Electron Capture by Protons in Hydrogen and Effect of an Electric Field

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By treating an electric field in the direction of the incident proton as a perturbation, the electron capture cross section in the Brinkman-Kramers approximation up to the first order in the field is obtained. The cross section for transition between principal quantum numbers, in particular for capture from the ground state into the ground state, is quadratic in the field. The experimental verification of this symmetry is desirable. The cross section in the zeroth-order approximation for transition between two Stark levels is independent of the quantum numbers of these levels and depends only on their principal quantum numbers. The inclusion of the first order, which is linear in the field, splits the cross section into different values. The simplicity of the zeroth-order cross-section formula between Stark levels allows through a transformation the evaluation of the cross section between the optical levels as a polynomial in the incident energy. A general expression for the capture from the state nl into the state $n'l'$ is given. An expression for the momentum distribution of the hydrogen atom in an electric field, correct up to the first order, is given. It is found that this distribution for the Stark levels of the atom in the zeroth order is the same as the known momentum distribution for their related principal quantum number. The momentum distributions for the principal quantum numbers are found to be quadratic in the field.

I. INTRODUCTION

THE momentum density distribution function for a bound electron occupying the state of the principal quantum number n and the azimuthal quantum number l in the Coulomb field of a nucleus of charge Ze has been found by Podolsky and Pauling[1] using the Fourier transform of the spatial wave functions, and by Fock[2] by solving the Schrödinger integral equation in the momentum space. Fock further has shown that when the momentum density distribution function is averaged over l, the following simple function results. Let $\mathbf{p}$ represent the momentum vector of the electron and $\mathbf{q}$ its propagation vector, then $\mathbf{p}=\hbar\mathbf{q}$ and this function is given by[3]

$$D(n,\mathbf{q})=\frac{1}{n^2}\sum_{l=0}^{n-1}(2l+1)D(nl,\mathbf{q})=\frac{8Z^2\alpha^3}{n^2\pi^2a_0^2}\frac{1}{(\alpha^2+q^2)^4}, \quad (1)$$

where

$$\alpha=Z/na_0. \quad (2)$$

The function $D(nl,\mathbf{q})$ is the distribution function for a given n and l, and a_0 is the Bohr radius. Equation (1) has also been given by May[4] by a different method.

It should be mentioned that a similar distribution to that given by (1) can be derived classically, provided we assume microcanonical distribution for the classical particle.[5] By application of the Bohr quantization rule, this distribution then becomes identical to the quantum-mechanical distribution.

The momentum distribution function of a particle in a Coulomb field, with states specified by nn_1n_2m where n_1 and n_2 are quantum numbers appropriate to parabolic coordinates and m is the absolute value of the magnetic quantum number, has not been considered before. These coordinates are appropriate for problems involving an electric field. It will be shown that the distribution function corresponding to these coordinates has a much simpler form than the analogous function $D(nl,\mathbf{q})$, and differs from $D(n,\mathbf{q})$ by a weighting factor.

The cross section for electron capture by protons in the hydrogen atom in the Born approximation in which the interaction between the nuclei is neglected, known also as the Brinkman-Kramers[6] approximation, is given as an integral over the product of the momentum density functions of the initial and final states of the atom. In this paper perturbed wave functions due to an electric field F, correct to the first order, for the initial and the final states are used to calculate the capture cross section. The electric field is taken to be parallel to the direction of the incident proton. It is found that for capture from nn_1n_2 into $n'n_1'n_2'$, the cross section in the zeroth-order approximation is independent of n_1, n_2, n_1', and n_2', and depends only on the principal quantum numbers n and n'. For capture from n into n', the cross section is quadratic in F and is therefore independent of the field up to the first order.

Since the capture cross section in parabolic coordinates has a simpler form, it may be convenient in cases where the capture cross section is spherical coordinates is desirable—e.g., where radiative transitions affect the population of the excited states with different l—to solve the problem in parabolic and then transform to spherical coordinates. This has been done here, and an expression in the form of a finite number of terms has been obtained for the capture cross section from any initial nl to any final $n'l'$. Previous results in this respect are in integral forms, and the present method may be used as an alternative. Similarly, the present method can be extended to electron capture in many-electron

[1] B. Podolsky and L. Pauling, Phys. Rev. **34**, 109 (1929).
[2] V. Fock, Z. Physik **98**, 145 (1935).
[3] Reference 2, Eq. (40).
[4] R. M. May, Phys. Rev. **136**, A669 (1964).
[5] See, for example, R. A. Mapleton, Proc. Phys. Soc. (London) **87**, 219 (1966); R. Abrines and I. C. Percival, *ibid.* **88**, 861 (1966).
[6] H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amsterdam **33**, 973 (1930).

atoms, provided that their wave function can be expressed as a sum of the hydrogenic wave functions, although this has not been done here.

II. MOMENTUM DISTRIBUTION IN PARABOLIC COORDINATES

The Schrödinger equation for a bound electron with position vector $\mathbf{r}$ in the field of a charge Ze located at the origin is given by

$$\left[-\tfrac{1}{2}\nabla^2-\frac{Z}{a_0r}\right]\psi(\alpha,\mathbf{r})=-\tfrac{1}{2}\alpha^2\psi(\alpha,\mathbf{r}), \quad (3)$$

with α defined in Eq. (2). The Fourier transform of $\psi(\alpha,\mathbf{r})$ is given by

$$U(\alpha,\mathbf{q})=(2\pi)^{-3/2}\int e^{i\mathbf{q}\cdot\mathbf{r}}\psi(\alpha,\mathbf{r})d\mathbf{r}. \quad (4)$$

We define in addition the function

$$V(\alpha,\mathbf{q})=(2\pi)^{-3/2}\int e^{i\mathbf{q}\cdot\mathbf{r}}\frac{Z}{r}\psi(\alpha,\mathbf{r})d\mathbf{r}. \quad (5)$$

Then by substituting $(Z/r)\psi(\alpha,\mathbf{r})$ from (3) into (5) and carrying out a partial integration, we obtain

$$U(\alpha,\mathbf{q})=\frac{2}{a_0(\alpha^2+q^2)}V(\alpha,\mathbf{q}). \quad (6)$$

The momentum density and also the electron capture cross section are given in terms of the squared modulus of $U(\alpha,\mathbf{q})$ summed over the magnetic quantum numbers. Since this quantity is a scalar and invariant under rotation of the coordinate system, for evaluation of $U(\alpha,\mathbf{q})$ we can take for convenience the z axis of the coordinate system along the $\mathbf{q}$; and we designate in this case the $U(\alpha,\mathbf{q})$ and $V(\alpha,\mathbf{q})$ by $U(\alpha,q)$ and $V(\alpha,q)$, respectively.

We now evaluate $V(\alpha,q)$ in parabolic coordinates. Recalling that in these coordinates $r=\frac{1}{2}(\xi+\eta)$, $z=\frac{1}{2}(\xi-\eta)$, $d\mathbf{r}=\frac{1}{4}(\xi+\eta)d\xi d\eta d\phi$, and expressing the spatial wave function as the product of two associated Laguerre functions,[7] we obtain from (5)

$$V(nn_1n_2m,q)=(2\pi)^{-3/2}\int e^{iqz}\frac{Z}{r}\psi(nn_1n_2m,\mathbf{r})d\mathbf{r}=0, \quad m\neq 0, \quad (7)$$

and

$$\begin{aligned}V(nn_1n_20,q)&=(2\pi)^{-3/2}\int e^{iqz}\frac{Z}{r}\psi(nn_1n_20,\mathbf{r})d\mathbf{r}\\&=\frac{1}{2\pi(2n)^{1/2}}\frac{Z\alpha^{3/2}}{n_1!n_2!}\int_0^\infty\int_0^\infty \exp\left[-\frac{\alpha}{2}(\xi+\eta)+\frac{iq}{2}(\xi-\eta)\right]L_{n_1}{}^0(\alpha\xi)L_{n_2}{}^0(\alpha\eta)d\xi d\eta\\&=\frac{1}{2\pi(2n)^{1/2}}\frac{Z\alpha^{3/2}}{n_1!n_2!}I(n_1)I^*(n_2)\end{aligned} \quad (8)$$

where

$$I(l)=\int_0^\infty \exp\left[-\left(\frac{\alpha}{2}-\frac{iq}{2}\right)\xi\right]L_l{}^0(\alpha\xi)d\xi. \quad (9)$$

Using the generating function of the associated Laguerre functions[8] it follows from (9) that

$$\sum_{l=0}^\infty\frac{s^lI(l)}{l!}=\frac{1}{1-s}\int_0^\infty \exp\left[-\left(\frac{\alpha}{2}-\frac{iq}{2}+\frac{\alpha s}{1-s}\right)\xi\right]d\xi$$
$$=\left[\tfrac{1}{2}(\alpha-iq)(1-s)+\alpha s\right]^{-1}=\frac{1}{\omega+\omega^*s} \quad (10)$$

where

$$\omega=\tfrac{1}{2}(\alpha-iq). \quad (11)$$

By expanding the right-hand side of (10) in terms of s and equating coefficients of equal powers of s on both sides, we obtain

$$I(l)=\frac{l!}{\omega}\left(-\frac{\omega^*}{\omega}\right)^l. \quad (12)$$

Equation (8) now becomes

$$V(nn_1n_20,q)=\frac{1}{2\pi(2n)^{1/2}}\frac{Z\alpha^{3/2}}{|\omega|^2}\left(-\frac{\omega^*}{\omega}\right)^{n_1-n_2}. \quad (13)$$

Since

$$n_1+n_2=n-1-m, \quad (14)$$

Eq. (13), if we neglect a constant phase factor, can be written

$$V(nn_1n_20,q)=\frac{1}{2\pi(2n)^{1/2}}\frac{Z\alpha^{3/2}}{|\omega|^2}\left(\frac{\omega^*}{\omega}\right)^{2n_1}. \quad (15)$$

From this equation and Eqs. (6), (11) we have similarly

$$U(nn_1n_20,q)=\frac{1}{2\pi(2n)^{1/2}}\frac{Z\alpha^{3/2}}{2a_0|\omega|^4}\left(\frac{\omega^*}{\omega}\right)^{2n_1}. \quad (16)$$

Equations (15) and (16) are the main equations from which the momentum distribution and electron capture cross sections are derived.

[7] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin, 1957), Sec. 6.
[8] Reference 7, Sec. 3.

The momentum density of an electron in the state nn_1n_2, summed over the magnetic quantum number, is given by

$$D(nn_1n_2,\mathbf{q})=\sum_m |U(nn_1n_2m,\mathbf{q})|^2 = |U(nn_1n_20,q)|^2=\frac{8Z^2\alpha^3}{n\pi^2a_0^2}\frac{1}{(\alpha^2+q^2)^4}, \quad (17)$$

which is independent of the sublevel quantum numbers n_1 and n_2.

The averaged momentum distribution of an electron in the shell n is given by averaging $D(nn_1n_2,\mathbf{q})$ over n_1 and n_2. Since there are n^2 states for a given n, we obtain

$$D(n,\mathbf{q})=n^{-2}\sum_{n_1=0}^{n-1} D(nn_1n_2,\mathbf{q})=n^{-1}D(nn_1n_2,\mathbf{q}) =\frac{8Z^2\alpha^3}{n^2\pi^2a_0^2}\frac{1}{(\alpha^2+q^2)^4}. \quad (18)$$

The integral with respect to $\mathbf{q}$ of $D(n,\mathbf{q})$ is normalized to unity which corresponds to an electron in the n shell:

$$\int D(n,\mathbf{q})d\mathbf{q}=\frac{32Z^2\alpha^3}{n^2\pi a_0^2}\int_0^\infty\frac{q^2dq}{(\alpha^2+q^2)^4} =\frac{32Z^2\alpha^3}{n^2\pi a_0^2}\frac{\pi}{32\alpha^5}=1. \quad (19)$$

The expression for $D(n,\mathbf{q})$ given in Eq. (18) is identical to the expression given in Eq. (1), derived by Fock using spherical coordinates, and to the classical momentum distribution of a particle in a Coulomb field with the assumption of the microcanonical distribution.

Equation (17) has the interesting meaning that in the zeroth order the Stark levels of the hydrogen atom within a given shell n have the same momentum distribution. The first-order correction to the momentum distribution will be given in Sec. VI.

III. CAPTURE CROSS SECTION IN AN ELECTRIC FIELD: ZEROTH-FIELD APPROXIMATION

Assume a nucleus of charge Z' and mass M' captures an electron from a single electron atom with nucleus of charge Z and mass M to form an atom with nucleus of charge Z' and mass M'. The capture cross section in the Born approximation with the interaction between the nuclei neglected is given by[9,10]

$$\sigma(i,f)=\frac{(2\pi)^7\mu^2e^2}{\hbar^4}\frac{v'}{v}\int_{-1}^{+1}|U(\alpha,\mathbf{q})|^2 \times|V(\alpha',\mathbf{q}')|^2d(\cos\theta), \quad (20)$$

where μ is the reduced mass of the system, e the absolute value of the electronic charge, v and v' the magnitudes of the initial and final velocities of relative motion of the nuclei, and θ the angle between $\mathbf{v}$ and $\mathbf{v}'$. From here on the unprimed symbols correspond to the initial states while the primed are for the final states. The vectors $\mathbf{q}$ and $\mathbf{q}'$ are related to the velocities $\mathbf{v}$ and $\mathbf{v}'$ through

$$\mathbf{q}=\frac{M}{M+m}\mathbf{k}-\mathbf{k}', \quad \mathbf{q}'=\mathbf{k}-\frac{M'}{M'+m}\mathbf{k}', \quad (21)$$

with

$$\mathbf{k}=\frac{M'(M+m)}{\hbar(M'+M+m)}\mathbf{v}, \quad \mathbf{k}'=\frac{M(M'+m)}{\hbar(M'+M+m)}\mathbf{v}'. \quad (22)$$

In the impact-parameter approximation the corresponding expression for the cross section is given by[4,11,12]

$$\sigma(i,f)=\frac{(2\pi)^5}{p^2}\int_0^\infty|U(\alpha,\mathbf{q})|^2\times|V(\alpha',\mathbf{q}')|^2\rho d\rho, \quad (23)$$

with p a dimensionless quantity defined by

$$p=\hbar v/e^2 \quad (24)$$

and ρ given by

$$\rho^2=q_x^2+q_y^2=q_x'^2+q_y'^2. \quad (25)$$

The validity of the second equality in (25) is implicit in the impact parameter approximation. Similarly by setting $q_z=\beta$, $q_z'=\beta'$ it is found that

$$\beta=\frac{1}{2a_0p}\left[p^2-\left(\frac{Z^2}{n^2}-\frac{Z'^2}{n'^2}\right)\right], \quad \beta'=\frac{-1}{2a_0p}\left[p^2+\left(\frac{Z^2}{n^2}-\frac{Z'^2}{n'^2}\right)\right], \quad (26)$$

with a_0 the Bohr radius and n and n' the principal quantum numbers of the initial and the final states of the electron.

Since the integral that appears in the impact parameter method is easier to evaluate, the cross sections below are evaluated according to this method. The difference between the two methods at high energies is probably negligible.

The capture cross section in the impact parameter approximation with the atom Z in the state nn_1n_2 and the atom Z' in the state $n'n_1'n_2'$, through Eqs. (15), (16), and (23), is given by

$$\sigma(nn_1n_2,n'n_1'n_2')=\frac{2\pi Z^2Z'^2(\alpha\alpha')^3}{16nn'a_0^2p^2}\int_0^\infty\frac{\rho d\rho}{|\omega|^8\times|\omega'|^4}. \quad (27)$$

Furthermore, through Eqs. (11), (2), (25), and (26) it is implied that

$$|\omega'|^2=\tfrac{1}{4}(\alpha'^2+q'^2)=\tfrac{1}{4}(\alpha^2+q^2)=|\omega|^2; \quad (28)$$

[9] D. R. Bates and A. Dalgarno, Proc. Phys. Soc. (London) **A66**, 972 (1953).

[10] J. D. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953).

[11] D. R. Bates, in *Atomic and Molecular Processes*, edited by D. R. Bates (Academic Press Inc., New York, 1962), p. 585. Equation (23) can be derived by some manipulation of Eqs. (135), (133), and (119) of this reference.

[12] M. H. Mittleman, Phys. Rev. **122**, 499 (1961).

consequently

$$\sigma(nn_1n_2,n'n_1'n_2')=\frac{2^9\pi(ZZ')^2(\alpha\alpha')^3}{nn'a_0^2p^2}\int_0^\infty\frac{\rho d\rho}{[\alpha^2+\beta^2+\rho^2]^6}$$
$$=\pi a_0^2\frac{2^8(ZZ')^5}{5(nn')^4p^2}\frac{1}{[(\alpha^2+\beta^2)a_0^2]^5}. \quad (29)$$

As was stated previously it is evident that $\sigma(nn_1n_2, n'n_1'n_2')$ is independent of $n_1n_2n_1'n_2'$. The transition $\sigma(nn_1n_2,n')$ is obtained by summing $\sigma(nn_1n_2,n'n_1'n_2')$ over $n_1'n_2'$. Noticing that only states with $m'=0$ contribute to the cross section, we obtain

$$\sigma(nn_1n_2,n')=n'\sigma(nn_1n_2,n'n_1'n_2')$$
$$=\pi a_0^2\frac{2^8(ZZ')^5}{5n^4n'^3p^2}\frac{1}{[(\alpha^2+\beta^2)a_0^2]^5}. \quad (30)$$

Finally the transition $\sigma(n,n')$ is obtained by averaging $\sigma(nn_1n_2,n')$ over the initial states. Only n states of the n^2 states of the initial states have nonvanishing cross section. Then

$$\sigma(n,n')=n^{-1}\sigma(nn_1n_2,n')$$
$$=\pi a_0^2\frac{2^8(ZZ')^5}{5n^5n'^3p^2}\frac{1}{[(\alpha^2+\beta^2)a_0^2]^5}. \quad (31)$$

This result is identical with the result obtained by May.[4]

IV. CAPTURE CROSS SECTION IN SPHERICAL COORDINATES

Let $\phi(nlm,\mathbf{r})$ represent the wave function of the hydrogen atom in spherical coordinates. Then we define the function $f(nlm,\mathbf{q})$ and $g(nlm,\mathbf{q})$ by

$$f(nlm,\mathbf{q})=(2\pi)^{-3/2}\int e^{i\mathbf{q}\cdot\mathbf{r}}\phi(nlm,\mathbf{r})d\mathbf{r}, \quad (32)$$

$$g(nlm,\mathbf{q})=(2\pi)^{-3/2}\int e^{i\mathbf{q}\cdot\mathbf{r}}\frac{Z}{r}\phi(nlm,\mathbf{r})d\mathbf{r}. \quad (33)$$

As before, we designate the $f(nlm,\mathbf{q})$ by $f(nlm,q)$ when $\mathbf{q}$ coincides with the coordinate z axis. Then by the invariance of the scalar quantities under rotation we have

$$\sum_{m=-l}^{l}|f(nlm,\mathbf{q})|^2=\sum_{m=-l}^{l}|f(nlm,q)|^2=|f(nl0,q)|^2. \quad (34)$$

Since the wave function of the hydrogen atom forms a complete set in each of the two spherical and parabolic coordinates, the wave function in spherical coordinates can be expressed as a linear combination of the wave functions in parabolic coordinates. In this transformation the principal and the magnetic quantum numbers n and m remain fixed:

$$\phi(nlm,\mathbf{r})=\sum_{n_1=0}^{n-1-m}a_{ln_1}\psi(nn_1n_2m,\mathbf{r}), \quad (35)$$

where a_{ln_1} are the elements of the transformation matrix. The same relationship holds between the Fourier transforms of ϕ and ψ. In our problem $m=0$, and by dropping n, m, n_2 from the indices in Eq. (35) and replacing n_1 by i, through Eqs. (4) and (32) we obtain

$$f(l,q)=\sum_{i=0}^{n-1}a_{li}U(i,q). \quad (36)$$

The determination of a_{li} for arbitrary n and m is worked out in Appendix A and the matrices for $n=1$, 2, 3, 4, 5 are given explicitly.

By Eq. (16) we now obtain

$$|f(l,q)|^2=\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}a_{li}a_{lj}U(i,q)U^*(j,q)$$
$$=\frac{Z^2\alpha^3}{32\pi^2a_0^2n|\omega|^8}\sum_{i,j}a_{li}a_{lj}\left(\frac{\omega^*}{\omega}\right)^{2i-2j}$$
$$=\frac{Z^2\alpha^3}{32\pi^2a_0^2n|\omega|^8}\sum_{i,j}a_{li}a_{lj}\frac{\mathrm{Re}[\omega^{*4|i-j|}]}{|\omega|^{4|i-j|}}, \quad (37)$$

where Re stands for the real part of $\omega^{*4|i-j|}$.

When a binomial expansion is made of this quantity in terms of α and q, [cf. Eq. (11)], we obtain

$$|f(l,q)|^2=\frac{8Z^2\alpha^3}{\pi^2a_0^2n(\alpha^2+q^2)^4}\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}\sum_{\lambda=0}^{2|i-j|}(-)^\lambda$$
$$\times a_{li}a_{lj}\binom{4|i-j|}{2\lambda}\frac{\alpha^{4|i-j|-2\lambda}q^{2\lambda}}{(\alpha^2+q^2)^{2|i-j|}}. \quad (38)$$

In a similar way, through Eq. (15),

$$|g(l,q)|^2=\frac{2Z^2\alpha^3}{\pi^2n(\alpha^2+q^2)^2}\sum_{i,j,\lambda}(-)^\lambda$$
$$\times a_{li}a_{lj}\binom{4|i-j|}{2\lambda}\frac{\alpha^{4|i-j|-2\lambda}q^{2\lambda}}{(\alpha^2+q^2)^{2|i-j|}}. \quad (39)$$

Replacement of $f(l,q)$ and $g(l',q')$ for $U(\alpha,q)$ and $V(\alpha',q')$ in Eq. (23) allows the integration in this equation to be carried out analytically. This is done in Appendix B and here we give the final results. Introduce the dimensionless A and A' as

$$A=\frac{\alpha^2}{\alpha^2+\beta^2},\quad A'=\frac{\alpha'^2}{\alpha^2+\beta^2}, \quad (40)$$

where α and β are given by (2) and (26). Then the capture cross section for a process in which the electron is initially in the state nl, averaged over m, and finally in the state $n'l'$, summed over m', is given as a polynomial in A and A':

$$\sigma(nl,n'l')=\frac{5n}{(2l+1)n'}\sigma(n,n') \times\sum_{\nu=0}^{2(n-1)}\sum_{\nu'=0}^{2(n'-1)} C(nl\nu,n'l'\nu')A^{\nu}A'^{\nu'}, \quad (41)$$

where $\sigma(n,n')$ is the cross section between n and n' and is given by (31), and

$$C(nl\nu,n'l'\nu')=\sum_{\gamma}\sum_{\gamma'}(1+\mu+\mu')^{-1} \times\binom{5+2(i-j+i'-j')}{1+\mu+\mu'}^{-1} \times D(\nu,\gamma)D(\nu',\gamma'), \quad (42)$$

$$D(\nu,\gamma)=[2-\delta(i,j)](-)^{\nu}a_{li}a_{lj}\binom{4i-4j}{2\lambda} \times\binom{\lambda}{\mu}\binom{\lambda-\mu}{\nu+\lambda-2(i-j)}, \quad (43)$$

where $\delta(i,j)$ is the Kronecker delta. In Eq. (42), γ stands for four integers i, j, λ, μ whose ranges are given by

$$\begin{aligned} &i=[\tfrac{1}{2}\nu],\ [\tfrac{1}{2}\nu]+1,\cdots,\ n-1;\\ &j=0,1,2,\cdots,\ i-[\tfrac{1}{2}\nu];\\ &\lambda=2(i-j)-\nu,\ 2(i-j)-\nu+1,\cdots,\ 2(i-j);\\ &\mu=0,1,2,\cdots,\ 2(i-j)-\nu;\\ &[\nu/2]=\begin{cases}\tfrac{1}{2}\nu, & \nu \text{ even},\\ \tfrac{1}{2}(\nu+1), & \nu \text{ odd}.\end{cases}\end{aligned} \quad (44)$$

A similar rule applies to γ' and other primed integers. Equation (41) then expresses the capture cross sections between two arbitrary states nl and $n'l'$ in terms of a finite number of terms, while previous results have been expressed in integral forms.

From Eqs. (41), (42), and (31), the following reciprocity equation results:

$$(2l'+1)p'^2\sigma(n'l',nl)=(2l+1)p^2\sigma(nl,n'l'). \quad (45)$$

As an example from Eq. (41) the following simple formulas are obtained for the electron capture cross sections with the ground state as the initial state and the sublevels of $n=1$, 2, 3, 4 as the final states. The prime in the final state is omitted for convenience

Type (I):

$$\sigma(1s,1s)=\sigma(1,1), \quad (46)$$

in agreement with the value given by Bates and Dalgarno,[9]

Type (II):

$$\sigma(1s,2s)=\sigma(1,2)\left(1-\frac{10}{3}A+\frac{20}{7}A^2\right), \quad (47)$$

$$\sigma(1s,2p)=\sigma(1,2)\left(\frac{10}{3}A-\frac{20}{7}A^2\right). \quad (48)$$

Type (III):

$$\sigma(1s,3s)=\sigma(1,3)\left(1-\frac{80}{9}A+\frac{1760}{63}A^2-\frac{320}{9}A^3+\frac{1280}{81}A^4\right). \quad (49)$$

$$\sigma(1s,3p)=\sigma(1,3)\left(\frac{80}{9}A-\frac{800}{21}A^2+\frac{160}{3}A^3-\frac{640}{27}A^4\right), \quad (50)$$

$$\sigma(1s,3d)=\sigma(1,3)\left(\frac{640}{63}A^2-\frac{160}{9}A^3+\frac{640}{81}A^4\right). \quad (51)$$

Equations (47) through (51) have also been obtained by May and Lodge[13] by explicit evaluation of the integrals in the impact parameter approximation.

Type (IV):

$$\sigma(1s,4s)=\sigma(1,4)\left(1-\frac{50}{3}A+\frac{740}{7}A^2-320A^3+\frac{4480}{9}A^4-384A^5+\frac{1280}{11}A^6\right), \quad (52)$$

$$\sigma(1s,4p)=\sigma(1,4)\left(\frac{50}{3}A-\frac{1060}{7}A^2+528A^3-\frac{2624}{3}A^4+\frac{3456}{5}A^5-\frac{2304}{11}A^6\right), \quad (53)$$

$$\sigma(1s,4d)=\sigma(1,4)\left(\frac{320}{7}A^2-240A^3+\frac{4160}{9}A^4-384A^5+\frac{1280}{11}A^6\right), \quad (54)$$

$$\sigma(1s,4f)=\sigma(1,4)\left(32A^3-\frac{256}{3}A^4+\frac{384}{5}A^5-\frac{256}{11}A^6\right). \quad (55)$$

Type (V):

$$\sigma(2s,2s)=4\sigma(2,2)\times\left(1-\frac{20}{3}A+\frac{120}{7}A^2-20A^3+\frac{80}{9}A^4\right), \quad (56)$$

$$\sigma(2s,2p)=4\sigma(2,2)\left(\frac{10}{3}A-\frac{100}{7}A^2+20A^3-\frac{80}{9}A^4\right), \quad (57)$$

$$\sigma(2p,2s)=\tfrac{1}{3}\sigma(2s,2p), \quad (58)$$

$$\sigma(2p,2p)=4\sigma(2,2)\left(\frac{80}{21}A^2-\frac{20}{3}A^3+\frac{80}{27}A^4\right). \quad (59)$$

As a check it can be verified that when averaging and summing are performed over the initial and final states, the corresponding $Q(n,n')$ results.

[13] R. M. May and J. G. Lodge, Phys. Rev. **137**, A699 (1965).

Extensive tabulation of the cross sections of the type (I)-(V) in the integral form are given by Hiskes.[14]

V. FIRST-ORDER WAVE FUNCTION IN AN ELECTRIC FIELD

Assume $\chi(nn_1n_2m,\mathbf{r})$ is the atomic wave function in an electric field of strength F. Then by writing

$$\chi(nn_1n_2m,\mathbf{r})=u_1(\xi)u_2(\eta)e^{\pm im\phi}/(2\pi)^{1/2}, \tag{60}$$

the Schrödinger equation for the system reduces to the following equations[15]:

$$\begin{aligned}\frac{d}{d\xi}\left(\xi\frac{du_1}{d\xi}\right)+\left(\frac{1}{2}E\xi+Z_1-\frac{m^2}{4\xi}\right)u_1&=\tfrac{1}{4}F\xi^2u_1,\\ \frac{d}{d\eta}\left(\eta\frac{du_2}{d\eta}\right)+\left(\frac{1}{2}E\eta+Z_2-\frac{m^2}{4\eta}\right)u_2&=-\tfrac{1}{4}F\eta^2u_2,\end{aligned} \tag{61}$$

where E is the energy of the system and

$$Z_1=\alpha a_0[n_1+\tfrac{1}{2}(m+1)],\quad Z_2=\alpha a_0[n_2+\tfrac{1}{2}(m+1)],\quad Z_1+Z_2=Z, \tag{62}$$

Z being the charge of the nucleus. The right-hand side of Eqs. (61) can be treated as a small perturbation. Then the first-order solution to the first of these equations can be written as

$$u_1=u_{n_1}+\sum_{n_1'\neq n_1}b_{n_1'}u_{n_1'}, \tag{63}$$

where u_{n_1} and $u_{n_1'}$ are the homogeneous solutions of this equation with Z_1 and Z_1' as their eigenvalues, and

$$b_{n_1'}=\frac{-\frac{1}{4}F\langle n_1|\xi^2|n_1'\rangle}{Z_1-Z_1'}. \tag{64}$$

The matrices in (64) are given by Bethe and Salpeter.[16] In this way we find that

$$\begin{aligned}b_{n_1-2}&=\frac{nF}{8Z\alpha^2}[n_1(n_1-1)(n_1+m)(n_1-1+m)]^{1/2},\\ b_{n_1-1}&=-\frac{nF}{2Z\alpha^2}(2n_1+m)[n_1(n_1+m)]^{1/2},\\ b_{n_1+1}&=\frac{nF}{2Z\alpha^2}(2n_1+2+m)[(n_1+1)(n_1+1+m)]^{1/2},\\ b_{n_1+2}&=-\frac{nF}{8Z\alpha^2}[(n_1+2)(n_1+1)(n_1+2+m)(n_1+1+m)]^{1/2},\end{aligned} \tag{65}$$

and $b_{n_1'}$ vanishes otherwise.

It is convenient to introduce a new function:

$$M(jm,x)=\frac{n}{4Z\alpha^2}\left[\frac{1}{2}(j+m)^2(j-1+m)^2L_{j-2+m}{}^m(x)-2(2j+m)(j+m)^2L_{j-1+m}{}^m(x)+2\frac{(2j+2+m)(j+1)}{j+1+m}L_{j+1+m}{}^m(x)-\frac{1}{2}\frac{(j+1)(j+2)}{(j+1+m)(j+2+m)}L_{j+2+m}{}^m(x)\right]; \tag{66}$$

then, expressing $u_{n_1'}$ as Laguerre functions, and combining (63) and (65) we obtain

$$u_1(\xi)=\frac{[(2/n)^{1/2}\alpha^{m+3/2}(n_1!)]^{1/2}}{[(n_1+m)!]^{3/2}}e^{-\alpha(\xi+\eta)/2}\xi^{m/2}[L_{n_1+m}{}^m(\alpha\xi)+FM(n_1m,\alpha\xi)]. \tag{67}$$

Similarly the solution to the second of Eqs. (61) is given by changing the index 1 to 2 in (63) and (65), and changing the sign of F in (65). Thus

$$u_2(\eta)=\frac{[(2/n)^{1/2}\alpha^{m+3/2}(n_2!)]^{1/2}}{[(n_2+m)!]^{3/2}}e^{-\alpha\eta/2}\eta^{m/2}[L_{n_2+m}{}^m(\alpha\eta)-FM(n_2m,\alpha\eta)]. \tag{68}$$

[14] J. R. Hiskes, Phys. Rev. **137**, A361 (1965).
[15] Reference 7, Sec. 51.
[16] Reference 7, Sec. 52.

In this way Eq. (60) can be written, to first order:

$$\chi(nn_1n_2m,\mathbf{r})=\frac{e^{\pm im\phi}}{(\pi n)^{1/2}}\frac{(n_1!n_2!)^{1/2}\alpha^{m+3/2}}{[(n_1+m)!(n_2+m)!]^{3/2}}e^{-\alpha(\xi+\eta)/2}(\xi\eta)^{m/2}$$
$$\times\{L_{n_1+m}{}^m(\alpha\xi)L_{n_2+m}{}^m(\alpha\eta)+F[M(n_1m,\alpha\xi)L_{n_2+m}{}^m(\alpha\eta)-M(n_2m,\alpha\eta)L_{n_1+m}{}^m(\alpha\xi)]\}. \quad (69)$$

As a special case the perturbed ground-state wave function is given by

$$\chi(1000,\mathbf{r})=\frac{\alpha^{3/2}e^{-\alpha(\xi+\eta)/2}}{\sqrt{\pi}}\{1+F[M(00,\alpha\xi)-M(00,\alpha\eta)]\}$$
$$=\frac{\alpha^{3/2}e^{-\alpha(\xi+\eta)/2}}{\sqrt{\pi}}\left\{1-\frac{F(\xi-\eta)}{4Z\alpha}\left[2+\frac{\alpha}{2}(\xi+\eta)\right]\right\}$$
$$=\frac{\alpha^{3/2}e^{-\alpha r}}{\sqrt{\pi}}\left[1-\frac{Fr\cos\theta}{2Z\alpha}(2+\alpha r)\right]. \quad (70)$$

In the special case of the ground state, the above equation can also be derived by solving the Schrödinger equation for the hydrogen atom perturbed by a weak electric field, using spherical coordinates.[17]

Expression (70) as the wave function of the perturbed hydrogen atom has been applied successfully by Temkin and Lamkin[18] to the problem of elastic scattering of electrons by the hydrogen atom. F in this case is due to the incident electron. This approach is named the method of polarized orbitals.

To the extent that the indices of each term in the product $M(n_1m,\alpha\xi)\times L_{n_2+m}{}^m(\alpha\eta)$ do not satisfy the condition (14), the terms on the right-hand side of (69), except for the first term, are not hydrogenic wave functions.

VI. FIRST-ORDER EFFECT ON THE CROSS SECTION DUE TO THE FIELD

By combining Eqs. (60) and (63) we can write to the first order

$$\chi(nn_1n_2m,\mathbf{r})=\psi(nn_1n_2m,\mathbf{r})+\sum_{n_1'\neq n_1}b_{n_1'}\psi(nn_1'n_2m,\mathbf{r})+\sum_{n_2'\neq n_2}b_{n_2'}\psi(nn_1n_2'm,\mathbf{r}). \quad (71)$$

Defining

$$F(nn_1n_2m,\mathbf{q})=(2\pi)^{-3/2}\int e^{i\mathbf{q}\cdot\mathbf{r}}\chi(nn_1n_2m,\mathbf{r})d\mathbf{r}, \quad (72)$$

$$G(nn_1n_2m,\mathbf{q})=(2\pi)^{-3/2}\int e^{i\mathbf{q}\cdot\mathbf{r}}\frac{Z}{r}\chi(nn_1n_2m,\mathbf{r})d\mathbf{r}, \quad (73)$$

it follows that

$$F(nn_1n_20,q)=U(nn_1n_20,q)+\sum_{n_1'}b_{n_1'}U(nn_1'n_20,q)+\sum_{n_2'}b_{n_2'}U(nn_1n_2'0,q), \quad (74)$$

$$G(nn_1n_20,q)=V(nn_1n_20,q)+\sum_{n_1'}b_{n_1'}V(nn_1'n_20,q)+\sum_{n_2'}b_{n_2'}V(nn_1n_2'0,q). \quad (75)$$

The coefficients b_{n_1}' are given by (65), and b_{n_2}' are obtained from b_{n_1}' by changing the index 1 to 2 and replacing F by $-F$.

The squared modulus of $F(nn_1n_20,q)$ gives the momentum distribution in an electric field. Through Eqs. (6), (13), and (74) the first-order term in the momentum distribution is given by

$$\left[|F(nn_1n_20,q)|^2\right]_1=\frac{Z^2\alpha^3}{16\pi^2a_0{}^2n|\omega|^8}\times\mathrm{Re}\left[\sum b_{n_1'}\left(-\frac{\omega^*}{\omega}\right)^{n_1-n_1'}+\sum b_{n_2'}\left(-\frac{\omega^*}{\omega}\right)^{n_2-n_2'}\right]. \quad (76)$$

For a given n, let us call the state specified by $n_1=j$ and $n_2=i$, with i and j two integers, the state conjugate to the state $n_1=i$ and $n_2=j$. Then from (76) it follows that the first-order correction to the momentum distribution of a conjugate state is the negative of this correction to the state itself. In particular when $n_1=n_2$, the first-order correction vanishes. The change in sign of F interchanges the first-order distribution for the two conjugate states. By averaging over n_1 and n_2 for a given n, the first-order terms drop out, and the momentum distribution for the principal quantum numbers becomes quadratic in F.

A similar consideration applies to the first-order correction to $G(nn_1n_20,q)$, and through Eq. (23) it follows that the capture cross section is quadratic in the field.

The evaluation of the cross section integral for the transition nn_1n_2 to $n'n_1'n_2'$, Eq. (23), is similar to the evaluation of this integral for the capture cross section in spherical coordinates. The final result is given below. Let Q represent the capture cross section is an electric

[17] R. M. Sternheimer, Phys. Rev. **96**, 951 (1954).

[18] A. Temkin and J. C. Lamkin, Phys. Rev. **121**, 788 (1960).

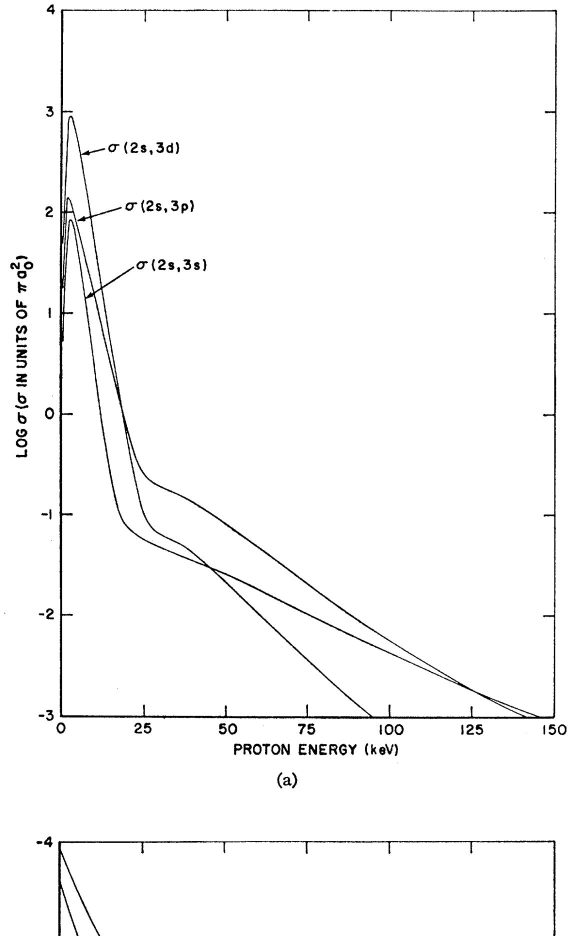

FIG. 1. Electron capture cross sections for the initial state $n=2$, $l=0$, and the final states $n'=3$.

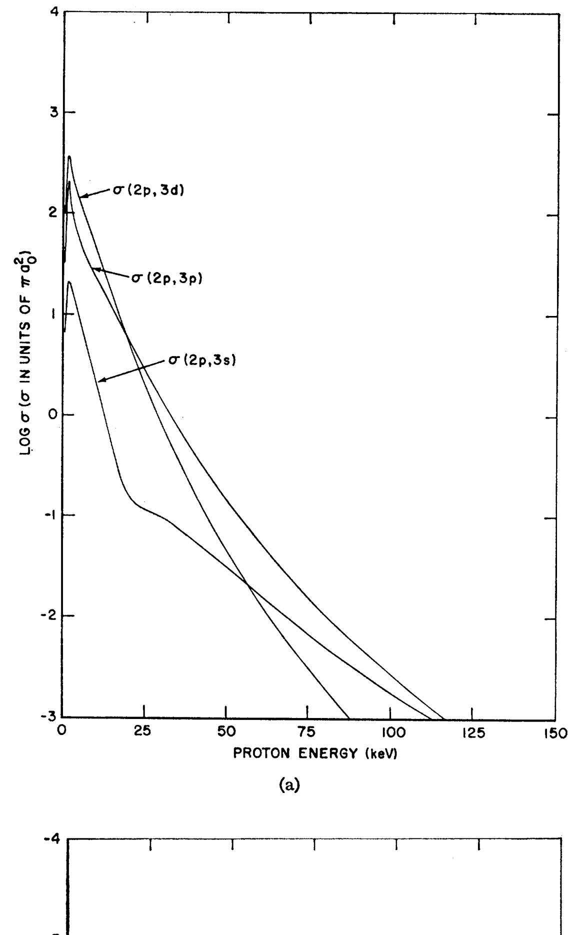

FIG. 2. Electron capture cross sections for the initial state $n=2$, $l=1$, and the final states $n'=3$.

field up to the first order. Then

$$Q(nn_1n_2,n'n_1'n_2')=\frac{n}{n'}\sigma(n,n')\times[1+P(n_1)+P(n_2)+P(n_1')+P(n_2')], \quad (77)$$

where $P(i)$ depend linearly on the electric field. Explicitly,

$$P(i)=10\sum_{\nu=0}^{2}C(i,\nu)A^{\nu}, \quad (78)$$

where A is defined in Eq. (40) and

$$C(i,\nu)=\sum_{j\lambda\mu}[1-\delta(i,j)]D(i,\nu,j,\lambda,\mu), \quad (79)$$

$$D(i,\nu,j,\lambda,\mu)=(-)^{\nu}(\mu+1)^{-1}\binom{5+|i-j|}{\mu+1}^{-1}\times\binom{2|i-j|}{2\lambda}\binom{\lambda}{\mu}\binom{\lambda-\mu}{\nu+\lambda-|i-j|}b_j, \quad (80)$$

$$\begin{aligned} &j=i-2,\quad i-1,\cdots,\quad i-\nu;\\ &\qquad i+\nu,\ i+\nu+1,\cdots,\quad i+2;\\ &\lambda=|i-j|-\nu,\quad |i-j|-\nu+1,\cdots,\quad |i-j|;\\ &\mu=0,\ 1,\ 2,\cdots,\quad |i-j|-\nu. \end{aligned} \quad (81)$$

The coefficients b_j depend linearly on F and are given by (65).

VII. DISCUSSION

As an example of the applicability of Sec. IV, in Figs. 1(a), 1(b), 2(a), and 2(b) the capture cross sections from the states $2s$ and $2p$ to the states $3s$, $3p$ and $3d$ are plotted as a function of the incident proton energies. The method of this section provides an easy way to calculate the electron capture by protons in any atomic or molecular gas, provided that the central field approximation can be applied to the particles of the gas, and that their wave functions can be expressed as hydrogenic wave functions.

The analysis of Sec. VI showed that the capture cross section between principal quantum numbers is quadratic in the field and invariant up to the second order under the change of sign of the field. Verification of this symmetry by experiment will provide a good test on the validity of the Brinkman-Kramers approximation.

Note added in proof. When in electron capture by a proton the interaction between the nuclei is included, the cross section will depend on $F(nn_1n_20,q)$, Eq. (74), as well as on its absolute value (cf. Ref. 10). Since the first-order correction to $F(nn_1n_20,q)$ does not vanish, the quadratic symmetry is destroyed in this approximation.

ACKNOWLEDGMENTS

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APPENDIX I: THE ELEMENTS OF THE TRANSFORMATION MATRIX BETWEEN THE WAVE FUNCTIONS IN SPHERICAL AND PARABOLIC COORDINATES

We require the transformation matrix which for a given principal quantum number n and absolute value of the magnetic quantum number m transforms the $n-m$ states in spherical coordinates to another set of $n-m$ states in parabolic coordinates. The simplest way to find the transformation matrix is by noticing that the matrix elements of interaction of an electric field with the hydrogen atom, taken with the unperturbed wave function of the atom, are diagonal in the parabolic coordinates representation. Let $\boldsymbol{\varepsilon}$ be this matrix and let $\mathbf{A}$ be the transformation matrix. We must then have

$$\mathbf{AH'A}^{-1}=\boldsymbol{\varepsilon}, \quad (A1)$$

where $\mathbf{H'}$ is the interaction matrix in spherical coordinates. $\boldsymbol{\varepsilon}$ is given by[19]

$$\begin{aligned}\epsilon_{ij}&=-\delta(i,j)\tfrac{3}{2}neFa_0(2j+1-n+m),\\ j&=0,\ 1,\ 2,\cdots,n-m-1,\end{aligned} \quad (A2)$$

with F the strength of the electric field. Similarly we can write

$$\begin{aligned}H_{ij}'&=-eF\int\phi_{ni\pm m}^*(\mathbf{r})r\cos\theta\phi_{nj\pm m}(\mathbf{r})d\mathbf{r}\\ &=-eF\int_0^\infty R_{ni}(r)R_{nj}(r)r^3dr\\ &\qquad\times\int Y_{i\pm m}(\Omega)Y_{j\pm m}(\Omega)\cos\theta d\Omega,\end{aligned} \quad (A3)$$

where i and j are the angular-momentum quantum numbers of the two states considered. It can be verified that

$$\int Y_{i\pm m}^*(\Omega)Y_{j\pm m}(\Omega)\cos\theta d\Omega=\left[\frac{i^2-m^2}{4i^2-1}\right]^{1/2}\delta(i,\ j+1)+\left[\frac{j^2-m^2}{4j^2-1}\right]^{1/2}\delta(i+1,\ j). \quad (A4)$$

Also[20]

$$\int_0^\infty R_{ni}R_{ni-1}r^3dr=\tfrac{3}{2}a_0n(n^2-i^2)^{1/2}. \quad (A5)$$

[19] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, New York, 1951), p. 399.
[20] Reference 19, p. 132.

TABLE I. Elements of the transformation matrices.

(I) $n=2,\ m=0$

$$\mathbf{a}(20)=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}.$$

(II) $n=3,\ m=0$

$$\mathbf{a}(30)=\frac{1}{\sqrt{3}}\begin{bmatrix}1 & 1 & 1\\ -\sqrt{(3/2)} & 0 & \sqrt{(3/2)}\\ \sqrt{\tfrac{1}{2}} & -\sqrt{2} & \sqrt{\tfrac{1}{2}}\end{bmatrix}.$$

(III) $n=3,\ m=1$

$$\mathbf{a}(31)=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}.$$

(IV) $n=4,\ m=0$

$$\mathbf{a}(40)=\frac{1}{2}\begin{bmatrix}1 & 1 & 1 & 1\\ -3/\sqrt{5} & -1/\sqrt{5} & 1/\sqrt{5} & 3/\sqrt{5}\\ 1 & -1 & -1 & 1\\ -1/\sqrt{5} & 3/\sqrt{5} & -3/\sqrt{5} & 1/\sqrt{5}\end{bmatrix}.$$

(V) $n=4,\ m=1$

$$\mathbf{a}(41)=\begin{bmatrix}\sqrt{(3/10)} & \sqrt{\tfrac{2}{5}} & \sqrt{(3/10)}\\ -\sqrt{\tfrac{1}{2}} & 0 & 1/\sqrt{2}\\ 1/\sqrt{5} & -\sqrt{\tfrac{3}{5}} & 1/\sqrt{5}\end{bmatrix}.$$

(VI) $n=4,\ m=2$

$$\mathbf{a}(42)=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}.$$

(VII) $n=5,\ m=0$

$$\mathbf{a}(50)=\frac{1}{\sqrt{5}}\begin{bmatrix}1 & 1 & 1 & 1 & 1\\ -\sqrt{2} & -\sqrt{\tfrac{1}{2}} & 0 & \sqrt{\tfrac{1}{2}} & \sqrt{2}\\ \sqrt{(10/7)} & -\sqrt{(5/14)} & -\sqrt{(10/7)} & -\sqrt{(5/14)} & \sqrt{(10/7)}\\ -\sqrt{\tfrac{1}{2}} & \sqrt{2} & 0 & -\sqrt{2} & \sqrt{\tfrac{1}{2}}\\ \sqrt{(1/14)} & -\sqrt{(8/7)} & \sqrt{(18/7)} & -\sqrt{(8/7)} & \sqrt{(1/14)}\end{bmatrix}.$$

(VIII) $n=5,\ m=1$

$$\mathbf{a}(51)=\begin{bmatrix}1/\sqrt{5} & \sqrt{(3/10)} & \sqrt{(3/10)} & \sqrt{\tfrac{1}{5}}\\ -\sqrt{(3/7)} & -\sqrt{(1/14)} & \sqrt{(1/14)} & \sqrt{(3/7)}\\ \sqrt{(3/10)} & -\sqrt{\tfrac{1}{5}} & -\sqrt{\tfrac{1}{5}} & \sqrt{(3/10)}\\ -\sqrt{(1/14)} & \sqrt{(3/7)} & -\sqrt{(3/7)} & \sqrt{(1/14)}\end{bmatrix}.$$

(IX) $n=5,\ m=2$

$$\mathbf{a}(52)=\begin{bmatrix}\sqrt{(2/7)} & \sqrt{(3/7)} & \sqrt{(2/7)}\\ -\sqrt{\tfrac{1}{2}} & 0 & \sqrt{\tfrac{1}{2}}\\ \sqrt{(3/14)} & -\sqrt{(4/7)} & \sqrt{(3/14)}\end{bmatrix}$$

(X) $n=5,\ m=3$

$$\mathbf{a}(53)=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}.$$

In this way we obtain

$$H_{ij}'=-\tfrac{3}{2}neFa_0[C_i\delta(i,\,j+1)+C_j\delta(i+1,\,j)],\qquad\text{(A6)}$$

with

$$C_j=\left[\frac{(n^2-j^2)(j^2-m^2)}{4j^2-1}\right]^{1/2},\quad m\leq j.\qquad\text{(A7)}$$

Equation (A1) can now be written

$$\sum_l A_{il}H_{lj}'=\epsilon_{ii}A_{ij},\qquad\text{(A8)}$$

which by means of Eqs. (A2) and (A6) reduces to

$$A_{ij+1}C_{j+1}+A_{ij-1}C_j=(2i+1-n+m)A_{ij}.\qquad\text{(A9)}$$

This is a recursion relationship for $\mathbf{A}$ by means of which all the elements of a row of $\mathbf{A}$ can be found once the first element of the row is given.

The unitary condition on $\mathbf{A}$ gives

$$\sum_{j=0}^{n-1} A_{ij}^2=1,\qquad\text{(A10)}$$

where we have assumed that the elements of $\mathbf{A}$ are real, and if a solution for $\mathbf{A}$ is found our assumption is justified.

Equations (A9) and (A10) are sufficient for the determination of $\mathbf{A}$ for any given n and m. In the text the inverse of $\mathbf{A}$ is needed. Let $\mathbf{a}$ be the inverse of $\mathbf{A}$,

$$\mathbf{a}=\mathbf{A}^{-1}=\tilde{A},\qquad\text{(A11)}$$

with $\tilde{A}$ the transpose of $\mathbf{A}$. Table I gives the values of $\mathbf{a}$ for $n=1$, 2, 3, 4, 5, and all possible values of m.

APPENDIX B

Since the interchange of i and j in (38) does not change the value of $|f(l,q)|^2$, we can write

$$|f(l,q)|^2=\frac{8Z^2\alpha^3}{\pi^2a_0^2n(\alpha^2+q^2)^4}\sum_{i=0}^{n-1}\sum_{j=0}^{i}\sum_{\lambda=0}^{2(i-j)}[2-\delta(i,j)]\times(-)^\lambda a_{li}a_{lj}\binom{4i-4j}{2\lambda}\frac{\alpha^{4(i-j)-2\lambda}q^{2\lambda}}{(\alpha^2+q^2)^{2(i-j)}}.\qquad\text{(B1)}$$

Similar considerations apply to $|g(l,q)|^2$ as given by Eq. (39). Making use of the expansion

$$q^{2\lambda}=(\rho^2+\beta^2)^\lambda=\sum_{\mu=0}^{\lambda}\binom{\lambda}{\mu}\beta^{2(\lambda-\mu)}\rho^{2\mu}\qquad\text{(B2)}$$

in Eqs. (38) and (39), and recalling Eq. (28), we obtain the capture cross section with the initial states nl and the final states $n'l'$, averaged over the initial states and summed over the final states. This is given by

$$\sigma(nl,n'l')=\frac{(2\pi)^5}{(2l+1)p^2}\int_0^\infty|f(l,q)|^2\times|g(l',q')|^2\rho d\rho$$
$$=\frac{2^9\pi(ZZ')^2(\alpha\alpha')^3}{(2l+1)a_0^2p^2nn'}\sum_\gamma\sum_{\gamma'}B(\gamma)B(\gamma')\times\int_0^\infty\frac{\rho^{2(\mu+\mu')+1}d\rho}{(\alpha^2+\beta^2+\rho^2)^{2(3+|i-j|+|i'-j'|)}},\qquad\text{(B3)}$$

where

$$B(\gamma)=[2-\delta(i,j)](-)^\lambda a_{li}a_{lj}\times\binom{4i-4j}{2\lambda}\binom{\lambda}{\mu}\alpha^{4i-4j-2\lambda}\beta^{2\lambda-2\mu};\qquad\text{(B4)}$$

γ stands for the set of 4 integers i, j, λ, μ which take on the following values:

$$\begin{aligned} &i=0, 1, 2, \cdots, n-1;\\ &j=0, 1, 2, \cdots, i;\\ &\lambda=0, 1, 2, \cdots, 2(i-j);\\ &\mu=0, 1, 2, \cdots, \lambda. \end{aligned} \tag{B5}$$

The integral appearing in Eq. (B3) is of the form

$$I(M,N)=\int_0^\infty \frac{\rho^{2M+1}d\rho}{(b^2+\rho^2)^N}, \tag{B6}$$

which, after integration by parts, yields

$$\begin{aligned} I(M,N)&=\binom{N-1}{M}^{-1} I(0, N-M)\\ &=\tfrac{1}{2}(M+1)^{-1}\binom{N-1}{M+1}^{-1} b^{-2(N-M-1)}. \end{aligned} \tag{B7}$$

In this way we obtain

$$\sigma(nl,n'l')=\frac{5n}{(2l+1)n'}\sigma(n,n')\sum_\gamma\sum_{\gamma'}\frac{B(\gamma)B(\gamma')}{(1+\mu+\mu')\binom{5+2(i-j+i'-j')}{1+\mu+\mu'}(\alpha^2+\beta^2)^{2(i-j+i'-j')-(\mu+\mu')}}, \tag{B8}$$

where $\sigma(n,n')$ is given by (31). Introducing

$$A=\alpha^2/(\alpha^2+\beta^2), \tag{B9}$$

it follows that

$$\begin{aligned} (\alpha^2+\beta^2)^{-2(i-j)+\mu}B(\gamma)&=[2-\delta(i,j)](-)^\lambda a_{li}a_{lj}\binom{4i-4j}{2\lambda}\binom{\lambda}{\mu}A^{2(i-j)-\lambda}(1-A)^{\lambda-\mu}\\ &=\sum_{\mu_1}^{\lambda-\mu}[2-\delta(i,j)](-)^{\lambda+\mu_1}a_{li}a_{lj}\binom{4i-4j}{2\lambda}\binom{\lambda}{\mu}\binom{\lambda-\mu}{\mu_1}A^{2(i-j)-\lambda+\mu_1}\\ &=\sum_\nu D(\nu,\gamma)A^\nu, \end{aligned} \tag{B10}$$

where

$$\nu=2(i-j)-\lambda+\mu_1 \tag{B11}$$

and

$$D(\nu,\gamma)=[2-\delta(i,j)](-)^\nu a_{li}a_{lj}\binom{4i-4j}{2\lambda}\binom{\lambda}{\mu}\binom{\lambda-\mu}{\nu+\lambda-2i+2j}. \tag{B12}$$

Thus we can write

$$\sigma(nl,n'l')=\frac{5n}{(2l+1)n'}\sigma(n,n')\sum_\gamma\sum_{\gamma'}(1+\mu+\mu')^{-1}\binom{5+2(i-j+i'-j')}{1+\mu+\mu'}^{-1}\sum_\nu\sum_{\nu'}D(\nu,\gamma)D(\nu',\gamma')A^\nu A'^{\nu'}. \tag{B13}$$

When summation between γ and ν are interchanged, we obtain

$$\sigma(nl,n'l')=\frac{5n}{(2l+1)n'}\sigma(n,n')\sum_{\nu=0}^{2(n-1)}\sum_{\nu'=0}^{2(n'-1)}C(nl\nu,n'l'\nu')A^\nu A'^{\nu'}, \tag{B14}$$

$$C(nl\nu,n'l'\nu')=\sum_{\gamma,\gamma'}(1+\mu+\mu')^{-1}\binom{5+2(i-j+i'-j')}{1+\mu+\mu'}^{-1}D(\nu,\gamma)D(\nu',\gamma'), \tag{B15}$$

where γ stands for i, j, λ, μ, and the range of i, j, λ, μ are given by Eq. (44) of the text.