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ABSTRACT

A method for dealing with the nuclear many-body problem is suggested. The approach is a refinement of the shell model in which the asymptotic boundary conditions are used as constraints in a variational calculation of the R-matrix. Since it is the R-matrix that is calculated, this method should provide a description of nuclear reactions and decays as well as of nuclear bound states.

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I. INTRODUCTION

This paper will describe a procedure for making an approximate calculation of the R-matrix. The suggested procedure is a modification of that used in shell model calculations. The R-matrix is defined in terms of exact eigenfunctions of the Hamiltonian of a many-body system which are consistent with a specified set of boundary conditions. It is proposed to approximate these exact eigenfunctions by finite linear combinations of known functions. The coefficients that appear in these linear combinations are treated as variational parameters. They are determined by seeking the extrema of the expectation value of the Hamiltonian with the boundary conditions as constraints. By the method described here it should be possible to calculate the properties of nuclear continuum states as well as the discreet states of nuclei. In this way shell model techniques can be applied to nuclear reactions and nuclear decays as well as to the bound states of nuclei. This method should also make possible improvements in bound state calculations.

II. THE R-MATRIX

Suppose we have a system of N nucleons which has an energy low enough so that there are no open three-or-more-body channels. Let us denote the channel wave functions for this system by χ_a, χ_b, etc. Each channel wave function will consist of three factors.

$$\chi_a = \chi_a^A(\hat{r}_a)\,\chi_a^B\,\chi_a^C \qquad (1)$$

χ_a^B is the wave function describing the internal degrees of freedom of n nucleons in a bound state while χ_a^C represents a bound state of the other

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N-n nucleons. χ_a^A is a function of the direction $\hat{r}_a$ of the vector $\underset{\sim}{r}_a$ giving the displacement of the center of mass of group B from the center of mass of group C. Finally let us make χ_a an eigenfunction of the total angular momentum by appropriately coupling the orbital angular momentum represented by χ_a^A with the spins of χ_a^B and χ_a^C, and let us make χ_a antisymmetric by applying an antisymmetrization operator to the product $\chi_a^B \chi_a^C$.

For each channel wave function χ_a we define a channel radius R_a such that when the magnitude r_a of the relative displacement $\underset{\sim}{r}_a$ is greater than R_a, then the nuclear interaction between the two channel $\underline{a}$ clusters is negligible. Let H be the Hamiltonian for our system of N nucleons. We now define a set of "R-matrix wave functions" Φ_n. These functions will be exact eigenfunctions of the Hamiltonian

$$H\Phi_n = E_n \Phi_n \tag{2}$$

which satisfy the following boundary condition

$$0 = \left\{ \frac{d}{dr_a} \left\langle \chi_a \middle| \Phi_n \right\rangle - \left(\frac{L_a - 1}{R_a}\right) \left\langle \chi_a \middle| \Phi_n \right\rangle \right\}_{r_a = R_a} \tag{3}$$

for each channel. The logarithmic derivatives L_a will be specified at a later stage of the discussion. The R-matrix can now be defined in the following way:

$$R_{ab} = \sum_n \frac{\gamma_{an} \gamma_{bn} A_n}{E - E_n} \tag{4}$$

where

$$\gamma_{an} = \left\langle \chi_a \middle| \Phi_n \right\rangle_{r_a = R_a} \sqrt{\frac{\hbar^2 R_a}{2M_a}}$$

M_a = the reduced mass in channel $\underline{a}$

$$A_n^{-1} = \left\langle \Phi_n^* \middle| \Phi_n \right\rangle_R = \int_0^R d\tau \, \Phi_n \Phi_n$$

The normalization integral A_n^{-1} is evaluated within a region whose boundaries are given by $r_a \leq R_a$, $r_b \leq R_b$, etc.

The R-matrix is related to the S-matrix. The S-matrix is descriptive of the asymptotic form of the solutions of our N-body Schroedinger equation.

$$H\Psi = E\Psi \tag{5}$$

In the asymptotic region

$$\Psi \rightarrow \sum_a B_a \sum_b \chi_b \left(U_b^{(2)}(r_b)\,\delta_{ba} + U_b^{(1)}(r_b)\,S_{ba}\right) \qquad (6)$$

where the B_a are constant coeficients and the S_{ba} are the elements of the S-matrix. The $U_b^{(2)}$ and $U_b^{(1)}$ are the unit-current radial wave functions of the incoming and outgoing types respectively. The relationship between the S-matrix and R-matrix can be shown to be of the form

$$\delta_{ba} - R_{ba}(L_a - g_a^{(2)}) = \sum_c S_{ca} \frac{U_c^{(1)}(R_c)}{U_a^{(2)}(R_a)} \left\{R_{bc}(L_c - g_c^{(1)}) - \delta_{bc}\right\} \qquad (7)$$

where

$$g_a^{(i)} = \left[r_a \frac{d}{dr_a} \ln r_a\, U_a^{(i)}(r_a)\right]_{r_a = R_a}$$

and

$$L_a = \left[r_a \frac{d}{dr_a} \ln r_a \left\langle \chi_a \mid \Phi_n \right\rangle\right]_{r_a = R_a}$$

for all Φ_n.

In the work of Wigner and his collaborators the logarithmic derivatives L_a are chosen to be zero. Then the R-matrix is real and equation (7) becomes

$$\delta_{ba} + R_{ba}\, g_a^{(2)} = -\sum_c S_{ca} \frac{U_c^{(1)}(R_c)}{U_a^{(2)}(R_a)} \left\{R_{bc}\, g_c^{(1)} + \delta_{bc}\right\}. \qquad (8)$$

In the work of Kapur and Peierls the logarithmic derivatives L_a are chosen to be equal to $g_a^{(1)}$. Then the parameters in the R-matrix become complex and dependent on E, but equation (7) is considerably simplified.

$$S_{ba} = \frac{U_a^{(2)}(R_a)}{U_b^{(1)}(R_b)} \left\{R_{ba}(g_a^{(1)} - g_a^{(2)}) - \delta_{ba}\right\} \qquad (9)$$

The S-matrix has poles on the real axis and in the lower half of the complex plane (in energy). In the vicinity of one of these poles the S-matrix has the form

$$S_{ba} = \frac{U_a^{(2)}(R_a)}{U_b^{(1)}(R_b)} \left\{\frac{i\sqrt{\Gamma_a \Gamma_b}}{E - E_0 + i\frac{\Gamma}{2}} - \delta_{ab}\right\} \qquad (10)$$

where Γ_a is the partial width for channel $\underline{a}$ and $\Gamma = \sum_a \Gamma_a$ is the total width.

Γ_a vanishes if channel $\underline{a}$ is closed. Each such pole is associated with a stable or metastable state of the N-nucleon system, and the width Γ is inversely proportional to the mean life of the state.

III. CALCULATION OF THE R-MATRIX WAVE FUNCTIONS

Suppose Φ_α, Φ_β, $\cdots$ are a set of known, linearly independent, anti-symmetrized, N-nucleon wave functions. We propose to approximate the R-matrix wave functions Ψ_n with linear combinations of these known functions.

$$\Psi_n = \sum_a B_a^n \Phi_a \tag{11}$$

The coefficients B_a^n are regarded as variational parameters which are adjusted to yield extrema for the expectation value of the Hamiltonian. The boundary conditions given by equation (3) will be constraints on the variation. In addition, the normalization and orthogonalization condition

$$\langle \Psi_n | \Psi_m \rangle_R = \delta_{n,m} \tag{12}$$

will also constrain the variation.

To facilitate the discussion of the procedure for constructing the R-matrix wave functions we introduce the following symbols:

$$\begin{aligned}
H_{\alpha\beta} &= \langle \Phi_\alpha | H | \Phi_\beta \rangle_R \\
G_{\alpha\beta} &= \langle \Phi_\alpha | \Phi_\beta \rangle_R \\
F_{\alpha a} &= \left[\frac{d}{dr_a} \langle \chi_a | \Phi_\alpha \rangle - \left(\frac{L_a - 1}{R_a} \right) \langle \chi_a | \Phi_\alpha \rangle \right]_{r_a = R_a} \\
M_{\alpha\beta}(E) &= H_{\alpha\beta} - E\, G_{\alpha\beta} \\
F_\alpha^n &= \left(\sum_\beta G_{\alpha\beta} B_\beta^n \right)^*
\end{aligned} \tag{13}$$

In terms of these quantities we have

$$\langle \Psi_n | H | \Psi_n \rangle = \sum B_\alpha^{n*} H_{\alpha\beta} B_\beta \tag{14}$$

for the expectation value of the Hamiltonian,

$$\delta_{mn} = \sum B_\alpha^{m*} G_{\alpha\beta} B_\beta \tag{15}$$

for the orthonormalization condition,

and

$$\sum_{\beta} B_{\beta} F_{\beta b} = 0 \tag{16}$$

for the boundary conditions.

To calculate the first or lowest energy R-matrix wave function we require

$$\delta \{ \sum_{\alpha\beta} (B_{\alpha}^{1\,*} H_{\alpha\beta} B_{\beta}^{1} - E_1 B_{\alpha}^{1\,*} G_{\alpha\beta} B_{\beta}^{1}) - \sum_{\alpha a} B_{\alpha}^{1\,*} F_{\alpha a}^{*} D_a - \sum_{\beta b} B_{\beta}^{1} F_{\beta b} D_b^{*} \} = 0 \tag{17}$$

where E_1 and D_a are Lagrange multipliers. The resulting equation for B_{α}^{1} is

$$\sum_{\beta} M_{\alpha\beta}(E_1) B_{\beta}^{1} = \sum_{a} F_{\alpha a}^{*} D_a \tag{18}$$

This is solved by inverting the matrix M.

$$B_{\alpha}^{1} = \sum_{\beta b} M_{\alpha\beta}^{-1}(E_1) F_{\beta b}^{*} D_b \tag{19}$$

The Lagrange multipliers D_a are determined by the equations that result from substituting equation (19) into equation (16)

$$\sum_{\alpha\beta b} F_{\alpha a} M_{\alpha\beta}(E_1) F_{\beta b}^{*} D_b = \sum N_{ab}(E_1) D_b = 0 \tag{20}$$

The solution of this equation is found by diagonalizing the matrix $N(E_1)$ for the smallest value of E_1 that causes det $N(E_1) = 0$. This procedure gives us E_1 and the D_a's to within a multiplicative constant. The normalization of the D_a's is fixed by the constraint

$$\begin{aligned} 1 = \langle \Phi_1 | \Phi_1 \rangle_R &= \sum B_{\alpha}^{1\,*} G_{\alpha\beta} B_{\beta}^{1} \\ &= \sum_{\substack{\alpha\beta a \\ \gamma\delta b}} F_{\beta b} M_{\alpha\beta}^{-1}(E_1)^{*} G_{\alpha\gamma} M_{\gamma\delta}^{-1}(E_1) F_{\delta a}^{*} D_b^{*} D_a \\ &= \sum_{ab} J_{ba} D_b^{*} D_a \end{aligned} \tag{21}$$

Substituting these D_a's and E_1 back into equations (11) and (19) then gives Φ_1.

To calculate Φ_2 we repeat the entire procedure outlined above except that the orthogonality of Φ_2 and Φ_1 provides an additional constraint. Thus the procedure for calculating Φ_{n+1} would yield the equations

$$B_a^{n+1} = \sum_\beta M_{a\beta}^{-1}(E_{n+1}) \left\{ \sum_b F_{\beta b}^* D_b + \sum_{\ell=1}^{n} F_\beta^{\ell *} D^\ell \right\} \qquad (22)$$

$$\sum_a B_a^{n+1} F_{aa} = 0 \qquad (23)$$

$$\sum_a B_a^{n+1} F_a^\ell = 0 \qquad (24)$$

$$\sum_{a\beta} B_a^{n+1*} G_{a\beta} B_\beta^{n+1} = 1 \qquad (25)$$

The equations for Φ_{n+1} are seen to have the same structure as those for Φ_1 except that there are n additional Lagrange multipliers to be determined in the process of finding Φ_{n+1}. There will, of course, be no more than N linearly independent Φ_n's that can be constructed in this way, where N is the number of Φ_a's used. In terms of these R-matrix wave functions the R-matrix will be

$$R_{ab} = \sum_n \frac{\langle \chi_a | \Phi_n \rangle_{r_a=R_a} \langle \chi_b | \Phi_n \rangle_{r_b=R_b} \sqrt{\frac{\hbar^4}{4} \frac{R_a R_b}{M_a M_b}}}{(E-E_n) \langle \Phi_n^* | \Phi_n \rangle_R}$$

$$= \sum_{n,\alpha,\beta} \frac{\sqrt{\frac{\hbar^4}{4} \frac{R_a R_b}{M_a M_b}} \langle \chi_a | \Phi_\alpha \rangle_{r_a=R_a} \langle \chi_b | \Phi_\beta \rangle_{r_b=R_b} B_a^n B_\beta^n}{(E-E_n) \sum_{\gamma,\delta} B_\gamma^n B_\delta^n \langle \Phi_\gamma^* | \Phi_\delta \rangle_R} \qquad (26)$$

IV. CLUSTERING AND THE NUCLEAR SURFACE

At this point we consider what choice would be best advised for the N known N-nucleon wave functions Φ_a to be used in constructing the R-matrix wave functions Φ_n. The first thing that comes to mind is the use of anti-symmetrized products of single particle orbitals just as is done in the shell model. Such a representation has proved itself to be very successful in describing the nuclear interior. However, the shell model gives a very inadequate picture of the nuclear surface. There are two reasons for this. First of all the harmonic oscillator wave functions customarily used for shell model orbitals fall off too rapidly in the asymptotic region. Secondly and most importantly clustering should occur at the nuclear surface where the nucleon density is reduced, and these enhanced correlations in the surface region cannot be adequately represented by a sum of a few products of single particle orbitals.

To take a shell model wave function and force it to be consistent with realistic boundary conditions by the procedure suggested in this paper will probably not lead to an important improvement and will quite likely result in a worse result than the usual shell model calculation. This is just because the products of harmonic oscillator single particle orbitals are so poorly adpated to describe the nuclear surface. In order to implement the approach suggested by this paper it would seem necessary to include in the set of wave functions Φ_a types which contain clustering and also are enhanced in the surface region. These types should serve to supplement and not displace the usual shellmodel types. At the very least, one should include clustering terms appropriate to each of the channels in which boundary conditions are specified.

V. DEFINITION OF THE INSIDE REGION

At various points in this paper symbols of the form $\langle \Phi | \mathcal{O} | \Psi \rangle_R$ have appeared. These are used to represent matrix elements of the type

$$\langle \Phi | \mathcal{O} | \Psi \rangle_R = \int_0^R d\tau \; \Phi^* \mathcal{O} \Psi .$$

The symbol R is used to show that the integration is limited to the so-called inside region: $r_a < R_a$, $r_b < R_b$, $\cdots$.

Now there is a certain ambiguity connected with the definition of the inside region, and this ambiguity is necessarily present in any practical application of R-matrix theory.

The two-body channel $\underline{a}$ is associated with a particular clustering of our N-nucleon system into two groups A_a and B_a. The internal states of these two groups of nucleons are represented by the wave functions $\chi_a^A(\xi^A)$ and $\chi_a^B(\xi^B)$. $\underset{\sim}{r}_a$ denotes the displacement of the center of mass of A from that of B, while ξ^A and ξ^B represents the internal coordinates appropriate for clusters A and B. The meaning of equation (16) would be clear if we could write

$$\int_0^R d\tau = \int_0^{R_a} d\underset{\sim}{r}_a \int d\xi^A \int d\xi^B \qquad (27)$$

for every channel $\underline{a}$. But this cannot be simultaneously true for every channel a, b, c, $\cdots$. However, if the various channel radii R_a, R_b, $\cdots$ are chosen to be sufficiently large and if the wave functions $\underline{\Phi}_a$, $\underline{\Phi}_\beta$, $\cdots$ are wisely selected, then the integrands of the integrals will always be negligible in the region where the several definitions of the inside region fail to correspond.

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