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AN ELEMENTARY ITERATION-VARIATION PROCEDURE  
FOR SOLVING THE SCHRÖDINGER EQUATION

PER-OLOV LÖWDIN

1. Introduction

Variation principle:  $\delta \langle H \rangle = 0$

$$\langle H \rangle \equiv \frac{\int \Phi^* H \Phi dV}{\int \Phi^* \Phi dV} = E \quad (1)$$

complete set:  $\{\phi_\mu\}$

$$\text{overlap matrix: } \Delta_{\mu\nu} = \int \phi_\mu^* \phi_\nu dV \quad (2)$$

matrix Hamiltonian:

$$H_{\mu\nu} = \int \phi_\mu^* H \phi_\nu dV \quad (3)$$

Expanding:

$$\Phi = \sum_\mu \phi_\mu c_\mu \quad (4)$$

$\underline{c}$ : column vector formed by  $c_\mu$

$\underline{c}^+$ : row vector formed by  $c_\mu^*$

$$(1): \quad \langle H \rangle = \frac{\underline{c}^+ H \underline{c}}{\underline{c}^+ \Delta \underline{c}} = E \quad (5)$$

Varying  $c_\mu$  and applying the var. princ.

$$\sum_\nu (H_{\mu\nu} - E \Delta_{\mu\nu}) c_\nu = 0 \quad (6)$$

The roots  $E_0, E_1, \dots$  of the associated secular eq.

$$\det(H_{\mu\nu} - E \Delta_{\mu\nu}) = 0 \quad (7)$$

give the eigen values  $E_0, E_1, E_2, \dots$ . Defining:

$$M_{\mu\nu} \equiv H_{\mu\nu} - E \Delta_{\mu\nu} \quad (8)$$

(6) is:

$$\underline{M} \underline{c} = 0 \quad (9)$$

the Schrödinger eq. ( $\underline{M}$  is hermitian).

## 2. Partitioning of the secular equation.

Let's divide the basic set  $\phi_{\mu}$  into two subsets (a) and (b).

$$\underline{M} = \begin{pmatrix} \underline{M}_{aa} & \underline{M}_{ab} \\ \underline{M}_{ba} & \underline{M}_{bb} \end{pmatrix} \quad \underline{C} = \begin{pmatrix} \underline{C}_a \\ \underline{C}_b \end{pmatrix} \quad (10)$$

From (9):

$$\begin{aligned} \underline{M}_{aa} \underline{C}_a + \underline{M}_{ab} \underline{C}_b &= 0 \\ \underline{M}_{ba} \underline{C}_a + \underline{M}_{bb} \underline{C}_b &= 0 \end{aligned} \quad (11)$$

Solving the 2nd:

$$\underline{C}_b = -\underline{M}_{bb}^{-1} \underline{M}_{ba} \underline{C}_a \quad (12)$$

provided  $\underline{M}_{bb}$  is non-sing. Then:

$$(\underline{M}_{aa} - \underline{M}_{ab} \underline{M}_{bb}^{-1} \underline{M}_{ba}) \underline{C}_a = 0 \quad (13)$$

## 3. Iterative solution of the partitioned secular equation.

Let's choose the subset (a) to consist of a single function, say  $\phi_1$ .

Provided  $C_1 \neq 0$  we obtain, from (13):

$$M_{11} - \underline{M}_{1b} \underline{M}_{bb}^{-1} \underline{M}_{b1} = 0 \quad (14)$$

which may be written as:

$$E = f(E) \quad (15)$$

where:

$$f(E) \equiv \frac{1}{\Delta_{11}} [H_{11} - (H_{1b} - E \Delta_{1b})(H_{bb} - E \Delta_{bb})^{-1} (H_{b1} - E \Delta_{b1})]$$

Introducing an iteration procedure based on the formula:

$$E^{(k+1)} = f(E^{(k)})$$



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$$f(E) = H_{11} + H_{1b} \frac{1}{E^{(0)} - H_{bb}} H_{b1} \quad H_{11} + H_{1b} C_b^{(0)} = E^{(0)}$$

$$f(E) = H_{11} + H_{1b} \frac{1}{(E^{(0)} - H_{bb})^2} H_{b1} \quad E = E^{(0)} +$$

$$C_b^{(1)} = (E - H_{11}) C_b^{(1)} = H_{1b}$$

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It is well known that the energy of a system with Hamiltonian

$$H = \sum_i H_1(i) + \frac{1}{2!} \sum_{i,j} H_2(i,j) + \frac{1}{3!} \sum_{i,j,k} H_3(i,j,k)$$

can be written in the form:

$$E = \text{tr } H_1 \rho_1(1;1') + \frac{1}{2!} \text{tr } H_2 \rho_2(1,2;1',2') + \frac{1}{3!} \text{tr } H_3 \rho_3(1,2,3;1',2',3')$$

where  $\rho_n(1,2,\dots,n; 1',2',\dots,n')$  is the reduced density matrix for  $n$  particles and is unnormalized so that  $\int \rho_n(1,2,\dots,n; 1',2',\dots,n') dx_1 dx_2 \dots dx_n$  is the probability of finding  $n$  particles simultaneously in (space-time) volume elements  $dx_1 dx_2 \dots dx_n$  at points  $1,2,\dots,n$  of configuration space.

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An Elementary Iteration-variation Procedure for solving the  
Schrödinger Equation.

Per-Olov Löwdin

I - Introduction

$$\mathcal{H}\Psi = E\Psi$$

var. princ.

$$\delta \langle \mathcal{H} \rangle_{\Psi} = 0$$

$$\langle \mathcal{H}_{op} \rangle_{\Psi} = \frac{\int \Psi^* \mathcal{H}_{op} \Psi dx}{\int \Psi^* \Psi dx} = E$$

$\{\phi_{\mu}\}$  complete set

$$\Delta_{\mu\nu} = \int \phi_{\mu}^* \phi_{\nu} dx \quad \text{overlap matrix.}$$

Then:

$$\mathcal{H}_{\mu\nu} = \int \phi_{\mu}^* \mathcal{H}_{op} \phi_{\nu} dx$$

Expanding:

$$\Psi = \sum_{\mu} \phi_{\mu} c_{\mu}$$

Truncating up to order  $n$ :

$$\underline{c} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad \underline{c}^{\dagger} = (c_1^* \ c_2^* \ \dots)$$

$$\langle \mathcal{H}_{op} \rangle_{\Psi} = \frac{\underline{c}^{\dagger} \underline{H} \underline{c}}{\underline{c}^{\dagger} \underline{\Delta} \underline{c}} = E$$

From var. princ.

$$\sum_{\nu} (H_{\mu\nu} - E \Delta_{\mu\nu}) C_{\nu} = 0 \quad (A)$$

the roots of

$$\det(H_{\mu\nu} - E \Delta_{\mu\nu}) = 0.$$

give the eigenvalues.  $E_0, E_1, \dots$

Setting:

$$H_{\mu\nu} \equiv H_{\mu\nu} - E \Delta_{\mu\nu}$$

(A) is

$$\underline{M} \underline{C} = 0.$$

$\underline{M}$  is hermitian:

II Partitioning of the secular eq.

Let's divide the set  $\phi_{\mu}$  into subsets (a) and (b).

$$\underline{M} = \begin{pmatrix} \underline{M}_{aa} & \underline{M}_{ab} \\ \underline{M}_{ba} & \underline{M}_{bb} \end{pmatrix} \quad \underline{C} = \begin{pmatrix} \underline{C}_a \\ \underline{C}_b \end{pmatrix}$$

$$\underline{M}_{aa} \underline{C}_a + \underline{M}_{ab} \underline{C}_b = 0 \quad (A')$$

$$\underline{M}_{ba} \underline{C}_a + \underline{M}_{bb} \underline{C}_b = 0$$

Solving:

$$\underline{C}_b = -\underline{M}_{bb}^{-1} \underline{M}_{ba} \underline{C}_a$$

provided  $\underline{M}_{bb}$  is non-sing.

$$(\underline{M}_{aa} - \underline{M}_{ab} \underline{M}_{bb}^{-1} \underline{M}_{ba}) \underline{C}_a = 0 \quad (A'')$$



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III Iterative sol. of the partitioned sec. eq.

Let's choose (a) as a single funct.  $\phi$ ,

$\underline{C}_a$  is a number  $C_1$  and provided  $C_1 \neq 0$  we obtain

$$H_{11} - \underline{M}_{1b} \underline{M}_{bb}^{-1} \underline{M}_{b1} = 0$$

which we can write as:

$$E = f(E).$$

(A''')

$$f(E) = \frac{1}{\Delta_{11}} \{ H_{11} - (H_{1b} - E \Delta_{1b})(H_{bb} - E \Delta_{bb})^{-1} (H_{b1} - E \Delta_{b1}) \}$$

$\underline{M}_{bb} - E \Delta_{bb}$  should be non-sing.

Now into solving the iteration procedure:

$$E^{k+1} = f\{E^k\}$$

and starting from an initial value  $E^{(0)}$  we get a series of values  $E^{(1)}, E^{(2)}, \dots$

a) Orthogonal Basis

$\phi_{\mu}$  is orthonormal  $\Delta = 1$

$$E = H_{11} + H_{1b} (E^{-1} \underline{M}_{bb} - \underline{M}_{bb})^{-1} H_{b1} \quad (A''')$$

This sol. is closely related to the Lippman-Schwinger int. eq. Expanding the inverse matrix  $(E^{-1} \underline{M}_{bb} - \underline{M}_{bb})^{-1}$  formally into a power series in the non-diagonal part  $\underline{M}_{bb}$  of the matrix  $\underline{M}_{bb}$  one obtains

the Schrödinger - Brillouin formula:

Date: 
$$\underline{C}_1 = (E \underline{H}_{11} + \underline{H}_{12})^{-1} \underline{H}_{21} C_1 \quad (B)$$

the characteristic quotient:

$$q = f'(E) = -\underline{H}_{12} (E \underline{H}_{11} + \underline{H}_{12})^{-2} \underline{H}_{21}$$

$$\therefore q = -\frac{\underline{C}_1^+ C_1}{C_1^+ C_1} \quad (C)$$

provided  $C_1 \neq 0$ , showing that the process is convergent  $|q| < 1$ , if the contribution from the function  $\phi_1$  to the state described by the exact wave function  $\Phi$  is larger than the contribution from all the other functions.

Starting out from an arbitrary value  $E^{(0)}$  we can derive  $\underline{C}_1^{(0)}$  according to (B), and we obtain:

$$E^{(1)} = \underline{H}_{11} + \frac{\underline{H}_{12} \underline{C}_1^{(0)}}{C_1} \quad (D)$$

Starting from  $E^{(1)}$  instead of  $E^{(0)}$  we obtain  $E^{(2)}$  and so on.

Applying the Newton-Raphson formula to the eq.

$$F(E) \equiv E - f(E) = 0 \quad \text{we obtain}$$

$$E^* = E^{(0)} + \frac{E^{(1)} - F^{(0)}}{1 - f'(E^{(0)})} \quad (D')$$

From (C),  $f'(E)$  is never positive:

$$\therefore f'(E) \leq -1 \quad \therefore E^{(0)} \leq E^* \leq E^{(1)}$$



From (C) and (D) we obtain:

$$E^* = \frac{\underline{C}_1^{(0)+} + \underline{H}_{12} \underline{C}_1^{(0)}}{\underline{C}_1^{(0)+} \underline{C}_1^{(0)}}$$

where:  $\underline{C}_1^{(0)}$  is: 
$$\underline{C}_1^{(0)} = \begin{pmatrix} C_1 \\ C_1^{(0)} \end{pmatrix}$$

This means that a 2nd order value  $E^*$  may be directly obtained applying the expectation value expression to the trial vector  $\underline{C}_1^{(0)}$ .

The connection with the eq.  $E = f(E)$  and the first order iterative procedure  $E^{(k+1)} = f\{E^{(k)}\}$ , there is an interesting "bracketing theorem". Putting  $E^{(k)} = E + \epsilon^{(k)}$  and using the mean-value theorem:

$$f\{E^{(k)}\} = f(E) + \epsilon^{(k)} f'\{E + \theta \epsilon^{(k)}\}$$

where  $0 < \theta < 1$  we obtain:

$$E^{(k+1)} = E + \epsilon^{(k)} f'\{E + \theta \epsilon^{(k)}\}$$

Since  $f' < 0$ , the errors  $\epsilon^{(k)}$  change sign in an alternating way.  $\therefore E^{(k)}$  are alternatingly upper and lower bounds to the solution  $E$ . In the series  $E^{(0)}, E^{(1)}, E^{(2)}, \dots$  there is hence at least one eigenvalue  $E$  between two consecutive numbers in the series and, if the series is convergent, i.e.  $|f'| < 1$ , the series

will converge towards the real  $E$  from two sides and "bracket" the true eigenvalue

### Convergence Properties of the 2nd Order process

Let's investigate the analytical character of the function  $y = F(E) = E - f(E)$  or:

$$y = E - H_{11} - H_{1b}(E H_{bb} - H_{bb})^{-1} H_{b1} \quad (D')$$

for real  $E$ -values. For  $E \rightarrow \pm\infty$  the function has the linear asymptote:

$$y = E - H_{11}$$

Note:  $y' \geq 1$  for all  $E$ -values.

It's assumed  $\underline{U}$  an unitary matrix, which brings  $\underline{H}_{bb}$  to diagonal form  $\underline{h}_{bb}$ , so that:

$$\underline{U}^+ \underline{H}_{bb} \underline{U} = \underline{h}_{bb} \quad (E)$$

where  $\underline{h}_{bb}$  has the eigenvalues  $h_1, h_2, \dots$

According to the sup. then the eigenvalues of  $\underline{H}_{bb}$  will always separate the eigenvalues of  $\underline{H}$ . If  $\underline{H}$  has a degenerate eigenvalue of mult.  $g$ ,  $\underline{H}_{bb}$  has also the same eigenvalue with multiplicity either  $g-1$  or  $g$ .

From (E):

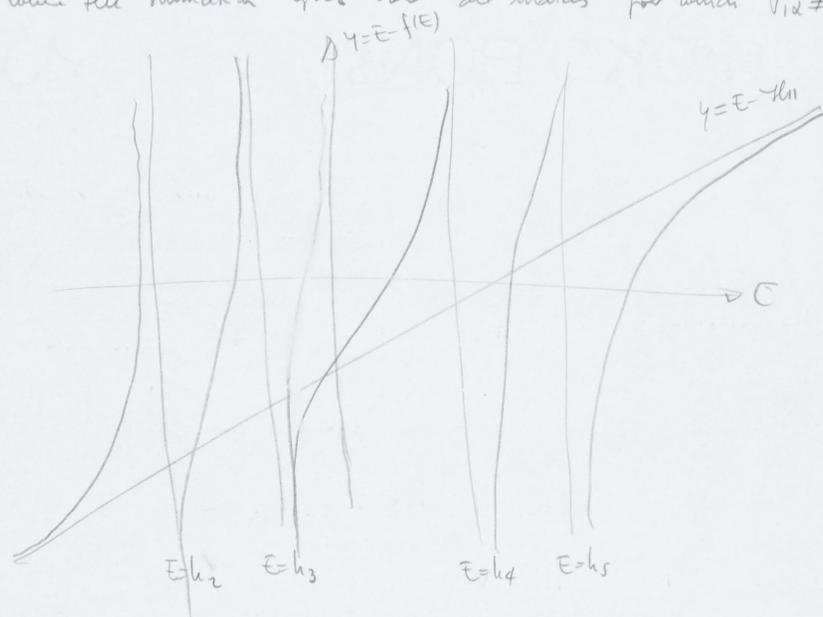
$$\underline{H}_{bb} = \underline{U} \underline{h}_{bb} \underline{U}^+$$

and calling:  $\underline{V}_{ib} = \underline{H}_{ib} \underline{U} \quad \underline{V}_{b1} = \underline{U}^+ \underline{H}_{b1}$



we get: 
$$y = E - H_{11} - \sum_{\alpha} \frac{|V_{1\alpha}|^2}{E - h_{\alpha}} \quad (F)$$

where the summation goes over all indices for which  $V_{1\alpha} \neq 0$ .



### Lost eigenvalues

We was assumed  $C_1 \neq 0$ . This implies that our theory does not give such eigenvalues  $E$  for which the associated eigenvalue has a vanishing coeff. for the partially selected  $\phi_1$ . Since one cannot know in advance about such accidentally vanishing coeff.,

there is a certain risk for lost eigenvalues

From (A') it follows that the matrices  $\underline{H}$  and  $\underline{H}_{bb}$  have a common eigenvalue. The corresponding eigenvectors are also the same except for the fact that the eigenvector to  $\underline{H}$  has an extra element  $C_1=0$ .

Let's study the influence in (D') and (F). Transmuting the total matrix  $\underline{H}$  by means of the unitary transf.

$$\begin{pmatrix} 1 & 0 \\ 0 & \underline{U} \end{pmatrix}$$

we obtain:

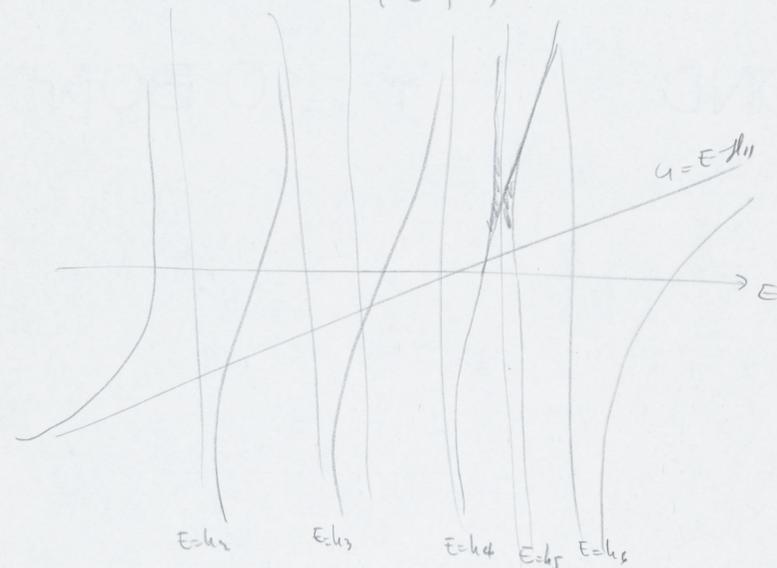
$$\begin{pmatrix} H_{11} & V_{1k} \\ \underline{V}_{b1} & \underline{H}_{bb} \end{pmatrix}$$

If a certain element  $V_{1k}$  happens to be zero, one can conclude that  $k$  must be a common eigenvalue to  $\underline{H}$  and its submatrix  $\underline{H}_{bb}$  and the associated eigenvector to  $\underline{H}$  is the same as the eigenvector to  $\underline{H}_{bb}$  with the addition of the single element  $C_1=0$ . This means that a lost eigenvalue, will wither away as a zero now as an asymptote to the curve, i.e. the eigenvalue is actually entirely lost.

Let's study the behavior of the curve  $y=F(E)$  when  $C_1 \rightarrow 0$ . The eigenvalue to  $\underline{H}$  corresponds to a zero and the eigenvalue to  $\underline{H}_{bb}$  to an asymptote, which get closer and closer together at the same time as the corresponding element  $V_{1k}$  approaches zero. The curve has a small interval of violent



change, which finally disappears for  $C_1=0$  and  $V_{1k}=0$ .  
 $\Delta y = E - f(E)$



### Multiple eigenvalues

Let's treat a 3rd order degeneracy. One could carry out the calculations by starting from the three different sub-vectors:

$$\underline{c}_a = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \underline{c}_b = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \underline{c}_c = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

in order to obtain three linearly indep. eigenvectors. The difficulty is that one does not know in advance the order of the degeneracies

which may occur

One essential advantage of the method described here is that it is not necessary to distinguish between single and multiple eigenvalues in the calculations. In both cases, it is possible to choose the subvector  $\underline{C}_k$  as consisting of a single element  $C_k$  and the iteration procedure based on (B) and (D\*) will still lead to the eigenvalues involved independent of their order of degeneracy. The curve  $y = F(E)$  will have the same characteristic behavior and usually one cannot, in fact, from the curve or the calculations lead to it find out whether an eigenvalue is degenerate or not.

The reason why the method does not break down in case of a degeneracy is simple. If the matrix  $\underline{H}$  has a degenerate eigenvalue of multiplicity  $g$ , the submatrix  $\underline{H}_{kk}$  has the same eigenvalues with the multiplicity  $g-1$  or  $g$ . The matrix  $(E\underline{H}_{kk} - \underline{H}_{kk})$  is then singular for this  $E$  value, the corresponding inverse matrix does not exist, and formula (B) is no longer valid in a strict sense. We note, however, that the subvector  $\underline{C}_k$  is in practice evaluated by solving the eq. syst.

$$(E\underline{H}_{kk} - \underline{H}_{kk})\underline{C}_k = \underline{H}_{kj} C_j \quad (9)$$

and that this has a unique solution as long as  $E$  is different from the eigenvalue. We may therefore use an iterative procedure



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which is defined uniquely by the choice of  $E^{(0)}$  and which does not break down when we approach a degenerate eigenvalue since the syst. (9) remains consistent. The system has a lower rank than its order, however, and one or more elements of  $\underline{C}_k$  may hence be chosen arbitrarily, which explains why the numerical procedure may lead to different limiting values of  $\underline{C}_k$  for different starting values  $E^{(0)}$ .

Except in the case of a lost eigenvalue, when  $C_k = 0$  for all the associated eigenvectors of the degenerate level, the iterative procedure leads therefore to a simple crossing point between the curve  $y = E + F(E)$  and the  $E$ -axis corresponding to a multiple eigenvalue and to a correct eigenvector  $\underline{C}_k$ , the special form of which depends on the limiting procedure and its starting point  $E^{(0)}$ .

The problem remains of determining some other eigenvectors  $\underline{C}_i$  such that those form a linearly independent set of order  $g$  spanning the subspace of the degeneracy. Putting  $C_k = 0$  we can find those eigenvectors by solving the homogeneous system

$$(E\underline{H}_{kk} - \underline{H}_{kk})\underline{C}_k = 0$$

for the  $E$  value under consideration. After getting a linearly independent set, the eigenvectors may be orthonormalized according to the Schmidt procedure.

In discussing the degeneracy problem one should distinguish between a true degeneracy and an approx. deg. It's assume true degeneracy of order  $g$ . Since there are  $g$  linearly indep. col  $\underline{C}$  there are  $g$  elements at our disposal and if the submatrix  $\underline{C}_a$  is chosen to be of order  $g$ , one can start from the choice

$$\underline{C}_a = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix} \dots$$

From (A'')

$$\underline{H}'_{aa} \underline{C}_a = \underline{E} \underline{C}_a$$

where:  $\underline{H}'_{aa} = \underline{H}_{aa} + \underline{H}_{ab} (\underline{E}_{bb} - \underline{H}_{bb})^{-1} \underline{H}_{ba}$  is of order  $g$ .

Subst. the 1st form for  $\underline{C}_a$ :

$$\underline{H}'_{aa} \underline{C}_1 = \underline{E} \underline{C}_1$$

and:

$$\underline{E} = \underline{H}_{aa} + \underline{H}_{ab} (\underline{E}_{bb} - \underline{H}_{bb})^{-1} \underline{H}_{ba}$$

which is (A''') with the only difference that the b-part has here been obtained by taking  $g$  away an a-part of order  $g$ . Instead of an algebraic eq. of order  $g$  one gets hence  $g$  eqs of type:

$$\underline{E} = \underline{H}_{kk} + \underline{H}_{kb} (\underline{E}_{bb} - \underline{H}_{bb})^{-1} \underline{H}_{bk}$$

which are, of course, all identical.

In principle, the treatment of an approx. linear dependency should be just as simple, since it should be possible to write



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the close-lying levels into a set of non-degenerate and truly degenerate levels which are then considered separately. However, since the curve  $q = E - f(E)$  will now have zero-points and vertical asymptotes lying very close to each other, the problem of numerical analysis is considerably more complicated.

### b) Non-Orthogonal Basis.

The 1st order process is based in eq. (A\*) and we can obtain for the characteristic quotient:

$$q = f'(E) = 1 - \frac{\underline{C}^+ \underline{\Delta} \underline{C}}{\underline{C}_1^+ \underline{\Delta}_{11} \underline{C}_1} \quad (V)$$

The convergence criterion for the 1st order process or the corresp. Schrödinger - Brillouin type formula is  $|q| < 1$

$$\text{i.e.} \quad \underline{C}_1^+ \underline{\Delta}_{11} \underline{C}_1 > \frac{1}{2} \underline{C}^+ \underline{\Delta} \underline{C}$$

Independent of whether this inequality is fulfilled or not we can now easily go over to the 2nd-order process. Starting out from an initial value  $E^{(0)}$ , evaluating  $\underline{C}_b^{(0)}$  by solving the linear system

$$\underline{M}_{bb}^{(0)} \underline{C}_b = - \underline{M}_{ba} \underline{C}_1 \quad (W)$$

$$\text{we define} \quad \underline{E}^{(2)} = \frac{\underline{C}_b^{(0) +} \underline{H} \underline{C}_b^{(0)}}{\underline{C}_b^{(0) +} \underline{\Delta} \underline{C}_b^{(0)}} \quad (X)$$

a bit.

#### IV - Condensed description of the numerical method

It is convenient to choose  $C_1=1$  and after choosing a starting value  $E^{(0)}$  and evaluating the matrix elements according to the formula:

$$M_{\mu\nu}^{(0)} = H_{\mu\nu} - \bar{E}^{(0)} \Delta_{\mu\nu}$$

we will determine  $\underline{C}_b^{(0)}$  by solving (W).

Since it may sometimes be feasible to ~~the~~ visualize the procedure by making a graph of the curve  $y = F(E) = E - f(E)$ , we note that:

$$E^{(1)} = f\{E^{(0)}\} = \frac{1}{\Delta_{11}} (H_{11} + M_{1b} \underline{C}_b^{(0)})$$

and that  $y^{(0)} = F\{E^{(0)}\} = E^{(0)} - E^{(1)}$  is given by:

$$y^{(0)} = -\frac{1}{\Delta_{11}} (M_{11}^{(0)} C_1 + M_{1b}^{(0)} \underline{C}_b^{(0)})$$

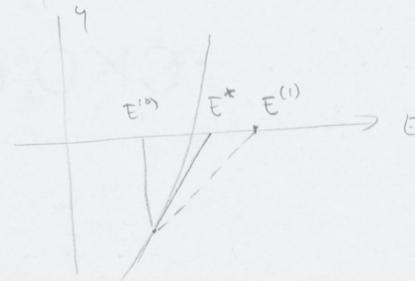
which is the left-hand side of (A'), divided by  $-\Delta_{11}$ .

We can now easily plot both the point  $(E^{(0)}, y^{(0)})$  and the tangent to the curve in this point, since  $E^*$  defined by the variational expression (X) gives the abscissa for the crossing



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point between this line and the E-axis



The numerical value of the derivative  $y'$  in the point  $E^{(0)}$  may also be obtained from (V) leading to:

$$y' = \frac{C_1^+ \Delta C_1}{C_1^+ \Delta_{11} C_1}$$

#### Appendix Properties of iterative procedure

Let's consider the sol. of the eq.  $x = f(x)$  by means of the iterative procedure.

$$x_{k+1} = f(x_k) \quad (1)$$

Putting  $x_k = x + \epsilon_k$  and using the Taylor expansion

$$\epsilon_{k+1} = \epsilon_k f'(x) + \frac{1}{2!} \epsilon_k^2 f''(x) + \frac{1}{3!} \epsilon_k^3 f'''(x) + \dots \quad (2)$$

The order of an iterative process is defined as the order of the first non-vanishing derivative of  $f(x)$  in the r.h.s of (2)

Let's study the 1<sup>st</sup> order process. Calling  $g = f'(x)$  one obtains by repeated use of (2):

$$E_{k+n} \approx E_k g^n$$

showing that the errors  $E_k = x_k - x$  form approx. a geometrical progression converging to zero if  $|g| < 1$  which is hence the convergence condition for a 1<sup>st</sup> order process. Since the quantities  $x_{k+1} - x_k = E_{k+1} - E_k$  form approx. a geom. series with the same quotient, one can try to calculate  $x$  by:

$$x = x_0 + (x_1 - x_0) + (x_2 - x_1) + \dots \approx x_0 + \frac{x_1 - x_0}{1 - g} \quad (5)$$

provided that  $|g| < 1$ . Since an approx. value of  $g$  is given by  $\frac{x_2 - x_1}{x_1 - x_0}$  we get:

$$x^* = x_0 + \frac{(x_1 - x_0)^2}{x_2 - 2x_1 + x_0}$$

as an approx. to  $x$ . If still higher accuracy is desired we can use  $x^*$  as a new initial value for the iterati (1) and derive  $x^{**}$  and  $x^{***}$  which may then be substituted into the right-hand side of (5)



Appendix Properties of iterative procedures.

Let's consider the sol. of the eq.  $x = f(x)$  by means of the iterati procedure:

$$x_{k+1} = f(x_k)$$

Putting  $x_k = x + E_k$  and using the Taylor expansion

$$f(x_k) = f(x) + E_k f'(x) + \frac{E_k^2}{2!} f''(x) + \dots$$

we obtain:

$$E_{k+1} = E_k f'(x) + \frac{1}{2!} E_k^2 f''(x) + \dots \quad (2)$$

The order of an iterative process is defined as the order of the 1<sup>st</sup> non-vanishing derivative of  $f(x)$  in the r.h.s of (2).

Let's study the 1<sup>st</sup> order process. Calling  $g = f'(x)$  we obtain:

$$E_{k+1} = E_k g + \frac{1}{2!} E_k^2 g^2 + \dots$$

$$E_{k+2} = E_{k+1} g + \frac{1}{2!} (E_{k+1})^2 g^2 + \dots =$$

$$= (E_k g + \frac{1}{2!} E_k^2 g^2) g + \frac{1}{2!} (E_k g + \frac{1}{2!} E_k^2 g^2)^2 g^2 + \dots$$

$$= E_k g^2 + \frac{1}{2!} E_k^2 g^3 + \dots$$

$$\dots \quad E_{k+n} = E_k g^n \quad (3)$$

showing that the errors  $E_k = x_k - x$  form approx. a geometrical progression converging towards zero if  $|g| < 1$  which is hence the convergence condition for a 1<sup>st</sup> order process.

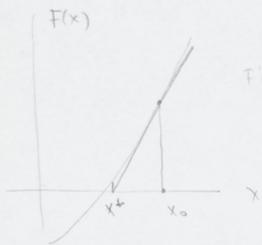
Let's consider the underlying eq.  $x=f(x)$  as a special case of the eq.

$$F(x) = 0.$$

with  $F(x) \equiv x - f(x) = 0$ .

If  $x_0$  is an approx root, the Newton-Raphson formula gives:

$$x^* = x_0 - \frac{F(x_0)}{F'(x_0)}$$



$$F'(x_0) = \frac{F(x_0)}{x_0 - x^*}$$

$$\text{or } x^* = x_0 + \frac{x_1 - x_0}{1 - f'(x_0)}$$

$$\text{if } f'(x_0) \approx \frac{x_2 - x_1}{x_1 - x_0}$$

$$x^* = x_0 + \frac{(x_1 - x_0)^2}{x_2 - 2x_1 + x_0}$$