QUANTUM THEORY PROJECT
FOR RESEARCH IN ATOMIC, MOLECULAR AND SOLID STATE
CHEMISTRY AND PHYSICS
UNIVERSITY OF FLORIDA, GAINESVILLE, FLORIDA

STUDIES IN PERTURBATION THEORY. XI
LOWER BOUNDS TO ENERGY EIGENVALUES, GROUND STATE AND EXCITED STATES

by

Per-Olov Löwdin*

PREPRINT NO. 68
June 15, 1964

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* Since the author is also connected with the Uppsala University, this report has been issued as Technical Note No. 121 from the Uppsala Quantum Chemistry Group.

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ABSTRACT

The bracketing theorem in the partitioning technique for solving the Schrödinger equation may be used in principle to determine upper and lower bounds to energy eigenvalues. Practical lower bounds of any accuracy desired may be evaluated by utilizing the properties of "inner projections" on finite manifolds in the Hilbert space. The method is here applied to the ground state and excited states of a Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \bar{V}$ having a positive definite perturbation $\bar{V}$. Even if inspiration is derived from the method of intermediate Hamiltonians, the final results are of bracketing type and independent of this approach. The method is numerically illustrated in some accompanying papers.

Author

I. INTRODUCTION

The problem of evaluating lower bounds to the energy eigenvalues E to the Schrödinger equation $\mathcal{H}\Psi = E\Psi$ is of great importance and, in a previous paper[1], we have given a short survey of the history of the problem and a summary of the results obtained so far. The fundamental importance of the work by Alexander Weinstein[2] and his school, Aronszajn[3], Fox and Bazley[4] et. al., and the strength of the idea of the "intermediate Hamiltonians" were emphasized. At the same time, it was shown that the problem could be approached in an entirely different way by using the so-called "bracketing function" $\mathcal{E}_1 = f(\mathcal{E})$, which is such that every interval $(\mathcal{E}_1, \mathcal{E})$ contains at least one true eigenvalue E. If $\mathcal{E}$ is chosen as an upper bound and $\mathcal{E}_1 < \mathcal{E}$, the quantity $\mathcal{E}_1$ is hence going to provide a lower bound to E.

The main problem in this approach is to evaluate the bracketing function $\mathcal{E}_1 = f(\mathcal{E})$ or a lower bound to this function for a given value of the variable $\mathcal{E}$. In this connection, it may be convenient to put the Hamiltonian in the form $\mathcal{H} = \mathcal{H}_0 + V$, where the "unperturbed" Hamiltonian $\mathcal{H}_0$ has the eigenvalues E_ω^0 and eigenfunctions Ψ_ω^0, and V is a not necessarily small "perturbation". In PT X, we studied the problem of evaluating a lower bound to the ground-state energy of $\mathcal{H}$, in case the conditions

$$V > 0 \,, \qquad \mathcal{E} < E_1^0 \tag{1}$$

were fulfilled. The first implies that the "perturbation" V should be positive definite, and the second that the ground-state energy of $\mathcal{H}$ should be situated between the two lowest eigenvalues of $\mathcal{H}_0$. In this paper, we are going to make ourselves free from the second restriction and to extend the treatment also to the excited states.

II. PROPERTIES OF BRACKETING FUNCTION

The partitioning technique[5] for solving the Schrödinger equation $\mathcal{H}\underline{\Psi} = E\underline{\Psi}$ is based on the use of a variable $\mathcal{E}$, a normalized reference function φ having $\langle\varphi|\varphi\rangle = 1$, and a reduced resolvent T. If $\mathbb{O} = |\varphi\rangle\langle\varphi|$ is the projection operator on the one-dimensional "reference space" and $P = 1 - \mathbb{O}$ is the projection operator for the orthogonal complement, one has the definition

$$T = P\left[\alpha\cdot\mathbb{O} + P(\mathcal{E}-\mathcal{H})P\right]^{-1}P \,, \tag{2}$$

for any $\alpha \neq 0$. This operator satisfies the following algebraic relations

$$\mathbb{O}T = T\mathbb{O} = 0 \,, \tag{3}$$

$$P(\mathcal{E}-\mathcal{H})T = P \,, \tag{4}$$

$$\frac{\partial T}{\partial \alpha} \equiv 0 \,, \qquad \text{for } \alpha \neq 0 \,, \tag{5}$$

$$\frac{\partial T}{\partial \mathcal{E}} = -T^2 \,, \tag{6}$$

and it has become customary to use the symbolic notation

$$T = \frac{P}{\mathcal{E}-\mathcal{H}} \tag{7}$$

The fundamental properties of T are studied in Appendix A. In order

to proceed, it is convenient to introduce the "trial" wave function $\underline{\Psi}_\varepsilon$ associated with the variable ε by the definition:

$$\underline{\Psi}_\varepsilon = \varphi + T\mathcal{H}\varphi \,. \tag{8}$$

It satisfies the intermediate normalization $\langle\varphi|\underline{\Psi}_\varepsilon\rangle = 1$ useful in all parts of the spectrum and, according to (4), the relation $P(\varepsilon-\mathcal{H})\underline{\Psi}_\varepsilon = 0$. This implies that

$$\begin{aligned}(\varepsilon-\mathcal{H})\underline{\Psi}_\varepsilon &= (\mathbb{O}+P)(\varepsilon-\mathcal{H})\underline{\Psi}_\varepsilon = \\ &= \mathbb{O}(\varepsilon-\mathcal{H})\underline{\Psi}_\varepsilon = \varphi\langle\varphi|\varepsilon-\mathcal{H}|\underline{\Psi}_\varepsilon\rangle = \\ &= \varphi\left(\varepsilon-\langle\varphi|\mathcal{H}|\underline{\Psi}_\varepsilon\rangle\right) = \varphi(\varepsilon-\varepsilon_1)\,,\end{aligned} \tag{9}$$

where we have used the notation $\varepsilon_1 = \langle\varphi|\mathcal{H}|\underline{\Psi}_\varepsilon\rangle$. It is clear that $\underline{\Psi}_\varepsilon$ satisfies an <u>inhomogeneous</u> differential equation closely associated with the Schrödinger equation and with a right-hand member proportional to the reference function φ :

$$(\mathcal{H}-\varepsilon)\underline{\Psi}_\varepsilon = (\varepsilon_1-\varepsilon)\varphi \tag{10}$$

Of particular interest is the quantity ε_1 given by the relation

$$\begin{aligned}\varepsilon_1 &= \langle\varphi|\mathcal{H}|\underline{\Psi}_\varepsilon\rangle = \\ &= \langle\varphi|\mathcal{H}+\mathcal{H}T\mathcal{H}|\varphi\rangle = \\ &= \langle\varphi|\mathcal{H}+\mathcal{H}\frac{P}{\varepsilon-\mathcal{H}}\mathcal{H}|\varphi\rangle \equiv f(\varepsilon)\,,\end{aligned} \tag{11}$$

and defining a function $\mathcal{E}_1 = f(\mathcal{E})$ of the variable $\mathcal{E}$, which will be studied over the real axis, $-\infty < \mathcal{E} < +\infty$. The values $\mathcal{E}$, for which $\mathcal{E}_1 = \mathcal{E} = E$, are of special importance, since the trial function $\Psi_\mathcal{E}$ will then satisfy the original Schrödinger equation $(\mathcal{H} - E)\Psi_E = 0$.

From now on, we will concentrate our interest to regions where the trial function (8) is normalizable, so that

$$\langle \Psi_\mathcal{E} | \Psi_\mathcal{E} \rangle = \langle \varphi | \varphi \rangle + \langle T\mathcal{H}\varphi | T\mathcal{H}\varphi \rangle \qquad (12)$$

exists. According to (6), one obtains further

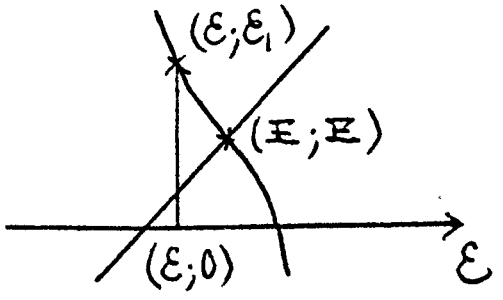
$$\frac{d\mathcal{E}_1}{d\mathcal{E}} = -\langle \varphi | \mathcal{H} T^2 \mathcal{H} | \varphi \rangle =$$

$$= -\langle T\mathcal{H}\varphi | T\mathcal{H}\varphi \rangle < 0, \qquad (13)$$

so that the derivative $f'(\mathcal{E})$ is negative. The curve for $\mathcal{E}_1 = f(\mathcal{E})$ is hence monotonously decreasing, and has further a series of vertical asymptotes for such $\mathcal{E}$-values as are eigenvalues of the operator $\overline{\mathcal{H}} = P\mathcal{H}P$ different from the eigenvalues of the operator $\mathcal{H}$ itself. For further details, see Appendix A and PT X.

Let us now consider a continuous part of the curve $\mathcal{E}_1 = f(\mathcal{E})$ associated with the eigenvalue E. Putting $\mathcal{E}_1 = E + \epsilon_1$ and $\mathcal{E} = E + \epsilon$, one obtains $E + \epsilon_1 =$

$$= f(E+\epsilon) = f(E) + \epsilon f'(E+\theta\epsilon),$$



where $0 < \theta < 1$, and this gives

$$\epsilon_1 = \epsilon\, f'(E+\theta\epsilon)\,, \qquad (14)$$

which implies that the "errors" ϵ and ϵ_1 have different signs and that the numbers $\mathcal{E}$ and $\mathcal{E}_1$ bracket at least one true eigenvalue E. For this reason, the function $\mathcal{E}_1 = f(\mathcal{E})$ will in the following be called the "bracketing function". For $\mathcal{E} = -\infty$, one has e.g. $\mathcal{E}_1 = \langle\varphi|\mathcal{H}|\varphi\rangle$, and the bracketing theorem says that there is at least one eigenvalue between $-\infty$ and $\langle\varphi|\mathcal{H}|\varphi\rangle$ -- a result familiar from the variation principle.

A study of the relations (12) and (14) shows that $\mathcal{E}_1$ is a <u>better bound</u> to E than $\mathcal{E}$, if and only if $|f'(E+\theta\epsilon)| < 1$, i.e.

$$\langle T\mathcal{H}\varphi \,|\, T\mathcal{H}\varphi\rangle < \langle\varphi|\varphi\rangle\,. \qquad (15)$$

According to (12), this means that the reference function φ must give a larger contribution than the orthogonal complement $T\mathcal{H}\varphi$ to the normalization integral $\langle\Psi_\mathcal{E}|\Psi_\mathcal{E}\rangle$, i.e. φ must contribute more than 50% of the wave function Ψ.

The bracketing procedure breaks down only if the reference function happens to be orthogonal to specific eigenfunction Ψ, in which case the associated eigenvalue E does not show up at all. Otherwise the reference function φ may be chosen quite arbitrarily, but it is clear that, if one wants a good upper bound $\mathcal{E}$ to give an even better lower bound $\mathcal{E}_1$, the function φ has to be carefully chosen. In the perturbation theory developed in PT X, the reference function φ was chosen to be an eigenfunction to $\mathcal{H}_0$ and, if the perturbation V is large, the condition (15) may not be satisfied at all. Since our practical evaluation of $\mathcal{E}_1$ is associated with writing the Hamiltonian in the

form $\mathcal{H} = \mathcal{H}_0 + V$, it is hence desirable to try to develop a modification of perturbation theory in which one can use an arbitrary reference function φ as a starting point and improve the bounds by improving this function itself.

III. PERTURBATION THEORY WITH ARBITRARY REFERENCE FUNCTION

Wave and Reaction Operators

If the Hamiltonian $\mathcal{H}$ is written as the sum of two terms $\mathcal{H} = \mathcal{H}_0 + V$, it is convenient to introduce a generalized reaction operator $\mathcal{K}$ and a wave operator W through the relations:

$$W = 1 + TV , \tag{16}$$

$$\mathcal{K} = VW = V + VTV , \tag{17}$$

Whereas in conventional perturbation theory, one tries to hit the true eigenvalue E at once, we will here only try to "bracket" such an eigenvalue in an interval $(\mathcal{E}_1 , \mathcal{E})$, and the operators $\mathcal{K}$ and W will hence depend on $\mathcal{E}$.

In order to proceed, it is now convenient to introduce the reduced resolvent T_0 associated with the operator $\mathcal{H}_0$ through the symbolic relation

$$T_0 = \frac{P}{\mathcal{E} - \mathcal{H}_0} , \tag{18}$$

analogous to (2) and (7). Using the operator identity $(A-B)^{-1} \equiv A^{-1} + A^{-1}B(A-B)^{-1}$, one obtains $T = T_0 + T_0 V T = T_0(1+VT)$, $TV = T_0 t$, $t = V + V T_0 t$, $(1 - V T_0)\, t = V$, and

$$t = (1 - V T_0)^{-1} V = V (1 - T_0 V)^{-1}, \tag{19}$$

$$W = (1 - T_0 V)^{-1} \tag{20}$$

If the perturbation V has a product form, $V = V_1 \cdot V_2$, one gets further the more general expression

$$t = V_1 (1 - V_2 T_0 V_1)^{-1} V_2, \tag{21}$$

which is easily shown to satisfy the basic equation $t = V + V T_0 t$ even if the factors V_1 and V_2 would not have any inverse operators. If finally V has an inverse, one obtains the simple relation

$$t^{-1} = V^{-1} - T_0, \tag{22}$$

which forms the starting point for PT X. For the reduced resolvent T, one obtains similarly $T = T_0 + T_0 V T$, $(1 - T_0 V)\, T = T_0$, and

$$T = (1 - T_0 V)^{-1} T_0, \tag{23}$$

$$T = T_0' + T_0 t T_0 \tag{24}$$

It should be observed that all the relations (16) - (24) are valid irrespective of the choice of the reference function φ which enters only through the projection operator $P = 1 - |\varphi\rangle\langle\varphi|$ for the orthogonal complement.

Transformation of the Wave Function Ψ_ε

According to (8), the trial wave function associated with the variable ε may be written in the form $\Psi_\varepsilon = (1 + T\mathcal{H})\,\varphi$ For the operator $(1 + T\mathcal{H})$, one gets now according to (23) and (20) the following transformation:

$$\begin{aligned} 1 + T\mathcal{H} &= 1 + (1 - T_0 V)^{-1} T_0 \mathcal{H} = \\ &= (1 - T_0 V)^{-1} \{ 1 - T_0 V + T_0 \mathcal{H} \} = \\ &= (1 - T_0 V)^{-1} (1 + T_0 \mathcal{H}_0) = W (1 + T_0 \mathcal{H}_0) \end{aligned} \tag{25}$$

Because of the factor $(1 + T_0 \mathcal{H}_0)$, which is going to occur frequently in the following, it is now convenient to introduce a <u>modified reference</u> $\overline{\varphi}$ through the relation

$$\overline{\varphi} = (1 + T_0 \mathcal{H}_0)\,\varphi \tag{26}$$

The problem of calculating this function is treated in Appendix B. Combination of (25) and (26) gives finally

$$\Psi_\varepsilon = W \overline{\varphi} \tag{27}$$

i.e. the trial wave function is obtained by letting the wave operator

W work on the modified reference function $\overline{\varphi}$. If the original reference function φ is chosen to be an eigenfunction Ψ_k° of $\mathcal{H}_0$, one has immediately $\overline{\varphi} = \Psi_k^\circ$, and one is back to the treatment in PT X.

Transformation of the Bracketing Function $\mathcal{E}_1 = f(\mathcal{E})$.

According to (11), the bracketing function is defined by the expression $\mathcal{E}_1 = \langle \varphi | \mathcal{H} + \mathcal{H} T \mathcal{H} | \varphi \rangle$. For the operator $\mathcal{H} + \mathcal{H} T \mathcal{H}$, one obtains, by using the relations $\mathcal{A} = V + V T V$, $TV = T_0 \mathcal{A}$, $VT = \mathcal{A} T_0$, and $T = T_0 + T_0 \mathcal{A} T_0$ treated above, the following transformation:

$$\mathcal{H} + \mathcal{H} T \mathcal{H} = \mathcal{H}_0 + V + (\mathcal{H}_0 + V) T (\mathcal{H}_0 + V) =$$

$$= \mathcal{H}_0 + V + \mathcal{H}_0 T \mathcal{H}_0 + \mathcal{H}_0 T V + V T \mathcal{H}_0 + V T V =$$

$$= \mathcal{H}_0 + \mathcal{A} + \mathcal{H}_0 (T_0 + T_0 \mathcal{A} T_0) \mathcal{H}_0 + \mathcal{H}_0 T_0 \mathcal{A} + \mathcal{A} T_0 \mathcal{H}_0 =$$

$$= (\mathcal{H}_0 + \mathcal{H}_0 T_0 \mathcal{H}_0) + (1 + \mathcal{H}_0 T_0) \mathcal{A} (1 + T_0 \mathcal{H}_0) \quad (28)$$

Substituting this expression into (11), we obtain

$$\mathcal{E}_1 = \langle \varphi | \mathcal{H}_0 | \overline{\varphi} \rangle + \langle \overline{\varphi} | \mathcal{A} | \overline{\varphi} \rangle =$$

$$= \langle \overline{\varphi} | \mathcal{H}_0 | \varphi \rangle + \langle \overline{\varphi} | \mathcal{A} | \overline{\varphi} \rangle \quad (29)$$

which is an expression closely analogous to the corresponding formula in PT X. Since $\varphi = (1 + T_0 \mathcal{H}_0)^{-1} \overline{\varphi}$, one obtains further

$$\mathcal{E}_1 = \langle \overline{\varphi} \,|\, \mathcal{H}_0 (1 + T_0 \mathcal{H}_0)^{-1} + \mathcal{A} \,|\, \overline{\varphi} \rangle \,, \tag{30}$$

which gives the bracketing function as an expectation value with respect to $\overline{\varphi}$. In this connection, however, it should be observed that the modified reference function $\overline{\varphi}$ is not properly normalized:

$$\langle \overline{\varphi} \,|\, \overline{\varphi} \rangle = \langle \varphi \,|\, 1 + \mathcal{H}_0 T_0^2 \mathcal{H}_0 \,|\, \varphi \rangle, \tag{31}$$

and that further $\overline{\varphi}$ depends on the variable $\mathcal{E}$. In the following, we will hence mainly use the form (29) for practical purposes.

IV. CASE OF POSITIVE DEFINITE PERTURBATION

Effect of Inner Projection

In this section, we will try to evaluate a lower bound to the bracketing function $\mathcal{E}_1 = f(\mathcal{E})$ defined by (29) in the case of a positive definite perturbation $V > 0$. For this purpose, we will utilize the method of forming "inner projections"[1,3,4].

Inner Projections

If $\mathbf{f} = (f_1, f_2, \cdots f_n)$ is a set of n linearly independent functions in Hilbert space having the metric $\Delta = \langle \mathbf{f} | \mathbf{f} \rangle$, i.e. $\Delta_{kl} = \langle f_k | f_l \rangle$, and spanning a subspace $\mathcal{M}_n$, then the

For the inner projection, one obtains according to (32) and (35) the following alternative expressions:

$$A' = A^{1/2}|f\rangle\langle f|f\rangle^{-1}\langle f|A^{1/2} = \tag{36}$$

$$= A|g\rangle\langle g|A|g\rangle^{-1}\langle g|A = \tag{37}$$

$$= |h\rangle\langle h|A^{-1}|h\rangle^{-1}\langle h| \tag{38}$$

The first form will be denoted as the standard inner projection, whereas the second will be called an Aronszajn projection, and the third a Bazley projection. It may also be convenient to refer to the manifold $f = (f_1, f_2, \ldots f_n)$ as the "standard space", to the manifold $g = (g_1, g_2, \ldots g_n)$ as an "Aronszajn space", and to the manifold $h = (h_1, h_2, \ldots h_n)$ as a "Bazley space". It should be observed that the form (37) was the first one to be introduced by Aronszajn[3], and some additional features of this projection are treated in Appendix C.

In PT X, it was shown that, if $\varphi = \Sigma_0^0$ and $\varepsilon < E_1^0$, the reaction operator t itself was positive definite and satisfied the inequality

$$0 < t < V \tag{39}$$

According to (36) - (38), it was then easy to construct an inner projection $t' = t^{\frac{1}{2}}Qt^{\frac{1}{2}}$ satisfying the inequality $t' < t$, which could be used to evaluate a lower bound to ε_1 and hence also to the ground state energy E_a. In the general case, however, t is not positive definite, and the problem must be approached in another way.

Treatment by an Intermediate Hamiltonian

Let us first see what happens, if the problem is temporarily treated by means of the method of intermediate Hamiltonians. In addition to $\mathcal{H} = \mathcal{H}_0 + V$, we will then consider an intermediate Hamiltonian $\mathcal{H}' = \mathcal{H}_0 + V'$, where $V' = V^{1/2} Q V^{1/2}$ is an inner projection of the perturbation V --defined by the relations (36) - (38). One has $\mathcal{H}' < \mathcal{H}$, from which follows the theorem $E'_k < E_k$ for the eigenvalues taken in order. If the ordering condition is fulfilled, the eigenvalues of $\mathcal{H}'$ are hence lower bounds to the eigenvalues of $\mathcal{H}$. The solution of the eigenvalue problem for $\mathcal{H}'$ is briefly surveyed in Appendix D.

Here we will instead proceed by bracketing the eigenvalues to $\mathcal{H}'$, and it is then necessary to evaluate the associated reaction operator t'. For the perturbation V', we will use the form (37):

$$V' = V|q\rangle \langle q|V|q\rangle^{-1} \langle q|V \tag{40}$$

which is considered to consist of two factors $V' = V'_1 \cdot V'_2$. We note that V' has no inverse. Substitution into (21) gives immediately

$$t' = V'_1 \{1 - V'_2 T_0 V'_1\}^{-1} V'_2 =$$

$$= V|q\rangle \langle q|V|q\rangle^{-1} \{1 - \langle q|V T_0 V|q\rangle \langle q|V|q\rangle^{-1}\}^{-1} \langle q|V =$$

$$= V|q\rangle \{\langle q|V|q\rangle - \langle q|V T_0 V|q\rangle\}^{-1} \langle q|V =$$

$$= V|q\rangle \langle q|V - V T_0 V|q\rangle^{-1} \langle q|V \tag{41}$$

which is a practically very useful form. Using (22) and introducing the Bazley space $h = Vq$, one obtains further the relation

$$t' = V|q\rangle\langle q|Vt^{-1}V|q\rangle^{-1}\langle q|V = \\ = |h\rangle\langle h|t^{-1}|h\rangle^{-1}\langle h| , \tag{42}$$

showing that t' has actually the same form as the Bazley projection of t. However, since t is not positive definite, one must not draw any conclusions which later cannot be properly verified. Substitution of (41) and (42) into (29) gives

$$\mathcal{E}_1' = \langle\varphi|\mathcal{H}_0|\bar{\varphi}\rangle + \langle\bar{\varphi}|t'|\bar{\varphi}\rangle =$$

$$= \langle\varphi|\mathcal{H}_0|\bar{\varphi}\rangle + \langle\bar{\varphi}|V|q\rangle\langle q|V - VT_0V|q\rangle^{-1}\langle q|V|\bar{\varphi}\rangle =$$

$$= \langle\varphi|\mathcal{H}_0|\bar{\varphi}\rangle + \langle\bar{\varphi}|h\rangle\langle h|V^{-1} - T_0|h\rangle^{-1}\langle h|\bar{\varphi}\rangle =$$

$$= \langle\varphi|\mathcal{H}_0|\bar{\varphi}\rangle + \alpha^{\dagger}A^{-1}\alpha , \tag{43}$$

where

$$\alpha = \langle q|V|\bar{\varphi}\rangle = \langle h|\bar{\varphi}\rangle , \tag{44}$$

$$A = \langle q|V - VT_0V|q\rangle = \\ = \langle h|V^{-1} - T_0|h\rangle . \tag{45}$$

One has hence the theorem that, provided $\mathcal{E}$ is a proper upper bound, $\mathcal{E}_1'$ is a lower bound to an eigenvalue of $\mathcal{H}'$ and hence also to an eigenvalue of $\mathcal{H}$. It seems simple and straightforward to apply this approach, but there is an inherent difficulty connected with the "ordering

theorem", which is at first sight not so obvious, but which shows up very strongly in the applications, particularly if $\mathcal{H}_0$ has a low-lying limiting point.

It has been shown by Gay[5] that, under the condition $\mathcal{E} < E_1^0$, the substitution $\mathcal{R} = (\mathcal{E} - \mathcal{H}_0)^{-1}$ greatly simplifies the study of the intermediate Hamiltonian and the evaluation of a lower bound for the ground state, and this approach has been further extended by Bright Wilson[5]. However, depending on the difficulties with the ordering theorem, there is for the moment no method to generalize this approach also to the excited states or to ground state levels situated above E_1^0. A good test case is the ground state of the H^- ion which, for $V = e^2/r_{12}$, has four unperturbed energy levels situated below the ground state energy.

The bracketing theorem tells us here that there is at least one eigenvalue to $\mathcal{H}'$ situated between $\mathcal{E}_1'$ and $\mathcal{E}$, but, unless one has additional information about the lower eigenvalues, it seems impossible to say whether the interval contains also an eigenvalue to $\mathcal{H}$. At this point, we will leave the method of "intermediate Hamiltonians" and try a more direct approach.

Direct Treatment Without an Intermediate Hamiltonian

In connection with the inner projections, it is interesting to observe that the form (36) exists only for a positive definite A, whereas the forms (37) and (38) may exist even if this is not the case. In (42), there appears actually a "Bazley projection" of the reaction operator t, in spite of the fact that this operator may not be positive definite. It may hence be worthwhile to study the reaction operator t' associated with the perturbation $V' = V^{1/2} Q V^{1/2}$ to see whether one can find some simple <u>sufficient</u> conditions for the inequality $t' < t$, which would then enable us to say that there is at least one eigenvalue to $\mathcal{H}$ situated in the interval between $\mathcal{E}_1'$ and $\mathcal{E}$.

Let us introduce the notation $V'' = V - V' > 0$. By using (19) and (22), we obtain

$$
\begin{aligned}
t' &= (1 - V' T_0)^{-1} V' = \\
&= \{ 1 - (V - V'') T_0 \}^{-1} (V - V'') = \\
&= \{ 1 + (V - V'')(t^{-1} - V^{-1}) \}^{-1} (V - V'') = \\
&= t \{ V - V'' (1 - V^{-1} t) \}^{-1} (V - V'' + V'' V^{-1} t - V'' V^{-1} t) = \\
&= t - t V^{-1} \{ 1 - V'' (V^{-1} - V^{-1} t V^{-1}) \}^{-1} V'' V^{-1} t = \\
&= t - t V^{-1} \{ 1 + V'' T \}^{-1} V'' V^{-1} t = \\
&= t - t V^{-1} \omega V^{-1} t ,
\end{aligned}
\tag{46}
$$

where

$$
\omega = (1 + V'' T)^{-1} V'' \tag{47}
$$

It is clear that $t' < t$, if ω is positive definite. Let us now assume that V'' can be written in product form, so that $V'' = V_1'' V_2''$. By using the same arguments as were used in transforming (19) into (21), one obtains

$$
\omega = V_1'' (1 + V_2'' T V_1'')^{-1} V_2'' \tag{48}
$$

Since $V'' = V - V' = V - V^{1/2} Q V^{1/2} = V^{1/2}(1-Q)V^{1/2}$ and $(1-Q)$ is idempotent, one can put $V''_1 = V^{1/2}(1-Q)$ and $V''_2 = (1-Q)V^{1/2} = (V''_1)^{\dagger}$. This implies that $\omega > 0$, if $1 + V''_2 T V''_1 > 0$. Using (17) and (21), one obtains the transformation $V^{1/2} T V^{1/2} = V^{-1/2} t V^{-1/2} - 1 = (1 - V^{1/2} T_0 V^{1/2})^{-1} - 1$, which gives

$$1 + V''_2 T V''_1 =$$

$$= 1 + (1-Q) V^{1/2} T V^{1/2} (1-Q) =$$

$$= Q + (1-Q)(1 - V^{1/2} T_0 V^{1/2})^{-1} (1-Q) > 0. \quad (49)$$

This implies that $t' < t$, if the operator $(1 - V^{1/2} T_0 V^{1/2})^{-1}$ is positive definite for the given value of $\mathcal{E}$ within the subspace of $(1-Q)$, i.e. within the orthogonal complement to the standard manifold $\mathbf{f} = (f_1, f_2, \cdots f_n)$.

It is perhaps interesting to observe that perturbation expansions of the Brillouin-tupe for t and W are possible, if and only if the convergence criterion

$$-1 < V^{1/2} T_0 V^{1/2} < +1 \quad (50)$$

is fulfilled. Since in such a case $1 - V^{1/2} T_0 V^{1/2} > 0$, one has further $(1 - V^{1/2} T_0 V^{1/2})^{-1} > 0$ over the entire space, and the condition (49) is automatically fulfilled.

Case of $\mathcal{E} < E^{0}_{\rho+1}$.

Let us now consider an energy level of $\tilde{\mathcal{H}}$ such that there is an upper bound $\mathcal{E}$ satisfying the inequality

$$\mathcal{E} < E^{0}_{\rho+1} \tag{51}$$

for a finite value of ρ . In such a case, it seems convenient to choose a minimum Aronszajn space consisting of all the unperturbed functions

$$\mathcal{Q} = \{ \Phi^{0}_{0}, \Phi^{0}_{1}, \Phi^{0}_{2}, \cdots \Phi^{0}_{\rho} \}, \tag{52}$$

and an arbitrary reference function φ within this space:

$$\varphi = \sum_{k=0}^{\rho} \Phi^{0}_{k} a^{0}_{k} \tag{53}$$

For T_0 , one obtains a spectral resolution of the form (see Appendix A):

$$T_0 = \sum_{k=0}^{\rho} \frac{|\bar{\Phi}^{0}_{k}\rangle\langle\bar{\Phi}^{0}_{k}|}{\mathcal{E} - \bar{E}^{0}_{k}} + \sum_{k=\rho+1}^{\infty} \frac{|\Phi^{0}_{k}\rangle\langle\Phi^{0}_{k}|}{\mathcal{E} - E^{0}_{k}} = \tag{54}$$

$$= T'_0 + T''_0$$

where the second term T''_0 is certainly negative definite: $T''_0 < 0$.

We note that the Aronszajn space has been chosen so that the functions $V^{1/2}|\Xi_k^0\rangle$ for $k = 0, 1, \ldots p$ all belong to Q, whereas the functions $V^{1/2}|\Xi_k^0\rangle$ for $k = p+1, p+2, \ldots$ all belong to $(1-Q)$. This gives

$$(1-Q)V^{1/2}\Gamma_0 V^{1/2} = V^{1/2}\Gamma_0'' V^{1/2} = \\ = V^{1/2}\Gamma_0'' V^{1/2}(1-Q) \tag{55}$$

By using the operator identity $(A-B)^{-1} \equiv A^{-1} + A^{-1}B(A-B)^{-1}$, we obtain further

$$(1-Q)(1-V^{1/2}\Gamma_0 V^{1/2})^{-1} = \\ = (1-Q) + (1-Q)V^{1/2}\Gamma_0 V^{1/2}(1-V^{1/2}\Gamma_0 V^{1/2})^{-1} = \\ = (1-Q) + V^{1/2}\Gamma_0'' V^{1/2}(1-Q)(1-V^{1/2}\Gamma_0 V^{1/2})^{-1}, \tag{56}$$

which gives

$$(1-Q)(1-V^{1/2}\Gamma_0 V^{1/2})^{-1} = (1-V^{1/2}\Gamma_0'' V^{1/2})^{-1}(1-Q) \tag{57}$$

and

$$(1-Q)(1-V^{1/2}\Gamma_0 V^{1/2})^{-1}(1-Q) = \\ = (1-Q)(1-V^{1/2}\Gamma_0'' V^{1/2})^{-1}(1-Q) > 0 \tag{58}$$

The condition (49) is hence fulfilled, and one has consequently $\omega > 0$ and $t' < t$. This implies also that, in the interval between $\mathcal{E}'_1$ and $\mathcal{E}$, there is situated at least one eigenvalue of the operator $\mathcal{H}$ itself, and no further ordering theorem is required. The lower bound $\mathcal{E}'_1$ is conveniently calculated by one of the relations (43).

Let us now keep the reference function φ fixed, but extend the Aronszajn space to a larger manifold $\mathcal{G}_1$, which contains the minimum space (52) previously defined. For the associated projection operator Q_1 for the "standard space", one has

$$Q_1 > Q \quad , \qquad Q_1 Q = Q \quad , \tag{59}$$

which gives the relations $(1 - Q_1) < (1 - Q)$ and

$$(1-Q_1)(1-Q) = (1-Q_1) \quad . \tag{60}$$

Multiplying (58) to the left and right by $(1 - Q_1)$, one obtains ·

$$(1-Q_1)\left(1-V^{1/2}\,T_0\,V^{1/2}\right)^{-1}(1-Q_1) > 0, \tag{61}$$

which shows that $\omega > 0$, $t' < t$ and $\mathcal{E}'_1 < \mathcal{E}_1$ also for the extended space. We note finally that ω goes to zero as Q approaches the identity, and that the convergence is essentially monotonous as soon as the space is extended, function for function, beyond the minimum space. Formula (43) provides hence a lower bound which can be indefinitely improved by choosing a better and better upper bound $\mathcal{E}$ and by properly extending the finite subspace used in the inner projection.

The practical treatment of the operator T_0 is outlined in Appendix A, and one may further simplify the calculations by some of the transformations described in PT X.

V. PERTURBATION EXPANSIONS

In conventional perturbation theory, the operators t and W are expanded in terms of infinite power series in the operator V. In PT X, we have studied the corresponding finite expansions with an estimate of the remainder term, and we will here briefly consider these expansions in the case of $V > 0$ and $\mathcal{E} < E_{p+1}^0$. By a proper choice of reference function φ and minimum Aronszajn space $\mathfrak{g}$ according to (52), one obtains a lower bound t' for the reaction operator t, so that $t' < t$. Here t' is defined by the expressions (41) and (42).

Using (22) and the symmetric expansion of the inverse[1], one obtains directly

$$\begin{aligned} t &= \left(V^{-1} - T_0\right)^{-1} = \\ &= V + VT_0V + VT_0tT_0V , \end{aligned} \tag{62}$$

and the lower bound

$$t > V + VT_0V + VT_0t'T_0V \tag{63}$$

More generally one has the finite expansion

$$\begin{aligned} t &= V\sum_{k=0}^{2m-1}(T_0V)^k + (VT_0)^m t (T_0V)^m > \\ &> V\sum_{k=0}^{2m-1}(T_0V)^k + (VT_0)^m t' (T_0V)^m . \end{aligned} \tag{64}$$

and substitution into (43) gives the estimate

$$\mathcal{E}_1 > \langle\Phi|\mathcal{H}_0|\bar{\Phi}\rangle + \langle\bar{\Phi}|V\sum_{k=0}^{2m-1}(T_0V)^k|\bar{\Phi}\rangle +$$

$$+\langle\bar{\Phi}|V(T_0V)^m|q\rangle\langle q|V-VT_0V|q\rangle^{-1}\langle q|(VT_0)^mV|\bar{\Phi}\rangle \tag{65}$$

This formula is a direct generalization of the corresponding relation in PT X to the case of an arbitrary reference function, and it remains still to be seen how useful expansions of this type can be.

VI DISCUSSION

In this paper, we have discussed the application of the partitioning technique and the evaluation of the bracketing function $\mathcal{E}_1 = f(\mathcal{E})$ in the case when the Hamiltonian can be written as the sum of two terms $\mathcal{H} = \mathcal{H}_0 + V$, one of which is positive definite. If the variable $\mathcal{E}$ is chosen as an upper bound, the quantity $\mathcal{E}_1$ will provide a lower bound to an eigenvalue E situated between $\mathcal{E}_1$ and $\mathcal{E}$. In PT X, the case $\mathcal{E} < E_1^0$ was studied in greater detail, and the treatment has here been extended to the case $\mathcal{E} < E_{p+1}^0$. It has been shown that, if the Aronszajn space q contains all the eigenfunctions $\Phi_0^0, \Phi_1^0, \ldots \Phi_p^0$, and the reference function Φ is a linear combination of them, the quantity

$$\mathcal{E}_1' = \langle\Phi|\mathcal{H}_0|\bar{\Phi}\rangle +$$

$$+\langle\bar{\Phi}|V|q\rangle\langle q|V-VT_0V|q\rangle^{-1}\langle q|V|\bar{\Phi}\rangle, \tag{66}$$

provides a lower bound to $\mathcal{E}_1$ and hence also to E. In PT X, we have discussed some transformations and methods which may be useful in evaluating quantities of this type. In arriving at the final results, we have not explicitly used the idea of the intermediate Hamiltonians and the associated ordering requirement as to the eigenvalues, which seems to be an advantage. However, the study of formula (46) should be considered only as a first rough approximation, and there is little doubt that the discussion of the conditions for the inequality $t' < t$ can be greatly refined. It is also desirable to remove the present restrictions on the reference function φ to be a <u>finite</u> sum of eigenfunctions to $\mathcal{H}_0$.

In conclusion, an alternative approach based on the use of a multidimensional projection $\mathcal{O}$ of order m should be briefly mentioned.[5] The operator

$$\overline{\mathcal{H}} = \mathcal{O}\left(\mathcal{H}+\mathcal{H}\mathcal{T}\mathcal{H}\right)\mathcal{O} = \overline{\mathcal{H}}(\mathcal{E}) \qquad (67)$$

may be represented by a finite matrix of order m having elements which are all functions of the variable $\mathcal{E}$. The secular equation for $\overline{\mathcal{H}}$ of order m defines a multi-valued function $\mathcal{E}_1, \mathcal{E}_2, \ldots \mathcal{E}_m$ of the variable $\mathcal{E}$, and there is again a bracketing theorem saying that each interval between $\mathcal{E}$ and $\mathcal{E}_\omega$ contains at least one true eigenvalue E of $\mathcal{H}$. In the case $\mathcal{E} < E_{p+1}^0$, it is convenient to define $\mathcal{O}$ so that the subspace contains the functions $\mathfrak{S}_0^0$, $\mathfrak{S}_1^0, \ldots \mathfrak{S}_p^0$, and the technique developed in PT X can then be applied. It should be observed that, even if the secular equation renders m roots for every value of $\mathcal{E}$, there is usually only one interval at a time which is of practical importance for bracketing an eigenvalue. This approach will be studied in greater detail in a forthcoming paper.

Some numerical applications of formula (66) and the technique developed in this paper are published in the accompanying papers by some

of my colleagues and co-workers, and the results seem to be very encouraging. The author is greatly indebted to Prof. Charles Reid, Prof. Darwin Smith, Dr. Jack Gay, and Mr. Osvaldo Goscinski for many interesting and valuable comments about this problem.

In conclusion the author would also like to express his sincere gratitude to Prof. Robert S. Mulliken for many fruitful discussions about the fundaments of quantum mechanics, including the problem of finding lower bounds to the energy levels.

APPENDIX A. PROPERTIES OF THE REDUCED RESOLVENTS T AND T_0.

The reduced resolvent T is defined by (2) and characterized by the relations (3) - (6). One has further $PT = TP = T$. The operator T has been evaluated if, for any given function f, one can determine the function

$$\chi = Tf \,, \tag{A1}$$

satisfying the relation $P\chi = \chi$. This problem can be attacked in several ways.

Spectral Resolution of T.

Let us assume that $\mathcal{H}$ has the eigenfunctions Φ_k and eigenvalues E_k satisfying the resolution of the identity $1 = \Sigma_k |\Phi_k\rangle\langle\Phi_k|$ and the spectral resolution $\mathcal{H} = \Sigma_k E_k |\Phi_k\rangle\langle\Phi_k|$. Let us further consider the "outer projection" $\overline{\mathcal{H}}$ defined by the relation[1)]

$$\overline{\mathcal{H}} = P\mathcal{H}P \,, \tag{A2}$$

The reference function φ is an eigenfunction of $\overline{\mathcal{H}}$ associated with the eigenvalue 0, which is of little interest to us, and instead we will concentrate on the eigenfunctions $\overline{\Phi}_k$ associated with the eigenvalues $\overline{E}_k$ situated in the subspace of P. One has the resolutions

$$P = \sum_k |\overline{\Phi}_k\rangle\langle\overline{\Phi}_k| \,, \tag{A3}$$

$$\overline{\mathcal{H}} = \sum_k E_k |\overline{\Phi}_k\rangle\langle\overline{\Phi}_k| \tag{A4}$$

Let us now study the transformation (A1). Applying the operator $P(\mathcal{E}-\mathcal{H})$ to both sides and using (4), one obtains

$$
\begin{aligned}
P(\mathcal{E}-\mathcal{H})\chi &= Pf\ ;\\
P(\mathcal{E}-\bar{\mathcal{H}})\chi &= Pf\ ;\\
(\mathcal{E}-\bar{\mathcal{H}})\chi - \varphi\langle\varphi|\mathcal{E}-\bar{\mathcal{H}}|\chi\rangle &= Pf\ ;\\
(\mathcal{E}-\bar{\mathcal{H}})\chi &= Pf\ ;\\
\chi = (\mathcal{E}-\bar{\mathcal{H}})^{-1}Pf &= \\
= \sum_k \frac{|\bar{\Psi}_k\rangle\langle\bar{\Psi}_k|P}{\mathcal{E}-\bar{E}_k} f &= \\
= \left(\sum_k \frac{|\bar{\Psi}_k\rangle\langle\bar{\Psi}_k|}{\mathcal{E}-\bar{E}_k}\right) f &\ , \qquad \text{(A5)}
\end{aligned}
$$

and

$$
T = \sum_k \frac{|\bar{\Psi}_k\rangle\langle\bar{\Psi}_k|}{\mathcal{E}-\bar{E}_k}\ , \qquad \text{(A6)}
$$

where $|\bar{\Psi}_k\rangle\langle\bar{\Psi}_k| = \bar{O}_k$ is a positive definite projection operator. This is the spectral resolution of T, in which one sums over all eigenfunctions $\bar{\Psi}_k$ to $\bar{\mathcal{H}}$ within the subspace of P. If the eigenvalues of $\bar{\mathcal{H}}$ in increasing order are $\bar{E}_1 < \bar{E}_2 < \bar{E}_3 < \dots$, one obtains, for $\mathcal{E} < \bar{E}_1$, the estimate:

$$
0 > T > \frac{P}{\mathcal{E}-\bar{E}_1} \qquad \text{(A7)}
$$

and more generally, for $\mathcal{E} < \overline{E}_{p+1}$:

$$\sum_{k=1}^{p} \frac{\overline{\mathbb{O}}_k}{\mathcal{E}-\overline{E}_k} > T > \sum_{k=1}^{p} \frac{\overline{\mathbb{O}}_k}{\mathcal{E}-\overline{E}_k} + \frac{P - \sum_{k=1}^{p} \overline{\mathbb{O}}_k}{\mathcal{E} - \overline{E}_{p+1}} \qquad (A8)$$

It is evident that the eigenvalues and eigenfunctions of $\overline{\mathcal{H}}$ play a large role in determining the properties of T

Eigenvalue Problem of $\overline{\mathcal{H}} = P\mathcal{H}P$.

Let us now study the eigenvalue problem

$$\overline{\mathcal{H}}\ \overline{\Phi} = \overline{E}\ \overline{\Phi} \qquad (A9)$$

where all the eigenfunctions $\overline{\Phi}$ should belong to the subspace P , so that $P\overline{\Phi} = \overline{\Phi}$. This is a typical Weinstein problem[2]. The eigenfunctions are also orthogonal to φ , so that $\langle\varphi|\overline{\Phi}\rangle = 0$. From (A9), one obtains

$$(\overline{\mathcal{H}} - \overline{E})\,\overline{\Phi} = 0 ;$$
$$P(\mathcal{H} - \overline{E})\,\overline{\Phi} = 0 ;$$
$$(\mathcal{H} - \overline{E})\,\overline{\Phi} = \mathbb{O}(\mathcal{H} - \overline{E})\,\overline{\Phi} ;$$
$$(\mathcal{H} - \overline{E})\,\overline{\Phi} = \varphi\langle\varphi|\mathcal{H} - \overline{E}|\,\overline{\Phi}\rangle ;$$
$$\overline{\Phi} = (\mathcal{H} - \overline{E})^{-1}\varphi\,\langle\varphi|\mathcal{H}|\,\overline{\Phi}\rangle .$$

(A10')

$$0 = \langle \varphi | \bar{\Psi} \rangle = \langle \varphi | (\mathcal{H} - \bar{E})^{-1} | \varphi \rangle \langle \varphi | \mathcal{H} | \bar{\Psi} \rangle , \qquad \text{(A10'')}$$

At this point, it is convenient to introduce the so-called Weinstein function:

$$W(\lambda) \equiv \langle \varphi | (\lambda - \mathcal{H})^{-1} | \varphi \rangle , \qquad \text{(A11)}$$

which is a simple special case of the Weinstein determinant[1]. It follows from (A10'') that, if $\langle \varphi | \mathcal{H} | \bar{\Psi} \rangle \neq 0$, the associated eigenvalue $\bar{E}$ is a zero-point of the Weinstein determinant. Since

$$W'(\lambda) = - \langle \varphi | (\lambda - \mathcal{H})^{-2} | \varphi \rangle < 0 , \qquad \text{(A12)}$$

the Weinstein function is monotonously decreasing with λ, but it should be observed that the curve for $W(\lambda)$ has a series of vertical asymptotes.

Expanding the given reference function φ in terms of the eigenfunctions Ψ_κ of $\mathcal{H}$, one has $\varphi = 1 \cdot \varphi = \left(\sum_\kappa |\Psi_\kappa\rangle\langle\Psi_\kappa| \right) \varphi = \sum_\kappa \Psi_\kappa \langle \Psi_\kappa | \varphi \rangle$, i.e.

$$\varphi = \sum_{\kappa=0}^{\infty} \Psi_\kappa a_\kappa , \qquad a_\kappa = \langle \Psi_\kappa | \varphi \rangle , \qquad \text{(A13)}$$

where the coefficients a_κ are well-defined and satisfy the relation $\sum_\kappa |a_\kappa|^2 = 1$. Using the spectral resolution of the resolvent:

$$(\lambda - \mathcal{H})^{-1} = \sum_{k=0}^{\infty} \frac{|\Phi_k\rangle\langle\Phi_k|}{\lambda - E_k} \quad , \tag{A14}$$

one obtains thus for the Weinstein function

$$W(\lambda) = \sum_{k=0}^{\infty} \frac{|a_k|^2}{\lambda - E_k} \quad , \tag{A15}$$

showing that the curve has a vertical asymptote for all values $\lambda = E_k$, for which $a_k = \langle \Phi_k | \varphi \rangle \neq 0$. The curve is illustrated below,

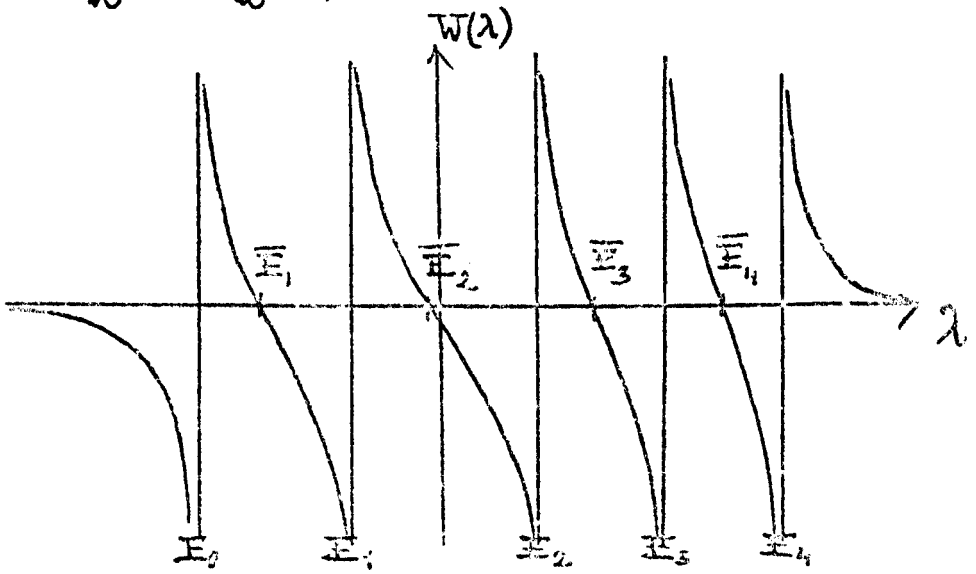


Fig. 2. Graphical illustration of the behaviour of the Weinstein function.

and we observe that the eigenvalues to $\overline{\mathcal{H}} = P\mathcal{H}P$ in order are upper bounds to the eigenvalues of $\mathcal{H}$; cf. reference 1.

If $\lambda < E_{\rho+1}$, one obtains directly the following estimate for the Weinstein function:

$$\sum_{k=0}^{\rho} \frac{|a_k|^2}{\lambda - E_k} > W(\lambda) > \sum_{k=0}^{\rho} \frac{|a_k|^2}{\lambda - E_{k+1}} + \frac{1 - \sum_{k=0}^{\rho} |a_k|^2}{\lambda - E_{\rho+1}} \qquad \text{(A16)}$$

If one puts the left-hand side equal to zero, the function $W(\lambda)$ will be negative, and the corresponding λ- values will then be upper bounds to the eigenvalues E . On the other hand, if one puts the right-hand side equal to zero, the function $W(\lambda)$ will be positive, and the corresponding λ - values will be lower bounds to E .

As an example of this technique, we will bracket the lowest eigenvalue E_1 of $\mathcal{H}$. For $\lambda < E_1$, one has according to (A16) for $\rho = 1$ and $\rho = 0$, respectively:

$$\frac{|a_0|^2}{\lambda - E_0} + \frac{|a_1|^2}{\lambda - E_1} > W(\lambda) > \frac{|a_0|^2}{\lambda - E_0} + \frac{1 - |a_0|^2}{\lambda - E_1} . \qquad \text{(A17)}$$

Putting the bounds equal to zero, one obtains the following bracketing:

$$E_0 \{1 - |a_0|^2\} + E_1 |a_0|^2 < E_1 < \frac{E_0 |a_1|^2 + E_1 |a_0|^2}{|a_0|^2 + |a_1|^2} . \qquad \text{(A18)}$$

If φ is a mixture of Φ_0 and Φ_1 only, these two bounds will coincide, and E_1 is exactly determined. In the case of a general reference function, the bounds may be improved by increasing the values of ρ used in the estimate (A16), until one reaches the accuracy desired.

It is interesting to observe that, according to the Eckart criterion, one has the operator inequality

$$1 - |\Psi_0\rangle\langle\Psi_0| < \frac{\mathcal{H} - E_0}{E_1 - E_0} \quad , \tag{A19}$$

which applied to the reference function φ gives

$$1 - |a_0|^2 \leq \frac{\langle\varphi|\mathcal{H}|\varphi\rangle - E_0}{E_1 - E_0} \tag{A20}$$

Substitution into the lower bound in (A18) gives

$$\bar{E}_1 > E_1 - (E_1 - E_0)(1 - |a_0|^2) \geq E_1 + E_0 - \langle\varphi|\mathcal{H}|\varphi\rangle \tag{A21}$$

and a rough but simple lower estimate of $\bar{E}_1$

Let us finally consider the eigenfunctions $\bar{\Psi}$ of the operator $\bar{\mathcal{H}} = \mathcal{P}\mathcal{H}\mathcal{P}$ in the case when $\langle\varphi|\mathcal{H}|\bar{\Psi}\rangle \neq 0$. According to (A10'), $\bar{\Psi}$ is proportional to $(\mathcal{H} - \bar{E})^{-1}\varphi$ and, using the spectral resolution (A14), one obtains

$$\bar{\Psi} = \text{Const.} \sum_\nu \frac{\Psi_\nu a_\nu}{E_\nu - \bar{E}} \tag{A22}$$

It is clear that all the quantities $\bar{\Psi}_i$ and $\bar{E}_i$ may be expressed in terms of the quantities Ψ_ν , E_ν , and a_ν , and, according to (A6), it should then be possible to express also $\mathcal{T}$ in terms of the latter quantities. We will now try to determine this expression directly.

Alternative Form of

Let us return to the basic relation (A1). Since $\chi = \mathcal{T} f$, one has $\langle \varphi | \chi \rangle = 0$. According to (4), one gets further

$$P(\mathcal{E} - \mathcal{H})\chi = Pf ;$$

$$(\mathcal{E} - \mathcal{H})\chi - \varphi \langle \varphi | \mathcal{E} - \mathcal{H} | \chi \rangle = f - \varphi \langle \varphi | f \rangle ;$$

$$(\mathcal{E} - \mathcal{H})\chi = f - \varphi \{ \langle \varphi | f \rangle + \langle \varphi | \mathcal{H} | \chi \rangle \} =$$

$$= f - \varphi \alpha ;$$

$$\chi = (\mathcal{E} - \mathcal{H})^{-1} f - (\mathcal{E} - \mathcal{H})^{-1} \varphi \alpha ; \tag{A23}$$

$$0 = \langle \varphi | \chi \rangle = \langle \varphi | (\mathcal{E} - \mathcal{H})^{-1} | f \rangle - \langle \varphi | (\mathcal{E} - \mathcal{H})^{-1} | \varphi \rangle \alpha \tag{A24}$$

This implies that, for the constant $\alpha = \langle \varphi | f + \mathcal{H} \chi \rangle$, one gets the value

$$\alpha = \frac{\langle \varphi | (\mathcal{E} - \mathcal{H})^{-1} | f \rangle}{\langle \varphi | (\mathcal{E} - \mathcal{H})^{-1} | \varphi \rangle} . \tag{A25}$$

Substitution into (A23) gives the explicit solution

$$\chi = (\mathcal{E} - \mathcal{H})^{-1} f - \frac{(\mathcal{E} - \mathcal{H})^{-1} | \varphi \rangle \langle \varphi | (\mathcal{E} - \mathcal{H})^{-1} | f \rangle}{\langle \varphi | (\mathcal{E} - \mathcal{H})^{-1} | \varphi \rangle} \tag{A26}$$

For the reduced resolvent $\mathcal{T}$, one obtains hence the following formula

$$\mathcal{T} = (\mathcal{E} - \mathcal{H})^{-1} - \frac{(\mathcal{E} - \mathcal{H})^{-1} \mathbb{O} (\mathcal{E} - \mathcal{H})^{-1}}{\langle \varphi | (\mathcal{E} - \mathcal{H})^{-1} | \varphi \rangle} \tag{A27}$$

We note that the quantity in the denominator is nothing but the Weinstein function $W(\mathcal{E})$ defined in (A11).

Let us now transform this expression. By using the spectral resolutions (A14) and (A15), one obtains for the numerator of (A27):

$$(\mathcal{E}-\mathcal{H})^{-1}\langle\varphi|(\mathcal{E}-\mathcal{H})^{-1}|\varphi\rangle - (\mathcal{E}-\mathcal{H})^{-1}\mathbb{O}(\mathcal{E}-\mathcal{H})^{-1} =$$

$$= \Big(\sum_\kappa \frac{\mathbb{O}_\kappa}{\mathcal{E}-E_\kappa}\Big)\Big(\sum_\ell \frac{|a_\ell|^2}{\mathcal{E}-E_\ell}\Big) - \Big(\sum_\kappa \frac{\mathbb{O}_\kappa}{\mathcal{E}-E_\kappa}\Big)\mathbb{O}\Big(\sum_\ell \frac{\mathbb{O}_\ell}{\mathcal{E}-E_\ell}\Big)$$

$$= \sum_{\kappa,\ell} \frac{\mathbb{O}_\kappa |a_\ell|^2 - \mathbb{O}_\kappa \mathbb{O} \mathbb{O}_\ell}{(\mathcal{E}-E_\kappa)(\mathcal{E}-E_\ell)} =$$

$$= \frac{1}{2}\sum_{\kappa,\ell} \frac{\mathbb{O}_\kappa |a_\ell|^2 + \mathbb{O}_\ell |a_\kappa|^2 - \mathbb{O}_\kappa \mathbb{O} \mathbb{O}_\ell - \mathbb{O}_\ell \mathbb{O} \mathbb{O}_\kappa}{(\mathcal{E}-E_\kappa)(\mathcal{E}-E_\ell)} . \tag{A28}$$

For the numerator of each term, one has further

$$\mathbb{O}_\kappa |a_\ell|^2 + \mathbb{O}_\ell |a_\kappa|^2 - \mathbb{O}_\kappa \mathbb{O} \mathbb{O}_\ell - \mathbb{O}_\ell \mathbb{O} \mathbb{O}_\kappa =$$

$$= |\underline{\Phi}_\kappa\rangle |a_\ell|^2 \langle\underline{\Phi}_\kappa| + |\underline{\Phi}_\ell\rangle |a_\kappa|^2 \langle\underline{\Phi}_\ell| -$$

$$- |\underline{\Phi}_\kappa\rangle a_\kappa a_\ell^* \langle\underline{\Phi}_\ell| - |\underline{\Phi}_\ell\rangle a_\ell a_\kappa^* \langle\underline{\Phi}_\kappa| =$$

$$= \big(|\underline{\Phi}_\kappa\rangle a_\ell^* - |\underline{\Phi}_\ell\rangle a_\kappa^*\big)\big(a_\ell \langle\underline{\Phi}_\kappa| - a_\kappa \langle\underline{\Phi}_\ell|\big) =$$

$$= \Omega_{\kappa\ell}^\dagger \Omega_{\kappa\ell} , \tag{A29}$$

where we have used the notation

$$\Omega_{\kappa\ell} = a_\ell \langle \Psi_\kappa | - a_\kappa \langle \Psi_\ell | = \langle a_\ell^* \Psi_\kappa - a_\kappa^* \Psi_\ell | = \tag{A30}$$

$$= \langle \Psi_\ell | \varphi \rangle \langle \Psi_\kappa | - \langle \Psi_\kappa | \varphi \rangle \langle \Psi_\ell | = -\Omega_{\ell\kappa} .$$

Substitution into (A27) gives finally

$$T = \{ W(\mathcal{E}) \}^{-1} \frac{1}{2} \sum_{\kappa,\ell} \frac{\Omega^\dagger_{\kappa\ell} \Omega_{\kappa\ell}}{(\mathcal{E} - E_\kappa)(\mathcal{E} - E_\ell)} , \tag{A31}$$

which is the explicit expression desired. The operator $\Omega^\dagger_{\kappa\ell} \Omega_{\kappa\ell}$ is positive definite and satisfies the relations

$$\frac{1}{2} \sum_{\kappa,\ell} \Omega^\dagger_{\kappa\ell} \Omega_{\kappa\ell} = P , \tag{A32}$$

$$\left(\Omega^\dagger_{\kappa\ell} \Omega_{\kappa\ell} \right)^2 = \{ |a_\kappa|^2 + |a_\ell|^2 \} \left(\Omega^\dagger_{\kappa\ell} \Omega_{\kappa\ell} \right) . \tag{A33}$$

The latter implies that, except for a constant factor, the operator ($\Omega^\dagger_{\kappa\ell} \Omega_{\kappa\ell}$) is also a projection operator. The form (A31) is such that one can easily give upper and lower estimates to T analogous to (A8).

We have here gone into some details to study the properties of the reduced resolvent T , which is the basic operator of the entire partitioning technique. We note that, at the same time, we have obtained a set of formulas for the operator T_0 which occurs in all the applications to perturbation theory. The only thing one has to do is to replace $\mathcal{H}$ by $\mathcal{H}_0$ and to add an upper index 0 to all the eigenfunctions

Ψ_k , all the eigenvalues E_k , and to all the coefficients a_k . In these applications, it is hence convenient to specify the reference function φ in terms of the eigenfunctions to $\mathcal{H}_0$, so that

$$\varphi = \sum_k \Psi_k^0 a_k^0 \,. \tag{A34}$$

APPENDIX B. CALCULATION OF THE MODIFIED REFERENCE FUNCTION

The simple formulas (27) and (29) for the trial wave function and the bracketing function $\mathcal{E}_1 = f(\mathcal{E})$ are both based on the use of the modified reference function $\overline{\varphi}$ defined by (26) or

$$\overline{\varphi} = (1 + T_0 \mathcal{H}_0)\varphi . \tag{B1}$$

It should be observed that $\overline{\varphi}$ depends only on $\mathcal{E}$, φ, and $\mathcal{H}_0$ and is entirely independent of the perturbation V. Note that $\langle \varphi | \overline{\varphi} \rangle = 1$. Letting the operator $P(\mathcal{E} - \mathcal{H}_0)$ work on both sides of (26) and applying (4), one obtains

$$P(\mathcal{E} - \mathcal{H}_0)\overline{\varphi} = P(\mathcal{E} - \mathcal{H}_0)\varphi + P\mathcal{H}_0\varphi = 0;$$

$$(\mathcal{E} - \mathcal{H}_0)\overline{\varphi} = \varphi \langle \varphi | \mathcal{E} - \mathcal{H}_0 | \overline{\varphi} \rangle = \varphi\beta;$$

$$\overline{\varphi} = (\mathcal{E} - \mathcal{H}_0)^{-1}\varphi\beta; \tag{B2}$$

$$1 = \langle \varphi | \overline{\varphi} \rangle = \langle \varphi | (\mathcal{E} - \mathcal{H}_0)^{-1} | \varphi \rangle \beta;$$

$$\beta = \langle \varphi | (\mathcal{E} - \mathcal{H}_0)^{-1} | \varphi \rangle^{-1} . \tag{B3}$$

Substitution of this β - value into (B2) gives the explicit formula:

$$\overline{\varphi} = \frac{(\mathcal{E} - \mathcal{H}_0)^{-1}\varphi}{\langle \varphi | (\mathcal{E} - \mathcal{H}_0)^{-1} | \varphi \rangle} \tag{B4}$$

which is also easily derived from (B1) by using the explicit expression (A27) for T_0 . The denominator is simply the Weinstein function $W_0(\mathcal{E})$ associated with the operator $\mathcal{H}_0$. Using (A34) and the spectral resolution for $(\mathcal{E}-\mathcal{H}_0)^{-1}$, one obtains:

$$\overline{\varphi} = \frac{\sum_{k=0}^{\infty} \frac{\Sigma_k^0 a_k^0}{\mathcal{E}-E_k^0}}{\sum_{k=0}^{\infty} \frac{|a_k^0|^2}{\mathcal{E}-E_k^0}} \qquad (B5)$$

which may be useful for practical purposes. If φ contains only a finite number of eigenfunctions to $\mathcal{H}_0$, the same applies to $\overline{\varphi}$.

It is interesting to observe that, if one could solve the <u>inhomogenous</u> differential equation

$$(\mathcal{E}-\mathcal{H}_0)\chi_0 = \varphi \,, \qquad (36)$$

and find a quadratically integrable solution $\chi_0 = (\mathcal{E}-\mathcal{H}_0)^{-1}\varphi$, one would simply have

$$\overline{\varphi} = \frac{\chi_0}{\langle\varphi|\chi_0\rangle} \qquad (37)$$

The problem of evaluating $\overline{\varphi}$ is hence closely associated with ordinary perturbation theory; see PT IX.[8] If the function χ_0 is introduced into the expression (A27) for $\mathcal{H}=\mathcal{H}_0$, one obtains the following formula for T_0 :

$$T_0 = \left\{1 - \frac{|\chi_0\rangle\langle\varphi_0|}{\langle\varphi|\chi_0\rangle}\right\}(\mathcal{E}-\mathcal{H}_0)^{-1}, \qquad (38)$$

which shows that any function $T_0 f$ may be evaluated either by using a suitable expression for the resolvent $(\mathcal{E} - \mathcal{H}_0)^{-1}$ or by solving an inhonogeneous equation of the same type as occurs in perturbation theory[8].

APPENDIX C. SOME PROPERTIES OF THE ARONSZAJN PROJECTION

Since Aronszajn[3] and Fox and Bazley[4] use projection operators which are not self-adjoint and hence of a rather different type, it is perhaps worthwhile to point out the main differences in terminology. The Aronszajn projection A' of a positive definite operator $A > 0$ on a manifold $q = (g_1, g_2, \ldots g_m)$ is defined by (37). Introducing the operator pair

$$\mathbb{O}_A = A\,|q\rangle\langle q|A|q\rangle^{-1}\langle q| \,, \tag{C1}$$

$$\mathbb{O}_A^\dagger = |q\rangle\langle q|A|q\rangle^{-1}\langle q|A \,, \tag{C2}$$

one can write the definition in the form

$$\begin{aligned} A' &= A\,|q\rangle\langle q|A|q\rangle^{-1}\langle q|A = \\ &= \mathbb{O}_A A = A\,\mathbb{O}_A^\dagger \,. \end{aligned} \tag{C3}$$

It is easily seen that $\mathbb{O}_A$ is a projection operator

$$\mathbb{O}_A^2 = \mathbb{O}_A \,, \tag{C4}$$

but we note that $\mathbb{O}_A \neq \mathbb{O}_A^\dagger$, which means that one is considering a non-orthogonal projection. Instead of (C3), one can then also use the more symmetric form

$$A' = \mathbb{O}_A A = A\,\mathbb{O}_A^\dagger = \mathbb{O}_A A\,\mathbb{O}_A^\dagger \,. \tag{C5}$$

The Aronszajn projection satisfies hence the characteristic relations

$$\mathbb{O}_A \, A \, (1-\mathbb{O}_A)^\dagger = (1-\mathbb{O}_A) \, A \, \mathbb{O}_A^\dagger = 0 \, . \qquad (C6)$$

Using the resolution of the identity $1 = \mathbb{O}_A + (1-\mathbb{O}_A)$, one obtains

$$A = 1 \cdot A \cdot 1 = [\mathbb{O}_A + (1-\mathbb{O}_A)] \, A \, [\mathbb{O}_A^\dagger + (1-\mathbb{O}_A^\dagger)] = \qquad (C7)$$
$$= \mathbb{O}_A \, A \, \mathbb{O}_A^\dagger + (1-\mathbb{O}_A) \, A \, (1-\mathbb{O}_A^\dagger) \, ,$$

i.e.

$$A - A' = (1-\mathbb{O}_A) \, A \, (1-\mathbb{O}_A^\dagger) > 0 \qquad (C8)$$

which gives another derivation of the fundamental inequality fulfilled by the Aronszajn projection A' . In conclusion, we note that

$$A' |q\rangle = A |q\rangle \qquad (C9)$$

which means that, within the manifold q , the operator A' has the same effect as A . Since further

$$A' (1-\mathbb{O}_A^\dagger) = 0 \, , \qquad (C10)$$

the operator A' has the effect of a zero-operator within the entire infinite subspace defined by the projection operator $(1-\mathbb{O}_A^\dagger)$.

APPENDIX D. SECULAR EQUATION IN METHOD OF INTERMEDIATE HAMILTONIANS.

Let us consider an intermediate Hamiltonian[2,3,4] of the type $\mathcal{H}' = \mathcal{H}_0 + V'$, where V' is an Aronszajn projection of the perturbation V which is assumed to be positive definite. One has $\mathcal{H}' < \mathcal{H}$, and the eigenvalues E'_ν of $\mathcal{H}'$ are lower bounds to the eigenvalues E_ν of $\mathcal{H}$, if they are arranged in order from below. According to (40) and (C5), one has the definition

$$V' = V|q\rangle\langle q|V|q\rangle^{-1}\langle q|V = \\ = \mathbb{O}_V V = V\mathbb{O}_V^\dagger = \mathbb{O}_V V \mathbb{O}_V^\dagger \tag{D1}$$

and, since $V'|q\rangle = V|q\rangle$, one has further $\mathcal{H}'|q\rangle = \mathcal{H}|q\rangle$. From the relation $V'(1-\mathbb{O}_V^\dagger) = 0$ follows that V' has the effect of a zero-operator within the entire subspace defined by the projection operator $(1-\mathbb{O}_V^\dagger)$ and, since V' is thus different from zero only within a finite subspace, it seems natural to approach the solution of the eigenvalue problem for $\mathcal{H}'$ by means of "localized perturbation theory".[9] There is a close resemblance between this technique developed to treat impurities in solid-state physics[10] and the methods used by the Weinstein school.

The eigenvalue problem $\mathcal{H}'\underline{\Psi}' = E'\underline{\Psi}'$ may be modified in the following way:

$$(\mathcal{H}_0 + V')\underline{\Psi}' = E'\underline{\Psi}';$$
$$(E' - \mathcal{H}_0)\underline{\Psi}' = V'\underline{\Psi}';$$
$$\underline{\Psi}' = (E' - \mathcal{H}_0)^{-1} V'\underline{\Psi}' \tag{D2}$$

This is the basic equation in localized perturbation theory[9,10]. In substituting the expression (D1) for V', it is convenient to introduce the notation $a = \langle q|V|q\rangle^{-1}\langle q|V|\Psi'\rangle$, and one obtains

$$\Psi' = (E'-\mathcal{H}_0)^{-1}V|q\rangle\langle q|V|q\rangle^{-1}\langle q|V|\Psi'\rangle = (E'-\mathcal{H}_0)^{-1}V|q\rangle a \,. \tag{D3}$$

Multiplying to the left by $\langle q|V|q\rangle^{-1}\langle q|V$, one gets further

$$a = \langle q|V|q\rangle^{-1}\langle q|V(E'-\mathcal{H}_0)^{-1}V|q\rangle a \,,$$

$$\{\langle q|V|q\rangle - \langle q|V(E'-\mathcal{H}_0)^{-1}V|q\rangle\}a = 0 \,,$$

and, for $a \neq 0$, the condition

$$\det\{\langle q|V - V(E'-\mathcal{H}_0)^{-1}V|q\rangle\} = 0 \,, \tag{D4}$$

which is the fundamental secular equation of the problem.

It should be observed that the operators $\mathcal{H}'$ and $\mathcal{H}_0$ are actually the same within the entire infinite subspace defined by the projection operator $(1 - Q_V^{\dagger})$. The solution of the secular equation (D4) gives only those eigenvalues E' of $\mathcal{H}'$ as are different from the eigenvalues of $\mathcal{H}_0$, but we note that, in order to be able to apply the ordering theorem used in the inequality

$$E'_k < E_k \,, \tag{D5}$$

one has to know <u>all</u> eigenvalues of $\mathcal{H}'$ in order from below up to the level under consideration. For a more complete discussion of this important problem, we will refer to the original papers[2,3,4].

Instead of solving the secular equation (D4), we have here tried to bracket the eigenvalues of $\mathcal{H}'$. However, since the influence of the ordering theorem is such that an eigenvalue E' may be a lower bound not to a close-lying level but to an eigenvalue E rather far away, we have here tried to avoid the idea of the intermediate Hamiltonian as far as possible and instead tried to bracket the eigenvalues of $\mathcal{H}$ directly. In connection with this change of approach, it seems particularly important to give full credit to the pioneering work carried out by Prof. Alexander Weinstein and his co-workers.

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