

for $k = 3, 2, 1, \dots, -2M+2$.

C. THE DETERMINATION OF THE SOLUTION OF THE SYSTEM OF EQUATIONS

The system of nonlinear algebraic equations described in the preceding section is considerably more difficult to solve than that encountered in Chapter II. The questions concerning the existence and uniqueness of the solution are not easily answered and the application of algebra is not capable of significantly reducing the system (for the case of M an arbitrary integer) into a tractable form. An operational procedure, proven successful for solving the system for various test cases, shall be described, which is based on the fixed point iteration technique. Fixed point methods typically require a reasonably accurate initial guess to the solution, in order to achieve convergence. The approach taken here to obtain the initial guess relies on the solution to the equations described in Chapter II and also requires the solution to the system described in the preceding section for the special case of $M = 1$.

For the case of $M = 1$, the system for which a solution is desired is given by

$$\begin{aligned}\tilde{S}(3,b) &= f_1' \omega_1'^3 + 2\gamma (b-\epsilon_0)^{-\frac{1}{2}} \\ \tilde{S}(2,b) &= f_1' \omega_1'^2 + \frac{2}{3}\gamma (b-\epsilon_0)^{-\frac{3}{2}} \\ \tilde{S}(1,b) &= f_1' \omega_1' + \frac{2}{5}\gamma (b-\epsilon_0)^{-\frac{5}{2}} \\ \tilde{S}(0,b) &= f_1' + \frac{2}{7}\gamma (b-\epsilon_0)^{-\frac{7}{2}}.\end{aligned}\tag{11}$$

In order to simplify the notation the following identifications shall be made:

$$\begin{aligned}f_1 &= f_1' \\ \omega_1 &= \omega_1' \\ \xi &= (b-\epsilon_0)\end{aligned}$$

$$\begin{aligned}
 A &= \tilde{S}(3, b) \\
 B &= \tilde{S}(2, b) \\
 C &= \tilde{S}(1, b) \\
 D &= \tilde{S}(0, b).
 \end{aligned}$$

Rewriting the system of equations (11) then gives

$$\begin{aligned}
 A &= f_1 \omega_1^3 + 2\gamma \xi^{-\frac{1}{2}} \\
 B &= f_1 \omega_1^2 + \frac{2}{3}\gamma \xi^{-\frac{3}{2}} \\
 C &= f_1 \omega_1 + \frac{2}{5}\gamma \xi^{-\frac{5}{2}} \\
 D &= f_1 + \frac{2}{7}\gamma \xi^{-\frac{7}{2}}.
 \end{aligned} \tag{12}$$

Straightforward algebra leads to a solution of ξ in terms of A, B, C and D as the roots of a sixth degree polynomial with coefficients expressed in terms of A, B, C and D. This sixth degree polynomial can be factored into the product of a fifth degree polynomial and a first degree polynomial, resulting in the equations

$$\begin{aligned}
 &15 [BD^2 - C^2D] \xi^5 + \left[\frac{125}{7} C^3 - \frac{90}{7} BCD - 5AD^2 \right] \xi^4 \\
 &+ \left[\frac{18}{7} B^2D - \frac{90}{7} BC^2 + \frac{72}{7} ACD \right] \xi^3 + \left[\frac{54}{7} BC^2 - \frac{24}{7} ABD - \frac{30}{7} AC^2 \right] \xi^2 \\
 &+ \left[\frac{90}{49} ABC - \frac{513}{245} B^3 + \frac{9}{35} A^2D \right] \xi + \left[\frac{9}{45} AB^2 - \frac{9}{45} A^2C \right] \\
 &= 0
 \end{aligned} \tag{13}$$

and

$$C\xi - \frac{3}{5}B = 0. \tag{14}$$

Once the desired solution to ξ is obtained, the solution to the remaining three unknowns, f_1 , ω_1 and γ , may be obtained using the relations

$$\gamma = \frac{(AC - B^2) \xi^{7/2} + \frac{35}{3} (C^2 - BD) \xi^{11/2}}{\frac{2}{5} A \xi - \frac{14}{3} B \xi^2 + \frac{34}{3} C \xi^3 - \frac{70}{9} D \xi^4} \quad (15)$$

$$f_1 = \frac{(C - \frac{28}{5} \xi^{-5/2})^2}{B - \frac{28}{3} \xi^{-3/2}} \quad (16)$$

and

$$\omega_1 = \frac{B - \frac{28}{3} \xi^{-3/2}}{C - \frac{28}{5} \xi^{-5/2}} \quad (17)$$

Clearly the only nontrivial part of this problem is determining the solution to ξ . Note that A, B, C and D are implicitly functions of ξ . The implicit dependence upon ξ in equations (13) and (14) may be eliminated by expanding A, B, C and D in terms of $S(0)$, $S(1)$, $S(2)$, $S_f(3)$, α , β and ξ . This expansion results in higher degree polynomials (in the variable $\xi^{1/2}$) which are straightforward to compute if so desired. The problem at this point is that any root to either equation (13) or (14) satisfies the original system and it is not obvious which solution is wanted. In order to proceed further, some criterion must be set to choose which root is needed. Physical considerations clearly require that ξ be real so all conjugate complex roots of the polynomials may be ruled out. Since only the real roots are of interest, the roots of equations (13) and (14) may be located using standard numerical techniques such as bisection or the Newton-Raphson method. After the set of real roots has been obtained, the most reasonable choice for the desired solution appears to be the largest root in the set. This seems to be the best choice because ξ determines the cut off energy for an approximation to the oscillator strength density which will probably be accurate only at high energies. Choosing the largest root then helps confine the approximate density to a high enough energy region where it is expected to be valid. This argument is rather rough, however choosing ξ to be the largest real root has achieved good

results for the calculations performed on atomic hydrogen.

The recommended numerical approach to obtaining the correct solution for ξ uses equations (13) and (14) directly, without eliminating the implicit dependence upon ξ . This is accomplished by assuming some value ξ' for the ξ which is contained implicitly in A, B, C and D. Then $A(\xi')$, $B(\xi')$, $C(\xi')$ and $D(\xi')$ are constants and equations (13) and (14) may be solved by bisection or the Newton-Raphson method. The largest real root of the polynomials involving $A(\xi')$, $B(\xi')$, $C(\xi')$ and $D(\xi')$ can then be easily obtained. This procedure is repeated over a range of values for ξ' , and the desired solution is the value of ξ' for which the largest root of the associated polynomials coincides with ξ' . This method is essentially a "graphical" approach which searches for the intersection of two curves and is easily computed using the bisection method. A completely pedestrian viewpoint will be taken concerning the existence of solutions, where the existence for a specific problem is proven by explicitly obtaining a numerical solution.

Having described the procedure for solving the $M = 1$ case of the system of equations developed in the last section, it is now possible to obtain a fairly accurate estimate of the solution for the general case of M equal to some arbitrary integer. The first step is to set up the system of equations given by

$$\tilde{S}(k, b') = \sum_{n=1}^{M+1} f'_n \omega_n'^k \quad (18)$$

for $k = 3, 2, 1, \dots, -2M+2$, where some reasonable value b' has been assumed for b . The system given by equation (18) can be solved by the techniques of Chapter II, leading to a collection of effective states consisting of f'_m and ω'_m for $m = 1, 2, 3, \dots, M+1$. For the following it is assumed that the states have been labeled such that the effective energy difference ω'_m monotonically increases as a function of the index m . Then the two highest energy effective states (f'_M, ω'_M and f'_{M+1}, ω'_{M+1}) are to be replaced by an effective state and an effective density using the procedure described previously to solve the system

given by equation (12). This replacement is accomplished by using the two highest effective states to determine values for the moments A, B, C and D appearing in the system described by equation (12), according to

$$\begin{aligned}
 A &= f'_M \omega'_M{}^3 + f'_{M+1} \omega'_{M+1}{}^3 \\
 B &= f'_M \omega'_M{}^2 + f'_{M+1} \omega'_{M+1}{}^2 \\
 C &= f'_M \omega'_M + f'_{M+1} \omega'_{M+1} \\
 D &= f'_M + f'_{M+1} .
 \end{aligned}
 \tag{19}$$

These constant values for A, B, C and D are then substituted into equations (13) and (14) and the largest real root is obtained using the usual methods. The largest root obtained for ξ is then compared with the value of $b' - \epsilon_0$ for the choice of b' assumed in equation (18). The entire above procedure is repeated over a range of values for b' , and the desired solution is the value of b' for which the largest root of the associated polynomial coincides with $b' - \epsilon_0$. This is again essentially equivalent to determining the intersection of two curves and can be computed using the bisection method.

The claim that the above procedure provides a good estimate for the actual desired solution is easily justified. The effective distribution which has been constructed is of the form specified in the last section, i.e. with M discrete states plus the continuous density. This distribution satisfies equation (10) exactly for $k = 0, 1, 2$ and 3 . The remaining equations for $k = -1, -2, \dots, -2M+2$ are more sensitive to the behavior of the low lying discrete states, so the conversion of the two highest discrete states into a discrete state plus a continuous density should not cause these equations to be violated too badly. Hence the above procedure should provide an adequate initial guess for the fixed point iteration technique described below. In practice this method has proved successful

for calculations performed on various test cases.

After dealing with the subtle problem of obtaining the initial guess, the task of implementing a fixed point iteration procedure on the system given in equation (10) is quite straightforward. The specific technique to be used is the well known multi-dimensional generalization of the Newton-Raphson method⁴. This method finds the values of x_1, x_2, \dots, x_N which satisfy the system of equations

$$\phi_i(x_1, x_2, \dots, x_N) = 0 \quad (20)$$

for $i = 1, 2, \dots, N$. The solution is obtained by iterating the transformation

$$\vec{x}' = \vec{x} - J^{-1}(\vec{x}) \vec{\phi}(\vec{x}) \quad (21)$$

until convergence is achieved, where $J(\vec{x})$ is the Jacobian matrix,

$$J(\vec{x}) = \begin{pmatrix} \frac{\partial \phi_1}{\partial x_1} & \frac{\partial \phi_1}{\partial x_2} & \dots & \frac{\partial \phi_1}{\partial x_N} \\ \frac{\partial \phi_2}{\partial x_1} & \frac{\partial \phi_2}{\partial x_2} & \dots & \vdots \\ \vdots & \vdots & \dots & \vdots \\ \frac{\partial \phi_N}{\partial x_1} & \dots & \dots & \frac{\partial \phi_N}{\partial x_N} \end{pmatrix} \quad (22)$$

and \vec{x} , \vec{x}' and $\vec{\phi}$ are column vectors. This procedure may be applied to the problem of interest by setting

$$\phi_i = \tilde{S}(4-i, b) - \sum_{n=1}^M f'_n \omega_n^{4-i} - \frac{\gamma}{i-\frac{1}{2}} (b - \epsilon_0)^{\frac{1}{2}-i} \quad (23)$$

for $i = 1, 2, 3, \dots, 2M+2$, and

$$\begin{aligned} x_1 &= \delta \\ x_2 &= b \\ x_j &= f'_{\left(\frac{j-1}{2}\right)} && \text{if } j \text{ odd, } (2M+2) \geq j > 2 \\ x_j &= \omega'_{\left(\frac{j}{2}-1\right)} && \text{if } j \text{ even, } (2M+2) \geq j > 2. \end{aligned} \quad (24)$$

The stability and the efficiency of the procedure can, however, be improved by reducing the dimensionality by the application of straightforward algebra. Using the first four equations, the variables δ , f'_M , and ω'_M may be eliminated through the relations

$$\delta = \frac{(A'C' - B'^2)\xi^{7/2} + \frac{35}{3}(C'^2 - B'D')\xi^{11/2}}{\frac{2}{5}A'\xi - \frac{14}{3}B'\xi^2 + \frac{34}{3}C'\xi^3 - \frac{70}{9}D'\xi^4} \quad (25)$$

$$f'_M = \frac{(C' - \frac{2\delta}{5}\xi^{-5/2})^2}{B' - \frac{2\delta}{3}\xi^{-3/2}} \quad (26)$$

and

$$\omega'_M = \frac{B' - \frac{2\delta}{3}\xi^{-3/2}}{C' - \frac{2\delta}{5}\xi^{-5/2}} \quad (27)$$

where

$$\begin{aligned} A' &= \tilde{S}(3, b) - \sum_{n=1}^{M-1} f'_n \omega_n'^3 \\ B' &= \tilde{S}(2, b) - \sum_{n=1}^{M-1} f'_n \omega_n'^2 \\ C' &= \tilde{S}(1, b) - \sum_{n=1}^{M-1} f'_n \omega_n' \\ D' &= \tilde{S}(0, b) - \sum_{n=1}^{M-1} f'_n \end{aligned} \quad (28)$$

Then the Newton-Raphson procedure may be implemented by setting

$$\phi_i = \tilde{S}(1-i, b) - \sum_{n=1}^M f'_n \omega_n'^{1-i} - \frac{\delta}{i + \frac{5}{2}} (b - \epsilon_0)^{-\frac{5}{2}-i} \quad (29)$$

for $i = 1, 2, 3, \dots, 2M-1$, and

$$\begin{aligned} x_1 &= b \\ x_j &= f'_{(\frac{j}{2}+1)} && \text{if } j \text{ even, } (2M-1) \geq j > 1 \\ x_j &= \omega'_{(\frac{j-1}{2})} && \text{if } j \text{ odd, } (2M-1) \geq j > 1. \end{aligned} \quad (30)$$

In equation (29) the variables γ , f'_M and ω'_M are of course defined in terms of the independent variables $x_1, x_2, \dots, x_{2M-1}$ through equations (25), (26) and (27).

D. RESULTS FROM THE EFFECTIVE DISTRIBUTIONS FOR ATOMIC HYDROGEN

Effective oscillator strength distributions have been constructed for atomic hydrogen using the procedure described in the previous section for the $M = 1, 2, 3$ and 4 cases. In addition, effective oscillator strength distributions have been constructed which include contributions from the first four physical excited states explicitly, with the remaining portion of the distribution constructed according to the usual procedure. This remaining portion of the distribution has also been calculated for the $M = 1, 2, 3$ and 4 cases and of course the moments which are used are those of the actual distribution minus the contributions of the first four physical excited states.

The moments and asymptotic coefficients are easily obtained for atomic hydrogen but will be listed here for completeness. The moments used, in atomic units, are

$$S_f(3) = 8 \ln 2 - \frac{8}{3}$$

$$S(2) = \frac{4}{3}$$

$$S(1) = \frac{2}{3}$$

$$S(0) = 1$$

$$S(-1) = 2$$

$$S(-2) = \frac{9}{2}$$

$$S(-3) = \frac{43}{4}$$

$$S(-4) = \frac{319}{12}$$

$$S(-5) = \frac{9673}{144}$$

$$S(-6) = \frac{297541}{1728} .$$

The coefficients of the first two asymptotic terms of the oscillator strength density are

$$\alpha = \frac{8\sqrt{2}}{3\pi}$$

and

$$\beta = -\frac{8}{3} .$$

The oscillator strengths and transition energies between the 1s state and the 2p, 3p, 4p, and 5p states were also used. These are given by

$$f_1 = 2^{13}/3^9$$

$$f_2 = 3^4/2^{10}$$

$$f_3 = 2^{18} \times 3^3 / 5^{12}$$

$$f_4 = 2^6 \times 5^5 / 3^{15}$$

$$\omega_1 = 3/8$$

$$\omega_2 = 4/9$$

$$\omega_3 = 15/32$$

$$\omega_4 = 12/25 .$$

The effective distributions have been used to obtain estimates of the logarithmic mean excitation energies by evaluating the $L(k)$ associated with the effective distributions, i.e.

$$\begin{aligned}
 & L(k) \\
 = & \sum_{n=1}^M f'_n \omega_n^k \ln \omega_n \\
 & + \frac{\alpha}{\frac{5}{2} - k} (b - \epsilon_0)^{k - 5/2} \ln(b - \epsilon_0) + \frac{\alpha}{(\frac{5}{2} - k)^2} (b - \epsilon_0)^{k - 5/2} \\
 & + \frac{\beta}{3 - k} (b - \epsilon_0)^{k - 3} \ln(b - \epsilon_0) + \frac{\beta}{(3 - k)^2} (b - \epsilon_0)^{k - 3} \\
 & + \frac{\gamma}{\frac{7}{2} - k} (b - \epsilon_0)^{k - 7/2} \ln(b - \epsilon_0) + \frac{\gamma}{(\frac{7}{2} - k)^2} (b - \epsilon_0)^{k - 7/2} \quad (31)
 \end{aligned}$$

Values for $L(2)$, $L(1)$, $L(0)$ and $L(-1)$ are listed below and compared with exact results. Table 13 lists the results for the effective distribution without actual oscillator strengths explicitly included and Table 14 lists the results with the first four oscillator strengths included. The logarithmic sum $L(0)$ is needed to compute the stopping power of fast charged particles scattering off atoms and molecules. A more common form for expressing the information contained in $L(0)$ is the quantity I , where

$$I = \exp(L(0)/S(0)) \quad (32)$$

with $L(0)$ calculated in units of electron volts. Tables 15 and 16 list results for I and δ , the coefficient of the third asymptotic term of the oscillator strength density in the expansion

$$\frac{df}{d\epsilon} = \alpha (\epsilon - \epsilon_0)^{-3.5} + \beta (\epsilon - \epsilon_0)^{-4} + \gamma (\epsilon - \epsilon_0)^{-4.5} + \dots \quad (33)$$

where ϵ_0 is the ground state energy. The exact value of δ listed

has been obtained by performing an expansion of the result obtained in Section E of Chapter III. The results obtained for the $L(k)$ are significantly better than those obtained using the technique described in Chapter II which did not utilize the information concerning $S_f(3)$ and the coefficients of the first two asymptotic terms of the oscillator strength distribution. The results obtained for I and $L(2)$ are also significantly better than those obtained using Garcia's interpolation scheme (note Garcia considered only I and $L(2)$).

The effective distributions obtained may also be of some interest. Table 17 includes the effective discrete oscillator strengths and transition energies and δ and $(b - \epsilon_0)$ to 5 digits for the distributions without physical states. Table 18 includes the same information for the distributions which included four states explicitly.

E. THE HIGH ENERGY PHOTOIONIZATION CROSS SECTION

The expansion given in equation (1) may be useful for estimating the photoionization cross section at high energies. The total photoionization cross section σ , in the dipole approximation, is related to the oscillator strength density $(df/d\epsilon)$ (when ϵ is given in atomic units) by⁵

$$\sigma = 2\pi^2 \alpha a_0^2 \frac{df}{d\epsilon} \quad (34)$$

where $\alpha = e^2/(\hbar c) \approx 137$ is the fine structure constant and $a_0 = \hbar^2/(me^2)$ is the Bohr radius.

Using the best value of δ obtained from Table 16 leads to the approximate expansion

$$\frac{df'}{d\epsilon} = \frac{8\sqrt{2}}{3\pi} (\epsilon - \epsilon_0)^{-3.5} - \frac{8}{3} (\epsilon - \epsilon_0)^{-4} + 3.51 (\epsilon - \epsilon_0)^{-4.5} \quad (35)$$

Comparing this with the exact expression for $(df/d\epsilon)$, one finds that equation (35) leads to a result approximately 10% too high at $(\epsilon - \epsilon_0) = 10$ a.u. and to a result approximately 1% too high at 20 a.u. The approximate σ corresponding to equation (35) is given by

$$\sigma = 2\pi^2 \alpha a_0^2 \left[\frac{8\sqrt{2}}{3\pi} (\epsilon - \epsilon_0)^{-3.5} - \frac{8}{3} (\epsilon - \epsilon_0)^{-4} + 3.51 (\epsilon - \epsilon_0)^{-4.5} \right] \quad (36)$$

and the associated dipole approximation to the differential photoion-

ization cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{3\pi}{4} \alpha a_0^2 \sin^2\theta \times \left[\frac{8\sqrt{2}}{3\pi} (\epsilon - \epsilon_0)^{-3.5} - \frac{8}{3} (\epsilon - \epsilon_0)^{-4} + 3.51 (\epsilon - \epsilon_0)^{-4.5} \right] \quad (37)$$

where the differential cross section has been averaged over both helicity states of the incoming photons and θ is measured from the direction of propagation of the light⁶.

The dipole approximation is certain to hold⁵ only for energies such that $(\epsilon - \epsilon_0) \ll (\epsilon_0/\alpha) \approx 68.5$ a.u. Beyond 20 a.u. it might be argued that the dipole approximation is being violated. However for the case of atomic hydrogen it can be shown⁶ that asymptotically, the differential cross section (including all multipoles) is given by

$$\frac{d\sigma}{d\Omega} = 2\sqrt{2} \alpha a_0^2 (\epsilon - \epsilon_0)^{-3.5} \sin^2\theta [1 + 4 \frac{v}{c} \cos\theta] \quad (38)$$

$$= 2\sqrt{2} \alpha a_0^2 (\epsilon - \epsilon_0)^{-3.5} \sin^2\theta [1 + 4\alpha \left(\frac{\epsilon - \epsilon_0}{\epsilon_0}\right)^{\frac{1}{2}} \cos\theta] \quad (39)$$

where v is the velocity of the ejected electron. This form for writing the asymptotic expansion is reasonable if $(v/c) \ll 1$, which is simply the assumption that only the nonrelativistic case is being considered (already required by the fact that the Schrodinger equation rather than the Dirac equation is being used). The expansion in equation (38) contains only two leading terms of an expansion which should be in powers of both $(\epsilon - \epsilon_0)^{-1/2}$ and (v/c) , i.e. terms of the type appearing in equation (37) should also be in the expansion. Equation (38), however, indicates the importance of the higher order multipoles to the actual expansion. For (v/c) sufficiently small, equation (37) should be a better expansion than equation (39). Note that the second term in equation (39) is small when $(\epsilon - \epsilon_0) \ll \epsilon_0/(16\alpha^2) \approx 586.5$ a.u. Therefore although the dipole approximation requirement that $(\epsilon - \epsilon_0) \ll 68.5$ a.u. is sufficient

for equation (37) to be useful, it is more stringent than necessary. Also note that when equation (39) is integrated over all solid angle to obtain the total cross section the second term in the expansion vanishes by virtue of the angular dependence. The next term in (v/c) will be of order $(v/c)^2$ and presumably will be less important than the first order term which appeared in the differential cross section. Therefore equation (36) should serve as a better approximation to the total cross section than equation (37) serves for the differential cross section. Finally note that the $(v/c)^2$ term can be shown⁵ to be of the same order as relativistic effects, so to proceed beyond this point the Dirac equation must be used. In conclusion, equations (36) and (37) should serve fairly well in the high energy region and it appears that this behavior should also hold true for other atoms.

Table 13

Without Physical States

M	L(-1)	L(0)	L(1)	L(2)
1	.15383	.15191	.7128	16.109
2	-.07493	.09907	.7545	15.978
3	-.07334	.09724	.7595	15.942
4	-.07326	.09704	.7606	15.929
Exact ^a	-.07325	.09698	.7612	15.915

Table 14

With 4 Physical States

M	L(-1)	L(0)	L(1)	L(2)
1	-.02252	.11701	.7372	16.042
2	-.07374	.09779	.7578	15.957
3	-.07328	.09709	.7603	15.934
4	-.07326	.09701	.7609	15.925
Exact ^a	-.07325	.09698	.7612	15.915

a. Reference (7).

Table 15

Without Physical States

M	I (in eV)	δ
1	15.838	3.07
2	15.023	3.25
3	14.995	3.37
4	14.992	3.46
Exact	14.992 ^a	3.73

Table 16

With 4 Physical States

M	I (in eV)	δ
1	15.295	3.15
2	15.004	3.32
3	14.993	3.43
4	14.992	3.51
Exact	14.992 ^a	3.73

a. Reference (7).

Table 17

Without Physical States

M			
1	$f'_1 = .95657$ $\gamma = 3.0717$	$\omega'_1 = .53956$ $b - \epsilon_0 = 2.1186$	
2	$f'_1 = .71186$ $f'_2 = .27125$ $\gamma = 3.2515$	$\omega'_1 = .40878$ $\omega'_2 = 1.0653$ $b - \epsilon_0 = 3.0560$	
3	$f'_1 = .53047$ $f'_2 = .36228$ $f'_3 = .099038$ $\gamma = 3.3748$	$\omega'_1 = .38345$ $\omega'_2 = .64955$ $\omega'_3 = 1.7247$ $b - \epsilon_0 = 4.0812$	
4	$f'_1 = .45542$ $f'_2 = .30593$ $f'_3 = .19051$ $f'_4 = .043580$ $\gamma = 3.4647$	$\omega'_1 = .37711$ $\omega'_2 = .53129$ $\omega'_3 = .96002$ $\omega'_4 = 2.4963$ $b - \epsilon_0 = 5.1958$	

Table 18

With 4 Physical States

M			
1	$f_1' = .43277$ $\delta = 3.1468$	$\omega_1' = .77731$ $b - \epsilon_0 = 2.4715$	
2	$f_1' = .30406$ $f_2' = .14621$ $\delta = 3.3169$	$\omega_1' = .58996$ $\omega_2' = 1.4117$ $b - \epsilon_0 = 3.5617$	
3	$f_1' = .19121$ $f_2' = .20725$ $f_3' = .057586$ $\delta = 3.4297$	$\omega_1' = .53821$ $\omega_2' = .86775$ $\omega_3' = 2.1879$ $b - \epsilon_0 = 4.7284$	
4	$f_1' = .12703$ $f_2' = .18926$ $f_3' = .11547$ $f_4' = .026751$ $\delta = 3.5109$	$\omega_1' = .51690$ $\omega_2' = .69371$ $\omega_3' = 1.2335$ $\omega_4' = 3.0744$ $b - \epsilon_0 = 5.9772$	

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CHAPTER VI
 THE LOGARITHMIC MEAN EXCITATION ENERGIES AND THE HIGH ENERGY
 PHOTOIONIZATION CROSS SECTION FOR ATOMIC HELIUM AND THE
 NEGATIVE HYDROGEN ION

A. INTRODUCTION

In Chapter V, a technique has been suggested for calculating the logarithmic mean excitation energies and the high energy photoionization cross section for atoms and molecules. The present work describes the application of the technique to evaluate these properties for atomic helium and the negative hydrogen ion. The moments $S(k)$ of the oscillator strength distribution, needed for implementing the method, have been taken from the literature. However, accurate values of $S_f(3)$ (the "finite" part of the third moment of the oscillator strength distribution), also needed, have not previously been available. In order to obtain $S_f(3)$ to the required accuracy calculations have been performed using a 162 term He ground state and a 162 term H^- ground state, both containing Fock terms in the wavefunction. The resulting calculations of the logarithmic mean excitation energies appear to be the only existing values for the negative hydrogen ion and the most accurate to date on $L(-1)$, $L(0)$ and $L(1)$ for atomic helium.

B. THE CALCULATION OF $S_f(3)$

The "finite" part of the third moment of the oscillator strength distribution, as shown in Chapter V, is expressed in terms of expectation values of the wavefunction according to

$$S_f(3) = \frac{4}{3} Z^3 N \rho(0) \left[\frac{1}{2} \ln 2 - \frac{1}{2} - C_{EM} \right] + \frac{2}{3} Z^2 \left[\sum_{i \neq j=1}^N \left\langle \Psi_0 \left| \frac{\vec{r}_i \cdot \vec{r}_j}{r_i^3 r_j^3} \right| \Psi_0 \right\rangle - N \int_0^\infty \ln r \frac{d^2 \rho}{dr^2} dr \right] \quad (1)$$

where $\rho(r)$ is the radial one-electron density and $C_{EM} = .5772\dots$, the Euler-Mascheroni constant. Note that $S_f(3)$ may be written in terms of what Schwartz¹ calls "C" through the relation

$$S_f(3) = \frac{2}{3} Z^2 N \rho(0) C. \quad (2)$$

Schwartz¹ has performed a calculation using an 18 term Kinoshita wavefunction and obtained $C = 5.18$ for atomic helium. Using Pekeris' result², $N\rho(0) = 45.501$, leads to $S_f(3) = 629$ for He, in substantial disagreement with the value obtained in the present work.

The wavefunction used for the present calculation is a modified version of a Fock type wavefunction due to C. W. Scherr and E. J. Shipsey (unpublished). The wavefunction is of the form

$$\Psi = e^{-\frac{\lambda}{2}(r_1+r_2)} P(r_1, r_2, r_{12}) \quad (3)$$

where

$$P = \sum_{\substack{p,q,l, \\ i,j}} A(p,q,l,i,j) r_1^p r_2^q r_{12}^l (r_1^2+r_2^2)^{i/2} [\ln(r_1^2+r_2^2)]^j \quad (4)$$

as specified by Fock³, where r_1 , r_2 and r_{12} are the Hylleraas variables. The symmetry of the ground state has been insured by requiring $A(p,q,l,i,j) = A(q,p,l,i,j)$. The standard Rayleigh-Ritz procedure⁴ has been employed to determine the values of $A(p,q,l,i,j)$ and λ for which the expectation value of the energy is minimized. The inclusion of the nonconventional half-power and logarithmic terms is necessary in order for the wavefunction to assume the correct analytic form when both electrons are near the nucleus. This type of wavefunction appears to be especially well suited for the present calculation since the expectation values necessary for the evaluation of $S_f(3)$ are clearly very sensitive to the behavior of the wavefunction near the nucleus. Tables 19 and 20 list ground state energies as a function of basis size. Energies are given in terms of atomic units.

Table 19

 H^-

Number of Terms Included	Energy
89	-.527750699
101	-.527750929
117	-.527750967
137	-.527750989
162	-.527751000
Actual	-.527751016 ^a

Table 20

He

Number of Terms Included	Energy
89	-2.903724376161
101	-2.903724376985
117	-2.903724377018
137	-2.903724377023
162	-2.903724377025
Actual	-2.903724377034 ^b

a. Reference (5).

b. Reference (6).

Table 21

 H^-

Number of Terms Included	$\int_0^\infty \frac{d^2 \rho}{dr^2} \ln r dr$	$\left\langle \sum_{i \neq j=1}^2 \frac{\vec{r}_i \cdot \vec{r}_j}{r_i^3 r_j^3} \right\rangle$
89	-5.355	-.05584
101	-5.363	-.05606
117	-5.354	-.05610
137	-5.347	-.05610
162	-5.350	-.05609
Best Estimate	-5.349	-.05609

Table 22

He

Number of Terms Included	$\int_0^\infty \frac{d^2 \rho}{dr^2} \ln r dr$	$\left\langle \sum_{i \neq j=1}^2 \frac{\vec{r}_i \cdot \vec{r}_j}{r_i^3 r_j^3} \right\rangle$
89	-180.941	-1.36700
101	-180.935	-1.36695
117	-180.940	-1.36694
137	-180.936	-1.36693
162	-180.937	-1.36693
Best Estimate	-180.937	-1.36693

Tables 21 and 22 contain results for the expectation values needed for the evaluation of $S_f(3)$ for H^- and He. The results have apparently converged to almost 4 digits for the negative hydrogen ion and to 6 digits for atomic helium. The accuracy achieved appears to be adequate for the present needs.

Using the "best estimate" results of the expectation values listed in Tables 21 and 22, $S_f(3)$ may readily be calculated for H^- and He once $N\rho(0)$ has been supplied. From the work of Pekeris the value of $N\rho(0)$ is known to be 4.136 for the negative hydrogen ion⁷ and 45.501 for atomic helium². Hence the value of $S_f(3)$ is found to be 3.066 for H^- and 606.76 for He.

C. THE CONSTRUCTION OF THE EFFECTIVE DISTRIBUTIONS

Effective distributions shall be constructed according to the prescription given in Chapter V. The effective distributions consist of a set of discrete effective oscillator strengths and a continuous oscillator strength density extending from infinity down to some cut off value of the energy. The effective oscillator strengths, energies and coefficients (in the expansion of the density) are determined such that the effective density has the correct asymptotic behavior for high energies and the moments of the effective distribution equal the moments of the actual distribution.

The coefficients α and β of the first two terms in the asymptotic expansion of the oscillator strength density,

$$\frac{df}{d\epsilon} = \alpha \epsilon^{-7/2} + \beta \epsilon^{-4} + \dots \quad (5)$$

and the moments of the oscillator strength distribution which can be obtained from sum rules are listed in Table 23 for H^- and Table 24 for He. The values of $S_f(3)$ listed are those which have been calculated in the present work. The values of $S(2)$, $S(1)$ and $S(-1)$ are expressible as expectation values of the wavefunction and have been

Table 23

H⁻

$$\alpha = (2^{3/2}/\pi) Z S(2) = 1.24112$$

$$\beta = -2 Z^2 S(2) = -2.75708$$

$$S_f(3) = 3.066$$

$$S(2) = 1.37854$$

$$S(1) = .747508$$

$$S(0) = 2.00000$$

$$S(-1) = 14.9685$$

Table 24

He

$$\alpha = (2^{3/2}/\pi) Z S(2) = 54.6204$$

$$\beta = -2 Z^2 S(2) = -242.672$$

$$S_f(3) = 606.76$$

$$S(2) = 30.3340$$

$$S(1) = 4.08373$$

$$S(0) = 2.00000$$

$$S(-1) = 1.50500$$

Table 25

H⁻

	Langhoff "a" ^a	Langhoff "b" ^a
S(-2)	206.0959	206.0744
S(-3)	3771.499	3767.879
S(-4)	80102.66	79941.35
S(-5)	1867814	1861477
S(-6)	46472740	46237640

Table 26

He

	Thakkar ^b	Langhoff "a" ^a	Langhoff "b" ^a
S(-2)	1.38312	1.383019	1.381584
S(-3)	1.41496	1.414911	1.413573
S(-4)	1.54210	1.542067	1.541327
S(-5)	1.74987	1.749849	1.749589
S(-6)	2.04044	2.040661	2.040570

a. Reference (8).

b. Reference (9).

taken from the work of Pekeris on the negative hydrogen ion⁷ and atomic helium². $S(0)$ is of course equal to the number of electrons in the system which is two for H^- and He.

Ab initio values of $S(-2)$, $S(-3)$, $S(-4)$, $S(-5)$ and $S(-6)$ have also been taken from the literature, however these quantities cannot be expressed as expectation values of the wavefunction. These moments must be calculated variationally hence the precision attained for $S(-2) - S(-6)$ is not likely to be as accurate as that of the $S_f(3)$, $S(2)$, $S(1)$ and $S(-1)$ calculations. In order to test the sensitivity of the effective distribution (and the properties derived from it) to errors in the $S(-2) - S(-6)$ moments, calculations were performed with two different sets of $S(-2) - S(-6)$ values for the negative hydrogen ion and with three different sets of $S(-2) - S(-6)$ values for atomic helium. Table 25 contains the "Spectrum a" and "Spectrum b" variational approximations to $S(-2) - S(-6)$ for H^- obtained by Langhoff et.al.⁸ Table 26 contains Thakkar's variational approximations⁹ to $S(-2) - S(-6)$ for He and the "Spectrum a" and "Spectrum b" variational approximations to $S(-2) - S(-6)$ for He obtained by Langhoff et.al.⁸

Tables 27 through 31 list the effective distributions obtained in the present work which satisfy the moments $S_f(3)$, $S(2)$, $S(1)$, ..., $S(2-2M)$ where M ranges over 1, 2, 3 and 4. The f'_n are the effective oscillator strengths and the ω'_n are the associated energy differences between the "effective states" and the ground state. The effective oscillator strength density is of the form

$$\frac{df'}{d\epsilon} = \alpha(\epsilon - \epsilon_0)^{-7/2} + \beta(\epsilon - \epsilon_0)^{-4} + \gamma(\epsilon - \epsilon_0)^{-9/2} \quad (6)$$

and extends over the energy range from b to ∞ . The α and β are obtained from Table 23 for H^- and Table 24 for He. The f'_n , ω'_n , γ and b are of course determined by solving the system of simultaneous equations described in Chapter V. Tables 27 and 28 contain the results

Table 27

 H^- (S(-2) - S(-6) from Langhoff "a")

M

1	$f_1' = 1.906$ $\gamma = 3.097$	$\omega_1' = .2640$ $b-\epsilon_0 = 1.629$
2	$f_1' = .7410$ $f_2' = 1.200$ $\gamma = 3.200$	$\omega_1' = .06092$ $\omega_2' = .4309$ $b-\epsilon_0 = 1.933$
3	$f_1' = .2139$ $f_2' = .8626$ $f_3' = .8818$ $\gamma = 3.277$	$\omega_1' = .04138$ $\omega_2' = .1049$ $\omega_3' = .5646$ $b-\epsilon_0 = 2.208$
4	$f_1' = .07482$ $f_2' = .4227$ $f_3' = .8195$ $f_4' = .6528$ $\gamma = 3.346$	$\omega_1' = .03543$ $\omega_2' = .06050$ $\omega_3' = .1662$ $\omega_4' = .7027$ $b-\epsilon_0 = 2.498$

Table 28

 H^- (S(-2) - S(-6) from Langhoff "b")

M

1	$f'_1 = 1.906$ $\gamma = 3.097$	$\omega'_1 = .2640$ $b - \epsilon_0 = 1.629$
2	$f'_1 = .7411$ $f'_2 = 1.199$ $\gamma = 3.200$	$\omega'_1 = .06093$ $\omega'_2 = .4310$ $b - \epsilon_0 = 1.933$
3	$f'_1 = .2134$ $f'_2 = .8601$ $f'_3 = .8847$ $\gamma = 3.276$	$\omega'_1 = .04139$ $\omega'_2 = .1045$ $\omega'_3 = .5630$ $b - \epsilon_0 = 2.205$
4	$f'_1 = .07392$ $f'_2 = .4145$ $f'_3 = .8086$ $f'_4 = .6717$ $\gamma = 3.339$	$\omega'_1 = .03543$ $\omega'_2 = .06006$ $\omega'_3 = .1619$ $\omega'_4 = .6880$ $b - \epsilon_0 = 2.464$

Table 29

He (S(-2) - S(-6) from Thakkar)

M

1	$f'_1 = 1.917$ $\gamma = 564.2$	$\omega'_1 = 1.592$ $b - \epsilon_0 = 7.690$
2	$f'_1 = 1.197$ $f'_2 = .7651$ $\gamma = 594.6$	$\omega'_1 = .9606$ $\omega'_2 = 2.983$ $b - \epsilon_0 = 10.34$
3	$f'_1 = .6853$ $f'_2 = .9540$ $f'_3 = .3401$ $\gamma = 617.0$	$\omega'_1 = .8399$ $\omega'_2 = 1.553$ $\omega'_3 = 4.623$ $b - \epsilon_0 = 13.17$
4	$f'_1 = .4874$ $f'_2 = .7506$ $f'_3 = .6132$ $f'_4 = .1386$ $\gamma = 640.9$	$\omega'_1 = .8060$ $\omega'_2 = 1.194$ $\omega'_3 = 2.434$ $\omega'_4 = 7.213$ $b - \epsilon_0 = 17.45$

Table 30

He (S(-2) - S(-6) from Langhoff "a")

M

1	$f'_1 = 1.917$ $\gamma = 564.2$	$\omega'_1 = 1.592$ $b-\epsilon_0 = 7.690$
2	$f'_1 = 1.197$ $f'_2 = .7646$ $\gamma = 594.6$	$\omega'_1 = .9608$ $\omega'_2 = 2.984$ $b-\epsilon_0 = 10.35$
3	$f'_1 = .6908$ $f'_2 = .9561$ $f'_3 = .3330$ $\gamma = 617.8$	$\omega'_1 = .8409$ $\omega'_2 = 1.564$ $\omega'_3 = 4.681$ $b-\epsilon_0 = 13.29$
4	$f'_1 = .4803$ $f'_2 = .7563$ $f'_3 = .6282$ $f'_4 = .1268$ $\gamma = 675.1$	$\omega'_1 = .8047$ $\omega'_2 = 1.188$ $\omega'_3 = 2.469$ $\omega'_4 = 7.735$ $b-\epsilon_0 = 19.36$

Table 31

He (S(-2) - S(-6) from Langhoff "b")

M		
1	$f'_1 = 1.917$ $\delta = 564.2$	$\omega'_1 = 1.592$ $b - \epsilon_0 = 7.690$
2	$f'_1 = 1.204$ $f'_2 = .7583$ $\delta = 595.0$	$\omega'_1 = .9634$ $\omega'_2 = 3.001$ $b - \epsilon_0 = 10.38$
3	$f'_1 = .7220$ $f'_2 = .9858$ $f'_3 = .2765$ $\delta = 627.9$	$\omega'_1 = .8464$ $\omega'_2 = 1.646$ $\omega'_3 = 5.286$ $b - \epsilon_0 = 14.69$
4	$f'_1 = .4876$ $f'_2 = .7652$ $f'_3 = .6613$ $f'_4 = -.007327$ $\delta = 789.6$	$\omega'_1 = .8059$ $\omega'_2 = 1.199$ $\omega'_3 = 2.607$ $\omega'_4 = 27.11$ $b - \epsilon_0 = 8.638$

for H^- obtained by using the Langhoff "a" and the Langhoff "b" values for $S(-2) - S(-6)$ respectively. Tables 29, 30, and 31 contain the results for He obtained by using the Thakkar, the Langhoff "a" and the Langhoff "b" values for $S(-2) - S(-6)$ respectively.

The effective distributions for the negative hydrogen ion obtained using the Langhoff "a" and the Langhoff "b" values for $S(-2) - S(-6)$ are fairly consistent. Although noticeable differences can be detected between the $M = 4$ distributions, the results appear to be reasonable. The atomic helium results are more sensitive to errors in the input, perhaps due to the different shape of the distribution. The distributions constructed using the Langhoff "b" values for $S(-2) - S(-6)$ appear to be unreliable (with an unreasonably large jump in the γ value for $M = 4$) and noticeable differences can be detected between all three of the $M = 4$ distributions.

D. RESULTS FROM THE EFFECTIVE DISTRIBUTIONS FOR THE NEGATIVE HYDROGEN ION AND ATOMIC HELIUM

The effective distributions constructed in the previous section have been used to compute the logarithmic mean excitation energies $L(k)$ associated with the effective distributions according to

$$\begin{aligned}
 L(k) = & \sum_{n=1}^M f'_n w'_n{}^k \ln w'_n \\
 & + \frac{\alpha}{\frac{5}{2}-k} (b-\epsilon_0)^{k-5/2} \ln(b-\epsilon_0) + \frac{\alpha}{(\frac{5}{2}-k)^2} (b-\epsilon_0)^{k-5/2} \\
 & + \frac{\beta}{3-k} (b-\epsilon_0)^{k-3} \ln(b-\epsilon_0) + \frac{\beta}{(3-k)^2} (b-\epsilon_0)^{k-3} \\
 & + \frac{\gamma}{\frac{7}{2}-k} (b-\epsilon_0)^{k-7/2} \ln(b-\epsilon_0) + \frac{\gamma}{(\frac{7}{2}-k)^2} (b-\epsilon_0)^{k-7/2}. \quad (7)
 \end{aligned}$$

Note that while the moments and effective distributions have been given in terms of atomic units, the logarithmic mean excitation ener-

gies shall be expressed in terms of Rydbergs.

Tables 32 through 36 contain the results for $L(-1)$, $L(0)$, $L(1)$, $L(2)$ and γ of the negative hydrogen ion. The Bethe theory for collisions of fast particles holds only for neutral atoms so apparently the values of $L(-1)$, $L(0)$ and $L(1)$ are of no practical importance for the negative hydrogen ion. The $L(2)$ value however can be used to estimate the Lamb shift of H^- . Tables 37 through 41 contain the results for $L(-1)$, $L(0)$, $L(1)$, $L(2)$ and γ of atomic helium. I is another quantity containing the information provided by $L(0)$ and is related to $L(0)$ (given in electron volts) by

$$I = \exp(L(0)/S(0)). \quad (8)$$

Results for I are presented in Table 42. The "best estimates" and associated error estimates are clearly subjective and are meant only to serve as a guide. The "best estimates" are an extrapolation of the $M = 1, 2, 3, 4$ results and have been influenced by the convergence behavior of results for atomic hydrogen presented in Chapter V. Also, for atomic helium the Langhoff "b" results (which gave an effective spectrum with anomalous behavior) were basically ignored. Despite the fact that the effective distributions constructed from the higher order M systems appear to be fairly sensitive to errors in the inputs the $L(k)$ are nevertheless fairly stable. Also note that γ seems to be more sensitive to errors in the inputs than the $L(k)$. For the case of atomic helium, the most reasonable distributions appear to be those given by Thakkar's values of $S(-2) - S(-6)$ and the $M = 4$ Thakkar distribution yields a value of $L(2)$ in best accordance with Schwartz's¹ accurate value of $L(2)$.

Finally, Table 43 compares the present work with results obtained earlier for atomic helium. It appears that the results obtained here for $L(-1)$, I , $L(0)$ and $L(1)$ are the most accurate to date. Apparently there is no earlier work for comparison with the results obtained here for the negative hydrogen ion.

Table 32

L(-1) of H⁻

M	Langhoff "a"	Langhoff "b"
1	-4.097	-4.097
2	-1.299	-1.299
3	-1.275	-1.276
4	-1.272	-1.273
Best Estimate	-1.270	-1.270
	<u>+3</u>	<u>+3</u>

Table 33

L(0) of H⁻

M	Langhoff "a"	Langhoff "b"
1	-1.072	-1.072
2	-1.636	-1.636
3	-1.695	-1.695
4	-1.711	-1.710
Best Estimate	-1.718	-1.718
	<u>+8</u>	<u>+8</u>

Table 34

L(1) of H^-

M	Langhoff "a"	Langhoff "b"
1	.2386	.2386
2	.3964	.3964
3	.4390	.4386
4	.4575	.4557
Best Estimate	.4725 <u>+75</u>	.4725 <u>+75</u>

Table 35

L(2) of H^-

M	Langhoff "a"	Langhoff "b"
1	16.98	16.98
2	16.78	16.78
3	16.68	16.68
4	16.62	16.63
Best Estimate	16.58 <u>+4</u>	16.58 <u>+4</u>

Table 36

 δ of H^-

M	Langhoff "a"	Langhoff "b"
1	3.10	3.10
2	3.20	3.20
3	3.28	3.28
4	3.35	3.34
Best Estimate	3.50	3.50
	<u>+15</u>	<u>+15</u>

Table 37

L(-1) of He

M	Thakkar	Langhoff "a"	Langhoff "b"
1	.8107	.8107	.8107
2	.6402	.6402	.6402
3	.6435	.6436	.6444
4	.6438	.6438	.6448
Best Estimate	.6440	.6440	.6440
	<u>+4</u>	<u>+4</u>	<u>+4</u>

Table 38

L(0) of He

M	Thakkar	Langhoff "a"	Langhoff "b"
1	2.478	2.478	2.478
2	2.278	2.278	2.278
3	2.268	2.268	2.266
4	2.267	2.267	2.262
Best Estimate	2.265 <u>+3</u>	2.265 <u>+3</u>	2.265 <u>+3</u>

Table 39

L(1) of He

M	Thakkar	Langhoff "a"	Langhoff "b"
1	14.04	14.04	14.04
2	14.48	14.48	14.48
3	14.55	14.55	14.57
4	14.57	14.58	14.64
Best Estimate	14.58 <u>+3</u>	14.58 <u>+3</u>	14.58 <u>+3</u>

Table 40

L(2) of He

M	Thakkar	Langhoff "a"	Langhoff "b"
1	537.0	537.0	537.0
2	532.9	532.9	532.9
3	531.5	531.5	531.0
4	530.8	531.4	528.1
Accurate ^a	530.2	530.2	530.2
	<u>+5</u>	<u>+5</u>	<u>+5</u>

Table 41

 γ of He

M	Thakkar	Langhoff "a"	Langhoff "b"
1	564	564	564
2	595	595	595
3	617	618	628
4	641	675	790
Best Estimate	680	680	680
	<u>+40</u>	<u>+40</u>	<u>+40</u>

a. Reference (1).

Table 42

I of He

M	Thakkar	Langhoff "a"	Langhoff "b"
1	46.97	46.97	46.97
2	42.50	42.50	42.50
3	42.29	42.29	42.25
4	42.27	42.27	42.16
Best Estimate	42.23	42.23	42.23
	<u>+6</u>	<u>+6</u>	<u>+6</u>

Table 43

Comparison of Values of $L(k)$ and I for Atomic Helium

	$L(-1)$	Source
	$.6456_{\pm}.0015$	Moment Theory ^a
	$.6440_{\pm}.0004$	Present Work
I	$L(0)$	Source
$42.03_{\pm}.32$	$2.256_{\pm}.015$	Moment Theory ^a
42.00	2.254	Variational Calculation ^b
42.12	2.260	Variational Calculation ^c
41.70	2.240	$S(k)$ Fit ^d
39.0	2.11	$S(k)$ Fit ^e
42.19	2.263	$S(k)$ Fit ^f
44.30	2.361	Experimental ^g
41.35	2.223	Experimental ^h
$42.23_{\pm}.06$	$2.265_{\pm}.003$	Present Work
	$L(1)$	Source
	$14.72_{\pm}.50$	Moment Theory ^a
	13.76	Variational Calculation ^c
	14.6	$S(k)$ Fit ^e
	$14.58_{\pm}.03$	Present Work

a. Reference (10).

b. Reference (11).

c. Reference (12).

d. Reference (13).

e. Reference (14).

f. Reference (15).

g. Reference (16).

h. Reference (17).

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