Predefined exponential basis set for half-bounded multi domain spectral method

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***Abstract*— A fast and efficient multi-domain spectral method (MDSM) based on wide range non-orthogonal predefined exponential basis set is presented. This method works extremely well for semi-infinite differential problems. It spans wide range of exponential decay rates with multi scaling and does not suffer from zero crossing. These two conditions are necessary for many physical problems. For comparison, the method is used to approximate different exponentially decaying functions and compared with Laguerre basis method. Also for comparison purpose, it is used to analyze arbitrary quantum wells (QW) and optical waveguides. The comparisons exhibit the accuracy and the efficiency of the presented method. In the analytical limit, the relative error in the quantized energy level of the studied QW is in the order of 10^{-12} with very small number of bases.**

I. Introduction

Spectral method is one of the weighted residual methods where the unknown functions are approximated by either an expansion of or interpolation by a selected basis set. In this paper, the functional expansion method is used. Spectral method works very well for homogeneous and smooth computational windows. But, it suffer from the Gibbs phenomenon if the structural function of the studied problem is not analytical. the Gibbs phenomenon is generally a peculiarity of any functional approximation at simple discontinuity. To avoid this problem, the computational window is divided into homogeneous domains where the discontinuities lie at the boundaries. Then, the spectral method is applied alone in each domain to build the matrices and vectors. These are then joined together by applying boundary conditions between domains. This approach is known as multi-domain spectral method (MDSM) [1]–[3].

In many real-valued physical system, the extensions toward infinities decay exponentially as:

$$f \propto e^{\pm \alpha x} \tag{1}$$

where $\pm$ is used to cover both $\mp\infty$ with positive α. In spectral and multi domain spectral methods, this is one of the main problems. A review paper by Shen and Wang discusses this in further details [4]. To overcome this problem, many techniques where used. They can be classified in the following three main categories:

- **Using exponentially decaying basis sets** such as physical Hermite and Laguerre functions and rational Chebyshev and Legendre polynomials. Some other basis sets are used as well. This predefines a narrow ranged decay rate and hence limit the generality. Some researchers adopted them in studying phenomena known that they can be analyzed using such functions. For example, Laguerre function is the base for radial extension of electron wave functions in hydrogenic atoms. So, it is expected to work for electronic distributions of some hydrogenic like atoms. Beside the narrow ranged predefined decay rate, this approach inherently forces many zero crossing since most of the used basis sets are forms of Jacobi polynomials which has N zeros for the N^{th} order polynomial. In many physical problems, this is expected and allowed. However, in physical system where the decay is behaving as described by Eq. (1), this should not be the case.
- **Truncating the numerical window;** this is used as well by many researchers. The unbounded window is truncated and additional boundary conditions are used to force an asymptotic exponential behavior, i.e. the function and its first derivatives vanish at the truncating points. This reduces the analytical accuracy of spectral methods by adding the truncation error. Also, this does not eliminate zero crossing and hence it doesn't fit the system with Eq. (1) exponential decay.
- **Single scaling of the coordinates;** This is similar to the first category; but with coordinate scaling where

  $$x \Rightarrow cx \tag{2}$$

  Therefore the predefined decay rate is also scaled. The scaling factor c is chosen intuitively to fit the studied problem. However, this results in losing the generality and missing many eigen solutions in eigenvalue problems where the decaying rates for the different eigenvalue solutions are generally different.

The presented method overcome zero-crossing and single scaling problems by approximating the decaying domain functions by exponential basis set with exponentially spanned decaying rates as follows:

$$f = \sum_{n=0}^{N} a_n u_n = \sum_{n=0}^{N} a_n e^{-\alpha_n x} \tag{3}$$

where

$$\alpha_n = b^{d_s + \frac{n}{N}(d_e - d_s)} \tag{4}$$

b is the used exponential base and d_s and d_e are the smallest and largest used powers respectively. They should be predefined intuitively based on the studied problem. Yet, they allow many possible decay rates with very small number of bases. For example, by setting $N = 10$, $b = 10$, $d_s = -5$, and $d_e = 5$, 11 bases can be used to approximate any exponential function with decay rates between 0.00001 and 100000.

II. Some applications

A. Approximating of distant exponentially decaying functions

In this subsection, the presented method is applied to approximate five exponentially decaying function and compared with Laguerre basis method. The used decaying rates are 0.00535, 0.0632, 0.752, 81.2, and 926. Fig.(1) shows the obtained approximation using unscaled modified Laguerre bases.

It is clear that with 25 used bases, only two function out of the five are approximated adequately. Yet, the method is converging but very slowly for the remaining functions. For $e^{-0.752x}$, very few bases are needed to approximate the function to an adequate accuracy. If scaling

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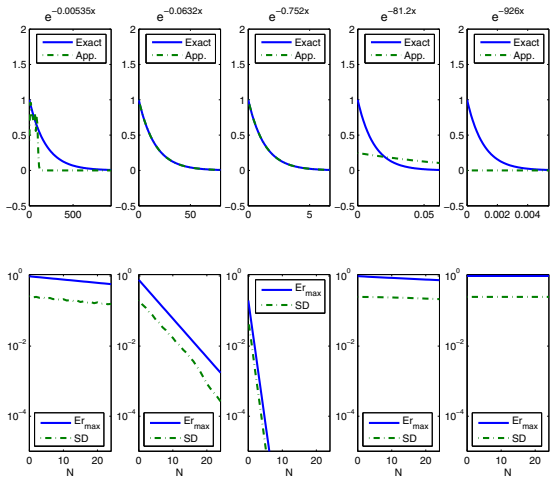

Fig. 1. Approximations (top) and maximum approximation errors and their standard deviations (bottom) of the five exponentially decaying functions using unscaled modified Laguerre bases. The used decaying rates are 0.00535, 0.0632, 0.752, 81.2, and 926.

was used, only two or mostly three functions would be approximated adequately depending on the scaling. For many eigenvalue problems, this is a very serious limitation where different eigenvalues have different decaying rates. So, only part of the eigenvalues can be obtained accurately. The same five functions are approximated using the presented method with $b = 10$, $d_s = -4$, and $d_e = 4$. The resulted approximations and their associated errors are shown in Fig.(2). All the five functions were approximated adequately using the same exponential bases and the convergence is geometric as can been seen.

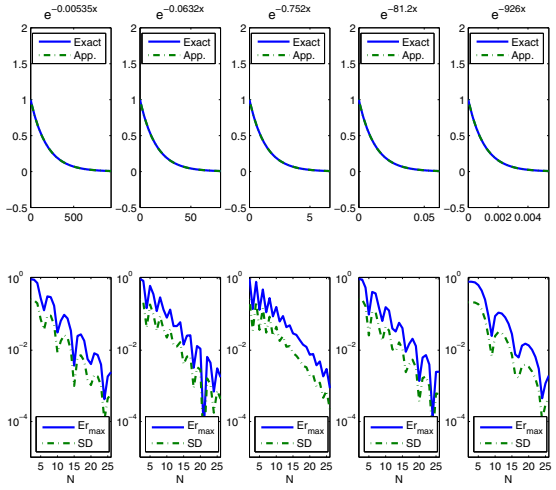

Fig. 2. Approximations (top) and maximum approximation errors and their standard deviations (bottom) of the five exponentially decaying functions using the presented method with the same bases. The used decaying rates are 0.00535, 0.0632, 0.752, 81.2, and 926.

In many applications, it is crucial to find many eigenvalues. By using the presented method, this can be done simultaneously. While by using the modified Laguerre bases, the algoritm should be repeated with different scaling and error detection to obtain the required number of eigenvalues. However for the set of eigenvalues that is obtained accurately using the modified Laguerre bases, the convergence is faster than the convergence of the presented method.

	Interval (nm)	m^*/m_0	$V(x)$ (meV)
D1	$(-\infty$,-10)	0.0919	225
D2	(-10,10)	0.067	0
D3	(10, ∞)	0.0919	225

TABLE I
THE STRUCTURAL PARAMETERS OF THE STUDIED QW

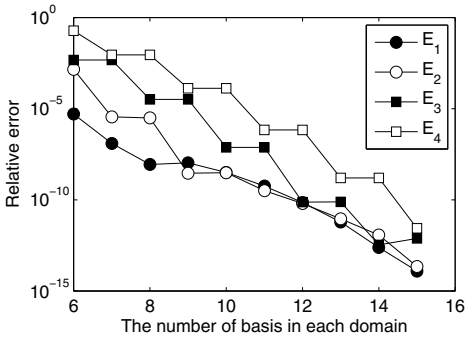

Fig. 3. The relative error of multi-domain spectral method and the exact solutions of the studied QW

B. Single QW without biasing field

The structure is simply a thin layer of GaAs sandwiched in $Al_{0.3}Ga_{0.7}As$. The width of the QW layer is 20 nm. The numerical window is divided into three domains. The structural parameters in each domain are shown in the Table-I This structure can be analyzed analytically, where the energy states are only the solutions of the following characteristic equation

$$\left(1+\gamma^2\right) e^{i\alpha L} - \left(1-\gamma^2\right) e^{-i\alpha L} = 0 \qquad (5)$$

where

$$\alpha = \sqrt{\mathcal{E}\frac{2m_w}{\hbar^2}} \qquad \beta = \sqrt{\left(V_b - \mathcal{E}\right)\frac{2m_b}{\hbar^2}} \qquad \gamma = i\frac{m_b}{m_w}\frac{\alpha}{\beta}$$

where m_b and m_w are the effective masses in the barrier and the well and L is the width of the well. The relative errors of the results obtained using the presented method and the exact solution are shown in Figure-3 against the number of the used bases in each domain. It is clear that acceptable results can be achieved with only 9 basis in each domain. In QWs, an accuracy tolerance of 0.001 meV is usually very sufficient. The speed of the method mainly depends on the largest used matrix in the analysis. We reach the machine accuracy with 15 basis in each domain where the largest matrix is only 45×45. This is handled very easily and rapidly. The whole analysis lasted about half a second.

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