Vol. XVIII, 3 REVISTA MEXICANA DE FISICA 1969

ENERGY VARIATION OF THE EFFECTIVE HAMILTONIAN*

J. Flores, M. Fortes and P.A. Mello
Instituto de Física, Universidad Nacional de México
(Recibido: 15 enero 1969)

RESUMEN

Se discuten algunas propiedades generales de los eigenvalores del Hamiltoniano efectivo, definido en un espacio finito. En particular, se demuestra que ignorar la autoconsistencia en el cálculo del Hamiltoniano efectivo puede llevar a conclusiones erróneas. Las propiedades arriba mencionadas se muestran en un ejemplo numérico.

ABSTRACT

Some general properties of the eigenvalues of the effective Hamiltonian, defined in a finite space, are discussed. In particular, it is shown that neg-

*Work supported by the Comisión Nacional de Energía Nuclear, México.

lecting self-consistency in the calculation of the effective Hamiltonian may lead to wrong conclusions. These properties are shown explicitly in a numerical example.

I. INTRODUCTION

In a many-body system, due to the complexity of the problem, one is usually forced to introduce a model. This provides a complete set of model wave functions, defined in a Hilbert space S, in terms of which the wave functions of the system are to be expanded. Due to the practical difficulties in dealing with the complete expansion, one usually truncates the model basis, defining in this way a subspace $\mathcal{S}$ of S; the goal is then to describe the system *within* $\mathcal{S}$. In other words, the problem consists in finding operators, defined in $\mathcal{S}$, such that their eigenvalues coincide with the true eigenvalues of the problem. These are the so-called effective operators[2].

For the case of the effective Hamiltonian it turns out that the effective operator is a function of the true eigenvalues of the problem, as is shown in section 2. As these eigenvalues are unknown a self-consistency problem arises.

Much attention has been given in the last few years to the analysis of effective operators in many branches of physics. In solid state theory very well known examples are provided by the dynamics of electrons in solids[4]. Another well known example is provided by the nuclear shell model. In this case the effective interaction has been calculated by at least two different approaches[5,6].

It is a common feature of all these calculations to assume that the self-consistency problem mentioned above can be ignored. It is the purpose of this work to study the dependence of the effective hamiltonian on the true energy eigenvalues and therefore to analize the consequences of ignoring self-consistency.

In section 2 we define the effective hamiltonian and in section 3 we analize some general properties of its energy dependence. What is discussed in these two sections is completely general, in the sense that the concept of an effective hamiltonian arises whenever one truncates the space. In other words the

discussion of the effective hamiltonian of sections 2 or 3 does not depend on the specific form of the hamiltonian, the number of particles, etc.

In order to show in specific examples the general properties of the effective hamiltonian discussed in sections 2 and 3 and to investigate how well can the effective hamiltonian reproduce the true results, we analize in section 4 the simplest possible case: a one-body problem described in a finite space.

II. DEFINITION OF THE EFFECTIVE HAMILTONIAN.

We consider a finite vector space S of dimension $p+q$, and make an orthogonal separation of it into a model space $\mathcal{S}$, of dimension p, and its complement of dimension q. This means that vectors in the model space are orthogonal to vectors in its complement. We now introduce the projection operators P and Q which project, respectively, onto the model space (P-space) and onto its complement (Q-space). The operators P and Q have, therefore, the following properties

$$P + Q = I$$

$$P^2 = P, \qquad Q^2 = Q \tag{2.1}$$

$$PQ = QP = 0.$$

Let us now consider a Hamiltonian H, defined in the complete vector space, with eigenvectors $|\Psi_i>$ and eigenvalues ϵ_i, i.e.

$$H|\Psi_i> = \epsilon_i|\Psi_i> . \tag{2.2}$$

For a given eigenvector $|\Psi_i>$ we construct its projection $P|\Psi_i>$ in the P-space and look for an effective Hamiltonian $\mathcal{H}$, defined in the model space only, with the property that $P|\Psi_i>$ is an eigenvector of $\mathcal{H}$ corresponding to the eigenvalue ϵ_i. In other words,

$$\mathcal{H} P \,|\Psi_i\rangle = \epsilon_i \, P \,|\Psi_i\rangle \quad . \tag{2.3}$$

We shall now obtain an expression for $\mathcal{H}$.

Using eqs. (2.1) it is simple to derive from eq. (2.2) the pair of coupled equations[1]

$$\begin{cases} (\epsilon_i - H_{PP})\, P\,|\Psi_i\rangle = H_{PQ}\, Q\,|\Psi_i\rangle & (2.4a) \\ (\epsilon_i - H_{QQ})\, Q\,|\Psi_i\rangle = H_{QP}\, P\,|\Psi_i\rangle \ , & (2.4b) \end{cases}$$

where

$$H_{PP} = PHP,\ H_{QQ} = QHQ,\ H_{PQ} = PHQ,\ H_{QP} = QHP \tag{2.5}$$

and

$$H_{PQ} = H_{QP}^{+} \tag{2.6}$$

the last eq. being valid since H is Hermitian. Solving (2.4b) for $Q\,|\Psi_i\rangle$ and substituting in (2.4a) one obtains, finally,

$$\left(H_{PP} + H_{PQ} \frac{1}{\epsilon_i - H_{QQ}} H_{QP} \right) \quad P\,|\Psi_i\rangle = \epsilon_i \, P\,|\Psi_i\rangle \ , \tag{2.7}$$

which defines the Hermitian effective Hamiltonian $\mathcal{H}$, as

$$\mathcal{H}(\epsilon_i) = H_{PP} + H_{PQ} \frac{1}{\epsilon_i - H_{QQ}} H_{QP} \quad . \tag{2.8}$$

In this equation we have explicitly indicated that $\mathcal{H}$ depends on the specific eigenvalue ϵ_i we want to reproduce. In other words, we need a different effective operator for each eigenvalue we want to adjust.

If we can separate H as $H^0 + V$, where H^0 commutes with P and Q, the ef-

fective Hamiltonian $\mathcal{H}$ can be written as

$$\mathcal{H} = H^0_{PP} + V_{PP} + V_{PQ} \frac{1}{\epsilon_i - H^0 - V_{QQ}} V_{QP}$$

$$= H^0_{PP} + \mathcal{V}_{PP} \tag{2.9}$$

Since $\mathcal{V}_{PP}$ can also be put in the form

$$\mathcal{V}_{PP} = V_{PP} + V_{PQ} \frac{1}{\epsilon_i - H^0} \mathcal{V}_{QP} \ ,$$

it coincides with the usual definition of the effective interaction[2]. We also see that the effective operator corresponding to H^0 is identical to H^0 itself and, therefore, it is not energy dependent.

In order to proceed with the analysis, we choose for the complete finite vector space a basis which diagonalizes H_{PP} and H_{QQ}, separately:

$$\begin{cases} H_{PP}|\lambda> = E_\lambda|\lambda> & \lambda = 1, \ldots, p \\ H_{QQ}|\mu> = E_\mu|\mu> & \mu = 1, \ldots, q \end{cases} \tag{2.10}$$

This is convenient and does not imply any lack of generality, since we are interested in diagonalizing $\mathcal{H}$ and any basis can be used for this purpose. Using the basis defined in eq. (2.10) the matrix elements of the operator $\mathcal{H}$ take the form,

$$<\lambda|\mathcal{H}|\lambda'> \equiv \mathcal{H}_{\lambda\lambda'} = E_\lambda \delta_{\lambda\lambda'} + \sum_\mu \frac{H_{\lambda\mu} H_{\mu\lambda'}}{\epsilon_i - E_\mu} \ , \tag{2.11}$$

where

$$H_{\lambda\mu} = \langle\lambda| H |\mu\rangle = \langle\lambda| PHQ |\mu\rangle = H^{*}_{\mu\lambda} \quad . \tag{2.12}$$

Since to construct $\mathcal{H}_{\lambda\lambda'}$ we need to know ϵ_i, the unknown eigenvalues of the total Hamiltonian H, we face a self-consistency problem. In general, this is very difficult to solve and what is usually done is to replace the eigenvalue ϵ_i in (2.11) by a parameter E, *hoping* that the eigenvalues and eigenvectors of $\mathcal{H}$ do not depend severely on the value of this parameter. The effective Hamiltonian matrix elements then become

$$\mathcal{H}_{\lambda\lambda'}(E) = E_\lambda \delta_{\lambda\lambda'} + \sum_{\mu} \frac{H_{\lambda\mu} H_{\mu\lambda'}}{E - E_\mu} \tag{2.13}$$

and it is the purpose of this paper to analyze the dependence of the eigenvalues $\mathcal{E}_i(E)$ of $\mathcal{H}$ on the parameter E. Before doing this it is interesting to discuss the following result.

We have seen that if we consider $E = \epsilon_i$ in eq. (2.13) we obtain an operator $\mathcal{H}(\epsilon_i)$, one of whose eigenvalues coincides with ϵ_i. We shall now show that those values of the parameter E such that

$$\mathcal{E}_i(E) = E \quad , \qquad i = 1, \ldots, p \quad , \tag{2.14}$$

(in other words, E is equal to what could be called a self-consistency energy) coincide with the eigenvalues ϵ_j of the Hamiltonian H, diagonalized in the *complete* vector space.

In order to prove this, let $|\Phi\rangle$ be the model eigenvector corresponding to one of the eigenvalues (2.14), i.e.

$$\mathcal{H}(E) |\Phi\rangle = E |\Phi\rangle \quad . \tag{2.15}$$

Let us now construct the vector $|\Psi>$

$$|\Psi> \equiv |\Phi> + \frac{1}{E - H_{QQ}} H_{QP} |\Phi> \tag{2.16}$$

that clearly has components in both P and Q-spaces. Acting with H on $|\Psi>$ we obtain

$$H|\Psi> = \mathcal{H}(E)|\Phi> + E \frac{1}{E - H_{QQ}} H_{QP}|\Phi> \ ,$$

where we have used the fact that H_{QQ} and Q commute, as well as eqs. (2.1). If we now use (2.15) we get

$$H|\Psi> = E|\Psi> \ ,$$

proving our statement.

III. BEHAVIOR OF THE EIGENVALUES OF $\mathcal{H}$ AS FUNCTIONS OF THE PARAMETER E.

The general behavior of the eigenvalues of $\mathcal{H}$ as functions of E is rather difficult to analyze for arbitrary values of p and q. Therefore, we shall start the analysis with the simplest possible case $p = 1$ and q arbitrary. We have in this case

$$\mathcal{E}_1(E) = E_\lambda + \sum_\mu \frac{|H_{\lambda\mu}|^2}{E - E_\mu} \ , \tag{3.1}$$

where $\mathcal{E}_1(E)$ and E_λ designate the only eigenvalue of $\mathcal{H}(E)$ and H_{PP}, respectively. The graph for $\mathcal{E}_1(E)$ is given in fig. 1. The energy origin is indicated in the abscissa with the point O and E_λ is taken to be negative, for definiteness. We

see that for $E \to \pm \infty$, $\mathcal{E}_1 \to E_\lambda$, and as E approaches each one of the E'_μs, $\mathcal{E}_1$ shows a pole. The intersections of the dotted line, drawn through the energy origin at 45 degrees, with the curve $\mathcal{E}_1(E)$ give, according to the result mentioned at the end of section 2, the $q+1$ eigenvalues of H in the complete vector space. We can adjust the parameter E to fit, for example, the lowest eigenvalue; the corresponding self-consistent value is given as ϵ_1 in fig. 1. One can see that the energy variation of $\mathcal{E}_1(E)$ is smooth for values of $E \ll E_{\mu_1}$ but is very strong when $E \to E_{\mu_1}$. If the value of ϵ_1 is in the vicinity of E_{μ_1} (as in fig. 1), the lack of self-consistency may lead us to an eigenvalue $\mathcal{E}_1(E)$ which differs considerably from the correct eigenvalue of H. Such difficulties arise in the general case (p arbitrary) as will be discussed later on.

A specific example of the danger of the lack of self-consistency is provided by a recent calculation by Arima et al.[3] They analyze, among other nuclei, F^{18}, restricting the nuclear shell-model space to the configuration $(1d_{5/2}, 2s_{1/2})$ and parametrizing the effective nucleon-nucleon interaction in terms of its two-body matrix elements, which are varied until a best fit to the spectra is obtained. Once a set of matrix elements of the effective interaction is obtained, the same set is used to fit all energy levels. This would correspond in our language to using the same value of the parameter E to fit all eigenvalues ϵ_i, therefore breaking self-consistency. They find that it is impossible to get a good fit to all existing data if the 1.7 MeV, 1^+ state of F^{18} is included in the least-square procedure. This state seems to have a different character from the other low-lying states. Indeed, rough energy estimates indicate that a 1^+ state with two $1p$ nucleons excited from the ^{16}O core, and therefore outside the model space, should occur at about 1 – 3 MeV excitation energy in F^{18}. In our language, this corresponds to having one of the E'_μs in the energy range of the ϵ'_is we want to adjust and as can be seen from a figure similar to fig. 1, the variation of the eigenvalues of $\mathcal{H}$ with respect to E may be very strong. Similar difficulties have been found by Brown and Green[7] and by Federman and Talmi[8].

We shall now analyze some properties of the general case p and q arbitrary. We first study the behavior of the eigenvalue curves, when the parameter E ap-

proaches one of the non-degenerate eigenvalues of H_{QQ}, say E_{μ_0}. We shall prove that in this case only one of the eigenvalues $\mathcal{E}_i(E)$ shows a singularity and the other $p-1$ eigenvalues of $\mathcal{H}$ tend to finite values in the limit $E \to E_{\mu_0}$.

First of all, since the trace of $\mathcal{H}$ is equal to

$$Tr\,\mathcal{H} = \sum_{\lambda} \left(E_\lambda + \sum_{\mu} \frac{|H_{\lambda\mu}|^2}{E - E_\mu} \right) , \tag{3.2}$$

which clearly tends to $\pm \infty$ when $E - E_{\mu_0} \to 0^{\pm}$, (provided $H_{\lambda\mu_0} \neq 0$) we see that at least one of the eigenvalues of $\mathcal{H}$ diverges in this limit.

As we shall give in the appendix the proof that only one eigenvalue diverges, we shall only present at this point an argument that makes the result plausible. Let us single out from expression (2.13) the term corresponding to μ_0, since this is the only one that goes to infinity when $E \to E_{\mu_0}$, and write $\mathcal{H}$ as

$$\mathcal{H} = \mathcal{H}^0 + \mathcal{V} \tag{3.3}$$

where

$$\mathcal{H}^0_{\lambda\lambda'} \equiv \frac{H_{\lambda\mu_0} H_{\mu_0\lambda'}}{E - E_{\mu_0}} \tag{3.4}$$

and

$$\mathcal{V}_{\lambda\lambda'} \equiv E_\lambda \delta_{\lambda\lambda'} + \sum_{\mu(\neq \mu_0)} \frac{H_{\lambda\mu} H_{\mu\lambda'}}{E - E_\mu} \quad . \tag{3.5}$$

It will be shown in the appendix that the matrix $\mathcal{H}^0$ has $p-1$ eigenvalues equal to zero and one eigenvalue different from zero, which goes to infinity in the limit. Since all the matrix elements $\mathcal{V}_{\lambda\lambda'}$ remain finite for $E \to E_{\mu_0}$, $\mathcal{V}$ represents a finite perturbation to $\mathcal{H}^0$ and although $\mathcal{H}$ will have, in general, all its eigenvalues different from zero, it seems plausible that it has still only one diverging eigenvalue.

Another general property of the curves $\mathcal{E}_i(E)$ can be readily obtained: the derivative $d\mathcal{E}_i(E)/dE \leq 0$. In order to prove this, we analyze the behavior of $\mathcal{E}_i(E)$ when we replace $\mathcal{H}(E)$ by $\mathcal{H}(E + \Delta E)$, where ΔE is taken small enough so that in the truncated Taylor expansion

$$\mathcal{H}(E + \Delta E) \approx \mathcal{H}(E) + \mathcal{H}'(E)\Delta E \tag{3.6}$$

the second term can be made as small as we want compared to the first one. This allows us to consider the effect of $\mathcal{H}'(E)\Delta E$ by means of first order perturbation theory. This is consistent with eq. (3.6), since only terms linear in ΔE are necessary to calculate the first derivative. Therefore, the change $\Delta\mathcal{E}_i$ in the i-th eigenvalue of $\mathcal{H}$ is

$$\Delta\mathcal{E}_i \approx \langle\phi^{(i)}|\,\mathcal{H}'(E)\,|\phi^{(i)}\rangle\,\Delta E \quad ,$$

where $|\phi^{(i)}\rangle$ is the i-th eigenvector of $\mathcal{H}(E)$ with components $C_\lambda^{(i)}$. Using eq. (2.13) we can now write

$$\frac{d\mathcal{E}_i(E)}{dE} \equiv \mathcal{E}_i'(E) = \sum_{\lambda\lambda'} C_\lambda^{(i)}\,\mathcal{H}'_{\lambda\lambda'}\,C_{\lambda'}^{(i)} = -\sum_\mu \frac{\left[\sum_\lambda H_{\lambda_\mu} C_\lambda^{(i)}\right]^2}{(E - E_\mu)^2} \leq 0 \tag{3.7}$$

which proves the theorem. This result is consistent with the fact that the trace of $\mathcal{H}(E)$ has a negative derivative with respect to E, as can be seen directly from eq. (2.13), i.e.

$$\frac{d}{dE}\left[Tr\,\mathcal{H}(E)\right] = -\sum_\mu \left(\frac{H_{\lambda_\mu}}{E - E_\mu}\right)^2 \leq 0 \quad . \tag{3.8}$$

It is interesting to notice that $\mathcal{E}_i'(E)$ is negative both for attractive and repulsive interactions. We can now use the result $\mathcal{E}_i' \leqslant 0$ to see that there exists a value of E (in the region of physical interest, i.e. $E < E_\mu$ for an attractive Hamiltonian) such that $\mathcal{H}(E)$ gives a closer result to the lowest p correct eigenvalues of H, than those obtained by diagonalizing H within the model space. From Ritz variational principle we know that the true eigenvalues ϵ_i lie lower than the corresponding E_{λ_i}. On the other hand, in the limit $E \to -\infty$, $\mathcal{H} \to H_{PP}$ (see eq. (2.8)) and $\mathcal{E}_i$ tends asymptotically to E_{λ_i}. When E becomes finite, the $\mathcal{E}_i$ decreases becoming a better approximation to ϵ_i.

More detailed properties of the eigenvalue curves can only be obtained through the explicit knowledge of the numerical values of the matrix elements of H. In the next section, we present some numerical results for simple cases, in which the effective Hamiltonian is calculated exactly.

IV. AN EFFECTIVE ONE-BODY HAMILTONIAN

As mentioned in the introduction, for any quantum mechanical system described by Schrodinger's equation in a given Hilbert space S, the concept of an effective Hamiltonian arises whenever we want to describe the system within a subspace $\mathcal{S}$ of S. The general characteristics of the effective Hamiltonian we have discussed in the previous sections, are valid for any system of an arbitrary number of particles, independently of the specific properties of the Hamiltonian H.

In order to show in specific examples the general features of H discussed in sections 2 and 3 and to investigate how well can the effective Hamiltonian reproduce the exact results for a given value of the parameter E (see eq. (2.13)), we shall analyze the simplest possible case: a one-body problem described in a finite space. We consider the one-body Hamiltonian

$$H = \frac{p^2}{2m} + V(r) \quad , \tag{4.1}$$

where $V(r)$ is a central potential. We now take a finite set of $d = p + q$ harmonic-oscillator states and construct the matrix of (4.1) with respect to this basis. The d eigenvalues of this matrix can be made to approach the true eigenvalues of (4.1) as closely as we want, by taking d large enough. For a given d, on the other hand, we shall consider the corresponding d eigenvalues as the "exact" results and call them ϵ_i. We analyze the same problem using an effective Hamiltonian defined in a smaller vector space, spanned by p harmonic-oscillator states.

In the numerical example we now discuss, the value $d = 10$ is used and p is varied from 1 to 5; $V(r)$ is taken as a 1-body Coulomb potential $V(r) = c/r$. We show in fig. 2 the energy variation of the eigenvalues $\mathcal{E}_i(E)$ of the effective Coulomb Hamiltonian $\mathcal{H}$ for the case $p = 5$. First of all, we observe that for $E \to \pm \infty$ the $\mathcal{E}_i$ approach the eigenvalues E_λ of H_{PP}. On the other hand, as E approaches the eigenvalues E_μ of H_{QQ} *only one* eigenvalue of $\mathcal{H}$ goes to infinity, while the other four remain finite and are continuous functions of E.

It is also apparent from the graph that the slope of the curves is always negative. We see in this specific example, therefore, that the curves $\mathcal{E}_i(E)$ have all the properties we have discussed in general before.

We now analyze how well can the effective Hamiltonian describe the exact solution of this problem. The ten "exact" eigenvalues ϵ_i are shown on the left-hand side of fig. 2. They are seen to coincide with the self-consistent values given by the intersection of the curves $\mathcal{E}_i(E)$ with the straight line drawn at 45 degrees. This is consistent with the discussion given at the end of section 2. Since by diagonalizing $\mathcal{H}(E)$ within the model space we obtain five eigenvalues only, we restrict our attention to the first five self-consistent eigenvalues, indicated in fig. 2 by the full circles. We see that they are spread in an energy range of 3 units and that there is no single value of E for which all five ϵ_i can be reasonably fit. In this case E_{μ_1} lies between ϵ_3 and ϵ_4, as can be seen from the graph and one must be rather careful in neglecting self-consistency in the present example. On the other hand, if we only take into account the three lowest eigenvalues, E_{μ_1} is no longer within the energy range of the ϵ_i's one wants to adjust, and a good fit can be obtained in the vicinity of $E = 0$

Finally in fig. 3 we show the energy variation of $\mathcal{E}_i(E)$ when $p = 3$. We see that the graph is qualitatively similar to the one corresponding to $p = 5$ and the same discussion applies to it.

CONCLUSIONS

We have shown that the following properties of the eigenvalues of the effective Hamiltonian $\mathcal{H}$ do not depend neither on the specitic torm ot the Hamiltonian H nor on the number of particles of the system:

1. When the parameter E is in the vicinity of one of the eigenvalues of H_{QQ}, one of the effective eigenvalues varies strongly with this parameter, while all others do not. This implies that if one of the eigenvalues of the Hamiltonian H_{QQ} is contained in the energy range of the true eigenvalues to be adjusted, the lack of self-consistency may lead to wrong conclusions.

2. The slope of the effective eigenvalue curves is less than or equal to zero. This implies, by Ritz variational principle, that one can always find values of the parameter E for which these eigenvalues represent a better approximation to the p lowest true eigenvalues ϵ_i than the E'_λs obtained by diagonalizing the original Hamiltonian H within the model space.

These general properties are explicitly shown in a numerical example, which also serves the purpose of indicating how well the effective Hamiltonian technique reproduces the true results.

ACKNOWLEDGEMENTS

We would like to thank Prof. M. Moshinsky for suggesting the numerical example.

APPENDIX

In this appendix we shall give the proof that in the limit $E \to E_{\mu_0}$ (E_{μ_0} being a non-degenerate eigenvalue of H_{QQ}) only one eigenvalue of $\mathcal{H}(E)$ diverges, all others remaining finite.

As was done in section 2, we single out from expression (2.13) the term corresponding to μ_0 and write $\mathcal{H}$ as

$$\mathcal{H} = \mathcal{H}^{\circ} + \mathcal{V} \tag{A.1}$$

where

$$\mathcal{H}^{\circ}_{\lambda\lambda'} \equiv \frac{H_{\lambda\mu_0} H_{\mu_0\lambda'}}{E - E_{\mu_0}} \tag{A.2}$$

and

$$\mathcal{V}_{\lambda\lambda'} \equiv E_{\lambda}\delta_{\lambda\lambda'} + \sum_{\mu(\neq\mu_0)} \frac{H_{\lambda\mu} H_{\mu\lambda'}}{E - E_{\mu}} \tag{A.3}$$

We shall now find the eigenvalues $\mathcal{E}_i^{(0)}$ and the eigenvectors $|\phi_i\rangle$ of $\mathcal{H}^{\circ}$, i.e.

$$\mathcal{H}^{\circ}|\phi_i\rangle = \mathcal{E}_i^{(0)}|\phi_i\rangle \ . \tag{A.4}$$

Calling $\gamma_{\lambda}^{(i)}$ the λ-th component of $|\phi_i\rangle$ and using (A.2), the eigenvalue eq. can be written explicitly as

$$\frac{H_{\lambda\mu_0}}{E - E_{\mu_0}} \sum_{\lambda'} H_{\mu_0\lambda'} \gamma_{\lambda'}^{(i)} = \mathcal{E}_i^{(0)} \gamma_{\lambda}^{(i)} \ . \tag{A.5}$$

From (A.5) we see that if

$$\sum_{\lambda'} H_{\mu_0 \lambda'} \gamma_{\lambda'}^{(i)} = 0 \ , \tag{A.6}$$

$\gamma_\lambda^{(i)}$ is an eigenvector of $\mathcal{H}^\circ$ corresponding to the eigenvalue

$$\mathcal{E}_i^{(0)} = 0 \ .$$

As we deal with a p-dimensional vector space, there exist $p-1$ eigenvectors $\gamma^{(i)}$, $i = 2, \ldots, p$ which fulfill eq. (A.6), showing that

$$\mathcal{E}_2^{(0)} = \mathcal{E}_3^{(0)} = \ldots = \mathcal{E}_p^{(0)} = 0 \ . \tag{A.7}$$

The remaining eigenvalue $\mathcal{E}_1^{(0)}$ corresponds to the case

$$\sum_{\lambda'} H_{\mu_0 \lambda'} \gamma_{\lambda'}^{(1)} \neq 0 \tag{A.8}$$

From (A.5), the normalized eigenvector $\gamma^{(1)}$ is given as

$$\gamma_\lambda^{(1)} = \frac{H_{\mu_0 \lambda}}{\left[\sum_\lambda |H_{\mu_0 \lambda}|^2\right]^{1/2}} \tag{A.9}$$

and $\mathcal{E}_1^{(0)}$ is obtained by multiplying both sides of (A.5) by $H_{\mu_0 \lambda}$ summing over λ and dividing through by expression (A.8), giving

$$\mathcal{E}_1^{(0)} = \frac{\sum_\lambda |H_{\lambda \mu_0}|^2}{E - E_{\mu_0}} \ . \tag{A.10}$$

In other words $\mathcal{H}^\circ$ has only one eigenvalue different from zero.

This is true, in general, for a matrix A, whose matrix elements are of the separable form $A_{ij} = A_i A_j$. Note that for a degenerate eigenvalue of H_{QQ} the matrix $\mathcal{H}^\circ$ is *not* separable, and this result does not hold. We note that for the non-degenerate case only one of the $\mathcal{E}_i^{(0)}$ can be made as large as we want, by choosing E close enough to E_{μ_0}, all others remaining equal to zero. Since in the limit $E \to E_{\mu_0}$, $U_{\lambda\chi}$ of eq. (A.3) remains finite, it seems plausible that only one eigenvalue of $\mathcal{H}$ diverges and that the remaining p-1 eigenvalues tend to finite values. We shall now prove that this is the case.

In order to do this, we make an orthogonal separation of the P-space into a one-dimensional R-space, containing the eigenvector $|\phi_1>$ (eq. (A.9)) and an S-space, spanned by $|\phi_i>$, $i = 2, \ldots, p$. This corresponds to the splitting of the projection operator P into two pieces,

$$P = R + S \tag{A.11}$$

where

$$R = |\phi_1><\phi_1| \quad .$$

If we now consider the "effective" Hamiltonian $\tilde{\mathcal{H}}$ in the R-space, defined by

$$\tilde{\mathcal{H}}(\mathcal{E}) = \mathcal{H}_{RR} + \mathcal{H}_{RS} \frac{1}{\mathcal{E} - \mathcal{H}_{SS}} \mathcal{H}_{SR} \quad , \tag{A.12}$$

it is clear that the values of $\mathcal{E}$ that satisfy the equation

$$<\phi_1 | \tilde{\mathcal{H}}(\mathcal{E}) | \phi_1> = \mathcal{E} \tag{A.13}$$

coincide with the eigenvalues $\mathcal{E}_i$ of $\mathcal{H}$, for a given value of E. (See the end of section 2). Now

$$\langle \phi_1 | \tilde{\mathcal{H}}(\mathcal{E}) | \phi_1 \rangle = E_1 + \sum_{\sigma} \frac{|\langle \phi_1 | \mathcal{H}_{RS} | \chi_\sigma \rangle|^2}{\mathcal{E} - E_\sigma} , \qquad (A.14)$$

where

$$\mathcal{H}_{SS} | \chi_\sigma \rangle = E_\sigma | \chi_\sigma \rangle , \quad \sigma = 2, \ldots, p \qquad (A.15)$$

and

$$E_1 = \langle \phi_1 | \mathcal{H} | \phi_1 \rangle = \mathcal{E}_1^{(0)} + \langle \phi_1 | U | \phi_1 \rangle , \qquad (A.16)$$

where $\mathcal{E}_1^{(0)}$ is given in eq. (A.10) and the matrix element $\langle \phi_1 | U | \phi_1 \rangle$ remains finite in the limit $E \to E_{\mu_0}$. Since, on the other hand,

$$\mathcal{H}_{SS} = \mathcal{H}^{\circ}_{SS} + U_{SS} = U_{SS}$$

is a bounded matrix in the limit, E_σ ($\sigma = 2, \ldots, p$) remain finite. Eq. (A.13) now reads

$$\sum_{\sigma} \frac{|\langle \phi_1 | \mathcal{H} | \chi_\sigma \rangle|^2}{\mathcal{E} - E_\sigma} = \mathcal{E} - E_1 \qquad (A.17)$$

which can be solved graphically. The solutions of (A.17) are indicated by the circles in fig. 4, for a given value of E. As $E - E_{\mu_0} \to 0^{\pm}$, E_σ ($\sigma = 2, \ldots, p$) will remain finite while E_1 tends $\pm \infty$ (see eq. (A.10)). Therefore, only one of the eigenvalues $\mathcal{E}_i$ of $\mathcal{H}$ shows a singularity, as stated before.

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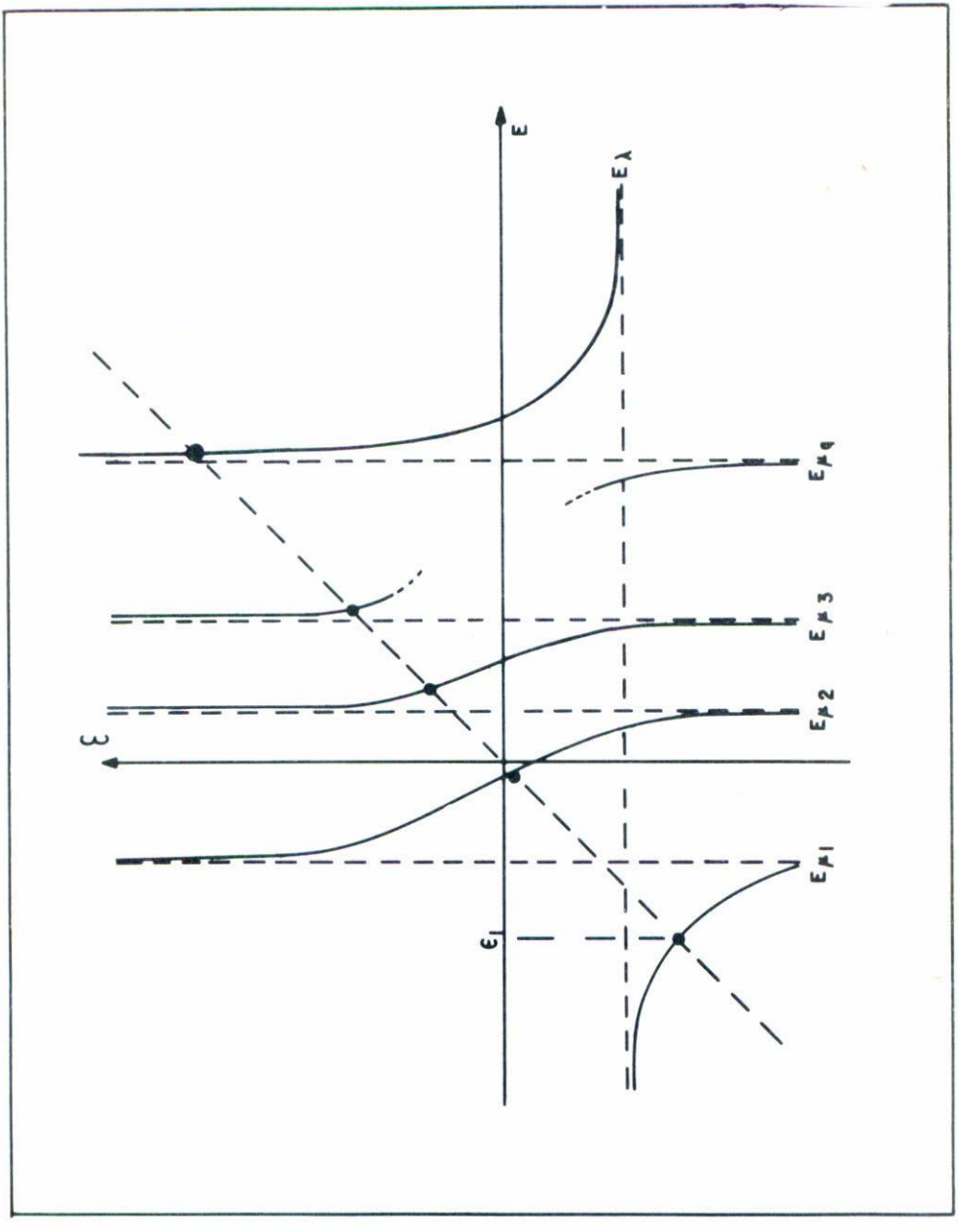

Fig. 1. Behaviour of the eigenvalue curve $\mathcal{E}_1(E)$ for the case $p = 1$ and q arbitrary.

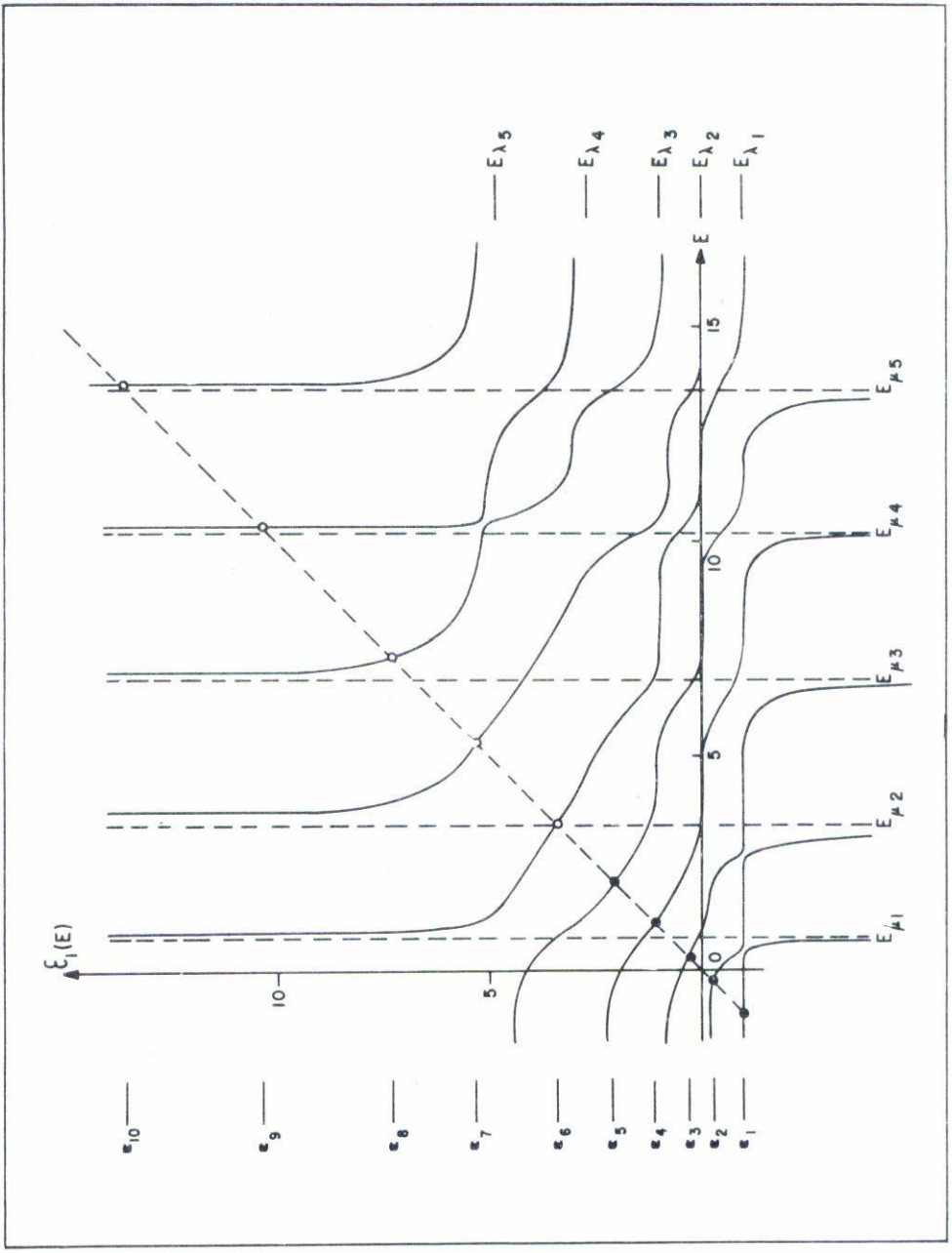

Fig. 2. Effective eigenvalue curves for the one-electron Coulomb problem for the case $p = 5$ and $q = 5$. The energy is given in units of the first Bohr orbit.

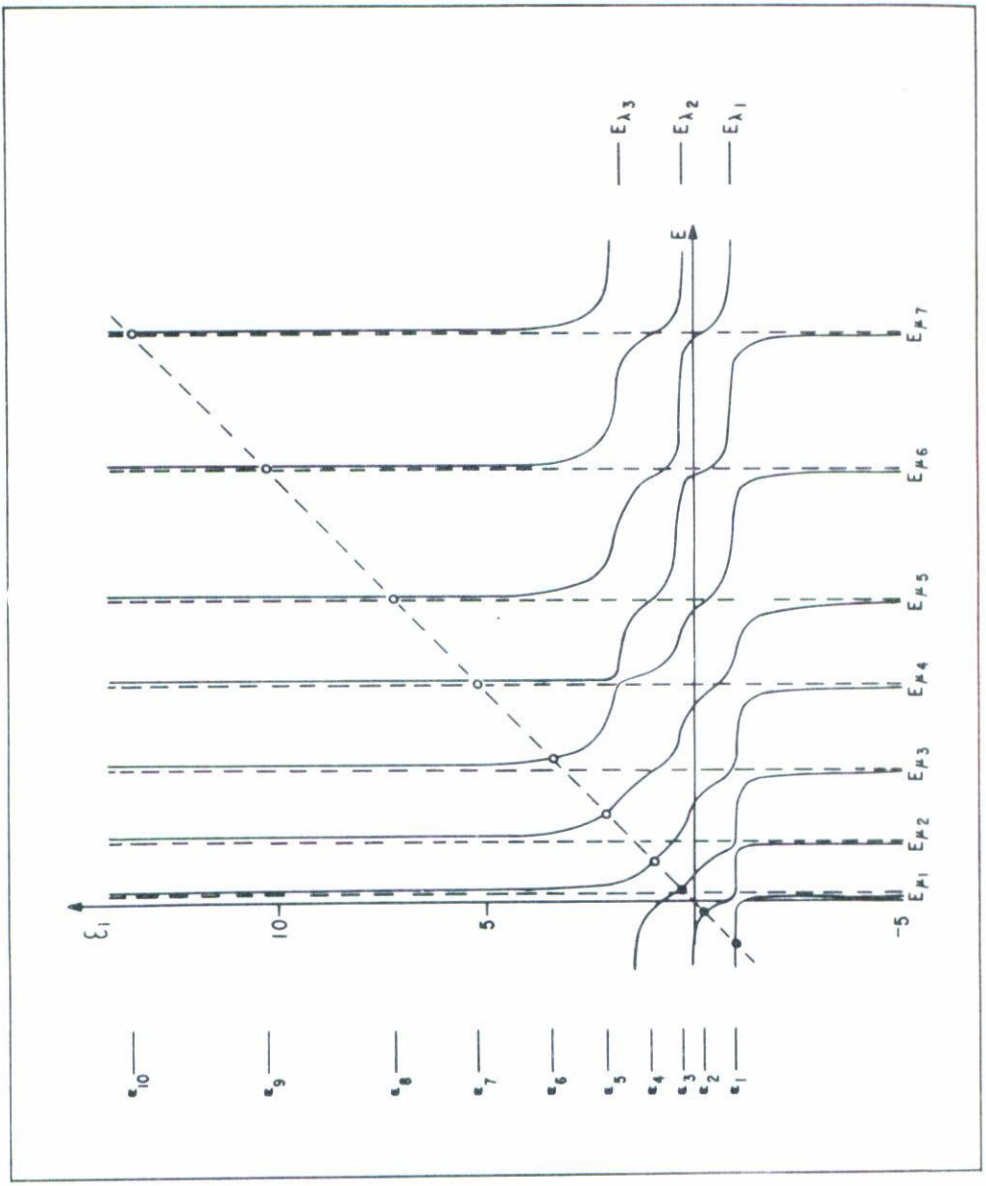

Fig. 3. Effective eigenvalue curves for the one-electron Coulomb problem for the case $p = 3$ and $q = 7$.

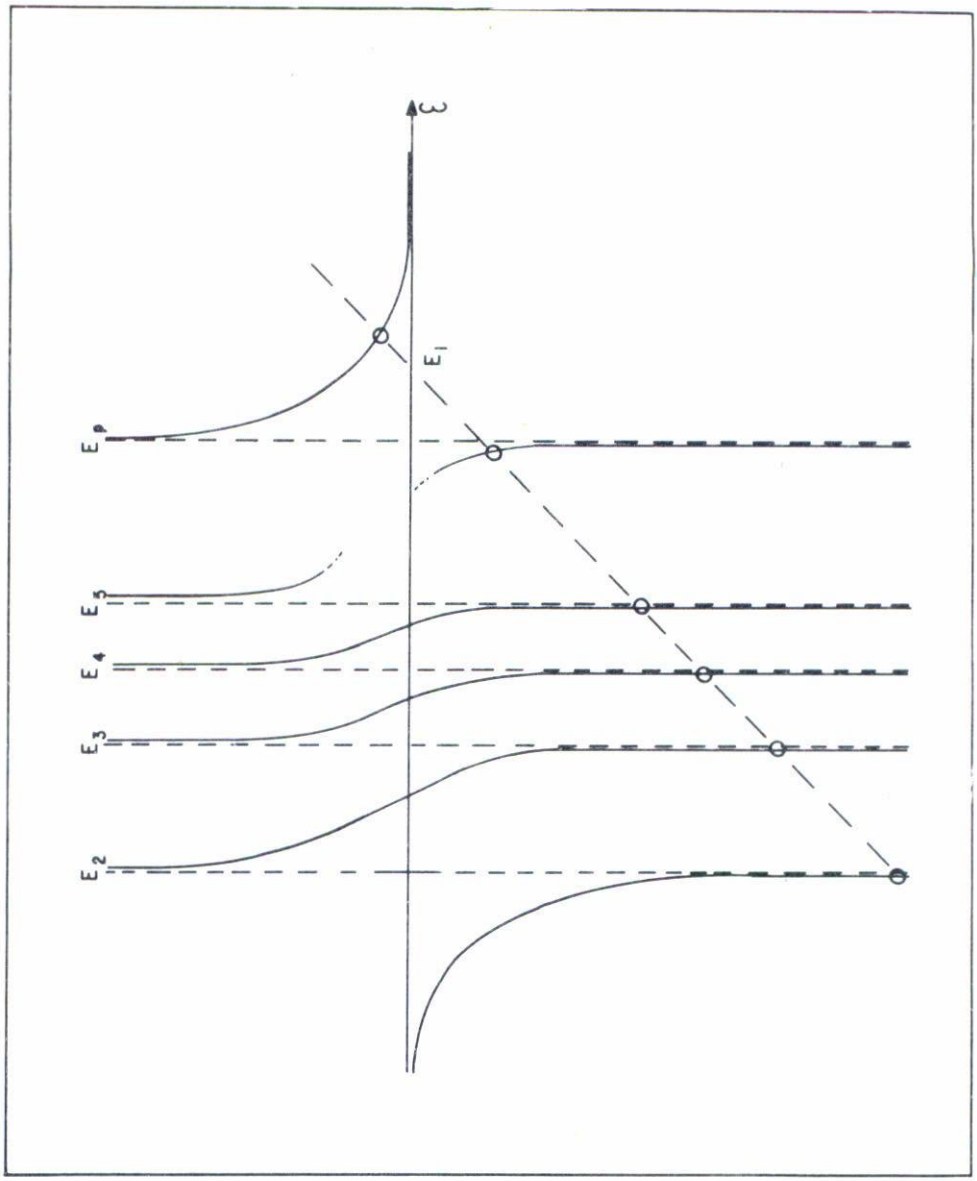

Fig. 4. Graphical solution of Eq. (A.17).