Integral form of energy matrix element

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The radial part of the matrix element of Goldhammer's Hamiltonian is expressed in the integral form. The variation principle is applied to give the maximum binding energy of the nuclear system. This results in a set of Morpurgo type coupled differential equations corresponding to each quantum of excitation.

[NUCLEAR STRUCTURE A mathematical model for binding energy calculations.]

The radial dependence of Goldhammer's two-body interaction[1] contains both Gaussian and Gartenhaus forms. In the appendixes, the radial parts of the matrix element of the central and tensor forces (in both forms of radial dependence) between two states of angular momentum L, L' and quanta of excitation M, M', respectively, are expressed in the integral form in terms of a set of hypergeometric functions. This is written as

$$V_{ML,M'L'} = I(ML, M'L') + J(ML, M'L'),$$

where $I(ML, M'L)$ and $J(ML, M'L')$ are given by Eqs. (C2) with (C3) and (C6) of Appendix C, respectively.

The kinetic energy operator T under the transformation to the internal coordinate system given in Appendix A becomes

$$T = \frac{-\hbar^2}{2\mu a_0^2}\,(\nabla_{a_1}^2 + \nabla_{a_2}^2 + \cdots + \nabla_{a_{p-1}}^2) = \frac{-\hbar^2}{2\mu a_0^2}\,\Delta_m$$

with

$$\Delta_m = \frac{1}{R^{m-1}}\,\frac{d}{dR}\left(R^{m-1}\,\frac{d}{dR}\right) - \frac{1}{R^2}\,L_m^2,$$

where L_m is the m dimensional angular momentum operator. To evaluate the eigenvalues of L_m^2 we consider a harmonic multidimensional function

$$S = R^k\, Y_m^{(k)L}$$

which satisfies $\Delta_m S = 0$, where $Y_m^{(k)L}$ is a hyperspherical harmonic defined by Eq. (B4) of Appendix B. Since

$$T|S\rangle = k(m+k-2)R^{k-2}Y_m^{(k)L} - R^{k-2}L_m^2 Y_m^{(k)L} = 0,$$

we get

$$L_m^2 Y_m^{(k)L} = k(m+k-2)Y_m^{(k)L}.$$

Therefore it follows that

$$T|U_{ML}^{(m)}(R)Y_m^{(M)L}\rangle = \frac{-\hbar^2}{2\mu a_0^2}\left[\frac{1}{R^{m-1}}\,\frac{d}{dR}\left(R^{m-1}\,\frac{d}{dR}\right)U_{ML}^{(m)}(R) - \frac{M(M+m-2)}{R^2}\,U_{ML}^{(M)}(R)\right]Y_m^{(M)L}$$

which shows that the kinetic energy operator does not affect the hyperspherical harmonic whose orthogonality gives

$$\langle U_{ML}^{(m)}(R)Y_m^{(M)L}|T|U_{M'L'}^{(m)}(R)Y_m^{(M')L'}\rangle = \langle \Psi_{ML}|T|\Psi_{M'L'}\rangle = \frac{-\hbar^2}{2\mu a_0^2}\int U_{ML}^{(m)}(R)\left[\frac{1}{R^{m-1}}\,\frac{d}{dR}\left(R^{m-1}\,\frac{d}{dR}\right)U_{M'L'}^{(m)}(R) - \frac{M'(M'+m-2)}{R^2}\times U_{M'L'}^{(m)}(R)\right]R^{m-1}\,dR\,\delta(M,M')\delta(L,L').$$

For these diagonal matrix elements we have

$$\langle \Psi_{ML}|T|\Psi_{M'L'}\rangle = \int G_{ML}(R)\left(\frac{d^2}{dR^2} - \frac{(m-3)(m-1)+4M(M+m-2)}{4R^2}\right)G_{ML}(R)\,dR,$$

where we have put

$$U_{ML}^{(m)}(R) = R^{(1-m)/2}G_{ML}(R).$$

The expectation value of the total Hamiltonian $H = T + V$, where V is the two-body interaction given by Goldhammer is now written as

$$\langle \Psi_{ML}|H|\Psi_{M'L'}\rangle = \frac{-\hbar^2}{2\mu a_0^2}\,\delta(M,M')\delta(L,L')\int G_{ML}(R)\left(\frac{d^2}{dR^2} - \frac{(m-3)(m-1)+4M(M+m-2)}{4R^2}\right),$$

$$G_{M'L'}(R)\,dR + \sum_{M',L'}\int G_{ML}(R)V_{ML,M'L'}\,G_{M'L'}(R)\,dR = E\int G_{ML}(R)G_{M'L'}(R)\,dR\,.$$

Integrating by parts and making use of the fact that $G_{ML}(R)(d/dR)G_{ML}(R)$ vanishes at both $R=0$ and $R=\infty$ we get

$$\frac{\hbar^2}{2\mu a_0^2}\int\left[\left(\frac{d}{dR}G_{ML}(R)\right)^2 + \frac{(m-3)(m-1)+4M(M+m-2)}{4R^2}\,G_{ML}^2(R)\right]dR$$

$$+\sum_{M'L'}\int G_{ML}(R)V_{ML,M'L'}G_{M'L'}(R)\,dR = E\int (G_{ML}^{(R)})^2\,dR\,.$$

The radial part of the total wave function is now varied to produce the maximum binding energy. This gives

$$\int \delta G_{ML}^{(R)}\left(\frac{d^2}{dR^2}G_{ML}^{(R)} + \frac{(m-3)(m-1)+4M(M+m-2)}{4R^2}\,G_{ML}^{(R)}\right.$$

$$\left.+\sum_{M',L'}\frac{2\mu a_0^2}{\hbar^2}V_{ML,M'L'}\,G_{M'L'}^{(R)} - \frac{2\mu a_0^2 E}{\hbar^2}\,G_{ML}^{(R)}\right)dR = 0\,.$$

Since $\delta G_{ML}^{(R)}$ is arbitrary we must have

$$\frac{d^2}{dR^2}G_{ML}^{(R)} + \frac{(m-3)(m-1)+4M(M+m-2)}{4R^2}\,G_{ML}^{(R)}$$

$$+\sum_{M',L'}\frac{2\mu a_0^2}{\hbar^2}V_{ML,M'L'}\,G_{M'L'}^{(R)} = \epsilon G_{ML}^{(R)}$$

with $\epsilon = 2\mu a_0^2 E/\hbar^2$. The last equation represents a set of coupled second order differential equations[2] corresponding to possible values of the total angular momentum L and the total quanta of excitation M. A numerical solution of the above set of differential equations will produce the binding energy of the nucleus E.

APPENDIX A: INTERNAL COORDINATE SYSTEM

An internal coordinate system is set up characterizing a $3(P-1)=m$ dimensional hyperspace. In this space the orbital part of the total wave function is constructed from products of single particle oscillator well wave functions which led to the definition of hyperspace spherical harmonics. This form of the total wave function will ensure the expression of the kinetic energy matrix element in the required integral form.

To eliminate the center of mass motion, the nondimensional vectors

$$\vec{\mathfrak{q}}_k = \vec{\mathfrak{r}}_k/a_0$$

are employed, where $\vec{\mathfrak{r}}_k$ is the position vector of the kth particle and a_0 is the oscillator well parameter. A set of orthonormal vectors $\vec{\mathfrak{a}}_1, \vec{\mathfrak{a}}_2, \ldots, \vec{\mathfrak{a}}_P$ is then built up as a linear combination of the vectors $\vec{\mathfrak{q}}_k$ transforming according to the representation $[P-1,1]$ of the permutation group S_P as given in Table I, where $1/\sqrt{N}$ is the normalizing factor. The last vector $\vec{\mathfrak{a}}_P$ is taken as the center of mass vector and the first $(P-1)$ vectors describe the internal motion of the P particles relative to the center of mass of the nucleus. These $(P-1)$ vectors characterize the $3(P-1) = m$ dimensional space in the following manner. The polar coordinates θ_{a_k} and Φ_{a_k} are introduced for each vector as

$$d\vec{\mathfrak{a}}_k = a_k^2\sin\theta_{a_k}\,d\theta_{a_k}\,d\Phi_{a_k} = a_k^2\,da_k\,dw_{ak}$$

with $0<\theta_{a_k}<\pi$, $0<\Phi_{a_k}<2\pi$, and $k=1,2,3,\ldots,(P-1)$.

The volume element in this space is

$$d\Omega = d\vec{\mathfrak{a}}_1 d\vec{\mathfrak{a}}_2\cdots d\vec{\mathfrak{a}}_{P-1}\,. \tag{A1}$$

Introducing the set of variables $R, \chi_1, \chi_2, \ldots \chi_{P-2}$ such that

$$a_1 = R\cos\chi_1\,,$$

$$a_2 = R\sin\chi_1\cos\chi_2\,,$$

$$a_3 = R\sin\chi_1\sin\chi_2\cos\chi_3\,,$$

$$\cdots$$

$$a_{p-1} = R\sin\chi_1\sin\chi_2\cdots\sin\chi_{P-2}$$

with $0<\chi_i<\pi/2$, $i=1,2,\ldots,(P-2)$, and

$$a_1^2 + a_2^2 + \cdots + a_{P-1}^2 = R^2$$

it follows that the volume element in the last $(P-1)$ dimensional space is

TABLE I. $[P-1, 1]$ representation of S_P.

	$\vec{q}_1$	$\vec{q}_2$	$\vec{q}_3$	$\vec{q}_4$	$\vec{q}_{p-3}$	$\vec{q}_{p-2}$	$\vec{q}_{p-1}$	$\vec{q}_p$	N
$\vec{a}_1$	1	1	1	1	1	1	1	$-(P-1)$	$P(P-1)$
$\vec{a}_2$	1	1	1	1	1	1	$-(P-2)$	0	$(P-1)(P-2)$
$\vec{a}_3$	1	1	1	1	1	$-(P-3)$	0	0	$(P-2)(P-3)$
$\vec{a}_4$	1	1	1	1	$-(P-4)$	0	0	0	$(P-3)(P-4)$
...	...	...	...	...	...	...	...	...	...
...									
...	...	...	...	...	...	...	...	...	...
$\vec{a}_{p-3}$	1	1	1	-3	0	0	0	0	12
$\vec{a}_{p-2}$	1	1	-2	0	0	0	0	0	6
$\vec{a}_{p-1}$	1	-1	0	0	0	0	0	0	2
$\vec{a}_p$	1	1	1	1	1	1	1	1	P

$$da_1 da_2 da_3 \cdots da_{P-1} = \frac{\partial(a_1 a_2 \cdots a_{P-1})}{\partial(R\chi_1\chi_2\cdots\chi_{P-2})}\, dR\, d\chi_1 d\chi_2 \cdots d\chi_{P-2}$$
$$= (R^{P-2}dR)(\sin^{P-3}\chi_1 d\chi_1)(\sin^{P-4}\chi_2 d\chi_2)\cdots(\sin\chi_{P-3}d\chi_{P-3})\,d\chi_{P-2}.$$

Substituting in Eq. (A1) we get the volume element in the m dimensional space as

$$d\Omega = (R^{m-1}dR)(\cos^2\chi_1 \sin^{m-4}\chi_1 d\chi_1)\,(\cos^2\chi_2 \sin^{m-7}\chi_2 d\chi_2)\cdots \times(\cos^2\chi_{p-2}\sin^2\chi_{p-2}d\chi_{p-2})(d\omega_{a_1}d\omega_{a_2}\cdots d\omega_{a_{p-1}})$$

or, in short,

$$d\Omega = R^{m-1}dR\, d\Omega_\chi\, d\omega_{a_1}d\omega_{a_2}\cdots d\omega_{a_{p-1}}.$$

Using

$$\int_0^{\pi/2} (\cos\chi)^\mu (\sin\chi)^\mu d\chi = \frac{1}{2}\,\frac{\Gamma(\frac{1}{2}(\mu+1))\Gamma(\frac{1}{2}(\nu+1))}{\Gamma(\frac{1}{2}(\mu+\nu+2))}$$

the surface area of a unit sphere in the m dimensional space is

$$\int d\Omega_m = (4\pi)^{P-1}\int d\Omega_\chi = \frac{2\pi^{m/2}}{\Gamma(\frac{1}{2}m)}$$

since

$$\int d\Omega_\chi = \frac{\pi^{\frac{1}{2}(P-1)}}{2^{2P-3}\Gamma(\frac{1}{2}m)}\,.$$

APPENDIX B: VECTOR COUPLED ORBITAL STATES

The oscillator well wave functions for a single particle that belong to the eigenvalue $\hbar^2/2ma_0^2(n+\frac{3}{2})$ is of the form

$$\Phi_{nlm}(a) = B_{nl}(a)Y_l^m(\theta,\Phi),$$

where

$$B_{nl}(a) = \left(\frac{2\Gamma(\frac{1}{2}(n-l+2))}{\Gamma(\frac{1}{2}(n+l+3))}\right)^{1/2} e^{-a^2/2}a^l\,\mathfrak{L}^{l+1/2}_{(n-l)/2}(a^2) \quad \text{(B1)}$$

and $Y_l^m(\theta,\Phi)$ is a three dimensional spherical harmonic with the normal quantum numbers n, l, and m. This wave function can be expressed in the shell model form using the relation

$$|\gamma^l(\vec{e})\rangle = \left(\frac{2l+1}{4\pi}\right)^{1/2}\left(\frac{(2l)!}{2^l P!P!}\right)^{1/2}|[\vec{e}^{\,l}]\,P\rangle,$$

where $\vec{e}$ is a unit vector. It follows that the general shell model state in the vector $\vec{a}_1$ can be written as

$$|(2r+l,l)\rangle = \left(\frac{r!\,(2l+1)(2l)!}{2\pi\Gamma(r+l+\frac{3}{2})2^l l!!}\right)^{1/2} \times e^{-2a_i^2}\mathfrak{L}_r^{l+1/2}(a_1^2)|[\vec{a}_i^{\,l}]\,l\rangle,$$

where $(2r+l)=M$ stands for the number of quanta of excitation. When such shell model states in the $(P-1)$ vectors are vector coupled together, the resulting total shell model states of angular momentum L in the hyperspace take the form

$$|(M_1)l_{a_1}, (M_2)l_{a_2}; L_2\cdots; (M_{p-2})l_{a_{p-2}}, L_{P-2}, (M_{P-1})l_{P-1}, L\rangle,$$

which could always be expressed as the sum of a number of terms each of which is of the form

$$\Psi_{ML} = U^{(M)}_{ML}(R)\,Y_R^{(M)L}, \quad \text{(B2)}$$

where $U^{(m)}_{ML}(R)$ is the multidimensional oscillator well radial dependence given by

$$U^{(M)}_{ML}(R) = \left(\frac{2[\frac{1}{2}(M-L)]!}{\Gamma(\frac{1}{2}(M+L+m))}\right)^{1/2} e^{-R^2/2}R^L\,\mathfrak{L}^{L+(m-2)/2}_{(M-L)/2}(R^2) \quad \text{(B3)}$$

satisfying the orthonormal relation

$$\int U_{ML}(R)U_{M'L'}(R)R^{m-1}dR = \delta(L,L')\delta(M,M')$$

and $Y_M^{(M)L}$ is a hyperspace spherical harmonic defined by

$$Y_m^{(M)L} = \frac{1}{(\int d\Omega_\chi)^{1/2}}\, Y_{a_1}^{(M_1)l_{a_1}} Y_{a_2}^{(M_2)l_{a_2}} \cdots Y_{a_{P-1}}^{(M_{P-1})l_{a_{P-1}}}. \tag{B4}$$

APPENDIX C: EVALUATION OF THE RADIAL INTEGRALS

The matrix element of a two-body interaction V with Gaussian radial dependence of the form

$$J_{ij} = \exp[-(1/\alpha)(-q_i + q_j)^2],$$

where α is a constant, can be written as

$$\langle \Phi_{ML} | V | \Phi_{M'L'} \rangle = \tfrac{1}{2}P(P-1)\langle \Phi | J_{P-1,P} | \Phi' \rangle,$$

where

$$J_{P-1,P} = \exp[-(2/\alpha)(a_{P-1}{}^2)]$$

and Φ and Φ' are identical shell model states in the particulars of the first $(P-2)$ particles; otherwise the matrix element is zero. This is because $J_{P-1,P}$ operates only on the coordinates of the last pair of particles (see the table). The problem of calculating the above matrix element is therefore reduced to the three dimensional problem of evaluating the radial integral:

$$I(ML, M'L') = \int_0^\infty U_{ML}^{(3)}(a) e^{-2a^2/\alpha} U_{M'L'}^{(3)}(a) a^2\, da.$$

Substitution from (B3) gives

$$I(ML, M'L') = A \int_0^\infty e^{-a^2/\beta} a^{(L+L'+2}\, \mathfrak{L}_{(M-L)/2}^{L+1/2}$$
$$\times \mathfrak{L}_{(M'-L')/2}^{L'+1/2}(a^2)\, da, \tag{C1}$$

where

$$\beta = \alpha/(\alpha+2)$$

and

$$A = \left(\frac{4[\tfrac{1}{2}(M-L)]!\,[\tfrac{1}{2}(M'-L')]!}{\Gamma(\tfrac{1}{2}(M+L+3))\Gamma(\tfrac{1}{2}(M'+L'+3))} \right)^{1/2}.$$

Putting $a^2 = \beta y$ we get

$$I(ML, M'L') = \frac{A}{2} \int_0^\infty e^{-y} (\beta y)^{L+L'+2} \mathfrak{L}_{(M-L)/2}^{L+1/2}(\beta y)$$
$$\times \mathfrak{L}_{(M'-L')/2}^{L'+1/2}(\beta y)\, d(\beta y).$$

Using

$$\mathfrak{L}_n^k(x) = \sum_{r=0}^{n} (-1)^r \frac{\Gamma(n+k+1)x^r}{\Gamma(n-r+1)\Gamma(k+r+1)\Gamma(r+1)}$$

we get

$$I(ML, M'L') = \frac{A}{2} \sum_{r=0}^{(M-L')/2} \sum_{s=0}^{(M'-L')/2} (-1)^{r+s} \beta^{1/2(L+L'+2r+2s+3)}$$
$$\times \frac{\Gamma(M+L+\tfrac{3}{2})\Gamma(M'+L'+\tfrac{3}{2}) \int_0^\infty e^{-y} y^{1/2(L+L'+2r+2s+1)} dy}{\Gamma(L+r+\tfrac{3}{2})\Gamma(L'+S+\tfrac{3}{2})\Gamma(\tfrac{1}{2}(M-L-2r+2))\Gamma(\tfrac{1}{2}(M'-L'-2s+2))L(r+1)\Gamma(s+1)}$$
$$= C \sum_{r=0}^{(M-L)/2} \sum_{s=0}^{(M'-L')/2} \frac{(-1)^{r+s}\beta^{1/2(L+L'+2r2s+3)}\Gamma(\tfrac{1}{2}(L+L'+2r+2s+3))}{\Gamma(L+r+\tfrac{3}{2})\Gamma(L'+s+\tfrac{3}{2})\Gamma(r+1)\Gamma(s+1)\Gamma(\tfrac{1}{2}(M-L-2r+2))\Gamma(\tfrac{1}{2}(M'-L'-2s+2))}, \tag{C2}$$

where $C = \tfrac{1}{2}A\,\Gamma(M+L+\tfrac{3}{2})\Gamma(M'+L'+\tfrac{3}{2})$. To express the final result (C2) in the integral form we use the following relations[3] for the hypergeometric function $\Phi(a, c, x)$:

(i)

$$\Phi(a, c, -x) = e^{-x}\Phi(c-a, a, x),$$

(ii)

$$\int_0^\infty e^{-sx} x^{c-1} \Phi(a, c, x)\, dx = \frac{\Gamma(c)}{S^c}\left(\frac{s}{s-1}\right)^a.$$

Combining these two we get

$$\int_0^\infty e^{-(s-1)x} x^{c-1} \Phi(a, c, -x)\, dx = \frac{\Gamma(c)}{S^c}\left(\frac{s}{s-1}\right)^{c-a}.$$

Putting $S = \tfrac{1}{2}(\alpha+2)$, i.e., $S/(S+1) = 1/\beta$, we get

$$\int_0^\infty e^{(\alpha/2)x} x^{c-1} \Phi(a, c, -x)\, dx = \frac{\Gamma(c)}{\tfrac{1}{2}(\alpha+2)^c}\beta^{a-c}.$$

Substituting $\alpha x = 2R^2$ we get

$$\int_0^\infty e^{-R^2} R^{2c-1} \Phi(a, c, -2R^2/\alpha)\, dR = \tfrac{1}{2}\Gamma(c)\beta^a;$$

putting $c = \tfrac{1}{2}(M+M'+m)$ we get

$$\beta^a = \Gamma(\tfrac{1}{2}(M+M'+m))$$
$$\times \int_0^\infty e^{-R^2} R^{M+M'+m-1} \Phi[a\tfrac{1}{2}(M+M'+m) - 2R^2/\alpha]\, dR,$$

but from (B3)

$$U^{(m)}_{MM}(R)=\left(\frac{2}{\Gamma(\frac{1}{2}(M+M'+m))}\right)^{1/2}e^{-R^2/2}R^M;$$

therefore,

$$\beta^a=\frac{[\Gamma(m+\frac{1}{2}m)\Gamma(M'+\frac{1}{2}m)]^{1/2}}{\Gamma(\frac{1}{2}(M+M'+m))}$$

$$\times\int_0^\infty U^{(m)}_{M'M'}(R)U^{(m)}_{MM}(R)$$

$$\times\Phi(a,\tfrac{1}{2}(M+M'+m),-2R^2/\alpha)R^{m-1}dR\,. \quad \text{(C3)}$$

Substitution of (C3) in (C2) would finally express the matrix element of a Gaussian radial dependence two-body interaction in the required integral form. Since the Gartenhaus radial dependence of a two-body interaction is of the form $(2a^2/\alpha)\times\exp[-(2a^2/\alpha)]$ we differentiate Eq. (C1) with respect to β to get

$$\frac{d}{d\beta}I(ML,M'L')=\frac{A}{\beta^2}\int_0^\infty e^{-a^2/\beta}(a)^{L+L'+4}\,\mathfrak{L}^{L+1/2}_{(M-L)/2}(a^2)$$

$$\times\mathfrak{L}^{L'+1/2}_{(M'-L')/2}(a^2)da\,. \quad \text{(C4)}$$

But the matrix element of a Gartenhaus radial dependence two-body interaction is

$$J(ML,M'L')=\int_0^\infty U^{(3)}_{ML}(a)U^{(3)}_{M'L'}(a)$$

$$\times[(2a^2/\alpha)e^{-2a^2/\alpha}]a^2da;$$

on substitution from (B3) it can be written as

$$J(ML,M'L')=A\left(\frac{1-\beta}{\beta}\right)\int_0^\infty e^{-a^2/\beta}(a)^{L+L'+4}$$

$$\times\mathfrak{L}^{L+1/2}_{(M-L)/2}(a^2)$$

$$\times\mathfrak{L}^{L'+1/2}_{(M'-L')/2}(a^2)da\,, \quad \text{(C5)}$$

$$J(ML,M'L')=\beta(1-\beta)I(ML,M'L')\,, \quad \text{(C6)}$$

which gives the matrix element of the Gartenhaus radial dependence two-body interaction in terms of that with a Gaussian radial dependence. The former, therefore, could be expressed in the integral form in terms of a new set of hypergeometric functions if we follow the same steps used to express the latter in that form.

[1]P. Goldhammer, Phys. Rev. 116, 676 (1959).
[2]G. Morpurgo, Nuovo Cimento 9, 461 (1952).
[3]*Higher Transcendental Functions* (Bateman Manuscript Project), edited by A. Erdélyi (McGraw-Hill, New York, 1953), Vol. 2.