The isotopic ratios $^7\mathrm{Li}/^6\mathrm{Li}$ and $^{11}\mathrm{B}/^{10}\mathrm{B}$ calculated using Rudstam's relation are shown in Tables VI and VII, together with the experimental values for those ratios. In fact, since $^6\mathrm{He}$ is a β emitter and $^7\mathrm{Be}$ decays by electron capture to $^7\mathrm{Li}$, we have determined also the isotopic ratio $(^7\mathrm{Li}+^7\mathrm{Be})/(^6\mathrm{He}+^6\mathrm{Li})$; such ratios are of interest for the study of nucleosynthesis of the Li, Be, and B elements. In a like manner, by assuming $^{10}\mathrm{B}$ to be the decay product of the $^{10}\mathrm{Be}$ isotope on a cosmic time scale ($\tau \sim 10^6$ yr), and since $^{10}\mathrm{C}$ and $^{11}\mathrm{C}$ are β emitters, we have determined the isotopic ratio $(^{11}\mathrm{B}+^{11}\mathrm{C})/(^{10}\mathrm{Be}+^{10}\mathrm{B}+^{10}\mathrm{C})$ in the case of boron.

CONCLUSION

Since the cross-section values determined for spallation reactions with α particles in medium-mass nuclei are greater than those values for protons, we point out that the contribution of the α particles to the synthesis of Li, Be, and B elements is not insignificant compared with that of protons, particularly near the threshold of formation, even though the universal abundance of helium is about 10%. For that reason, it is interesting to study the cross sections for the production of Li, Be, and B elements by α particles at different energies.

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Discussion of a New Technique for Solving the Bethe-Goldstone Equation

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The new method of Truelove and Nicholls for obtaining reaction matrix elements for nuclear-structure calculations is discussed. In this method, the Bethe-Goldstone wave function is expanded in terms of eigenfunctions of two interacting nucleons bound in a common potential well. The Bethe-Goldstone equation, which is written in terms of an expansion over noninteracting two-particle states, is then solved iteratively. In practice, the method is most easily applied when a harmonic-oscillator basis is used; the Pauli operator Q can then be treated exactly. The convergence of the Truelove-Nicholls iteration scheme and of the above two expansions is investigated. It is shown that the original method is incorrect for nucleon-nucleon potentials with an infinite hard core. A simple way of correcting the method is presented.

I. INTRODUCTION

Nuclear-structure calculations based on realistic nucleon-nucleon potentials are, in general, perturbation expansions involving the nuclear reaction matrix G. The precise form of the expansion can vary depending upon the particular nuclear properties being calculated and the model space in which one chooses to work, but in all cases a central task is the evaluation of the appropriate reaction matrix elements to use in the expansion.

The defining equation for G can always be cast in the form

$$G(\omega) = V + V \frac{Q}{\omega - H_0} G(\omega) . \tag{1}$$

Here V is the nucleon-nucleon potential, the Pauli operator Q forbids scattering into states within the model space, H_0 is the sum of two single-particle Hamiltonians which define the basis states of the perturbation expansion, and the energy parameter ω is specified by the particular problem being studied.

A fundamental problem facing reaction matrix calculations is the choice of the unperturbed Hamiltonian H_0. This should be chosen so that the perturbation expansion (either Brueckner-Goldstone or Bloch-Horowitz) converges as rapidly as possible *and* so that the reaction matrix elements can be easily and accurately calculated. The final solution of this problem must await more accurate evaluation of three-body cluster and higher-order diagrams. However, both of the above criteria can probably be satisfied by taking H_0 to be a harmonic-oscillator (HO) Hamiltonian with arbitrary shifts in the oscillator eigenvalues.[1,2]

A second problem which arises is purely a numerical one. The nucleon-nucleon potential V is usually defined in the relative coordinate system, while the Pauli operator Q is diagonal in the direct product space of two single-particle states. The usual approximation made is to treat Q as diagonal in relative and center-of-mass (rcm) coordinates. Some studies[3] and improvements[1] on this approximation indicate that the errors involved might be quite large.

The above two problems are related because Q and H_0 appear only in the ratio $Q/(\omega - H_0)$. When $(\omega - H_0)$ is small, any error in Q becomes more important. In addition, errors in the treatment of Q mask the dependence of $G(\omega)$ on H_0. Clearly one needs a method of finding $G(\omega)$ which treats Q exactly.

Equation (1) for $G(\omega)$ is generally not solved directly. The usual approach is to define a perturbed wave function $\Psi_\alpha^{\mathrm{BG}}(\omega)$, known as the Bethe-Goldstone (BG) wave function, such that[4]

$$\langle\phi_\beta|G(\omega)|\phi_\alpha\rangle = \langle\phi_\beta|V|\Psi_\alpha^{\mathrm{BG}}(\omega)\rangle \; . \tag{2}$$

It then follows from Eqs. (1) and (2) that $\Psi_\alpha^{\mathrm{BG}}(\omega)$ satisfies the equation

$$\Psi_\alpha^{\mathrm{BG}}(\omega) = \phi_\alpha + \sum_\mu^\infty \frac{Q_\mu \phi_\mu \langle\phi_\mu|V|\Psi_\alpha^{\mathrm{BG}}(\omega)\rangle}{\omega - \epsilon_\mu} \; . \tag{3}$$

Here the basis function ϕ_μ is a two-particle eigenstate of H_0 with eigenvalue ϵ_μ, and $Q_\mu = 0$ or 1 depending upon whether the state ϕ_μ is inside or outside the model space, respectively. The wave function $\Psi_\alpha^{\mathrm{BG}}(\omega)$ and the matrix elements $\langle\phi_\mu|V|\Psi_\alpha^{\mathrm{BG}}(\omega)\rangle$ depend *implicitly* on the energy parameter ω.[5] The problem of evaluating G matrix elements now becomes the problem of solving Eq. (3) for $\Psi_\alpha^{\mathrm{BG}}(\omega)$.

Recently Truelove and Nicholls[6] (TN) have proposed a new method of solving the BG equation, which treats Q exactly in a HO basis. Their procedure follows a suggestion by Butler *et al.*[7] that $\Psi_\alpha^{\mathrm{BG}}(\omega)$ be expanded in terms of the eigenfunctions of $H_0 + V$, rather than in terms of eigenfunctions of H_0 alone. Since the basis eigenfunctions thereby already contain the effects of the short-range correlations caused by V, it is expected that this expansion for $\Psi_\alpha^{\mathrm{BG}}(\omega)$ will converge rapidly. TN then solve Eq. (3) by iteration.

The TN method is interesting for a number of reasons. First the summation over intermediate states ϕ_μ in Eq. (3) is carried out explicitly. Consequently, the Pauli operator Q may be treated exactly and the energies ϵ_μ can be shifted by an arbitrary amount in a straightforward manner. In addition, the convergence of this summation can show how important the highly-excited intermediate states are in a calculation of $\Psi_\alpha^{\mathrm{BG}}(\omega)$ and $G(\omega)$. Secondly the method generates the coefficients of a rapidly converging expansion for the BG wave function, $\Psi_\alpha^{\mathrm{BG}}(\omega)$, as mentioned in the previous paragraph. Finally the method gives a completely independent check on the results of other calculations that use different approximations.

In Sec. II of this paper we briefly review the methods of Butler *et al.* and TN and then show how the latter may be extended to include arbitrary energy shifts in the intermediate-state spectrum. Next we discuss the convergence of the summation over intermediate states in the TN method. It is shown that the sum can be truncated at some upper limit, *provided* this upper limit is chosen with regard to the point of truncation of the eigenfunction expansion of the BG wave function. Finally we show that the convergence of the TN iteration scheme is closely related to that of an iterative procedure for finding the inverse of a matrix. A condition for the convergence of this inversion procedure is given.

In Sec. III, we use the differential form of the BG equation to show that the expressions for the G matrix elements given by Butler *et al.* and TN are incorrect for potentials with infinite hard cores but are valid for all other potentials. The reason for this error is that the above authors effectively interchange two limiting processes in a nonuniformly convergent sum for the G matrices. We conclude the section by extending the TN method to treat potentials with infinite hard cores.

II. ITERATIVE METHOD FOR SOLVING THE BETHE-GOLDSTONE EQUATION

To obtain a solution of the BG equation [Eq. (3)] in a HO basis, Butler *et al.*[7] and TN[6] expand the BG wave function $\Psi_\alpha^{\mathrm{BG}}(\omega)$ in terms of the complete set of eigenfunctions ψ_i ,

$$\Psi_\alpha^{\mathrm{BG}}(\omega)=\sum_i^\infty a_{i\alpha}(\omega)\psi_i \, . \tag{4}$$

In the above equation

$$a_{i\alpha}(\omega)=\langle\psi_i|\Psi_\alpha^{\mathrm{BG}}(\omega)\rangle , \tag{5}$$

and ψ_i is an eigenfunction of the Schrödinger equation,

$$(H_0+V)\psi_i=E_i\psi_i \, , \tag{6}$$

for two interacting particles bound in a HO well. The eigenvalues and eigenfunctions of the two-particle HO Hamiltonian H_{ho} are given by

$$H_0\phi_\alpha\equiv H_{\mathrm{ho}}\phi_\alpha=\epsilon_\alpha\phi_\alpha \, . \tag{7}$$

Because H_0+V is separable in rcm coordinates, the wave function ψ_i may be written as the product of a HO wave function for the c.m. coordinates and an eigenfunction for the relative part of Eq. (6).[8] The latter function and the eigenvalues E_i can be found numerically. It follows from Eqs. (4)–(7) that Eq. (3) can be written in the form[6]

$$a_{i\alpha}(\omega)=b_{i\alpha}+\sum_\mu^\infty \frac{Q_\mu b_{i\mu}G_{\mu\alpha}(\omega)}{\omega-\epsilon_\mu} \, , \tag{8}$$

where $G_{\mu\alpha}(\omega)$ is the reaction matrix defined by Eq. (2), and

$$b_{i\alpha}=\langle\psi_i|\phi_\alpha\rangle \, . \tag{9}$$

For states i which are *not coupled* by the tensor force in the nucleon-nucleon interaction, the quantity $b_{i\alpha}$ is obtained simply by multiplying the usual Talmi-Moshinsky bracket by the radial overlap integral of the relative part of ψ_i with a relative HO wave function with the same angular momentum. For coupled states i, $b_{i\alpha}$ is the sum of two such terms. It can also be shown that for potentials *without an infinite hard core*[7]

$$G_{\beta\alpha}(\omega)=\sum_i^\infty a_{i\alpha}(\omega)b_{i\beta}(E_i-\epsilon_\beta) \, . \tag{10}$$

In practice, the sums over i in Eqs. (4) and (10) are truncated at some upper limit $i_{\max}$. This will be discussed further in Sec. III.

At this stage Butler *et al.* make the approximation

$$a_{i\alpha}=n_\alpha b_{i\alpha} \, , \tag{11}$$

where

$$n_\alpha\sum_i^{i_{\max}} b_{i\alpha}{}^2=1 \, , \tag{12}$$

and use Eq. (10) to calculate the reaction matrix elements. Equation (12) follows from the requirement $\langle\phi_\alpha|\Psi_\alpha^{\mathrm{BG}}\rangle=1$, which in turn follows from Eq. (3). This simple approximation gives G matrix elements and BG wave functions with no dependence on ω and is thus of limited applicability. Truelove and Nicholls, however, truncate the sum over μ in Eq. (8) and then use this equation together with Eq. (10) and the self-consistency equations for ω to set up an iteration scheme to solve for $a_{i\alpha}(\omega)$, $G_{\mu\alpha}(\omega)$, and ω. Obviously their procedure can readily be adapted to solve for $a_{i\alpha}(\omega)$ and $G_{\mu\alpha}(\omega)$ for any specified value of ω.

We now observe that it is also possible to trivially modify the TN method to deal with the shifted HO Hamiltonian

$$H_0\equiv H_{\mathrm{ho}}+\sum_\beta C_\beta|\phi_\beta\rangle\langle\phi_\beta| \, . \tag{13}$$

Because

$$\Big(H_{\mathrm{ho}}+\sum_\beta C_\beta|\phi_\beta\rangle\langle\phi_\beta|\Big)\phi_\alpha=(\epsilon_\alpha+C_\alpha)\phi_\alpha , \tag{14}$$

the eigenfunctions ϕ_α of this Hamiltonian are identical to those of H_{ho}, but the corresponding eigenvalues are e_α, where

$$e_\alpha=\epsilon_\alpha+C_\alpha \, . \tag{15}$$

The original TN method cannot be used directly with this new H_0, because it does not separate readily into rcm coordinates. This problem can be overcome by continuing to define the eigenfunctions ψ_i using the *unshifted* HO Hamiltonian H_{ho} rather than H_0 itself in Eq. (6). The form of Eq. (10) remains unchanged, but $a_{i\alpha}(\omega)$ is now given by the equation obtained by replacing ϵ_μ by e_μ in Eq. (8).

We now turn our attention to the truncation of the infinite sum over μ in Eq. (8). Assuming that the sum over i in Eq. (10) has *already* been truncated at the upper limit $i_{\max}$, we substitute Eq. (10) into Eq. (8) and interchange the orders of summation to obtain

$$a_{i\alpha}(\omega)=b_{i\alpha}+\sum_j^{i_{\max}} B_{ij}(\omega)a_{j\alpha}(\omega) \, , \tag{16}$$

where

$$B_{ij}(\omega)=\sum_\mu^\infty\left(\frac{E_j-\epsilon_\mu}{\omega-\epsilon_\mu}\right)Q_\mu b_{i\mu}b_{j\mu} \, . \tag{17}$$

The interchange is valid provided the sum in Eq. (17) is absolutely convergent. For large ϵ_μ , the terms of this sum fall into two categories. The first category contains terms corresponding to states μ which consist of one particle in an excluded single-particle state and the other in a highly excited one; these terms are zero because Q_μ is zero. The terms in the second category have both particles in excited states and are approximately equal to $b_{i\mu}b_{j\mu}$, since Q_μ is 1 and the energy-difference ratio tends to unity for ϵ_μ much larger than E_j and ω. Therefore, it can easily be shown, using the Schwartz inequality, that the sum is indeed absolutely convergent.

In order to perform numerical calculations, one must truncate the infinite sum over μ in Eq. (17) at some upper bound $\mu_{\max}$. It is obvious that this upper bound can be chosen independently for each i,j pair. However, the iterative procedure used in the TN method forces one to select a *fixed* value of $\mu_{\max}$ for *all* i and j less than $i_{\max}$. Since it is found empirically that for any given j the overlaps $b_{j\mu}$ are largest when ϵ_μ is approximately equal to E_j and since the maximum possible value of E_j increases with $i_{\max}$, a higher value of $\mu_{\max}$ should be used if $i_{\max}$ is increased. It is probable that the anomalous convergence of the TN procedure as a function of $\mu_{\max}$ for two different values of $i_{\max}$ (see Fig. 1 of Ref. 6) is a result of choosing these upper limits independently. The above discussion is also applicable to the shifted Hamiltonian of Eq. (13).

We conclude this section with a discussion of the convergence of the TN iteration scheme. We first recast the theory in matrix form; Eq. (16) then becomes

$$[\underline{\mathrm{I}}-\underline{\mathrm{B}}(\omega)]\underline{\mathrm{a}}_\alpha(\omega)=\underline{\mathrm{b}}_\alpha\,, \tag{18}$$

where the matrix elements of $\underline{\mathrm{B}}$ are given by Eq. (17). Provided the energy ω is specified, the expansion coefficients $a_{i\alpha}(\omega)$ can be found by matrix inversion. For large matrices, it is more convenient to solve Eq. (18) iteratively, using the scheme

$$\begin{aligned}\underline{\mathrm{a}}_\alpha^{(0)}&=\underline{\mathrm{b}}_\alpha\,,\\ \underline{\mathrm{a}}_\alpha^{(n)}&=\underline{\mathrm{b}}_\alpha+\underline{\mathrm{B}}(\omega)\underline{\mathrm{a}}_\alpha^{(n-1)}\,.\end{aligned} \tag{19}$$

For a fixed ω, the above scheme reduces to

$$\underline{\mathrm{a}}_\alpha^{(n)}=(\underline{\mathrm{I}}+\underline{\mathrm{B}}+\cdots+\underline{\mathrm{B}}^n)\underline{\mathrm{b}}_\alpha\,, \tag{20}$$

which is a variant of the familiar Gauss-Seidel iterative method[9] for solving matrix equations. A sufficient condition for the convergence of this method is that all of the eigenvalues of $\underline{\mathrm{B}}$ have modulus less than unity. On the other hand, if we determine ω, and hence $\underline{\mathrm{B}}(\omega)$, at each iteration step, Eq. (19) is precisely the TN iteration scheme. Since the matrix $\underline{\mathrm{B}}(\omega)$ is not altered appreciably by changes in ω within the range of interest for a shell-model calculation, the convergence of this latter scheme would be expected to be essentially equivalent to that of Eq. (20).

III. TREATMENT OF INFINITE HARD-CORE POTENTIALS

If the reaction matrix elements defined by Eq. (2) are to be finite for potentials with an infinite hard core, the wave function $\Psi_\alpha^{\mathrm{BG}}(\omega)$ must be zero within the region of the hard core, and $V\Psi_\alpha^{\mathrm{BG}}(\omega)$ within this region must be specified by a limiting process. This, in turn, implies that the reaction matrix elements, the BG wave function, and the coefficients $a_{i\alpha}$ are also determined by this same limiting process. It is clear that we should study the limit of these quantities for potentials V^F with large but finite repulsive cores of the same range c as that of V, but which are otherwise equivalent to V. Quantities calculated using V^F will be denoted by a superscript F.

We first transform the BG equation for the potential V^F into an integrodifferential equation by operating on both sides of Eq. (3) with $(\omega-H_0)$ to obtain[10]

$$(\omega-H_0)[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F=(\omega-\epsilon_\alpha)\phi_\alpha+\sum_\mu Q_\mu\phi_\mu\langle\phi_\mu|V^F|[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F\rangle\,. \tag{21}$$

Because the ϕ_μ form a complete set, we have after rearrangement

$$(H_0+V^F-\omega)[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F=(\epsilon_\alpha-\omega)\phi_\alpha+\sum_\mu(1-Q_\mu)\phi_\mu\langle\phi_\mu|V^F|[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F\rangle\,. \tag{22}$$

By dividing the range of integration of the *relative* coordinate in Eq. (2) into two regions, i.e., $r\equiv|\vec{\mathrm{r}}_1-\vec{\mathrm{r}}_2|\leqslant(c+\epsilon)$ and $r>(c+\epsilon)$, where ϵ represents an infinitesimal distance, we can use Eq. (22) to derive the relation

$$\begin{aligned}G_{\beta\alpha}^F(\omega)&=\langle\phi_\beta|V^F|[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F\rangle\\ &=\iint_{r<c}d\vec{\mathrm{r}}\,d\vec{\mathrm{R}}\{(\omega-\epsilon_\beta)\phi_\beta{}^*[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F\\ &\quad+(\epsilon_\alpha-\omega)\phi_\beta{}^*\phi_\alpha+\sum_\mu(1-Q_\mu)\\ &\quad\times\langle\phi_\mu|V^F|[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F\rangle\,\phi_\beta{}^*\phi_\mu\}\\ &\quad+\frac{\hbar^2}{m}\iint d\Omega(\hat{r})d\vec{\mathrm{R}}\{r^2\phi_\beta{}^*\frac{\partial}{\partial r}[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F\\ &\quad-r^2[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F\frac{\partial}{\partial r}\phi_\beta{}^*\}|_{c+\epsilon}\\ &\quad+\iint_{r>c}d\vec{\mathrm{r}}\,d\vec{\mathrm{R}}\,\phi_\beta{}^*V^F[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F\,,\end{aligned} \tag{23}$$

where the integrations over $\vec{\mathrm{r}}$ are confined to the specified regions and include spin summations; $\Omega(\hat{r})$ has been used to denote the angular coordinates of $\vec{\mathrm{r}}$; and $\vec{\mathrm{R}}$ denotes the c.m. coordinates.[11]

If we now define the reaction matrix elements for the infinite hard-core potential V by

$$G_{\beta\alpha}(\omega)=\lim_{V^F\to V}G_{\beta\alpha}^F(\omega)\,, \tag{24}$$

Eq. (23) can be used to establish a definition of

$V\Psi_\alpha^{\mathrm{BG}}(\omega)$ for $r \leqslant c$, i.e.,

$$V\Psi_\alpha^{\mathrm{BG}}(\omega) = (\epsilon_\alpha - \omega)\phi_\alpha + \sum_\mu (1 - Q_\mu)\phi_\mu G_{\mu\alpha}(\omega) \qquad r < c\,, \tag{25}$$

$$V\Psi_\alpha^{\mathrm{BG}}(\omega) = \frac{\hbar^2}{m} \lim_{V^F \to V} \frac{\partial}{\partial r}\,[\Psi_\alpha^{\mathrm{BG}}(\omega)]^F|_{r=c+\epsilon}\,\delta(r - c)\,, \qquad r = c\,,$$

since $\Psi_\alpha^{\mathrm{BG}}(\omega) = 0$ for $r \leqslant c$. This expression is the same as that for the corresponding quantity in the reference-spectrum approach,[12] apart from the term involving the sum over μ, which represents the Pauli correction.

Having established the appropriate limiting behavior of $V\Psi_\alpha^{\mathrm{BG}}(\omega)$, we now consider the expansion of $\Psi_\alpha^{\mathrm{BG}}(\omega)$ in terms of known eigenfunctions, as discussed in Sec. II. If V is an infinite hard-core potential, then we can write

$$\Psi_\alpha^{\mathrm{BG}}(\omega) = \lim_{V^F \to V} [\Psi_\alpha^{\mathrm{BG}}(\omega)]^F = \lim_{V^F \to V} \sum_i^\infty a_{i\alpha}^F(\omega)\psi_i^F\,, \tag{26}$$

where ψ_i^F is the eigensolution of

$$(H_0 + V^F)\psi_i^F = E_i^F \psi_i^F\,, \tag{27}$$

and the infinite sum over i is uniformly convergent with respect to the height of the core of V^F for all r. Since the sum is uniformly convergent, we can interchange the limit and the sum, so that

$$\Psi_\alpha^{\mathrm{BG}}(\omega) = \sum_i^\infty a_{i\alpha}(\omega)\psi_i\,, \tag{28}$$

where $a_{i\alpha}(\omega)$ and ψ_i are the limits as $V^F \to V$ of $a_{i\alpha}^F(\omega)$ and ψ_i^F, respectively. Consequently, no problems arise in the expansion for $\Psi_\alpha^{\mathrm{BG}}(\omega)$ in the limit of infinite hard-core potentials.

Unfortunately a similar statement is not true for the product of $V\Psi_\alpha^{\mathrm{BG}}(\omega)$. Expressing $V\Psi_\alpha^{\mathrm{BG}}(\omega)$ as above, i.e.,

$$V\Psi_\alpha^{\mathrm{BG}}(\omega) = \lim_{V^F \to V} \sum_i^\infty a_{i\alpha}^F(\omega)V^F\psi_i^F\,, \tag{29}$$

we see that it is invalid to interchange the limiting process with the infinite sum for $r < c$, because this would lead to the spurious result $V\Psi_\alpha^{\mathrm{BG}}(\omega) = 0$ for $r < c$. This spurious result follows from Eq. (27) and the fact that

$$\lim_{V^F \to V} \psi_i^F = 0 \quad \text{for } r \leqslant c\,. \tag{30}$$

Since this interchange would be permitted if the sum had a finite number of terms, *any* truncation of the sum in Eq. (28) automatically leads to the omission of the contribution to the reaction matrix element from the region $r < c$, i.e., the "inner-core" term. On the other hand, if we take a sufficient number of terms in the i sums to give an adequate representation of $\Psi_\alpha^{\mathrm{BG}}(\omega)$ in the region $r > c$, the contributions to the reaction matrix element from $r > c$ and from the "core edge," $r = c$, will be included properly. The latter result follows directly from Eq. (25), which implies that the "core-edge" term depends only on the form of $\Psi_\alpha^{\mathrm{BG}}(\omega)$ immediately outside the core.

The "inner-core" term can be included in the following manner. We write Eq. (28) in the form

$$\Psi_\alpha^{\mathrm{BG}}(\omega) = \underline{\Psi}_\alpha(\omega) + \sum_i^{i_{\max}} a_{i\alpha}(\omega)\psi_i\,, \tag{31}$$

where the i sum is truncated at some upper bound $i_{\max}$ and $\underline{\Psi}_\alpha(\omega)$ represents the remainder of the sum. Then

$$V\Psi_\alpha^{\mathrm{BG}}(\omega) = V\underline{\Psi}_\alpha(\omega) + \sum_i^{i_{\max}} a_{i\alpha}(\omega)V\psi_i\,, \tag{32}$$

where

$$V\underline{\Psi}_\alpha(\omega) = \lim_{V^F \to V} \sum_{i > i_{\max}}^\infty a_{i\alpha}^F(\omega)V^F\psi_i^F\,. \tag{33}$$

Because Eq. (28) is uniformly convergent, by a suitable choice of $i_{\max}$ we can make $\underline{\Psi}_\alpha(\omega)$ arbitrarily small for all values of r. Then for $r \geqslant c$, $V\underline{\Psi}_\alpha(\omega)$ can be approximated by zero. For $r < c$ we have the exact result

$$V\underline{\Psi}_\alpha(\omega) = (\epsilon_\alpha - \omega)\phi_\alpha + \sum_\mu (1 - Q_\mu)\phi_\mu G_{\mu\alpha}(\omega)\,, \qquad r < c\,, \tag{34}$$

which follows from Eqs. (25) and (32). It should be noted that it is the eigenstates which have energies approximately equal to the height of the repulsive core of the potential that give the inner-core term, because only these eigenfunctions are appreciable and slowly varying in the region of the core.

Substitution of Eq. (32) into the definition (24) of the reaction matrix gives[13]

$$G_{\beta\alpha}(\omega) = (\epsilon_\alpha - \omega)O_{\beta\alpha} + \sum_\mu (1 - Q_\mu)O_{\beta\mu}G_{\mu\alpha}(\omega) + \sum_i^{i_{\max}} a_{i\alpha}(\omega)b_{i\beta}(E_i - \epsilon_\beta)\,, \tag{35}$$

where

$$O_{\beta\alpha} = \iint_{r<c} d\vec{r}\, d\vec{R}\, \phi_\beta{}^*\phi_\alpha\,. \tag{36}$$

The first two terms of Eq. (35) were omitted in the inert-core shell-model calculations of Refs. 6 and 7. However, it should be noted that these "inner-core" contributions to G are usually a very small fraction of the total reaction matrix element, and their inclusion would not affect the results of the shell-model calculations. On the other hand, in calculations of the total binding energy or calculations involving off-energy-shell G-matrix elements, the relative importance of the inner-core terms increases, and they should be included.

The inner-core term in Eq. (35) could be calculated by truncating the sum over μ and solving the resultant set of equations by matrix inversion. Because of the small size of the overlaps $O_{\beta\alpha}$, it is probably more than adequate to substitute

$$G_{\mu\alpha}(\omega)\approx(\epsilon_\alpha-\omega)O_{\mu\alpha}+\sum_{i}^{i_{\max}}a_{i\alpha}(\omega)b_{i\mu}(E_i-\epsilon_\mu) \tag{37}$$

into the right-hand side of Eq. (35) to obtain

$$\begin{aligned}G_{\beta\alpha}(\omega)\approx(\epsilon_\alpha-\omega)\Big[O_{\beta\alpha}&+\sum_{\mu}^{\mu_{\max}}(1-Q_\mu)O_{\beta\mu}O_{\mu\alpha}\Big]\\&+\sum_{i}^{i_{\max}}a_{i\alpha}(\omega)\Big[b_{i\beta}(E_i-\epsilon_\beta)\\&+\sum_{\mu}^{\mu_{\max}}(1-Q_\mu)O_{\beta\mu}b_{i\mu}(E_i-\epsilon_\mu)\Big]\,.\end{aligned} \tag{38}$$

This last equation can be used to calculate directly the nth approximation to the coefficients $a_{i\alpha}$. The TN method can, therefore, be extended to infinite hard-core potentials by replacing Eq. (10) by Eq. (38) in the iteration procedure.

Finally, we observe that it is still possible to include arbitrary shifts in the intermediate-state energies. However, the procedure involves more than simple changes in the energy denominators. Our final expression, Eq. (35), for the G matrix must be modified by adding the extra term

$$-\sum_{\mu}Q_\mu C_\mu O_{\beta\mu}(\omega-e_\mu)^{-1}G_{\mu\alpha} \tag{39}$$

to the right-hand side, leaving all other terms unchanged.

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[7] S. T. Butler, R. G. L. Hewitt, B. H. J. McKellar, I. R. Nicholls, and J. S. Truelove, Phys. Rev. 186, 963 (1969).

[8] The italic letters i, j,... will be used to denote all the quantum numbers of the rcm states that are eigensolutions of Eq. (6).

[9] See for example, J. Todd, *Survey of Numerical Analysis* (McGraw-Hill Book Company, Inc., New York, 1963), p. 230.

[10] Mathematically this is a well-defined procedure, since $(\omega-H_0)$ commutes with the projection operator and since ω can be taken to be complex, making $(\omega-H_0)$ a bounded and well-defined operator. Since $(\omega-H_0)^{-1}$ has only discrete poles, no problems are encountered in taking the limit of ω approaching the real axis.

[11] The derivation of Eq. (23) for the full reaction matrix is similar to that used in Refs. 2 and 12 for the reference-spectrum reaction matrix.

[12] H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. 129, 225 (1963).

[13] Equation (35) for $G_{\beta\alpha}(\omega)$ can also be obtained by an alternate method that starts with Eq. (23). Substituting the expansion for $[\Psi_\alpha^{BG}(\omega)]^F$ in terms of ψ_i^F into the outer-core term in Eq. (23), then using Eq. (27) and partially integrating twice, one obtains the last term in Eq. (35) along with a term which cancels the core-edge contribution to Eq. (23). If one now applies the limit of Eq. (24) to Eq. (23), one obtains the expression given in Eq. (35) for $G_{\beta\alpha}(\omega)$.