equation for our system is

$$(E-H)\psi=\sum_\alpha D_\alpha\zeta_\alpha. \quad (11)$$

The formal solution to this equation is

$$\psi=\sum_\alpha(E-H)^{-1}\zeta_\alpha D_\alpha. \quad (12)$$

The Lagrange multipliers D_α are determined by applying the constraint conditions to this solution:

$$\begin{aligned}0&=\sum_\alpha\langle\zeta_\beta^*|(E-H)^{-1}|\zeta_\alpha\rangle D_\alpha\\&=\sum_\alpha\mathfrak{M}_{\beta\alpha}D_\alpha.\end{aligned} \quad (13)$$

Let us introduce a complete set of real orthonormal wave functions φ_n for our system. Then Eqs. (12) and (13) become

$$\psi=\sum_{n,m}\varphi_n\langle\varphi_n|(E-H)^{-1}|\varphi_m\rangle\sum_\alpha\gamma_\alpha{}^m(\lambda_\alpha{}^m-\mathfrak{L}_\alpha)D_\alpha, \quad (14)$$

$$0=\sum_{n,m}(\lambda_\beta{}^n-\mathfrak{L}_\beta)\gamma_\beta{}^n\langle\varphi_n|(E-H)^{-1}|\varphi_m\rangle\times\sum_\alpha\gamma_\alpha{}^m(\lambda_\alpha{}^m-\mathfrak{L}_\alpha)D_\alpha, \quad (15)$$

where we have defined

$$\gamma_\alpha{}^n=(\hbar^2R_\alpha/2m_\alpha)^{1/2}(\Phi_\alpha|\varphi_n)_{R_\alpha} \quad (16)$$

and

$$\lambda_\alpha{}^n=[r_\alpha(d/dr_\alpha)\ln r_\alpha(\Phi_\alpha|\varphi_n)]_{R_\alpha} \quad (17)$$

so that

$$\langle\zeta_\alpha^*|\varphi_n\rangle=\gamma_\alpha{}^n(\lambda_\alpha{}^n-\mathfrak{L}_\alpha). \quad (18)$$

If the functions φ_n are eigenfunctions of H,

$$(E_n-H)\varphi_n=0, \quad (19)$$

then Eqs. (14) and (15) simplify to

$$\psi=\sum_{n,\alpha}\varphi_n(E-E_n)^{-1}\gamma_\alpha{}^n(\lambda_\alpha{}^n-\mathfrak{L}_\alpha)D_\alpha=\sum_n\varphi_nB_n \quad (20)$$

and

$$0=\sum_{n,\alpha}(\lambda_\beta{}^n-\mathfrak{L}_\beta)\gamma_\beta{}^n(E-E_n)^{-1}\gamma_\alpha{}^n(\lambda_\alpha{}^n-\mathfrak{L}_\alpha)D_\alpha=\sum_\alpha\mathfrak{M}_{\beta\alpha}D_\alpha. \quad (21)$$

The bound-state spectrum is found by determining the roots of

$$\det\mathfrak{M}=0. \quad (22)$$

Corresponding to each root $E^{(j)}$ of this equation there is a solution $D_\alpha{}^{(j)}$ of Eq. (21). Substituting these $D_\alpha{}^{(j)}$ back into Eq. (20) gives the associated bound-state wave function $\psi^{(j)}$.

In the conventional shell-model approach one diagonalizes the Hamiltonian H in the space spanned by a finite number of Slater determinants. This is the prescription provided by our variational principle if we ignore the boundary-condition constraints and seek the best representation of the wave function in terms of the finite set of Slater determinants. Including the constraints leads instead to Eqs. (14) and (15), where now the φ_n are the given Slater determinants and the sums over m and n include only members of the given finite set. If instead of this we let the φ_n represent the different linear combinations of the Slater determinants which are eigenfunctions of H in the space spanned by the finite set of Slater determinants, then we have Eqs. (20) and (21).

The imposition of boundary condition constraints on a shell-model calculation is thus seen to be a very straightforward procedure. First, one does a conventional shell-model calculation to determine a set of approximate eigenvalues E_n and eigenfunctions φ_n of the Hamiltonian. From the φ_n the reduced widths $\gamma_\alpha{}^n$ and logarithmic derivatives $\lambda_\alpha{}^n$ are calculated. These quantities are then substituted into Eqs. (20) and (21) together with the energies E_n and the constraint logarithmic derivatives $\mathfrak{L}_\alpha$. From Eq. (22) we find the bound-state eigenvalue spectrum. Then Eq. (21) is solved for the $D_\alpha{}^{(j)}$, which are substituted into Eq. (20) to give the wave functions $\psi^{(j)}$.

IV. THE GREEN'S-THEOREM METHOD

We seek a solution to the Schrödinger equation

$$(E-H)\psi=0 \quad (23)$$

which will be regular everywhere in the inside region $\mathfrak{R}$ and which satisfies the boundary conditions

$$\langle\zeta_\alpha^*|\psi\rangle=0. \quad (24)$$

We will formally solve the Schrödinger equation with the help of the Green's function G.

$$[E-H(y)]G(x,y)=I(x,y), \quad (25)$$

where I is the identity operator. Combining Eqs. (23) and (25) we find

$$\psi(x)=\langle G(x,y)|H(y)\psi(y)\rangle_{\mathfrak{R}}-\langle H(y)G(x,y)|\psi(y)\rangle_{\mathfrak{R}}, \quad (26)$$

where the subscript $\mathfrak{R}$ on the matrix elements indicates that the configuration space integral is limited to the inside region $\mathfrak{R}$. The Hamiltonian consists of a kinetic energy T and an interaction energy V,

$$H=T+V. \quad (27)$$

We assume that the interaction energy is Hermitian in the matrix elements of Eq. (26). Thus,

$$\psi(x)=\langle G(x,y)|T(y)\psi(y)\rangle_{\mathfrak{R}}-\langle T(y)G(x,y)|\psi(y)\rangle_{\mathfrak{R}}. \quad (28)$$

Now the kinetic energy has the form of a $3A$-dimen-

sional Laplacian

$$T=\sum_{i=1}^{A}(-\hbar^2/2m_i)\nabla_i^2=-\sum_{n=1}^{3A}(\partial^2/\partial x_n^2). \quad (29)$$

Application of Green's theorem allows us to replace the two matrix elements on the right of Eq. (28) by an integral over the $(3A-1)$-dimensional hypersurface $\mathcal{S}$ separating the inside region from the outside region. We assume that ψ is negligible everywhere on this hypersurface except at those portions corresponding to the two-particle channel entrances. Thus

$$\begin{aligned}\psi(x)&\approx\sum_\alpha\frac{\hbar^2R_\alpha^2}{2m_\alpha}\left\{(\Phi_\alpha|\psi)\frac{\partial}{\partial r_\alpha'}(G(x,x')|\Phi_\alpha(x'))-(G(x,x')|\Phi_\alpha(x'))\frac{\partial}{\partial r_\alpha'}(\Phi_\alpha|\psi)\right\}_{r_\alpha'=R_\alpha}\\&\approx\sum_\alpha\left(\frac{\hbar^2R_\alpha}{2m_\alpha}\right)^{1/2}\gamma_\alpha\left\{\frac{\partial}{\partial r_\alpha'}r_\alpha'(G(x,x')|\Phi_\alpha(x'))-\lambda_\alpha(G(x,x')|\Phi_\alpha(x'))\right\}_{r_\alpha'=R_\alpha}\\&\approx-\textstyle\sum_\alpha\gamma_\alpha\langle G(x,x')|\xi_\alpha(x')\rangle. \quad (30)\end{aligned}$$

We have succeeded in expressing the wave function in the interior of the inside region $\mathcal{R}$ in terms of its reduced widths γ_α and logarithmic derivatives λ_α on the hypersurface $\mathcal{S}$. We now impose the asymptotic boundary conditions by requiring

$$\gamma_\alpha=\delta_{\alpha\omega}\gamma_\alpha^{(2)}+S_{\alpha\omega}\gamma_\alpha^{(1)} \quad (31)$$

and

$$\gamma_\alpha\lambda_\alpha=\delta_{\alpha\omega}\gamma_\alpha^{(2)}\lambda_\alpha^{(2)}+S_{\alpha\omega}\gamma_\alpha^{(1)}\lambda_\alpha^{(1)}, \quad (32)$$

where

$$\gamma_\alpha^{(i)}=(\hbar^2R_\alpha/2m_\alpha)^{1/2}u_\alpha^{(i)}(R_\alpha) \quad (33)$$

and

$$\lambda_\alpha^{(i)}=[r_\alpha(d/dr_\alpha)\ln r_\alpha u_\alpha^{(i)}(r_\alpha)]_{R_\alpha}. \quad (34)$$

$u_\alpha^{(1)}$ is the unit current outgoing radial wave function for channel α and $u_\alpha^{(2)}$ is the unit current incoming radial wave function. The coefficients $S_{\alpha\omega}$ will be called the elements of the S matrix. Subscript ω refers to the incident channel. For the bound-state case $u_\alpha^{(1)}$ becomes an exponentially decaying function. For the bound-state case we set $\gamma_\alpha^{(2)}=0$ and ignore the second subscript on the S-matrix elements.

We can now find explicit expressions for the S matrix elements. Using Eq. (30) to evaluate the reduced width γ_α gives

$$\gamma_\alpha=\sum_\beta\left(\frac{\hbar^4R_\alpha R_\beta}{4m_\alpha m_\beta}\right)^{1/2}\gamma_\beta\left[\left(\frac{\partial}{\partial r_\beta}r_\beta-\lambda_\beta\right)(\Phi_\alpha|G|\Phi_\beta)\right]_{R_\alpha,R_\beta}. \quad (35)$$

Substituting Eqs. (31) and (32) into Eq. (35) results in

$$\begin{aligned}&(\delta_{\alpha\omega}\gamma_\alpha^{(2)}+S_{\alpha\omega}\gamma_\alpha^{(1)})\\&=\sum_\beta\left(\frac{\hbar^4R_\alpha R_\beta}{4m_\alpha m_\beta}\right)^{1/2}\Big[(\delta_{\beta\omega}\gamma_\beta^{(2)}+S_{\beta\omega}\gamma_\beta^{(1)})\\&\quad\times\frac{\partial}{\partial r_\beta}r_\beta(\Phi_\alpha|G|\Phi_\beta)-(\delta_{\beta\omega}\lambda_\beta^{(2)}\gamma_\beta^{(2)}+S_{\beta\omega}\lambda_\beta^{(1)}\gamma_\beta^{(1)})\\&\qquad\times(\Phi_\alpha|G|\Phi_\beta)\Big]_{R_\alpha,R_\beta}. \quad (36)\end{aligned}$$

By rearranging the terms, this expression can be rewritten to read

$$-Z_{\alpha\omega}^{(2)}=\textstyle\sum_\beta Z_{\alpha\beta}^{(1)}S_{\beta\omega}, \quad (37)$$

where

$$Z_{\alpha\beta}^{(i)}=\delta_{\alpha\beta}\gamma_\beta^{(i)}-\left(\frac{\hbar^4R_\alpha R_\beta}{4m_\alpha m_\beta}\right)^{1/2}\times\gamma_\beta^{(i)}\left[\left(\frac{\partial}{\partial r_\beta}r_\beta-\lambda_\beta^{(i)}\right)(\Phi_\alpha|G|\Phi_\beta)\right]_{R_\alpha,R_\beta}. \quad (38)$$

For the bound-state case $Z^{(2)}$ is set equal to zero. Equation (37) provides a set of linear equation which may be solved for the elements of the S matrix. For the bound-state case there is the additional requirement

$$\det Z^{(1)}=0, \quad (39)$$

which determines the energy spectrum.

For the purpose of constructing more explicit expressions we introduce a complete set of eigenfunctions of the Hamiltonian

$$(E_n-H)\varphi_n=0. \quad (40)$$

These functions are to be defined for a region $\mathcal{R}'$ large enough to contain our inside region $\mathcal{R}$. Let these functions satisfy homogeneous boundary conditions on the boundary $\mathcal{S}'$ of this region $\mathcal{R}'$. Then we can make this set orthonormal

$$\langle\varphi_n^*|\varphi_m\rangle_{\mathcal{R}'}=\delta_{nm} \quad (41)$$

and have the following representation for the Green's function valid inside region $\mathcal{R}'$

$$\begin{aligned}G(x,y)&=[E-H(y)]^{-1}I(x,y)\\&=\textstyle\sum_n|\varphi_n(x)\rangle(E-E_n)^{-1}\langle\varphi_n(y)^*|. \quad (42)\end{aligned}$$

Substituting this into Eq. (38) gives

$$\begin{aligned}Z_{\alpha\beta}^{(i)}&=\delta_{\alpha\beta}\gamma_\beta^{(i)}\\&\quad-\textstyle\sum_n(\gamma_\alpha^n\gamma_\beta^n/(E-E_n))(\lambda_\beta^n-\lambda_\beta^{(i)})\gamma_\beta^{(i)}, \quad (43)\end{aligned}$$

where

$$\gamma_\alpha{}^n=(\hbar^2R_\alpha/2m_\alpha)^{1/2}(\Phi_\alpha|\,\varphi_n)_{R_\alpha} \tag{44}$$

and

$$\lambda_\alpha{}^n=[r_\beta(d/dr_\alpha)\,\ln r_\alpha(\Phi_\alpha|\,\varphi_n)]_{R_\alpha}. \tag{45}$$

With the help of the $Z_{\alpha\beta}{}^{(i)}$ we can evaluate the S matrix and the bound-state energy spectrum. The wave function for the inside region is given by

$$\begin{aligned}\psi(x)&=\sum_{\alpha,n}(\varphi_n(x)\gamma_\alpha{}^n/(E-E_n))(\lambda_\alpha{}^n-\lambda_\alpha)\gamma_\alpha\\&=\sum_{\alpha,n}(\varphi_n(x)\gamma_\alpha{}^n/(E-E_n))\\&\quad\times\{\delta_{\alpha\omega}(\lambda_\alpha{}^n-\lambda_\alpha{}^{(2)})\gamma_\alpha{}^{(2)}+S_{\alpha\omega}(\lambda_\alpha{}^n-\lambda_\alpha{}^{(1)})\gamma_\alpha{}^{(1)}\}.\end{aligned} \tag{46}$$

The above expressions represent a generalization of the R-matrix theory of nuclear reactions.[3] If we choose the region $\mathcal{R}'$ to coincide with the inside region $\mathcal{R}$, then all the logarithmic derivatives $\lambda_\alpha{}^n$ will have the same value, say $\bar{\lambda}_\alpha$, since the φ_n all satisfy the same homogeneous boundary conditions on the boundary $\mathcal{S}'$ of $\mathcal{R}'$. Then

$$Z_{\alpha\beta}{}^{(i)}=\delta_{\alpha\beta}\gamma_\beta{}^{(i)}-R_{\alpha\beta}(\bar{\lambda}_\beta-\lambda_\beta{}^{(i)})\gamma_\beta{}^{(i)}, \tag{47}$$

where

$$R_{\alpha\beta}=\sum_n\gamma_\alpha{}^n(E-E_n)^{-1}\gamma_\beta{}^n \tag{48}$$

are the elements of the R matrix. In the Kapur-Peierls[4] treatment $\bar{\lambda}_\alpha$ is set equal to $\lambda_\alpha{}^{(1)}$, while in the Wigner-Eisenbud[5] treatment the $\bar{\lambda}_\alpha$ are all required to vanish.

The formulas of R-matrix theory are somewhat simpler in form than those generated by our generalization of R-matrix theory. However, there are no convenient approximations available for the R-matrix theory eigenfunctions φ_n. By using our generalization of R-matrix theory, we can use the wave functions resulting from a conventional shell-model calculation to provide a useful approximation to the φ_n.

V. MUTUAL CONSISTENCY OF THE TWO METHODS

An alternative set of equations for the S matrix can be derived by using Eq. (30) to evaluate the logarithmic derivative:

$$\begin{aligned}\gamma_\beta\lambda_\beta&=\sum_\alpha\left(\frac{\hbar^4R_\beta R_\alpha}{4m_\beta m_\alpha}\right)^{1/2}\\&\quad\times\gamma_\alpha\left[\frac{\partial}{\partial r_\beta}r_\beta\left(\frac{\partial}{\partial r_\alpha}r_\alpha-\lambda_\alpha\right)(\Phi_\beta|G|\Phi_\alpha)\right]_{R_\alpha,R_\beta}.\end{aligned} \tag{49}$$

Use of Eqs. (31) and (32) then leads to

$$-Y_{\beta\omega}{}^{(2)}=\sum_\alpha Y_{\beta\alpha}{}^{(1)}S_{\alpha\omega}, \tag{50}$$

where

$$\begin{aligned}Y_{\alpha\beta}{}^{(i)}&=\delta_{\alpha\beta}\gamma_\beta{}^{(i)}\lambda_\beta{}^{(i)}-\left(\frac{\hbar^4R_\alpha R_\beta}{4m_\alpha m_\beta}\right)^{1/2}\\&\quad\times\gamma_\beta{}^{(i)}\left[\frac{\partial}{\partial r_\alpha}r_\alpha\left(\frac{\partial}{\partial r_\beta}r_\beta-\lambda_\beta{}^{(i)}\right)(\Phi_\alpha|G|\Phi_\beta)\right]_{R_\alpha,R_\beta}\\&=\delta_{\alpha\beta}\gamma_\beta{}^{(i)}\lambda_\beta{}^{(i)}-\sum_n\frac{\lambda_\alpha{}^n\gamma_\alpha{}^n\gamma_\beta{}^n}{E-E_n}(\lambda_\beta{}^n-\lambda_\beta{}^{(i)})\gamma_\beta{}^{(i)}.\end{aligned} \tag{51}$$

Combining Eqs. (37), (43), (50), and (51) gives

$$\begin{aligned}&(\lambda_\alpha{}^{(1)}Z_{\alpha\omega}{}^{(2)}-Y_{\alpha\omega}{}^{(2)})\\&\qquad=-\sum_\beta(\lambda_\alpha{}^{(1)}Z_{\alpha\beta}{}^{(1)}-Y_{\alpha\beta}{}^{(1)})S_{\beta\omega}\end{aligned} \tag{52}$$

or

$$\delta_{\alpha\omega}J_\omega+N_{\alpha\omega}=-\sum_\beta M_{\alpha\beta}S_{\beta\omega}, \tag{53}$$

where

$$\begin{aligned}M_{\alpha\beta}&=\sum_n\gamma_\alpha{}^{(1)}(\lambda_\alpha{}^n-\lambda_\alpha{}^{(1)})\gamma_\alpha{}^n(E-E_n)^{-1}\\&\qquad\times\gamma_\beta{}^n(\lambda_\beta{}^n-\lambda_\beta{}^{(1)})\gamma_\beta{}^{(1)},\end{aligned} \tag{54}$$

$$\begin{aligned}N_{\alpha\beta}&=\sum_n\gamma_\alpha{}^{(1)}(\lambda_\alpha{}^n-\lambda_\alpha{}^{(1)})\gamma_\alpha{}^n(E-E_n)^{-1}\\&\qquad\times\gamma_\beta{}^n(\lambda_\beta{}^n-\lambda_\beta{}^{(2)})\gamma_\beta{}^{(2)},\end{aligned} \tag{55}$$

$$J_\alpha=\gamma_\alpha{}^{(1)}(\lambda_\alpha{}^{(1)}-\lambda_\alpha{}^{(2)})\gamma_\alpha{}^{(2)}. \tag{56}$$

For the scattering case $J_\omega=i\hbar$ while for the bound-state case $J_\omega=0$.

Equations (53), (54), and (55) are remarkable for the symmetry they display. In addition, they coincide in form with the result of the constrained variation calculation. For the bound-state case $J_\omega=0$ and $N_{\alpha\omega}=0$. In addition $\mathcal{L}_\alpha=\lambda_\alpha{}^{(1)}$ for all channels. Then comparison with Eq. (21) leads to

$$0=\sum_\beta M_{\alpha\beta}S_\beta=\sum_\beta\gamma_\alpha{}^{(1)}\mathfrak{M}_{\alpha\beta}\gamma_\beta{}^{(1)}S_\beta. \tag{57}$$

Identifying $\gamma_\alpha{}^{(1)}S_\alpha$ with D_α makes Eqs. (57) and (21) identical.

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