Hyperspherical harmonics and electric dipole sum rules for the triton

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We use expansions in hyperspherical harmonics to calculate electric dipole transitions in the triton photoeffect. Gunn's ground state wave function is used with a Born approximation; the resulting cross section is compared with sum-rule calculations. We also use Ballot's ground state wave function for the spin-independent Volkov potential, in Born approximation, and combined with a continuum wave function for grand orbital one for the Volkov potential assumed to have Wigner character. The latter assumption gives an integrated cross section only 6% larger than the Thomas-Reiche-Kuhn sum rule; i.e., the severe truncation has only a small effect.

[NUCLEAR REACTIONS Triton; calculated photoeffect; hyperspherical harmonics; sum rules.]

I. INTRODUCTION

The trinucleon photoeffect for electric dipole transitions has been calculated by Gunn and Irving[1], Delves[2], Barbour and Phillips[3], Fabre and Levinger[4,5] and Gibson and Lehman[6] using different choices of the potential and different formalisms. In this paper we use the hyperspherical formalism of Delves as extended by Simonov[7] and Fabre[8]. We choose Volkov's model potential[9], which is independent of the spin or the parity of the nucleon-nucleon pair, so that we can compare our integrated cross section with the Thomas-Reiche-Kuhn (TRK) sum rule[10]. The actual nucleon-nucleon potential does depend on spin and parity, and also contains a noncentral force; therefore, we do not expect our model calculation to agree with experiment.

In the next section expansions in hyperspherical harmonics (h.h.) are introduced and used to evaulate several dipole sum rules. In the third section Gunn's Born approximation calculation for three-body breakup of the trinucleon is repeated and the results compared with sum rules. The Born approximation is also applied to the triton ground state wavefunction[11] for Volkov's potential. In the fourth section the triton photoeffect is calculated using Volkov's potential for the continuum, truncated at the lowest hyperspherical harmonic of grand orbital one; we find an integrated cross section only 6% higher than that given by the TRK sum rule. Our results are discussed in the final section.

II. PHOTOEFFECT USING HYPERSPHERICAL HARMONICS

The triton cross section for electric dipole transitions from initial state $|i\rangle$ to final state $|f\rangle$ with density of states ρ_f is

$$d\sigma(E_\gamma) = (4\pi^2/\hbar c)E_\gamma \langle i|D|f\rangle^2 \rho_f. \quad (2.1)$$

The photon, assumed polarized along the z-axis, interacts with the proton, chosen as the third nucleon. The dipole operator D is given by

$$D = e(z_3 - Z), \quad (2.2)$$

where Z is a component of the center of mass of the triton.

Moments of the cross section for the photoeffect are defined by

$$\sigma_p = \int_0^\infty \sigma(E_\gamma)\, E_\gamma{}^p dE_\gamma. \quad (2.3)$$

The moment for p = -1 is found from eq. (2.1) by summing over all final states

$$\sigma_{-1} = (4\pi^2/\hbar c)\langle i|D^2|i\rangle. \quad (2.4)$$

Note that σ_{-1} is independent of the shapes of the wavefunctions of the final states $|f\rangle$; we use only the property that the $|f\rangle$ form a complete set. Eq. (2.4) serves as a check on the numerical accuracy of our calculations.

The TRK sum rule is found using the Heisenberg relation

$$E_\gamma\langle i|D|f\rangle = -\langle i|[H,D]|f\rangle, \quad (2.5)$$

where H is the Hamiltonian. Applying the Heisenberg relation twice gives

$$\sigma_0 = -(2\pi^2/\hbar c)\langle i|[[H,D],D]|i\rangle. \quad (2.6)$$

If the potential energy term in H commutes with D, only the kinetic energy $\sum_i p_i^2/2M$ contributes to σ_0. Eq. (2.6) gives the nuclear TRK result

$$\sigma_0 = (4\pi^2/3)\alpha(\hbar^2/M) = 39.8 \text{ MeV mb}. \quad (2.7)$$

The Heisenberg relation is also used twice in obtaining the first moment

$$\sigma_1 = (4\pi^2/\hbar c)|\langle i|[H,D]^2|i\rangle|. \tag{2.8}$$

Again assuming that the potential energy commutes with D, we have the simple result that σ_1 is proportional to the expectation value of the kinetic energy.

Jacobi coordinates are defined following Fabre's notation[8] as

$$\vec{\xi} = \vec{r}_1 - \vec{r}_2,$$

$$\vec{\eta} = 3^{\frac{1}{2}}(\vec{r}_3 - \vec{R}), \tag{2.9}$$

where $\vec{R}$ is the position of the center of mass. Following Morse and Feshbach[12], and Fano,[13] $\vec{\xi}$ and $\vec{\eta}$, the two vectors in three dimensional space, are expressed in terms of one length r and five angles (θ_1, ϕ_1, θ_1, ϕ_2, Φ) which are collectively designated as Ω. θ_1 and ϕ_1 are the angles of the unit vector $\hat{\xi}$ in spherical polar coordinates, and θ_2 and ϕ_2 are the angles of $\hat{\eta}$. The lengths ξ and η are transformed to the polar coordinates r and Φ:

$$\eta = r \sin\Phi,$$

$$\xi = r \cos\Phi. \tag{2.10}$$

Fabre[8] and Morse and Feshbach[12] give the solution of the six-dimensional Helmholtz equation

$$(\nabla_\xi{}^2 + \nabla_\eta{}^2)\psi(r,\Omega) + k^2\psi(r,\Omega) = 0,$$

as

$$\psi(r,\Omega) = (kr)^{-2}\, J_{L+2}(kr)\, H_{[L]}(\Omega) \tag{2.11}$$

where the kinetic energy of the nucleons is $E = \hbar^2 k^2/M$. Here Fabre's "grand orbital" $L = \ell_1 + \ell_2 + 2n$, where n is a non-negative integer. The hyperspherical harmonics $H_{[L]}$, called K-harmonics by Simonov[7], are given by

$$H_{[L]}(\Omega) = N \cos^{\ell_1}\Phi \sin^{\ell_2}\Phi\, P_n^{\ell_1+\frac{1}{2},\ell_2+\frac{1}{2}}(\cos 2\Phi)\, Y_{\ell_1}^{m_1}(\theta_1,\phi_1)\, Y_{\ell_2}^{m_2}(\theta_2,\phi_2). \tag{2.11a}$$

$P_n^{\ell_1+\frac{1}{2},\ell_2+\frac{1}{2}}(\cos 2\Phi)$ is a Jacobi polynomial.

The notation [L] stands for the five quantum numbers (L, ℓ_1, m_1, ℓ_2, m_2). For the triton ground state, Simonov chooses a linear combination of the $H_{[L]}$ giving total orbital angular momentum zero, even parity, and complete symmetry for particle exchange. These linear combinations are designated $\mathcal{Y}_L^{(o)}(\Omega)$. Only even L are included in $\mathcal{Y}_L^{(o)}(\Omega)$, since the parity $(-1)^{\ell_1+\ell_2}$ is just $(-1)^L$ from the definition of the grand orbital. Simonov shows that the terms with L=2 are missing in the $\mathcal{Y}_L^{(o)}(\Omega)$.

Simonov[7], Erens[14] and Beiner[11] used h.h. to find the triton ground state wave function. The wave function $|i\rangle$ and the potential energy V were expanded in h.h.; the coefficient of a given h.h. was $r^{-5/2}\, u_L(r)$ for the wave function, and a "hypermultipole" $V_L(r)$ for the potential. Substituting these expansions into the Schroedinger equation, they obtained an infinite set of coupled differential equations for $u_L(r)$, which they truncated at a maximum grand orbital L_M.

Delves[2] and Fabre[4] pointed out that the dipole operator D from Eq. (2.2) is a h.h. with grand orbital one,

$$D = e\eta_z/3^{\frac{1}{2}} = e(\pi/18)^{\frac{1}{2}} r\, H_{1,0,1}^{0,0}(\Omega). \tag{2.12}$$

The three subscripts give the values of L, ℓ_1 and ℓ_2 respectively; the two superscripts give the values of m_1 and m_2.

Since the h.h. obey the same "triangle rule" as the spherical harmonics, electric dipole transitions take us from a truncated expansion for $|i\rangle$ to one for $|f\rangle$ (or vice versa). Specifically, if, following Gunn[1] we use only grand orbital zero in the h.h. expansion of $|i\rangle$, then transitions take us to $|f\rangle$ with grand orbital one. Alternately, if, following Fabre[4] we truncate the expansion of $|f\rangle$ at grand orbital one, then only transitions from grand orbital zero contribute for the initially completely symmetric S state.

The initial state wave function is

$$\psi_i(r,\Omega) = u_o(r)\, H_{0,0,0}^{0,0}(\Omega) r^{-5/2},$$

$$= u_o(r)\pi^{-3/2}\, r^{-5/2}. \tag{2.13}$$

The final free wave function is expanded in an infinite series of h.h. (see Ref. 4, Eq. (2.14)). The single term A which gives a non-zero matrix element for electric dipole transitions is

$$A = (2\pi)^3\, iJ_3(kr)(kr)^{-2} H_{1,0,1}^{0,0}(\Omega)\cdot H_{1,0,1}^{0,0*}(\Omega_k). \tag{2.14}$$

The integrations over the five-dimensional $d^5\Omega$ are done analytically. Define the radial matrix element

$$r_{if}^B = \int_o^\infty u_o(r) r(\pi kr/2)^{\frac{1}{2}}\, J_3(kr)dr. \tag{2.15}$$

The density of final states is

$$\rho_f = \tfrac{1}{2}(M/\hbar^2)\, (2\pi)^{-6}\, k^4 d^5\Omega_k. \tag{2.16}$$

Substitution of Eqs. (2.13) through (2.16) into (2.1) gives the differential cross section

$$d\sigma^B/d^5\Omega_k = (2\pi/9)\alpha(E_\gamma/k)(M/\hbar^2)(r_{if})^2|H^{0,0}_{1,0,1}(\Omega_k)|^2. \quad (2.17)$$

Integration over the five-dimensional solid angle d Ω_k in momentum-space gives the total cross section

$$\sigma^B = (2\pi/9)\alpha(E_\gamma/k)(M/\hbar^2)(r_{if})^2. \quad (2.18)$$

We note that our cross section is twice as large as Fabre's[4], since we use both isospin final states. Also, Fabre uses a mixed symmetry S' state in ψ_i, and therefore includes $u_2(r)$ in the calculation of the radial matrix element r_{if}. For our spin-independent potential, $u_2(r) = 0$.

The above calculations should be modified to include the effect of a hyperpotential $U_1^{(1)}(r)$ acting in the final state with grand orbital one. The wave function $u_1(r)$ obeys the differential equation[4]

$$(-d^2/dr^2 + 35/4r^2)u_1(r) + (M/\hbar^2)U_1^{(1)}(r)u_1(r) = k^2u_1(r). \quad (2.19)$$

At large r, $U_1^{(1)}(r)$ is negligible. The wave function is normalized to an asymptotic solution[5]

$$u_1(r) = (\pi kr/2)^{\frac{1}{2}}(\cos\delta\, J_3(kr) - \sin\delta\, Y_3(kr)). \quad (2.20)$$

Here δ is the phase shift for three-body to three-body scattering[2,5,14]. This wave function is used in (2.15) to evaluate the radial matrix element r_{if}.

For calculation of wave function, dipole matrix elements, and cross sections, it is convenient to truncate the wave function expansions in h.h.. However, for sum rule calculations of the integrated cross section σ_0, it is more convenient to truncate the h.h. expansion of the potential energy $V(r,\Omega)$. Suppose we use the same potential for both initial and final states; then we should find agreement with the TRK sum rule. But if we use different potentials for the initial and final states, then the potential V does not commute with the dipole operator D, giving us an extra term in Eq. (2.6).

The sum rules (2.4), (2.6) and (2.8) for σ_{-1}, σ_0, and σ_1 respectively, can be evaluated using h.h. For the first one, (2.12) is used to express the dipole operator in terms of η_z. For a completely symmetric S state,

$$\langle i|\eta_z^2|i\rangle = \langle i|r^2|i\rangle/6. \quad (2.21)$$

Expanding the initial wave function in h.h. and using their orthonormality to integrate over the five angles,

$$\sigma_{-1} = (\pi^2/9)\alpha\langle i|r^2|i\rangle = (\pi^2/9)\alpha\int_0^\infty (u_0^2 + u_4^2 + \ldots)r^2\,dr. \quad (2.22)$$

This infinite series converges very rapidly: a single term contributes about 99% of the sum rule, because its weight is 99.3% of the wave function[11].

Equation (2.7) gives the model-independent value of the integrated cross section for a potential that commutes with the dipole operator. In Born approximation, the double commutator of the potential energy and the dipole operator in Eq. (2.6) gives

$$\langle i|[[V,D],D]|i\rangle = 2\langle i|VD^2|i\rangle. \quad (2.23)$$

Since both V and $|i\rangle$ are completely symmetric,

$$\sigma_0^B = (4\pi^2/3)\,\alpha\{(\hbar^2/M) - \langle i|Vr^2|i\rangle/6\}. \quad (2.24)$$

If we make a different truncation of the potential for states $|i\rangle$ and $|f\rangle$, we need to replace the total potential V in (2.24) by the difference V' for the two states. For instance, the Volkov potential is truncated at about 24 for state $|i\rangle$ while in Section IV the final state $|f\rangle$ is truncated at L = 0. Then[11]

$$V'(r,\Omega) = \sum_{L=4}^{24} U_L^{(L)}(r)a_L\mathcal{Y}_L^{(o)}(\Omega). \quad (2.25)$$

III. BORN APPROXIMATION CALCULATIONS

The results of the previous section are applied to find the Born approximation cross section $\sigma^B(E_\gamma)$, the moment σ^B_{-1}, and the integrated cross section σ_0^B using two different ground state wave functions: the analytical form of Gunn-Irving[1] and the numerical results by Beiner[11] for the Volkov[9] potential.

Gunn's ground state wave function rewritten in h.h. contains only grand orbital zero:

$$u_0(r) = (8/3)^{\frac{1}{2}}\mu^2r^{3/2}\exp(-\mu r). \quad (3.1)$$

We assume $-h^2\mu^2/M$ = the triton energy. With the matrix element r_{if}, evaluated from (2.15), Eq. (2.18) gives Gunn's result

$$\sigma^B(E_\gamma) = (200\pi^2/3)\ \alpha(M/\hbar^2)E_\gamma\mu^4k^6(\mu^2 + k^2)^{-7}. \tag{3.2}$$

With these analytical expressions, σ_{-1} can be found in analytical form using either the definition (2.3) or the sum rule result (2.22). They agree[4].

The two calculations of the integrated cross section are done in an analogous manner. Using (2.3) and (3.2),

$$\sigma_0^B = (10\pi^2/3)\ \alpha(\hbar^2/M). \tag{3.3}$$

Note that σ_0^B is 2.5 times that of the TRK sum rule, (2.7); the extra integrated cross section comes from the expectation value of Vr^2 in (2.24). Gunn's ground state potential V(r) is found by substituting his wave function into the differential equation for the triton,

$$-d^2u_o/dr^2 + (15/4r^2)u_o + \mu^2u_o + (M/\hbar^2)V(r)u_o=0. \tag{3.4}$$

Thus,

$$V(r) = -(\hbar^2/M)(3/r^2 + 3\mu/r). \tag{3.5}$$

Note the "long tail" on the potential, as compared to the $1/r^3$ tail for a short-range two-body potential. This long tail is due to the incorrect behavior of Gunn's wave function at large r: u_o should fall off as an exponential, <u>without</u> his extra $r^{3/2}$ factor[16]. Substituting (3.5) into the sum rule equation (2.24) gives the result (3.3) for the integrated cross section.

We now turn to a somewhat more realistic example, Volkov's spin-independent potential, using Beiner's numerical solution for the triton ground state wave function, u_o.

Beiner and Fabre (private communication) have provided a tabulation of $u_o(r)$ out to 15 fm. u_o was extrapolated to large r using

$$u_0(r) \simeq 2.15\ r^{\frac{1}{2}}\ K_2(\mu r)\ \exp(-\beta^2/r^2). \tag{3.6}$$

The parameter β = 5.7 fm, and K_2 is a Kelvin function.

The matrix element r_{if} of (2.15) was evaluated numerically, giving the cross sections shown in Table I. The unusual values of photon energy were chosen to facilitate numerical integration of the cross section to obtain σ_{-1}, σ_0 and σ_1. Using Stagat's[17] 10-point Gauss-Gegenbauer integration formula

$$\int_0^\infty f(E_\gamma)dE_\gamma \simeq \sum_{i=1}^{10} w_i f(E_{\gamma_i}) \tag{3.7}$$

Stagat used the behavior of the asymptotic forms of the integrand at both lower and upper limits. The weights w_i are given in Table I.

The cross sections given in Table I were used with these weights to give the moments shown in Table II. Comparison with the sum rule values serves as a check on the accuracy of our calculations. From (2.22), σ_{-1} = 2.87 mb, in excellent agreement with our result found from the cross sections.

The sum rule (2.24) for the integrated cross section was evaluated by expanding both the potential and the wave function |i> in h.h.. Thus,

$$r^{5/2} < r,\Omega|i> = u_o(r)Y^{(o)}(\Omega) + u_4(r)Y_4^{(o)}(\Omega) + \dots , \tag{3.8}$$

$$\pi^{-3/2}V(r,\Omega) = 3V_o(r)Y^{(o)}(\Omega) + 3^{3/2}V_4(r)Y_4^{(o)}(\Omega) + \dots . \tag{3.9}$$

The "hypermultipole" $V_L(r)$ is defined by Fabre[4,8]. The factor 3 enters since there are 3 nucleon pairs.

Substitution and integration over the 5 angles gives

$$<i|Vr^2|i> = 3\int_0^\infty (u_0{}^2 + \dots)V_0(r)r^2dr + 6(3)^{\frac{1}{2}}\int_0^\infty(u_0u_4V_4r^2dr + \dots). \tag{3.10}$$

These integrals were evaluated numerically, using the h.h. expansion for Volkov's two-body potential, $V(r_{ij})$:

$$V(r_{ij}) = 144.86\ \exp(-(r_{ij}/0.82)^2) - 83.4\ \exp(-(r_{ij}/1.60)^2), \tag{3.11}$$

$$V_{2K}(r) = 289.72\ \exp(-x)\ I_{K+1}(x)/x - 166.8\ \exp(-x')I_{K+1}(x')/x',$$
$$x = \tfrac{1}{2}(r/0.82)^2;\ x' = \tfrac{1}{2}(r/1.60)^2. \tag{3.12}$$

Table I

Cross section for triton photoeffect

Photon Energy E_γ (MeV)	Weight[a] w_i	Born Approximation σ^B (mb)	Cross Section σ (mb)	Phase Shift[b] δ (deg)
8.84	0.501	0.0028	0.018	14.4
9.51	0.867	0.035	0.36	28.3
10.61	1.37	0.180	2.46	50.7
12.33	2.13	0.563	6.29	88.6
15.02	3.36	1.24	4.08	122.6
19.38	5.60	1.98	1.33	136.7
26.99	10.2	2.13	.296	137.8
41.79	21.2	1.52	.0356	129.0
76.92	56.7	0.426	6.88×10^{-4}	108.8
201.7	262.	0.00196	1.10×10^{-4}	69.0

a. See Eq. (3.7).
b. See Eq. (2.20).

Here $I_{K+1}(x)$ is a modified Bessel function.

Evaluating (3.12) numerically and substituting into (2.24) gives the numerical result

$$\sigma_0^B = 39.8 + 54.1 + 2.4 + \ldots \quad 96.3 \text{ MeVmb}. \tag{3.13}$$

The first term on the right is the TRK result, and the latter two are contributions from the two terms in (3.10). Comparison with $\sigma_0^B = 95.3$ MeV mb is remarkably good.

IV. CALCULATION FOR VOLKOV POTENTIAL

Another unreasonable assumption is substituted for the Born approximation: that we have a Wigner force, with indentical two-body forces in the ground and continuum states. We do not expect agreement with this experiment. Our purpose in performing this model calculation was to find the effect of truncation of the h.h. expansion for the continuum by comparison with the TRK sum rule results. The moment σ_1 was also checked against sum rule results; the value of σ_{-1} was used as a check on our numerical accuracy.

The continuum wave function $u_1(r)$ is a solution of (2.19) with normalization (2.20). The hyperpotential $U_1^{(1)}(r) = 3V_0(r)$ where $V_0(r)$ is given by (3.12) for the Volkov potential.

This differential equation was solved numerically and normalized by comparison with (2.20) at two large values or r.

Our result for the cross section and the phase shift are given in Table I. (These numerical results were given earlier[18] at the Delhi conference, where the cross section for final isospin 3/2 states is just half the value for the total cross section evaluated in this paper.)

The effect of using the potential in the final state is shown in Table I: the broad peak for the Born approximation is narrowed and pulled to lower energy. The attractive potential for the final state wave function "pulls in" the wave function, giving a significant increase in the cross section at low energies. At high energies, this "pulling in" leads to destructive interference so the calculation with a potential gives a lower cross section than that for Born approximation. The large values of the phase shift also show that (for this model) the Born approximation can be expected to be rather poor.

Table II shows that the integrated cross section $\sigma_0 = 42.2$ MeV mb is only 6% higher than the TRK value of 39.8 MeV mb. That is, our drastic truncation to a single term in the hypermultipole expansion of the final state potential is surprisingly accurate. The results of

Table II

Comparison with sum rules

Moment[a]	Born Approximation Cross Section	Born Approximation Sum Rule[b]	Volkov Potential Cross Section	Volkov Potential Sum Rule[b]
σ_{-1}	2.87 mb	2.87 mb	2.86 mb	2.87 mb
σ_0	95.3 MeV mb	96.3 MeV mb	42.2 MeV mb	42.2, 39.8 MeV mb
σ_1	4200 MeV^2 mb		677. MeV^2 mb	580 MeV^2 mb
$\sigma_1\sigma_{-1}/(\sigma_0)^2$	1.33		1.09	

a. See Eq. (2.3).
b. See Eqs. (2.7), (2.22), (3.13), and (4.1).

neglected terms can be studied in two different ways. First, we can calculate the final state wave function using coupled h.h. with grand orbitals of one and three. Fang finds[18] that the cross section curve is shifted to a slightly lower peak energy, σ_{-1} is unchanged, and σ_0 is decreased from our 42.2 MeV mb to 41.0 MeV mb. Second, we can evaluate the series (3.13), this time omitting the term proportional to the expectation value of $3V_0r^2$, since we included the term $3V_0(r)$ in finding the final state wave function u (r). This sum rule calculation gives $\sigma_0 = 39.8 + 2.4 + \ldots \simeq 42.2$ MeV mb. The agreement with 42.2 MeV mb from the cross sections is quite good.

The cross section curve gives $\sigma_1 =$ 677 MeV^2 mb. Evaluating the sum rule (2.8) for a potential that commutes with the dipole operator gives

$$\sigma_1 = (8\pi^2/9)\alpha(\hbar^2/M)\langle i|T|i\rangle. \tag{4.1}$$

The ground state expectation value of the kinetic energy operator T is evaluated using $T = H - V(r,\Omega)$. The hypermultipole expansion of $V(r,\Omega)$ was truncated at the first term. Numerical evaluation gives $\langle i|T|i\rangle = 21.9$ MeV, and from (4.1), $\sigma_1 = 580$ MeV^2 mb. Comparison with 677 MeV^2 mb in Table II shows that our cross sections give a value of σ_1 17% higher than the approximate sum rule result.

Table II also shows $\sigma_{-1}\sigma_1/(\sigma_0)^2$ evaluated from the cross sections. This quantity is always larger than unity. It is close to unity for the Volkov potential, since the photoeffect curve has a narrow resonance[10].

V. DISCUSSION

The calculations of electric dipole transitions in the photoeffect for the Volkov potential, truncating the continuum wave function to a single term, show that this truncation is surprisingly good. While the Born approximation gives an integrated cross section 140% larger than the Thomas-Reiche-Kuhn value, Table II shows that the use of a single h.h. in the continuum reduces the integrated cross section to a value only 6% above the TRK value. This six percent difference is understood in terms of the expectation value of neglected terms in the h.h. expansion of the potential energy, starting with grand orbital four.

Convergence may be poor for the h.h. expansions of $V(r,\Omega)$ and $\psi_f(r,\Omega)$ for the potential energy and continuum wave function. However, calculations of the total cross section for the photoeffect show rapid convergence of the h.h. expansion, due to the dominance of the lowest term $u_0(r)$ in the ground state triton wave function [4,11].

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