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L. C. Biedenharn
M. E. Rose

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COULOMB EXCITATION OF NUCLEAR LEVELS

L. C. Biedenharn* and M. E. Rose

I. INTRODUCTION

The excitation of nuclear levels by means of the Coulomb field of incident particles has been a particularly useful tool for obtaining nuclear information[1]. The interpretation of the experimental information obviously requires that properties of the probe, the electric excitation, be readily available and clearly understood. At present, the most feasible procedure has been to use the classical approximation to the electric excitation, i.e., to consider the charged particles as travelling in a definite classical Kepler orbit, with the Coulomb field causing the nuclear transition[2]. This approach, as is well known, suffers from two defects: (1) to be valid it requires that $\eta = \frac{z_1 z_2 e^2}{\hbar v} \gg 1$, which is not the case in many experimental investigations (where η may be ~ 2 or 3) and (2) the energy required for the nuclear transition must be small compared to the energy of the incident particles. Letting $\rho \equiv \frac{k_2}{k_1} = \sqrt{\frac{E_f}{E_i}}$, this condition may be expressed as $1 - \rho \ll 1$. This condition also fails in many practical cases. In fact, it is clear that this classical approach must necessarily be invalid both for large ($\eta \sim 1$) <u>and</u> small ($\rho \sim 1$) bombarding energies.

Finally, it should be mentioned that deviations from the classical approach are apparently found experimentally[3]. This, of course, is the over-

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riding fact and furnishes the principal motivation in the present undertaking.

The program for which the present considerations provide an initial formulation, is to take the Coulomb field into account rigorously in a quantum mechanical perturbation treatment. This would provide an essentially exact result. In this connection it is of interest to note that for dipole transitions, the problem was long ago completely solved, in effect, by Sommerfeld[4]. The cases of greatest interest are, however, the quadrupole transitions, and, after having the beautifully complete result of Sommerfeld for the dipole problem, it is surprising how difficult and laborious this task proves to be. In fact, it proves quite futile to proceed along the lines Sommerfeld marked out, using the Coulomb wave functions in parabolic coordinates, and recourse to the spherical representation is indicated.

In the following, we set up the problem in the spherical representation and obtain a formal answer to both the total cross-section and angular distribution problems. The principal problem involved in this formulation is the construction of a Coulomb field wave function which asymptotically defines a definite direction of motion. Exactly this problem was solved in another connection.[5] The problem considered in reference 5 was the internal conversion process. The differences between that situation and the one of interest in the Coulomb excitation problem are formal. Thus, while previously a transition between a bound state and one in the continuum was considered here the transition is

between two continuum states. Moreover, for one of these, the final state, there is no coherent mixing of different angular momenta because (in accordance with the usual experimental arrangement) it will be assumed that this state is not observed - see B. below.

In this report the reduction of the problem to the task of evaluating radial integrals is presented. This task of numerical evaluation is formidable, to say the least. Complete discussion and a procedure for numerical evaluation on the ORACLE will be presented in a forthcoming report. The coding of the problem on the ORACLE is under way at present, and it is hoped results will be available in the not too distant future.

II. FORMAL DEVELOPMENT

The problem to be discussed is the following: A (Coulomb distorted) plane wave of particles, of wave vector $\vec{k}_1$ and charge z_1 is incident upon nuclei of charge z_2. By means of the electrostatic coupling between the nucleus and incident particle the nucleus undergoes a quadrupole electromagnetic transition from a state $J_i \pi_i$ to a state J_f, π_f, the incident particles emerging at infinity as a (Coulomb distorted) plane wave of wave vector $\vec{k}_2$. Here J, π represent the nuclear angular momentum and parity. In the sequel the explicit assumption that the nucleus is very much heavier than the target particle will be made.

We seek to find the total cross-section for this process, averaged over the directions of $\vec{k}_2$, and, moreover, the angular correlation of a subsequent

nuclear radiation with the incident direction $\vec{k}_1$, similarly averaged over $\vec{k}_2$.

A. Cross-Section

Let us consider the total cross-section first. It will be assumed to begin with that the interaction is primarily electrostatic. Hence, for the quadrupole case, the interaction is:

$$H = \frac{4\pi}{5} z_1 z_2 e^2 \sum_{i,\mu} r_i^2 r^{-3} Y_2^{\mu *} (\theta_i \varphi_i) Y_2^{\mu} (\vartheta, \varphi) \tag{1}$$

Here $(r_i, \theta_i, \varphi_i)$ refer to the coordinates of the ith proton in the nucleus, and (r, ϑ, φ) are the coordinates of the projectile. The nucleus is considered to have negligible extension. The usual perturbation treatment then leads to the result:

$$\sigma = \frac{k_2}{k_1} \frac{m^2}{4\pi^2 \hbar^4} \mathcal{S} \int d\hat{k}_2 \left| \langle \psi_2 (\vec{k}_2, \vec{r}) \Psi_f | H | \Psi_i \psi_1 (\vec{k}_1, \vec{r}) \rangle \right|^2 \tag{2}$$

In (2) $\mathcal{S}$ denotes the appropriate summation over final states and averaging over magnetic substates of the initial nuclear state (wave functions Ψ_f and Ψ_i respectively). Also,

$$\psi_1 (\vec{k}_1, \vec{r}) = \left(\frac{2\pi \eta_1}{e^{2\pi \eta_1} - 1} \right)^{\frac{1}{2}} e^{i\vec{k}_1 \cdot \vec{r}} \, {}_1F_1(-i\eta_1; 1; i(k_1 r - \vec{k}_1 \cdot \vec{r})) \tag{3}$$

$$\eta_1 \equiv \frac{z_1 z_2 e^2}{\hbar v_1} \tag{4}$$

$$\psi_2(\vec{k}_2,\vec{r}) = \left(\frac{2\pi\eta_2}{e^{2\pi\eta_2} - 1}\right)^{\frac{1}{2}} e^{+i\vec{k}_2\cdot\vec{r}} \; {}_1F_1(i\eta_2;\, 1;\, -i\,(k_2 r + \vec{k}_2\cdot\vec{r})) \qquad (5)$$

These latter wave functions are exact wave functions of a particle of mass m and charge z_1 in the field of a fixed charge z_2 as given in detail by Sommerfeld[4]. They reduce to distorted plane waves at infinity, with the appropriate out- and in-going spherical parts respectively.

Evaluating the nuclear integral formally we have:

$$\int d\tau_N \sum_i r_i^2\, Y_2^{\mu}(\theta_i\, \varphi_i)\, \Psi_f^*\, \Psi_i \equiv C(J_i 2 J_f; M_i \mu M_f)\, (f \| 2 \| i) \qquad (6)$$

Thus:

$$\sigma = \frac{k_2}{k_1}\, \frac{m^2}{4\pi^2\hbar^4}(z_1 z_2 e^2)^2 \left(\frac{4\pi}{5}\right)^2 \cdot \left|(f\|2\|i)\right|^2 \cdot \frac{2J_f+1}{2J_i+1} \cdot \frac{1}{5} \cdot$$

$$\times \int d\hat{k}_2 \sum_{\mu} \left|\langle \psi_2 \left| r^{-3}\, Y_2^{\mu}(\hat{r}) \right| \psi_1 \rangle\right|^2 \qquad (7)$$

Recourse to the spherical representation is necessary to proceed further, as mentioned above. This uses:

$$\psi_1(\vec{k}_1,\vec{r}) = \sum_{\ell,m} \sqrt{4\pi(2\ell+1)}\, \frac{e^{i(\sigma_\ell - \sigma_0)}}{k_1 r}\, F_\ell(k_1 r)\, D^{\ell}_{m,0}(\hat{k}_1)\, i^{\ell}\, Y_\ell^m(\vartheta,\varphi) \qquad (8)$$

$$\psi_2(\vec{k},\vec{r}) = \sum_{\bar{\ell},\bar{m}} \sqrt{4\pi(2\bar{\ell}+1)}\, \frac{F_{\bar{\ell}}(k_2 r)}{k_2 r}\, e^{-i(\sigma_{\bar{\ell}} - \sigma_0)}\, D^{\bar{\ell}}_{\bar{m},0}(\hat{k}_2)^*\, i^{\bar{\ell}}\, Y_{\bar{\ell}}^{\bar{m}*}(\hat{r}) \qquad (9)$$

Here D^{ℓ}_{mm} is the $2\ell+1$ dimensional representation of the rotation group. Thus the integral in Eq. (7) becomes:

$$(\psi_2 | r^{-3} Y_2^{\mu}(\hat{r}) | \psi_1)$$

$$= 4\pi \sum_{\ell\bar{\ell}} \sum_{m\bar{m}} \sqrt{(2\ell+1)(2\bar{\ell}+1)}\, e^{i(\sigma_\ell - \sigma_0)+i(\sigma_{\bar{\ell}} - \sigma_0)} D^{\bar{\ell}}_{\bar{m},0}(\hat{k}_2)\, D^{\ell}_{m,0}(\hat{k}_1)$$

$$(-)^{\bar{\ell}}\, i^{\ell+\bar{\ell}} \int d\Omega\, Y_\ell^m\, Y_{\bar{\ell}}^{\bar{m}}\, Y_2^{\mu} \int_0^\infty r^2 dr\, \frac{F_\ell(k_1 r)}{k_1 r}\, \frac{F_{\bar{\ell}}(k_2 r)}{k_2 r}\, r^{-3} \tag{10}$$

Upon using the result,

$$\int d\Omega\, Y_\ell^m\, Y_{\bar{\ell}}^{\bar{m}}\, Y_2^{\mu} = \sqrt{\frac{5(2\ell+1)}{4\pi(2\bar{\ell}+1)}}\; C(\ell\, 2\bar{\ell};00)\, C(\ell\, 2\bar{\ell};m\mu)\, (-)^{\bar{m}}\, \delta_{-\bar{m},m+\mu} \tag{11}$$

the integral assumes the form:

$$(\psi_2 | r^{-3} Y_2^{\mu} | \psi_1) =$$

$$\sqrt{20\pi} \sum_{\ell\bar{\ell}m} \frac{(2\ell+1)}{k_1 k_2} \cdot e^{i(\sigma_\ell - \sigma_0)+i(\sigma_{\bar{\ell}} - \sigma_0)} \cdot i^{\ell-\bar{\ell}} \cdot C(\ell\, 2\bar{\ell};00)$$

$$C(\ell 2\bar{\ell};m\mu)\, (-)^{m+\mu} \cdot D^{\bar{\ell}}_{-m-\mu;0}(\hat{k}_2)\, D^{\ell}_{m,0}(\hat{k}_1). \tag{12}$$

$$\times \int_0^\infty r^{-3} F_\ell(k_1 r)\, F_{\bar{\ell}}(k_2 r)\, dr$$

and finally

$$\int d\hat{k}_2 \sum_{\mu} \left| (\psi_2 \left| r^{-3} Y_2^{\mu} \right| \psi_1) \right|^2 = \frac{80\pi^2}{(k_1 k_2)^2} \sum_{\ell\bar{\ell}} (2\ell+1) \cdot c^2(\ell\, 2\, \bar{\ell}\,; 00)$$

$$\times \left[\int_0^{\infty} r^{-3} F_{\ell}(k_1 r)\, F_{\bar{\ell}}(k_2 r)\, dr \right]^2 \tag{13}$$

Use:

$$c^2(\ell\, 2\, \ell\,; 00) = \frac{\ell(\ell+1)}{(2\ell-1)(2\ell+3)}$$

$$c^2(\ell\, 2\, \ell-2; 00) = \frac{3\ell(\ell-1)}{2(2\ell-1)(2\ell+1)}$$

$$c^2(\ell\, 2\, \ell+2; 00) = \frac{3(\ell+1)(\ell+2)}{2(2\ell+1)(2\ell+3)}$$

$$\int d\hat{k}_2 \sum_{\mu} \left| (\psi_2 \left| r^{-3} Y_2^{\mu} \right| \psi_1) \right|^2 = \frac{80\pi^2}{(k_1 k_2)^2} \sum_{\ell} \left\{ \frac{\ell(\ell+1)(2\ell+1)}{(2\ell-1)(2\ell+3)} \left[\int_0^{\infty} r^{-3} F_{\ell}(k_1 r)\, F_{\ell}(k_2 r)\, dr \right]^2 \right.$$

$$\left. + \frac{3\ell(\ell-1)}{2(2\ell-1)} \left[\int_0^{\infty} r^{-3} F_{\ell}(k_1 r)\, F_{\ell-2}(k_2 r)\, dr \right]^2 + \frac{3}{2} \frac{(\ell+1)(\ell+2)}{(2\ell+3)} \left[\int_0^{\infty} r^{-3} F_{\ell}(k_1 r) F_{\ell+2}(k_2 r)\, dr \right]^2 \right\}$$

Hence:

$$\sigma = \frac{64\pi^2}{25} \frac{m^2}{\hbar^4} \frac{(z_1 z_2 e^2)^2}{k_1^3 k_2} \frac{2J_f+1}{2J_i+1} (f \| 2 \| i)^2$$

$$\times \sum_{\ell=0}^{\infty} \left\{ \frac{\ell(\ell+1)(2\ell+1)}{(2\ell-1)(2\ell+1)} \left[\int_0^\infty r^{-3} F_\ell (k_1 r) F_\ell (k_2 r) dr \right]^2 \right.$$

$$+ \frac{3\ell(\ell-1)}{2(2\ell-1)} \left[\int_0^\infty r^{-3} F_\ell (k_1 r) F_{\ell-2} (k_2 r) dr \right]^2$$

$$\left. + \frac{3(\ell+1)(\ell+2)}{2(2\ell+3)} \left[\int_0^\infty r^{-3} F_\ell (k_1 r) F_{\ell+2} (k_2 r) dr \right]^2 \right\} \qquad (14)$$

B. Angular Correlation

To calculate the angular correlation between the incident projectile beam and the direction of a subsequent γ-ray emitted by the nucleus, it is convenient to make use of the result that if we know the γ-ray angular correlation for the nuclear transitions $J_i \rightarrow J_f$ by E2 (excitation), and then $J_f \rightarrow J_i'$, by emission of 2^L pole radiation, it is only necessary to multiply the Legendre polynomials $P_\nu (\cos \theta)$ in this correlation by the "particle parameters" b_ν to obtain the particle - γ correlation. This result is discussed in detail elsewhere[6]. The problem reduces then to computing the b_ν and standard techniques are available. In effect, the (virtual) E2 γ-transition of the nucleus, is represented by the incident projectile's transition between Coulomb orbits. As mentioned earlier, the problem at hand is an analogue to the internal conversion correlation problem discussed at length in reference

(5). The calculation given below exploits this similarity, but for brevity does not reproduce details which can be found in that reference. Since the Coulomb excitation is (in a sense) the inverse to the internal conversion calculation, it should be mentioned that care should be taken in interpreting the words "initial" and "final" in comparing the two problems.

The particle parameters, b_ν, are the ratio of the tensor parameters of the projectile to the tensor parameters of the E2 gamma ray, normalized such that $b_o = 1$. To obtain the tensor parameters of the projectile we couple the tensor parameters of the observed initial state and the tensor parameters of the unobserved final state. The latter are simple, being random and, therefore, scalar.

The tensor parameters of the initial state are:

$$R_i(\nu q;\, \ell \ell' \pi) = 4\pi \left[(2\ell+1)(2\ell'+1)\right]^{\frac{1}{2}} (-)^{\ell-q}\, C(\ell \ell' \nu\, ;000)$$

$$e^{i(\sigma_\ell - \sigma_{\ell'})}\, D^{\nu}_{q,0}(\hat{k}_1) \tag{15}$$

The tensor parameters of the final state are simply

$$R_f(\nu q) = \delta_{0\nu}\, \delta_{0q} \tag{16}$$

Defining the reduced matrix elements, $Q(\bar{\ell}, \ell)$, for the transition between Coulomb states by:

$$\langle \bar{\ell}\, \bar{m} \,|\, r^{-3}\, Y_2^{\mu} \,|\, \ell m \rangle \equiv Q(\bar{\ell}, \ell)\, C(\bar{\ell}\, 2\, \ell; \bar{m} \mu m) \tag{17}$$

one then obtains for the coupled tensor parameters,

$$R(\nu q) = \sum_{\ell\ell'\bar{\ell}} Q(\bar{\ell}\ell)\, Q^*(\bar{\ell}\ell') \cdot \sqrt{(2\ell+1)(2\ell'+1)}$$

$$\times\, W(\ell\bar{\ell}\nu\, 2;2\ell')\, R_1(\nu q;\, \ell\ell'). \tag{18}$$

Now the matrix elements $Q(\ell\bar{\ell})$ can be simplified further:

$$Q(\ell,\bar{\ell}) = \frac{1}{k_1 k_2} \int_0^\infty r^{-3}\, F_{\bar{\ell}}(k_2 r)\, F_\ell(k_1 r)\, dr \cdot \sqrt{\frac{5}{4\pi}}\, C(\ell\, 2\, \bar{\ell};000) \tag{19}$$

Using this, and discarding irrelevant constants, we get:

$$R(\nu q) \sim \sum_{\ell\ell'\bar{\ell}} (2\ell+1)(2\ell'+1)\, (-)^{\ell-q}\, C(\ell\ell'\nu;000)\, C(\ell\, 2\, \bar{\ell};000)\, C(\ell' 2\bar{\ell};000)$$

$$\times e^{i(\sigma_\ell - \sigma_{\ell'})} \left[\int_0^\infty F_{\bar{\ell}}(k_2 r)\, F_\ell(k_1 r)\, r^{-3}\, dr\right]\left[\int_0^\infty F_{\bar{\ell}}(k_2 r)\, F_{\ell'}(k_1 r)\, r^{-3}\, dr\right]$$

$$\times\, W(\ell\bar{\ell}\nu 2;2\ell')\, D^{\nu}_{q,0}(\hat{k}_1) \tag{20}$$

Since the tensor parameters of the E2 γ-transition are,

$$R_\nu(\nu q) \sim (-)^{q+1}\, C(22\nu;1\text{-}1)\, D^{\nu}_{q0}(\hat{\gamma}) \tag{21}$$

one then obtains for the unnormalized particle parameters,

$$\bar{b}_\nu = - C^{-1}(22\,\nu;1\text{-}1)$$

$$\times \sum_{\ell\ell'\bar{\ell}} (2\ell+1)(2\ell'+1) \cdot C(\ell 2\bar{\ell};00)\, C(\ell' 2\bar{\ell};00) \cdot e^{i(\sigma_\ell - \sigma_{\ell'})}$$

$$\times \left[\int_0^\infty F_{\bar{\ell}}(k_2 r)\, F_\ell(k_1 r)\, r^{-3}\, dr \right] \left[\int_0^\infty F_{\bar{\ell}}(k_2 r)\, F_{\ell'}(k_1 r)\, r^{-3}\, dr \right]$$

$$\times \quad W(\ell\bar{\ell}\nu 2;2\ell') \cdot (-)^\ell \quad C(\ell\ell'\nu;00) \tag{22}$$

By virtue of the triangular relationship which must exist between the first three arguments of the C coefficients it is clear that for a given value of $\bar{\ell}$, ℓ and ℓ' are restricted to the values $\bar{\ell}$ and $\bar{\ell} \pm 2$. Hence in the triple sum over ℓ, ℓ' and $\bar{\ell}$ only one of these (over $\bar{\ell}$ say) is an infinite summation. The other two are three-fold sums. As a consequence, it follows that for <u>both</u> the total cross section, (cf. Eq. (14)), and the angular correlation the primary task is the computation of essentially the same radial integrals so that the latter is, for all practical purposes, no more difficult to obtain than the former.

For $\nu = 0$ the W coefficient vanishes unless $\ell = \ell'$. That is

$$W(\ell\bar{\ell}\,02;2\ell') = \delta_{\ell\ell'} \frac{1}{\sqrt{5(2\ell+1)}}$$

Also:

$$C(\ell\ell'\,0;00) = \delta_{\ell\ell'}(-)^\ell / \sqrt{2\ell+1}$$

Hence:

$$\bar{b}_o = \sum_{\ell\bar{\ell}} (2\ell+1)\, C^2(\ell\, 2\,\bar{\ell};000) \left[\int_0^\infty F_{\bar{\ell}}(k_2 r)\, F_\ell(k_1 r)\, r^{-3}\, dr \right]^2 \qquad (23)$$

which is seen to agree, to within a factor independent of ℓ and $\bar{\ell}$, with the result for the total cross section (cf. Eq. (14)), as it must, of course.

It is customary to normalize the particle parameters so that $b_o = 1$. Thus one finds that the quantities of interest are:

$$b_\nu = \bar{b}_\nu / \bar{b}_o. \qquad (24)$$

It is more convenient to perform this normalization at the end.

III. CONCLUDING REMARKS

As developed above the calculation of the total cross section and the b as well reduces to the computation of the integrals:

$$I(\ell, \ell'; k_1, k_2) \equiv \int_0^\infty r^{-3}\, F_\ell(k_1 r)\, F_{\ell'}(k_2 r)\, dr$$

(where $\ell' = \ell, \ell \pm 2$). One of the major difficulties is that, unlike the internal conversion problem, the number of ℓ's that enter is unrestricted. In practice the summation to be carried out must be a finite one. It is essential, therefore, to get an idea of how many ℓ's can enter in a significant way.

To a sufficient approximation this can be done as follows. For large values of ℓ, the magnitude of F_ℓ at the turning point (that is, $kr \cong \ell$) is a constant times $\ell^{1/6}$.[7] Crudely one can say that the magnitude is the same

for all ℓ (say unity). Inside the turning point, the F_ℓ functions behave like $(r/\ell)^{\ell+1}$. Thus the contribution from $r < \ell$ is of the order of ℓ^{-3}. Outside the turning point, the F_ℓ's oscillate and an over-estimate is to neglect the phase difference between the two F_ℓ's and take their product to be of the order of unity everywhere. Thus, the outside contribution is of the order of ℓ^{-2}, and one gets as a rough estimate that $I \sim \ell^{-2}$, in general. We have evaluated some special cases exactly and this estimate is found to be quite precise.

Using this estimate in the summation for the total cross-section, it is clear that the sum will involve, in the limit of large ℓ, a summation over terms that behave like ℓ^{-3}, and thus this part of the sum will be of the order of ℓ^{-2}. For reasonable accuracy one should expect something like one hundred ℓ's to occur. The computation of the $\bar{b}_\nu$ is clearly a sizeable task, and it is essential to simplify the work as far as possible. As a computational procedure, it would appear quite inadvisable to compute the F_ℓ's first and then perform the integration numerically since the functions oscillate and a great many oscillations must be integrated before asymptotic formulae are applicable. Rather it seems more feasible to use the properties of the F_ℓ's to cast the required integrals in a more tractable form. Since the steps involved are not completely trivial (the integrals are apparently discontinuous functions of the parameters, for example) we shall present the work in some detail in a subsequent report which, it is to be hoped, will contain numerical results.

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