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Nonexistence of a Positron–Hydrogen-Atom Bound State*

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One needs a *necessary* condition (rather than a sufficient condition, such as that of Rayleigh-Ritz) to even attempt to prove that a given bound state cannot exist. We use an adiabaticlike method to show that a positron (e^+) and a hydrogen atom (H) cannot form a bound state. The separation r (but *not* $\vec{r}$) of the proton (p) and e^+ is fixed; working in a subspace of zero total angular momentum, we calculate the lowest energy $E_{e1}(r)$ of the electron in the field of e^+ and p. An effective one-body $p+e^+$ potential is then defined by $V^{(1)}(r)=E_{e1}(r)+e^2/r+e^2/2a_0$. The necessary condition for the existence of a bound state of the true $\mathrm{H}+e^+$ system is the existence of a bound state of an artificial $p+e^+$ system with an interaction $V^{(1)}(r)$. This one-body problem is readily solved, and we find that it (and therefore the true problem) has no bound state. The proof is not rigorous since $E_{e1}(r)$ is not determined exactly, but the accuracy attained is such as to make the existence of an $\mathrm{H}+e^+$ bound state extremely unlikely. A by-product of the calculation is the determination of an improved lower bound on the ground-state energy of H^-.

I. INTRODUCTION

An approach based on the use of adiabaticlike potentials was used recently to obtain rigorous lower bounds on the ground-state energy of a compound system.[1,2] When a bound state of the compound system does in fact exist, the rigorous lower bound may well be rather crude; the primary significance of the method lies in the possibility of proving that the lower bound is zero, that is, in proving that no bound state exists. [The nonexistence of a bound state *cannot* be proved by means of a Rayleigh-Ritz (RR) approach no matter how accurately one performs the calculation.] The adiabaticlike approach was applied to a number of cases and, among other results, it was shown that a positron cannot be bound to a helium atom. A (crude) lower bound was obtained on the binding energy of the electron-atomic-hydrogen ($\mathrm{H}+e^-$) singlet ground state. In the case of the positron–atomic-hydrogen ($\mathrm{H}+e^+$) system, where extensive RR calculations make it almost certain (on reasonability grounds only—the result is in no sense rigorous) that no bound state exists, the adiabaticlike method failed to prove the nonexistence of a bound state; a lower bound on the energy of the bound state, if a bound state exists, was obtained.

The lowest-energy state of a three-body system with central two-body interactions is of course a state of zero angular momentum, i.e., $L=0$. For the case of interest, for which one of the three particles is effectively infinitely massive, it was pointed out[1,2] that this fact could be used to obtain improved results for the $H + e^+$ and $H + e^-$ systems. Using this suggestion, we have in fact been able to effectively prove the nonexistence of a bound state for the $H + e^+$ system. Though of much less interest conceptually, it is little extra work and we have therefore also obtained an improved, though still crude, lower bound on the binding energy for the negative hydrogen ion.

II. METHOD

Following the approach noted earlier,[1,2] we begin by writing the Hamiltonian for a zero total angular momentum state as

$$H(r_1, r_2, \theta_{12}) = t(r_1) + t(r_2) + \tfrac{1}{2}(1/m_1 r_1^2 + 1/m_2 r_2^2)\,\mathcal{L}^2 + V, \tag{1}$$

where r_1 and r_2 are the distances of the positron and electron, respectively, from the (infinitely heavy) proton, and θ_{12} is the angle between $\vec{r}_1$ and $\vec{r}_2$. V is given by

$$V = e^2/r_1 - e^2/r_2 - e^2/r_{12}\,,$$
$$t(r_i) = -\frac{\hbar^2}{2m_i}\,\frac{1}{r_i^2}\,\frac{\partial}{\partial r_i}\,r_i^2\,\frac{\partial}{\partial r_i}\,, \tag{2}$$

and

$$\mathcal{L}^2 = -\frac{\hbar^2}{\sin\theta_{12}}\,\frac{\partial}{\partial \theta_{12}}\sin\theta_{12}\,\frac{\partial}{\partial\theta_{12}}\,. \tag{3}$$

(For the $H + e^-$ case, the signs of the first and third terms of V are reversed.) Separating off the kinetic energy term $t(r_1)$, we write

$$H(r_1, r_2, \theta_{12}) = t(r_1) + H_a(r_2, \theta_{12}; r_1), \tag{4}$$

which defines H_a. Letting $E_{a0}(r_1)$ be the lowest eigenvalue of H_a for r_1 fixed, it is clear that[1,2]

$$H_a(r_2, \theta_{12}; r_1) \geqslant \hat{1}(r_2, \theta_{12}) E_{a0}(r_1), \tag{5}$$

where $\hat{1}(r_2, \theta_{12})$ is the unit operator in the function space of the coordinates r_2 and θ_{12}. If E_{thr} is the energy of the deepest continuum threshold of H, it follows that

$$H(r_1, r_2, \theta_{12}) - E_{\mathrm{thr}} \geqslant \hat{1}(r_2, \theta_{12}) H^{(1)}(r_1), \tag{6}$$

where the one-body Hamiltonian

$$H^{(1)}(r_1) \equiv t(r_1) + V^{(1)}(r_1) \tag{7}$$

contains the one-body potential

$$V^{(1)}(r_1) \equiv E_{a0}(r_1) - E_{\mathrm{thr}}\,. \tag{8}$$

Thus, if $E_{a0}(r_1)$ is known or can be obtained, one need only solve a one-dimensional Schrödinger equation to find a lower bound on $H(r_1, r_2, \theta_{12})$, and if $V^{(1)}(r_1)$ is incapable of supporting a bound state, the three-body bound-state system cannot exist.

The method just described represents the second of two approaches described previously.[1,2] It is superior to the first method in that it differs from the first by the non-negative angular momentum term $\mathcal{L}^2/(2m_1 r_1^2)$ in H_a and will therefore generate an improved lower bound. The price one has to pay in using the second (improved) method is that one must evaluate $E_{a0}(r_1)$; the corresponding energy function required for the use of the first method is known for a number of simple cases. Only the first method was used in Ref. 1.

If $E_{a0}(r_1)$ cannot be obtained exactly, a lower bound on $E_{a0}(r_1)$ will maintain a rigorous lower bound on H. We will use the RR method to determine $E_{a0}(r_1)$. This gives an upper bound on $E_{a0}(r_1)$, but the results obtained are reasonably accurate and for the moment $E_{a0}(r_1)$ will be thought of as known exactly. (We will return to this point later.) The trial function used is of the form

$$\psi_t(r_2, \theta_{12}; r_1) = \sum_{l,i} c_{li}\, r_2^{\,l+n_{li}}\, e^{-a_{li} r_2}\, P_l(\cos\theta_{12}), \tag{9}$$

where the $c_{li}(r_1)$ are linear parameters, the $a_{li}(r_1)$ are nonlinear parameters, and the n_{li} are non-negative integers, to be chosen arbitrarily. The P_l are the Legendre polynomials. We solve

$$\det(\overleftrightarrow{\mathrm{H}}_a - E_a \overleftrightarrow{\mathrm{J}}) = 0 \tag{10}$$

for the lowest-energy eigenvalue, where

$$H_{a\,ij} = (\psi_{it}, H_a \psi_{jt}) \tag{11}$$

and

$$J_{ij} = (\psi_{it}, \psi_{jt}). \tag{12}$$

For each value of l the best value of a_{li} was searched for, and then successive values of l were added. An example is given in Table I for $r_1 = 2a_0$

TABLE I. Convergence of E_{el}, the adiabaticlike energy excluding the Coulomb interaction energy of the two fixed particles, as a function of the number of terms n used in the trial function of Eq. (9) for the $l_i = 0$ case, for $r_1 = 2.0a_0$. $E_{\mathrm{el}}(r_1, +)$ and $E_{\mathrm{el}}(r_1, -)$ are the results for the $H + e^+$ and $H + e^-$ systems, respectively. E_{el} is in rydbergs (1 Ry = 13.6 eV). Note that these numbers have not been corrected by the method described in the text.

n	$E_{\mathrm{el}}(r_1, +)$	$E_{\mathrm{el}}(r_1, -)$
1	− 1.945 05	− 0.039 57
2	− 1.952 33	− 0.053 69
3	− 1.955 84	− 0.082 32
4	− 1.956 11	− 0.085 83
5	− 1.956 23	− 0.086 75
6	− 1.956 38	− 0.086 76
7	− 1.956 39	− 0.086 78
8	− 1.956 40	− 0.086 83
9	− 1.956 41	− 0.086 87
10	− 1.956 43	− 0.086 88
11	− 1.956 44	− 0.086 88
12	− 1.956 44	− 0.086 88

TABLE II. Convergence of E_{el} as a function of l_i, for $r_1 = 2.0a_0$. Seven terms were used for $l_i = 0$ and five terms for the other l_i's. The entry in the l_{max} column specifies a trial function containing all terms up to and including the l_{max} term. $E_{el}(r_1, +)$ and $E_{el}(r_1, -)$ are the results for the $H + e^+$ and $H + e^-$ systems, respectively. E_{el} is in rydbergs. Note that these numbers have not been corrected by the method described in the text.

l_{max}	$E_{el}(r_1, +)$	$E_{el}(r_1, -)$
0	−1.9564	−0.086 78
1	−2.0259	−0.145 93
2	−2.0510	−0.148 77
3	−2.0618	−0.149 38
4	−2.0670	−0.149 59
5	−2.0697	−0.149 68
6	−2.0712	−0.149 72
7	−2.0721	−0.149 74
8	−2.0727	−0.149 75
9	−2.0731	−0.149 75

(where a_0 is the Bohr radius) of convergence in n, the number of functions for $l = 0$; in Table II we study the convergence in l, where we used seven functions for $l = 0$ and five functions for each l for l from 1 through 9. E_{el} represents the adiabaticlike energy excluding the Coulomb interaction energy of the two fixed particles, and is given by $E_{el} = E_{a0} \mp e^2/r_1$, where the minus and plus signs refer to the $H + e^+$ and $H + e^-$ cases, respectively.

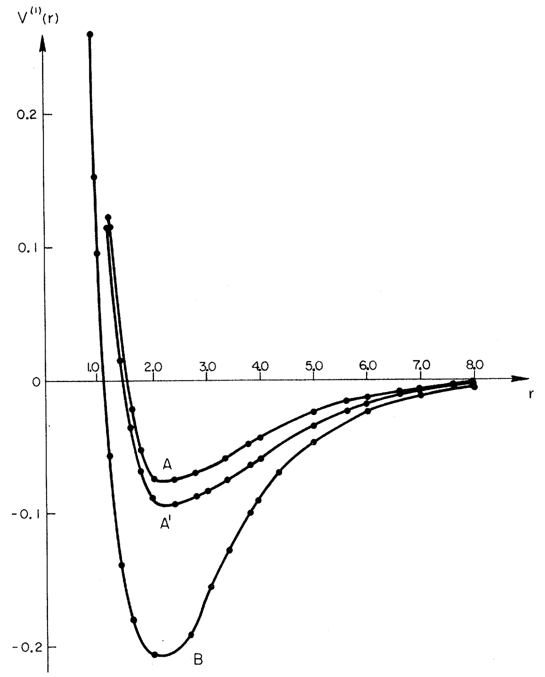

FIG. 1. Comparison between the present improved uncorrected adiabaticlike approximation (A), the improved corrected adiabaticlike approximation (A′), and the adiabatic approximation (B) used in Ref. 3 of the potential $V^{(1)}(r)$ [see Eq. (8) and opening paragraph of Sec. II A] for $H + e^+$. $V^{(1)}(r)$ is in rydbergs and $r = r_1/a_0$.

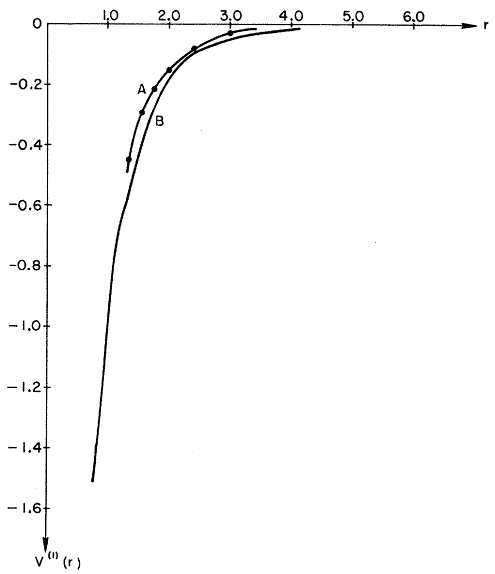

FIG. 2. Comparison between the present improved adiabaticlike approximation (A) and the adiabatic approximation (B) used in Ref. 4 of the potential $V^{(1)}(r)$ [see Eq. (8)] for $H + e^-$. $V^{(1)}(r)$ is in rydbergs and $r = r_1/a_0$.

It is interesting to note that, as expected, the $l = 1$ term is of much greater significance in the $H + e^-$ case than in the $H + e^+$ case; in the $H + e^-$ case, where one fixes the proton and one of the electrons, the monopole moment is identically zero and the leading multipole is the dipole. The very considerable effect of the $l = 1$ contribution in the $H + e^-$ case can be seen from Table II, the energy for states including $l = 0$ and $l = 1$ being almost double that for an $l = 0$ state only. (One might expect the effect of the $l = 2$ state to be relatively significant for the $H + e^+$ case, where the fixed proton and positron generate a reasonable quadrupole moment as well as a monopole moment, but the effect is small.)

Comparisons of our adiabaticlike energies with the adiabatic energies of Wind[3] and Wallis *et al.*[4] are given in Figs. 1 and 2 for the $H + e^+$ and for $H + e^-$. The presence of the angular momentum term in our Hamiltonian is seen to make the potential significantly less attractive in the $H + e^+$ case.

A. $H + e^+$

The variational estimate of $E_{a0}(r_1)$ can be expected to be quite accurate, but, unfortunately, it is ultimately the influence of $V^{(1)}(r_1)$ that must be considered, and it is trivial to check that a very slight error in $E_{a0}(r_1)$ can lead to a significant error in $V^{(1)}(r_1)$. A careful estimate of the accuracy of the results for E_{a0} is therefore called for. To make such an estimate, we deleted the angular momentum term $\mathcal{L}^2/2m_1r_1^2$ from H_a and repeated the calculation of E_{a0}, using the same form of trial function as with the angular momentum present. Our results should then agree with those obtained by Wind[3] for the hydrogen molecular ion. (Fixing two protons or fixing a proton and a positron will of course give the same energy.) Wind used an expansion technique and his results should be extremely reliable. Our results for $E_{a0}(r_1)$ are very close to those of Wind for almost all r, but in some regions of r they do deviate by about 1%. (Being a RR calculation, our values are not as deep as those of Wind.) A 1% error in $E_{a0}(r_1)$ can generate errors an order of magnitude larger in $V^{(1)}(r_1)$ and must be corrected for. Since the angular momentum term contributes only a few percent to the value of $E_{a0}(r_1)$, we took the difference between our results with and without the angular momentum term as the contribution of the angular momentum term. This difference was then added on to Wind's results to obtain a corrected $E_{a0}(r_1)$. The result should be reliable; further, if anything, it should make $V^{(1)}(r_1)$ slightly more attractive than in fact it is. If then the $V^{(1)}(r_1)$ we use cannot support a bound state, the exact $V^{(1)}(r_1)$ can *a fortiori* not support a bound state.

A necessary condition for the existence of a bound state for a potential $V(r)$ is the Bargmann-Schwinger result[2]

$$(2m/\hbar^2)\int_0^\infty r[-V_-(r)]dr \geq 1, \tag{13}$$

where $V_-(r)$ is defined as equal to $V(r)$ where $V(r)$ is negative, and equal to zero where $V(r)$ is non-negative. We find that the above integral, with $V^{(1)}(r)$ of Eq. (8) as the potential and with m the mass of an electron, gives 1.07. Since this is larger than 1, it does not follow that there is no bound state of $\mathrm{H}+e^+$. It does follow, though, that the smallest mass for which a bound state can possibly exist is $(1.07)^{-1}m$, which is $0.93m$. [The calculation in Ref. 1, using $E_{a0}(r_1)$ from Ref. 3, gave $1.8m$ for the value of the integral in (13), corresponding to a smallest mass at which a bound state could possibly exist of $0.56m$, a much poorer result.]

An improved result for the smallest mass of a particle with the charge equal to that of a positron that can be bound to H is obtained by solving the one-dimensional Schrödinger equation with the Hamiltonian given by (7). We obtain a mass of $1.46m$. This then proves that the positron cannot be bound to the hydrogen atom. (The calculation in Ref. 1, using the Schrödinger equation approach, found that no bound state exists for a mass of $0.75m$, and was unable to prove the nonexistence of a bound state of $\mathrm{H}+e^+$.) Our result, that a mass less than $1.46m$ cannot be supported by a H atom, is of course consistent with the result of Rotenberg and Stein,[5] obtained by a RR calculation, that a mass greater than $2.2m$ can be supported by a H atom. The actual value of the mass that can just be supported should be quite close to the $2.2m$ result. The proof we give for the nonexistence of the bound state is not completely rigorous, since $E_{a0}(r)$ is not determined exactly, but the accuracy attained is such as to make the existence of the $\mathrm{H}+e^+$ bound state extremely unlikely.

It is important to distinguish between the various roles played by the RR approach in the different calculations. We have stressed that a direct application of an RR approach to the original problem of $m^- + \mathrm{H}$ represents a sufficient but not a necessary condition for the existence of a bound state—a particle of mass greater than the lowest mass obtained for which the particle will be bound to the H atom will also be bound. The method of the present paper presumably generates a necessary but not a sufficient condition for the existence of a bound state; yet in the course of its application a RR calculation was used to estimate a potential. The difference is one of practice rather than principle. In our case the RR calculation is applied not to the original three-body problem but to a very much simpler two-body problem; furthermore, we are using the RR approach simply to calculate a potential energy curve, and the subtle problems that can arise when one is directly studying conditions for which a bound state just appears are not present.

To make the matter concrete, we note that a RR calculation[6] using no less than 84 parameters found that a particle of mass $m^+ = 2.625m$ was bound by 0.000 54 eV. If one uses Fig. 1 of Ref. 5 to extrapolate to that mass, one finds a binding energy of 0.026 eV. Thus, while the RR result provides an upper bound on the energy, the upper bound is off by about a factor of 50, despite the 84 variational parameters. Thus, had an attempt been made by the authors of Ref. 6 to estimate the necessary mass for binding (no such attempt was in fact made), a very bad result would have been obtained. The fact that an estimate of the mass obtained in this way is itself variational[2] helps, but not all that much.

It is of course clear *now* why the energy obtained[6] is so far off. As the binding energy of the additional particle approaches zero, the wave function of the system extends to greater and greater distances and cannot readily be approximated by a standard Hylleraas-type trial function. The beauty of the work of Rotenberg and Stein is that a term was added to the usual form of trial function to account for the asymptotic form of the wave function.

Some recent work[7] on the ground-state energies of three-particle systems using the Faddeev equations indicated that the positron was bound to the hydrogen atom by about 0.9 eV. The authors had some doubts about the validity of that result; the

TABLE III. Conditions on the mass of a particle if it is to be possible for that particle to form a bound state with a hydrogen atom. We consider a particle with a charge equal to that of an electron and a mass m^-, and also a particle with a charge equal to that of a positron and a mass m^+. (I) refers to the first method described in Ref. 1 and to the method actually applied in Ref. 1. (II) refers to the second method described in Ref. 1 and to the method applied in the present paper. "Integral" refers to the use of the theorem quoted in connection with Eq. (13), while "Schr" refers to the improved result obtained by explicit solution of the one-body Schrödinger equation. RR refers to the Rayleigh-Ritz result. The RR result is a sufficient condition. All of the other results are necessary conditions. m is the mass of an electron.

	System	
Method	$H+m^+$	$H+m^-$
Integral (I)	$\geq 0.56m$	$\geq 0.4m$
Integral (II)	$\geq 0.93m$	$\geq 0.4m$
Schr (I)	$\geq 0.75m$	$\geq 0.66m$
Schr (II)	$\geq 1.46m$	$\geq 0.72m$
RR[a]	$2.2m$	

[a]See Ref. 5.

present calculations make it clear that the result is not valid.

A further result is readily obtained from scaling considerations.[1] We consider three charged particles with charges equal in magnitude to the charge on an electron and with masses $M^+=\infty$, m^+, and m^-, the superscripts denoting the sign of the charge. We know that if there exists a state with energy $E(m^+, m^-)$ in which both m^+ and m^- are bound, then

$$E(bm^+, bm^-) = bE(m^+, m^-) \tag{14}$$

for b a positive constant. We also have for the energy E_{thr} of the hydrogenic $m^- M^+$ bound state

$$E_{\text{thr}}(bm^-) = bE_{\text{thr}}(m^-). \tag{15}$$

Choosing $b=(1.46)^{-1}=0.69$, $m^+=1.46m$, and $m^-=m$, it follows that

$$E(m^+, 0.69m^-) - E_{\text{thr}}(0.69m^-) = 0.69[E(1.46m^+, m^-) - E_{\text{thr}}(m^-)] = 0. \tag{16}$$

Thus, if we increase the mass of the particle of negative charge rather than decrease the mass of the particle of positive charge, we find that a proton, a positron, and a negatively charged particle of mass $0.69m$ cannot form a bound state.

B. $H+e^-$

Since the negative hydrogen ion is known to exist in a singlet state, we can only obtain an improved lower bound on the energy of the bound state. In this case also we checked the accuracy of our results for E_{a0} by deleting the angular momentum term and comparing the resulting numbers with those of Wallis *et al.*[4] The results checked to within 0.01%. We then find that

$$(2m/\hbar^2)\int_0^\infty r[-V_-^{(1)}(r)]\,dr = 2.49\,, \tag{17}$$

so that a particle with the charge of that of an electron and of mass smaller than $0.4m$ cannot attach itself to the hydrogen atom. Upon solving the one-body Schrödinger equation, we find that the electron is bound by at most 1.64 eV. From this result it follows[1] that the energies of both the first excited singlet state and the triplet ground state lie above $\frac{1}{2}(-1.64 \text{ eV})$ or -0.82 eV. Our results in this case are not appreciably better than those of Ref. 1 (see Table III). The solution of the one-body Schrödinger equation gives the improved result that a particle with the charge of that of an electron must have a mass of at least $0.72m$ to be bound to a hydrogen atom.

The reason for the much more considerable improvement in our calculation for the $H+e^+$ case than for the $H+e^-$ case is a consequence of the fact that the electronic energy E_{el} is larger in the important region of r in the $H+e^+$ case than in the $H+e^-$ case. Thus the increase in the potential due to the angular momentum term, while being proportionally about the same in both cases, makes a much greater difference in the absolute potential, and thus leads to a significant improvement.

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Does the Coster-Kronig Transition Probability f_{23} Have a Radiative Component?*

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The radiative magnetic dipole transition rate between $2p_{3/2}$ and $2p_{1/2}$ single-particle electron states has been calculated with relativistic screened hydrogenic wave functions for seven elements with $70 \leqslant Z \leqslant 93$ and is found to contribute only $\sim 10^{-5}$ of the total L_2 level width. The result has been corroborated by an experimental study of the Pb M x-ray spectrum in coincidence with $K\alpha_1$ and $K\alpha_2$ x rays, establishing a limit $\omega_{23} \lesssim (1.4 \pm 3.0) \times 10^{-3}$ for the radiative part of the L_2-L_3X Coster-Kronig transition probability in Pb.

I. THEORY

Existing measurements[1-6] of the L_2-L_3X Coster-Kronig transition probability f_{23} for $Z \geqslant 70$ exceed theoretical results derived from screened hydrogenic wave functions[7] and from a self-consistent-field (SCF) approach[8] (Fig. 1). The question arises whether radiative spin-flip transitions could contribute measurably to f_{23}. The L_1-L_3 radiative Coster-Kronig transition has recently been observed,[9] as has the K-L_1 spin-flip transition.[10]

We calculate the radiative magnetic dipole transition rate between $2p_{3/2}$ and $2p_{1/2}$ single-particle electron states following the formalism of Scofield,[11] but with relativistic screened hydrogenic wave functions. The use of analytic wave functions is justified since only an order-of-magnitude result is desired. The initial and final states are characterized by the quantum numbers $\kappa_i = -2$, $\kappa_f = 1$ [$\kappa = \mp (j + \frac{1}{2})$ for $j = l \pm \frac{1}{2}$]. The transition rate is

$$\Gamma_{fi} = 2\alpha\omega^2(2j_i+1) f_1(m)$$
$$= 2\alpha\omega(2j_i+1) B(-\kappa_i,\, \kappa_f,\, 1) R_1^2(m)\,, \qquad (1)$$

where α is the fine-structure constant and ω is the transition energy, in units such that $\hbar = m = c = 1$. The quantity B, which vanishes unless $J = L + \bar{l}_i + l_f$ is even and L, j_i, and j_f form a triangle, is defined as

$$B(-\kappa_i,\, \kappa_f, L) = [(2\bar{l}_i+1)(2l_f+1)/L(L+1)]$$
$$\times C^2(\bar{l}_i,\, l_f,\, L\,; 0, 0) W^2(j_i \bar{l}_i j_f l_f; \tfrac{1}{2}L), \qquad (2)$$

where $\bar{l} = -\kappa$ if $\kappa < 0$ and $\bar{l} = \kappa - 1$ if $\kappa > 0$. In the present case, $B(2,\, 1,\, 1) = \frac{1}{4}$, whence

$$\Gamma_{fi} = 2\alpha\omega\, R_1^2(m)\,. \qquad (3)$$

The radial matrix element is

$$R_1(m) = (\kappa_i + \kappa_f) \int dr\, j_1(kr)\, (F_f G_i + G_f F_i)$$

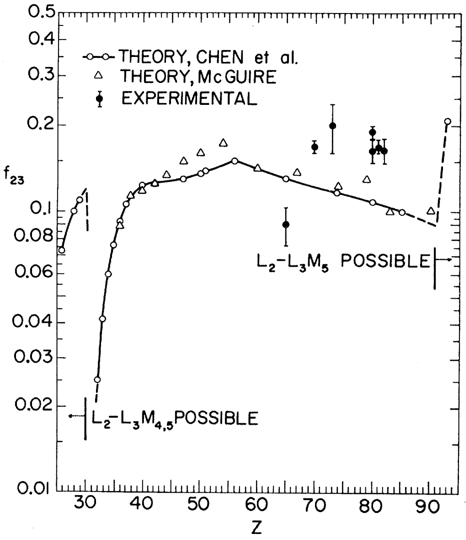

FIG. 1. Theoretical L_2-L_3X Coster-Kronig transition probability f_{23} calculated by Chen, Crasemann, and Kostroun (Ref. 7) from hydrogenic wave functions and by McGuire (Ref. 8) through an SCF approach, compared with experimental points (Refs. 1–6).