Studies in Perturbation Theory. X. Lower Bounds to Energy Eigenvalues in Perturbation-Theory Ground State*

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The eigenvalue problem $H\Psi=E\Psi$ in quantum theory is conveniently studied by means of the partitioning technique. It is shown that, if ε is a real variable, one may construct a function $\varepsilon_1=f(\varepsilon)$ such that each pair ε and ε_1 always bracket at least one true eigenvalue E. If ε is chosen as an upper bound by means of, e.g., the variation principle, the function ε_1 is hence going to provide a lower bound. The reaction operator t associated with the perturbation problem $H=H_0+V$ for a positive-definite perturbation V is studied in some detail, and it is shown that a lower bound to t may be constructed in a finite number of operations by using the idea of "inner projection" closely associated with the Aronszajn projection previously utilized in the method of intermediate Hamiltonians. By means of truncated basic sets one can now obtain not only upper bounds but also useful lower bounds which converge towards the correct eigenvalues when the set becomes complete. The method is applied to the Brillouin-type perturbation theory, and lower bounds may be obtained either by pure expansion methods, by inner projections, or by a combination of both approaches leading to perturbation expansions with estimated remainders. The applications to Schrödinger's perturbation theory are also outlined. The method is numerically illustrated by a study of lower bounds to the ground-state energies of the helium-like ions: He, Li^+, B^{+2}, etc.

1. INTRODUCTION

IN quantum theory, the energy values of the stationary states of a physical system are determined by the eigenvalues E of the time-independent Schrödinger equation

$$H\Psi=E\Psi\,, \tag{1}$$

where the Hamiltonian H is a self-adjoint operator ($H^\dagger=H$). For atomic and molecular systems, the ground state and lower excited states correspond to a set of discrete energy levels; the associated Hamiltonian is hence bounded from below, and the spectrum starts with a set of discrete eigenvalues. In addition to the closed stationary states, there may further be scattering states connected with a continuous part of the spectrum, but we will here focus our interest on the discrete energy levels.

In general, it is very difficult to solve the Schrödinger Eq. (1) exactly, and it is then very important to be able to "bracket" the exact eigenvalues E by means of upper and lower bounds. Let us denote the eigenvalues in increasing order by E_0 $E_1, F_2, \cdots$ and the associated normalized eigenfunctions by $\Psi_0, \Psi_1, \Psi_2, \cdots$, respectively. Convenient upper bounds are provided by the Rayleigh-Ritz variation principle,[1] which says that the expectation value

$$\langle H_{\rm op}\rangle_{\rm av}=\frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} \tag{2}$$

gives an upper bound to E_0 for arbitrary wave functions Φ, and that it further gives an upper bound to E_1, if Φ is restricted to functions orthogonal to Ψ_0, an upper bound to E_2, if Φ is restricted to functions orthogonal to Ψ_0 and Ψ_1, etc. In the treatment of the excited states, the exact wave functions for the lower states are apparently involved, and a practically more useful formulation which avoids this difficulty has been given by Hylleraas and Undheim[2] and by MacDonald.[3] Introducing an arbitrary orthonormal set $\Phi_1, \Phi_2, \Phi_3\cdots\Phi_n$ of order n and the associated nth-order energy matrix having the elements

$$H_{kl}=\langle\Phi_k|H|\Phi_l\rangle\,, \tag{3}$$

they have shown that its n eigenvalues are, in order, upper bounds to the true eigenvalues $E_0, E_1, E_2, \cdots E_{n-1}$.

The problem of finding convenient lower bounds to the eigenvalues E_k seems to be considerably more difficult, and it has been approached in many different ways. In matrix theory, there are several theorems available about localization of characteristic roots, and the most well known is the Hadamard-Gershgorin theorem[4] which says that, in each one of the complex circles

$$|z-H_{kk}|=\sum_{l\neq k}|H_{kl}|\,, \tag{4}$$

there is at least one eigenvalue E. For generalizations and surveys of the rich literature in this field, we will refer to the recent papers by Minc[5] and Householder.[6]

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[5] H. Minc, Report from the Mathematics Department, University of Florida, 1961 (unpublished).

[6] A. S. Householder, Mathematics Research Center, U. S. Army, University of Wisconsin, Publication No. 12, 1963 (unpublished).

It is evident that this approach is useful in connection with the Schrödinger equation only if the underlying basis is complete and one deals with infinite matrices.

Other studies are based on the concept of the width ΔH of the Hamiltonian defined by the expression

$$(\Delta H)^2=\int|(H\Phi-\langle H\rangle\Phi)|^2(dx) \\ =\langle H\Phi|H\Phi\rangle-\langle\Phi|H|\Phi\rangle^2\geq 0, \tag{5}$$

with $\langle\Phi|\Phi\rangle=1$. This quantity vanishes if and only if Φ is an eigenfunction to H. Introducing the value E_1 of the first excited state, Temple[7] has given the following lower bound:

$$E_0\geq\langle H\rangle-\frac{(\Delta H)^2}{E_1-\langle H\rangle}, \tag{6}$$

provided that the approximation is so good that $\langle H\rangle<E_1$. Using a similar approach, D. H. Weinstein[8] has shown that the eigenvalue E_k situated closest to $\langle H\rangle$ satisfies the relation

$$\langle H\rangle-\Delta H\leq E_k\leq\langle H\rangle+\Delta H. \tag{7}$$

Another modification has been given by Stevenson.[9] Formulas of these types have been used in determining lower bounds for the ground-state energy of the helium atom.[10] Some illustrative examples have further been given by Bailey and Kinsey.[11]

An entirely different approach to the problem of lower bounds has been taken by Alexander Weinstein[12] and his school by using the method of so-called "intermediate" Hamiltonians. There is constructed a set of operators $H^{(1)}\leq H^{(2)}\leq H^{(3)}\leq\cdots\leq H$ converging towards the given Hamiltonian, and the associated eigenvalues in order then fulfill the inequalities

$$E_k^{(1)}\leq E_k^{(2)}\leq E_k^{(3)}\leq\cdots\leq E_k, \tag{8}$$

providing a set of lower bounds converging towards the exact eigenvalue. The method is very forceful and may be applied to systems with various types of constraint. For a Hamiltonian of the form $H=H_0+V$, where V is a positive-definite perturbation, one may consider the intermediate Hamiltonians:

$$H^{(n)}=H_0+V^{1/2}O^{(n)}V^{1/2}, \tag{9}$$

where $O^{(n)}$ is the operator for the orthogonal projection on an arbitrary subspace of order n, which for $n\rightarrow\infty$ converges towards the identity operator.[13] Many fundamental problems in quantum theory have, in this way, been studied by Bazley and Fox.[14]

In this paper, we will use a new tool in the study of upper and lower bounds to energy eigenvalues. In the partitioning technique[15] for solving the Schrödinger equation, there exists a first-order iteration procedure $\mathcal{E}_{k+1}=f\{\mathcal{E}_k\}$ which generates a set of numbers $\mathcal{E}_0$, $\mathcal{E}_1$, $\mathcal{E}_2$, $\mathcal{E}_3$, $\cdots$ such that between any two consecutive numbers there is at least one true eigenvalue E. Such a series provides hence upper and lower bounds, and the main problem is to evaluate the quantities involved.

2. OUTER AND INNER PROJECTIONS; ORDERING THEOREMS FOR EIGENVALUES

Outer projections. Let O be an arbitrary projection operator characterized by the relations

$$O^2=O,\quad O^\dagger=O,\quad \mathrm{Tr}(O)=n, \tag{10}$$

and which selects a certain subspace of the Hilbert space of finite or infinite order n. For the moment, it is not necessary to specify the explicit form of this operator. Let us further consider a self-adjoint operator A bounded from below having the eigenvalues a_k and the normalized eigenfunctions u_k:

$$Au_k=a_ku_k. \tag{11}$$

We will define the "outer projection" $\bar{A}$ of this operator with respect to the subspace O by the relation

$$\bar{A}=OAO. \tag{12}$$

It is evident that every function in the complementary subspace associated with the projection operator $(1-O)$ is an eigenfunction of $\bar{A}$ associated with the eigenvalue 0, but these functions are usually of little use. Instead we will concentrate our interest on the eigenfunctions $\bar{u}_k$ situated within the subspace O:

$$\bar{A}\bar{u}_k=\bar{a}_k\bar{u}_k,\quad O\bar{u}_k=\bar{u}_k,\quad\langle\bar{u}_k|\bar{u}_k\rangle=1. \tag{13}$$

For these functions, one has the theorem that the eigenvalues of $\bar{A}$ are upper bounds to the eigenvalues of A

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in order:

$$a_k \leq \bar{a}_k. \tag{14}$$

The proof is very simple. According to the variation principle, one has

$$a_1 = \langle u_1 | A | u_1 \rangle \leq \langle \bar{u}_1 | A | \bar{u}_1 \rangle = \langle \bar{u}_1 | O^\dagger A O | \bar{u}_1 \rangle = \langle \bar{u}_1 | \bar{A} | \bar{u}_1 \rangle = \bar{a}_1. \tag{15}$$

Next, we will consider the auxiliary function $\varphi = \bar{u}_1\beta_1 + \bar{u}_2\beta_2$ subject to the conditions

$$\begin{aligned} \langle u_1 | \varphi \rangle &= \langle u_1 | \bar{u}_1 \rangle \beta_1 + \langle u_1 | \bar{u}_2 \rangle \beta_2 = 0, \\ \langle \varphi | \varphi \rangle &= |\beta_1|^2 + |\beta_2^2| = 1, \end{aligned} \tag{16}$$

and satisfying the relation $O\varphi = \varphi$. Since φ is assumed orthogonal to u_1, the variation principle gives

$$\begin{aligned} a_2 &\leq \langle \varphi | A | \varphi \rangle = \langle O\varphi | A | O\varphi \rangle = \langle \varphi | O^\dagger A O | \varphi \rangle \\ &= \langle \varphi | \bar{A} | \varphi \rangle = \langle \bar{u}_1\beta_1 + \bar{u}_2\beta_2 | \bar{A} | \bar{u}_1\beta_1 + \bar{u}_2\beta_2 \rangle \\ &= \bar{a}_1 |\beta_1|^2 + \bar{a}_2 |\beta_2|^2 \leq \bar{a}_2. \end{aligned} \tag{17}$$

Next, we will consider the auxiliary function $\varphi = \bar{u}_1\beta_1 + \bar{u}_2\beta_2 + \bar{u}_3\beta_3$ subject to the conditions $\langle u_1 | \varphi \rangle = \langle u_2 | \varphi \rangle = 0$, $\langle \varphi | \varphi \rangle = 1$, and satisfying the relation $O\varphi = \varphi$, and the variation principle gives immediately

$$a_3 \leq \bar{a}_3, \quad \text{etc.} \tag{18}$$

The projection operator O may be defined in different ways. If $\mathbf{f} = (f_1, f_2, f_3, \cdots f_n)$ is a set of n linearly independent vectors in Hilbert space having the metric matrix $\boldsymbol{\Delta} = \mathbf{f}^\dagger\mathbf{f}$, i.e., $\Delta_{kl} = \langle f_k | f_l \rangle$, and spanning the subspace M_n, then the projection operator associated with this manifold is given by the relation

$$\begin{aligned} O &= \mathbf{f}\boldsymbol{\Delta}^{-1}\mathbf{f}^\dagger \\ &= \sum_{kl} |f_k\rangle \Delta^{-1}{}_{kl} \langle f_l| \end{aligned} \tag{19}$$

(see Appendix A). The infinite set $(f_1, f_2, f_3, \cdots)$ is complete, if and only if the associated projection operator is identical with the identity operator, in which case (19) represents a "resolution of the identity."

It is often convenient to choose an orthonormal basis $\boldsymbol{\Phi} = (\Phi_1, \Phi_2, \Phi_3, \cdots \Phi_n)$ with $\langle \Phi_k | \Phi_l \rangle = \delta_{kl}$, and the projection operator has then the form $O = \boldsymbol{\Phi}\boldsymbol{\Phi}^\dagger = \sum_k |\Phi_k\rangle\langle\Phi_k|$. Within this subspace the outer projection $\bar{A} = OAO$ is then exactly represented by the nth-order matrix $\bar{A}$ having the elements $A_{kl} = \langle \Phi_k | A | \Phi_l \rangle$, obtained by truncation from the infinite-order matrix A. In this case, the ordering theorem (14) says that the characteristic roots $\bar{a}_k$ of any finite matrix are, in order, upper bounds to the n lowest eigenvalues a_k and that, further, these upper bounds decrease with increasing order of the matrix. This gives a new proof of the previously quoted theorem by Hylleraas and Undheim[2] and by MacDonald.[3]

In conclusion, we note that the eigenvalue problem (13) for the operator $\bar{A} = OAO$ is also closely associated with the problem of finding the extreme values of the integral $I = \langle \bar{u} | A | \bar{u} \rangle / \langle \bar{u} | \bar{u} \rangle$ for functions $\bar{u}$ which belong to the subspace of O, i.e., satisfying the condition $O\bar{u} = \bar{u}$. This problem is further discussed in Appendix B.

Inequalities for operators. Let us consider two self-adjoint operators A and B which are both bounded from below. One is using the inequality notation

$$A < B, \tag{20}$$

if $\langle \varphi | A | \varphi \rangle < \langle \varphi | B | \varphi \rangle$ for all possible φ, and, further, the domain of B belongs entirely to the domain of A. If the eigenvalues of A and B are denoted by a_k and b_k, respectively, one has the theorem

$$a_k < b_k, \tag{21}$$

in order. We note that (21) is a consequence of (20), whereas the reverse is in general not true. The proof of (21) is simple and starts from the eigenvalue relations

$$Au_k = a_k u_k, \quad Bv_k = b_k v_k. \tag{22}$$

The variation principle gives immediately

$$a_1 \leq \langle v_1 | A | v_1 \rangle < \langle v_1 | B | v_1 \rangle = b_1. \tag{23}$$

Next one considers the auxiliary function $\varphi = v_1\beta_1 + v_2\beta_2$ subject to the conditions $\langle u_1 | \varphi \rangle = 0$, $\langle \varphi | \varphi \rangle = 1$. Since φ is orthogonal to u_1, the variation principle gives

$$\begin{aligned} a_2 &\leq \langle \varphi | A | \varphi \rangle < \langle \varphi | B | \varphi \rangle \\ &= \langle v_1\beta_1 + v_2\beta_2 | B | v_1\beta_1 + v_2\beta_2 \rangle \\ &= b_1 |\beta_1|^2 + b_2 |\beta_2|^2 \leq b_2. \end{aligned} \tag{24}$$

Next one considers the auxiliary function $\varphi = v_1\beta_1 + v_2\beta_2 + v_3\beta_3$, subject to the conditions $\langle u_1 | \varphi \rangle = \langle u_2 | \varphi \rangle = 0$, $\langle \varphi | \varphi \rangle = 1$, and the variation principle gives

$$a_3 \leq b_3, \quad \text{etc.} \tag{25}$$

The ordering theorem (21) is of fundamental importance in Weinstein's approach using the method of intermediate problems.[12]

Inner projections. Let us consider a self-adjoint operator A, which is also assumed to be positive-definite so that $A > 0$. If the eigenvalues and eigenfunctions are denoted by a_k and u_k, respectively, one has the spectral resolution

$$A = \sum_k a_k |u_k\rangle\langle u_k|, \tag{26}$$

where $a_k > 0$. One can further define the "positive square root" by the relation

$$A^{1/2} = \sum_k a_k^{1/2} |u_k\rangle\langle u_k|, \tag{27}$$

and this operator may then be used to define the so-called "inner projection"

$$A' = A^{1/2} O A^{1/2}, \tag{28}$$

which satisfies the important inequality

$$0 < A' < A. \tag{29}$$

In order to prove this statement, we observe that every

projection operator O satisfying (10) is necessarily positive-definite:

$$\langle\varphi|O|\varphi\rangle=\langle\varphi|O^2|\varphi\rangle=\langle\varphi|O^\dagger O|\varphi\rangle =\langle O\varphi|O\varphi\rangle\geq 0. \tag{30}$$

Since the same applies to the projection operator for the orthogonal complement $P=1-O\geq 0$, one gets finally the inequality

$$0\leq O\leq 1, \tag{31}$$

i.e., $0\leq\langle\varphi|O|\varphi\rangle\leq\langle\varphi|\varphi\rangle$. Replacing φ by $A^{1/2}\varphi$, this gives $0\leq\langle\varphi|A^{1/2}OA^{1/2}|\varphi\rangle\leq\langle\varphi|A|\varphi\rangle$, which proves theorem (29).

The inner projection on a linear manifold M_n characterized by the projection operator (19) is hence

$$A'=A^{1/2}\mathbf{f}\boldsymbol{\Delta}^{-1}\mathbf{f}^\dagger A^{1/2}, \tag{32}$$

where $\boldsymbol{\Delta}=\mathbf{f}^\dagger\mathbf{f}=\langle\mathbf{f}|\mathbf{f}\rangle$ is a finite matrix of order n. Making the substitution $\mathbf{f}=A^{1/2}\mathbf{g}$, one obtains the alternative form

$$A'=A\,\mathbf{g}\boldsymbol{\Delta}^{-1}\mathbf{g}^\dagger A, \tag{33}$$

where $\boldsymbol{\Delta}^{-1}$ is now the inverse of the matrix $\boldsymbol{\Delta}=\mathbf{g}^\dagger A\,\mathbf{g}=\langle\mathbf{g}|A|\mathbf{g}\rangle$. This important form is due to Aronszajn,[13] who derived it by considering a linear space having a scalar product $[g_k,g_l]=\langle g_k|A|g_l\rangle$. If one instead makes the substitution $\mathbf{f}=A^{-1/2}\mathbf{h}$, one obtains another form

$$A'=\mathbf{h}\boldsymbol{\Delta}^{-1}\mathbf{h}^\dagger, \tag{34}$$

where $\boldsymbol{\Delta}=\mathbf{h}^\dagger A^{-1}\mathbf{h}=\langle\mathbf{h}|A^{-1}|\mathbf{h}\rangle$, which has been used particularly by Bazley.[14] We note that the three forms (32), (33), and (34) are essentially equivalent, except for the domains of the operators involved. In Eq. (9) one has utilized the inner projection of a positive-definite perturbation V and, according to (29), one has

$$H^{(1)}<H^{(2)}<H^{(3)}<\cdots<H. \tag{35}$$

The ordering theorem (21) gives then

$$E_k^{(1)}<E_k^{(2)}<E_k^{(3)}<\cdots<E_k, \tag{36}$$

i.e., a set of lower bounds converging towards the true eigenvalue. These relations form the essential basis for the work carried out by Bazley and Fox.[14]

The method of "intermediate Hamiltonians" based on the inequalities (20) and (21) is a very powerful tool for determining lower bounds, but it has the difficulty that one necessarily must know the eigenvalues a_k and b_k *in order*, since otherwise (21) becomes meaningless. In the following, we will utilize the ideas of outer and inner projections at the same time as we will try avoiding a specific ordering of the eigenvalues.

3. PARTITIONING TECHNIQUE; BRACKETING THEOREM

In order to solve the Schrödinger equation (1), we will introduce a normalized *reference function* φ, $\langle\varphi|\varphi\rangle=1$, and the associated projection operator $O=|\varphi\rangle\langle\varphi|$, satisfying the relations

$$O^2=O,\quad O^\dagger=O,\quad \mathrm{Tr}(O)=1. \tag{37}$$

It is further convenient to introduce the projection operator $P=1-O$ for the orthogonal complement satisfying the relations

$$P^2=P,\quad P^\dagger=P,\quad OP=PO=0. \tag{38}$$

The key operator[15] in the treatment is the "reduced resolvent" T defined strictly by the equation

$$T=P[\alpha\cdot O+P(\mathcal{E}-H)P]^{-1}P, \tag{39}$$

for $\alpha\neq 0$, and given the symbolic notation

$$T=P/(\mathcal{E}-H), \tag{40}$$

where $\mathcal{E}$ is a variable which may vary over the real axis or over the entire complex plane. It is easily shown that it satisfies the following equations:

$$OT=TO=0, \tag{41}$$

$$P(\mathcal{E}-H)T=P. \tag{42}$$

Let us now consider the auxiliary function $\phi=\phi_\mathcal{E}$, defined by the relation

$$\phi_\mathcal{E}=TH\varphi. \tag{43}$$

Multiplying (43) to the left by the operator $P(\mathcal{E}-H)$ and using (42), one obtains $P(\mathcal{E}-H)\phi_\mathcal{E}=PH\varphi$. Substituting $P=1-O=1-|\varphi\rangle\langle\varphi|$, one gets, further,

$$(\mathcal{E}-H)\phi+\varphi\langle\varphi|H|\phi_\mathcal{E}\rangle=H\varphi-\varphi\langle\varphi|H|\varphi\rangle, \tag{44}$$

where we have utilized the fact that $\langle\varphi|\phi(\mathcal{E})\rangle=0$ according to (41). Introducing the new notation

$$\mathcal{E}_1=\langle\varphi|H|\varphi\rangle+\langle\varphi|H|\phi_\mathcal{E}\rangle, \tag{45}$$

one can write (44) in the simple form

$$(H-\mathcal{E})(\varphi+\phi(\mathcal{E}))=(\mathcal{E}_1-\mathcal{E})\varphi. \tag{46}$$

The function $\Psi_\mathcal{E}=\varphi+\phi_\mathcal{E}$ may be denoted as the "trial wave function" associated with the parameter $\mathcal{E}$ and characterized by the "intermediate" normalization $\langle\varphi|\Psi_\mathcal{E}\rangle=1$, which is valid both for the discrete and continuous part of the spectrum. Here we will concen-

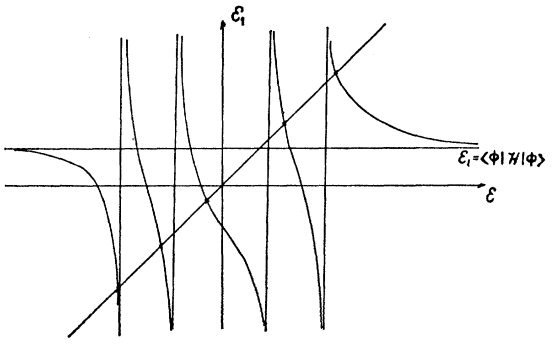

FIG. 1. The bracketing function $\mathcal{E}_1=f(\mathcal{E})$.

trate our interest on the discrete levels. We note that Ψ_ε satisfies the Schrödinger equation (1), if and only if $\mathcal{E}_1=\mathcal{E}=E$:

$$(H-E)\Psi_E=0. \tag{47}$$

In general, $\mathcal{E}_1$ is a function of $\mathcal{E}$ defined by (43) and (45) or by the relation

$$\mathcal{E}_1=\langle\varphi|H+H(P/(\mathcal{E}-H))H|\varphi\rangle\equiv f(\mathcal{E}). \tag{48}$$

The eigenvalues satisfy the equation $E=f(E)$. By means of (46), one now finds easily the expectation value of H with respect to the trial function Ψ_ε:

$$\begin{aligned}\langle H_{op}\rangle_{av}&=\mathcal{E}+\frac{\langle\Psi_\varepsilon|H-\mathcal{E}|\Psi_\varepsilon\rangle}{\langle\Psi_\varepsilon|\Psi_\varepsilon\rangle}\\&=\mathcal{E}+(\mathcal{E}_1-\mathcal{E})/(1+\langle\phi_\varepsilon|\phi_\varepsilon\rangle).\end{aligned} \tag{49}$$

If one constructs the curve corresponding to $\mathcal{E}_1=f(\mathcal{E})$, it has a series of vertical asymptotes usually situated at the eigenvalues of the outer projection PHP and the horizontal asymptote $\mathcal{E}_1=\langle\varphi|H|\varphi\rangle$; see Fig. 1. For the derivative, one obtains

$$\begin{aligned}f'(\mathcal{E})&=-\langle\varphi|H(P/(\mathcal{E}-H)^2)H|\varphi\rangle\\&=-\langle\phi_\varepsilon|\phi_\varepsilon\rangle<0;\end{aligned} \tag{50}$$

i.e., the derivative is always negative and the curve descending. On each branch of the curve, there is exactly one crossing point $(E;E)$ between the line $\mathcal{E}_1=\mathcal{E}$ and the curve $\mathcal{E}_1=f(\mathcal{E})$. The geometrical construction shows that, for any value of $\mathcal{E}$ associated with a particular branch, there is a value $\mathcal{E}_1$ such that the pair $(\mathcal{E},\mathcal{E}_1)$ brackets the true eigenvalue E of the branch involved.

Analytically this may be proven by putting $\mathcal{E}_1=E+\epsilon_1$ and $\mathcal{E}=E+\epsilon$, and the use of Lagrange's mean-value theorem gives then

$$\begin{aligned}&E+\epsilon_1=f(E)+\epsilon f'(E+\theta\epsilon),\\ \text{and}\qquad&\\&\epsilon_1=\epsilon f'(E+\theta\epsilon),\end{aligned} \tag{51}$$

where $0\leq\theta\leq1$. This formula indicates that ϵ and ϵ_1 have different signs, which proves the bracketing theorem.

The function (48) may be used to construct a first-order iteration process. Starting out from a specific number $\mathcal{E}_0$, one defines the set

$$\begin{aligned}\mathcal{E}_1&=f(\mathcal{E}_0),\\ \mathcal{E}_2&=f(\mathcal{E}_1),\\ &\cdots\cdots\cdots\\ \mathcal{E}_{k+1}&=f(\mathcal{E}_k).\end{aligned} \tag{52}$$

According to (51), any two consecutive values $\mathcal{E}_k$ and $\mathcal{E}_{k+1}$ are then going to "bracket" a true eigenvalue E. The series is convergent if $|f'|<1$, whereas it is divergent if $|f'|>1$. In both cases, the first-order process may be replaced by a second-order iteration process

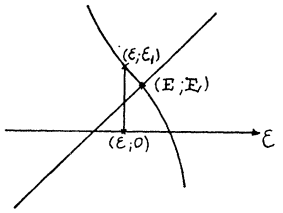

FIG. 2. Graphical demonstration of the bracketing theorem.

based on the Aitken-Samuelson formula[16]:

$$\mathcal{E}_0^*=\mathcal{E}_0-\frac{(\mathcal{E}_1-\mathcal{E}_0)^2}{\mathcal{E}_0-2\mathcal{E}_1+\mathcal{E}_2}, \tag{53}$$

and the iterations take the form $\mathcal{E}_0$, $\mathcal{E}_1$, $\mathcal{E}_2$; $\mathcal{E}_0^*$, $\mathcal{E}_1^*$, $\mathcal{E}_2^*$; $\mathcal{E}_0^{**}$, $\mathcal{E}_1^{**}$, $\mathcal{E}_2^{**}$; etc. An alternative procedure is based on Newton-Raphson's tangential method for solving an equation of the type $F(E)=0$:

$$\mathcal{E}^*=\mathcal{E}-F(\mathcal{E})/F'(\mathcal{E}). \tag{54}$$

Putting $F(\mathcal{E})=\mathcal{E}-f(\mathcal{E})=\mathcal{E}-\mathcal{E}_1$ and using (50), one obtains $F'(\mathcal{E})=1+\langle\phi_\varepsilon|\phi_\varepsilon\rangle$, and (54) leads then to an expression identical with the expectation value (49), so that

$$\mathcal{E}^*=\frac{\langle\Psi_\varepsilon|H|\Psi_\varepsilon\rangle}{\langle\Psi_\varepsilon|\Psi_\varepsilon\rangle}. \tag{55}$$

There is hence a close connection between the tangential construction in (54) and the quantum-mechanical variation principle.[15]

Resolvent Operator Formulas. In the previous section, we have used the "reduced" resolvent T defined by (39) and (40), and the question is whether similar formulas can be derived using the full resolvent $(\mathcal{E}-H)^{-1}$. For this purpose, we will introduce the function

$$\chi=(\mathcal{E}-H)^{-1}\varphi, \tag{56}$$

subject to the condition that the scalar products $\langle\varphi|\chi\rangle$ and $\langle\chi|\chi\rangle$ should exist. If the Hamiltonian H has the eigenvalues E_k and the eigenfunctions Ψ_k, and the latter are associated with the projection operators $O_k=|\Psi_k\rangle\langle\Psi_k|$, one has the fundamental relations

$$1=\sum_k O_k,\quad H=\sum_k E_kO_k, \tag{57}$$

corresponding to the "resolution of the identity" and the spectral resolution of the operator H, respectively. A function $f(H)$ of the operator H is defined by the relation $f(H)=\sum_k f(E_k)O_k$, and for the resolvent one

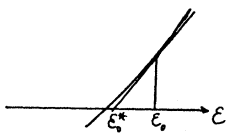

FIG. 3. Application of the Newton-Raphson method.

[16] A. C. Aitken, Proc. Roy. Soc. (Edinburgh) **46**, 289 (1925); P. A. Samuelson, J. Math. & Phys. **24**, 131 (1945).

has particularly

$$(\mathcal{E}-H)^{-1}=\sum_k(\mathcal{E}-E_k)^{-1}O_k. \tag{58}$$

If $\mathcal{E}$ is approaching a particular eigenvalue E_n, the coefficient for the associated projection operator O_n is "blowing up," and one obtains

$$\lim_{\mathcal{E}\to E_n}\frac{\chi}{\langle\varphi|\chi\rangle}=\frac{\Psi_n}{\langle\varphi|\Psi_n\rangle}, \tag{59}$$

showing that the function $\chi/\langle\varphi|\chi\rangle$ goes over into an eigenfunction.

The connection between the two approaches is rendered by Eq. (46) which gives

$$\begin{aligned}\Psi(\mathcal{E})&=(\mathcal{E}-\mathcal{E}_1)(\mathcal{E}-H)^{-1}\varphi,\\&=(\mathcal{E}-\mathcal{E}_1)\chi,\end{aligned} \tag{60}$$

i.e., the previous trial function $\Psi(\mathcal{E})$ is proportional to χ. Further, since $1=\langle\varphi|\Psi_\mathcal{E}\rangle=(\mathcal{E}-\mathcal{E}_1)\langle\varphi|\chi\rangle$, one obtains

$$\begin{aligned}\mathcal{E}_1&=\mathcal{E}-\langle\varphi|\chi\rangle^{-1},\\&=\mathcal{E}-\langle\varphi|(\mathcal{E}-H)^{-1}|\varphi\rangle^{-1},\end{aligned} \tag{61}$$

which relation replaces (48) and gives

$$\Psi_\mathcal{E}=\chi/\langle\varphi|\chi\rangle. \tag{62}$$

By means of (61), it is easily proven that $\mathcal{E}$ and $\mathcal{E}_1$ bracket a true eigenvalue E. Introducing the function

$$F(\mathcal{E})=\langle\varphi|\chi\rangle^{-1}=\langle\varphi|(\mathcal{E}-H)^{-1}|\varphi\rangle^{-1}, \tag{63}$$

one finds that the eigenvalues satisfy the relation $F(E)=0$ and that the Newton-Raphson rule (54) takes the form

$$\mathcal{E}^*=\mathcal{E}-\langle\varphi|\chi\rangle/\langle\chi|\chi\rangle. \tag{64}$$

In summary, we have hence the following four relations:

$$\begin{aligned}(\mathcal{E}-H)\chi&=\varphi;\\\Psi_\mathcal{E}&=\langle\varphi|\chi\rangle^{-1}\chi;\\\mathcal{E}_1&=\mathcal{E}-\langle\varphi|\chi\rangle^{-1};\\\mathcal{E}^*&=\mathcal{E}-\langle\varphi|\chi\rangle\langle\chi|\chi\rangle^{-1}.\end{aligned} \tag{65}$$

The first is an inhomogeneous equation defining the function χ, the second defines the trial function $\Psi(\mathcal{E})$, the third is connected with the bracketing theorem, and the fourth with the variation principle. It is hence possible to develop a theory based on the use of the complete resolvent $(\mathcal{E}-H)^{-1}$ but, from practical points of view, it is often more convenient to carry out the limiting procedure $\mathcal{E}\to E_k$ in a formalism based on the "reduced" resolvent $T=P/(\mathcal{E}-H)$. This applies particularly to the considerations in perturbation theory.[16a]

4. PERTURBATION THEORY. WAVE AND REACTION OPERATORS

In perturbation theory, one assumes that the Hamiltonian may be written in the form $H=H_0+V$, where the perturbation V is here not necessarily assumed to be small. As reference function φ, we will choose the normalized eigenfunction φ_0 of H_0 associated with the unperturbed eigenvalue E_0 under consideration, so that $H_0\varphi_0=E_0\varphi_0$. It is here not necessary to introduce all the eigenfunctions to H_0; for our considerations it is sufficient to introduce a single eigenfunction φ_0, the associated projection operator $O=|\varphi_0\rangle\langle\varphi_0|$, and the projection operator for the orthogonal complement $P=1-O$. Since $T\varphi_0=0$, one gets the simplification $TH\varphi_0=T(H_0+V)\varphi_0=T(E_0+V)\varphi_0=TV\varphi_0$. Using (43) and (48), one obtains the reduced formulas

$$\Psi_\mathcal{E}=\varphi_0+TH\varphi_0=(1+TV)\varphi_0, \tag{66}$$

$$\begin{aligned}\mathcal{E}_1&=\langle\varphi_0|H+HTH|\varphi_0\rangle\\&=E_0+\langle\varphi_0|V+VTV|\varphi_0\rangle.\end{aligned} \tag{67}$$

In this connection, it is convenient to introduce the *wave operator* W and the *reaction operator* t through the relations

$$W=1+TV, \tag{68}$$

$$t=V+VTV=VW, \tag{69}$$

and (66) and (67) can then be written in the form

$$\Psi_\mathcal{E}=W\varphi_0,\quad \mathcal{E}_1=E_0+\langle\varphi_0|t|\varphi_0\rangle. \tag{70}$$

The operators W and t will here be considered as functions of the parameter $\mathcal{E}$, and $\mathcal{E}$ and $\mathcal{E}_1$ will be used to bracket the true eigenvalues E. According to (49) and (55), one obtains, further, the expectation value

$$\begin{aligned}\mathcal{E}^*=\langle H_{\rm op}\rangle_{\rm av}&=\mathcal{E}+\frac{\mathcal{E}_1-\mathcal{E}_0}{1+\langle\varphi_0|VT^2V|\varphi_0\rangle}\\&=E_0+\frac{\langle\varphi_0|V+VTV+(\mathcal{E}-E_0)VT^2V|\varphi_0\rangle}{1+\langle\varphi_0|VT^2V|\varphi_0\rangle}.\end{aligned} \tag{71}$$

We note that, for $\mathcal{E}_1=\mathcal{E}=E$, the wave operator transforms the unperturbed eigenfunction into the perturbed one, whereas the expectation value of the reaction operator gives the energy shift.

In addition to T, it is now feasible to introduce the reduced resolvent T_0 for the unperturbed Hamiltonian H_0:

$$T_0=P/(\mathcal{E}-H_0). \tag{72}$$

The notation is, of course, symbolic, and T_0 is more strictly defined by the relation

$$T_0=P[\alpha\cdot O+P(\mathcal{E}-H_0)P]^{-1}P$$

analogous to (39). For an inverse operator, one has the identity

$$(A-B)^{-1}\equiv A^{-1}+A^{-1}B(A-B)^{-1}, \tag{73}$$

which is easily proven by multiplying both members to the right by $(A-B)$. Putting $A=\alpha\cdot O+P(\mathcal{E}-H_0)P$ and $B=PVP$ in (39), one obtains the identity

$$T=T_0+T_0VT=T_0(1+VT). \tag{74}$$

[16a] G. Speisman, Phys. Rev. **107**, 1180 (1957); W. H. Young and N. H. March, Phys. Rev. **109**, 1854 (1957); R. Yaris, J. Chem. Phys. **40**, 1891 (1964).

By means of (69), this gives, further

$$TV=T_0t, \tag{75}$$

$$t=V+VT_0t. \tag{76}$$

The last relation is the well-known Lippmann-Schwinger equation[17] which is here presented in a derivation given by Ohno.[18] From (76), one obtains $(1-VT_0)t=V$ and $(V^{-1}-T_0)t=1$, provided V^{-1} exists. Hence one has

$$t=(V^{-1}-T_0)^{-1}, \tag{77}$$

which relation forms the starting point for our treatment of lower and upper bounds for the energy eigenvalues.

5. UPPER AND LOWER BOUNDS FOR THE REACTION OPERATOR

Estimates of T_0. In order to treat T_0, it may temporarily be convenient to introduce the eigenvalues E_k^0 to H_0, the eigenfunctions φ_k^0, and the associated projection operators $O_k^0=|\varphi_k^0\rangle\langle\varphi_k^0|$. Assuming that the set of eigenfunctions $|\varphi_k^0\rangle$ is complete, one has the following resolution of the identity:

$$1=\sum_{k=0}^{\infty} O_k^0. \tag{78}$$

The summation sign implies that one should sum over the discrete eigenvalues and integrate over the continuous part of the spectrum. Analogous to (58), one obtains for the reduced resolvent

$$T_0=\frac{P}{\mathcal{E}-H_0}=\sum_{k=1}^{\infty}\frac{O_k^0}{\mathcal{E}-E_k^0}, \tag{79}$$

where we have omitted the term associated with φ_0 because of the operator P. In the following, we will assume that φ_0 is associated with the *ground state* of H_0 and that the variable $\mathcal{E}$ is subject to the condition

$$\mathcal{E}<E_1^0. \tag{80}$$

This implies that all the denominators in (79) are negative and that T_0 is hence a negative-definite operator

$$T_0<0. \tag{81}$$

Arranging the eigenvalues in order, $E_0^0<E_1^0\leq E_2^0\leq E_3^0\leq\cdots$, one has

$$1/(E_1^0-\mathcal{E})\geq 1/(E_2^0-\mathcal{E})\geq 1/(E_3^0-\mathcal{E})\geq\cdots. \tag{82}$$

Hence one obtains the estimate

$$-T_0=\sum_{k=1}^{\infty}\frac{O_k^0}{E_k^0-\mathcal{E}}\leq\sum_{k=1}^{\infty}\frac{O_k^0}{E_1^0-\mathcal{E}}=\frac{1}{E_1^0-\mathcal{E}}(1-O_0^0);\qquad T_0\geq -P/(E_1^0-\mathcal{E}). \tag{83}$$

A still better bound is rendered by keeping p terms in the sum (79) intact and estimating the remainder:

$$\begin{aligned}-T_0&=\sum_{k=1}^{p}\frac{O_k^0}{E_k^0-\mathcal{E}}+\sum_{k=p+1}^{\infty}\frac{O_k^0}{E_k^0-\mathcal{E}}\\&\leq\sum_{k=1}^{p}\frac{O_k^0}{E_k^0-\mathcal{E}}+\frac{1}{E_{p+1}^0-\mathcal{E}}\sum_{k=p+1}^{\infty}O_k^0\\&=\sum_{k=1}^{p}\frac{O_k^0}{E_k^0-\mathcal{E}}+\frac{1}{E_{p+1}^0-\mathcal{E}}\{P-\sum_{k=1}^{p}O_k^0\}\equiv -T_0(p).\end{aligned} \tag{84}$$

The quantity $-T_0(p)$ for $p=0, 1, 2, \cdots$ gives hence a convenient upper bound for the operator $-T_0$; we note that this approach is closely analogous to the "method of truncation" of H_0 introduced by Bazley and Fox.[14] The formula (84) may be used to obtain a lower bound for T_0 if an exact evaluation for some reason turns out to be difficult.

Some inequalities for operators. Let us start by considering two self-adjoint operators A and B which satisfy the inequality

$$A>B, \tag{85}$$

according to the definition in (20), so that $\langle\varphi|A|\varphi\rangle>\langle\varphi|B|\varphi\rangle$. Replacing φ by $\Omega\varphi$, where Ω is an arbitrary linear operator, one obtains $\langle\varphi|\Omega^\dagger A\Omega|\varphi\rangle>\langle\varphi|\Omega^\dagger B\Omega|\varphi\rangle$, i.e.,

$$\Omega^\dagger A\Omega>\Omega^\dagger B\Omega, \tag{86}$$

which is a very useful theorem.

Previously we have considered the identity (73), and we will now study the two identities for $(A-B)^{-1}$ which are valid for the left-inverse and right-inverse, respectively:

$$(A-B)^{-1}\equiv A^{-1}+A^{-1}B(A-B)^{-1}, \tag{87}$$

$$(A-B)^{-1}\equiv A^{-1}+(A-B)^{-1}BA^{-1}. \tag{88}$$

They are easily proven by multiplying the two relations by $(A-B)$ to the right and left, respectively. Substituting the second identity into the right-hand member of the first, one obtains the "symmetric" identity

$$(A-B)^{-1}\equiv A^{-1}+A^{-1}BA^{-1}+A^{-1}B(A-B)^{-1}BA^{-1}, \tag{89}$$

which will be used to derive upper and lower bounds for operators.

Let us start by considering two operators A and B which are positive-definite and satisfy the inequality

$$A>B>0. \tag{90}$$

It follows that the operators A^{-1} and B^{-1} exist, are positive, and satisfy the inequality

$$A^{-1}<B^{-1}. \tag{91}$$

A simple proof is based on the symmetric identity (89) which gives

$$\begin{aligned}B^{-1}&\equiv[A-(A-B)]^{-1}\\&\equiv A^{-1}+A^{-1}(A-B)A^{-1}\\&\quad+A^{-1}(A-B)B^{-1}(A-B)A^{-1}.\end{aligned} \tag{92}$$

[17] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).
[18] K. Ohno, Lecture in Uppsala, 1957 (unpublished).

Since $(A-B)$ and B^{-1} are positive-definite, the two last terms are positive-definite, which proves that $B^{-1}>A^{-1}$.

Upper and lower bounds to the reaction operator. According to (70), the two quantities $\mathcal{E}$ and $\mathcal{E}_1$, which bracket a true eigenvalue E, are connected by the relation

$$\mathcal{E}_1=E_0+\langle\varphi_0|t|\varphi_0\rangle. \tag{93}$$

It is easy to give upper and lower bounds for the last term in the case when the reaction operator t is *positive-definite.* As before, we will assume that $\mathcal{E}<E_1^0$, i.e., that the condition (80) is fulfilled, which implies that T_0 is negative-definite. According to (77), one has the relation

$$t^{-1}=V^{-1}-T_0, \tag{94}$$

which means that t^{-1} (and hence t) will be positive definite, if and only if

$$V^{-1}>T_0. \tag{95}$$

In the following, we will mainly consider the case of a *positive definite perturbation* V, and the inequality (95) is then always fulfilled. From (94) follows that $t^{-1}=V^{-1}-T_0>V^{-1}>0$, and application of (91) gives then immediately

$$0<t<V. \tag{96}$$

The perturbation V is hence an upper bound for the reaction operator t.

Next we will try to improve the lower bound for t. Putting $a=t^{1/2}\varphi_0$ and $b=t^{-1/2}\varphi_0$ into Schwarz inequality $|\langle a|b\rangle|^2\leq\langle a|a\rangle\langle b|b\rangle$, one obtains

$$1=|\langle\varphi_0|\varphi_0\rangle|^2=|\langle t^{1/2}\varphi_0|t^{-1/2}\varphi_0\rangle|^2\leq\langle\varphi_0|t|\varphi_0\rangle\langle\varphi_0|t^{-1}|\varphi_0\rangle,$$

and further

$$\langle\varphi_0|t|\varphi_0\rangle\geq\langle\varphi_0|t^{-1}|\varphi_0\rangle^{-1}, \tag{97}$$

for any positive-definite operator t. Substituting the expression (94) for t^{-1} and observing that $T_0\varphi_0=0$, one gets the lower bound

$$\langle\varphi_0|t|\varphi_0\rangle\geq\langle\varphi_0|V^{-1}|\varphi_0\rangle^{-1}. \tag{97'}$$

This means that the quantity $E_0+\langle\varphi_0|V^{-1}|\varphi_0\rangle^{-1}$ is a lower bound to the true ground-state energy. The formula is useful if V^{-1} is a simple operator as, for instance, in the He atom and the H_2 molecule with $V=e^2/r_{12}$. This lower bound was first derived by Bazley[14] using the method of intermediate Hamiltonians.

Still better lower bounds for t may be derived by using the idea of the "inner projection" as developed in connection with formulas (32), (33), and (34). Introducing a linear manifold $\mathbf{f}=(f_1,f_2,f_3,\cdots f_n)$ with the metric matrix $\mathbf{\Delta}=\mathbf{f}^\dagger\mathbf{f}$, one can define the inner projection t' of t with respect to this subspace by the formula

$$t'=t^{1/2}\mathbf{f}\mathbf{\Delta}^{-1}\mathbf{f}^\dagger t^{1/2}. \tag{98}$$

This operator is positive-definite and satisfies the inequality $t'<t$, so it provides actually a lower bound for t. Making the substitutions

$$t^{-1/2}\mathbf{f}=\mathbf{g}, \quad t^{1/2}\mathbf{f}=\mathbf{h}, \tag{99}$$

one obtains the alternative forms

$$t'=t\mathbf{g}\mathbf{\Delta}^{-1}\mathbf{g}^\dagger t, \quad \mathbf{\Delta}=\mathbf{g}^\dagger t\mathbf{g}, \tag{100}$$

$$t'=\mathbf{h}\mathbf{\Delta}^{-1}\mathbf{h}^\dagger, \quad \mathbf{\Delta}=\mathbf{h}^\dagger t^{-1}\mathbf{h}. \tag{101}$$

The form (100) will be called the Aronszajn projection,[13] and we will call the space $\mathbf{g}=(g_1,g_2,\cdots g_n)$ an Aronszajn space, whereas the form (101) will be called a Bazley projection and the associated space $\mathbf{h}=(h_1,h_2\cdots h_n)$ a Bazley space.

Because of the simplicity of relation (94), it seems as if the Bazley projection would be of particular importance in evaluating lower bounds. One has

$$\langle\varphi_0|t|\varphi_0\rangle\geq\langle\varphi_0|t'|\varphi_0\rangle$$
$$=\langle\varphi_0|\mathbf{h}\mathbf{\Delta}^{-1}\mathbf{h}^\dagger|\varphi_0\rangle=\sum_{k,l=1}^{n}\langle\varphi_0|h_k\rangle(\Delta^{-1})_{kl}\langle h_l|\varphi_0\rangle, \tag{102}$$

where Δ^{-1} is the inverse of the nth-order matrix

$$\begin{aligned}\mathbf{\Delta}&=\langle\mathbf{h}|t^{-1}|\mathbf{h}\rangle\\&=\langle\mathbf{h}|V^{-1}-T_0|\mathbf{h}\rangle.\end{aligned} \tag{103}$$

The entire problem is thus here reduced to the evaluation of the finite set $(V^{-1}-T_0)\mathbf{h}$ for an arbitrary choice of the set $\mathbf{h}$. This problem may be handled in several different ways, and a few hints for the practical treatment will be indicated below.

Evaluation of lower bounds. If the exact treatment of the operator T_0 turns out to be practically difficult, it may be feasible to use the relation (84), which together with (94) leads to the inequality

$$0<t^{-1}\leq V^{-1}-T_0(p), \tag{104}$$

where $-T_0(p)$ is an upper bound to $-T_0$, which may be evaluated if one knows the eigenfunctions φ_α^0 for $\alpha=1,2,\cdots p$ and the eigenvalues E_α^0 for $\alpha=1,2,\cdots p,p+1$:

$$-T_0(p)=\sum_{\alpha=1}^{p}\frac{|\varphi_\alpha^0\rangle\langle\varphi_\alpha^0|}{E_\alpha^0-\mathcal{E}}+\frac{1}{E_{p+1}^0-\mathcal{E}}\{P-\sum_{\alpha=1}^{p}|\varphi_\alpha^0\rangle\langle\varphi_\alpha^0|\}. \tag{105}$$

Using (86) and (91), one obtains finally

$$0<\mathbf{\Delta}=\mathbf{h}^\dagger t^{-1}\mathbf{h}\leq\mathbf{h}^\dagger(V^{-1}-T_0(p))\mathbf{h}, \tag{106}$$

and

$$t'=\mathbf{h}\mathbf{\Delta}^{-1}\mathbf{h}^\dagger\geq\mathbf{h}\langle\mathbf{h}|V^{-1}-T_0(p)|\mathbf{h}\rangle^{-1}\mathbf{h}^\dagger, \tag{107}$$

which gives a convenient lower bound for the operator t'. All these expressions may further be transformed to alternative forms by suitable linear transformations of the set $\mathbf{h}=(h_1,h_2,\cdots h_n)$.

Substitution $\mathbf{h}=V\mathbf{i}$. The introduction of the transformation $\mathbf{h}=V\mathbf{i}$ into (101) and (107) leads to the

relations

$$t'=V\mathbf{i}\Delta^{-1}\mathbf{i}^{\dagger}V;\quad \Delta=\mathbf{i}^{\dagger}(V-VT_0V)\mathbf{i}; \tag{108}$$

$$t'\geq V\mathbf{i}\langle\mathbf{i}|\,V-VT_0(p)V\,|\mathbf{i}\rangle^{-1}\mathbf{i}^{\dagger}V. \tag{109}$$

The elements of the matrix,

$$\langle\mathbf{i}|\,V-VT_0(p)V\,|\mathbf{i}\rangle = \langle\mathbf{i}|\,V\,|\mathbf{i}\rangle+\sum_{i=1}^{p}\frac{\langle\mathbf{i}|\,\varphi_\alpha{}^0\rangle\langle\varphi_\alpha{}^0|\,\mathbf{i}\rangle}{E_\alpha{}^0-\mathcal{E}}+\frac{1}{E_{p+1}{}^0-\mathcal{E}} \times\{\langle\mathbf{i}|\,V^2\,|\mathbf{i}\rangle-\sum_{\alpha=0}^{p}\langle\mathbf{i}|\,V\,|\varphi_\alpha{}^0\rangle\langle\varphi_\alpha{}^0|\,V\,|\mathbf{i}\rangle\}, \tag{110}$$

are of the same type as those occurring in perturbation theory and are comparatively easily evaluated. If the operator H_0 has a completely discrete spectrum, one can improve the accuracy of (110) to any degree desired, but if part of the spectrum has continuous character, the treatment of the associated integrals requires a great deal of care and may cause additional difficulties.

Substitution $\mathbf{h}=(a-H_0)\mathbf{j}$. There exists a transformation $\mathbf{h}=(a-H_0)\mathbf{j}$, where a is an arbitrary constant, by means of which it is possible to partly eliminate the effect of the denominator in the reduced resolvent $T_0=P/(\mathcal{E}-H_0)$. Substitution of this transformation into (101) gives the alternative form

$$t'=(a-H_0)\mathbf{j}\Delta^{-1}\mathbf{j}^{\dagger}(a-H_0), \tag{111}$$

$$\Delta=\langle\mathbf{j}|\,(a-H_0)V^{-1}(a-H_0) -(a-H_0)T_0(a-H_0)\,|\mathbf{j}\rangle. \tag{112}$$

One has

$$(a-H_0)T_0=(a-\mathcal{E})T_0+(O+P)(\mathcal{E}-H_0)T_0 =(a-\mathcal{E})T_0+O(\mathcal{E}-E_0)T_0+P=(a-\mathcal{E})T_0+P,$$

and further

$$(a-H_0)T_0(a-H_0)=(a-\mathcal{E})^2T_0+P(2a-\mathcal{E}-H_0) =(a-\mathcal{E})^2T_0+(2a-\mathcal{E}-H_0)-(2a-\mathcal{E}-E_0)O, \tag{113}$$

which leads to the formula

$$\Delta=\langle\mathbf{j}|\,(a-H_0)V^{-1}(a-H_0)\,|\mathbf{j}\rangle -(a-\mathcal{E})^2\langle\mathbf{j}|\,T_0\,|\mathbf{j}\rangle-\langle\mathbf{j}|\,2a-\mathcal{E}-H_0\,|\mathbf{j}\rangle +(2a-\mathcal{E}-E_0)\langle\mathbf{j}|\,\varphi_0\rangle\langle\varphi_0|\,\mathbf{j}\rangle. \tag{114}$$

There is still a term containing T_0, but it may be estimated by using (105) and diminished by using a value of the constant a close to the upper bound $\mathcal{E}$; one may actually put $a=\mathcal{E}$. These examples may be enough to illustrate how one can derive alternative forms for the operator t'. We note that it is necessary that the sets $\mathbf{f}$, $\mathbf{g}$, $\mathbf{h}$, $\mathbf{i}$, and $\mathbf{j}$ belong to the proper domains of the operators involved, but that they otherwise may be chosen arbitrarily. The lower bounds are going to vary with the choice of the subspace, but as a rule it is not worthwhile to try to optimize the choice—instead it is usually more practical to extend the subspace by increasing its order.

6. UPPER AND LOWER BOUNDS FOR EIGENVALUES IN THE BRILLOUIN-TYPE PERTURBATION THEORY

For the sake of simplicity, we will in this section limit ourselves to consider only positive-definite perturbations $V>0$, but many of the arguments may be extended to a more general case. We will further assume that the parameter $\mathcal{E}$ fulfills the condition $\mathcal{E}<E_1{}^0$, so that $-T_0>0$ according to (81); the reaction operator t is then also positive definite and fulfills the inequality

$$0<t<V. \tag{115}$$

The Brillouin-type perturbation series is based on relation (76):

$$t=V+VT_0t=V+tT_0V =V+VT_0V+VT_0tT_0V. \tag{116}$$

Iteration leads to the formula

$$t=V\sum_{k=0}^{2n-1}(T_0V)^k+(VT_0)^nt(T_0V)^n, \tag{117}$$

which is a geometrical series with a remainder term. For $n=\infty$, one obtains the infinite series

$$t=V\sum_{k=0}^{\infty}(T_0V)^k =V+VT_0V+VT_0VT_0V+\cdots. \tag{118}$$

We note that the terms of odd order have a factor V in the middle and that, according to (86), they are positive-definite, whereas the terms of even order have a T_0 in the middle and are negative-definite. For $V>0$, the Brillouin-type expansion is hence an alternating series.

In order to investigate the convergence of (118), it is convenient to use the more symmetric form

$$t=V^{1/2}\sum_{k=0}^{\infty}(V^{1/2}T_0V^{1/2})^kV^{1/2}, \tag{119}$$

having the self-adjoint "quotient" $V^{1/2}T_0V^{1/2}$, which is negative-definite. The series is convergent, if and only if

$$-1<V^{1/2}T_0V^{1/2}<+1, \tag{120}$$

where the right-hand part is automatically fulfilled. For $V>0$, this gives the condition $-T_0<V^{-1}$ and, according to (94), $t^{-1}=V^{-1}-T_0<2V^{-1}$, i.e.,

$$t>\tfrac{1}{2}V. \tag{121}$$

This result implies e.g., that the operator series (118) may be convergent only if the energy shift is larger than $\frac{1}{2}\langle\varphi_0|\,V\,|\varphi_0\rangle$. The convergence criterion will be further studied in Appendix C.

Substituting the infinite power-series expansions in T_0V into Eqs. (70), one obtains the fundamental formulas in the Brillouin-type perturbation theory:

$$\Psi\varepsilon=(1+T_0V+T_0VT_0V+\cdots)\varphi_0,$$
$$\mathcal{E}_1=E_0+\langle\varphi_0|V+VT_0V+VT_0VT_0V+\cdots|\varphi_0\rangle. \tag{122}$$

Introducing the notations

$$\chi_k=(T_0V)^k\varphi_0, \quad \varepsilon_{k+1}=\langle\varphi_0|V|\chi_k\rangle, \tag{123}$$

one has consequently

$$\Psi\varepsilon=\sum_{k=0}^{\infty}\chi_k, \quad \mathcal{E}_1=E_0+\sum_{k=1}^{\infty}\varepsilon_k, \tag{124}$$

provided that the two series are convergent. The functions $\chi_0, \chi_1, \chi_2, \chi_3, \cdots$ are interrelated by the recursion formula $\chi_{k+1}=T_0V\chi_k$. According to (72), one has $P(\mathcal{E}-H_0)T_0=P$, which leads to the relation

$$P(\mathcal{E}-H_0)\chi_{k+1}=PV\chi_k$$

or

$$(\mathcal{E}-H_0)\chi_{k+1}=V\chi_k-\varepsilon_{k+1}\varphi_0. \tag{125}$$

This implies that, starting from $\chi_0=\varphi_0$, one may successively derive the functions $\chi_1, \chi_2, \chi_3, \cdots$ by solving inhomogeneous equations of the type (125). The quantities introduced in this way may now be used in estimating lower bounds to the energy.

Let us return to the exact relation (117), which is valid regardless of whether the infinite expansion is convergent or not. From (115) and (86) follows that

$$0<(VT_0)^nt(T_0V)^n<(VT_0)^nV(T_0V)^n, \tag{126}$$

which leads to the inequality

$$V\sum_{k=0}^{2n-1}(T_0V)^k<t<V\sum_{k=0}^{2n}(T_0V)^k, \tag{127}$$

which shows that lower and upper bounds for the reaction operator t are provided by the partial sums of the Brillouin expansion (118) to even and odd orders in V, respectively. This theorem is, of course, true only for $V>0$, whereas, for a negative-definite perturbation $V<0$, all terms in (118) would be negative-definite, and the partial sums would form a monotonically decreasing set of operators.

If $\mathcal{E}$ is chosen as an upper bound to the energy E, the quantity $\mathcal{E}_1=E_0+\langle\varphi_0|t|\varphi_0\rangle$ is going to be a lower bound to the same energy and, using (124) and (127), one obtains

$$\mathcal{E}_1>E_0+\sum_{k=1}^{2n}\varepsilon_k. \tag{128}$$

The partial sums of even orders form hence a set of lower bounds to $\mathcal{E}_1$ and hence also to the energy E.

A still better lower bound for the remainder in (117) may be obtained by using the relation $t'<t$, where t' is the inner projection of t defined by the Eqs. (98)–(101). One obtains

$$V\sum_{k=0}^{2n-1}(T_0V)^k+(VT_0)^nt'(T_0V)^n<t<V\sum_{k=0}^{2n}(T_0V)^k. \tag{129}$$

For the evaluation of the term containing t', one may use anyone of the methods developed in the previous section. The result implies that it is possible to obtain a lower bound for t to any accuracy desired. Formula (129) is based on a combination of the perturbation results expressed in (127) with Aronszajn's idea[13] of obtaining a lower bound by means of an "inner projection."

It is possible to get an estimate of the remainder by using only such quantities which normally enters into Brillouin's perturbation theory. Using formula (108) and making the special choice $\mathbf{i}=\mathbf{X}=(\chi_0,\chi_1,\chi_2\cdots\chi_{m-1})$, we obtain

$$\langle\varphi_0|(VT_0)^nt'(T_0V)^n|\varphi_0\rangle = \langle\varphi_0|(VT_0)^nV|\mathbf{X}\rangle\boldsymbol{\Delta}^{-1}\langle\mathbf{X}|V(T_0V)^n|\varphi_0\rangle = \boldsymbol{\alpha}^\dagger\boldsymbol{\Delta}^{-1}\boldsymbol{\alpha}, \tag{130}$$

where $\boldsymbol{\alpha}^\dagger=\langle\varphi_0|(VT_0)^nV|\mathbf{X}\rangle=(\varepsilon_{n+1},\varepsilon_{n+2},\cdots,\varepsilon_{n+m})$ is a row vector of order m, and $\boldsymbol{\Delta}=\langle\mathbf{X}|V-VT_0V|\mathbf{X}\rangle$ is a matrix of order $m\times m$ with the elements ($k, l=0, 1, 2, \cdots, m-1$).

$$\Delta_{kl}=\varepsilon_{k+l+1}-\varepsilon_{k+l+2}, \tag{131}$$

so that

$$\boldsymbol{\Delta}=\begin{bmatrix}\varepsilon_1-\varepsilon_2, & \varepsilon_2-\varepsilon_3, & \cdots, & \varepsilon_m-\varepsilon_{m+1}\\ \varepsilon_2-\varepsilon_3, & \varepsilon_3-\varepsilon_4, & \cdots, & \varepsilon_{m+1}-\varepsilon_{m+2}\\ \cdots & \cdots & \cdots & \cdots\\ \varepsilon_m-\varepsilon_{m+1}, & \varepsilon_{m+1}-\varepsilon_{m+2}, & \cdots, & \varepsilon_{2m}-\varepsilon_{2m+1}\end{bmatrix}. \tag{132}$$

According to (129), this gives the estimate

$$\mathcal{E}_1>E_0+\sum_{k=1}^{2n}\varepsilon_k+\boldsymbol{\alpha}^\dagger\boldsymbol{\Delta}^{-1}\boldsymbol{\alpha}. \tag{133}$$

For $n=m=1$, one has, for instance,

$$\mathcal{E}_1>E_0+\varepsilon_1+\varepsilon_2+\varepsilon_1^2/(\varepsilon_1-\varepsilon_2). \tag{134}$$

It is easily shown that, for a given m, the formulas (133) for $n=0, 1, 2, \cdots, m$ are all identical. This depends on a simple identity valid for $n\leq m$:

$$(\varepsilon_{n+1},\varepsilon_{n+2},\cdots,\varepsilon_{n+m})\boldsymbol{\Delta}^{-1}\begin{bmatrix}\varepsilon_{n+1}\\ \varepsilon_{n+2}\\ \vdots\\ \varepsilon_{n+m}\end{bmatrix} = \sum_{k=2n+1}^{2m}\varepsilon_k+(\varepsilon_{m+1},\varepsilon_{m+2},\cdots,\varepsilon_{2m})\boldsymbol{\Delta}^{-1}\begin{bmatrix}\varepsilon_{m+1}\\ \varepsilon_{m+2}\\ \vdots\\ \varepsilon_{2m}\end{bmatrix}, \tag{135}$$

which is proven in Appendix D. For a given n, on the other hand, one obtains an increasing series of lower bounds by successively choosing $m=1, 2, 3, 4, \cdots$, respectively. We note that, in formula (133) for $m=n$, only the quantities ε_k up through $k=2n+1$ are involved.

In conclusion, we note that we are here dealing with a Brillouin-type perturbation theory which contains a variable parameter $\mathcal{E}$ and a function $\mathcal{E}_1=E_0+\langle\varphi_0|t|\varphi_0\rangle$ defined by (70) such that the pair $\mathcal{E}$, $\mathcal{E}_1$ bracket a true eigenvalue E. The quantity $\mathcal{E}_1$ will hence provide a lower bound to E, if $\mathcal{E}$ is chosen as an upper bound to E, for instance, by means of the variation principle. By using convenient lower bounds to the operator t, one can then obtain lower estimates of the number $\langle\varphi_0|t|\varphi_0\rangle$ leading to such practically useful lower bounds to E as are given by (128) and (133). We note that the conventional Brillouin perturbation theory is limited to the point $\mathcal{E}_1=\mathcal{E}=E$, and that our results may be applied to the partial sums also in this case.

7. UPPER AND LOWER BOUNDS FOR EIGENVALUES IN THE SCHRÖDINGER-TYPE PERTURBATION THEORY

The Schrödinger-type perturbation theory is based on the use of a reduced resolvent of the form

$$R_0=P/(E_0-H_0). \tag{136}$$

Instead of expanding T in powers of V, it is now convenient to expand T in powers of the quantity

$$V'=V-(\mathcal{E}-E_0). \tag{137}$$

By means of (40) and the use of the identity (87), one obtains

$$T=P/(\mathcal{E}-H)=\frac{P}{(E_0-H_0)-V'}, \tag{138}$$

$$=R_0+R_0V'T=R_0\sum_{k=0}^{\infty}(V'R_0)^k.$$

For the reaction operator (69), one is hence led to the expansion

$$t=V+VR_0\sum_{k=0}^{\infty}(V'R_0)^kV. \tag{139}$$

Of particular interest is the value of the variable $\mathcal{E}$ for which $\mathcal{E}_1=\mathcal{E}=E=E_0+\langle\varphi_0|t|\varphi_0\rangle$. This special value may be found from (139) by iteration. Arranging the terms in powers of V, one obtains

$$t=t_1+t_2+t_3+t_4+\cdots, \tag{140}$$

$$\langle\varphi_0|t|\varphi_0\rangle=\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4+\cdots, \tag{141}$$

with the notation $\epsilon_k=\langle\varphi_0|t_k|\varphi_0\rangle$. A study of the right-hand member of (139) gives immediately the result

$$\begin{aligned}
&t_1=V, && \epsilon_1=\langle\varphi_0|V|\varphi_0\rangle,\\
&t_2=VR_0V, && \epsilon_2=\langle\varphi_0|VR_0V|\varphi_0\rangle,\\
&t_3=VR_0(V-\epsilon_1)R_0V, && \cdots\\
&t_4=VR_0(V-\epsilon_1)R_0(V-\epsilon_1)R_0V-\epsilon_2VR_0^2V,\\
&\qquad\cdots.
\end{aligned} \tag{142}$$

The corresponding formula for the wave operator $W=1+W_1+W_2+W_3+\cdots$ is directly obtained from the relation $t=VW$, which gives

$$\begin{aligned}
&W_1=R_0V,\\
&W_2=R_0(V-\epsilon_1)R_0V,\\
&W_3=R_0(V-\epsilon_1)R_0(V-\epsilon_1)R_0V-\epsilon_2VR_0^2V,\\
&\qquad\cdots.
\end{aligned} \tag{143}$$

Analogous to (79), one has the following spectral resolution of the reduced resolvent:

$$R_0=\sum_{k=1}^{\infty}\frac{|\varphi_k^0\rangle\langle\varphi_k^0|}{E_0-E_k^0}, \tag{144}$$

and substituting this expression into (142) and (143), one obtains the conventional formulas for the energy $E=E_0+\epsilon_1+\epsilon_2+\epsilon_3+\cdots$ and the eigenfunction $\Psi=W\varphi_0$ in Schrödinger's perturbation theory.

In order to derive lower bounds for the energy in terms of the quantities occurring in Schrödinger's perturbation theory, we will keep $\mathcal{E}$ as a variable parameter and study the function $\mathcal{E}_1$. Utilizing the "symmetric" identity (89) for the expansion of T, we get

$$T=R_0+R_0V'R_0+R_0V'TV'R_0. \tag{145}$$

This relation indicates that it is important to obtain rough upper and lower bounds for T, since they may then be used to derive improved bounds, etc.

As before, we will consider the case of a positive-definite perturbation $V>0$ which is such that one can determine an upper bound $\mathcal{E}$ to the ground state which satisfies the inequality $\mathcal{E}<E_1^0$. This is, for instance, the case if $E_0^0+\langle\varphi_0|V|\varphi_0\rangle<E_1^0$. Using (69) and the fact that V^{-1} exists, one obtains

$$T=V^{-1}tV^{-1}-V^{-1}. \tag{146}$$

According to (96), one has the inequality $0<t<V$ and, consequently, one obtains the rough bounds

$$-V^{-1}<T<0, \tag{147}$$

showing that T is a negative-definite operator. If more detailed properties of the fundamental operator T are needed, it is usually more convenient to study T directly without reference to the reaction operator t, and such an investigation will be carried out in a forthcoming paper. However, the considerations given are sufficient for our purpose here.

Substitution of the lower bound $-V^{-1}$ for the operator T in (147) into the expression for the reaction operator t based on (145)

$$t=V+VR_0V+VR_0V'R_0V+VR_0V'TV'R_0V, \tag{148}$$

leads to formulas for lower bounds to $\mathcal{E}_1$ and the energy E, which are practically useful if V^{-1} is a simple operator. However, since they contain terms which usually do not appear in Schrödinger's perturbation theory e.g., of the form $(\mathcal{E}-E_0)^2VR_0V^{-1}R_0V$, we will try also a different approach.

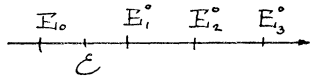

FIG. 4. Situation of some characteristic points on the energy axis.

Let us instead start from formula (74) which together with the relation $VT=tT_0$ gives

$$T=T_0+T_0tT_0. \tag{149}$$

The previous inequality for t leads immediately to the relation $T_0<T<T_0+T_0VT_0$ and combination with the upper bound from (147) leads to the simple estimate

$$T_0<T<0. \tag{150}$$

However, since Schrödinger's perturbation theory works in terms of R_0 and not T_0, it is necessary to modify even this lower bound. For this purpose, it is convenient to compare the spectral resolutions of T_0 and R_0 term for term.

Comparison between the operators T_0 and R_0. If the unperturbed Hamiltonian H_0 has the eigenvalues E_k^0 and the eigenfunctions φ_k^0 with the associated projection operators $O_k^0=|\varphi_k^0\rangle\langle\varphi_k^0|$ which form a resolution of the identity, one has according to (79) and (144) the following spectral resolutions:

$$\begin{aligned} T_0&=\frac{P}{\mathcal{E}-H_0}=\sum_{k=1}^{\infty}\frac{O_k^0}{\mathcal{E}-E_k^0},\\ R_0&=\frac{P}{E_0-H_0}=\sum_{k=1}^{\infty}\frac{O_k^0}{E_0-E_k^0}. \end{aligned} \tag{151}$$

As before, we will assume that the upper bound $\mathcal{E}$ is situated in the interval $E_0^0<\mathcal{E}<E_1^0$, which implies that all the terms in T_0 and R_0 are negative-definite (see Fig. 4). Let us now introduce a set of positive numbers κ_k defined by the relation

$$\kappa_k=(E_k^0-E_0)/(E_k^0-\mathcal{E})=1+(\mathcal{E}-E_0)/(E_k^0-\mathcal{E}). \tag{152}$$

Since the eigenvalues to H_0 are arranged in increasing order, one has immediately the inequality

$$\kappa_1\geq\kappa_2\geq\kappa_3\geq\cdots>1. \tag{153}$$

This gives the transformation

$$\begin{aligned} T_0=\sum_{k=1}^{\infty}\kappa_k\frac{O_k^0}{E_0-E_k^0}&=\kappa_1\sum_{k=1}^{\infty}\frac{\kappa_k}{\kappa_1}\frac{O_k^0}{E_0-E_k^0}\\ &\geq\kappa_1\sum_{k=1}^{\infty}(O_k^0/(E_0-E_k^0))=\kappa_1R_0, \end{aligned}$$

i.e.,

$$T_0>\kappa_1R_0. \tag{154}$$

According to (150), we have thus the inequality

$$\kappa_1R_0\leqq T<0, \tag{155}$$

which gives a rough but still convenient lower bound to T. The coefficient κ_1 defined by (152) or the alternative expression

$$\kappa_1=(1-(\mathcal{E}-E_0)/(E_1^0-E_0))^{-1}, \tag{156}$$

contains only quantities which anyway occur in the Schrödinger perturbation theory, and one obtains the estimate

$$\begin{aligned} (1-(E-E_0)/(E_1^0-E_0))^{-1}&\leq\kappa_1\\ &\leq(1-\epsilon_1/(E_1^0-E_0))^{-1}. \end{aligned} \tag{157}$$

The quantity κ_1 will hence be close to 1, only if the energy shift is small in comparison to the difference $(E_1^0-E_0^0)$.

Lower bounds to the energy. By means of the lower bound for T in (155), one may now derive a series of lower bounds of increasing accuracy for the reaction operator t. Starting from the definition (69), one obtains directly

$$t=V+VTV>V+\kappa_1VR_0V. \tag{158}$$

For the quantity $\mathcal{E}_1=E_0+\langle\varphi_0|t|\varphi_0\rangle$, this gives the lower bound

$$\mathcal{E}_1>E_0+\epsilon_1+\kappa_1\epsilon_2, \tag{159}$$

where the variable $\mathcal{E}$ in κ_1 has to be an upper bound e.g., $\mathcal{E}=E_0+\epsilon_1$. One can now refine this result by proceeding with the power series expansion in V'. Substituting (155) into (148), one gets

$$t>V+VR_0V+VR_0V'R_0V+\kappa_1VR_0V'R_0V'R_0V. \tag{160}$$

In order to insert a proper upper bound, we calculate the expectation value of H for the first-order wave function $(1+R_0V)\varphi_0$ which gives the result

$$\mathcal{E}=E_0+\epsilon_1+(\epsilon_2+\epsilon_3)/(1+\delta_2), \tag{161}$$

where $\delta_2=\langle\varphi_0|VR_0^2V|\varphi_0\rangle$. Using this value for $\mathcal{E}$ and (160), one obtains a lower bound to $\mathcal{E}_1$ and to the energy correct to the fourth order.

Repeated use of (145) and the definition (69) leads finally to the general formulas

$$T=R_0\sum_{k=0}^{2n-1}(V'R_0)^k+(R_0V')^nT(V'R_0)^n, \tag{162}$$

$$t>V+VR_0\sum_{k=0}^{2n-1}(V'R_0)^kV+\kappa_1VR_0(V'R_0)^{2n}V. \tag{163}$$

Using the value of the upper bound $\mathcal{E}$ corresponding to the expectation value of H with respect to the nth-order wave function $(1+W_1+W_2+\cdots+W_n)\varphi_0$ according to (143), one obtains a lower bound to $\mathcal{E}_1$ and the ground-state energy which is correct to the order $(2n+2)$.

In contrast to the Brillouin theory, the even-order approximations to the energy in the Schrödinger theory do not usually form true lower bounds but there are always remainders of higher order which cannot be neglected. However, it should be observed that the discussion of the lower bound of T given here is only

meant to be a first sketch, and that the results certainly can be highly improved. This question will be further discussed in a forthcoming paper.

8. LOWER BOUNDS TO THE GROUND-STATE ENERGIES OF THE He-LIKE IONS

As an illustrative example of the methods described here, we will now derive lower bounds for the ground-state energies of the He-like ions: He, Li^+, Be^{2+}, etc. This problem has previously been treated by several authors,[10] by means of formulas of the type (6) and (7) given by Temple and D. H. Weinstein. Using the method of intermediate Hamiltonians developed by A. Weinstein,[12] the problem has further been studied by Bazley and Fox[14] and recently by Gay.[19]

The He-like ions have a nonrelativistic Hamiltonian which in atomic units[20] takes the form

$$H_{\rm op}=-\tfrac{1}{2}\nabla_1^2-\tfrac{1}{2}\nabla_2^2-Z/r_1-Z/r_2+1/r_{12}, \quad (164)$$

where $Z=1, 2, 3, 4, \cdots$ is the atomic number. It is convenient to make the following separation:

$$\begin{aligned} H_0&=(-\tfrac{1}{2}\nabla_1^2-Z/r_1)+(-\tfrac{1}{2}\nabla_2^2-Z/r_2);\\ V&=1/r_{12}, \end{aligned} \quad (165)$$

and we note that the perturbation V is positive-definite. The unperturbed Hamiltonian H_0 is separable, and the eigenfunctions are products of hydrogen-like wave functions associated with the following eigenvalues:

$$-\tfrac{1}{2}Z^2(1/n^2+1/m^2), \quad (166)$$

for $n, m=1, 2, 3, \cdots$, i.e., with the spectrum

$$-Z^2, \quad -0.625Z^2, \quad -0.555\cdots Z^2, \quad -0.53125Z^2, \cdots. \quad (167)$$

The unperturbed function φ_0 is given by the expression

$$\varphi_0=(Z^3/\pi)e^{-Z(r_1+r_2)}, \quad (168)$$

and one obtains particularly the integral $\langle\varphi_0|V|\varphi_0\rangle=\frac{5}{8}Z$. The expectation value of H with respect to φ_0 gives hence the upper bound for the ground-state energy

$$\mathcal{E}=-Z^2+\tfrac{5}{8}Z, \quad (169)$$

showing that the ground-state energy will certainly lie below the energy of the first excited unperturbed state $-0.625Z^2$ if $Z>5/3$. One can hence apply the theory developed in this paper to the case of $Z=2, 3, 4, 5, \cdots$, whereas the case $Z=1$ has to be treated separately and will be studied in a forthcoming paper.

Lower bounds to the ground-state energy are here given by the formula (70) which will be used in the form

$$\mathcal{E}_1=E_0+\langle\varphi_0|t|\varphi_0\rangle>E_0+\langle\varphi_0|t'|\varphi_0\rangle, \quad (170)$$

where t' is an "inner projection" of t according to (98). Because of the particularly simple form of the operator $V^{-1}=r_{12}$, we will here apply formulas (111)–(114) for $a=\mathcal{E}$ and an arbitrary space $\mathbf{j}=(j_1, j_2, \cdots j_n)$, which gives

$$\langle\varphi_0|t'|\varphi_0\rangle=(\mathcal{E}-E_0)^2\langle\varphi_0|\mathbf{j}\rangle\mathbf{\Delta}^{-1}\langle\mathbf{j}|\varphi_0\rangle, \quad (171)$$

where $\mathbf{\Delta}^{-1}$ is the inverse of the nth order matrix

$$\mathbf{\Delta}=\langle\mathbf{j}|(\mathcal{E}-H_0)V^{-1}(\mathcal{E}-H_0)|\mathbf{j}\rangle-\langle\mathbf{j}|\mathcal{E}-H_0|\mathbf{j}\rangle+(\mathcal{E}-E_0)\langle\mathbf{j}|\varphi_0\rangle\langle\varphi_0|\mathbf{j}\rangle. \quad (172)$$

In the evaluation of (171) we will use the same type of function j_k as has previously been introduced by Hylleraas[21] in studying the upper bounds

$$s^\mu t^{2\nu}u^\sigma e^{-\eta s}, \quad (173)$$

where $s=r_1+r_2$, $t=r_1-r_2$, $u=r_{12}$, and η is scale parameter. We will here report the results of some calculations based on a $\mathbf{j}$ space of order $n=10$ spanned by the following basic elements:

$$\begin{aligned} p_1&=e^{-\eta s}, & p_2&=ue^{-\eta s},\\ p_3&=t^2e^{-\eta s}, & p_4&=se^{-\eta s},\\ p_5&=s^2e^{-\eta s}, & p_6&=u^2e^{-\eta s},\\ p_7&=sue^{-\eta s}, & p_8&=t^2ue^{-\eta s},\\ p_9&=u^3e^{-\eta s}, & p_{10}&=t^2u^2e^{-\eta s}. \end{aligned} \quad (174)$$

The functions selected are those previously found most effective in a tenth-order upper-bound calculation on helium.[22] The integrals have been evaluated by methods similar to those used by Wilets and Cherry.[23]

The lower bound in (170) for $Z=2$ is shown as a function of the scale parameter η for $n=1, 2, 3, \cdots 10$, in Fig. 1, and we note the nice optimum properties. The best results for $n=10$ are collected in Table I and render good lower bounds obtained with a comparatively small amount of effort. The numerical calculations were performed by Dr. J. G. Gay on the IBM 709 computer at the University of Florida, and his skillful assistance is gratefully acknowledged.

Further lower-bound applications concluded at the

TABLE I. Ground states of helium and helium-like positive ions; atomic units.

System	Lower bound[a]	Upper bound[b]
He	−2.90592	−2.903721
Li^+	−7.28444	−7.279910
Be^{2+}	−13.66269	−13.655563
B^{3+}	−22.04074	−22.030968
C^{4+}	−32.41864	−32.406243

[a] Results of this paper. Calculations were of tenth order optimized with respect to η.
[b] Quoted from E. A. Hylleraas and J. Midtdal,[2] Phys. Rev. **109**, 1013 (1958).

[19] J. G. Gay, University of Florida Quantum Theory Project, Report 49, 1964 (unpublished); Phys. Rev. **135**, A1220 (1964).
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[23] L. W. Wilets and I. J. Cherry, Phys. Rev. **103**, 112 (1956).

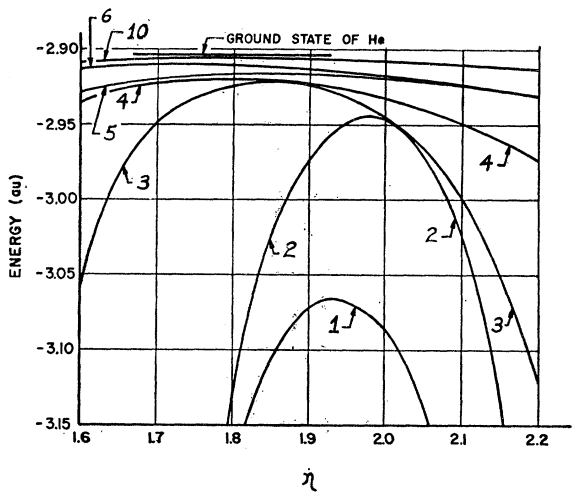

FIG. 5. Lower bounds to the helium ground state as a function of the scaling parameter η. The numbers associated with each curve indicate the order of the calculation, i.e., the number of elements in the basis **j**.

University of Florida include a study of the symmetric and asymmetric anharmonic oscillators by Professor Charles Reid and an investigation of the double-minimum potential problem by Carlos and Annik Bunge. The results obtained so far have been greatly encouraging, and further work is in progress.

9. DISCUSSION

The bracketing theorem in the partitioning technique for treating eigenvalue problems is here used to construct lower bounds for the energy eigenvalues. Our study is partly inspired by the excellent work by Professor Alexander Weinstein[12] and his school, and particularly by the recent papers by Bazley and Fox.[14] Even if we have here tried to avoid the use of the "intermediate Hamiltonians" in order to escape the explicit ordering of the eigenvalues, we have utilized Aronszajn's idea[13] for constructing lower bounds to a positive-definite operator by means of an "inner projection." In the Brillouin-type perturbation theory for $V>0$, the even-order approximations turn out to give lower bounds, but the inner-projection technique renders still a powerful tool for estimating the remainders.

The results indicate that, if one only has a truncated basic set in Hilbert space at disposal for solving a specific eigenvalue problem, one can determine upper bounds by means of the variation principle and lower bounds by using the method described. Some of the disadvantages connected with the fact that every basis has to be truncated in the numerical applications have hence been removed.

Our study is only meant as a first sketch which leaves room for many improvements. In the treatment of the perturbed Hamiltonian $H=H_0+V$, we have, e.g., chosen the unperturbed eigenfunction φ_0 as our reference function φ without questioning whether such a choice is feasible. The general considerations in connection with relation (51) indicate that one will get improved upper and lower bounds in the series $\mathcal{E}$, $\mathcal{E}_1$, $\mathcal{E}_2$, $\mathcal{E}_3$, $\cdots$, only if $\langle\phi|\phi\rangle<1$, i.e., if the reference function φ contributes more than 50% to the eigenfunction desired. It seems hence worthwhile to try to modify the perturbation treatment, so that one can choose a reference function φ which is a good approximation to the true eigenfunction as a starting point for evaluating lower bounds. This problem will be treated in a forthcoming paper.

We have here concentrated our interest on a study of lower bounds for ground-state energies in the case of positive definite perturbations V, which satisfy the relation $E_0+\langle\varphi_0|V|\varphi_0\rangle<E_1^0$. The method breaks down and has to be modified, if there are several unperturbed energies of the same symmetry type situated below the ground-state energy of the perturbed system. Another important problem is associated with the evaluation of lower bounds also for the excited states of the perturbed system. In both cases, one may proceed either by making a more careful choice of the reference function φ or by increasing the order of the associated linear manifold described by the projection operator O. These problems will be further discussed elsewhere.

APPENDIX A: PROJECTION OPERATORS ON A LINEAR MANIFOLD

Let us consider a linear manifold M_n of order n which is spanned by a set of n linearly independent vectors $\mathbf{f}=(f_1,f_2,f_3,\cdots f_n)$ having the metric matrix $\mathbf{\Delta}=\mathbf{f}^\dagger\mathbf{f}$ with the elements $\Delta_{kl}=\langle f_k|f_l\rangle$ and the properties $\mathbf{\Delta}^\dagger=\mathbf{\Delta}$ and $\mathbf{\Delta}>0$. Let further F be an element which does not necessarily belong to the subspace M_n, and let us try to express F in the form

$$F=\sum_{k=1}^{n} f_k a_k+g, \tag{A1}$$

where we will determine the coefficients a_k, which are conveniently arranged in a column vector **a**, so that the length of the "remainder" g becomes a minimum:

$$\langle g|g\rangle=\text{minimum}. \tag{A2}$$

In this connection it is feasible to introduce a column **c** defined by the relation

$$\mathbf{c}=\mathbf{\Delta}^{-1}\mathbf{f}^\dagger F, \tag{A3}$$

or $c_k=\sum_l(\Delta^{-1})_{kl}\langle f_l|F\rangle$. This implies also the relations $\mathbf{f}^\dagger F=\mathbf{\Delta c}$ and $F^\dagger\mathbf{f}=\mathbf{c}^\dagger\mathbf{\Delta}$. From (A1)–(A3), one obtains directly

$$\begin{aligned}\langle g|g\rangle&=(F-\mathbf{fa})^\dagger(F-\mathbf{fa})\\&=F^\dagger F-F^\dagger\mathbf{fa}-\mathbf{a}^\dagger\mathbf{f}^\dagger F+\mathbf{a}^\dagger\mathbf{f}^\dagger\mathbf{fa}\\&=F^\dagger F-\mathbf{c}^\dagger\mathbf{\Delta a}-\mathbf{a}^\dagger\mathbf{\Delta c}+\mathbf{a}^\dagger\mathbf{\Delta a}\\&=F^\dagger F-\mathbf{c}^\dagger\mathbf{\Delta c}+(\mathbf{c}-\mathbf{a})^\dagger\mathbf{\Delta}(\mathbf{c}-\mathbf{a}).\end{aligned} \tag{A4}$$

The last term in (A4) is positive-definite, and one has

hence the inequality

$$\langle g|g\rangle \geq \langle F|F\rangle - \mathbf{c}^\dagger \boldsymbol{\Delta} \mathbf{c} \geq 0. \tag{A5}$$

The minimum is achieved for the special choice $\mathbf{a}=\mathbf{c}=\boldsymbol{\Delta}^{-1}\mathbf{f}^\dagger F$, and we note the relation

$$\langle F|F\rangle \geq \sum_{k,l=1}^{n} c_k^* \Delta_{kl} c_l, \tag{A6}$$

which is a generalization of Bessel's inequality to a nonorthogonal basis. Substituting $\mathbf{a}=\mathbf{c}$ in (A1), we obtain the expansion

$$\begin{aligned} F &= \mathbf{f}\boldsymbol{\Delta}^{-1}\mathbf{f}^\dagger F + g_{\min} \\ &= OF + g_{\min}, \end{aligned} \tag{A7}$$

where we have introduced the operator

$$O = \mathbf{f}\boldsymbol{\Delta}^{-1}\mathbf{f}^\dagger. \tag{A8}$$

It satisfies the fundamental relations

$$O^2 = O, \quad O^\dagger = O, \quad \mathrm{Tr}(O) = n, \tag{A9}$$

and it will be characterized as the projection operator on the linear manifold M_n spanned by the set $\mathbf{f}=(f_1, f_2, \cdots f_n)$. According to (A7), one has further $g_{\min}=(1-O)F$ and

$$\langle g_{\min}|OF\rangle = 0, \tag{A10}$$

showing that $g_{\min}$ is orthogonal to the projection OF (see Fig. 6). Formula (A7) gives hence the resolution of an arbitrary element F into its projection on a given linear manifold M_n and a remainder which is orthogonal to this manifold.

By means of (A3) and (A8), one finds that $\mathbf{c}^\dagger\boldsymbol{\Delta}\mathbf{c} = F^\dagger \mathbf{f}\boldsymbol{\Delta}^{-1}\boldsymbol{\Delta}\boldsymbol{\Delta}^{-1}\mathbf{f}^\dagger F = F^\dagger OF$. According to (A5), one may hence write the generalization of Bessel's inequality in the form $F^\dagger F \geq F^\dagger OF$, or

$$\langle F|F\rangle \geq \langle F|O|F\rangle. \tag{A11}$$

An infinite set $\mathbf{f}=(f_1, f_2, f_3, \cdots)$ is finally said to be complete if, for all elements F having a norm, one has

$$\lim_{n\to\infty} \langle F|1-O_n|F\rangle = 0, \tag{A12}$$

where O_n is the projection operator for the finite set $(f_1, f_2, f_3, \cdots f_n)$. This is a direct generalization of Parseval's relation, and it may also be written in the form

$$\lim_{n\to\infty} \|F - O_n F\| = 0, \tag{A13}$$

defining the concept of "convergence in mean." Of a different character is the "resolution of identity"

$$1 = \lim_{n\to\infty} O_n, \tag{A14}$$

since it corresponds to the actual expansion theorem.

It should be observed that the physical interpretations of quantum theory are as a rule based on Parseval's relation and the concept of the convergence in mean. For the sake of simplicity, one is still often using the expansion theorem, the resolution of the identity or the spectral resolution of an operator, but a closer investigation often reveals that one is using tools which are unnecessarily strong for physical results to be obtained. In our study, however, we will follow the conventional pattern.

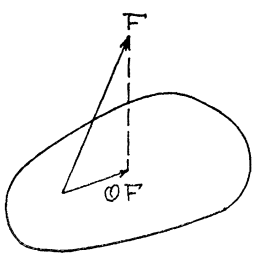

FIG. 6. Projection of an arbitrary vector F on a given subspace.

APPENDIX B: VARIATIONS SUBJECT TO A CONSTRAINT

Let A be a self-adjoint operator bounded from below, and let us consider the extreme values of the integral

$$I = \langle \bar{u}|A|\bar{u}\rangle / \langle \bar{u}|\bar{u}\rangle, \tag{B1}$$

when $\bar{u}$ is subject to the constraint that it should belong to the subspace of O, i.e., $O\bar{u}=\bar{u}$, where O is the projection operator for a given linear manifold. Introducing an arbitrary function u, one can put $\bar{u}=Ou$, which gives

$$I = \frac{\langle u|O^\dagger A O|u\rangle}{\langle u|O|u\rangle} = \frac{\langle u|\bar{A}|u\rangle}{\langle u|O|u\rangle}. \tag{B2}$$

The variation principle $\delta I = 0$ leads immediately to the relation $(\bar{A}-IO)u=0$ or

$$\bar{A}\bar{u} = I\bar{u}, \tag{B3}$$

i.e., an eigenvalue problem of the type (13). The extreme values of I are hence given by the eigenvalues $\bar{a}_1, \bar{a}_2, \bar{a}_3, \cdots$ of the operator $\bar{A}$ and, according to (14), they fulfill the inequality $\bar{a}_k \geq a_k$, which means that the constraint raises the eigenvalues and hence also the extreme values of the integral I.

Following Weinstein,[12] one can reformulate the problem by putting $(1-O)\bar{u}=0$, i.e., by requesting that the functions $\bar{u}$ are orthogonal to the manifold described by the projection operator $P=1-O$. This is particularly convenient if the manifold associated with O is of infinite order, whereas the manifold associated with P is of finite order, say n. If the latter is spanned by a linearly independent set of elements

$$\mathbf{p} = (p_1, p_2, p_3, \cdots p_n)$$

with the metric matrix $\boldsymbol{\Delta} = \mathbf{p}^\dagger\mathbf{p}$, the projection operator P has the form

$$P = \mathbf{p}\boldsymbol{\Delta}^{-1}\mathbf{p}^\dagger. \tag{B4}$$

The constraint $P\bar{u}=0$ implies that $\bar{u}$ should be orthogonal to the given functions $p_1, p_2, \cdots p_n$, i.e., a finite number of conditions. Equation (B3) now takes the form $(1-P)A\bar{u}=I\bar{u}$, i.e.,

$$(A-I)\bar{u}=PA\bar{u}=\mathbf{pa}, \tag{B5}$$

where $\mathbf{a}=\mathbf{\Delta}^{-1}\mathbf{p}^{\dagger}A\bar{u}$ is a column vector of order n. For all values of I different from the eigenvalues of A, the operator $(A-I)^{-1}$ exists, and one obtains $\bar{u}=(A-I)^{-1}\mathbf{pa}$. However, since the orthogonality constraint may be given the form $\mathbf{p}^{\dagger}\bar{u}=0$, one gets immediately

$$\mathbf{p}^{\dagger}(A-I)^{-1}\mathbf{pa}=0, \tag{B6}$$

which is a linear equation system in the unknown vector $\mathbf{a}$ of order n. It has a nontrivial solution if and only if $\det\{\mathbf{p}^{\dagger}(A-I)^{-1}\mathbf{p}\}=0$, i.e.,

$$\det\{\langle p_k|(A-I)^{-1}|p_l\rangle\}=0, \tag{B7}$$

where $k, l=1, 2, 3, \cdots n$. This equation in the unknown quantity I gives the eigenvalues to the operator $\bar{A}$. The determinant in the left-hand member is known as Weinstein's determinant, and the associated function in the complex variable I has been studied in great detail.[12]

APPENDIX C: CONVERGENCE OF THE BRILLOUIN EXPANSION

The Brillouin-type perturbation theory is based on the infinite expansion (119), which is convergent if and only if the criterion (120) is fulfilled:

$$-1<V^{1/2}T_0V^{1/2}<+1. \tag{C1}$$

Since T_0 is negative-definite, one has only to study the left-hand part which may be written in the form $V^{1/2}(-T_0)V^{1/2}<1$. For the positive-definite operator $-T_0$, we have previously derived a decreasing series of upper bounds $-T_0(p)$ for $p=0, 1, 2, \cdots$ which are given by relation (84):

$$\begin{aligned}-T_0(0)&=P/(E_1^0-\mathcal{E}),\\ -T_0(1)&=\frac{|\varphi_1^0\rangle\langle\varphi_1^0|}{E_1^0-\mathcal{E}}+\frac{P-|\varphi_1^0\rangle\langle\varphi_1^0|}{E_2^0-\mathcal{E}},\end{aligned} \tag{C2}$$

where $P=1-|\varphi_0\rangle\langle\varphi_0|$. If the inequality

$$-V^{1/2}T_0(p)V^{1/2}<1 \tag{C3}$$

would be fulfilled for any p, one could hence be sure that the convergence criterion (C1) would be satisfied. For $p=0$, the relation (C3) takes the form $V^{1/2}PV^{1/2}<E_1^0-\mathcal{E}$, or

$$V-V^{1/2}OV^{1/2}<E_1^0-\mathcal{E}, \tag{C4}$$

where $O=|\varphi_0\rangle\langle\varphi_0|$ and $\mathcal{E}$ is an upper bound smaller than or equal to $E_0+\langle\varphi_0|V|\varphi_0\rangle$. Relaxing this condition one step more, one can say that the convergence criterion (C1) is certainly satisfied, if the positive perturbation V fulfills the inequality

$$V<E_1^0-\mathcal{E}, \tag{C5}$$

for any upper bound $\mathcal{E}$. A more detailed study of the convergence properties of the Brillouin series is desired.

APPENDIX D: AN ALGEBRAIC IDENTITY

According to the definitions in connection with relation (130), the quantity $\mathbf{a}^{\dagger}=(\varepsilon_{n+1},\varepsilon_{n+2},\cdots\varepsilon_{n+m})$ is a row vector of order m, for which we temporarily will use the more specific symbol $\mathbf{a}^{\dagger}(n,m)$ stating the two indices involved. The quantity of interest is of the form

$$\boldsymbol{\alpha}^{\dagger}\mathbf{\Delta}^{-1}\boldsymbol{\alpha}=\sum_{k,l=0}^{m-1}\varepsilon_{n+k+1}(\mathbf{\Delta}^{-1})_{kl}\varepsilon_{n+l+1}. \tag{D1}$$

Using (131), one obtains for $n\leq m$ the identity

$$\begin{aligned}\varepsilon_{n+l+1}&=(\varepsilon_{n+l+1}-\varepsilon_{n+l+2})+(\varepsilon_{n+l+2}-\varepsilon_{n+l+3})\\ &\quad+\cdots+(\varepsilon_{m+l}-\varepsilon_{m+l+1})+\varepsilon_{m+l+1}\\ &=\sum_{r=0}^{m-n-1}\Delta_{l,n+r}+\varepsilon_{m+l+1};\end{aligned} \tag{D2}$$

which leads to the relations

$$\sum_{l=0}^{m-1}(\Delta^{-1})_{kl}\varepsilon_{n+l+1}=\sum_{r=0}^{m-n-1}\delta_{k,n+r}+\sum_{l=0}^{m-1}\varepsilon_{m+l+1}, \tag{D3}$$

$$\begin{aligned}&\sum_{k,l=0}^{m-1}\varepsilon_{n+k+1}(\Delta^{-1})_{kl}\varepsilon_{n+l+1}\\ &=\sum_{r=0}^{m-n-1}\varepsilon_{2n+r+1}+\sum_{k,l=0}^{m-1}\varepsilon_{n+k+1}(\Delta^{-1})_{kl}\varepsilon_{m+l+1}\\ &=\sum_{s=0}^{m-n-1}\varepsilon_{2n+r+1}+\sum_{s=0}^{m-n-1}\varepsilon_{n+m+s+1}\\ &\qquad+\sum_{k,l=0}^{m-1}\varepsilon_{m+k+1}(\Delta^{-1})_{kl}\varepsilon_{m+l+1}.\end{aligned}$$

Hence, one has for $n\leq m$ the algebraic identity

$$\begin{aligned}&\boldsymbol{\alpha}^{\dagger}(n,m)\mathbf{\Delta}^{-1}\boldsymbol{\alpha}(n,m)\\ &\qquad=\sum_{k=2n+1}^{2m}\varepsilon_k+\boldsymbol{\alpha}^{\dagger}(m,m)\mathbf{\Delta}^{-1}\boldsymbol{\alpha}(m,m),\end{aligned} \tag{D4}$$

which is the result desired.