

doi 10.26089/NumMet.v23r315

## The Kantorovich projection method in the generalized quadratic spectrum approximation

**Somia Kamouche**

University 08 May 1945, Department of Mathematics,  
Laboratory of Applied Mathematics and Modeling,  
Guelma, Algeria

ORCID: 0000-0002-8396-0570, e-mail: [soumia.kamouche@gmail.com](mailto:soumia.kamouche@gmail.com)

**Hamza Guebbai**

University 08 May 1945, Department of Mathematics,  
Laboratory of Applied Mathematics and Modeling,  
Guelma, Algeria

ORCID: 0000-0001-8119-2881, e-mail: [guebbaihamza@yahoo.fr](mailto:guebbaihamza@yahoo.fr)

**Mourad Ghiat**

University 08 May 1945, Department of Mathematics,  
Laboratory of Applied Mathematics and Modeling,  
Guelma, Algeria

ORCID: 0000-0002-4484-2504, e-mail: [mourad.ghi24@gmail.com](mailto:mourad.ghi24@gmail.com)

**Muhammet Kurulay**

Yildiz Technical University, Faculty of Chemistry and Metallurgy,  
Department of Mathematics Engineering,  
Istanbul, Turkey

ORCID: 0000-0002-9276-9989, e-mail: [muhammetkurulay@yahoo.com](mailto:muhammetkurulay@yahoo.com)

**Abstract:** The objective of this paper is to construct a generalized quadratic spectrum approximation based on the Kantorovich projection method which allows us to deal with the spectral pollution problem. For this purpose, we prove that the property U (see Eq. 3) holds under weaker conditions than the norm and the collectively compact convergence. Numerical results illustrate the effectiveness and the convergence of our method.

**Keywords:** spectral pollution, spectral approximation, Kantorovich projection, eigenvalue

**For citation:** S. Kamouche, H. Guebbai, M. Ghiat and M. Kurulay, “The Kantorovich projection method in the generalized quadratic spectrum approximation,” *Numerical Methods and Programming*. **23** (3), 240–247 (2022). doi 10.26089/NumMet.v23r315.



## Метод проекции Канторовича в приближении обобщенного квадратичного спектра

**Сумайя Камуш**

Университет 08 Мая 1945, факультет математики,  
 лаборатория прикладной математики и моделирования, Гельма, Алжир  
 ORCID: 0000-0002-8396-0570, e-mail: [soumia.kamouche@gmail.com](mailto:soumia.kamouche@gmail.com)

**Хамза Гибби**

Университет 08 Мая 1945, факультет математики,  
 лаборатория прикладной математики и моделирования, Гельма, Алжир  
 ORCID: 0000-0001-8119-2881, e-mail: [guebaihamza@yahoo.fr](mailto:guebaihamza@yahoo.fr)

**Мурад Гият**

Университет 08 Мая 1945, факультет математики,  
 лаборатория прикладной математики и моделирования, Гельма, Алжир  
 ORCID: 0000-0002-4484-2504, e-mail: [mourad.ghi24@gmail.com](mailto:mourad.ghi24@gmail.com)

**Мухаммед Курулай**

Технический университет Йылдыз, факультет химии и металлургии,  
 кафедра математической инженерии, Стамбул, Турция  
 ORCID: 0000-0002-9276-9989, e-mail: [muhammetkurulay@yahoo.com](mailto:muhammetkurulay@yahoo.com)

**Аннотация:** Целью данной работы является построение обобщенной квадратичной аппроксимации спектра на основе проекционного метода Канторовича, которая позволяет справиться с проблемой спектрального загрязнения. Для этого мы доказываем, что свойство U (см. (3)) выполняется при более слабых условиях, чем норма и коллективно компактная сходимость. Численные результаты иллюстрируют эффективность и сходимость нашего метода.

**Ключевые слова:** спектральное загрязнение, аппроксимация спектра, проекция Канторовича, собственное значение

**Для цитирования:** Камуш С., Гибби Х., Гият М., Курулай М. Метод проекции Канторовича в приближении обобщенного квадратичного спектра // Вычислительные методы и программирование. 2022. **23**, № 3. 240–247. doi 10.26089/NumMet.v23r315.

**1. Introduction.** The eigenvalue problem is one of the key issues in the modern investigations. For instance, the solution of this problem constitutes the basis of chemist’s and physicist’s studies on finding a stable electron orbits in atoms and molecules. The stable states of electrons are described by eigenvectors whose eigenvalues correspond to energy states. This kind of studies allows to simulate 3D molecules shape and to determine the possible reactions between two molecules using the density functional theory “DFT” [1–3].

In our work we are interested in the generalized quadratic eigenvalue problem associated to three bounded linear operators  $(A, B, I + D)$  from a Banach space  $\mathcal{B}$  into itself (see also [4]), where  $I$  is the identity operator of  $\mathcal{B}$ . It is formulated by the following way: it is necessary to find the couple  $(\lambda, x) \in \mathbb{C} \times \mathcal{B} \setminus \{0\}$  such that

$$\lambda^2 Ax + \lambda Bx + (I + D)x = 0, \tag{1}$$

where  $\lambda$  is a generalized quadratic eigenvalue of operators  $(A, B, I + D)$  and  $x$  is the corresponding eigenvector.

This problem appears in the mathematical modeling of real engineering tasks such as the vibration analysis of structural systems, vibro-acoustics and the study of the linear stability of flows in fluid mechanics [5]. In addition, it arises in the spectral approximation of quadratic pencil of the Sturm-Liouville and Schrödinger operators [6, 7].

In order to build an accurate method and to avoid the spectral pollution [8–11], we construct an approximation of the operators  $A, B$ , and  $D$  using the Kantorovich projection method [12–14] which allows us to satisfy the property U under weaker conditions than those used in [15–17]. The authors in [4] proved that property U

holds for the quadratic spectral problem of three bounded operators  $A, B$  and  $C$ , which may be written in the following form

$$\text{Find } (\lambda, x) \in \mathbb{C} \times \mathcal{B} \setminus \{0\} : \lambda^2 Ax + \lambda Bx + Cx = 0, \tag{2}$$

under the norm convergence and the collectively compact convergence of the sequences of bounded linear operators  $\{A_n\}_{n \in \mathbb{N}}, \{B_n\}_{n \in \mathbb{N}}$  and  $\{C_n\}_{n \in \mathbb{N}}$ , which means that

$$\text{If } \lambda_n \in \text{sp}(A_n, B_n, C_n) \text{ and } \lambda_n \rightarrow \lambda, \text{ then } \lambda \in \text{sp}(A, B, C). \tag{3}$$

**2. The Kantorovich projection in the generalized quadratic spectrum approximation.** Let  $A, B$  and  $D$  be three bounded linear operators defined on a Banach space  $(\mathcal{B}, \|\cdot\|)$  into itself. We determine the generalized quadratic resolvent set denoted by  $\text{re}(A, B, I + D)$  as a set of the complex numbers  $\lambda$  such that  $\lambda^2 A + \lambda B + (I + D)$  is bijective one from  $\mathcal{B}$  into  $\mathcal{B}$  and its inverse expression is bounded, i.e.  $[\lambda^2 A + \lambda B + (I + D)]^{-1} \in \text{BL}(\mathcal{B})$ , where  $\text{BL}(\mathcal{B})$  is the Banach space of all linear bounded operators defined on  $\mathcal{B}$  into itself, equipped with the following norm

$$\forall K \in \text{BL}(\mathcal{B}) : \| \|K\| \| = \sup_{\|x\|=1} \|Kx\|. \tag{4}$$

The complementary of  $\text{re}(A, B, I + D)$  in  $\mathbb{C}$  is the generalized quadratic spectrum  $\text{sp}(A, B, I + D)$ , i.e.

$$\text{sp}(A, B, I + D) = \mathbb{C} \setminus \text{re}(A, B, I + D). \tag{5}$$

Let  $\{A_n^K\}_{n \in \mathbb{N}}, \{B_n^K\}_{n \in \mathbb{N}}$  and  $\{D_n^K\}_{n \in \mathbb{N}}$  be sequences in  $\text{BL}(\mathcal{B})$ , where  $A_n^K, B_n^K, D_n^K$  are the approximate operators by the Kantorovich projection method given by equalities

$$A_n^K = \pi_n A, \quad B_n^K = \pi_n B, \quad D_n^K = \pi_n D, \tag{6}$$

where  $\pi_n \in \text{BL}(\mathcal{B})$  is a bounded projection such as  $\pi_n^2 = \pi_n$  [12], [14]. In this paper, we do not require that  $A, B$  and  $D$  to be compact operators.

Let  $G$  and  $H \in \text{BL}(\mathcal{B})$ . We suppose that

**(S1)**  $\pi_n x$  converges to  $x$  for all  $x \in \mathcal{B}$ .

**(S2)**  $GH$  is a compact operator, where  $G, H \in \{A, B, D\}$ .

The assumption **(S2)** is important in our study because it improves the previous results [16], where the compactness of the operators  $(A, B, D)$  was required to get the spectrum convergence. In order to show the significance of **(S2)**, we consider the Cauchy integral operator  $H$ , defined as

$$H^2 x(s) = \oint_0^1 \frac{x(t)}{t-s} dt = \lim_{\varepsilon \rightarrow 0} \left[ \int_0^{s-\varepsilon} \frac{x(t)}{t-s} dt + \int_{s+\varepsilon}^1 \frac{x(t)}{t-s} dt \right], \quad 0 \leq s \leq 1. \tag{7}$$

We know that  $H$  is a bounded no compact operator in  $L^2(0, 1)$  (see [18]), but  $H^2$  is compact. In fact,

$$Hx(t) = \oint_0^1 R(t, \theta)x(\theta)d\theta, \quad 0 \leq t \leq 1, \tag{8}$$

where  $R(t, \theta)$  is a continuous function defined on  $]0, 1[^2$  by

$$R(t, \theta) = \oint_0^1 \frac{ds}{(s-t)(\theta-s)} = \frac{\ln|t| - \ln|\theta|}{t-\theta} + \frac{\ln|1-\theta| - \ln|1-t|}{t-\theta}, \quad 0 < \{t, \theta\} < 1, \quad t \neq \theta. \tag{9}$$

The authors in [14] showed that the Kantorovich projection method converges in the norm sense, i.e. if  $T \in \text{BL}(\mathcal{B})$  is a compact, then  $T_n^K \xrightarrow{n} T$ , i.e.  $\|T_n^K - T\| \rightarrow 0$ . They also mentioned that the norm convergence implies the  $\nu$ -convergence, which is denoted as  $T_n^K \xrightarrow{\nu} T$ , i.e.

$$\| \|T_n^K\| \| \text{ is bounded, } \| \| (T_n^K - T)T \| \| \rightarrow 0 \text{ and } \| \| (T_n^K - T)T_n^K \| \| \rightarrow 0. \tag{10}$$

The assumptions **(S1)** and **(S2)** proved that the sequences  $\{A_n^K\}_{n \in \mathbb{N}}, \{B_n^K\}_{n \in \mathbb{N}}$  and  $\{D_n^K\}_{n \in \mathbb{N}}$  converge in the  $\nu$ -convergence sense.



**Theorem 1** *If the hypotheses (S1) and (S2) are satisfied, then for all  $\lambda \in \mathbb{C}$   $\lambda^2 A_n^K + \lambda B_n^K + D_n^K$  converges in  $\nu$ -convergence sense to  $\lambda^2 A + \lambda B + D$ .*

*Proof* Firstly, we prove that  $\| \lambda^2 A_n^K + \lambda B_n^K + D_n^K \|$  is bounded. Since  $A, B, D \in \text{BL}(\mathcal{B})$ , we have

$$\| \lambda^2 A_n^K + \lambda B_n^K + D_n^K \| \leq \| \lambda^2 A + \lambda B + D \| \cdot \| \pi_n \|.$$

Using now the Uniform Boundedness Principle (see [19]), we find that  $\| \pi_n \|$  is bounded, which allows us to obtain the result.

Secondly, we show that  $\| [(\lambda^2 A_n^K + \lambda B_n^K + D_n^K) - (\lambda^2 A + \lambda B + D)] (\lambda^2 A + \lambda B + D) \| \rightarrow 0$ . For this aim, we write down the following inequality:

$$\begin{aligned} & \| [(\lambda^2 A_n^K + \lambda B_n^K + D_n^K) - (\lambda^2 A + \lambda B + D)] (\lambda^2 A + \lambda B + D) \| \\ & \leq \| \lambda^4 (A_n^K - A) A \| + \| \lambda^3 (B_n^K - B) A \| + \| \lambda^2 (D_n^K - D) A \| \\ & + \| \lambda^3 (A_n^K - A) B \| + \| \lambda^2 (B_n^K - B) B \| + \| \lambda (D_n^K - D) B \| \\ & + \| \lambda^2 (A_n^K - A) D \| + \| \lambda (B_n^K - B) D \| + \| (D_n^K - D) D \|. \end{aligned} \tag{11}$$

For all  $n \in \mathbb{N}$ , we have

$$\begin{aligned} \| (A_n^K - A) A \| & = \| (\pi_n A - A) A \| = \| (\pi_n - I) A^2 \| = \sup_{x \in \mathcal{B}} \| (\pi_n - I) A^2 x \| \\ & \leq \sup_{z \in A^2(\omega(0,1))} \| (\pi_n - I) A^2 z \| \leq \sup_{z \in \bar{\omega}(0,1)} \| (\pi_n - I) A^2 z \| \rightarrow 0. \end{aligned}$$

Proceeding in a similar way with other parts of inequality (11), we arrive to the analogous results, namely  $\| (A_n^K - A) L \| \rightarrow 0$ ,  $\| (B_n^K - B) L \| \rightarrow 0$  and  $\| (D_n^K - D) L \| \rightarrow 0$ , where  $L \in \{A, B, D\}$ .

Finally, we demonstrate that  $\| [(\lambda^2 A_n^K + \lambda B_n^K + D_n^K) - (\lambda^2 A + \lambda B + D)] (\lambda^2 A_n^K + \lambda B_n^K + D_n^K) \| \rightarrow 0$ . Indeed,

$$\begin{aligned} & \| [(\lambda^2 A_n^K + \lambda B_n^K + D_n^K) - (\lambda^2 A + \lambda B + D)] (\lambda^2 A_n^K + \lambda B_n^K + D_n^K) \| \\ & \leq \| \lambda^4 (A_n^K - A) A_n^K \| + \| \lambda^3 (B_n^K - B) A_n^K \| + \| \lambda^2 (D_n^K - D) A_n^K \| \\ & + \| \lambda^3 (A_n^K - A) B_n^K \| + \| \lambda^2 (B_n^K - B) B_n^K \| + \| \lambda (D_n^K - D) B_n^K \| \\ & + \| \lambda^2 (A_n^K - A) D_n^K \| + \| \lambda (B_n^K - B) D_n^K \| + \| (D_n^K - D) D_n^K \|. \end{aligned} \tag{12}$$

For all  $n \in \mathbb{N}$ , we have

$$\| (A_n^K - A) A_n^K \| = \| (\pi_n A - A) \pi_n A \| = \| (\pi_n - I) A \pi_n A \|. \tag{13}$$

Since the projection  $\pi_n$  is a finite rank approximation, then  $\text{rank}(A \pi_n A)$  is a finite one as well. This fact leads to  $\| (\pi_n - I) A \pi_n A \| \rightarrow 0$ . For the rest terms in (12) we get the following similar outcomes:  $\| (A_n^K - A) L_n^K \| \rightarrow 0$ ,  $\| (B_n^K - B) L_n^K \| \rightarrow 0$ ,  $\| (D_n^K - D) L_n^K \| \rightarrow 0$ , where  $L_n^K \in \{A_n^K, B_n^K, D_n^K\}$ .

**Theorem 2** *If the assumptions (S1) and (S2) are valid,  $\lambda_n \in \text{sp}(A_n^K, B_n^K, I + D_n^K)$  and  $\lambda_n \rightarrow \lambda$  for all  $n \in \mathbb{N}$ , then  $\lambda \in \text{sp}(A, B, I + D)$ .*

*Proof* Let us define

$$T_n^K = \lambda^2 A_n^K + \lambda B_n^K + D_n^K \text{ for all } n \in \mathbb{N} \text{ and } T = \lambda^2 A + \lambda B + D.$$

We suppose that  $\lambda \in \text{re}(A, B, D + I)$ , i.e. that  $(\lambda^2 A + \lambda B + D + I)^{-1} = (T + I)^{-1}$  is bounded. It implies that  $\lambda = -1$  is a resolvent value of  $T$ . On the other hand,  $\lambda_n \in \text{sp}(A_n^K, B_n^K, I + D_n^K)$ , then  $\lambda_n = -1 \in \text{sp}(T_n^K)$ . The first theorem proves that  $T_n^K \xrightarrow{\nu} T$  and  $\lambda_n \rightarrow -1$ , since the property U associated to the standard spectral problem, implies that  $\lambda_n \rightarrow \lambda$ . Indeed, if  $\lambda_n \in \text{sp}(T_n^K)$  and  $\lambda_n \rightarrow \lambda$ , then  $\lambda \in \text{sp}(T)$  (see [6]). As a result, we obtain that  $\lambda = -1 \in \text{sp}(T)$ , which contradicts our assumption at the beginning of the proof. Therefore,  $\lambda$  must be in  $\text{sp}(A, B, D + I)$ .

**3. The Kantorovich projection application.** In this section, we provide an example demonstrating the efficiency of the Kantorovich projection method in the generalized quadratic spectrum approximation. Let us apply our method to compute the generalized quadratic spectrum of the quadratic pencil of Schrödinger’s operator, generated in  $L^2([0, +\infty[)$  by

$$(\mathcal{P}) \begin{cases} -x'' + t^2x + 2\lambda x - \lambda^2x = 0, & t \in [0, +\infty[, \\ x(0) = 0. \end{cases}$$

The spectrum of this operator contains only the eigenvalues that are given by  $\{1 \pm 2\sqrt{k}, k \in \mathbb{N}^*\}$ . Using the same technique as in [4], we transform the problem  $(\mathcal{P})$  to the quadratic spectral problem, which is formulated in the following way: for all  $x \in L^2(0, a)$  it is necessary to find such values  $\lambda \in \mathbb{C}$  that  $\lambda^2Ax(t) + \lambda Bx(t) + (I + D)x(t) = 0$ , where  $A, B, C$  are integral operators given by

$$Ax(t) = \int_0^a k_1(t, s)x(s)ds, \quad Bx(t) = \int_0^a k_2(t, s)x(s)ds, \quad Dx(t) = \int_0^a k_3(t, s)x(s)ds.$$

Here  $I$  is the identity operator of  $L^2(0, a)$  and the kernels  $k_1, k_2, k_3$  read:

$$\begin{aligned} k_1(t, s) &= \begin{cases} t(s - a)/a, & \text{if } 0 \leq t \leq s \leq a, \\ s(t - a)/a, & \text{if } 0 \leq s \leq t \leq a, \end{cases} \\ k_2(t, s) &= \begin{cases} 2t(a - s)/a, & \text{if } 0 \leq t \leq s \leq a, \\ 2s(a - t)/a, & \text{if } 0 \leq s \leq t \leq a, \end{cases} \\ k_3(t, s) &= \begin{cases} s^2t(a - s)/a, & \text{if } 0 \leq t \leq s \leq a, \\ s^3(a - t)/a, & \text{if } 0 \leq s \leq t \leq a. \end{cases} \end{aligned}$$

We define a uniform discretization of  $[0, a]$  by

$$\Sigma_n = \left\{ n \geq 2, \quad h_n = \frac{a}{n - 1}, \quad t_j = (j - 1)h_n, \quad 1 \leq j \leq n \right\}. \tag{14}$$

Firstly, we apply the Kantorovich projection on the operators  $A, B, D$  to define the approximate operators  $A_n^K, B_n^K, D_n^K$ :

$$\begin{aligned} A_n^K x(t) &= \sum_{j=1}^n Ax(t_j)e_j(t) = \sum_{j=1}^n \left[ \int_0^a k_1(t_j, s)x(s)ds \right] e_j(t) = \sum_{j=1}^n \alpha_j e_j(t), \\ B_n^K x(t) &= \sum_{j=1}^n Bx(t_j)e_j(t) = \sum_{j=1}^n \left[ \int_0^a k_2(t_j, s)x(s)ds \right] e_j(t) = \sum_{j=1}^n \beta_j e_j(t), \\ D_n^K x(t) &= \sum_{j=1}^n Dx(t_j)e_j(t) = \sum_{j=1}^n \left[ \int_0^a k_3(t_j, s)x(s)ds \right] e_j(t) = \sum_{j=1}^n \gamma_j e_j(t), \end{aligned}$$

where  $\alpha_j = \int_0^a k_1(t_j, s)x(s)ds, \quad \beta_j = \int_0^a k_2(t_j, s)x(s)ds, \quad \gamma_j = \int_0^a k_3(t_j, s)x(s)ds$



and  $\{e_j\}_{j=1}^n$  are the hat functions, defined in the following form for all  $2 \leq j \leq n - 1$ :

$$\begin{aligned}
 e_j(t) &= \begin{cases} \frac{t - t_{j-1}}{h}, & \text{if } t_{j-1} \leq t \leq t_j, \\ \frac{t_{j+1} - t}{h}, & \text{if } t_j \leq t \leq t_{j+1}, \\ 0, & \text{otherwise,} \end{cases} \\
 e_1(t) &= \begin{cases} \frac{t_2 - t}{h}, & \text{if } t_1 \leq t \leq t_2, \\ 0, & \text{otherwise,} \end{cases} \\
 e_n(t) &= \begin{cases} \frac{t - t_{n-1}}{h}, & \text{if } t_{n-1} \leq t \leq t_n, \\ 0, & \text{otherwise.} \end{cases}
 \end{aligned}$$

Taking into account the aforesaid, the quadratic spectral problem may be rewritten in the form of the following finite dimension quadratic eigenvalue problem:

$$\lambda^2 \sum_{j=1}^n \alpha_j e_j(t) + \lambda \sum_{j=1}^n \beta_j e_j(t) + \sum_{j=1}^n \gamma_j e_j(t) + x(t) = 0. \tag{15}$$

Secondly, multiplying (15) by  $k_1(t_i, s)$ ,  $k_2(t_i, s)$  and  $k_3(t_i, s)$  respectively and integrating then it over  $[0, a]$ , we arrive to the system:

$$\begin{aligned}
 \lambda^2 \sum_{j=1}^n P_1(i, j) \alpha_j + \lambda \sum_{j=1}^n P_1(i, j) \beta_j + \sum_{j=1}^n P_1(i, j) \gamma_j + \alpha_i &= 0, \\
 \lambda^2 \sum_{j=1}^n P_2(i, j) \alpha_j + \lambda \sum_{j=1}^n P_2(i, j) \beta_j + \sum_{j=1}^n P_2(i, j) \gamma_j + \beta_i &= 0, \\
 \lambda^2 \sum_{j=1}^n P_3(i, j) \alpha_j + \lambda \sum_{j=1}^n P_3(i, j) \beta_j + \sum_{j=1}^n P_3(i, j) \gamma_j + \gamma_i &= 0,
 \end{aligned}$$

where new functions, included in this system, are defined for all  $1 \leq \{i, j\} \leq n$  by the following way:

$$\begin{aligned}
 P_1(i, j) &= \int_0^a k_1(t_i, s) e_j(s) ds, \\
 P_2(i, j) &= \int_0^a k_2(t_i, s) e_j(s) ds, \\
 P_3(i, j) &= \int_0^a k_3(t_i, s) e_j(s) ds.
 \end{aligned}$$

Thirdly, we rewrite the previous system in a block matrix form:

$$\lambda_n^2 \begin{bmatrix} P_1 & 0 & 0 \\ P_2 & 0 & 0 \\ P_3 & 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} + \lambda_n \begin{bmatrix} 0 & P_1 & 0 \\ 0 & P_2 & 0 \\ 0 & P_3 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} + \begin{bmatrix} I_n & 0 & P_1 \\ 0 & I_n & P_2 \\ 0 & 0 & P_3 + I_n \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}. \tag{16}$$

Finally, we compute the quadratic eigenvalues  $\lambda_n$ . To show that the problem of the spectral pollution is solved, we will need the following definition:

$$\lambda_n \text{ is called } \varepsilon\text{-acceptable eigenvalue if } \text{dist}(\lambda_n, \text{sp}(A, B, I + D)) < \varepsilon. \tag{17}$$

Firstly, to calculate  $P_1, P_2$ , and  $P_3$  we set  $a = 1$ . Then, we use the function **polyeig** in Matlab to compute the quadratic eigenvalues of the quadratic pencil presented in (16). In addition, fixing  $\varepsilon = 10^{-2}$ , we find the

number of acceptable eigenvalues denoted as  $VP_{acc}$  and satisfied by (17). The corresponding numerical results are shown in Table 1, where  $VP_{app}$  represents the number of the eigenvalues obtained by our method, and  $P\%$  is the ratio between  $VP_{acc}$  and  $VP_{app}$ .

*Comments.* We notice that if the value of  $n$  is increased, the number of acceptable eigenvalues also grows. This means that these values converge to the exact eigenvalues. In this regard, the application of the generalized quadratic spectrum approximation method allows for avoiding the problem of spectral pollution.

**4. Conclusion.** The theoretical study of the generalized quadratic spectrum approximation, based on the Kantorovich projection method, is carried out under weak hypotheses compared to those used in previous researches. We have built the new approximation method of the generalized quadratic spectrum which allows us to avoid spectral pollution. This method enables to transform the spectral problem defined in infinite dimension into a finite dimensional matrix problem. Numerical tests show the effectiveness of the studied approach for computing of the generalized quadratic eigenvalues.

Table 1. Numerical results

$n$	$VP_{app}$	$VP_{acc}$	$P\%$
100	196	166	8.69%
200	396	366	92.42%
300	596	568	95.30%
400	796	764	95.98%
500	996	968	97.19%

## References

1. M. Cheriet, R. Djemil, A. Khellaf, and D. Khatmi, “Dopamine Family Complexes With  $\beta$  Cyclodextrin: Molecular Docking Studies,” *Polycyclic Aromatic Compounds*, 1–10, (2021). doi [10.1080/10406638.2021.1970588](https://doi.org/10.1080/10406638.2021.1970588).
2. E. Engel and R. M. Dreizler, *Density functional theory* (Springer, 2013).
3. X. Hua, X. Chen, and W. Goddard, “Generalized generalized gradient approximation: An improved density-functional theory for accurate orbital eigenvalues,” *Physical Review B*, **55** (24), 16103 (1997). doi [10.1103/PhysRevB.55.16103](https://doi.org/10.1103/PhysRevB.55.16103).
4. S. Kamouche, H. Guebbai, M. Ghiat, and S. Segni, “Generalized quadratic spectrum approximation in bounded and unbounded cases,” *Probl. anal.Issues Anal.*, **10(28)** (3), 53–70 (2021). doi [10.15393/j3.art.2021.10150](https://doi.org/10.15393/j3.art.2021.10150).
5. F. Tisseur and K. Meerbergen, “The Quadratic Eigenvalue Problem,” *SIAM review*, **43** (2), 235–286 (2001). doi [10.1137/S0036144500381988](https://doi.org/10.1137/S0036144500381988).
6. E. Bairamov, Ö. Çakar, and A. O. Çelebi, “Quadratic Pencil of Schrödinger Operators With Spectral Singularities: Discrete Spectrum And Principal Functions,” *Journal of Mathematical Analysis and Applications*, **216** (2), 303–320 (1997). doi [10.1006/jmaa.1997.5689](https://doi.org/10.1006/jmaa.1997.5689).
7. H. Koyunbakan, “Inverse problem for a quadratic pencil of Sturm–Liouville operator,” *Journal of mathematical analysis and applications*, **378** (2), 549–554 (2011). doi [10.1016/j.jmaa.2011.01.069](https://doi.org/10.1016/j.jmaa.2011.01.069).
8. E. Cancès, V. Ehrlacher, and Y. Maday, “Periodic Schrödinger operators with local defects and spectral pollution,” *SIAM Journal on Numerical Analysis*, **50** (6), 3016–3035 (2012). doi [10.1137/110855545](https://doi.org/10.1137/110855545).
9. P. D. Hislop and I. M. Sigal, *Introduction to spectral theory: With applications to Schrödinger operators*, Vol. 113: (Springer Science and Business Media, 2012).
10. M. Levitin, and E. Shargorodsky, “Spectral pollution and second-order relative spectra for self-adjoint operators,” *IMA journal of numerical analysis*, **24** (3), 393–416 (2004). doi [10.1093/imanum/24.3.393](https://doi.org/10.1093/imanum/24.3.393).
11. M. Lewin and É. Séré, “Spectral pollution and how to avoid it,” *Proceedings of the London mathematical society*, **100** (3), 864–900 (2010). doi [10.1112/plms/pdp046](https://doi.org/10.1112/plms/pdp046).
12. K. E. Atkinson, *The Numerical Solution of Integral Equations of The Second Kind* (Cambridge University Press, 1996).
13. M. T. Nair, *Linear operator equations: approximation and regularization* (World Scientific, 2009).
14. M. Ahues, A. Largillier, and B. Limaye, *Spectral Computations For Bounded Operators* (CRC Press, 2001).
15. H. Guebbai, “Generalized Spectrum Approximation And Numerical Computation of Eigenvalues For Schrödinger’s Operators,” *Lobachevskii Journal of Mathematics*, **34** (1), 45–60 (2013). doi [10.1134/S1995080213010058](https://doi.org/10.1134/S1995080213010058).
16. A. Khellaf, W. Merchela, and H. Guebbai, “New Sufficient Conditions For The Computation of Generalized Eigenvalues,” *Russian Mathematics*, **65**(2), 65–68(2021). doi [10.3103/S1066369X21020067](https://doi.org/10.3103/S1066369X21020067).



17. A. Khellaf and H. Guebbai, “A Note On Generalized Spectrum Approximation,” *Lobachevskii Journal of Mathematics*, **39** (9), 1388–1395 (2018). doi [10.1134/S1995080218090263](https://doi.org/10.1134/S1995080218090263).
18. M. Ahues and A. Mennouni, “A Collocation Method for Cauchy Integral Equations in  $L^2$ ”. *Integral Methods in Science and Engineering*. Birkhäuser Boston, 1–5 (2011). doi [10.1007/978-0-8176-8238-5\\_1](https://doi.org/10.1007/978-0-8176-8238-5_1).
19. B. V. Limaye, *Functional Analysis* (New age international LTD. Delhi, 2006).

Received  
June 1, 2022

Accepted for publication  
June 23, 2022

### Information about the authors

*Somia Kamouche* — Ph.D., Researcher; University 08 May 1945, Department of Mathematics, Laboratory of Applied Mathematics and Modeling, P. 401, 24000, Guelma, Algeria.

*Hamza Guebbai* — Professor, Leading Scientist; University 08 May 1945, Department of Mathematics, Laboratory of Applied Mathematics and Modeling, P. 401, 24000, Guelma, Algeria.

*Mourad Ghait* — M.C.A., Leading Scientist; University 08 May 1945, Department of Mathematics, Laboratory of Applied Mathematics and Modeling, P. 401, 24000, Guelma, Algeria.

*Muhammet Kurulay* — Professor, Researcher; Yildiz Technical University, Faculty of Chemistry and Metallurgy, Department of Mathematics Engineering, Davutpasa Campus Esenler, 34220, Istanbul, Turkey.