

**ON SIMULTANEOUS APPROXIMATION OF SEVERAL
EIGENVALUES OF A SEMI-DEFINITE SELF-ADJOINT
LINEAR OPERATOR IN A HILBERT SPACE**

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ABSTRACT. A lower semi-definite self-adjoint linear operator in a Hilbert space is taken whose discrete spectrum is not empty and comprises at least several eigenvalues $\lambda_{\min} = \lambda_1 \leq \dots \leq \lambda_m < \sigma_{\text{ess}}$. The problem of approximation of these eigenvalues by eigenvalues of some linear operator in a finite-dimensional space of the dimension s is considered and solved. The accuracy of the approximation obtained becomes unlimitedly high as $s \rightarrow \infty$.

1. INTRODUCTION.

The interest to Hilbert spaces and to linear operators in them is mainly due to their applications in quantum mechanics where the spaces of square integrable complex functions $L_2(\mathbb{C}, \mathbb{R}^{3N})$ and differential operators in them are considered. The most important of them is the energy operator which is called the Hamiltonian in general case and is called the Schrödinger operator in the case of particles in potential fields. In many cases the Schrödinger operator appears to be self-adjoint and semi-definite. With the quantum mechanical applications in view, Reed and Simon in their book [1] give the following theorem (see § 2 in Chapter XIII of [1]).

Theorem 1.1. *Let F be a lower semi-definite self-adjoint linear operator with the domain $D(F)$ in a Hilbert space H such that its discrete spectrum is not empty and λ_{\min} is its minimal eigenvalue¹. Let X be an eigenvector of F associated with the eigenvalue λ_{\min} . Assume that the eigenvector X is expanded in some orthonormal basis $\{h_i\}_{i=1, \dots, \infty}$ of the Hilbert space H :*

$$X = \lim_{n \rightarrow \infty} X_n, \quad \text{where } X_n = \sum_{i=1}^n x^i h_i. \quad (1.1)$$

Assume that $h_i \in D(F)$ for all $i = 1, \dots, \infty$ and suppose that

$$\exists \lim_{n \rightarrow \infty} \langle X_n | F X_n \rangle = \lambda_{\min} \|X\|^2.$$

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¹ It is implicitly assumed that λ_{\min} is below the lower limit of the essential spectrum $\sigma_{\text{ess}}(F)$ of the operator F .

Under these assumptions we have the equality

$$\lambda_{\min} = \lim_{n \rightarrow \infty} \hat{\mu}_1^{(n)},$$

where $\hat{\mu}_1^{(n)}$ is the minimal eigenvalue of the Hermitian $n \times n$ matrix $\Phi^{(n)}$ whose elements are $\Phi_{ij} = \langle h_i | F h_j \rangle$.

The angular brackets $\langle \bullet | \bullet \rangle$ in Theorem 1.1 mean the standard sesquilinear scalar product of the Hilbert space H . The formula (1.1) in Theorem 1.1 means convergence of the series

$$X = \sum_{i=1}^{\infty} x^i h_i, \quad (1.2)$$

with respect to the norm in H , while the coefficients x^i in (1.1) and (1.2) are denoted according to the Einstein's tensorial notation (see § 20 of Chapter I in [2]), i. e. using the upper index i for the coordinates of the vector X .

Theorem 1.1 is in background of almost all numerical methods of quantum chemistry, though it is used without recognition and without references to it. The goal of this paper is

- 1) to extend Theorem 1.1 to the case of several consecutive eigenvalues of the operator F taken in the non-decreasing order starting from the lowest one;
- 2) exclude the orthonormal basis from it;
- 3) replace the domain $D(F)$ of the operator F by the domain $Q(F)$ of the corresponding sesquilinear form $q_F(X, Y) = \langle X | F Y \rangle$.

2. STANDARD DEFINITIONS AND PREREQUISITES.

A Hilbert space H is a complex (generally speaking infinite-dimensional) linear vector space with some fixed positive sesquilinear form $\langle X | Y \rangle = \overline{\langle Y | X \rangle}$ that defines the norm $\|X\| = \sqrt{\langle X | X \rangle}$ and thus defines the topology of a complete metric space in H . With the quantum mechanical applications in view, all Hilbert spaces in this paper are implicitly assumed to be separable.

The form $\langle X | Y \rangle$ in H is assumed to be linear in its second argument Y and to be conjugate linear with respect to the first argument X . This convention is used in quantum mechanics (see. [3, 4]). The form $\langle X | Y \rangle$ is called the standard scalar product in H .

A linear operator F in a Hilbert space H is usually given along with its domain $D(F)$ which is assumed to be a dense subspace of H . The graph of a linear operator F is the following subset of the Cartesian product $H \times H$:

$$\Gamma(F) = \{(X, Y) \in H \times H : X \in D(F) \text{ and } Y = FX\}.$$

Definition 2.1. A linear operator F in a Hilbert space H is called closed, if its graph $\Gamma(F)$ is closed in $H \times H$.

An extension of an operator F is another operator with the domain bigger than $D(F)$ which upon restricting to $D(F)$ coincides with F .

Definition 2.2. A linear operator F in a Hilbert space H is called closable if it has at least one closed extension in H . The minimal closed extension of a closable

operator F is its closed extension with the minimal domain. It is denoted through \bar{F} and is shortly called the closure of F .

The minimal closed extension \bar{F} of a closable operator F is constructed by closing its graph: $\Gamma(\bar{F}) = \overline{\Gamma(F)}$. This yields the following theorem.

Theorem 2.1. *For any closable operator F in a Hilbert space H a vector X belongs to the domain $D(\bar{F})$ if and only if there is a sequence of vectors $X_n \in D(F)$ such that the following relationships hold:*

$$\lim_{n \rightarrow \infty} X_n = X, \quad \exists \lim_{n \rightarrow \infty} FX_n = Y \in H.$$

Limits here are in the sense of convergence with respect to the norm in H , while the vector Y is the value of the operator \bar{F} applied to the vector X , i. e. $\bar{F}X = Y$.

Definition 2.3. Let F be a linear operator in a Hilbert space H . The linear operator F^* with the domain

$$D(F^*) = \{X \in H: \exists Y \in H: \langle X|FZ \rangle = \langle Y|Z \rangle \forall Z \in D(F)\} \quad (2.1)$$

given by the formula $F^*X = Y$, where the element $Y \in H$ is uniquely fixed by the condition $\langle X|FZ \rangle = \langle Y|Z \rangle \forall Z \in D(F)$ from (2.1), is called the conjugate operator for the operator F .

In the book [5] the following theorem is given (see § 1 of Chapter VIII in [5]).

Theorem 2.2. *Let F be a linear operator in a Hilbert space H . Then*

- 1) *the conjugate operator F^* is closed;*
- 2) *the operator F is closable if and only if $D(F^*)$ is dense in H and $\bar{F} = F^{**}$ in such a case;*
- 3) *if the operator F is closable, then $(\bar{F})^* = F^*$.*

Definition 2.4. A linear operator F in a Hilbert space H is called symmetric if the conjugate operator F^* is an extension of F .

Practically the definition 2.4 can be replaced with a more simple and equivalent definition.

Definition 2.5. A linear operator F in a Hilbert space H is called symmetric if $\langle X|FY \rangle = \langle FX|Y \rangle$ for all $X, Y \in D(F)$.

Theorem 2.3. *Each symmetric operator F in a Hilbert space H is closable. Its closure \bar{F} itself is a symmetric operator in H .*

Definition 2.6. A linear operator F in a Hilbert space H is called self-adjoint if $F^* = F$, i. e. if F is symmetric and $D(F) = D(F^*)$.

Definition 2.7. A symmetric operator F in a Hilbert space H is called essentially self-adjoint if its closure \bar{F} is a self-adjoint operator in H .

Each linear operator F in a Hilbert space H is associated with the sesquilinear form $q_F(X, Y) = \langle X|FY \rangle$ which is defined for all X and Y in $D(F)$. In the case of a symmetric operator F the form q_F is symmetric, i. e. the following relationship holds: $q_F(X, Y) = \overline{q_F(Y, X)}$ for all $X, Y \in D(F)$.

Definition 2.8. A symmetric linear operator F in a Hilbert space H is called lower semi-definite if its form q_F is lower semi-definite, i. e. if there is a real constant C such that $q_F(X, X) = \langle X|FX \rangle \geq C \|X\|^2$ for all $X \in D(F)$. If $C = 0$, such an operator F is called non-negative.

In the case of a self-adjoint operator F , using the spectral theorem, the form q_F is extended from $D(F)$ to the bigger set

$$Q(F) = D(\sqrt{|F|}) \quad (2.2)$$

(see § 6 of Chapter VIII in [5] and § 53 of Part XV in [6]), preserving its symmetry:

$$q_F(X, Y) = \overline{q_F(Y, X)} \text{ for all } X, Y \in Q(F).$$

In the case of a lower semi-definite self-adjoint linear operator F the set (2.2) and the values of the form q_F in it admit a more constructive description.

Theorem 2.4. *Let F be a lower semi-definite self-adjoint linear operator in a Hilbert space H . Then a vector X belongs to the domain $Q(F)$ of the corresponding sesquilinear form q_F if and only if there is a sequence of vectors X_n in the domain $D(F)$ of the operator F such that*

- 1) $\|X_n - X\| \rightarrow 0$ as $n \rightarrow \infty$;
- 2) $\langle X_n - X_m | F(X_n - X_m) \rangle \rightarrow 0$ as $n, m \rightarrow \infty$.

Theorem 2.5. *Under the assumptions of Theorem 2.4 let X and Y be two vectors from $Q(F)$ and let X_n and Y_n be two sequences of vectors from $D(F)$ approximating X and Y in the sense of Theorem 2.4. Then*

$$q_F(X, Y) = \lim_{n \rightarrow \infty} \langle X_n | FY_n \rangle.$$

3. MINIMAX PRINCIPLE.

Theorem 3.1. *Let F be a lower semi-definite self-adjoint operator with the domain $D(F)$ in a Hilbert space H . For some positive integer n denote*

$$\mu_n(F) = \sup_{X_1, \dots, X_{n-1}} \inf_{\substack{X \in D(F), \|X\|=1 \\ X \perp X_1, \dots, X \perp X_{n-1}}} \langle X | FX \rangle. \quad (3.1)$$

Then exactly one of the two options holds:

- 1) *there exist n eigenvalues of the operator F below the lower limit of its essential spectrum $\sigma_{\text{ess}}(F)$ and the number $\mu_n(F)$ in (3.1) coincides with λ_n , provided that each eigenvalue of the operator F in the non-decreasing sequence*

$$\lambda_{\min} = \lambda_1 \leq \dots \leq \lambda_n$$

is repeated according to its multiplicity, except for maybe the last one;

- 2) *the number $\mu_n(F)$ in (3.1) coincides with the lower limit of of the essential spectrum $\sigma_{\text{ess}}(F)$ of the operator F . In this case there are not more than $n - 1$ eigenvalues of the operator F below $\sigma_{\text{ess}}(F)$, each being counted with its multiplicity, and $\mu_m(F) = \mu_n(F)$ for all $m > n$.*

Theorem 3.1 expresses the minimax principle for linear operators in Hilbert spaces. Its statement and its proof are given in the book [1] (see § 1 of Chapter XIII).

Remark. In [1] it is said that in Theorem 3.1 the domain $D(F)$ of the operator F can be replaced with the domain $Q(F)$ of its sesquilinear form q_F (see (2.2)). At the same time the quantity $\langle X|FX \rangle$ is replaced by the value of the form $q_F(X, X)$.

The case $n = 1$ in Theorem 3.1 is somewhat different from others. In this case the formula (3.1) simplifies and takes the form

$$\mu_1(F) = \inf_{X \in D(F), \|X\|=1} \langle X|FX \rangle. \tag{3.2}$$

The next theorem is a corollary of Theorem 3.1.

Theorem 3.2. *If a lower semi-definite self-adjoint operator F with the domain $D(F)$ in a Hilbert space H has a non-empty discrete spectrum below $\sigma_{\text{ess}}(F)$, then its minimal eigenvalue $\lambda_{\min} = \mu_1(F)$ is given by the formula (3.2).*

Remark. The domain $D(F)$ of the operator F in the formula (3.2) can be replaced by the domain $Q(F)$ of its sesquilinear form q_F (see (2.2)). At the same time the quantity $\langle X|FX \rangle$ is replaced by the value of the form $q_F(X, X)$.

4. MINIMUM PRINCIPLE.

In the case $n = 1$ the minimax principle is expressed by the formula (3.2). It transforms into minimum principle. A similar minimum principle can be formulated for the case $n > 1$.

Theorem 4.1. *Let F be a lower semi-definite self-adjoint linear operator with the domain $D(F)$ in a Hilbert space H whose discrete spectrum below $\sigma_{\text{ess}}(F)$ comprises at least n eigenvalues arranged in the non-decreasing order*

$$\lambda_{\min} = \lambda_1 \leq \dots \leq \lambda_{n-1} \leq \lambda_n$$

so that each eigenvalue in the sequence is repeated according to its multiplicity, except for maybe the last one. Let X_1, \dots, X_{n-1} be linearly independent eigenvectors for the initial $n - 1$ eigenvalues in this non-decreasing sequence. Then the quantity $\mu_n(F) = \lambda_n$ is given by the formula

$$\mu_n(F) = \inf_{\substack{X \in D(F), \|X\|=1 \\ X \perp X_1, \dots, X \perp X_{n-1}}} \langle X|FX \rangle.$$

The minimum principle similar to Theorem 4.1 for symmetric operators in a finite-dimensional Euclidean space can be found in the book [7]. For the Laplace operator it is formulated in [8]. The proof of Theorem 4.1 can be found in [9]. In this paper Theorem 4.1 is given for the sake of completeness of our preliminary review. It is not used in what follows.

5. THE RAYLEIGH-RITZ METHOD.

Theorem 5.1. *Let F be a lower semi-definite self-adjoint linear operator with the domain $D(F)$ in a Hilbert space H , let $V \subset D(F)$ be a finite-dimensional subspace of the dimension n in $D(F)$, and let P be the orthogonal projector onto V . The*

composite operator $P \circ F \circ P$ is lower semi-definite and self-adjoint. Its restriction F_V to the subspace V has exactly n eigenvalues $\hat{\mu}_1, \dots, \hat{\mu}_n$ that can be arranged in the non-decreasing order $\hat{\mu}_1 \leq \dots \leq \hat{\mu}_n$ where each eigenvalue is repeated according to its multiplicity. Under these assumptions the following inequalities hold:

$$\mu_m(F) \leq \hat{\mu}_m, \quad \text{where } m = 1, \dots, n. \quad (5.1)$$

The quantities $\mu_m(F)$ in the left hand side of the inequalities (5.1) are given by the formula (3.1). They do not depend on the choice of the subspace V in Theorem 5.1. The statement and the proof of Theorem 5.1 are given in the book [1] (see § 2 of Chapter XIII).

Remark. As we already noted above, the domain $D(F)$ of the operator F when computing $\mu_m(F)$ in the formula (3.1) can be replaced by the domain $Q(F)$ of its sesquilinear form q_F (see (2.2)). At the same time the quantity $\langle X|FX \rangle$ is replaced by the value of the form $q_F(X, X)$. In Theorem 5.1 the domain $D(F)$ can also be replaced by the domain $Q(F)$. Although then we should define the operator F_V in a different way through the restriction of the form q_F to the subspace $V \subset Q(F)$.

Theorem 5.2. *Let F be a lower semi-definite self-adjoint linear operator in a Hilbert space H whose associated sesquilinear form is q_F and the domain of q_F is $Q(F)$. Let $V \subset Q(F)$ be a finite-dimensional subspace of the dimension n in $Q(F)$ and let F_V be a linear operator in the subspace V defined by the restriction of the form q_F to V according to the formula*

$$\langle Y|F_V X \rangle = q_F(Y, X) \quad \text{for all } X, Y \in V.$$

The operator F_V has exactly n eigenvalues $\hat{\mu}_1, \dots, \hat{\mu}_n$ that can be arranged in the non-decreasing order $\hat{\mu}_1 \leq \dots \leq \hat{\mu}_n$ where each eigenvalue is repeated according to its multiplicity. Under these assumptions the following inequalities hold:

$$\mu_m(F) \leq \hat{\mu}_m, \quad \text{where } m = 1, \dots, n. \quad (5.2)$$

Proof. Applying the minimax principle expressed by Theorem 3.1 to the operator F_V in the finite-dimensional space V , from (3.1) we derive

$$\begin{aligned} \hat{\mu}_m &= \sup_{X_1, \dots, X_{m-1} \in V} \inf_{\substack{X \in V, \|X\|=1 \\ X \perp X_1, \dots, X \perp X_{m-1}}} \langle X|F_V X \rangle = \\ &= \sup_{X_1, \dots, X_{m-1} \in V} \inf_{\substack{X \in V, \|X\|=1 \\ X \perp X_1, \dots, X \perp X_{m-1}}} q_F(X, X). \end{aligned} \quad (5.3)$$

Let P be the orthogonal projector onto the subspace V . Then (5.3) implies

$$\begin{aligned} \hat{\mu}_m &= \sup_{X_1, \dots, X_{m-1} \in H} \inf_{\substack{X \in V, \|X\|=1 \\ X \perp PX_1, \dots, X \perp PX_{m-1}}} q_F(X, X) = \\ &= \sup_{X_1, \dots, X_{m-1} \in H} \inf_{\substack{X \in V, \|X\|=1 \\ X \perp X_1, \dots, X \perp X_{m-1}}} q_F(X, X) \geq \\ &\geq \sup_{X_1, \dots, X_{m-1} \in H} \inf_{\substack{X \in Q(F), \|X\|=1 \\ X \perp X_1, \dots, X \perp X_{m-1}}} q_F(X, X) = \mu_m(F). \end{aligned} \quad (5.4)$$

The inequality in (5.4) arises since we replace V in the left hand side of the inequality by a larger subspace $Q(F)$ in the right hand side of this inequality. The last equality in (5.4) is due to the remark to Theorem 3.1 on page 5. \square

Theorems 5.1 and 1.1 constitute a base for the Rayleigh-Ritz method. Its application to the experimental confirmation of the Lamb shift is described in [1] (see § 2 of Chapter XIII therein). See also [10–17].

6. APPROXIMATION OF SEVERAL EIGENVALUES.

Theorem 6.1. *Let F be a lower semi-definite self-adjoint linear operator with the domain $D(F)$ in a Hilbert space H whose discrete spectrum below $\sigma_{\text{ess}}(F)$ is not empty and comprises at least m eigenvalues arranged in the non-decreasing order $\lambda_{\min} = \lambda_1 \leq \dots \leq \lambda_m$ so that each eigenvalue is repeated according to its multiplicity, except for maybe the last one. Let X_1, \dots, X_m be linearly independent eigenvectors corresponding to the eigenvalues $\lambda_{\min} = \lambda_1 \leq \dots \leq \lambda_m$ and assume that for each eigenvector X_k a sequence of vectors X_{kn} from the domain $Q(F)$ of the associated with F sesquilinear form q_F is given so that*

$$X_k = \lim_{n \rightarrow \infty} X_{kn} \quad \text{and} \quad \lim_{n \rightarrow \infty} q_F(X_{kn}, X_{qn}) = \langle X_k | F X_q \rangle, \quad (6.1)$$

where $1 \leq k, q \leq m$. Under these assumptions

$$\lambda_k = \lim_{n \rightarrow \infty} \hat{\mu}_k^{(n)} \quad \text{for all } k = 1, \dots, m, \quad (6.2)$$

where $\hat{\mu}_{\min}^{(n)} = \hat{\mu}_1^{(n)} \leq \dots \leq \hat{\mu}_m^{(n)}$ are initial m eigenvalues of the operator F_{V_n} generated by the restriction of the form q_F to the finite-dimensional subspace

$$V_n = \text{Span}(\{X_{ks}, \text{ where } 1 \leq k \leq m, 1 \leq s \leq n\}) \subset Q(F) \quad (6.3)$$

taken in the non-decreasing order so that each eigenvalue is repeated according to its multiplicity, except for maybe the last one.

Proof. The eigenvectors X_1, \dots, X_m belong to the domain $D(F)$. They are linearly independent. Their span

$$\mathcal{V} = \text{Span}(X_1, \dots, X_m) \subset D(F) \subset Q(F) \quad (6.4)$$

is an m -dimensional subspace in $D(F)$ and in $Q(F)$. Let \mathcal{P} be the orthogonal projector onto the subspace (6.4). We set

$$F_{\mathcal{V}} = \mathcal{P} \circ F \circ \mathcal{P} \Big|_{\mathcal{V}}. \quad (6.5)$$

In other words, we denote through $F_{\mathcal{V}}$ the restriction of the composite operator $\mathcal{P} \circ F \circ \mathcal{P}$ to the subspace (6.4). The eigenvectors X_1, \dots, X_m of the operator F are eigenvectors of the operator (6.5), while the corresponding eigenvalues coincide with $\lambda_{\min} = \lambda_1 \leq \dots \leq \lambda_m$. Therefore the matrix of the operator (6.5) in the basis of the eigenvectors X_1, \dots, X_m is

$$\mathcal{F} = \left\| \begin{array}{ccc} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_m \end{array} \right\|. \quad (6.6)$$

The operator (6.5) is generated by the restriction of the form q_F to the subspace (6.4), therefore the matrix (6.6) obeys the relationships

$$\mathcal{H} = G \mathcal{F}, \quad \mathcal{F} = G^{-1} \mathcal{H}, \quad (6.7)$$

where \mathcal{H} and G are two Hermitian matrices with the components

$$\mathcal{H}_{sk} = q_F(X_s, X_k) = \langle X_s | F X_k \rangle, \quad g_{sq} = \langle X_s | X_q \rangle. \quad (6.8)$$

The matrix G is the Gram matrix of the basis of vectors X_1, \dots, X_m . Since these vectors are linearly independent, $\det G \neq 0$ and hence the matrix relationships (6.7) are consistent.

Let's consider the vectors X_{1n}, \dots, X_{mn} . According to the first condition in (6.1) these vectors approximate X_1, \dots, X_m in the sense of convergence with respect to the norm in the Hilbert space H . This means that for all sufficiently large n the vectors X_{1n}, \dots, X_{mn} are linearly independent. We set

$$\mathcal{V}_n = \text{Span}(X_{1n}, \dots, X_{mn}) \subset Q(F). \quad (6.9)$$

The subspace (6.9) is analogous to the subspace (6.4). For all sufficiently large n the dimensions of these subspaces do coincide:

$$\dim \mathcal{V}_n = \dim \mathcal{V} = m. \quad (6.10)$$

Generally speaking, the subspace (6.9) is not enclosed in $D(F)$. Therefore we cannot write a formula similar to (6.5). But we can consider the operator $F_{\mathcal{V}_n}$ generated by the restriction of the sesquilinear form q_F to the subspace (6.9). Let $\mathcal{F}^{(n)}$ be the matrix of such operator in the basis X_{1n}, \dots, X_{mn} . It is similar to the matrix (6.6), though it is not diagonal. The matrix $\mathcal{F}^{(n)}$ obeys the relationships which are similar to the relationships (6.7):

$$\mathcal{H}^{(n)} = G^{(n)} \mathcal{F}^{(n)}, \quad \mathcal{F}^{(n)} = (G^{(n)})^{-1} \mathcal{H}^{(n)}. \quad (6.11)$$

In (6.11) we see two Hermitian matrices $\mathcal{H}^{(n)}$ and $G^{(n)}$. Their components are defined by the formulas similar to (6.8):

$$\mathcal{H}[n]_{sk} = q_F(X_{sn}, X_{kn}) = \langle X_{sn} | F_{\mathcal{V}_n} X_{kn} \rangle, \quad g[n]_{sq} = \langle X_{sn} | X_{qn} \rangle. \quad (6.12)$$

The matrix $G^{(n)}$ in (6.11) is the Gram matrix for the basis composed by the vectors X_{1n}, \dots, X_{mn} . For all sufficiently large n the matrix $G^{(n)}$ is non-degenerate, which is in agreement with (6.10). Hence the relationships (6.11) are consistent.

Now we consider the conditions (6.1). Applying them to (6.8) and (6.12), we get

$$\lim_{n \rightarrow \infty} g[n]_{sq} = g_{sq}, \quad \lim_{n \rightarrow \infty} \mathcal{H}[n]_{sk} = \mathcal{H}_{sk}. \quad (6.13)$$

In the matrix form the relationships (6.13) are written as follows:

$$\lim_{n \rightarrow \infty} G^{(n)} = G, \quad \lim_{n \rightarrow \infty} \mathcal{H}^{(n)} = \mathcal{H}. \quad (6.14)$$

The first relationship (6.14) yields $\lim_{n \rightarrow \infty} \det G^{(n)} = \det G \neq 0$. Hence

$$\exists \lim_{n \rightarrow \infty} (G^{(n)})^{-1} = G^{-1}. \quad (6.15)$$

Let's combine (6.15) with the second relationship (6.14) and then take into account (6.11). This yields the following relationship

$$\exists \lim_{n \rightarrow \infty} \mathcal{F}^{(n)} = \mathcal{F}. \quad (6.16)$$

The eigenvalues of the matrix \mathcal{F} are the eigenvalues of the operator (6.5), coinciding with $\lambda_{\min} = \lambda_1 \leq \dots \leq \lambda_m$. They are presented explicitly in (6.6). The eigenvalues of the matrix $\mathcal{F}^{(n)}$ in (6.16) are the eigenvalues of the self-adjoint operator $F_{\mathcal{V}_n}$ in m -dimensional space \mathcal{V}_n . We denote them

$$\hat{\lambda}_{\min}^{(n)} = \hat{\lambda}_1^{(n)} \leq \dots \leq \hat{\lambda}_m^{(n)}. \quad (6.17)$$

From (6.16) for the eigenvalues (6.17) we derive

$$\exists \lim_{n \rightarrow \infty} \hat{\lambda}_k^{(n)} = \lambda_k \quad \text{for all } k = 1, \dots, m. \quad (6.18)$$

In the next step we consider the subspace (6.3). The sesquilinear form q_F produces the self-adjoint operator F_{V_n} whose initial m eigenvalues in Theorem 6.1 are denoted through $\hat{\mu}_{\min}^{(n)} = \hat{\mu}_1^{(n)} \leq \dots \leq \hat{\mu}_m^{(n)}$. We can apply Theorem 5.2 to the subspace (6.3). Applying this theorem, we get

$$\mu_k(F) \leq \hat{\mu}_k, \quad \text{where } k = 1, \dots, m. \quad (6.19)$$

Moreover, in our case the operator F is such that for all $\mu_k(F)$ from (6.19) the first of the two alternative options from Theorem 3.1 is realized. This means that

$$\mu_k(F) = \lambda_k \quad \text{for all } k = 1, \dots, m. \quad (6.20)$$

Comparing (6.19) and (6.20), we derive

$$\lambda_k \leq \hat{\mu}_k \quad \text{for all } k = 1, \dots, m. \quad (6.21)$$

In order to complete the proof of Theorem 6.1 we compare the subspaces (6.3) and (6.9) along with the self-adjoint operators F_{V_n} and $F_{\mathcal{V}_n}$ in them. It is easy to see that $\mathcal{V}_n \subset V_n$. If we denote through \mathcal{P}_n the orthogonal projector onto the smaller subspace \mathcal{V}_n , we can easily derive the relationship

$$F_{\mathcal{V}_n} = \mathcal{P}_n \circ F_{V_n} \circ \mathcal{P}_n \Big|_{\mathcal{V}_n}. \quad (6.22)$$

Due to the inclusion $\mathcal{V}_n \subset V_n$ and the relationship (6.22) we can apply Theorem 5.1 to the subspace \mathcal{V}_n and to the operator F_{V_n} in the enclosing subspace V_n . Applying this theorem, we derive the inequalities

$$\mu_k(F_{V_n}) = \hat{\mu}_k \leq \hat{\lambda}_k^{(n)} \quad \text{for all } k = 1, \dots, m. \quad (6.23)$$

From (6.21) and (6.23) we derive double inequalities:

$$\lambda_k \leq \hat{\mu}_k \leq \hat{\lambda}_k^{(n)} \quad \text{for all } k = 1, \dots, m. \quad (6.24)$$

Now, applying (6.18) to (6.24), we get the required result expressed by the formula (6.2). Theorem 6.1 is proved. \square

7. CONCLUSIONS

The main result of this paper is expressed by Theorem 6.1. As a mathematical result it has independent value. As for its application to quantum mechanics and quantum chemistry, it means that the Rayleigh-Ritz method can be used not only for computing the ground energy level of atoms and molecules, but for several consecutive excited energy levels along with the ground level. A way of applying Theorem 6.1 to quantum chemistry using polylinear splines is described in [9].

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