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¹³J. A. Bearden, Rev. Mod. Phys. **39**, 78 (1967).¹⁵M. Krause, private communications and to be published.¹⁴J. A. Bearden and A. F. Burr, Rev. Mod. Phys. **39**,EXCITATION OF $n=2$ STATES IN HYDROGEN BY ELECTRON IMPACT

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A possible source of incompleteness is pointed out in the most recent close-coupling calculations for the excitation cross sections of the $n=2$ levels in hydrogen, some of the results of which disagree with experiment. We present a method which removes this difficulty by the implicit inclusion of all important effective polarization potential terms of order α/r^4 .

A serious discrepancy presently exists between rather refined theoretical and experimental determinations of the total $1s-2s$ excitation cross section.¹ The purpose of this note is to suggest a possible source of incompleteness in the most recent calculations² which lies in their failure to include the full effective polarizabilities that arise. Methods for incorporating the full ground-state polarizability into low-energy calculations for the elastic-scattering cross section have been given,³ and in the following we present the extension to the excitation of the $n=2$ states.

Starting with the complete set of radial coupled equations, we specialize at once to the case where the only open channels are those containing the $1s$, $2s$, and $2p$ atomic states. The asymptotic forms of the closed-channel radial functions may be expressed in terms of the open-channel functions, since they provide an oscillatory asymptotic coupling.⁴ When they are substituted into the right-hand side of the open-channel equations, one obtains the following set of asymptotic relations between the four open-channel radial functions:

$$\left(\mathfrak{L}_L + \frac{\alpha(1s-p-1s)}{r^4} + k_1^2\right)F_0 = -\frac{\alpha(1s-p-2s)}{r^4}F_1 + \frac{2}{r^2} \frac{\langle u_{10} r u_{21} \rangle}{[3(2L+1)]^{1/2}} [L^{1/2}F_2 - (L+1)^{1/2}F_3], \quad (1)$$

$$\left(\mathfrak{L}_L + \frac{\alpha(2s-p-2s)}{r^4} + k_2^2\right)F_1 = -\frac{\alpha(2s-p-1s)}{r^4}F_0 + \frac{2}{r^2} \frac{\langle u_{20} r u_{21} \rangle}{[3(2L+1)]^{1/2}} [L^{1/2}F_2 - (L+1)^{1/2}F_3], \quad (2)$$

$$\begin{aligned} \left(\mathfrak{L}_{L-1} - \frac{2(L-1)}{5(2L+1)} \frac{\langle u_{21} r^2 u_{21} \rangle}{r^3} + \frac{1}{(2L+1)r^4}\right) \left\{ L\alpha(2p-s-2p) + \frac{7L+3}{5} \alpha(2p-d-2p) \right\} + k_2^2 F_2 \\ = \frac{2}{r^2} \left[\frac{L}{3(2L+1)} \right]^{1/2} [\langle u_{21} r u_{10} \rangle F_0 + \langle u_{21} r u_{20} \rangle F_1] - \frac{6[L(L+1)]^{1/2}}{5(2L+1)} \frac{\langle u_{21} r^2 u_{21} \rangle}{r^3} F_3, \end{aligned} \quad (3)$$

$$\begin{aligned} \left(\mathfrak{L}_{L+1} - \frac{2(L+2)}{5(2L+1)} \frac{\langle u_{21} r^2 u_{21} \rangle}{r^3} + \frac{1}{(2L+1)r^4}\right) \left\{ (L+1)\alpha(2p-s-2p) + \frac{7L+4}{5} \alpha(2p-d-2p) \right\} + k_2^2 F_3 \\ = -\frac{2}{r^2} \left[\frac{L+1}{3(2L+1)} \right]^{1/2} [\langle u_{21} r u_{10} \rangle F_0 + \langle u_{21} r u_{20} \rangle F_1] - \frac{6[L(L+1)]^{1/2}}{5(2L+1)} \frac{\langle u_{21} r^2 u_{21} \rangle}{r^3} F_2, \end{aligned} \quad (4)$$

where

$$\mathfrak{L}_L = \frac{d^2}{dr^2} - \frac{L(L+1)}{r^2}.$$

The notation is as follows: The channel indices 0, 1, 2, and 3 refer to the combinations of quantum numbers $nl'l'L=10LL$, $20LL$, $21L-1L$, and $21L+1L$, respectively, where nl are the atomic principal and orbital quantum numbers (radial function u_{nl}), l' is the free-electron orbital angular momentum, and L is the total coupled orbital angular momentum. The above asymptotic equations apply to both singlet and triplet scattering since the exchange terms in the close-coupling equations fall off more rapidly than the ones included. Only the leading asymptotic term in each of the coupling

coefficients between F_i and F_j has been included, and all diagonal potential terms up to α/r^4 have been included on the left-hand sides of (1)-(4). The effective polarizabilities are

$$\begin{aligned}\alpha(1s \rightarrow p \rightarrow 1s) &= \frac{2}{3} \sum_{n=3}^{\infty} \frac{\langle u_{10} r u_{n1} \rangle^2}{E_n - E_1}; & \alpha(1s \rightarrow p \rightarrow 2s) &= \frac{2}{3} \sum_{n=3}^{\infty} \frac{\langle u_{10} r u_{n1} \rangle \langle u_{n1} r u_{20} \rangle}{E_n - E_2}; \\ \alpha(2s \rightarrow p \rightarrow 2s) &= \frac{2}{3} \sum_{n=3}^{\infty} \frac{\langle u_{20} r u_{n1} \rangle^2}{E_n - E_2}; & \alpha(2s \rightarrow p \rightarrow 1s) &= \frac{2}{3} \sum_{n=3}^{\infty} \frac{\langle u_{20} r u_{n1} \rangle \langle u_{n1} r u_{10} \rangle}{E_n - E_1}; \\ \alpha(2p \rightarrow s \rightarrow 2p) &= \frac{2}{3} \sum_{n=3}^{\infty} \frac{\langle u_{21} r u_{n0} \rangle^2}{E_n - E_2}; & \alpha(2p \rightarrow d \rightarrow 2p) &= \frac{2}{3} \sum_{n=3}^{\infty} \frac{\langle u_{21} r u_{n2} \rangle^2}{E_n - E_2};\end{aligned}$$

where the sums also contain an integral over continuum states and atomic units are used throughout (E in double Rydbergs).

In the vicinity of the $n=2$ threshold (both above and below) where $|k_2|^2 \ll 1$, it is important that the full effective polarizability be present in the left-hand side of (2). For $L=1$ it is also clearly the dominant diagonal potential term in (3). It can also be easily seen that (for other L 's) although the r^{-3} term is the asymptotically dominant diagonal potential term in (3) and (4), its magnitude exceeds that of the r^{-4} term only at very large distances. The role of the α 's in the asymptotic cross-coupling coefficients is apparently not as important as the direct coupling terms ($\sim r^{-2}$ or r^{-3}), but they could possibly lead to appreciable interference effects. It is known that the r^{-2} coupling between the degenerate channels 1, 2, and 3 results in finite excitation cross sections at threshold. However, shorter range terms will affect the actual magnitude the cross section has at threshold, and it is this uncertainty in magnitude which characterizes the present discrepancies between theory and experiment. The calculations of Burke, Ormonde, and Whitaker include only the $n=3$ terms of each of the above infinite sums, and the calculation of Taylor and Burke has each α vanishing (although this is compensated to an unknown extent by their short-range correlation terms).

The most important α 's in the threshold region ($2s \rightarrow p \rightarrow 2s$, $2p \rightarrow s \rightarrow 2p$, and $2p \rightarrow d \rightarrow 2p$) may be readily evaluated by the implicit summation technique. Here we seek bound solutions to the inhomogeneous equations

$$\left(-\mathcal{E}_1 - \frac{2}{r} - 2E_2 \right) u_p = \frac{2(E_p - E_2)}{\langle u_p r u_{20} \rangle} \{ r u_{20} - \langle u_{21} r u_{20} \rangle u_{21} \}, \quad (5)$$

$$\left(-\mathcal{E}_0 - \frac{2}{r} - 2E_2 \right) u_s = \frac{2(E_s - E_2)}{\langle u_s r u_{21} \rangle} \{ r u_{21} - \langle u_{10} r u_{21} \rangle u_{10} - \langle u_{20} r u_{21} \rangle u_{20} \}, \quad (6)$$

$$\left(-\mathcal{E}_2 - \frac{2}{r} - 2E_2 \right) u_d = \frac{2(E_d - E_2)}{\langle u_d r u_{21} \rangle} r u_{21}. \quad (7)$$

In terms of these u 's it may be easily verified that the α 's become

$$\begin{aligned}\alpha(1s \rightarrow p \rightarrow 2s) &= \frac{2}{3} \frac{\langle u_{10} r u_p \rangle \langle u_p r u_{20} \rangle}{E_p - E_2}; & \alpha(2s \rightarrow p \rightarrow 2s) &= \frac{2}{3} \frac{\langle u_{20} r u_p \rangle^2}{E_p - E_2}; \\ \alpha(2p \rightarrow s \rightarrow 2p) &= \frac{2}{3} \frac{\langle u_{21} r u_s \rangle^2}{E_s - E_2}; & \alpha(2p \rightarrow d \rightarrow 2p) &= \frac{2}{3} \frac{\langle u_{21} r u_d \rangle^2}{E_d - E_2}.\end{aligned} \quad (8)$$

The remaining α 's can be evaluated by the same technique, but we will omit these details. The orthonormalized solutions and the effective energy levels in (5), (6), and (7) are

$$u_p = \frac{1}{2}(5/26)^{\frac{1}{2}} e^{-\frac{1}{2}r} r^2 (1-r^2/30); \quad E_p = -5/104 = -0.04808; \quad (9)$$

Table I. Effective polarizabilities in the $n=2$ excitation.

Effective polarizabilities	Exact value (in units of a_0^3)	Percent contained in Burke-Ormonde-Whitaker calculation	Percent contained in proposed calculation
$\alpha(1s \rightarrow p \rightarrow 1s)$	1.54	26.0	56.9
$\alpha(1s \rightarrow p \rightarrow 2s)$	24.8	61.2	100.0
$\alpha(2s \rightarrow p \rightarrow 2s)$	120.0	75.0	100.0
$\alpha(2s \rightarrow p \rightarrow 1s)$	4.97	47.8	84.9
$\alpha(2p \rightarrow s \rightarrow 2p)$	11.0	77.1	100.0
$\alpha(2p \rightarrow d \rightarrow 2p)$	260.0	83.2	100.0

$$u_s = \left(\frac{3}{2}\right)^{\frac{1}{2}} [57 - (2/9)(\frac{4}{3})^9]^{-\frac{1}{2}} r \{ e^{-\frac{1}{2}r} (1 - \frac{1}{2}r - \frac{1}{2}r^2 + \frac{1}{12}r^3) + \frac{1}{2}(\frac{4}{3})^6 e^{-r} \},$$

$$E_s = [3 + \frac{1}{9}(\frac{4}{3})^8] [57 - (2/9)(\frac{4}{3})^9]^{-1} - (\frac{1}{8}) = -0.04895; \quad (10)$$

$$u_d = \frac{1}{8}(55) e^{-\frac{1}{2}r} r^3 (1 + \frac{1}{8}r), \quad E_d = -9/176 = -0.05114; \quad (11)$$

where u_p is orthogonal to u_{21} and u_s is orthogonal to u_{10} and u_{20} . The effective energies all lie slightly above the hydrogenic level $E_3 = -0.05556$.

It can be seen that a close-coupling calculation with exchange in which the six basis wave functions for the target system,

$$\frac{1}{r}[u_{10}(r), u_{20}(r), u_s(r)]Y_{00}(\hat{r}), \quad \frac{1}{r}[u_{21}(r), u_p(r)]Y_{1m}(\hat{r}), \quad \frac{1}{r}u_d(r)Y_{2m}(\hat{r}), \quad (12)$$

are included will have built into it the exact values of the effective polarizabilities given in (8). In Table I we compare the exact values of the effective polarizabilities with those that arise in the Burke-Ormonde-Whitaker and in the presently proposed six-state close-coupling calculations. Note that the 17% of $\alpha(2p-d-2p)$ omitted in the previous calculation has a magnitude of about ten times the ground-state polarizability of hydrogen ($4.5a_0^3$).

The above procedure can be applied to any higher threshold. The applicability of minimum principles⁵ is preserved, allowing for the systematic improvement of results, say, by the addition of short-range correlation terms.

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