Stationary and Quasistationary Bounds on Arbitrary Bound-State Matrix Elements*

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Rigorous upper and lower bounds on the diagonal and off-diagonal bound-state matrix elements of an arbitrary Hermitian operator W are derived which represent a significant improvement over previous results in that all first-order error terms are eliminated. These bounds do, however, contain error terms of the three-halves power of the errors in the trial functions used; they are therefore termed "quasistationary bounds." In the particular but important case of the diagonal bound-state matrix elements of non-negative (nonpositive) Hermitian operators, true stationary lower (upper) bounds are obtained; the errors are of second order in the errors of the trial functions used. All trial functions can contain variational parameters. The results obtained are tested by computing upper and lower bounds on the expectation value of r_1+r_2 for the ground state of helium, and a substantial improvement over previous bounds is obtained.

I. INTRODUCTION

Rigorous upper and lower bounds on diagonal and off-diagonal bound-state matrix elements have been obtained.[1-3] The bounds are functionals of one or more trial functions which may contain parameters that can be varied to obtain the best possible bound for the given form of the trial functions. Further, the bounds are "global"—they are valid not only for trial functions which are close to the true functions but for arbitrary trial functions. (The bounds will of course be poor for poor trial functions.) Unfortunately, the bounds are nonstationary, in that the error, the difference between the bound and the true value, is of first order in the errors in the trial functions.

Variational, or rather stationary, principles for the estimation of diagonal and off-diagonal bound- (and continuum) state matrix elements also exist.[4-7] The stationary principles contain not first but only second-order error terms, but the sign of the error is unknown. The stationary principles are functionals of trial wave functions and of trial "auxiliary functions"; the latter can be thought of as Lagrange undetermined multipliers introduced to account for the constraints imposed upon the wave function.[6] A significant step was recently taken in these stationary principles, it having been shown[7] that it is possible to characterize the trial auxiliary functions as the functions which extremize specified functionals.

It will be our purpose in this paper to obtain results, where possible, which combine the advantages of the two above results, the bound and the stationary property. The approach is rather simple. Rather than bound the matrix element in question directly, we recast the matrix element into the sum of a calculable approximation and a formal higher-order error term, and we bound the error term. We could, in fact, begin with a "variational identity"[8] in which the matrix element is expressed as the sum of a (calculable) stationary principle for the matrix element plus an explicit but noncalculable second-order term, and proceed to bound the second-order term; the result would be the same as that obtained below by a slightly different approach.

The matrix elements to be bounded are of the form

$$W_{nm} \equiv (\psi_n,\, W\psi_m), \tag{1.1}$$

with a Hermitian inner product, where W is an arbitrary (except as noted) Hermitian operator with respect to the (orthonormal) bound-state eigenfunctions ψ_n defined by

$$(H-E_n)\psi_n=0, \quad (\psi_n,\, \psi_n)=1. \tag{1.2}$$

The global bounds will be functionals of normalized trial wave functions ψ_{nt} and ψ_{mt} and of trial auxiliary functions L_{nt} and L_{mt}. L_{nt} and L_{mt} are estimates of "hybrid auxiliary functions" L_n and L_m patterned after but slightly different from the auxiliary functions appearing in stationary principles.[4] L_n and L_m will be defined in Sec. II. We introduce the errors $\delta\psi_n$ and δL_n defined by

$$\delta\psi_n=\psi_{nt}-\psi_n, \quad \delta L_n = L_{nt}-L_n, \tag{1.3}$$

and refer to them as of first order, though there is no guarantee, of course, that they are small.

For the particular but important case of $n=m$ and $W>0$, we can, as shown in Sec. III, obtain results which combine all of the advantages of the bound and the stationary principles; we obtain a global lower bound on W_{nn} which is a functional of ψ_{nt} and L_{nt} (which may contain variational parameters) and for which the (second-order) error is given by $O(\delta\psi_n^2)+O(\delta\psi_n \delta L_n)$. For this special case, then, we have results for a non-negative but otherwise arbitrary operator which are of the same character as the results for matrix elements of the operator H, including the Rayleigh–Ritz theorem for the ground-state energy, the Hylleraas–Undheim theorem for excited-state energies,[9] and scattering parameters, including scattering lengths[10] and elements of the K matrix.[11]

The more general case of upper and lower bounds on W_{nm} for $n \neq m$ and/or for W not of well-defined sign is treated in Sec. IV. The bounds contain an error term of $O((\delta\psi)^{3/2})$ and possibly of $O((\delta\psi)(\delta L)^{1/2})$ as well, depending upon the details of the procedure used. We refer to such bounds as quasistationary.

Finally, in Sec. V, we explore the quality of the bounds derived by computing upper and lower bounds on the expectation value of r_1+r_2 for the ground state of helium, and compare the results with the "true value" as determined by Pekeris[12] with the use of a 1078-parameter wave function.

We assume in Secs. II–V that all matrix elements are real. This restriction is not at all necessary, as shown in Appendix A; we need not even restrict ourselves to systems which are invariant under time reversal and rotation, for which it is always possible[13] to choose the radial functions to be real.

II. BASIC UPPER- AND LOWER-STATIONARY BOUND FORMULAS

We begin by deriving stationary upper- and lower-bound formulas for the overlap of ψ_n with a quadratically integrable but otherwise arbitrary function Φ,

$$M_n \equiv (\psi_n, \Phi). \tag{2.1}$$

For the moment, we assume Φ to be known.

The trial auxiliary function $\hat{L}_{nt}$ that arises naturally in the stationary principle for M_n is an approximation to $\hat{L}_n$ defined by[8]

$$(H-E_n)\hat{L}_n = -\Phi + M_n\psi_n .$$

This involves only the exact (*unknown*) entities E_n and ψ_n. The differential equation defining $\hat{L}_{nt}$, on the other hand, must involve only *known* entities, including ψ_{nt} and E_{nt}. For present purposes it is convenient to introduce the hybrid auxiliary function L_n, defined by

$$(H-E_n)L_n = -\Phi + M_n\psi_{nt}/S_n , \tag{2.2}$$

where

$$S_n \equiv (\psi_n, \psi_{nt}) \tag{2.3}$$

is the overlap integral of the trial and true wave functions. We refer to L_n as hybrid since its defining equation involves both the unknown E_n and ψ_n and the known ψ_{nt}.

L_n is defined by (2.2) only to within a multiple of ψ_n. L_n can be made unique by requiring that $(L_n, \psi_n) = 0$.

The ultimate justification of the introduction of L_n via (2.2) is that it will enable us to obtain a bound on M_n, a bound which becomes exact as ψ_{nt} approaches ψ_n or as our approximation L_{nt} to L_n approaches L_n. However, (2.2) is by no means the only form of equation which can lead to a bound. While not an essential element, we note that the right-hand side of (2.2) has the nice property of being independent of the normalizations of ψ_n and of ψ_{nt}.

It will almost always be possible, theoretically or experimentally or by a combination, to obtain accurate upper and lower bounds on both E_n and S_n,[14] and therefore to replace E_n and S_n by the appropriate bound in any final bounds on M_n. For purposes of discussion, it will be convenient to think of E_n and S_n as known. Our unknowns are ψ_n and L_n.

In line with the discussion in the Introduction, we write the unknown M_n as a known term plus an unknown term of lower order; thus, using (1.3), we have

$$M_n = (\psi_{nt}, \Phi) - (\delta\psi_n, \Phi). \tag{2.4}$$

Carrying this one step further, we use (1.3) and (2.2) to write

$$-(\delta\psi_n, \Phi) = (\psi_{nt}, [H-E_n]L_{nt}) - (\delta\psi_n, [H-E_n]\delta L_n) - (1-S_n)M_n/S_n ;$$

to arrive at this, we also used

$$(H-E_n)\delta\psi_n = (H-E_n)\psi_{nt} ,$$

the quadratic integrability[7] of L_n, and the resulting hermiticity of H. The appearance of the unknown quantity M_n in the expression for $(\delta\psi_n, \Phi)$ causes no difficulty. Thus, we can insert the expression for $(\delta\psi_n, \Phi)$ into (2.4) and rearrange and square to find

$$(\delta\psi_n, [H-E_n]\delta L_n)^2 = [\alpha - (M_n/S_n)]^2, \tag{2.5}$$

where

$$\alpha \equiv (\psi_{nt}, \Phi) + (\psi_{nt}, [H-E_n]L_{nt}). \tag{2.6}$$

α is nothing other than the (calculable) stationary estimate for M_n, a quantity that could almost certainly have been expected to appear.

The problem of determining a stationary bound on M_n has thereby been reduced to the problem of obtaining a nonstationary bound on the second-order term on the left of (2.5). To do so, the Gram-determinant approach will suffice. The Gram-determinant inequality[15] formed from the three functions $\delta\psi_n$, $[H-E_n]\delta L_n$, and ψ_n is found to be

$$(\delta\psi_n, [H-E_n]\,\delta L_n)^2 \le (1-S_n^2)\,([H-E_n]\,\delta L_n, [H-E_n]\,\delta L_n). \quad (2.7)$$

With the help of (1.3) and (2.2), we find that

$$([H-E_n]\,\delta L_n, [H-E_n]\,\delta L_n) = \beta - (2\alpha S_n/M_n) + (M_n/S_n)^2, \quad (2.8)$$

where

$$\beta \equiv (\Phi,\Phi) + 2(\Phi, [H-E_n]\,L_{nt}) + (L_{nt}, [H-E_n]^2 L_{nt}). \quad (2.9)$$

From (2.5), (2.7), and (2.8), we find

$$[\alpha - (M_n/S_n)]^2 \le (1-S_n^2)[\beta - (2\alpha M_n/S_n) + (M_n/S_n)^2]$$

or

$$M_n^2 - 2\alpha S_n M_n - [(1-S_n^2)\beta - \alpha^2] \le 0$$

or, finally,

$$M_n \lesseqgtr S_n\,\alpha \pm [(1-S_n^2)(\beta-\alpha^2)]^{1/2}. \quad (2.10)$$

It is shown in Appendix B that $\beta - \alpha^2$ is non-negative so that the bounds (2.10) always exist. (We always have $S_n^2 \le 1$.)[16] It is also shown in Appendix B, as is to be expected from the nature of the derivation, that the right-hand side of (2.10) differs from M_n by quantities of second order so that the bounds are stationary ones.

The fundamental stationary bounds provided by (2.10) require the choice of an L_{nt}. In the development of a stationary principle for $(\phi_n, W\phi_n)$, one must be able to find an L_{nt} which differs from L_n in first order, and the problem there is first to find an appropriate differential equation defining L_{nt} and then a technique enabling one to approximate the L_{nt} so defined. The present approach, providing a global bound, does not require a defining differential equation for L_{nt}. One can simply guess at a form for L_{nt} which contains variational parameters and one can then vary the parameters to do as well as one can.

If Φ is indeed known, we have a calculable stationary bound on M_n. Φ is known for many problems, including, for example, the problem of the determination of the central density ρ_c of a star[6] for which the pressure P is of the form $P = K\rho^\gamma$, with K and γ constants. If Φ is not known, the bounds are only formal, and terms involving Φ must in turn be bounded. It is simple to bound terms such as (ψ_{nt}, Φ) when, for example, Φ is chosen to be $W\psi_n$, viz., by using (2.10) with $\Phi = W\psi_{nt}$. The more difficult problem of bounding (Φ, Φ) is considered in Sec. IV. We will first show that it is possible to obtain stationary lower bounds on W_{nn} for $W \ge 0$ with Φ chosen to be a known function.

III. VARIATIONAL STATIONARY LOWER BOUND ON W_{nn} FOR $W \ge 0$

If $W \ge 0$, the Schwartz inequality permits us to write

$$W_{nn} \ge \frac{(\psi_n, W\psi_{nt})^2}{(\psi_{nt}, W\psi_{nt})} \equiv \frac{(W_{n,nt})^2}{W_{nt,nt}}. \quad (3.1)$$

It is readily verified that the first-order error terms in (3.1) cancel, that is, that (3.1) is a stationary (though formal) bound. The unknown quantity $W_{n,nt}$ must still be bounded from below. A stationary lower bound on $W_{n,nt}$ is readily found from (2.10) on choosing $\Phi = W\psi_{nt}$. We assume that that lower bound is found to be a positive number, as will almost always be the case. We thereby obtain the stationary lower bound, one of the main results of the present paper,

$$W_{nn} \ge \{S_n\alpha - [(1-S_n^2)(\beta-\alpha^2)]^{1/2}\}^2 / W_{nt,nt}. \quad (3.2)$$

For ψ_{nt} fixed, the right-hand side of (3.1) represents the very best lower bound obtainable by means of Eq. (3.2). As we vary more and more parameters in more and more sophisticated approximations to L_n, the further inequality utilized in going from (3.1) to (3.2) will approximate an equality and our lower bound on W_{nn} will converge on $(W_{n,nt})^2/W_{nn}$. This statement is, of course, a purely formal one since we do not normally know ψ_n or, therefore, $W_{n,nt}$. It will be interesting to consider the rate of convergence of our lower stationary bound for the simple solvable problem of the expectation value $\langle r\rangle_{00} = \frac{3}{2}$ for the ground state of hydrogen. With $\hbar = m = e = 1$, we choose

$$\psi_t(r) = (Z_1^3/\pi)^{1/2}\, e^{-Z_1 r}. \quad (3.3)$$

Equation (2.2) becomes

$$\left(-\tfrac{1}{2}\nabla^2 - \frac{1}{r} + \tfrac{1}{2}\right) L = \left(-r + \frac{3}{Z_1+1}\right)\psi_t, \quad (3.4)$$

the solution of which is

$$L = \frac{2}{(Z_1+1)(Z_1-1)^2}\left(\frac{Z_1^3}{\pi}\right)^{1/2} \times \{-e^{-r} + [1+(Z_1-1)r]e^{-Z_1 r}\}. \quad (3.5a)$$

The term in e^{-r} has been added in order to guarantee that L has a well-defined limit as Z_1 approaches unity. In fact, we find

$$L(Z_1 = 1) = -\tfrac{1}{2}(1/\pi)^{1/2} r^2 e^{-r}. \quad (3.5b)$$

For various values of Z_1 we approximated the true L of Eq. (3.5) by L_t given by

$$L_t = \sum_{i=1}^{M} (c_i r^{i-1}) r^2 e^{-3r/2}, \quad (3.6)$$

where the choice of $\frac{3}{2}$ in the exponent is arbitrary.

TABLE I. Convergence of the stationary lower bound on $\langle r\rangle_{00}$ for hydrogen. ψ_t and L_t are given by Eqs. (3.3) and (3.6), respectively. M is the number of variational parameters contained in L_t. The exact value, in units of a_0, is 1.5.

Z_1 \ M	0	1	2	3	∞
1.001	1.4964	1.4978	1.4992	1.4997	1.49999+
1.05	1.330	1.401	1.462	1.484	1.496
1.25	.75	1.09	1.28	1.34	1.43

The choice $M=0$ corresponds to $L_t=0$; as M gets large, L_t converges on L of (3.5) and the bound on W_{nn} converges on

$$\frac{(W_{0,0t})^2}{W_{0t,0t}}=\frac{(\psi, r\psi_t)^2}{(\psi_t, r\psi_t)}=\frac{[24Z_1^{3/2}/(Z_1+1)^4]^2}{\frac{3}{2}Z_1}.$$

The results shown in Table I show reasonable convergence rates even for a rather poor ψ_t.

IV. QUASISTATIONARY UPPER AND LOWER BOUNDS ON W_{nn} AND W_{nm}

As always, we demand that W be Hermitian, but we drop the requirement imposed in Sec. III that W be of well-defined sign. Choosing

$$\Phi=W\psi_m, \tag{4.1}$$

where m may or may not be equal to n, α and β contain unknown quantities which must be bounded if we are to bound W_{nm}. The character of the bounds on α and β (simple zeroth-order errors, quasistationary, or stationary) will determine the character of the bounds on W_{nm}. With $X^{(\pm)}$ denoting upper and lower bounds on X, we can replace (2.10) by

$$W_{nm}\lesseqgtr S_n\,\alpha^{(\pm)}\pm\{(1-S_n^2)[\beta^{(+)}-(\alpha^2)^{(-)}]\}^{1/2}. \tag{4.2}$$

From the definitions of α and β, (2.6) and (2.9), respectively, we clearly have

$$\alpha^{(\pm)}=W_{nt,m}^{(\pm)}+(\psi_{nt},[H-E_n]L_{nt}), \tag{4.3}$$

$$\beta^{(+)}=(W^2)_{mm}^{(+)}+2(\psi_m, W[H-E_n]L_{nt})^{(+)}+(L_{nt},[H-E_n]^2L_{nt}). \tag{4.4}$$

The determination of bounds on α and β, and therefore on W_{nm}, is thereby reduced to the determination of the three quantities with superscripts on the right-hand sides of (4.3) and (4.4).

Stationary upper and lower bounds on both $W_{nt,m}$ and $(\psi_m, W[H-E_n]L_{nt})$ are readily obtained from Eq. (2.10) by setting $n=m$ and choosing $\Phi=W\psi_{nt}$ and $\Phi=W[H-E_n]L_{nt}$, respectively. Unfortunately, a stationary upper bound on W_{mm}^2 cannot be obtained. A nonstationary upper bound on W_{mm}^2 can be obtained by methods described previously,[3] for example, by means of a simple bound on W_{mm}^4; the nonstationary bound contains an error of order $\delta\psi_m$. Since $1-S_n^2$ is of order $\delta\psi_n^2$, the error in W_{nm} is of order $\delta\psi_n\,\delta\psi_m^{1/2}$. The bound is therefore superior, in principle, to the previous bounds with their first-order errors but inferior, in principle, to the bounds of Sec. III, when applicable, with their second-order errors. A concrete example of a quasistationary bound will be given in Sec. V.

By definition, simple bounds[3] contain zeroth-order error terms; their use for $W_{mm}^{2(+)}$ would cause the bound $\beta^{(+)}$ of (4.2), and therefore the bound of (4.2) on W_{nm}, to be of first order; the bound (4.2) would therefore be of the same accuracy as the nonstationary bounds[1-3] obtained previously and would be more difficult to calculate.

V. NUMERICAL EXAMPLE

In order to explore the quality of the bounds derived in preceding sections, upper and lower bounds on $\langle r_1+r_2\rangle_{00}$, the expectation value of r_1+r_2 for the ground state of helium, were calculated. We choose

$$W=s\equiv r_1+r_2, \tag{5.1}$$

and note that $\langle r_1\rangle_{00}=\frac{1}{2}\langle s\rangle_{00}$. We use Hylleraas coordinates s, $t=r_1-r_2$, and $u=r_{12}$. The trial wave functions were chosen to be the energy-optimized three-parameter Hylleraas function[17] $\psi_{0t}(3)$ and the energy-optimized ten-parameter function $\psi_{0t}(10)$ of Chandrasekhar *et al.*[18] The ψ_{0t}'s therefore contained no variational parameters. The trial auxiliary function L_{0t} does contain variational parameters. The form of L_{0t} chosen is based roughly on the realization that the Hamiltonian H for helium can be approximated by a sum of hydrogenlike Hamiltonians; L_{0t} should then, crudely, be a product of hydrogenlike L_0's, which are known. [See Eq. (3.5b).]

The upper bound on S_0 was always chosen to be unity. The lower bound on S_0, which plays a more significant role, was obtained from Weinhold's formula,[1,14]

$$(\psi_0,\psi_{0t}(N))\geq(\psi_0,\psi_{0t}(N'))\,(\psi_{0t}(N),\psi_{0t}(N'))-\{[1-(\psi_0,\psi_{0t}(N'))^2][1-(\psi_{0t}(N),\psi_{0t}(N'))]\}^{1/2}. \tag{5.2}$$

$\psi_{0t}(N)$ is the trial wave function being used; $\psi_{0t}(N')$ is some better trial wave function whose overlap with ψ_0 has been bounded. Thus, we choose $N'=10$ for $N=3$ and $N'=18$ for $N=10$, where $\psi_{0t}(18)$ is the 18-parameter energy-optimized trial wave function of Chandrasekhar *et al.*[19] In all cases, the required bound on $(\psi_0,\psi_{0t}(N'))$ has been obtained by means of the Eckart criterion,[20]

$$(\psi_0, \psi_{0t}(N'))^2 \geq \frac{E_1 - (\psi_{0t}(N'), H\psi_{0t}(N'))}{E_1 - E_0} . \quad (5.3)$$

Lower bounds on $\langle r_1 \rangle_{00}$ were calculated by means of Eq. (3.2), with $\Phi = s\,\psi_{0t}$. Equation (3.2) is then calculable as it stands.

Equation (4.2), with $m = n = 0$, was used for the upper-bound calculation; the same choice of Φ was made. Equation (4.2) then reads

$$(r_1)_{00} \leq \tfrac{1}{2}\{\alpha^{(+)} + [(1 - S_0^2)(\beta^{(+)} - (\alpha^2)^{(-)}]^{1/2}\},$$
$$\alpha^{(\pm)} = s_{0,0t}^{(\pm)} + (\psi_{0t}, (H - E_0)L_{0t})$$
$$\beta^{(+)} = s_{00}^{2(+)} + 2(\psi_{0t}, s(H - E_0)L_{0t})^{(+)} + \|(H - E_0)L_{0t}\|^2.$$

The required upper bound on s_{00}^2 was calculated from[1]

$$s_{00}^{2(+)} = s_{0,0t}^{2(+)} + \{(1 - S_0^2)(s_{00}^4 - [(s_{0,0t}^2)^{(-)}]^2\}^{1/2}, \quad (5.4a)$$

$$s_{0,0t}^{2(\pm)} = s_{0t,0t}^2 \pm \{(1 - S_0^2)[s_{0t,0t}^4 - (s_{0t,0t}^2)^2]\}^{1/2}. \quad (5.4b)$$

The required bound on s_{00}^4 could be taken as a simple bound, as mentioned earlier. This can be improved upon by using the relationship

$$s_{00}^4 \leq 16(r_1^4)_{00},$$

along with the upper bound

$$(r_1^4)_{00} \leq 4.81004$$

obtained by methods described in our previous paper.[3]

It is to be noted that the bounds (5.4b) are nonstationary, although stationary bounds for this term could have been obtained by the method described in the last paragraph of Sec. II. This was not considered to be worthwhile because only nonstationary bounds were available for s_{00}^2. For the same reason, the nonstationary bound

$$(\psi_{0t}, s(H - E_0)L_{0t})^{(+)} = (\psi_{0t}, s(H - E_0)L_{0t})$$
$$+ \{(1 - S_0^2)[\|s(H - E_0)L_{0t}\|^2 - (\psi_{0t}, s(H - E_0)L_{0t})^2]\}^{1/2}$$

was used. The resulting upper bound (5.3) is then quasistationary in character as described in the previous section.

Referring to Table II, it can be seen that the upper and lower bounds are of almost identical quality, despite the fact that the former is quasistationary, while the latter is a true stationary bound. This is a consequence of the relatively crude choices of L_t. More elaborate choices can be expected to result in a more rapid convergence of the stationary lower bound than the quasistationary upper bound.

APPENDIX A: MODIFICATION FOR COMPLEX MATRIX ELEMENTS

The Gram-determinant inequality for three arbitrary complex vectors ϕ, η, and χ can be expressed as

$$\|\phi\|^2|(\eta, \chi)|^2 + \|\chi\|^2|(\phi, \eta)|^2 + \|\eta\|^2|(\phi, \chi)|^2$$
$$- 2\,\mathrm{Re}[(\phi, \eta)(\eta, \chi)(\chi, \phi)] - \|\phi\|^2\|\eta\|^2\|\chi\|^2 \leq 0. \quad (A1)$$

Choose

$$\phi = \delta\psi_n, \quad \eta = (H - E_n)\delta L_n, \quad \chi = \psi_n.$$

Then $(\eta, \chi) = 0$, $\|\chi\|^2 = 1$, and (A1) becomes

$$|(\delta\psi_n, [H - E_n]\delta L_n)|^2 \leq [(\delta\psi_n, \delta\psi_n) - |(\delta\psi_n, \psi_n)|^2]$$
$$\times (\delta L_n, [H - E_n]^2 \delta L_n). \quad (A2)$$

Defining

$$S_n \equiv (\psi_n, \psi_{nt}),$$

so that

$$S_n^* = (\psi_{nt}, \psi_n),$$

it follows that

$$(\delta\psi_n, \delta\psi_n) = (\psi_{nt} - \psi_n, \psi_{nt} - \psi_n) = 2 - S^* - S,$$
$$|(\delta\psi_n, \psi_n)|^2 = |(\psi_{nt} - \psi_n, \psi_n)|^2 = |S_n^* - 1|^2$$
$$= |S_n|^2 - S_n^* - S_n + 1.$$

Thus, (A2) can be written as

$$|(\delta\psi_n, [H - E_n]\delta L_n)|^2 \leq (1 - |S_n|^2)$$
$$\times (\delta L_n, [H - E_n]^2 \delta L_n). \quad (A3)$$

We have

$$([H - E_n]L_n, [H - E_n]L_n)$$
$$= \|\phi\|^2 - 2\,\mathrm{Re}\,\frac{M_n^*}{S_n^*}(\psi_{nt}, \Phi) + \frac{|M_n|^2}{|S_n|^2}.$$

We also have

$$-([H - E_n]L_n, [H - E_n]L_{nt}) - ([H - E_n]L_{nt}, [H - E_n]L_n)$$
$$= 2\,\mathrm{Re}[(\Phi, [H - E_n]L_{nt})] - 2\,\mathrm{Re}\,\frac{M_n^*}{S_n^*}(\psi_{nt}, [H - E_n]L_{nt}).$$

TABLE II. Upper and lower bounds on $\langle r_1 \rangle_{00}/a_0$ for helium. N is the number of parameters in the trial wave function ψ_{0t} and L_t is the auxiliary trial function. The "true" value is 0.930 (Ref. 12).

		Parameters			
N	$L_t/e^{-c_1 s}$	Lower bound	Upper bound	Lower bound	Upper bound
3	$c_2 s^2$	$c_1 = 1.37$ $c_2 = -0.04$	$c_1 = 1.91$ $c_2 = -0.12$	0.913	0.946
3	$c_2(s^2 + t^2)$	$c_1 = 1.62$ $c_2 = -0.14$	$c_1 = 1.93$ $c_2 = -0.30$	0.917	0.943
3	$c_2 s^2 + c_3 t^2$	$c_1 = 1.51$ $c_2 = -0.104$ $c_3 = -0.239$	$c_1 = 1.80$ $c_2 = -0.226$ $c_3 = -0.325$	0.920	0.943
10	$c_2(s^2 + t^2)$	$c_1 = 1.78$ $c_2 = -0.215$	$c_1 = 1.71$ $c_2 = -0.170$	0.925	0.935

We can therefore write that

$$(\delta L_n, [H-E_n]^2 \delta L_n)$$
$$= \|\Phi\|^2 + 2\,\mathrm{Re}(\Phi, [H-E_n]L_{nt}) + (L_{nt}, [H-E_n]^2 L_{nt})$$
$$- 2\,\mathrm{Re}\left[\frac{M_n^*}{S_n^*}(\psi_{nt}, \Phi) + \frac{M_n^*}{S_n^*}(\psi_{nt}, [H-E_n]L_{nt})\right]$$
$$+ \frac{|M_n|^2}{|S_n|^2}. \qquad \text{(A4)}$$

Similarly we find that

$$|(\delta\psi_n, [H-E_n]\delta L_n)|^2$$
$$= |(\psi_{nt}, \Phi) + (\psi_{nt}, [H-E_n]L_{nt})|^2 + \frac{|M_n|^2}{|S_n|^2} - 2\,\mathrm{Re}$$
$$\times\left[\frac{M_n^*}{S_n^*}(\psi_{nt}, \Phi) + \frac{M_n^*}{S_n^*}(\psi_{nt}, [H-E_n]L_{nt}\right]. \qquad \text{(A5)}$$

Using these results in (A3) shows that

$$|(\psi_n, \Phi)|^2 - 2|S_n||\alpha||(\psi_n, \Phi)|$$
$$-[(1-|S_n|^2)\beta - |\alpha|^2] \leq 0$$

or

$$|(\psi_n, \Phi)| \substack{\leq \\ \geq} |S_n||\alpha| \pm \{(1-|S_n|^2)(\beta - |\alpha|^2)\}^{1/2}, \qquad \text{(A6)}$$

where

$$\alpha = (\psi_{nt}, \Phi) + (\psi_{nt}, [H-E_n]L_{nt}),$$
$$\beta = \|\Phi\|^2 + 2|(\Phi, [H-E_n]L_{nt})| + (L_{nt}, [H-E_n]^2 L_{nt}).$$

Equation (A6) is the complex equivalent of the basic bound (2.10).

If Φ is known, (A6) is calculable as it stands. If Φ is not known, $|\alpha|$ and β must be replaced by appropriate bounds. Thus

$$|\alpha|^{(\pm)} = |(\psi_{nt}, \phi)|^{(\pm)} \pm |(\psi_{nt}, [H-E_n]L_{nt})|,$$
$$\beta^{(+)} = (||\Phi||^2)^{(+)} + 2|(\Phi, [H-E_n]L_{nt})|^{(+)}$$
$$+ (L_{nt}, [H-E_n]^2 L_{nt}).$$

No assumptions were made about the form of ψ_n in obtaining (A6) which is valid regardless of the behavior of the system under time reversal and under rotation.

APPENDIX B: EXISTENCE AND STATIONARY CHARACTER OF THE BASIC BOUNDS OF (2.10)

Using (1.3) and (2.2), Eq. (2.6) defining α can be rewritten as

$$\alpha = (M_n/S_n) + (\delta\psi_n, [H-E_n]\delta L_n). \qquad \text{(B1)}$$

Equations (2.8) and (B1) give

$$\beta = 2\alpha(M_n/S_n) - (M_n/S_n)^2 + (\delta L_n, [H-E_n]^2 \delta L_n)$$
$$= (M_n/S_n)^2 + 2(M_n/S_n)(\delta\psi_n, [H-E_n]\delta L_n)$$
$$+ (\delta L_n, [H-E_n]^2 \delta L_n). \qquad \text{(B2)}$$

From (B1) and (B2), we have

$$\beta - \alpha^2 = (\delta L_n, [H-E_n]^2 \delta L_n) - (\delta\psi_n, [H-E_n]\delta L_n)^2. \qquad \text{(B3)}$$

It follows immediately from (2.7) that $\beta - \alpha^2$ is non-negative and, therefore, the bounds of (2.10) always exist.

Further, we see by inspection of (B3) that $\beta - \alpha^2$ is of second order. Since $(1 - S_n^2)$ is also of second order (and remains so after bounding),[14] $[(1-S_n^2)(\beta - \alpha^2)]^{1/2}$ is of second order. Since S_n differs from unity by a second-order term and since α is a stationary estimate of M_n, $S_n\alpha - M_n$ is of second order and the bounds provided by (2.10) are stationary bounds.

We discuss finally the statement made in Sec. II that both bounds of (2.10) reduce to the exact value M_n as either $\delta\psi_n$ or δL_n approach zero. It is clear by inspection of (B3) that $\beta - \alpha^2 \to 0$ as $\delta\psi_n \to 0$ or $\delta L_n \to 0$. Both bounds (2.10) therefore approach $S_n\alpha$, and $\alpha \to M_n/S_n$ under these circumstances, which proves the statement.

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Diffraction Radiation from a Charged Particle Moving through a Penetrable Sphere*

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The formal exact solution to the problem of the radiation of a charged particle traveling with a constant velocity through a dielectric sphere is obtained. The electromagnetic field may be expressed in terms of an infinite number of spherical normal modes. It is found that radiation may be emitted for arbitrarily small particle velocities. For larger spheres (i.e., $ka \gg 1$ when k is the wave number and a is the radius of the sphere) the radiated field is predominantly Čerenkov-type radiation when the velocity of the particle is above the Čerenkov threshold velocity. For small spheres $(ka \gg 1)$ and low particle velocities the radiation is shown to be mainly of transition type. Numerical results are presented to illustrate the behavior of the spectra of the various lower-order radiative modes as the velocity of the particle is varied.

I. INTRODUCTION

When a charged particle moves with constant velocity through or by an obstacle, there are three (macroscopic) mechanisms by which radiation may be emitted. Radiation of the Čerenkov type[1,2] is expected if the particle moves along or through a region in which the phase velocity of light is less than the speed of the particle. For radiation of this type to occur, the speed of the particle must be greater than the smallest phase velocity encountered. Transition radiation,[3-6] and diffraction radiation,[7-9] on the other hand, may be expected to occur at any particle speed. Transition radiation which occurs when the particle passes from one electrical medium to another, and diffraction radiation which occurs when the particle moves in the vicinity of a localized inhomogeneity in a medium, may be thought of as being emitted by the accelerated motion of the induced image charges. Since the nonuniform motion of the images will occur even if the moving charged particle is traveling slowly, there is no velocity threshold for transition or diffraction radiation.

Most previous studies[8] on diffraction radiation were carried out for perfectly conducting (impenetrable) bodies such as conducting half-planes, screens, or gratings, open ends of metallic waveguides, or conducting spheres. The important problem of diffraction radiation due to the presence of dielectric (penetrable) bodies has not been considered. It is expected that, owing to the presence of multiple reflections within the penetrable obstacles, the radiation characteristics for a uniformly moving charged particle passing by or through such penetrable obstacles will be quite different from those for the impenetrable case. An important feature of diffraction radiation is that the sources in general excite a continuous spectrum of frequencies; hence, it is essential that exact solutions to the problems of diffraction radiation be obtained. In this paper we shall treat the problem of diffraction radiation from a uniformly moving charged particle passing through a dielectric sphere. Exact solutions are obtained by expanding the incident fields due to the moving charge in terms of spherical harmonics and by matching the incident field and diffracted field with the interior field at the boundary of the dielectric sphere. In other words, the electromagnetic field excited by the passage of the charged particle may be expressed in terms of an infinite number of