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Inelastic transition form factors in the H atom

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Arbitrary inelastic transition form factors in the H atom have been exactly evaluated in closed form by a group-theoretical method. The final expression contains exactly known $O(4)$ and $O(2,1)$ representation functions and a single trivial finite sum. We also give the square of the form factors summed over l and l' and obtain as a special case the result of Massey and Mohr.

I. INTRODUCTION

The arbitrary inelastic excitation form factor of the hydrogen atom is an important quantity in atomic theory and in many applications, especially astrophysics, involving highly excited states. Therefore an exact closed expression for this quantity (and hence for the oscillator strengths and cross-section formulas) is quite essential. This goal has been partially achieved through various degrees of approximations.[1] Massey and Mohr[2] were first to evaluate the excitation of the H atom from its ground state to an arbitrary state by using explicitly the spatial wave functions. However, the general expressions for arbitrary transitions become too complicated to compute by this method.

In a previous paper[3] an algebraic approach was used to evaluate the arbitrary transition form factors, and general expressions were given, however, as complicated sums over certain Clebsch-Gordan coefficients. The purpose of the present paper is to considerably simplify these expressions by using the exactly known $O(4)$ and $O(2,1)$ representation functions. The final expression is reduced to a single finite sum. We further sum the square of the inelastic form factors over l and l', the initial and final angular momenta. The result is again a single finite sum over known functions. Finally, we show how in the special case our formulas reduce to the Massey-Mohr result, and relate the singularities of the form factor via anomalous threshold to the binding energy [cf. discussion after Eq. (20)]. The final results are analytic in n and hence valid also for noninteger n values; the latter occur for scattering states for which n is pure imaginary.

Besides the Massey-Mohr result,[2] there are a number of other, more recent papers dealing with the same topic. Holt considers bound-free transitions from $2s$ and $2p$ levels to continium.[4] Sobeslavsky[5] gives a semiclassical treatment of transitions for large n values. In two papers Beigman and co-workers[6,7] start from a general integral representation of the form factors obtained from Coulomb Green's functions and make expansions in powers of $1/n$ and $1/n'$, i.e., for large n and Δn. The bound-free transitions have also been considered in detail by Matzusawa.[1]

II. PRELIMINARIES

We give here a brief discussion of the significance and interpretation of the relatively new algebraic techniques used in Sec. III. A detailed technical introduction to the subject can be found in the recent book by Englefield,[8] and in Ref. 9. More specifically, the derivation of the algebraic form of the current operator from the Schrödinger picture has been recently described in detail.[10]

The algebraic description of the spin states and more generally the states of the H atom for fixed energy by the representations of the groups SO(3) and SO(4), respectively, is well known. It turns out that the totality of states of the atom for all energies also belongs to the representation space of a group—this time the noncompact group SO(4, 2). This group also contains the current operator and is called the *dynamical group* of the system; it incorporates all of the information about the atom and its electromagnetic interactions. The dynamical group of a system is determined as follows: From the dynamical variables of the theory (e.g., $\vec{r}$ and $\vec{p}$, in the spinless case) and their enveloping algebra (i.e., r, r^2, $\vec{r}\times\vec{p}$, p^2, etc.), we construct a Lie algebra L such that the Hamiltonian H of the system is a function of the Lie algebra (i.e., a function of the generators or their combinations). If this is the case then H acts on an irreducible representation of L, and this representation provides a complete set of states for the problem. The calculation of matrix elements can then be reduced to those of the group elements in the carrier space of the representation, which we call the space of the *group states*. Next, for problems involving external interactions there remains the identification of the interaction terms as a function of the group elements. For the interaction of the *bound* electron with an external electromagnetic field $A(x)$ we start from the two-body problem with the interaction term $-(e/2m_e)[\vec{p}_e\cdot\vec{A}(x_e)+\vec{A}(x_e)\cdot\vec{p}_e]$. The transformation between the dynamical variables $\vec{r}_e$, $\vec{p}_e$, etc., and the generators L_{AB} of the dynamical group leads easily to the form of the current given below in Eq. (2), which is the starting point of this paper. Because we start in general from a two-body problem the masses of an electron and a proton appear in the formulas, but for the nonrelativistic form factors of the bound electron the final results depend only on reduced mass.

The significance of the dynamical group SO(4, 2) does not end in providing methods of calculations of matrix elements. The group contains the symmetry group SO(4) of H as a subgroup, as well as the transformations corresponding to Galilean or Lorentz transformations, and provides a natural way of describing a composite system in a covariant way as a single "elementary entity." This point of view has been useful in the physics of fundamental particles, where we are aware of the composite nature of the particles (say a proton) but cannot yet identify the constituents or the forces that hold the constituents together.

III. CALCULATION OF THE FORM FACTORS

We present thus an exact evaluation of the four-vector vertex function

$$F_\lambda(q)=\int \psi^*_{n'l'm'}(\vec{x})e^{i(\mu/m_e)\vec{q}\cdot\vec{x}}J_\lambda\psi_{nlm}(\vec{x})\,d^3x \qquad (1)$$

by group-theoretical methods (μ is the reduced mass).

Equation (1) admits three different interpretations: (i) Fourier transform of the charge and current distribution of the atom; (ii) the inelastic transition matrix element of the interaction in an external electromagnetic plane wave of momentum q; and (iii) the imparting to the outgoing atom in the final state $(n'l'm')$ a momentum $\vec{q}$ (boost) by the external field, from an initial state (nlm) at rest. The last interpretation provides the algebraic reformulation. The coordinates $\vec{x}'=(\mu/m_e)\vec{x}$ are the generators of the Galilean-boosts transformations. In fact, the most concise and elegant formulation of the Kepler problem leads to the group $O(4,2)$, the conformal group, with its 15 generators $L_{AB}=-L_{BA}(A,B=1,2,3,4,5=0,6)$ composed of $\vec{J}$ (angular momentum), $\vec{A}$ (Lenz vector), $\vec{M}$ (boost operators), Γ_μ (a current four vector), and a dilation operator T plus a scalar S. The theory is relativistic and one can also evaluate the relativistic counterpart of (1), but we shall perform here the nonrelativistic calculation.

As described in earlier papers[3,9] the current operator J_μ in (1) with components

$$J_\mu=\{1;\ \vec{q}/2m_e\}$$

is represented in algebraic formulation by

$$\left\{\frac{1}{a}(L_{56}-L_{46});\ \frac{1}{m_e}L_{i6}+\frac{q_i}{2m_e}\frac{1}{a}(L_{56}-L_{46})\right\},\qquad i=1,2,3\ , \quad (2)$$

where a is an arbitrary scale parameter and the boost generators are represented by

$$M_i=-(m_p/a)(L_{i5}-L_{i4})\ , \qquad (3)$$

where m_p is the proton mass. The operators L_{AB} act on the physical states denoted by

$$|\overline{n}lm\rangle=(1/n)e^{-i\theta_n L_{45}}|nlm\rangle,\quad \theta_n=\ln(n)\ , \qquad (4)$$

where $|nlm\rangle$ are the "group states." With these notations the vertex function (1) can be written as the matrix element of a general group element

$$F_\mu=(1/nn')\langle n'l'm'|e^{i\theta_{n'}L_{45}}e^{i(K/a)(L_{35}-L_{34})}\times J_\mu e^{-i\theta_n L_{45}}|nlm\rangle\ , \qquad (5)$$

where we have assumed, without loss of generality, a boost in the z direction and have put $K=q_3 m_p$. Equation (5) is the starting point of our investigation.

We shall denote the charge form function F_0 by

$$I^{n'l'm'}_{nlm}=(1/ann')\langle n'l'm'|e^{i\theta_{n'}L_{45}}e^{i(K/a)(L_{35}-L_{34})}\times(L_{56}-L_{46})e^{-i\theta_n L_{45}}|nlm\rangle\,.$$

We simplify this equation by using the operator identity

$$e^{\theta A}Be^{-\theta A}=B+\theta[A,B]+(\theta^2/2\,!)[A,[A,B]]+\cdots$$

and the Lie commutation relation

$$[L_{AB},L_{CD}]=-i[g_{AC}L_{BD}+g_{BD}L_{AC}-g_{BC}L_{AD}-g_{AD}L_{BC}]$$

to obtain

$$I^{n'l'm'}_{nlm}=(1/n')\langle n'l'm'|G(L_{56}-L_{46})|nlm\rangle\ , \qquad (6)$$

where

$$G=e^{-i\theta_{n'n}L_{45}}e^{iKn(L_{35}-L_{34})},\quad \theta_{n'n}=\ln(n/n')\,.$$

The action of the $O(4,2)$-group generators on the canonical basis $|nlm\rangle$ are discussed in detail elsewhere.[9,11] We quote here the relevant expressions:

$$L_{56}|nlm\rangle = n|nlm\rangle\ ,$$

$$L_{46}|nlm\rangle = \tfrac{1}{2}[(n-l)(n+l+1)]^{1/2}|n+1,l,m\rangle + \tfrac{1}{2}[(n+l)(n-l-1)]^{1/2}|n-1,l,m\rangle\ .$$

Therefore

$$\begin{aligned} I_{nlm}^{n'l'm'} = (1/n')\{&n\langle n'l'm'|G|nlm\rangle \\ &-\tfrac{1}{2}[(n-l)(n+l+1)]^{1/2} \\ &\times\langle n'l'm'|G|n+1,l,m\rangle \\ &-\tfrac{1}{2}[(n+l)(n-l-1)]^{1/2} \\ &\times\langle n'l'm'|G|n-1,l,m\rangle\}\ . \end{aligned}$$

The matrix elements of the finite transformations $G = e^{-i\theta_{n'n}L_{45}}e^{iKn(L_{35}-L_{34})}$ can be very easily evaluated, especially because the operators L_{45}, $-L_{35}$, and L_{34} form an $O(2,1)$ subalgebra. The technique is standard and quite straightforward.[9] One usually parametrizes G in terms of Euler angles α, β, and γ such that

$$G = e^{-i\theta_{n'n}L_{45}}e^{iKn(L_{35}-L_{34})} = e^{-i\alpha L_{34}}e^{-i\beta L_{45}}e^{-i\gamma L_{34}}\ , \tag{7}$$

uses the 2×2 quaternion representation of $O(2,1)$, and evaluates both sides explicitly to get the angles α, β, and γ in terms of $\theta_{n'n}$ and Kn, i.e., one uses the two-dimensional representation

$$L_{45} = \tfrac{1}{2}i\sigma_1,\quad L_{35} = -\tfrac{1}{2}i\sigma_2,\quad L_{34} = \tfrac{1}{2}\sigma_3\ ,$$

where the σ_i are the usual Pauli matrices. Using these on both sides of the expression for G and comparing the coefficients of unity and of the σ_i matrices we obtain the following four equations ($\theta \equiv \theta_{n'n}$):

$$\cosh\tfrac{1}{2}\theta = \cosh\tfrac{1}{2}\beta\cos\tfrac{1}{2}(\alpha+\gamma)\ ,$$

$$\sinh\tfrac{1}{2}\theta = \sinh\tfrac{1}{2}\beta\cos\tfrac{1}{2}(\alpha-\gamma)\ ,$$

$$\tfrac{1}{2}nk(\coth\tfrac{1}{2}\theta - 1)\sinh\tfrac{1}{2}\theta = \sinh\tfrac{1}{2}\beta\sin\tfrac{1}{2}(\alpha-\gamma)\ ,$$

$$\tfrac{1}{2}nk(\coth\tfrac{1}{2}\theta - 1)\sinh\tfrac{1}{2}\theta = \cosh\tfrac{1}{2}\beta\sin\tfrac{1}{2}(\alpha+\gamma)\ .$$

Solving these equations, we get

$$\begin{aligned} \sinh\tfrac{1}{2}\beta &= [1/2(n'n)^{1/2}][(n'-n)^2+K^2n'^2n^2]^{1/2}\ , \\ \cosh\tfrac{1}{2}\beta &= [1/2(n'n)^{1/2}][(n'+n)^2+K^2n'^2n^2]^{1/2}\ , \\ \sin\alpha &= Kn/\sinh\beta\ , \\ \cos\alpha &= \frac{1}{2n'n}(n'^2-n^2+K^2n'^2n^2)\frac{1}{\sinh\beta} \\ &= \tanh\tfrac{1}{2}\beta - \frac{1}{n'}(n-n')\frac{1}{\sinh\beta} \\ &= \coth\tfrac{1}{2}\beta - \frac{1}{n'}(n+n')\frac{1}{\sinh\beta}\ , \\ \sin\gamma &= -Kn'/\sinh\beta\ , \\ \cos\gamma &= -\frac{1}{2n'n}(n^2-n'^2+K^2n'^2n^2)\frac{1}{\sinh\beta} \\ &= -\tanh\tfrac{1}{2}\beta + \frac{1}{n}(n'-n)\frac{1}{\sinh\beta} \\ &= -\coth\tfrac{1}{2}\beta + \frac{1}{n}(n'+n)\frac{1}{\sinh\beta}\ . \end{aligned} \tag{8}$$

Also, the matrix elements of $G = e^{-i\alpha L_{34}}e^{-i\beta L_{45}}e^{-i\gamma L_{34}}$ can be easily derived in a parabolic basis in which the operator L_{34} is diagonal, and one can express[12] these matrix elements (they exist only when $m = m'$) in terms of $O(4)$ and $O(2,1)$ representation functions, i.e.,

$$\langle n'l'm|G|nlm\rangle = \sum_{\tau} D(-\alpha)^{[n'-1,0]}_{l',|m|+\tau,|m|}\ V(\beta)^{|m|+1+\tau}_{n',n}\ D(-\gamma)^{[n-1,0]}_{l,|m|+\tau,|m|}\ ,\quad 0\leqslant\tau\leqslant\min(n-|m|-1,n'-|m|-1)\ , \tag{9}$$

where the $O(4)$ representation function

$$D(\theta)^{[P,Q]}_{j,j',m} = e^{i\theta m}[(2j+1)(2j'+1)]^{1/2}\sum_{m_1}\begin{pmatrix}\frac{1}{2}(P+Q) & \frac{1}{2}(P-Q) & j' \\ m_1 & m-m_1 & -m\end{pmatrix}\begin{pmatrix}\frac{1}{2}(P+Q) & \frac{1}{2}(P-Q) & j \\ m_1 & m-m_1 & -m\end{pmatrix}e^{-i2\theta m_1} \tag{10}$$

and the $O(2,1)$ representation function

$$\begin{aligned} V(\beta)^k_{m,n} &= \frac{1}{(m-n)!}\left[\frac{(m-k)!\,(m+k-1)!}{(n-k)!\,(n+k-1)!}\right]^{1/2}(\tanh\tfrac{1}{2}\beta)^{m-n}(\cosh\tfrac{1}{2}\beta)^{-2n}{}_2F_1(k-n,\,1-n-k;\,1+m-n;\,-\sinh^2\tfrac{1}{2}\beta)\quad (m\geqslant n) \\ &= \left[\frac{(n-k)!\,(m+k-1)!}{(m-k)!\,(n+k-1)!}\right]^{1/2}(\tanh\tfrac{1}{2}\beta)^{m-n}(\cosh\tfrac{1}{2}\beta)^{-2k}P^{m-n,\,2k-1}_{n-k}[1-2\tanh^2\tfrac{1}{2}\beta]\ , \end{aligned} \tag{11}$$

in which the Jacobi polynomial is defined as

$$P(x)^{\mu,\nu}_{\rho} = \sum_{\delta=0}^{\rho}\begin{pmatrix}\rho+\mu \\ \rho-\delta\end{pmatrix}\begin{pmatrix}\rho+\nu \\ \delta\end{pmatrix}\left(\frac{x-1}{2}\right)^{\delta}\left(\frac{x+1}{2}\right)^{\rho-\delta},\quad P(x)^{\mu,\nu}_0 = 1\ .$$

Therefore using Eq. (9) we obtain

$$
\begin{aligned}
I_{nlm}^{n'l'm} = \frac{1}{n'} \Bigg(n & \sum_{\tau=0}^{\min(n'-|m|-1,\, n-|m|-1)} D(-\alpha)^{[n'-1,0]}_{l',|m|+\tau,|m|} V(\beta)^{|m|+1+\tau}_{n',n} D(-\gamma)^{[n-1,0]}_{l,|m|+\tau,|m|} \\
& -\tfrac{1}{2}[(n-l)(n+l+1)]^{1/2} \sum_{\tau=0}^{\min(n'-|m|-1,\, n-|m|)} D(-\alpha)^{[n'-1,0]}_{l',|m|+\tau,|m|} V(\beta)^{|m|+1+\tau}_{n',n+1} D(-\gamma)^{[n,0]}_{l,|m|+\tau,|m|} \\
& -\tfrac{1}{2}[(n+l)(n-l-1)]^{1/2} \sum_{\tau=0}^{\min(n'-|m|-1,\, n-|m|-2)} D(-\alpha)^{[n'-1,0]}_{l',|m|+\tau,|m|} V(\beta)^{|m|+1+\tau}_{n',n-1} D(-\gamma)^{[n-2,0]}_{l,|m|+\tau,|m|} \Bigg) .
\end{aligned}
\tag{12}
$$

This expression can be written in a more compact form as

$$
I_{nlm}^{n'l'm} = \frac{1}{n'} \sum_{\tau=0}^{\min(n'-|m|-1,\, n-|m|-1)} \sum_{\epsilon=0,\pm 1} a_\epsilon(n,l) D(-\alpha)^{[n'-1,0]}_{l',|m|+\tau,|m|} V(\beta)^{|m|+1+\tau}_{n',n+\epsilon} D(-\gamma)^{[n-1+\epsilon,0]}_{l,|m|+\tau,|m|} ,
\tag{13}
$$

where

$$a_0(n,l) = n, \quad a_{\pm 1}(n,l) = -\tfrac{1}{2}[n(n\pm 1) - l(l+1)]^{1/2} .$$

Furthermore, in the above expression it is understood that the function $V(\beta)^k_{m,n}$ vanishes when $n, m < k$. [This is also clear from Eq. (11).]

Equation (13) is the exact expression for the charge form factor of the H atom and it can be readily computed using Eqs. (8), (10), and (11). For large n, n', l, and l' one could make use of the standard computer programs for the CG coefficients of Eq. (10), because this coefficient involves only a finite sum,[12] i.e.,

$$
\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} = (-1)^{l_2-l_1-m} \Delta \left(\frac{(l+l_2+m_1)!}{(l_1-l_2-m)!} \right) {}_3F_2(-l-m, -l+l_1-l_2, l_1-m_1+1; l_1-l_2-m+1, -l-l_2-m_1; 1) ,
$$

where

$$
\Delta = \left(\frac{(l+l_1-l_2)!(-l+l_1+l_2)!(l-m)!(l_1-m_1)!}{(l-l_1+l_2)!(l+l_1+l_2+1)!(l+m)!(l_1+m_1)!(l_2-m_2)!(l_2+m_2)!} \right)^{1/2} (-1)^{l_2+m_2}
$$

or

$$
\begin{aligned}
(2l+1)^{1/2} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} &= (-1)^{l_2+m_2-(l+m)} \left(\frac{(l+m)!(l_1+l_2-l)!(l-m)!(l-l_1+l_2)!(l+l_1-l_2)!}{(l_1+l_2+l+1)!(l_1-m_1)!(l_1+m_1)!(l_2-m_2)!(l_2+m_2)!} \right)^{1/2} \\
&\quad \times \sum_{Z=M}^{N} \frac{(-1)^Z (l+l_2-m_1-Z)!(l_1+m_1+Z)!}{Z!(l-m-Z)!(l-l_1+l_2-Z)!(l_1-l_2+m+Z)!} ,
\end{aligned}
$$

where

$$M = \max\{0, l_2-l_1-m\}, \quad N = \max\{l-m, l-l_1+l_2\} .$$

However, one might find it convenient to use the integral form of the self-conjugate $O(4)$ representation function $D(\alpha)^{[P,0]}_{l',j,m}$ derived by Vilenkin.[13] We quote here his result:

$$
D(\alpha)^{[P,0]}_{l',j,m} = a^P_{l',j,m} \int_0^\pi (\cos\alpha + i\cos\theta \sin\alpha)^{P-m} C^{m+1/2}_{j-m} \left(\frac{\cos\alpha \cos\theta + i\sin\alpha}{\cos\alpha + i\sin\alpha\cos\theta} \right) C^{m+1/2}_{l'-m}(\cos\alpha)(\sin\alpha)^{2m+1}\, d\theta ,
\tag{14}
$$

where

$$
a^P_{l',j,m} = \frac{i^{j-l'}}{\pi} 2^{2m-1} (m-\tfrac{1}{2})!(m-\tfrac{1}{2})! \left(\frac{(P-l')!(j-m)!(l'-m)!(P+l'+1)!(2l'+1)(2j+1)}{(P-j)!(j+m)!(l'+m)!(P+j+1)!} \right)^{1/2}
$$

and $C^\nu_n(\cos\phi)$ is the Gegenbauer polynomial.[14] For practical computation one might find the following identity[13] useful:

$$(\cos\alpha + i\cos\theta\sin\alpha)^{P-m} C_{j-m}^{m+1/2}\left(\frac{\cos\alpha\cos\theta + i\sin\alpha}{\cos\alpha + i\sin\alpha\cos\theta}\right) = \frac{\sqrt{\pi}}{2^{P+m}}\frac{j!(j+m)!(P-j)!}{(m-\frac{1}{2})!}(1+\cos\theta)^{P-m}e^{i(P-m)\alpha}$$
$$\times\sum_{s=0}^{P-m} b_{l',m,s}^{P}\, e^{-2is\alpha}\left(\frac{1-\cos\theta}{1+\cos\theta}\right)^{s},$$

where

$$b_{j,m,s}^{P} = \sum_{t=\max(0,s+j-P)}^{\min(j-m,s)} \frac{(-1)^t}{(s-t)!(P-j-s+t)!(j-t)!(j-m-t)!;(m+t)!t!}.$$

Next, we want to deduce from Eq. (12) the expression for the form factor for excitation to an arbitrary $(n'l'0)$ state from the ground state (100). We obtain

$$I_{100}^{n'l'0} = \frac{1}{n'}[D(-\alpha)_{l',0,0}^{[n'-1,0]}V(\beta)_{n',1}^{1}D(-\gamma)_{0,0,0}^{[0,0]} - (1/\sqrt{2})D(-\alpha)_{l',0,0}^{[n'-1,0]}V(\beta)_{n',2}^{1}D(-\gamma)_{0,0,0}^{[1,0]}$$
$$-(1/\sqrt{2})D(-\alpha)_{l',1,0}^{[n'-1,0]}V(\beta)_{n',2}^{2}D(-\gamma)_{0,1,0}^{[1,0]}]. \tag{15}$$

The special values of $O(4)$ and $O(2,1)$ representation functions can be very easily computed[12] from Eqs. (10) and (11). We here quote the final results:

$$D(-\gamma)_{0,0,0}^{[0,0]} = 1,\quad D(-\gamma)_{0,0,0}^{[1,0]} = \cos\gamma,\quad D(-\gamma)_{0,1,0}^{[1,0]} = -i\sin\gamma,$$
$$D(-\alpha)_{l',0,0}^{[n'-1,0]} = (-i)^{l'}2^{l'}(2l'+1)^{1/2}l'!\left(\frac{(n'-l'-1)!}{n'(n'+l')!}\right)^{1/2}(\sin\alpha)^{l'}C(\cos\alpha)_{n'-1-l'}^{l'+1},$$
$$D(-\alpha)_{l',1,0}^{[n'-1,0]} = (-i)^{l'}2^{l'}(2l'+1)^{1/2}l'!\left(\frac{-3(n'-l'-1)}{(n'+1)(n'-1)n'(n'+l')!}\right)^{1/2}$$
$$\times[l'(\sin\alpha)^{l'-1}(\cos\alpha)C(\cos\alpha)_{n'-1-l'}^{l'+1} - 2(l'+1)(\sin\alpha)^{l'+1}C(\cos\alpha)_{n'-2-l'}^{l'+2}], \tag{15'}$$
$$V(\beta)_{n',1}^{1} = \sqrt{n'}\,(\tanh\tfrac{1}{2}\beta)^{n'-1}(\cosh\tfrac{1}{2}\beta)^{-2},$$
$$V(\beta)_{n',2}^{1} = (1/\sqrt{2})\sqrt{n'}\,(n'-1)(\tanh\tfrac{1}{2}\beta)^{n'-2}(\cosh\tfrac{1}{2}\beta)^{-4} - \sqrt{2}\sqrt{n'}\,(\tanh\tfrac{1}{2}\beta)^{n'}(\cosh\tfrac{1}{2}\beta)^{-2},$$
$$V(\beta)_{n',2}^{2} = (1/\sqrt{6})[(n'-1)n'(n'+1)]^{1/2}(\tanh\tfrac{1}{2}\beta)^{n'-2}(\cosh\tfrac{1}{2}\beta)^{-4}.$$

One can also easily derive Eq. (15′) by substituting the following identity[13] into Vilenkin's formula, Eq. (14), for $j=m$:

$$(\sin\alpha)^{l'-m}C(\cos\alpha)_{P-l'}^{l'+1} = \frac{(-1)^{m-l'}}{\sqrt{\pi}}\frac{i^{l'-m}}{2^{l'-m+1}}\frac{(l'-m)!(m-1/2)!(P+l'+1)!}{(P-m)!(l'+m)!l'!}$$
$$\times\int_0^{\pi}(\cos\alpha + i\sin\alpha\cos\theta)^{P-m}C(\cos\theta)_{l'-m}^{m+1/2}(\sin\theta)^{2m+1}\,d\theta,$$

with

$$C_0^{\nu}(Z) = 1.$$

Therefore, using the special values of the representation functions, we obtain

$$I_{100}^{n'l'0} = \frac{1}{n'}(-i)^{l'}2^{l'}(2l'+1)^{1/2}l'!\left[\frac{(n'-l'-1)!}{(n'+l')!}\right]^{1/2}(\sin\alpha)^{l'}\frac{(\tanh\frac{1}{2}\beta)^{n'}}{(\cosh\frac{1}{2}\beta\sinh\frac{1}{2}\beta)^3}\frac{1}{8n'}$$
$$\times\{[(\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta)^2 8n' - 4n'(n'-1)\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta\cos\gamma + 8n'(\sinh\tfrac{1}{2}\beta)^3\cosh\tfrac{1}{2}\beta\cos\gamma$$
$$-4n'l'\cos\alpha\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta\sin\gamma/\sin\alpha]\,C(\cos)_{n'-1-l'}^{l'+1}$$
$$+8n'(l'+1)\sin\alpha\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta\sin\gamma)C(\cos\alpha)_{n'-2-l'}^{l'+2}\}. \tag{16}$$

In this equation we take the fourth and the fifth terms in the curly bracket together and for the fourth term we substitute the recurrence relation

$$(n+2\nu)C(\cos\alpha)_n^\nu = 2\nu C(\cos\alpha)_n^{\nu+1} - 2\nu(\cos\alpha)C(\cos\alpha)_{n-1}^{\nu+1}$$

and get

$$\begin{aligned}(\text{terms }4+5) = {} & 4n'(n'+1)\cos\alpha\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta(\sin\gamma/\sin\alpha)C(\cos\alpha)_{n'-1-l'}^{l'+1} \\ & - 8n'(l'+1)\cos\alpha\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta(\sin\gamma/\sin\alpha)C(\cos\alpha)_{n'-1-l'}^{l'+2} \\ & + 8n'(l'+1)\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta(\sin\gamma/\sin\alpha)C(\cos\alpha)_{n'-2-l'}^{l'+2}\,. \end{aligned} \tag{16a}$$

We then substitute the recurrence formula

$$(n+\nu)C(\cos\alpha)_n^\nu = \nu C(\cos\alpha)_n^{\nu+1} - \nu C(\cos\alpha)_{n-2}^{\nu+1} \tag{17}$$

into the first term of Eq. (16a) and make some rearrangements to obtain

$$\begin{aligned}(\text{terms }4+5) = {} & [4n'(n'+1)(l'+1)(\sinh\tfrac{1}{2}\beta)^2C(\cos\alpha)_{n'-1-l'}^{l'+2} + 4n'(n'-1)(l'+1)(\cos\tfrac{1}{2}\beta)^2C(\cos\alpha)_{n'-1-l'}^{l'+2} \\ & + 8n'(l'+1)\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta(\sin\gamma/\sin\alpha)C(\cos\alpha)_{n'-2-l'}^{l'+2}] \\ & - [8n'(n'+1)(l'+1)(\sinh\tfrac{1}{2}\beta)^2 + 8n'(l'+1)\cos\alpha\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta(\sin\gamma/\sin\alpha)] \\ & \times C(\cos\alpha)_{n'-1-l'}^{l'+2} - 2n'(n^{2\prime}-1)C(\cos\alpha)_{n'-1-l'}^{l'+1} \\ & + [8n'(l'+1)(\sinh\tfrac{1}{2}\beta)^2 - 4n'(n'-1)(l'+1)]C(\cos\alpha)_{n'-3-l'}^{l'+2}\,. \end{aligned}$$

We then substitute the above into Eq. (16), use the values of $\cos\alpha$, $\sin\alpha$, $\cos\gamma$, and $\sin\gamma$ from Eq. (8), apply Eq. (17) very generously to enjoy many cancellations, and eventually obtain

$$\begin{aligned} I_{100}^{n'l'0} = {} & \frac{1}{8n'^2}(-i)^{l'}2^{l'}(2l'+1)^{1/2}(l'+1)!\left(\frac{(n'-l'-1)!}{(n'+l')!}\right)^{1/2}(\sin\alpha)^{l'}\frac{(\tanh\frac{1}{2}\beta)^{n'}}{(\cosh\frac{1}{2}\beta\sinh\frac{1}{2}\beta)^3} \\ & \times[4n'(n'+1)(\sinh\tfrac{1}{2}\beta)^2C(\cos\alpha)_{n'-1-l'}^{l'+2} - 8n'^2(\sinh\tfrac{1}{2}\beta\cosh\tfrac{1}{2}\beta)C(\cos\alpha)_{n'-2-l'}^{l'+2} \\ & + 4n'(n'-1)(\cosh\tfrac{1}{2}\beta)^2C(\cos\alpha)_{n'-3-l'}^{l'+2}]\,. \end{aligned} \tag{18}$$

From Eq. (8) we get

$$\begin{aligned} & (\sin\alpha)^{l'} = 2^{l'}K^{l'}n'^{l'}[(n'-1)^2+K^2n'^2]^{-l'/2}/[(n'+1)^2+K^2n'^2]^{l'/2}\,, \\ & (\tanh\tfrac{1}{2}\beta)^{n'} = \{[(n'-1)^2+K^2n'^2]/[(n'+1)^2+K^2n'^2]\}^{n'/2}\,, \\ & 1/(\cosh\tfrac{1}{2}\beta\sinh\tfrac{1}{2}\beta)^3 = 2^6n'^3[(n'-1)^2+K^2n'^2]^{-3/2}/[(n'+1)^2+K^2n'^2]^{3/2}\,. \end{aligned}$$

Therefore Eq. (18) becomes

$$\begin{aligned} I_{100}^{n'l'0} = {} & (-i)^{l'}2^{2l'+3}(n')^{l'+1}(2l'+1)^{1/2}(l'+1)!\left[\frac{(n'-l'-1)!}{(n'+l')!}\right]^{1/2}K^{l'}\frac{[(n'-1)^2+K^2n'^2]^{(n'-l'-3)/2}}{[(n'+1)^2+K^2n'^2]^{(n'+l'+3)/2}} \\ & \times\{(n'+1)[(n'-1)^2+K^2n'^2]C(\cos\alpha)_{n'-1-l'}^{l'+2} - 2n'[(n'-1)^2+K^2n'^2]^{1/2}[(n'+1)^2+K^2n'^2]^{1/2}C(\cos\alpha)_{n'-2-l'}^{l'+2} \\ & + (n'-1)[(n'+1)^2+K^2n'^2]C(\cos\alpha)_{n'-3-l'}^{l'+2}\}\,, \end{aligned} \tag{19}$$

where

$$\cos\alpha = (n^2-1+K^2n'^2)/[(n'-1)^2+K^2n'^2]^{1/2}[(n'+1)^2+K^2n'^2]^{1/2}\,.$$

As expected, apart from the phase $(-i)^{l'}$, Eq. (19) is exactly the same expression derived by Massey and Mohr,[2] who made explicit use of the spatial wave functions of the hydrogen atom. The phase term $(-i)^l$ does not matter, since after all what we measure is the absolute square of the amplitude. One can even get rid of this phase by associating it with the definition of $O(4)$ harmonic functions just as the way Vilenkin[13] does, and in that case it will not appear in Eq. (15′). The exact derivation of the Massey-Mohr formula from our general expression Eq. (12) assures the exactness of the latter.

Furthermore, we find that from Eqs. (12) and (11) the form factor $I_{nlm}^{n'l'm}$ becomes singular at $\cosh\frac{1}{2}\beta = 0$. This means by Eq. (8)

$$K^2 = -(n'+n)^2/n'^2n^2 = 2[\sqrt{B_n}+\sqrt{B_{n'}}]^2\,, \tag{20}$$

where $B_n = -1/2n^2$ is the binding energy of the states $|nlm\rangle$. This value of K^2 exactly coincides with the anomalous threshold of the triangular diagram[3] (Fig. 1), which can be easily evaluated using the Cutkosky rules.[15] Looking at Fig. 1 one would have expected a singularity of the form factor at a momentum transfer squared equal to $(2m_e c^2)^2$. This is not so because of the special values of the masses in the triangular diagram of Fig. 1. Equation (20) means that the form factors have the correct singularity structure as required by the general principles of S-matrix theory. Conversely, the position of the singularity determines the binding energy and hence the mass formula for the composite system.

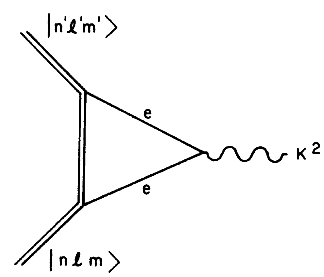

FIG. 1. Feynman diagram for scalar three-point function which gives an anomalous threshold the same as Eq. (20).

Finally, we derive an expression for the inelastic cross section. For this we substitute the following two recursion relations[12] of the $O(4)$ rotation functions ($t \equiv \tau + |m|$) in Eq. (12):

$$
\begin{aligned}
[(n-l)(n+l+1)]^{1/2} D(-\gamma)^{[n,0]}_{l,t,|m|} = {} & [(n-t)(n+t+1)]^{1/2} (\cos\gamma) D(-\gamma)^{[n-1,0]}_{l,t,|m|} \\
& + i\left(\frac{(t+|m|+1)(t-|m|+1)}{(2t+1)(2t+3)}(n-t)(n-t-1)\right)^{1/2} (\sin\gamma) D(-\gamma)^{[n-1,0]}_{l,t+1,|m|} \\
& + i\left(\frac{(t+|m|)(t-|m|)}{(2t+1)(2t-1)}(n+t)(n+t+1)\right)^{1/2} (\sin\gamma) D(-\gamma)^{[n-1,0]}_{l,t-1,|m|}
\end{aligned}
$$

and

$$
\begin{aligned}
[(n+l)(n-l-1)]^{1/2} D(-\gamma)^{[n-2,0]}_{l,t,|m|} = {} & [(n+t)(n-t-1)]^{1/2} (\cos\gamma) D(-\gamma)^{[n-1,0]}_{l,t,|m|} \\
& - i\left[\frac{(t+|m|+1)(t-|m|+1)}{(2t+1)(2t-3)}(n+t)(n+t+1)\right]^{1/2} (\sin\gamma) D(-\gamma)^{[n-1,0]}_{l,t+1,|m|} \\
& - i\left[\frac{(t+|m|)(t-|m|)}{(2t+1)(2t-1)}(n-t)(n-t-1)\right]^{1/2} (\sin\gamma) D(-\gamma)^{[n-1,0]}_{l,t-1,|m|} .
\end{aligned} \tag{21}
$$

After substitution and simplification we obtain

$$
\begin{aligned}
I^{n'l'm}_{nlm} = {} & \frac{A}{n'} \sum_{t=0}^{\min(n'-1,\,n-1)} D(-\alpha)^{[n'-1,0]}_{l',t,|m|} V(\beta)^{t+1}_{n',n} D(-\gamma)^{[n-1,0]}_{l,t,m} \\
& - \frac{i}{2n'} \sin\gamma \sum_{t=0}^{\min(n'-1,\,n-1)} \Bigg[\left(\frac{(t+1)^2-|m|^2}{(2t+1)(2t+3)}\right)^{1/2} D(-\alpha)^{[n'-1,0]}_{l',t,|m|} [b_1 V(\beta)^{t+1}_{n',n+1} - b_2 V(\beta)^{t+1}_{n',n-1}] D(-\gamma)^{[n-1,0]}_{l,t+1,|m|} \\
& + \left(\frac{t^2-|m|^2}{(2t+1)(2t-1)}\right)^{1/2} D(-\alpha)^{[n'-1,0]}_{l',t,|m|} [b_2 V(\beta)^{t+1}_{n',n+1} - b_1 V(\beta)^{t+1}_{n',n-1}] D(-\gamma)^{[n-1,0]}_{l,t-1,|m|} \Bigg] ,
\end{aligned} \tag{22}
$$

where we have used the following relation:

$$
[n-K+1)(n+K)]^{1/2} V(\beta)^K_{m,n+1} + [(n-K)(n+K-1)]^{1/2} V(\beta)^K_{m,n-1} = \frac{2}{\sinh\beta}[(m-n) - 2n\sinh^2\tfrac{1}{2}\beta] V(\beta)^K_{m,n} ,
$$

which can be easily derived using Eq. (11), and the identity

$$
c(c-1)\,{}_2F_1(a-1;b-1;c-1;x) - abx(1-x)\,{}_2F_1(a+1;b+1;c+1;x) + c[(a+b-1)x-(c-1)]\,{}_2F_1(a,b;c;x) = 0 .
$$

Also, in Eq. (22) the coefficients a_1, b_1, and b_2 are given by

$$
A = n - (\cos\gamma/\sinh\beta)[(n'-n) - 2n\sinh^2\tfrac{1}{2}\beta] = (1/n)4n'^4 n^4 K^2/[(n'+n)^2 + n'^2 n^2 K^2][(n'-n)^2 + n'^2 n^2 K^2] , \tag{23}
$$

$$
b_1 = [(n-t)(n-t-1)]^{1/2}, \quad b_2 = [(n+t)(n+t+1)]^{1/2} . \tag{24}
$$

One might notice that in Eq. (22)

$$[b_2 V(\beta)^{t+1}_{n',n+1} - b_1 V(\beta)^{t+1}_{n',n-1}] = [b_1 V(\beta)^{t+1}_{n',n+1} - b_2 V(\beta)^{t+1}_{n',n-1}]_{(t+1)\to -t},$$

since

$$V(\beta)^{K}_{m,n} = V(\beta)^{1-K}_{m,n}$$

[see Eq. (11)].

In order to obtain the excitation cross section, we square Eq. (22), sum over all final states (l', m), and average over the initial states (l, m). The summations over l' and l ($0 \leq l' \leq n'-1$; $0 \leq l \leq n-1$) can be very easily performed (with fixed value of m) using the orthogonality condition of the $O(4)$ rotation functions, i.e.,

$$\sum_{j} D(\theta)^{[P,Q]}_{j,j',m} D(-\theta)^{[P,Q]}_{j,j'',m} = \delta_{j'j''}. \qquad (25a)$$

But the summation over m is not easy here, unless there exist some recursion relations of the D functions which would absorb the terms $(t+1)^2 - |m|^2$ and $t^2 - |m|^2$ and give other D functions with coefficients independent of l, l', and $|m|$. In the latter situation one can perform the summation over l', l, and $|m|$ using the general orthogonality relation

$$\sum_{j,m} D(\theta)^{[P,Q]}_{j,j',|m|} D(-\theta)^{[P,Q]}_{j,j'',|m|} = \delta_{j'j''}. \qquad (25b)$$

Because the above-mentioned recursion relations of the D functions are not yet known, we use Eq. (25a) by keeping $|m|$ fixed for the summation over l' and l. We obtain

$$Q^{n',|m|}_{n,|m|} \equiv |I^{n',|m|}_{n,|m|}|^2 = \frac{A^2}{n^2 n'^2} \sum_{t=0}^{\min(n'-1,n-1)} V(\beta)^{t+1}_{n',n} V(\beta)^{t+1}_{n',n} + \frac{1}{4n^2 n'^2}\sin^2\gamma \sum_{t=0}^{\min(n'-1,n-1)} [A_1(t) V(\beta)^{t+1}_{n',n+1} V(\beta)^{t+1}_{n',n+1} + A_2(t) V(\beta)^{t+1}_{n',n-1} V(\beta)^{t+1}_{n',n-1} + A_3(t) V(\beta)^{t+1}_{n',n+1} V(\beta)^{t+1}_{n',n-1}], \qquad (26)$$

where

$$A_1(t) = \frac{(t+1)^2 - |m|^2}{(2t+1)(2t+3)}(n-t)(n-t-1) + \frac{t^2 - |m|^2}{(2t+1)(2t-1)}(n+t)(n+t+1),$$

$$A_2(t) = \frac{(t+1)^2 - |m|^2}{(2t+1)(2t+3)}(n+t)(n+t+1) + \frac{t^2 - |m|^2}{(2t+1)(2t-1)}(n-t)(n-t-1),$$

and

$$A_3(t) = -2[(n+t)(n+t+1)(n-t)(n-t-1)]^{1/2}\left(\frac{(t+1)^2 - |m|^2}{(2t+1)(2t+3)} + \frac{t^2 - |m|^2}{(2t+1)(2t-1)}\right).$$

Equation (26) is the exact analytic expression for the (n', n) excitation cross section for fixed direction of polarization. The corresponding generalized oscillator strength[1] is given by

$$f(K^2)^{n',|m|}_{n,|m|} = \frac{(E_{n'} - E_n)}{\mathcal{R} a_0^2} \frac{1}{K^2} Q(K^2)^{n',|m|}_{n,|m|}, \qquad (27)$$

where $\mathcal{R} = m_e e^4/2\hbar^2$ is the Rydberg energy and $a_0 = \hbar^2/m_e e^2$ is the Bohr radius. The optical (dipole) oscillator strength is obtained at the limit of zero momentum transfer, i.e.,

$$f^{n',|m|}_{n,|m|} = \lim_{K^2\to 0} f(K^2)^{n',|m|}_{n,|m|}. \qquad (28)$$

In this limit, various quantities appearing in Eq. (26) will acquire the following values:

$$\tanh^2 \tfrac{1}{2}\beta \approx [(n'-n)/(n'+n)]^2 + O(K^2), \quad \cosh^2 \tfrac{1}{2}\beta \approx (n'+n)^2/4n'n + O(K^2), \quad \sinh^2 \tfrac{1}{2}\beta \approx (n'-n)^2/4n'n + O(K^2), \qquad (29)$$

$$\sin^2\gamma \approx [n'^4 n^2/(n'-n)^2(n'+n)^2]K^2 + O(K^4), \quad A^2 \approx (1/n^2)[16n'^8 n^8/(n'+n)^4(n'-n)^4]K^4 + O(K^6),$$

$$V(\beta)^{t+1}_{n',n} \simeq \frac{(-1)^{n-t}}{(2t+1)!}\left(\frac{(n'+t)!\,(n+t)!}{(n'-t-1)!\,(n-t-1)!}\right)^{1/2}\left(\frac{n'-n}{n'+n}\right)^{n'+n}\left(\frac{(n'+n)^2}{4n'n}\right)^{-(t+1)}$$

$$\times {}_2F_1(t+1-n, t+1-n'; 2t+2; -4n'n/(n'-n)^2).$$

In order to obtain the last expression we have used the following identity in Eq. (11):

$${}_2F_1(-a,b;c;x) = \left(\frac{(a+b-1)!\,(c-1)!}{(a+c-1)!\,(b-1)!}\right)(-x)^a\,{}_2F_1(-a,1-a-c;1-a-b;1/x).$$

Clearly, for the optical oscillator strength $f^{n',|m|}_{n,m}$ [Eq. (28)] the first term in Eq. (26) does not contribute (vanishes as K^2) and only the second term contributes, i.e.,

$$f^{n',|m|}_{n,|m|} = \frac{1}{n^2}\frac{1}{4}\left(\frac{n'^2 n^2}{(n'-n)^2(n'+n)^2}\right)$$
$$\times \sum_{t=0}^{\min(n'-1,n-1)} [A_1(t)V(\beta)^{t+1}_{n',n+1}V(\beta)^{t+1}_{n',n+1} + A_2(t)V(\beta)^{t+1}_{n',n-1}V(\beta)^{t+1}_{n',n-1} + A_3(t)V(\beta)^{t+1}_{n',n+1}V(\beta)^{t+1}_{n',n-1}], \tag{30}$$

where $V(\beta)^{t+1}_{n',n}$ is given by Eq. (29). The summation over t may be performed according to whether one is interested in the emission ($n'<n$) or absorption ($n'>n$) oscillator strength.

We may also see the behavior of the excitation cross section in the infinite-momentum limit ($K^2\to\infty$) and for large values of n and n' ($n,n'\to\infty$) from Eq. (26). We can express each V function in Eq. (26) in terms of Jacobi polynomials such as $P^{n'-n,\rho}_n(1-2\tanh^2\frac{1}{2}\beta)$, using Eq. (11). If we use the identity

$$P^{a,b}_d(x) = (-1)^d P^{b,a}_d(-x)$$

and Stirling's formula $[x! \simeq \sqrt{(2\pi)}\,x^{x+1/2}e^{-x}]$ for the asymptotic limits $n,n'\to\infty$, then each term $(1/n')V(\beta)^{\rho}_{n',n}$ in Eq. (26) behaves as

$$n^{-\rho}P^{\rho,n'-n}_n\left(1-\frac{(2/K)^2}{2n^2}\right),$$

since, from Eq. (8),

$$\tanh^2\tfrac{1}{2}\beta \approx 1-4/K^2n^2$$

and

$$\cosh^2\tfrac{1}{2}\beta \approx Kn\tfrac{1}{2}(1+2/K^2n^2).$$

Now one can use the Mehler-Heine type asymptotic formula,

$$\lim_{d\to\infty} d^{-b}P^{b,a}_d(1-x^2/2d^2) = (\tfrac{1}{2}x)^{-b}J_b(x),$$

and infer that the total excitation cross section would behave asymptotically as the product of two Bessel functions $J_\rho(2/K)$. Similar conclusions have also been reached by Beigman *et al.*[6] This reduction is in fact expected, because in the infinite-momentum limit the orthogonal subgroup $O(2,1)$ contracts[11] to the Euclidean subgroup $E(2)$ and consequently the Jacobi polynomials become Bessel functions.

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