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# A Novel Boundary Integral Formulation for Quantum Energy Eigenvalue Analysis and Its Application in a Model-Based Systems Engineering Framework for Quantum Systems Development

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# A NOVEL BOUNDARY INTEGRAL FORMULATION FOR QUANTUM ENERGY EIGENVALUE ANALYSIS AND ITS APPLICATION IN A MODEL-BASED SYSTEMS ENGINEERING FRAMEWORK FOR QUANTUM SYSTEMS DEVELOPMENT

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*To Amin,*

*my love, my life, and my light.*

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## TABLE OF CONTENTS

## LIST OF TABLES

## LIST OF FIGURES

Appendix Figure Page

# ABSTRACT

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In recent decades, the development and utilization of high-end technologies have increased noticeably. This progress has become possible by finding a complete understanding of physical rules in microscopic scales, such as quantum mechanics. Quantum technologies can be applied to various fields, including optics, superconduction, computing and simulation, precision measurement, and biomedical imaging to enhance the performance of relevant devices and systems. However, the complexity which emerges in the procedure of developing such devices can prevent one from taking advantage of potential quantum technologies to effectively develop these devices. In the current research, an attempt has been made to find a solution for this problem.

Based on the various benefits of using systems engineering techniques in managing the complexities of developing such systems, a model-based systems engineering methodology has been employed towards the development of quantum systems. In this research, quantum dot solar cells are chosen as a typical quantum system, and four main stages of system analysis, design, manufacturing, and verification, validation, and testing are considered and studied during the product lifecycle. By integrating systems engineering tools with domain engineering tools, it

is verified that the use of appropriate models can facilitate the overall procedure of system development.

Moreover, by focusing on the system design and analysis phases, a novel boundary integral formulation was developed in this research to accelerate the procedure of system development. This approach decreases the computation burden required to solve the governing equation of quantum devices and accomplishes the design procedure more effectively and accurately. Various case studies have demonstrated that the proposed technique can enhance both the accuracy and computational-efficiency in the design of new quantum devices.

# CHAPTER I

# INTRODUCTION, MOTIVATION, AND OBJECTIVES

## 1.1 Introduction

Living in a modern society is associated with efficiency and speed, two features that are possible using high-end technologies. Progress in this area is only possible through a complete understanding of microscopic systems and the relevant physical rules for the behavior of light and matter, including quantum mechanics. The application of quantum mechanics can be witnessed in various fields and systems, including chemistry, optics, semiconductors, transistors and diodes, medical imaging, quantum computing, etc. In this regard, Max Planck [1] and Albert Einstein [2] had an important role in the emergence of this new field by establishing the fundamental quantum theories, including an introduction to the new concept of photons. It was stated that the energy of light consists of quantized bundles, known as photons. This great discovery has enabled us to provide descriptions for some important phenomena which were difficult to understand, like the emission of radiation from an object in thermal equilibrium within the atomic domain [3]. Later in 1924, based on Einstein's theory regarding the quanta of light, Louis de Broglie stated that all particles are quanta and show wave-particle duality [4]. According to the fact that particles have wave-like behavior, a wave function can be defined for them using the linear partial differential equation introduced by Schrödinger in 1926 [5]. Generally, the Schrödinger equation is a function of time

and the particle position. This function illustrates the state of a quantum mechanical system and includes its known information. In order to find system states, the time-dependent Schrödinger equation must be solved. The first step in this process is to derive the stationary states of the system and employ them to calculate other system states [6]. These stationary states can be obtained by using the simplified form of the Schrödinger equation in which the potential function is independent of time (known as the time-independent Schrödinger equation). In this regard, dynamic models including a moving particle in a region, which are known as quantum billiards, are used to study the behavior of such systems. The main reason for considering these billiards as models for the simulation of quantum systems is that the motion of electrons and also the relevant energy conservation in such systems is similar to that of the particles in quantum billiards.

One of the main characteristics of the quantum systems that can be identified using the previously mentioned system states is the system energy. This can be achieved by solving the energy eigenvalue problem of the time-independent Schrödinger equation. It is crucial to solve the eigenvalue problem of the Schrödinger equation precisely, because this solution provides the required information regarding quantum systems. There are several approaches towards solving this equation, such as analytical and numerical methods. The analytical techniques can only help to solve a small number of simple quantum systems, mostly single-electron ones [7]. It is also worthwhile to note that analytical methods become inefficient when the geometry or the boundary conditions considered for the system are complicated [3]. This is the main reason why numerical solutions are implemented to solve the aforementioned equation. The boundary element method (BEM) is one of the numerical procedures which is successfully utilized to solve a wide range of engineering and science problems governed by the time-independent

Schrödinger equation [8]. Technically, boundary element analysis (BEA) is used to reduce the partial differential equation associated with a given problem to a boundary integral equation by employing Green's theorem and the relevant fundamental solution [9]. The most significant advantage of this technique over other similar approaches, like the finite element method (FEM), is that only the system boundary has to be discretized instead of the whole physical domain. So, it is possible to handle domains with more complicated geometries using this methodology. Although using the BEM to solve the eigenvalue problem of the time-independent Schrödinger equation has several advantages compared to other similar techniques, there are some challenges and concerns that should be considered in order to achieve appropriate results. The issues that may occur in this regard are briefly discussed in Section 1.2, while more information will be presented in Chapter II. In summary, it is very important to calculate the energy eigenvalues of the time-independent Schrödinger equation accurately and effectively, especially for quantum systems. These eigenvalues can be employed in the design and analysis of various physical systems. Therefore, using a more precise methodology to obtain the mentioned eigenvalues leads to the successful design and analysis of such systems.

Nowadays, systems engineering can be applied to develop the majority of physical systems that are seen around the world. It is an approach that takes many factors into account, from a high-level understanding of user's requirements to the detailed design of individual components as parts of a system. One of the main purposes in systems engineering is to study complex systems in a more convenient way. A complex system can be defined as a system such that its behavior and characteristics are difficult to be anticipated [10]. Therefore, by considering this definition, quantum systems can be identified as complex systems and systems engineering can be implemented to handle the complexity of these systems. In this

regard, model-based systems engineering (MBSE) is an emerging approach that can be used to integrate systems using models based on systems engineering concepts in order to develop systems more conveniently [11]. The following definition is provided by the International Council on Systems Engineering (INCOSE) for MBSE: "The formalized application of modeling to support system requirements, design, analysis, verification and validation activities beginning in the conceptual design phase and continuing throughout development and later life cycle phases" [12]. That is to say, in order to develop complex, interdisciplinary systems meeting user requirements, an organized, convergent, iterative, and repeatable methodology can be obtained by using MBSE [13]. Technically, MBSE can play an important role in describing complex systems, their relevant lifecycle, and integration when combined with SysML or any other modeling languages. MBSE can facilitate the communication procedure by connecting all of the information produced during the system development [14]. In addition to the INCOSE definition, MBSE can also contribute to quality improvement, productivity increases, risk reduction, and better communication [15]. So, analysis and design of complex systems like quantum systems can be improved noticeably using MBSE.

## 1.2 Problem Statement

The significant role of quantum mechanics in modern technology was discussed in the previous section. Although quantum systems form a considerable portion of the recently-developed physical systems, and it is clear that these systems are categorized as complex systems, to the best of the author's knowledge, there has not been any research carried out in order to analyze, design, and develop quantum systems using MBSE. In other words, MBSE has not been employed to cope with the complexity of quantum systems. Therefore, it is vital to understand and

demonstrate the benefits of MBSE in analysis, design, manufacturing, integration, and verification, validation, and testing (VV&T) quantum systems in general. So, by representing the overall concept of MBSE in developing quantum systems, any complex quantum system can be handled using this tool more conveniently.

Various researches have been conducted in order to apply MBSE to the different stages of each product lifecycle from requirements analysis to system retirement. However, this technique has not yet been implemented to quantum systems. So, it is crucial to perform a similar process for the quantum systems to use MBSE in the analysis, design, manufacturing, and testing stages during system development. The main focus of this research is on the analysis and design areas of the MBSE for quantum systems. In particular, using appropriate models in this procedure can help to obtain a better understanding of these complex systems, and perform the system design and evaluation more accurately. Consequently, this research can help to develop high-level tools for the design of physical systems using the potential quantum technologies. The design of a quantum system is associated with several important steps. One of these main steps is to identify the governing equation of the quantum system. Since the time-independent Schrödinger equation, that was introduced in the previous chapter, is the governing equation of most quantum systems, the key element in the analysis and design of these systems is to compute the energy eigenvalues of this equation. It is worthwhile to mention that by solving this eigenvalue problem, the important features of the quantum system like its energy levels can be obtained which are required for the design stage. As mentioned in the previous section, the BEM methodology can be employed to solve the eigenvalue problem of the above-mentioned equation.

Principally, by implementing the boundary integral equations (BIE), a system of equations like $\mathbf{Ax} = \mathbf{b}$ will be obtained, where $\mathbf{A}$ is the matrix of

coefficients, $\mathbf{x}$ is the vector of unknown parameters, and $\mathbf{b}$ is the vector of known parameters based on the assumed boundary conditions. In case of the energy eigenvalue problem, the above system of equations becomes $\mathbf{Ax} = \mathbf{0}$. This equation has a trivial solution ($\mathbf{x} = 0$), but its non-trivial solution can be obtained by solving $\det(\mathbf{A}) = 0$. In this equation, $\mathbf{A}$ is a function of wave number value, $k$. One of the main methods implemented by most researchers to solve this equation is scanning the wave number amounts to find the local minima of the coefficients' matrix determinant in the BEM system of equations. These local minima represent the eigenvalues of the time-independent Schrödinger equation. However, the major drawback of this methodology is that the implemented standard searching technique is extremely time-consuming because of its iterative nature. Therefore, a non-iterative technique should be developed to alleviate this problem, and improve the efficiency of the procedure.

Recently, researchers have tried to provide fast algorithms to make use of the BEM method in solving partial differential equations more efficiently. Series expansion methods are the main methodologies which can accelerate the process of finding the eigenvalues of the time-independent Schrödinger equation. In spite of more efficiency with these methods, the results may not have an acceptable accuracy compared to analytical solutions. It is essential to develop an improved technique which has an appropriate speed compared to iterative techniques and a desirable accuracy in comparison with the current series expansion methods.

## 1.3 Research Objectives and Hypothesis

The main purpose of the current research is to develop an MBSE methodology which can be used to support the analysis, design, manufacture, and verification and validation of quantum systems. Then this technique will be applied

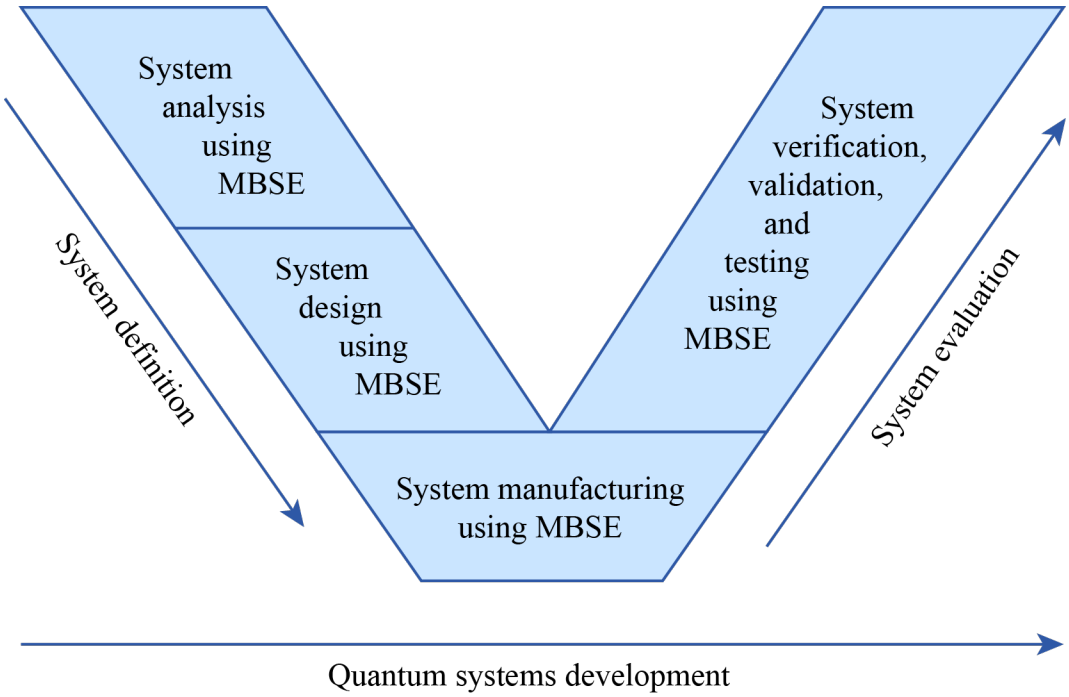


Figure 1. Systems engineering Vee for quantum systems development.

to the new generation of quantum dot solar cells as an example of quantum systems. This research is performed with the original idea of finding a complete understanding of the quantum systems performance by providing a working simulation model. This goal will be achieved through using MBSE in every stage of the quantum systems development from requirements definition to systems integration, verification, validation and testing, as depicted in Fig. 1. The results obtained in this research will help other researchers to gain a broader overview and a better understanding of the relationship between the performance and the design of complex systems like quantum ones.

The other purpose of this research is to propose a more effective method to calculate the energy eigenvalues required for the analysis and design of most quantum systems governed by the time-independent Schrödinger equation. As described in the previous section, most current approaches used to solve the energy

eigenvalue problem of the time-independent Schrödinger equation are based on iterative methods, and are very time-consuming. So, it is required to provide a more efficient technique in this regard. This is the main reason researchers are trying to propose acceleration methodologies to deal with the drawbacks of previous approaches. One of the proposed methods in this regard is utilizing the series expansion method. According to Section 1.2, the energy eigenvalues of the time-independent Schrödinger equation can be obtained by finding the roots of $\det(\mathbf{A}) = 0$. These roots demonstrate the so-called energy eigenvalues of the time-independent Schrödinger equation. Since $\mathbf{A}$ is a function of wave number, $k$, and the conventional iterative methods require scanning $k$, numerous recalculations of $\det(\mathbf{A})$ are required in order to find the local minima of this determinant. However, in series expansion methods, the attempt is to make the BEM integrand independent of $k$ and save computational costs by avoiding iterative calculations. Although the series expansion methods have increased the efficiency of solving these problems noticeably, there are some concerns regarding the accuracy of the results. For instance, fictitious eigenvalues can be produced because of using the real-valued fundamental solution of the Laplace equation instead of the complex-valued fundamental solution of the time-independent Schrödinger or Helmholtz equation[1]. More details regarding the researches performed in this field will be discussed in the next chapter.

## 1.4 Contributions

This research will contribute to the investigation of quantum systems as follows:

[1] In the absence of further potentials in the dynamical systems like quantum billiards, the relevant time-independent Schrödinger equation is related to the acoustical problems that only involve the Helmholtz equation. The difference between the fundamental solution of the Helmholtz and the time-independent Schrödinger equation is in a coefficient.

- *Dealing with the complexity of quantum systems more conveniently and effectively:* Quantum systems can be categorized as complex systems, because it is not convenient to model such systems and anticipate their behavior. However, in this research it is proposed to develop a general approach to cope with the complexity of these systems. By implementing the suggested methodology, researchers in this area can develop complex quantum systems more easily.

- *Proposing a complete MBSE approach for quantum dot solar cells:* Solar power plays a very important role in the field of sustainability, especially in developing countries. Solar energy is more reliable, useful, cost-effective, and healthier for both humans and the environment [16]. Nevertheless, one of the disadvantages of the solar cells is their low efficiency. However, this parameter can be increased by considering quantum dots in the design of these devices (Fig. A.14). Quantum dot solar cells are environmentally-friendly and have acceptable performance [17]. Since quantum dot solar cells can be considered as complex quantum systems, and it is difficult to design, develop, and evaluate these complex systems, model-based systems engineering can be employed as a strong tool for this purpose. In this regard, an MBSE methodology is described in Chapter III to show the contribution of this research to study the quantum dot solar cells as an example of a complex quantum system.

- *Proposing an accurate and efficient numerical technique to find the energy eigenvalues of quantum systems:* The iterative procedures that are employed to calculate the energy eigenvalues of various quantum systems are very time-consuming and inefficient. The numerical technique proposed in this research can help in finding these parameters, and can be used for the design

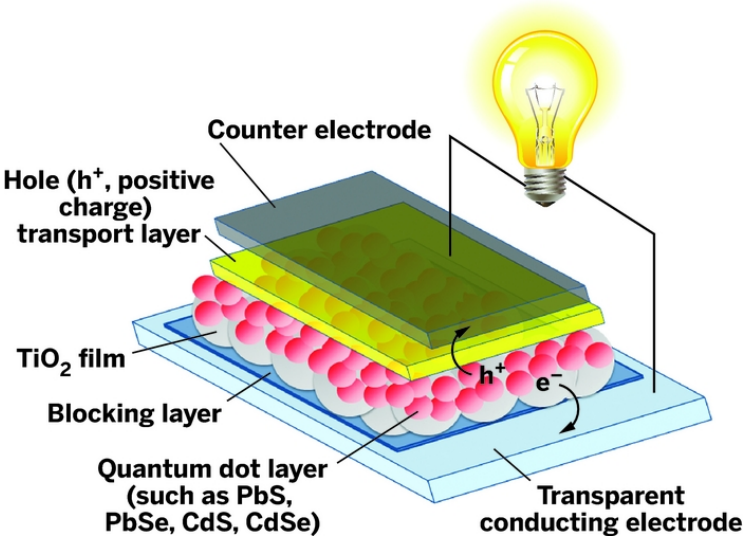


Figure 2. The structure of a typical quantum dot solar cell [18].

of most quantum systems. It is also worthwhile to mention that the accuracy of this process is higher in comparison to similar methods suggested in the literature.

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# CHAPTER II
# LITERATURE REVIEW

In this chapter, the previously performed researches in three main fields are discussed. In the first section, the important role of model-based systems engineering is shown in various engineering fields, particularly in the investigation of complex physical systems. It is observed that there is a special need for such a beneficial approach in the development of quantum systems. Despite the fact that MBSE has not been exploited to study quantum systems, the significant impact of using models on the investigation of these complex systems is clear. Consequently, quantum billiards are employed as dynamic models to facilitate the study of quantum systems that are discussed in the second section. The third section considers the necessity for obtaining energy eigenvalues for the design of most quantum systems, and summarizes a noticeable number of researches that are devoted to implementing numerical methods like the BEM for solving the energy eigenvalue problem of the Helmholtz and time-independent Schrödinger equations. As mentioned in the previous chapter, these equations play an important role in quantum mechanics since they are the governing equations of a wide range of quantum systems.

## 2.1 Model-Based Systems Engineering

Model-based systems engineering serves to highlight the role of modeling in various activities in the system lifecycle, from the conceptual design stage to the

product end life, including development of system requirements, analysis, design, and verification and validation [1]. When using document-based methodologies, some inconsistency may appear in the documentation. This inconsistency can be alleviated by employing MBSE and relevant models for the systems [2]. Another advantage of MBSE is to improve communications between the participants who contribute to the system development, such as stakeholders and engineers. Moreover, better system quality and productivity in addition to lower risks and expenses are other merits of using this method for industrial purposes [3]. According to the INCOSE systems engineering handbook, the MBSE methodology is associated with several other advantages. For one, all the information obtained will be gathered in a standardized format, so obtaining access and reusing the knowledge achieved during systems development will be improved. For another, a representative model of a system will be prepared which can be used in the next stages in the system lifecycle, like maintenance, retirement, and legacy system development [4]. In this regard, the authors in [5] took advantage of an MBSE technique for addressing all the required system information in order to optimize the cost, schedule, and overall performance of the system. According to these mentioned points, it is noticeably advantageous for designers and manufacturers to apply MBSE for developing complex systems because the complexities in the system architecture can be communicated more effectively by using models [3]. Various researches show the applicability of the MBSE in the investigation on complex systems. For instance, Masior et al. studied the development of MBSE techniques and technologies in the context of complexity and relevant methodologies including virtual models and informational and process consistency [6]. These authors also proposed an MBSE method which provides a basis for consistent and integrated system models to deal with complex systems of small or large companies. In

another research, Inkermann et al. introduced a concept to find the requirements for developing automotive systems using MBSE [7]. For this purpose, five partial models including use-cases, functions, function realization, system structure, and product structure were used. Then a case study on an electrical vehicle was performed to verify the capability of the proposed method in the development of such products. Akhundi and Lopez represented the current need for an MBSE technique to address complexities in the manufacturing phase of the system design process [3]. Scherer et al. also tried to reduce system complexity by proposing a modular-structured approach in the MBSE area [8]. Wang emphasized the importance of using models in the whole product lifecycle in order to develop complex systems more economically and efficiently [9]. In addition, a noticeable number of complex systems that are going to be developed may be exposed to cyber attacks in the future. MBSE can be implemented to alleviate the probable risks existing in this regard. In fact, MBSE is superior to other approaches, since it can reduce security risks of the system at the initial steps of its development procedure. Consequently, cyber-security risks will be addressed during the system design stage [10]. Altogether, according to the researches performed in this area, the favorable impact of the MBSE method in the development of complex systems is clear. However, there is no research which uses MBSE approach to cope with complex quantum systems in general. So, it is crucial to propose an appropriate methodology for quantum systems development via MBSE.

## 2.2 Quantum Billiards

As mentioned before, the importance of implementing models for the investigation of complex systems is clear. This is the main reason why dynamic models known as quantum billiards are introduced to study quantum systems.

Billiards are models considered for a wide range of physical systems, including moving particles in a vessel which hit the walls or collide with each other. Due to various wall shapes of these containers, the billiards will demonstrate different dynamic properties. They can become entirely regular and integrable or fully chaotic [11, 12]. The chaotic behavior of billiards was studied by Sinai for the first time in 1970 [11]. This behavior of particles are similar to that of the electrons in quantum devices. As a result, quantum billiards have often been employed to model particles moving inside nanodevices, such as quantum dots and pn-junctions. In several researches carried out using quantum billiards, analytical approaches are employed in order to calculate the relevant eigenvalues and eigenfunctions. For example, Heller used an analytical approach to obtain the bound-state eigenfunctions of chaotic systems [13]. The main disadvantage of these methods is that it is difficult, or sometimes impossible, to apply them to complex problems including complicated geometries or boundary conditions. Thus, the necessity of using numerical methods for solving these problems is undeniable. One of the popular numerical techniques is iterative boundary element methods (BEM), although it is a time-consuming approach. For instance, Ree and Reichl studied the quantum dynamics of circular billiards with a straight cut using an iterative BEM [14]. Similarly, this technique was implemented by Kosztin and Schulten to compute the stationary states of quantum billiards [15]. In this regard, the relevant energy eigenvalues were found by calculating the roots of the Fredholm determinants. Furthermore, in this investigation, the chaotic features of the circular and stadium billiards were studied, but in order to study chaos, the authors had to consider more than a thousand eigenvalues to construct the histogram of energy level distribution, which was a computationally-inefficient procedure. The inefficiency of the iterative BEM approach is discussed with more details in the next section. Another aspect of

solving the eigenvalue problem of quantum billiards is the boundary geometry. Several researchers studied only regions with smooth boundaries [13, 16], like circular billiards, while sharp corners in the billiards may lead to singularity and ineffectiveness of the approach. Thus, it is required to establish a more efficient BEM technique and also take advantage of dynamic billiards as models to solve the energy eigenvalue problems, and then use these eigenvalues to design and develop quantum systems with arbitrary geometries.

## 2.3 Energy Eigenvalues of the Time-Independent Schrödinger Equation

As mentioned in Chapter I, the Schrödinger equation is a partial differential equation which governs the behavior of a quantum mechanical system. Most investigations on quantum systems try to obtain the energy eigenvalues of this equation using iterative procedures. These techniques scan the wave number to find the local minima of the determinant obtained from boundary integral equations, as discussed in the previous chapter. However, these methods are time-consuming and inefficient. Therefore, considerable effort has been made to accelerate the process of solving the eigenvalue problem of the time-independent Schrödinger equation. The main approach in this regard is to make the BEM integrand independent of the wave number in order to avoid a huge amount of recalculations required for the iterative methodologies. In addition, there are several other fast techniques proposed in the literature, such as the fast multipole method, the adaptive cross approximation technique, etc. The advantages and also the limitations of these approaches are discussed in this section.

### 2.3.1 Wave Number Scanning Method

One of the conventional methods to find the energy eigenvalues of the Helmholtz equation is the iterative method. This approach scans the wave number range in order to find the relevant eigenvalues, and is well-studied by several scholars. For instance, Tai and Shaw employed this technique to achieve the eigenvalues and eigenmodes of the homogeneous Helmholtz equation for closed regions in two and three dimensions [17]. In this effort, the problem was solved under the first order homogeneous boundary conditions for domains with arbitrary geometries. It is shown that the results obtained in the case of an isosceles right triangle are in agreement with analytical results. In another study, De Mey used the same procedure to determine the eigenvalues of the two-dimensional Helmholtz equation for circular and rectangular domains [18]. Although the results obtained are accurate compared to analytical solutions, the author admitted that the main disadvantage of this method is its iterative nature, as a conclusive point. In another investigation carried out by this author, a real particular solution of the Helmholtz function was used instead of the conventional Green's function to find the first eigenvalue of a circular region, taking the drawback mentioned into account [19]. Adeyeye et al. employed three numerical collocation treatments to calculate the eigenvalues of the Helmholtz equation under Dirichlet boundary conditions [20]. The problem was successfully solved for various geometries, including circular, elliptic, and square domains. Nevertheless, despite the ability of the scanning approach to find the energy eigenvalues of the Helmholtz equation, its major demerit is computational ineffectiveness. The next two sections discuss procedures to cope with this issue.

### 2.3.2 Series Expansion Method

As mentioned in previous sections, several researches were performed in order to make the BEM integrand independent of the wave number by employing static fundamental solutions. In this regard, the multiple reciprocity method (MRM) was proposed by Nowak and Brebbia [21] to convert the domain integrals to boundary integrals. After that, Kamiya and Andoh found a more effective approach to find the eigenvalues of the Helmholtz equation by using the MRM method, considering the real-valued fundamental solution of the Laplace equation [22]. The problem was solved for two-dimensional regions under various homogenous boundary conditions, and the performance of this method was compared with techniques mentioned in Section 2.3.1. A similar approach was employed by Kamiya et al. to find the eigenvalues of the 2-D Helmholtz equation for three-dimensional regions [23]. In this research, a Newton iteration method was developed using the lower-upper (LU) decomposition process, instead of applying the standard-type eigenvalue problem [24]. The results show that the overall computational cost decreased compared to the wave number scanning methods, as expected. Later, Sladek et al. represented the applicability of the MRM method in finding the eigenvalues of the 3-D Helmholtz equation [25]. These authors verified the higher efficiency of this procedure when seeking a large number of eigenvalues in the boundary value problems.

The series expansion method was employed by Kamiya et al. to find the eigenvalues of the scalar-valued Helmholtz equation using the complex-valued fundamental solution [26]. The authors derived a polynomial in terms of $k^2$ for just the real part of the coefficient matrix. Since they were not able to make the whole integrand independent of the wave number, they had to apply an iterative procedure, like Newton iteration method, to calculate the relevant eigenvalues.

Therefore, despite using the series expansion procedure, an iterative method was implemented to find the eigenvalues. In another investigation, a new MRM approach, which was equivalent to using the complex-valued fundamental solution, was developed by Yeih et al. for one-, two-, and three-dimensional forms of the Helmholtz equation [27]. It was also explained how to deal with the spurious eigenvalues obtained by this process. Later, Kirkup and Amini proposed a polynomial approximation for the BEM coefficient integrand with respect to the wave number in order to convert the non-linear eigenvalue problem into a standard one [28]. This method was applied to a two-dimensional square and a three-dimensional sphere under axisymmetric boundary conditions. The series expansion method was also implemented by Wang et al. to solve the multi-frequency acoustical problems governed by the Helmholtz equation [29]. The authors formed BEM matrices independent of $k$, which led to an overdetermined system of equations, and numerical examples showed the effectiveness of this approach. It was also stated that this method is appropriate for small and medium numbers of the wave numbers because of higher data storage space required for larger systems. In a more recent study, Xie and Liu developed a model order reduction method on the basis of an offline-online structure [30]. In the offline phase, the boundary integral kernels were made independent of the wave number by applying Taylor's theorem. Then by summing up the offline reduced matrices in the online phase, a reduced-order model can be produced for the three-dimensional fundamental solution in order to solve the multi-frequency acoustic wave problems. Altogether, researches in this category can be summarized into two groups. The first group uses the real-valued Laplace fundamental solution instead of the complex-valued Helmholtz fundamental solution, which leads to obtaining fictitious eigenvalues and reduces the accuracy of the results. The second group uses the

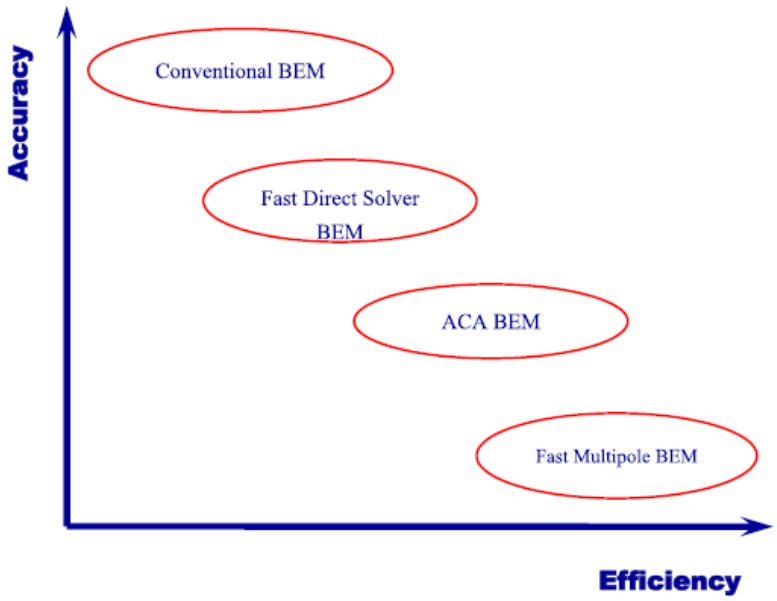


Figure 3. A comparison among the effectiveness of the three acceleration methods [32].

complex-valued fundamental solution, but because they were not able to make the BEM integrand independent of the wave number, they had to use the inefficient iterative method to achieve the eigenvalues.

### 2.3.3 Other BEM Acceleration Methods

In the past three decades, significant effort has been devoted to find a fast method for solving the BEM problems, especially in the field of acoustics [31]. These acceleration techniques include the fast multipole method (FMM) [32], adaptive cross approximation (ACA) [33], and fast direct solvers [34]. The FMM method tries to accelerate the matrix-vector calculation required for the BEM system of equations in iterative methods. This approach was implemented to solve the Helmholtz equation in different researches [35, 36, 37]. Besides that, Bebendorf et al. suggested using ACA method to solve the BEM problems with respect to matrix algebra. It is a kernel-independent method and is more convenient to be implemented in comparison with the FMM approach [38]. The main idea regarding

the algorithms associated with the fast direct solvers is to consider a low-rank approximation for specific submatrices of the main BEM coefficient matrix. A comparison among the precision and effectiveness of these three methods is illustrated in Fig. 3.

Recently, a new technique called contour integral method (CIM) is developed to solve the nonlinear eigenvalue problems of the Helmholtz equation via BEM [39]. This process converts the nonlinear eigenvalue problems into ordinary ones. In order to accelerate the solution procedure, Zheng et al. implemented a combination of the CIM and FFM methods to reduce the overall solution cost of the boundary element system of equations. However, it is worthwhile to note that using this combination is more complicated in comparison with the series expansion methodology.

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# CHAPTER III
# ARTICLE 1 – A MODEL-BASED SYSTEMS ENGINEERING FRAMEWORK FOR QUANTUM DOT SOLAR CELLS DEVELOPMENT

## 3.1 Supplementary material

This paper[1] introduces a model-based systems engineering (MBSE) framework for dealing with the complexity of developing quantum systems. More details relevant to the material described in this article are provided in Appendix A.

## 3.2 Abstract

Nowadays, a wide range of newly designed devices are based on high-end quantum technologies. To successfully design a quantum system, it is necessary to appropriately address the increasing complexity which exists in the development procedure of the system. A suitable approach to deal with this problem is to employ systems engineering models and integrate them with domain engineering tools. The model-based systems engineering (MBSE) methodology is commonly used to analyze, design, manufacture, and test various complex systems. In this paper, the MBSE approach is chosen towards the development of quantum dot solar cells as a typical quantum system and to deal with the complexity existing in this procedure.

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The analysis, manufacturing, and verification, validation, and testing (VV&T) for this system are described using SysML in Cameo Systems Modeler software to represent the role of models in this regard. Then a detailed design is performed in MATLAB and integrated with SysML to identify how changing various parameters during the system development process affects the overall system performance. This technique facilitates the communication between different engineering teams and helps to manage the complexity in the entire system lifecycle.

## 3.3 Introduction

Living in a modern society is associated with using complex technologies, based on the procedure of developing complicated systems as well as integrating these systems together, which makes this area even more complex. A similar trend can be seen in development of quantum technologies and the relevant devices. Discovering the concept of photons and the wave-particle duality behavior was the first revolution in the field of quantum mechanics, which led to finding the relevant underlying technologies. On the other hand, the second quantum revolution is happening in the $21^{st}$ century, the result of which will be the development of a wide range of devices based on quantum technologies [1]. It is worthwhile to mention that the main purpose in the development of quantum technologies is not merely providing new products. Quantum technologies have the potential to play the most important role in establishing new physics-based tools that can be used in design, engineering, and even architecture [2]. Most people think of the quantum computing field as the main application of quantum technologies; however, there are a vast number of other applications, including semiconductors, optics, navigation, cryptography, precise timing, gravity sensors, and imaging systems or similar devices for biomedical purposes. Many other applications that can be mentioned for

quantum technologies indicate the basis for a technological revolution [3]. In spite of noticeable advantages considered for quantum technologies, the complexity existing in using the potential quantum technologies to develop novel systems and devices is a major problem that may prevent developing such systems as efficiently as expected. One way to cope with this problem is to use systems engineering tools.

Nowadays, systems engineering can be applied to develop the majority of physical systems seen in the world. It is an approach that takes many factors into account, from a high-level understanding of user's requirements to the detailed design of individual components as parts of a system. One of the main purposes in systems engineering is to study complex systems in a more convenient way. A complex system can be defined as a system such that its behavior and characteristics are difficult to be anticipated [4]. Therefore, by considering this definition, quantum systems are identified as complex systems and systems engineering tools should be implemented to handle the complexity of these systems. Model-based systems engineering (MBSE) is an emerging approach in systems engineering that can be used to integrate systems using models based on systems engineering concepts in order to develop systems more conveniently [5]. In other words, to develop complex and interdisciplinary systems meeting user requirements, an organized, convergent, iterative, and repeatable methodology can be obtained by using MBSE [6]. Technically, MBSE can play an important role in describing complex systems and their relevant lifecycle and integration when combined with Systems Modeling Language (SysML which is a systems engineering adaptation of unified modeling language originated by software development [6]) or any other modeling language. MBSE can facilitate communication by connecting all the information produced during the system development [7]. In addition, a noticeable number of complex systems that are going to be developed may be exposed to

cyber-attacks in the future. MBSE can be implemented to alleviate the probable risks existing in this regard. In fact, MBSE has a superiority over other approaches, since it can reduce security risks of the system at the initial steps of its development procedure. Consequently, cyber-security risks will be addressed during the system design stage [8]. According to the mentioned points, it is noticeably advantageous for designers and manufacturers to apply MBSE for developing complex systems because the complexities in the system architecture can be communicated more effectively by using models [9].

Model-based systems engineering serves to highlight the role of modeling in various activities in the system lifecycle, from the conceptual design stage to the product end life, including development of system requirements, analysis, design, and verification and validation [10]. For instance, Wang emphasized the importance of using models in the whole product lifecycle in order to develop complex systems more economically and efficiently [11]. Scherer et al. also tried to reduce the system complexity by proposing a modular-structured approach in the MBSE area [12]. When it is required to develop a new system, various engineering teams should work together using different tools to accomplish this goal successfully. As mentioned before, the use of models can facilitate the communication between these teams, so MBSE can be applied to develop complex systems more effectively. MBSE can also help the engineers in these teams to understand better the relationship between the various subsystems of a complex system, and figure out how changing the design of one part affects the entire system. As a result of this stage, the optimized design for a system can be achieved (Fig. 4). Managing and sharing the resulting data more conveniently and ensuring the requirement traceability are other goals that can be achieved by using MBSE. Altogether, according to the researches performed in this area, the favorable impact of the MBSE method in the development of complex

systems is clear. To the best of authors' knowledge, there is no research which uses MBSE approach to cope with complex quantum systems. So, it is crucial to propose an appropriate methodology for quantum systems development via MBSE. The main purpose of this paper is to cover this gap.

In this research, an MBSE approach is suggested to develop quantum systems more effectively. As previously mentioned, MBSE can be applied to the whole product lifecycle, but the focus in this paper is on the simulation stage. By doing so, the requirements verification for each design can be performed before prototyping and investing too much time and money on designs that may not meet the requirements. For this purpose, quantum dot solar cells are chosen in this research as a typical quantum system to study the MBSE approach and its application in quantum systems development. In the remainder of this paper, the system analysis, design, manufacturing, and verification, validation and testing (VV&T) procedures for the development of quantum dot solar cells using MBSE are described.

### 3.4 Quantum dot solar cells

Today, energy concerns are a significant challenge in the development of modern civilizations. Although fossil fuels have not yet been exhausted, their negative environmental effects are undeniable. The pollution and the greenhouse gases arise from burning these fuels for harnessing their inner energy threaten human society [13]. Therefore, replacing fossil fuels by alternative energy sources to protect the planet, supply growing energy demands, and enhance the standard of living is crucial [14]. In this approach, solar power is a renewable energy resource which is easily available in almost all parts of the world. If all the solar energy reaching the atmosphere could be absorbed, it would be more than enough to satisfy the energy demands of the whole world for an entire year [15]. So,

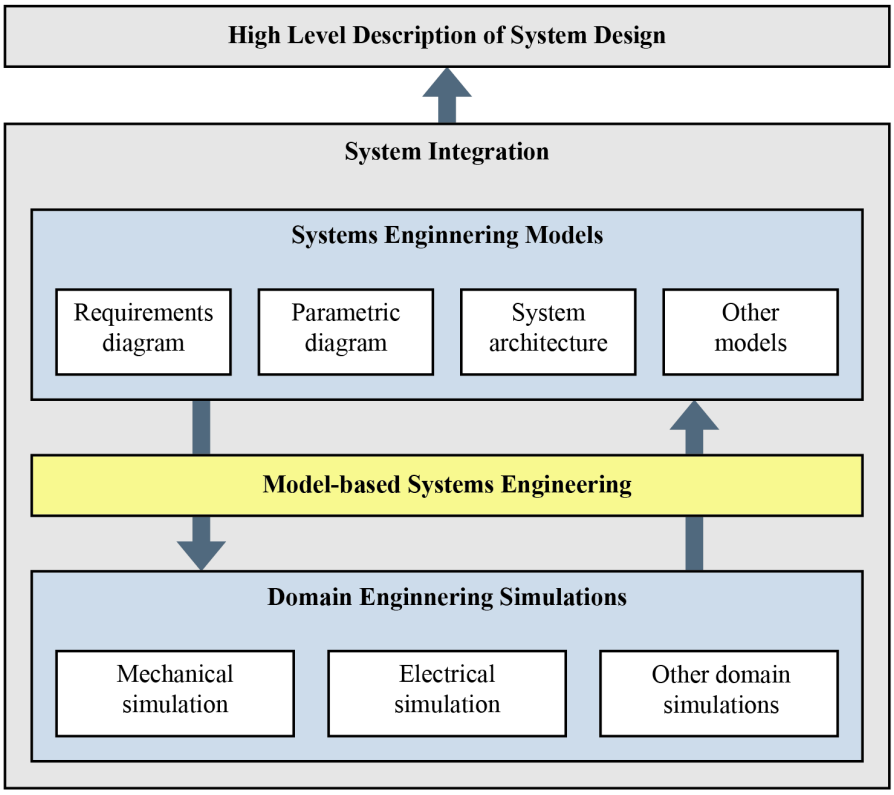


Figure 4. Model-based systems engineering.

researchers in the last few decades have focused on finding the most efficient and cost-effective methods to make use of solar energy as much as possible. Solar power plays an important role in the field of sustainability, especially in developing countries. Solar energy is more reliable, useful, cost-effective, and healthier for both humans and the environment [16]. By capturing the solar irradiation and converting it into a useful form of energy, such as electricity, a sustainable and clean energy system can be achieved. This energy conversion can be performed using so-called solar cells. Technically, a solar cell is a semiconductor device that directly converts solar energy into electricity via a physical and chemical phenomenon, called the photovoltaic effect [17]. When photons hit a solar cell, electrons of the cell are separated from their atoms. If each side of the cell is connected to an electrical load

by electrical conductors, the released electrons can freely flow through this closed circuit, and thus an electrical current is generated, and the electrical load is successfully supplied. Multiple solar cells are integrated into a group to create a solar panel which can be used in residential, commercial, or industrial buildings [18]. Nevertheless, one of the disadvantages of solar cells is their low efficiency. However, their efficiency can be improved by using quantum technologies.

Potentially, each type of material can absorb a different range of solar irradiation, and the rest of the solar energy cannot be converted to electricity. One way to cope with this problem is to use multi-junction solar cells, where different materials are put together layer-by-layer to successfully harvest multiple portions of the solar spectrum. To achieve this goal, a variety of materials is required, such that each one has the ability to absorb a specific portion of the solar spectrum. With the recent development of quantum mechanics, the property of a material can be modified by using quantum dots. Principally, quantum dot are particles of a semiconducting material with tiny diameters in the range of 2 to 10 nanometers (about 10 to 50 atoms). They have unique electronic properties which can be tuned during manufacturing by simply changing the dot shape and size [19]. A quantum dot solar cell is obtained by incorporating quantum dots into the absorbing photovoltaic material [20]. Using a well-tuned solar cell, it is possible to absorb a wide range of the solar spectrum which is typically difficult to achieve by conventional solar cells, and thus the efficiency of the solar cell is eventually enhanced [21]. Since quantum dot solar cells are considered as a complex quantum system, and it is difficult to design, develop, and evaluate these complex systems, MBSE can be employed as a strong tool for this purpose. In this regard, an MBSE methodology is described in the next sections to show the contribution of this

research to study the quantum dot solar cells as an example of a complex quantum system.

## 3.5 System analysis

Nowadays, one of the aims in quantum mechanics is to accelerate the application of potential quantum technologies into physical devices, because of the importance of these apparatus in modern technology. Hence, it is essential to find the needs in this field, and also figure out the disadvantages and limitations of the current systems in order to be improved. As discussed in Section 3.4, quantum dot solar cells are an application of quantum technologies in the field of renewable energy. However, one of the main challenges regarding the use of renewable energy sources is to convince people to use these new energies instead of conventional sources [22]. In fact, one of the problems that may have influence on making this decision is the point that the required time for return of investment for using solar cells is much higher than expected if their efficiency is not high enough. On the other hand, making consumers aware of the generated amount of electrical power from their installed solar cell systems continually can motivate them to become renewable energy users. Therefore, as one of the initial steps in the system analysis, the stakeholder requirements can be derived using the above-mentioned desirements as follows:

- The user shall be able to monitor the generated electricity remotely.
- The time of return of investment shall be decreased to less than half.

It should be noted that conventional solar cells were made of crystalline silicon, and were able to attain an efficiency of up to 26%, which led to long time of return of investment. However, by using quantum dot solar cells with an optimized design, it

is possible to achieve much higher efficiencies, which makes it possible to successfully satisfy the stakeholder requirements.

The next step in the system analysis is to capture the interactions between the system of interest (quantum dot solar cell) and the active and passive stakeholders by preparing a domain diagram. Namely, a domain diagram can be considered as a SysML version of a context diagram. This diagram is noticeably useful for the analysis of complex quantum systems because it provides a common understanding of the modeling scope. Additionally, it helps to define system interfaces and boundaries, which is a difficult procedure for most quantum systems. Figure 5 illustrates the interactions between a solar cell system and its stakeholders and environment.

In the next step, the uses and functions of the quantum system and also the actors or other systems with which the system of interest (quantum dot solar cell) interacts are captured. These uses are depicted in Fig. 6 using SysML in the form of a use case diagram. According to this diagram, electrical power generation is identified as the basic functionality of the quantum dot solar cell based on the defined system purpose or usage. Furthermore, a system monitoring feature is added as per the user requirements. Finally, the functions of other stakeholders, like the solar cell owner and maintainer, are also indicated. It is worthwhile to mention that this diagram only shows the top-level functionalities of the system.

One of the main phases in a system development is to derive the system requirements based on the stakeholder requirements. Basically, each stakeholder requirement will be converted into several system requirements. In Fig. 7, the system requirements of quantum dot solar cells are demonstrated using SysML. As is shown, the system requirements are categorized into five main groups. The most important one is the system requirement that will lead to increasing the solar

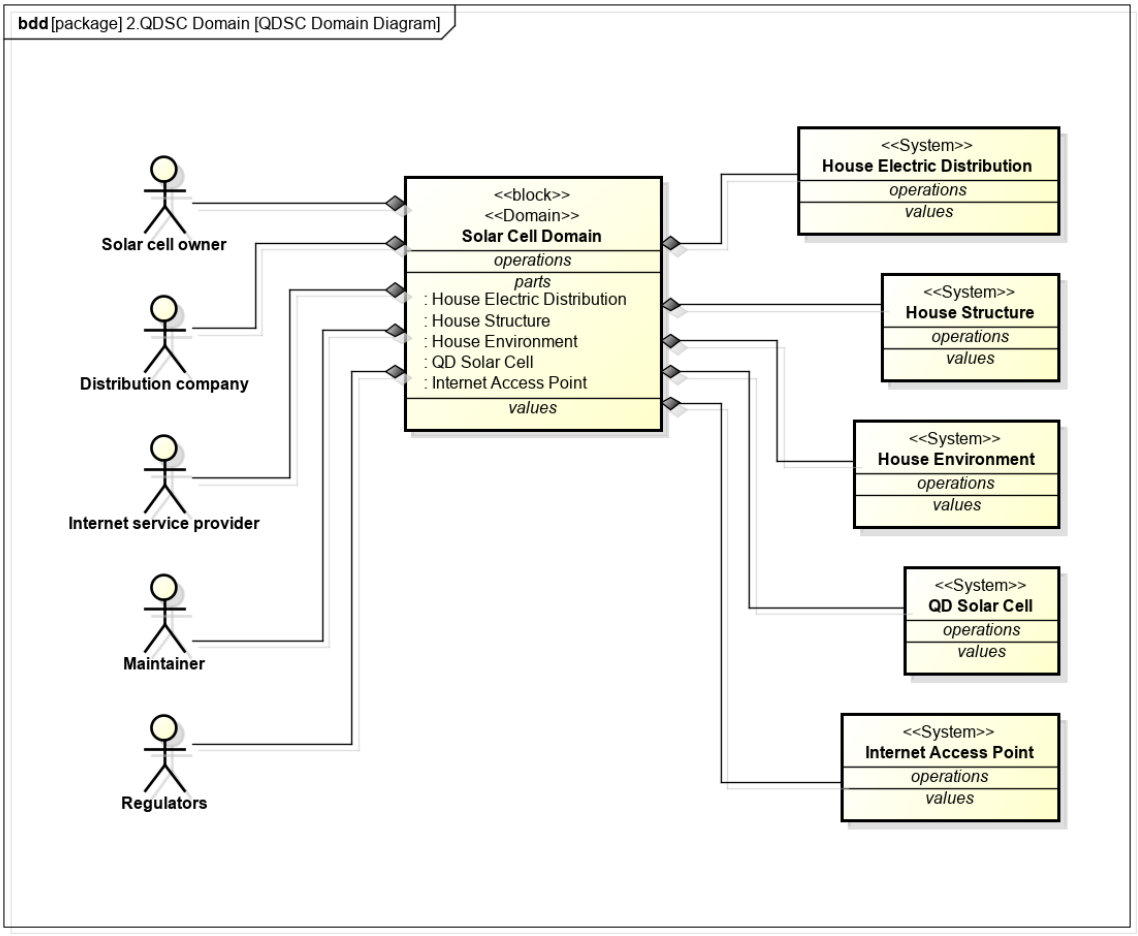


Figure 5. The domain diagram of a quantum dot solar cell.

system efficiency. As previously mentioned, the efficiency of a quantum dot solar cell depends on its material and its geometrical parameters. Thus, as shown in Fig. 9, by optimizing the material (i.e. the substrate material and the quantum dot material of the solar cell) and the geometrical characteristics (i.e. the shape, the size, and the inter-dot spacing between quantum dots), the efficiency of the quantum dot solar cell can be enhanced. The other points to improve the efficiency are to distribute the quantum dots uniformly in the solar cell structure, to consider a design for the quantum dot solar cell that increases its photon absorption rate. Note that the other requirements are defined to provide the monitoring and

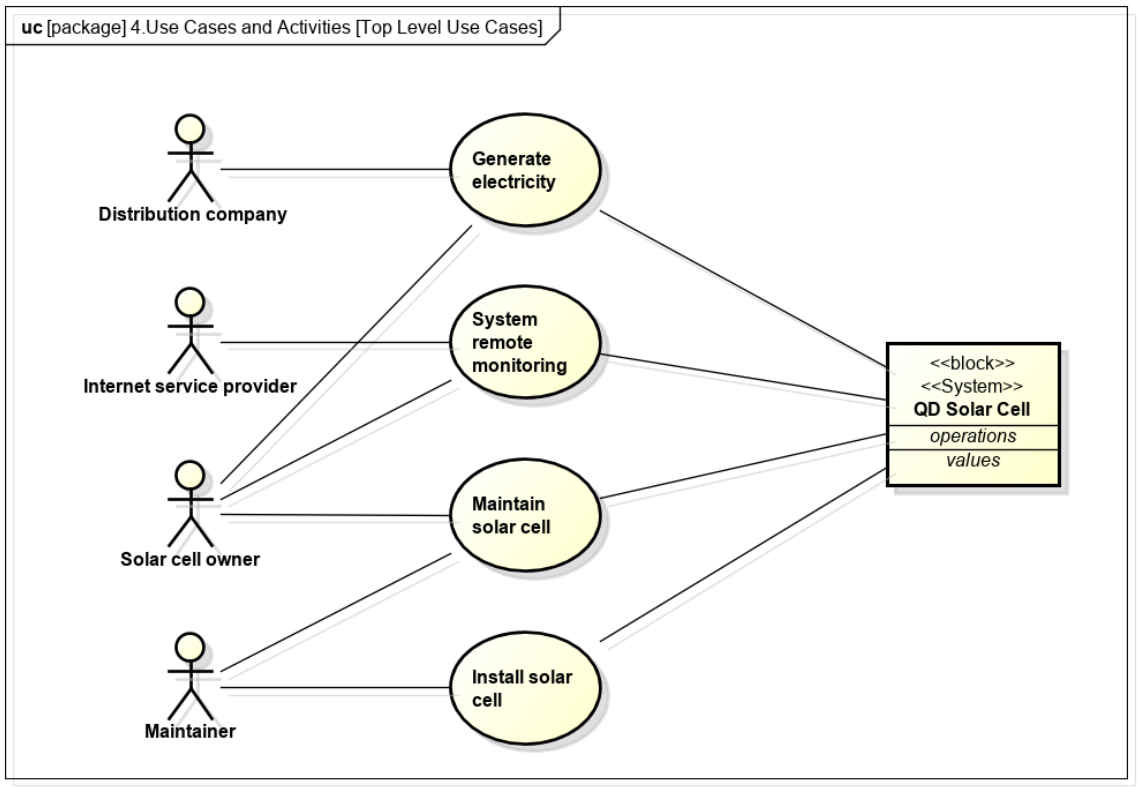


Figure 6. The use case diagram of a quantum dot solar cell.

maintenance outputs of the solar cell system. Now that the system requirements are obtained, the system design can be performed in order to meet these requirements.

## 3.6 System design

One of the main objectives which should be considered in the design and development of any system, especially quantum systems, is to design a system that operates with a desired accuracy and a low chance of failure. Namely, the reliability aspect is crucial in this regard [3]. In order to design a quantum system to meet the reliability requirement, a complete understanding of the system as well as its operation and also the relevant system failure possibilities should be determined. The MBSE methodology paves the way to find such an understanding. For instance, some quantum features, like entanglement, may cause unexpected system failure

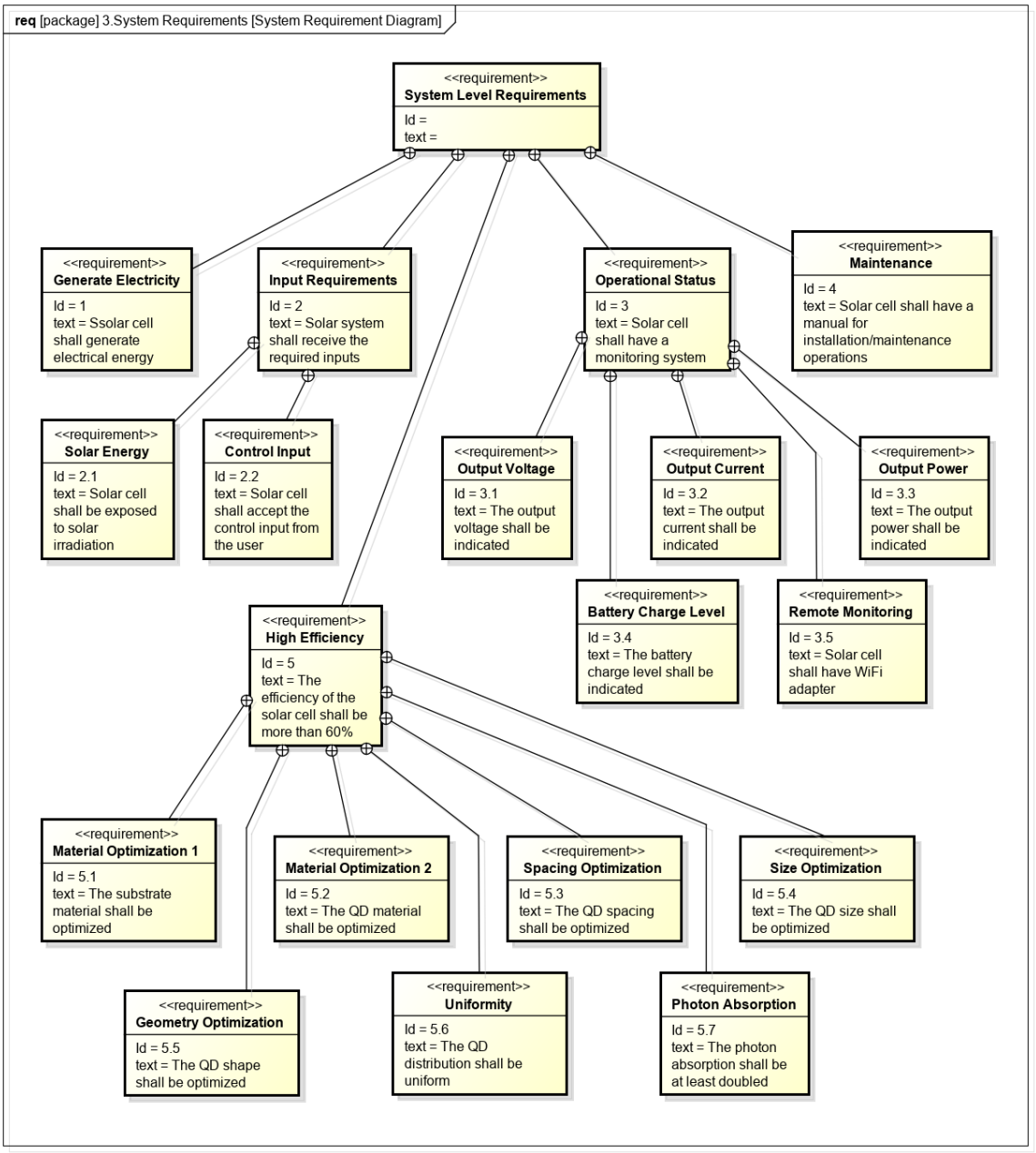


Figure 7. System requirement diagram of the quantum dot solar cell.

modes. Quantum entanglement is a feature representing the underlying relationship between the subsystems of an entire quantum system, which cannot be defined in terms of classical mechanics [23]. In other words, although quantum systems are more likely to fail because of their entangled nature, by taking advantage of systems engineering techniques like MBSE, it is possible to design systems to avoid failure.

### 3.6.1 System design using engineering tools

It is considerably difficult to construct a precise model for quantum systems. Thus, an approximate model can be developed based on the statistical data obtained from experimental tests and relevant quantum theories. Quantum systems design can also be performed based on this model. By employing computer-aided engineering, the design of systems based on advanced technologies, such as quantum technologies, can be accelerated. However, implementation of the newly developed physical rules in the systems development and the employment of a combination of quantum technologies and the relevant classical feedback are still big challenges. Therefore, new computational methods should be developed to provide design tools for quantum systems [3]. For instance, in order to accelerate the application of potential quantum technologies into physical devices, the novel boundary integral techniques [24, 25] for computing the quantum energy eigenvalues can be employed in the proposed MBSE framework to effectively and accurately evaluate the efficiency of quantum dot solar cells. In other words, these numerical methodologies can be employed to solve the governing equation for the mentioned solar cells more efficiently. According to these points, a design model is proposed in this research with the aid of MBSE and the aforementioned boundary integral techniques, which is depicted in Fig. 8. The design process for quantum dot solar cells can be described as follows:

- The governing equation of the system should be identified first, which is the time-independent Schrödinger equation.
- A model should be prepared based on the selected governing equation and the experimental results.
- The energy eigenvalue problem of the time-independent Schrödinger equation is solved using the boundary integral techniques mentioned above (the results of this stage can be evaluated by comparing them with analytical results).
- The derived energy eigenvalues can be used to develop a quantum dot solar cell in order to meet the requirements.

In order to use the boundary integral techniques to accelerate the design procedure of quantum dot solar cells, a MATLAB script is prepared based on a model developed by Aouami et al. [20]. The simplified 2-D model for the solar cells with spherical and cubic quantum dots is shown in Fig. 9. As mentioned previously, one of the system requirements is to increase the photon absorption rate of the solar cell. Technically, there is a group of solar cells that can generate two or three energy carriers, known as excitons, by receiving a single photon from solar irradiation. In this study, it is assumed that the quantum dot solar cell belongs to this group and is categorized as a multi-exciton solar cell. The solar cell substrate material is GaN, and the quantum dots are from $\mathrm{In}_x\mathrm{Ga}_{(1\text{-}x)}\mathrm{N}$, where $x$ shows the Indium content. The size, shape, and interdot spacing of these quantum dots, and also their material, are the main parameters that affect the solar cell efficiency. The MATLAB script receives these input variables, and computes the solar cell efficiency using boundary integral techniques. Thus, the calculated efficiency based on the geometrical and material inputs will be the output of this stage.

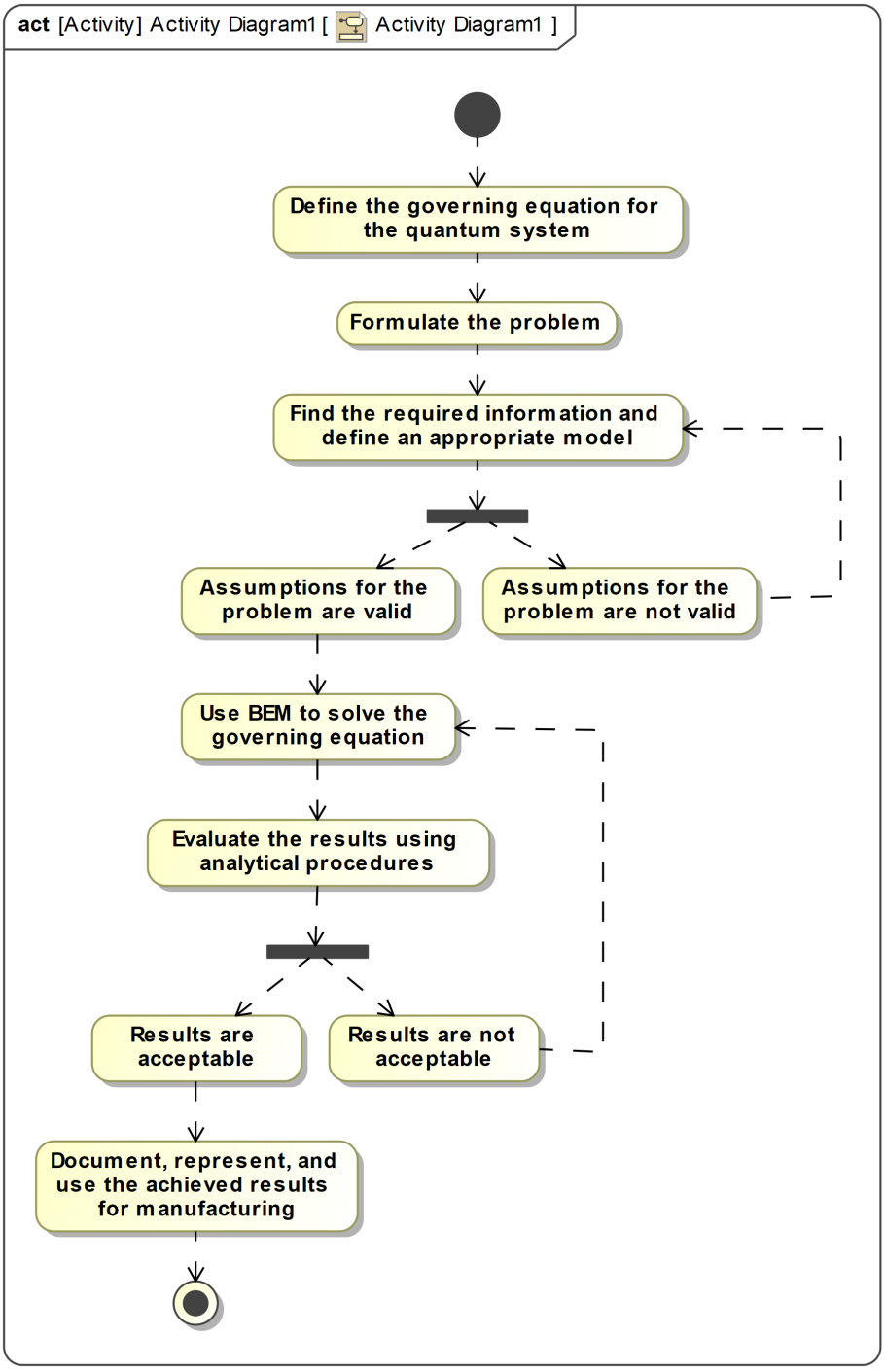


Figure 8. The system design model for a quantum dot solar cell.

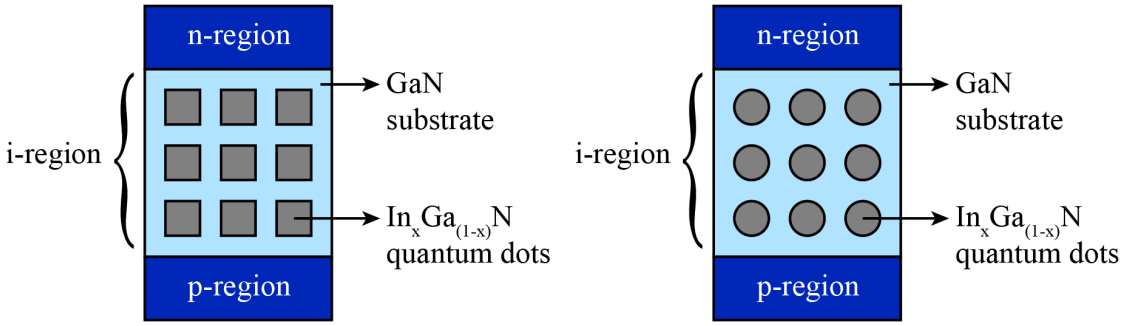


Figure 9. The simplified model of a typical quantum dot solar cell.

### 3.6.2 Integrating SysML with MATLAB

During quantum systems development, various teams work together. The most important point in this regard is to integrate the activities performed by domain engineering teams with the tasks prepared in the systems engineering tools. So, every person who is involved in the analysis, design, and VV&T procedure can understand how making a change in each parameter will influence the other parts and the final system performance. In this study, the system models created using SysML in Cameo System Modeler software [26] are integrated with the MATLAB script described in the previous section. A parametric diagram is developed to link the geometrical and material properties of the quantum dot solar cell to its efficiency, as depicted in Fig. 10. Therefore, the impact of changing each parameter on the efficiency can be easily identified, and it is possible to check whether the newly considered values for the system design will meet the system requirements or not. Furthermore, the parametric diagram of the design process can be connected to test parameters to check whether the design output is in conformity with the test results. It shows the accuracy of the assumptions considered during the design phase. The procedure of manufacturing the designed quantum dot solar cell and measuring its efficiency via a test process are described in the next section.

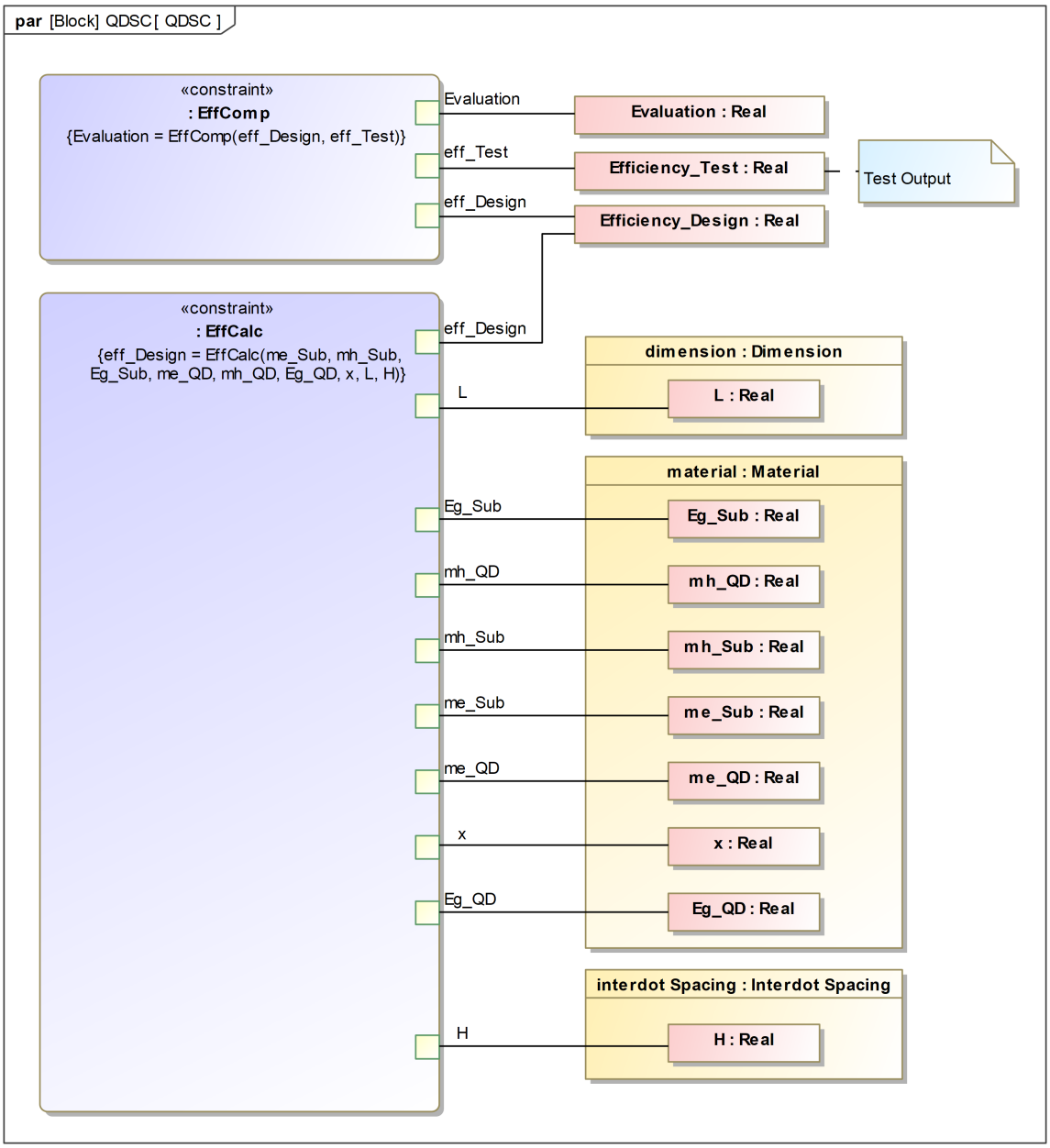


Figure 10. The parametric diagram of a quantum dot solar cell.

### 3.7 System manufacturing and testing

Recently, a transition from document-based approaches to the model-based ones is crucial in order to successfully address complexities in the manufacturing industry. The main reason is inconsistencies occurring during the design information exchange process [9]. When it comes to the development of quantum systems, the complexity level is further increased. Therefore, using MBSE to cope with such complexities becomes inevitable. In this section, it is described how SysML can be applied to provide a manufacturing model for quantum dot solar cells. The process of manufacturing quantum dot solar cells under this study is described in [27]. According to this procedure, in the first step, a layer of Sapphire is prepared as a template for the solar cell. Then a layer of GaN is grown on this template, which acts as the substrate of the solar cell. Next, a layer of $In_xGa_{(1-x)}N$ is grown on the GaN substrate by using metalorganic vapor phase epitaxy (MOVPE) technique. The sample is capped with a layer of GaN, and then it is coated with a layer of aluminum. In the next step, a mask pattern of quantum dots is fabricated on the sample surface using the electron-beam lithography method based on geometrical parameters. By employing the $SiCl_4$ reactive ion etching technique, the pattern is transferred to create quantum dots. Now, the ohmic contacts are deposited on the solar cell surface, after which the sample is annealed with $NH_3$ and $N_2$ to improve its surface morphology. Finally, an anti-reflection coating layer is added to the solar cell to enhance the absorption of solar irradiation. By using model-based techniques, every detail considered in this regard will be followed carefully, and the probability of system failure due to complexity will decrease significantly. An activity diagram representing the manufacturing process is shown in Fig. 11. Similar SysML diagrams can also be employed for modeling the product and also the required manufacturing facilities.

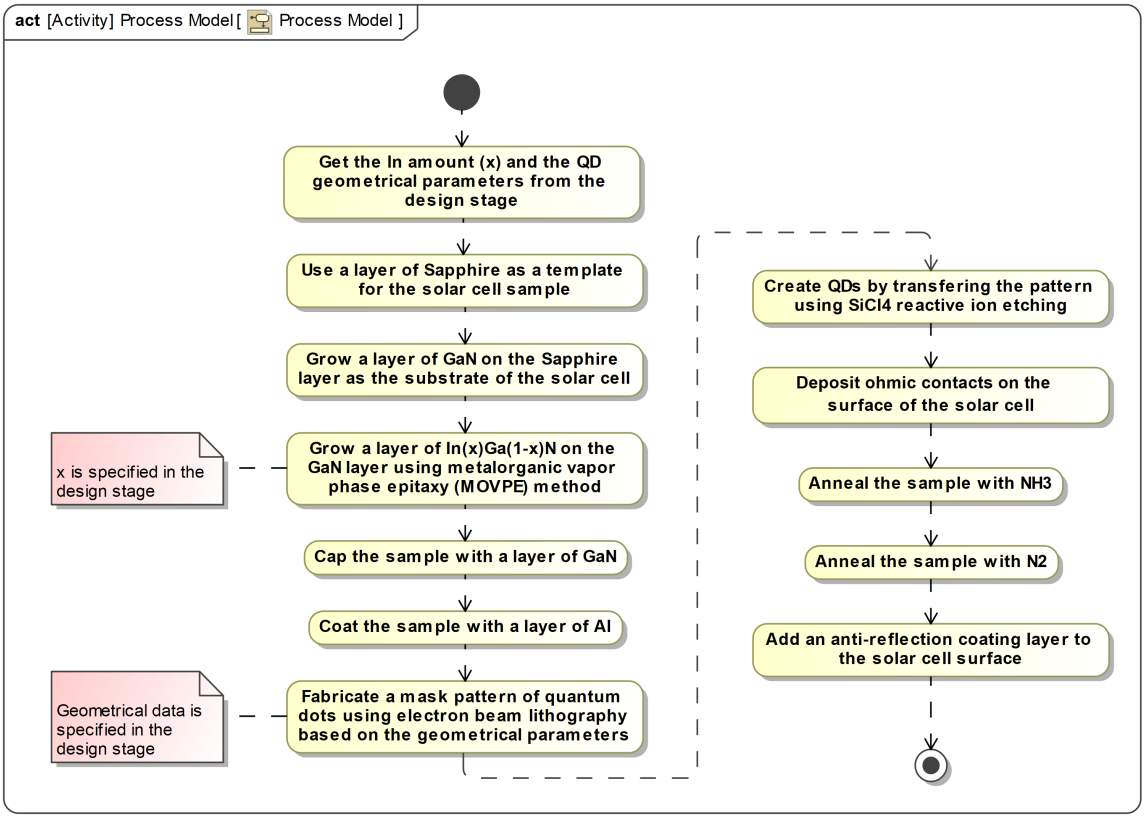


Figure 11. The manufacturing process model for a quantum dot solar cell.

Because of the delicacy existing in the measurement of quantum systems and other similar issues, it is difficult to develop a method to test such systems. Some researches have been conducted to help perform the testing and certification of quantum systems based on quantum statistics [28, 29]. In these methods, the quantum system is assumed to be a black box, and the main focus is the inputs and outputs of the experiments. The methods suggested in these investigations can be applied to both theoretical and numerical models [3]. The testing process that can help to validate and verify the design for the quantum dot solar cells is discussed in several articles [30, 31]. In these articles, the efficiency testing process is described as is shown in Fig. 13. The first step in this process is to prepare the electrical circuit for testing the solar cell (Fig. 12). The initial value of the variable resistor is

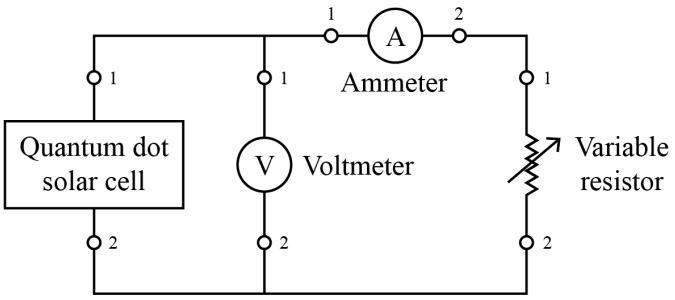


Figure 12. The testing circuit for a quantum dot solar cell.

set to zero. By exposing the quantum dot solar cell to solar irradiation, the voltage and current of the circuit are measured using the voltmeter and ammeter, respectively. Then the variable resistor is increased gradually and the voltage and current measurements are recorded until the amount of current shown by the ammeter is zero. Next, the obtained voltage and current values are plotted in an I-V plain. Finally, by using the area of the largest rectangle that can be fitted inside the I-V curve, the efficiency of the quantum dot solar cell can be calculated by $\eta = (V_m I_m)/P_{in}$, where $V_m I_m$ is the area of the aforementioned rectangle and $P_{in}$ is the input solar power. The VV&T procedure for the model developed for the quantum dot solar cells can be performed to confirm whether the theoretical efficiency sought for the solar cell system is in conformance with the expected value of this parameter or not. As described in Section 3.6.2, a parametric diagram can also be prepared for the testing phase, which makes it possible to check the conformity between the efficiency resulting from the design process and the measured amount achieved from the efficiency testing process (Fig. 10). For this purpose, simulators for the atomistic structure of the chosen materials and the manufacturing process (i.e. MAPS, SILVACO TCAD, etc.) can be used for the verification and validation of the designed quantum dot solar cells. Furthermore, a prototype of the quantum dot solar cell can also be manufactured if the relevant

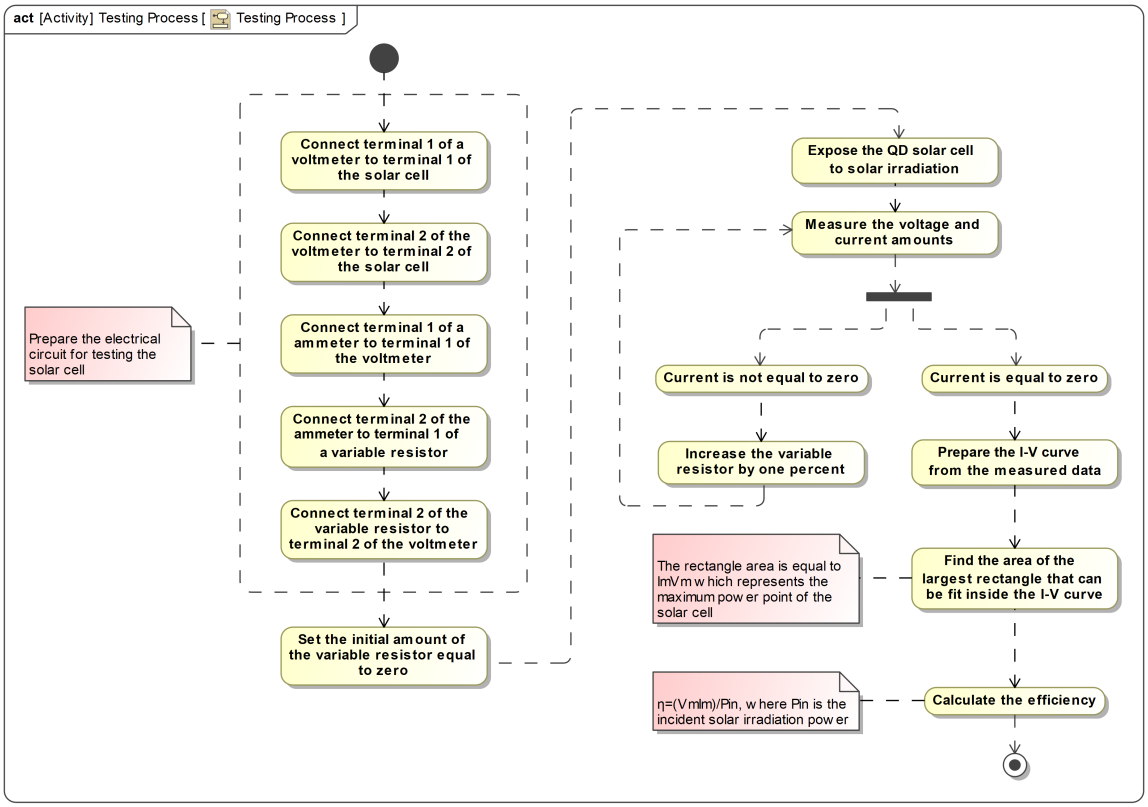


Figure 13. The testing process model for a quantum dot solar cell.

expenses are reasonable. Hence, by performing simulations and experimental tests, as per the diagram shown in Fig. 13, it can be verified that the system requirements and specifications are met using this model for the design process. In addition, it can be validated that the solar cell will operate under the assumed conditions to generate electrical power with the efficiency specified as the system requirement.

The importance of the proposed framework can be witnessed through the traceability enhancement. In other words, by developing an MBSE approach for integration purpose in the system design and testing stages, all system requirements can be traced and verified whether they have been met through the procedure of system development or not. This capability is essential when a complex quantum system with a high number of system requirements is going to be developed. By

using the current method, every system requirement can be traced from the beginning point of the system analysis and design to the testing stage. In addition to the benefits that this approach brings for systems engineers to trace the technical requirements, it also helps domain engineers to take advantage of systems engineering.

## 3.8 Conclusion

In this paper, one of the main challenges in quantum systems development, which is dealing with the existing complexity in this process, was studied. MBSE plays an important role in investigating and creating complex systems. Here, an MBSE methodology is employed in the analysis, design, manufacturing, and VV&T of a typical quantum system, namely a quantum dot solar cell system. Although quantum technologies can be applied to various fields, the role of these novel technologies in the energy area is inevitable. Therefore, because of the importance of the energy field in today's world, quantum dot solar cells which are the new generation of solar cells are chosen for this purpose. All the models for these stages were prepared using SysML in Cameo Systems Modeler integrated with MATLAB scripts prepared for the detailed design procedure. The integration process for all these steps were carried out using a parametric diagram to show the impact of each parameter on the overall system performance. The technique described shows the importance of using models in quantum systems development and paves the way for future investigations on quantum systems using MBSE in order to manage the complexity of these systems.

## 3.9 Acknowledgements

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## 3.10 Conflict of Interest

The authors declare that they have no conflict of interest.

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# CHAPTER IV
# ARTICLE 2 – A STANDARD ENERGY EIGENVALUE PROBLEM FOR DIRECTLY SOLVING THE STATIONARY STATES OF QUANTUM BILLIARDS VIA BOUNDARY INTEGRAL ANALYSIS

## 4.1 Supplementary material

This paper[1] and the related paper in Chapter V presented novel numerical techniques for effectively and accurately solving the energy eigenvalue problem of the time-independent Schrödinger equation (or Helmholtz equation) which are the governing equations for a wide range of quantum systems under various boundary conditions. Further mathematical details required to gain a better understanding of the calculations in these two papers are provided in Appendix B based on [1].

## 4.2 Abstract

By using the series expansions of the Bessel functions for the real and imaginary parts of the free particle Green's function for the two-dimensional stationary states of quantum billiards, it can be shown that some components of the Green's function are redundant which can be eliminated to make the boundary integral equation for the wave function of free particles inside quantum billiards independent of the wave numbers. This development leads to a much faster search

[1] A.-V. Phan and M. Karimaghaei, "A standard energy eigenvalue problem for directly solving the stationary states of quantum billiards via boundary integral analysis", *Forces in Mechanics*, Vol. 4, p. 100027, 2021. https://doi.org/10.1016/j.finmec.2021.100027

for the energy eigenvalues of quantum billiards by scanning their wave numbers or the formulation of the standard eigenvalue problem which can directly be solved for the energy eigenvalues. Some numerical examples were used to demonstrate that the proposed technique is accurate, computationally effective and straightforward to be applied in practice.

## 4.3 Introduction

The uniform motion of a particle in a domain, which has a piecewise smooth boundary, creates a dynamical system known as a billiard [2]. One of the methods to study quantum version of billiards is to replace the classical Hamiltonian equation for billiards by the stationary-state Schrodinger equation for a particle with zero potential. In this case, the wave function does not exist on the billiard boundary [3]. Quantum billiards are an important topic of research as they can serve as models of nanoelectronic devices, *e.g.*, [4]. There is an interest in understanding the chaotic behavior of a quantum billiard due to the irregularity of its boundary. A research direction concerning this interest is the study of the change of the energy levels of a quantum billiard, *e.g.*, [5]. The energy spectrum of a quantum billiard can be constructed from the energy eigenvalues obtained by solving the aforementioned Schrodinger equation.

Energy eigenvalues for quantum billiards have been determined by repeatedly searching for the local minima of a determinant derived from a boundary element analysis (BEA), *e.g.*, [1]. As this determinant is a function of the wave number $k$, the entire BEA has to be repeated for every value of the wave number within the range of search which is quite computationally expensive (conventional search method) [1]. By using a sequence of higher-order fundamental solutions of the Laplace equation within the multiple reciprocity method (MRM), the coefficient

matrix of the boundary element system of equations can be expressed as a polynomial matrix in terms of the wave number [6, 7, 8, 9], thus Newton iteration and LU decomposition can be utilized [6, 7] or a standard eigenvalue problem can be formulated [8] for finding the eigenvalues in a more computationally effective manner. However, this MRM technique also produces fictitious eigenvalues [8] as it employs the higher-order real-valued fundamental solutions of the Laplace equation instead of the higher-order complex-valued fundamental solutions of the Helmholtz equation. In addition, the technique using Newton iteration and LU decomposition is an iterative process and requires a good initial guess for quick convergence toward the eigenvalues. In the group using the boundary element method with the complex-valued fundamental solution of the Helmholtz equation, Kamiya *et al.* [10] made use of series expansions for the fundamental solutions of the Helmholtz equation for obtaining a polynomial matrix in $k^2$ and applied Newton iteration to compute the eigenvalues, Itagaki and Brebbia [11] utilized an iterative method to find the maximum eigenvalue, while Kirkup and Amini [12] used a polynomial approximation with respect to the wave number $k$ for the BEA system of equations to formulate the standard eigenvalue problem. The latter required the user to choose a degree for the polynomial approximation and intervals of $k$s containing the eigenvalues to be sought before these eigenvalues were found from solving the standard eigenvalue problem for each of the aforementioned intervals.

In the current work, the series expansions of the Bessel functions are applied to the real and imaginary parts of the complex-valued free-particle Green's function. As a result, the boundary integral equation (BIE) for the time-independent wave function of free particles inside quantum billiards becomes independent of the wave number. Following a numerical implementation of this BIE using boundary elements, the system of equations emerges as a polynomial matrix equation whose

variable is the square of the wave number. There are two options to be implemented with this polynomial matrix equation: (a) search for the local minima of the determinant of the polynomial matrix for the eigenvalues; (b) formulation of the standard eigenvalue problem to directly solve for the energy eigenvalues. These two options should be much more computationally effective than the conventional search method mentioned earlier as the entire BEA does not have to be repeated. In addition, no fictitious eigenvalues should be expected to be produced by the proposed technique.

### 4.4 Boundary integral formulation for energy eigenvalue problem

For particles moving freely inside a hard-wall quantum billiard, the wave function $\psi$ should vanish along its boundary $\Gamma$. The BIE for two-dimensional quantum billiards with Dirichlet boundary conditions is written as

$$\int_{\Gamma} G(P,Q)\, u(Q)\, \mathrm{d}Q = 0. \tag{IV.1}$$

where $P$ and $Q$ are source and field points, respectively, $u(Q) = \dfrac{\partial \psi(Q)}{\partial \boldsymbol{n}}$, $\boldsymbol{n} = \boldsymbol{n}(Q)$ denotes the unit outward normal to the boundary $\Gamma$, $\mathrm{d}Q$ is an infinitesimal boundary length, and the Green's function $G(P,Q)$ is given by

$$G(P,Q) = -\frac{m}{\pi\hbar^2} K_o(-ikr). \tag{IV.2}$$

In this equation, $m$ and $\hbar$ are the particle's mass and reduced Planck's constant, respectively, $K_o$ is the modified Bessel function of the second kind and order zero, $k = \sqrt{2Em}/\hbar$ is the wave number of the particle of energy $E$, $i$ is the imaginary unit, and $r$ is the distance between $P$ and $Q$.

### 4.4.1 Searching for the energy eigenvalues by scanning $k$

The simplest technique for finding the energy eigenvalues is reviewed first. A numerical implementation of Eq. (IV.1) with $N$ boundary elements results in

$$\sum_{i=1}^{N} A_{ij}(k)\, u_j = \boldsymbol{A}(k)\boldsymbol{u} = \boldsymbol{0}. \tag{IV.3}$$

To obtain non-trivial solutions for $\boldsymbol{u}$ which is the vector of nodal $\dfrac{\partial \psi}{\partial \boldsymbol{n}}$ on $\Gamma$, the following condition must be met:

$$\det[\boldsymbol{A}(k)] = 0. \tag{IV.4}$$

and the energy eigenvalues in terms of $k$ can be found as the real roots of this equation.

In most practices, finding the roots of Eq. (IV.4) has been replaced by finding the local minima of $|\det[\boldsymbol{A}(k)]|$ by scanning $k$ within intervals $[k_{\min}, k_{\max}]$ using a small step size $\Delta k$. The two primary drawbacks of this technique are: (a) it is quite computationally expensive, especially with very small $\Delta k$, as it requires the calculation of $\boldsymbol{A}$ for each value of $k$; (b) the iterative search could miss some eigenvalues if $\Delta k$ is not small enough at certain location within the range of interest.

### 4.4.2 Formulation of the standard energy eigenvalue problem

The Green's function in Eq. (V.3) can be rewritten in terms of the Bessel function of the first kind and order zero $J_o$ and the Bessel function of the second kind and order zero $Y_o$ as

$$G(P,Q) = \frac{m}{2\hbar^2}\Big(Y_o(kr) - iJ_o(kr)\Big). \tag{IV.5}$$

By using Eq. (V.5) in Eq. (IV.1), one gets

$$\int_\Gamma \Big(Y_o(kr) - iJ_o(kr)\Big)\, u(Q)\, \mathrm{d}Q = 0. \tag{IV.6}$$

which implies that

$$\int_\Gamma Y_o(kr)\, u(Q)\, \mathrm{d}Q = 0 \tag{IV.7}$$

and

$$\int_\Gamma J_o(kr)\, u(Q)\, \mathrm{d}Q = 0 \tag{IV.8}$$

The series expansions of $Y_o$ and $J_o$ are known to be

$$Y_o(kr) = \frac{2}{\pi}\Big(\gamma + \ln\frac{k}{2}\Big)J_o(kr) + \frac{2}{\pi}\sum_{j=0}^{\infty} F_j(\ln r - S_j)r^{2j} \tag{IV.9}$$

and

$$J_o(kr) = \sum_{j=0}^{\infty} F_j r^{2j} \tag{IV.10}$$

where $\gamma$ is the Euler-Mascheroni constant, and

$$F_j = \frac{k^{2j}}{(-4)^j (j!)^2}\ ; \quad S_j = \sum_{\ell=1}^{j}\frac{1}{\ell}$$

Use of Eq. (V.10) in Eq. (IV.7) while taking Eq. (IV.8) into account results in

$$\int_\Gamma Y_o(kr)\, u(Q)\, \mathrm{d}Q = \frac{2}{\pi}\sum_{j=0}^{\infty} F_j \int_\Gamma (\ln r - S_j) r^{2j}\, u(Q)\, \mathrm{d}Q = 0 \tag{IV.11}$$

Substitution of Eq. (V.11) in Eq. (IV.8) yields

$$\int_\Gamma J_o(kr)\, u(Q)\, \mathrm{d}Q = \sum_{j=0}^{\infty} F_j \int_\Gamma r^{2j}\, u(Q)\, \mathrm{d}Q = 0 \tag{IV.12}$$

By using Eqs. (IV.11) and (IV.12) in Eq. (IV.6), one gets

$$\sum_{j=0}^{\infty} \lambda^j \int_{\Gamma} \bar{G}_j(P,Q)\, u(Q)\, \mathrm{d}Q = 0 \tag{IV.13}$$

where $\lambda = k^2$ and

$$\bar{G}_j(P,Q) = \frac{\Big(2(S_j - \ln r) + i\pi\Big) r^{2j}}{(-4)^j (j!)^2} \tag{IV.14}$$

$\bar{G}_j$ is called the adjusted Green's function which, unlike the Green's function $G$, is independent of $k$. $\bar{G}_j$ is logarithmic singular when $r = 0$ and $j = 0$. However, within numerical implementation, the related singular integrals can be straightforwardly evaluated by using the following conversion:

$$\int_0^1 f(\xi)\, \ln \xi \, \mathrm{d}\xi = -\int_0^1 \int_0^1 f(\xi\eta)\, \mathrm{d}\xi \, \mathrm{d}\eta \tag{IV.15}$$

where $f$ is a nonsingular function.

It is sufficient to use a finite number of terms in the series in Eq. (V.4) to achieve convergence. Using the first $(m+1)$ terms and discretizing Eq. (V.4) with boundary elements results in

$$\sum_{j=0}^{m} \lambda^j \, \boldsymbol{B}_j \boldsymbol{u}_0 = \boldsymbol{0} \tag{IV.16}$$

where $\boldsymbol{u}_0$ is the vector of nodal $\dfrac{\partial \psi}{\partial \boldsymbol{n}}$ along $\Gamma$.

The energy eigenvalues $k$ can also be found as the local minima of $|\det[\sum_{j=0}^{m} \lambda^j \, \boldsymbol{B}_j]|$. To search for the energy eigenvalues within the interval $[k_{\min}, k_{\max}]$ using a step size of $\Delta k$, the number of required iterations is $N_k = (k_{\max} - k_{\min})/\Delta k$. For the conventional search method presented in Section 2.1, as matrix $\boldsymbol{A}(k)$ in Eq. (IV.4) is dependent of $k$, one would need to recalculate $\boldsymbol{A}(k)$ at each iteration for a total of $N_k$ times. In order to avoid missing any

potential energy eigenvalues, $\Delta k$ must be small enough which makes $N_k$ very large, especially for wide intervals $[k_{\min}, k_{\max}]$. However, as $\boldsymbol{B}_j$ in Eq. (IV.16) is independent of $k$, the search for the eigenvalues using this equation only requires matrix $\boldsymbol{B}_j$ to be computed $(m+1)$ times and typically, $m \leq 50$ is sufficient for obtaining highly accurate eigenvalues for many problems. For each value of $k$ used at each iteration, the polynomial matrix $\sum_{j=0}^{m} \lambda^j \boldsymbol{B}_j = \sum_{j=0}^{m} k^{2j} \boldsymbol{B}_j$ can be recalculated very quickly. Therefore, the use of the adjusted Green's function (V.22) would eliminate the first drawback of the conventional search technique outlined in Section 2.1.

To formulate the standard energy eigenvalue problem, rewrite Eq. (IV.16) as,

$$\sum_{j=0}^{m} \lambda^j \boldsymbol{B}_j \boldsymbol{u}_0 = \sum_{j=0}^{m} \boldsymbol{B}_j \boldsymbol{u}_j = \boldsymbol{0} \tag{IV.17}$$

where $\boldsymbol{u}_i = \lambda \boldsymbol{u}_{i-1}$, thus $\boldsymbol{u}_j = \lambda^j \boldsymbol{u}_0$.

Premultiplying Eq. (IV.17) by $-\boldsymbol{B}_m^{-1}$ yields

$$-\boldsymbol{B}_m^{-1} \sum_{j=0}^{m-1} \boldsymbol{B}_j \boldsymbol{u}_j = \boldsymbol{B}_m^{-1} \boldsymbol{B}_m \boldsymbol{u}_m = \boldsymbol{I} \boldsymbol{u}_m = \lambda \boldsymbol{u}_{m-1} \tag{IV.18}$$

From $\boldsymbol{u}_i = \lambda \boldsymbol{u}_{i-1}$, one can write

$$\begin{array}{lll} \boldsymbol{I}\boldsymbol{u}_{m-1} + \boldsymbol{0}\boldsymbol{u}_{m-2} + & \cdots + \boldsymbol{0}\boldsymbol{u}_1 + \boldsymbol{0}\boldsymbol{u}_0 & = \lambda \boldsymbol{u}_{m-2} \\ \vdots & \ddots & \vdots \\ \boldsymbol{0}\boldsymbol{u}_{m-1} + \boldsymbol{0}\boldsymbol{u}_{m-2} + & \cdots + \boldsymbol{I}\boldsymbol{u}_1 + \boldsymbol{0}\boldsymbol{u}_0 & = \lambda \boldsymbol{u}_0 \end{array} \tag{IV.19}$$

Equations (IV.18) and (IV.19) form the following system:

$$\begin{bmatrix} -\boldsymbol{B}_m^{-1}\boldsymbol{B}_{m-1} & -\boldsymbol{B}_m^{-1}\boldsymbol{B}_{m-2} & \cdots & -\boldsymbol{B}_m^{-1}\boldsymbol{B}_1 & -\boldsymbol{B}_m^{-1}\boldsymbol{B}_0 \\ \boldsymbol{I} & \boldsymbol{0} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \vdots & & \ddots & & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{I} & \boldsymbol{0} \end{bmatrix} \begin{Bmatrix} \boldsymbol{u}_{m-1} \\ \boldsymbol{u}_{m-2} \\ \boldsymbol{u}_{m-3} \\ \vdots \\ \boldsymbol{u}_0 \end{Bmatrix} = \lambda \begin{Bmatrix} \boldsymbol{u}_{m-1} \\ \boldsymbol{u}_{m-2} \\ \boldsymbol{u}_{m-3} \\ \vdots \\ \boldsymbol{u}_0 \end{Bmatrix} \tag{IV.20}$$

which represents an eigenvalue problem of the standard form $\boldsymbol{D}\boldsymbol{u} = \lambda\boldsymbol{u}$. Numerical techniques for large scale eigenvalue problems with sparse matrices can be employed to directly find the energy eigenvalues in terms of $\lambda = k^2$ for quantum systems.

### 4.5 Numerical examples

Two numerical examples, involving a circular billiard and a stadium billiard, are shown in this work to demonstrate the accuracy and effectiveness of the proposed technique. MATLAB scripts were developed to implement the boundary integral and standard eigenvalue formulations of the new technique. The scripts were run to compute the energy eigenvalues for the circular and stadium quantum billiards. Equation (V.4) was numerically implemented using quadratic boundary elements. The eigenvalues $k$ obtained from solving Eq. (V.37) are complex numbers, including multiple roots. As the energy eigenvalues are real numbers, only numerical results for $k$ with a small imaginary part relative to its real part (*e.g.*, $|\text{imag}(k)| < 10^{-3}\text{real}(k)$) are chosen as the results sought.

The MATLAB scripts used `eig(D)` which is based on the LAPACK [13] routine `ZGEEV` for computing eigenvalues. If matrix $\boldsymbol{B}_m$ in Eq. (V.37) is close to singular (ill-conditioned), the standard eigenvalue problem can be recasted in the

form of the generalized eigenvalue problem $\boldsymbol{A}\boldsymbol{u} = \lambda \boldsymbol{B}\boldsymbol{u}$ and MATLAB function `eig(A,B,'qz')` based on the QZ algorithm can be used to find the eigenvalues.

### 4.5.1 Circular billiard

As the first example, consider a circular billiard of unit radius. The circular boundary was discretized with 24 uniform quadratic elements. The analytical solution for this problem is known to be the roots of the Bessel function of the first kind and integer order.

To accurately obtain the first 20 distinct energy eigenvalues using the proposed standard eigenvalue problem (SEVP) method represented by Eq. (V.37), a selected value of $m = 36$ is sufficient. When rounding off to the nearest ten thousandth, the SEVP numerical results and those obtained from searching for the local minima of $|\det[\sum_{j=0}^{36} \lambda^j \boldsymbol{B}_j]|$ are identical. The local minima within the interval $k = [2, 13.2]$ are shown in Fig. 14. Table 4 compares the numerical results with their analytical counterparts. An excellent agreement can be observed where the maximum error is 0.02%.

### 4.5.2 Bunimovich stadium billiard

The Bunimovich stadium billiard shown in Fig. 15 , where $R = L = 1$, was chosen as the second example. Each of the semicircles and line segments are discretized with five and three uniform quadratic elements, respectively. The Bunimovich stadium billiard represents a chaotic quantum system, *e.g.*, [14].

To demonstrate the effectiveness and accuracy of the proposed technique, consider the use of the following three methods to find the first 10 energy eigenvalues $k$: the search for the local minima of $|\det[\boldsymbol{A}(k)]|$ (conventional search method) and $|\det[\sum_{j=0}^{m} \lambda^j \boldsymbol{B}_j]|$ (proposed search method where $m = 40$) described in Sections 2.1 and 2.2, respectively, and the SEVP method. The searches were

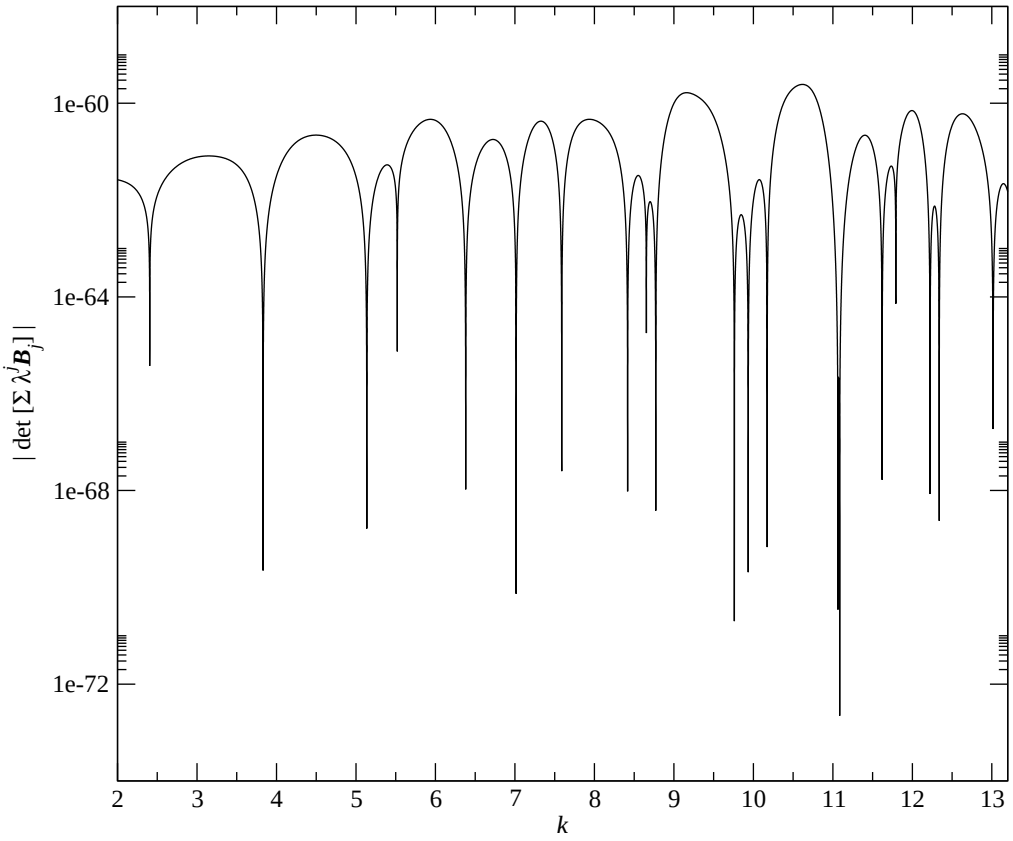


Figure 14. Plot of $|\det[\sum_{j=0}^{36} \lambda^j \, \boldsymbol{B}_j]|$ for the circular billiard.

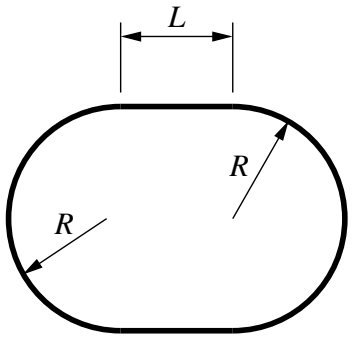


Figure 15. Bunimovich stadium billiard.

Table 1. The first 20 distinct eigenvalues $k$ for the circular billiard.

| SEVP or $\min(\lvert\det[\sum_{j=0}^{36}\lambda^j \boldsymbol{B}_j]\rvert)$ | Analytical Solution | % error | SEVP or $\min(\lvert\det[\sum_{j=0}^{36}\lambda^j \boldsymbol{B}_j]\rvert)$ | Analytical Solution | % error |
|---|---|---|---|---|---|
| 2.4048 | 2.4048 | 0.000 | 9.7610 | 9.7610 | 0.000 |
| 3.8317 | 3.8317 | 0.000 | 9.9355 | 9.9346 | 0.006 |
| 5.1356 | 5.1356 | 0.000 | 10.1735 | 10.1735 | 0.000 |
| 5.5201 | 5.5201 | 0.000 | 11.0646 | 11.0647 | 0.001 |
| 6.3801 | 6.3802 | 0.002 | 11.0851 | 11.0864 | 0.012 |
| 7.0156 | 7.0156 | 0.000 | 11.6199 | 11.6198 | 0.001 |
| 7.5883 | 7.5883 | 0.000 | 11.7916 | 11.7915 | 0.001 |
| 8.4173 | 8.4172 | 0.001 | 12.2227 | 12.2251 | 0.020 |
| 8.6537 | 8.6537 | 0.000 | 12.3382 | 12.3386 | 0.003 |
| 8.7712 | 8.7715 | 0.003 | 13.0156 | 13.0152 | 0.003 |

conducted over the interval $k = [1.5, 5.7]$ with step sizes $\Delta k = 10^{-3}$ and $10^{-4}$ being employed for the conventional and proposed search methods, respectively. In the order given, this selection of $\Delta k$ resulted in the numerical energy eigenvalues accurate up to three and four decimal places as shown in Table 5. While the number of search iterations for the conventional search method is 10 times less than the proposed search method ($N_k = 4,200$ vs 42,000), its CPU time measured on the computer used to search for just the first 10 eigenvalues for this work was already about 252 times larger. Note that, as the matrix of the standard eigenvalue problem for this example is ill-conditioned, the form of the generalized eigenvalue problem with $m = 40$ was used instead to find the first 10 energy eigenvalues. There is a very good agreement between the numerical results obtained from these three methods as it can be seen in Table 5. Actually, the eigenvalues obtained from both the search methods are identical if $\Delta k = 10^{-4}$ is also chosen for the conventional search

Table 2. The first 10 distinct energy eigenvalues $k$ for the stadium billiard.

| $\min(\lvert\det[\boldsymbol{A}(k)]\rvert)$ | $\min(\lvert\det[\sum_{j=0}^{40} \lambda^j \boldsymbol{B}_j]\rvert)$ | SEVP |
|---|---|---|
| 1.954 | 1.9537 | 1.9537 |
| 2.778 | 2.7780 | 2.7780 |
| 3.404 | 3.4036 | 3.4036 |
| 3.721 | 3.7207 | 3.7208 |
| 4.056 | 4.0562 | 4.0564 |
| 4.678 | 4.6783 | 4.6792 |
| 4.880 | 4.8797 | 4.8666 |
| 4.922 | 4.9218 | 4.9227 |
| 5.493 | 5.4931 | 5.4870 |
| 5.635 | 5.6352 | 5.6522 |

method. For this case, the CPU time for the conventional search method is about 300 times larger than that for the SEVP method.

The ill-conditioned matrix in the standard eigenvalue problem of this example prevents the solver to produce a large number of accurate eigenvalues. To resolve this issue, quadruple precision from ADVANPIX multiprecision computing toolbox [15] for MATLAB was employed. Table 6 depicts the first 40 distinct energy eigenvalues $k$ obtained from using quadruple precision for solving the standard eigenvalue problem represented by Eq. (V.37) and from using the proposed search method for locating the local minima of $|\det[\sum_{j=0}^{m} \lambda^j \boldsymbol{B}_j]|$. Here, a larger value of $m$ ($m = 50$) was needed for both methods in order to produce at least 40 accurate energy eigenvalues. It was not necessary to use the conventional search method here for the purpose of validation as it would produce the same numerical results while requiring an extremely large amount of computing time.

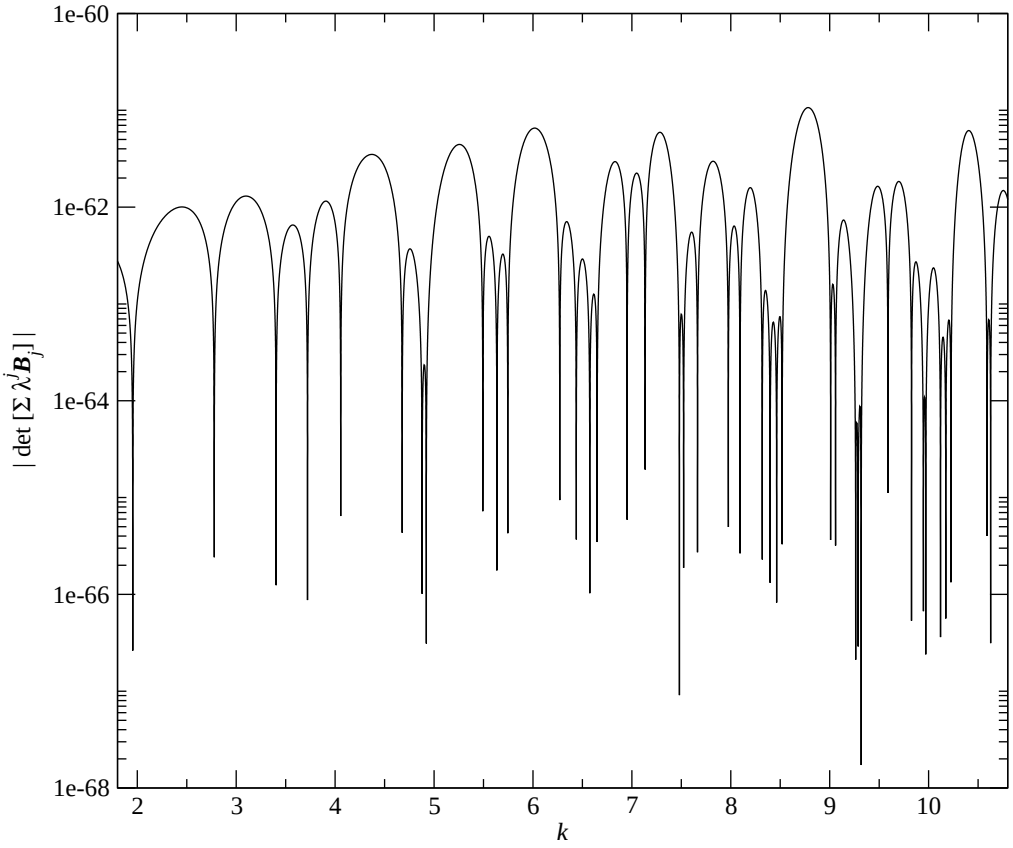


Figure 16. Plot of $|\det[\sum_{j=0}^{50} \lambda^j \, \boldsymbol{B}_j]|$ for the Bunimovich stadium billiard.

The graphical result from this search within the interval $k = [1.5, 11]$ is depicted in Fig. 16. It can be seen that the numerical results using four decimal places are practically identical which demonstrates the accuracy of the proposed technique. Note in Ref. [1] that the iterative process for searching for the local minima of $|\det[\boldsymbol{A}(k)]|$ (conventional search method) was employed to find the eigenvalues for this example. By comparing the results reported in [1] with those in Table 6, it is observed that the first eigenvalue ($k = 1.9537$) was absent from their results.

Table 3. The first 40 distinct energy eigenvalues $k$ for the stadium billiard.

| SEVP | $\min(\lvert\det[\sum_{j=0}^{50} \lambda^j \boldsymbol{B}_j]\rvert)$ | SEVP | $\min(\lvert\det[\sum_{j=0}^{50} \lambda^j \boldsymbol{B}_j]\rvert)$ |
|---|---|---|---|
| 1.9537 | 1.9537 | 7.9754 | 7.9754 |
| 2.7780 | 2.7780 | 8.0935 | 8.0935 |
| 3.4036 | 3.4036 | 8.3183 | 8.3183 |
| 3.7207 | 3.7207 | 8.3978 | 8.3978 |
| 4.0562 | 4.0562 | 8.4635 | 8.4635 |
| 4.6783 | 4.6783 | 8.5193 | 8.5193 |
| 4.8797 | 4.8797 | 9.0093 | 9.0093 |
| 4.9218 | 4.9218 | 9.0590 | 9.0590 |
| 5.4931 | 5.4931 | 9.2624 | 9.2624 |
| 5.6352 | 5.6352 | 9.2877 | 9.2877 |
| 5.7452 | 5.7452 | 9.3187 | 9.3187 |
| 6.2708 | 6.2708 | 9.5891 | 9.5891 |
| 6.4384 | 6.4384 | 9.8274 | 9.8274 |
| 6.5743 | 6.5743 | 9.9474 | 9.9474 |
| 6.6491 | 6.6491 | 9.9711 | 9.9711 |
| 6.9521 | 6.9521 | 10.1202 | 10.1202 |
| 7.1345 | 7.1345 | 10.1734 | 10.1734 |
| 7.4807 | 7.4807 | 10.2260 | 10.2260 |
| 7.5230 | 7.5230 | 10.5916 | 10.5916 |
| 7.6638 | 7.6638 | 10.6268 | 10.6268 |

## 4.6 Summary

A series of adjusted Green's functions which are independent of the wave number was derived in this work for formulating the standard eigenvalue problem (SEVP method) for quantum billiards. In case a very large number of energy

eigenvalues (typically in the order of thousands) is required to determine the quantum energy spectrum, the adjusted Green's functions can also be employed to conduct a much faster search (compared to the conventional search method) for the eigenvalues sought by scanning the wave numbers over a wide scan range to locate the local minima of $|\det[\sum_{j=0}^{m} \lambda^j \boldsymbol{B}_j]|$ (see Eq. (IV.16)). Via two numerical examples, the proposed technique has shown to be accurate and computationally effective in determining the energy eigenvalues for quantum billiards. The technique is readily expanded to eigenvalue analysis of the Helmholtz equation in general and standard eigenvalue problems for three-dimensional quantum billiards in particular. The large scale standard eigenvalue problem given by Eq. (V.37) should stimulate interest in developing effective algorithms for accurately finding a large number of eigenvalues for this type of sparse matrix.

## 4.7 Acknowledgements

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## 4.8 Conflict of Interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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# CHAPTER V

# ARTICLE 3 – BOUNDARY INTEGRAL FORMULATION OF THE STANDARD EIGENVALUE PROBLEM FOR THE 2-D HELMHOLTZ EQUATION

## 5.1 Abstract

In this paper[1], a boundary integral formulation is presented for obtaining the standard eigenvalue problem for the two-dimensional (2-D) Helmholtz equation. The formulation is derived by using the series expansions of zero-order Bessel functions for the fundamental solution to the Helmholtz equation. The proposed approach leads to a series of new fundamental functions which are independent of the wave number $k$ of the Helmholtz equation. The coefficient matrix of the resulting homogeneous system of boundary element equations is of the form of a polynomial matrix in $k$ which allows a much faster search for the eigenvalues by scanning $k$ over an interval of interest or the standard eigenvalue problem to be formulated for directly solving for the eigenvalues without resort to iterative methods. The proposed technique was used to solve some known problems with available analytical solutions: 2-D domains with circular and rectangular geometries

[1]M. Karimaghaei and A.-V. Phan, "Boundary integral formulation of the standard eigenvalue problem for the 2-D Helmholtz equation ", *Engineering Analysis with Boundary Elements*, Vol. 132, p. 281–288, 2021. https://doi.org/10.1016/j.enganabound.2021.07.013

under Dirichlet and/or Neumann boundary conditions. The outcomes demonstrate that the proposed approach is computationally efficient and highly accurate[2].

## 5.2 Introduction

The method of scanning the wave number $k$ to locate the local minima of the eigenvalue determinant obtained via boundary element analysis (BEA) has been utilized to find the eigenvalues of the Helmholtz equation. For example, Tai and Shaw [1] employed this technique to obtain eigenvalues and eigenmodes of the homogeneous Helmholtz equation for closed 2-D and 3-D domains of arbitrary shape. De Mey [2] also used this method for circular and rectangular geometries. In a following work carried out by De Mey [3], only a real particular solution of the Helmholtz equation was employed to find the lowest eigenvalue for a circular domain. Adeyeye *et al.* [4] presented three numerical treatments for the BEA of the Helmholtz equation under Dirichlet boundary conditions to compute the first (lowest) eigenvalue for some circular, elliptic and square domains. In general, the technique of scanning $k$ is straightforward. However, it suffers a major drawback: as the determinant is a function of $k$, it requires the entire BEA to be repeated for every value of $k$ which is quite computationally ineffective.

Subsequent efforts in Helmholtz eigenvalue analysis were devoted to using static fundamental solutions which are independent of $k$. Through the use of the multiple reciprocity method (MRM) with a sequence of higher-order fundamental solutions of the real-valued Laplace operator, the coefficient matrix of the BEA system of equations can be expressed as a polynomial function in terms of $k$ which allows the eigenvalues of the Helmholtz equation to be found more effectively than from the techniques mentioned above, *e.g.*, [5, 6, 7, 8] for two dimensions, and [9] for

[2]This paper is dedicated to the memory of Professor Frank Rizzo whose pioneering contributions to boundary integal method have an enormous impact on the growth of the subject area

three dimensions. Among these works, the standard eigenvalue problem was formulated [6] or Newton iteration and LU decomposition was employed [7, 8] to solve for the Helmholtz eigenvalues. Nevertheless, the use of higher-order fundamental solutions of the Laplace equation is known for producing fictitious eigenvalues [6] as the fundamental solutions of the Laplace equation lack the imaginary part of the complex-valued fundamental solutions of the Helmholtz equation.

For research groups using BEA based upon the complex-valued fundamental solution of the Helmholtz equation, Kamiya *et al.* [10] used series expansions for the 2-D fundamental solution of the Helmholtz operator to derive a polynomial in terms of $k^2$ for the real part of the coefficient matrix of the BEA system of equation and applied Newton iteration for calculating the eigenvalues, Itagaki and Brebbia [11] employed an iterative power method to obtain the maximum eigenvalue (2-D), Yeih *et al.* [12] developed a new MRM formulation which is fully equivalent to the use of the complex-valued fundamental solution (1-, 2- and 3-D), Kirkup and Amini [13] made use of a polynomial approximation with respect to $k$ for the BEA coefficient matrix to formulate a standard eigenvalue problem (2- and 3-D), Wang *et al.* [14] employed series expansion for the 3-D fundamental solution to derive boundary element matrices independent of the wave number which leads to an overdetermined system of equations for the multi-frequency calculation of acoustical pressures. Xie and Liu [15] applied model order reduction methods to frequency-decoupled system matrices resulted from applying Taylor's theorem to the 3-D fundamental solution to solve multi-frequency acoustic wave problems.

Recently, the contour integral method (CIM) has been employed to solve nonlinear eigenvalue problems governed by the Helmholtz equation and formulated via the method of fundamental solutions [16], the plane wave method [16], and the

boundary element method [17]. CIM was also used with the boundary element formulation of the Helmholtz equation to compute the sensitivities of eigenfrequencies for both interior and exterior acoustic systems [18].

In this work, the boundary integral equation of the Helmholtz equation is expressed in the form of a limit as a source point exterior to the domain under consideration as it approaches the boundary. The use of the series expansions for the fundamental solution to the Helmholtz equation under this limit form yields a new equation composed of a series of boundary integrals which are independent of the wave number $k$. A discretization with boundary elements and homogeneous boundary conditions results in a BEA system of equations whose coefficient matrix is of the form of a polynomial function in terms of $k$. Thus, the search for the eigenvalues by scanning $k$ using this technique is much less time-consuming than by using the method mentioned in the first paragraph of this section where the boundary integrals have to be re-evaluated for each value of $k$ within the range of search. Also, the resulting BEA system of equations can be recast to formulate the standard or generalized eigenvalue problems for solving the eigenvalues without resort to iterative methods. This work is an extension of a previous work on the 2-D Helmholtz equation under Dirichlet conditions along the domain boundary [19]. Several numerical examples were presented to demonstrate the effectiveness and accuracy of the proposed technique.

For exterior (*e.g.*, [20]) and multiply connected domains (*e.g.*, [21]), it has been shown that BEA of the Helmholtz equation yields fictitious/spurious eigenvalues, even if the complex-valued fundamental solution is employed. Fictitious eigenvalues for multiply connected domains were found to depend upon not only the inner boundary [21] but also the outer boundary [22] and, like in case of exterior domains, they can be eliminated by using the Burton-Miller method. As pointed

out in [23], the Burton-Miller formulation does not actually eliminate the fictitious eigenvalues but rather shifts them from the real axis to a region in the complex plane so these eigenfrequencies do not cause any problems for acoustic wave analysis.

Recent work based upon the CIM and BEA formulation of the Helmholtz equation [22] showed that fictitious eigenfrequencies also appear in the numerical results for interior acoustic problems. However, as expected, no fictitious eigenvalues exist in the numerical results for the interior domains considered in the four examples studied in this work.

### 5.3 Boundary element formulation for the standard eigenvalue problem

Consider the Helmholtz equation in a two-dimensional (2-D) domain having boundary $\Gamma$,

$$\nabla^2\psi + k^2\psi = 0 \tag{V.1}$$

where $\nabla^2$, $\psi$ and $k$ are the Laplacian, a scalar function and the wavenumber, respectively.

By using its fundamental solution, Eq. (V.1) can be solved via the following boundary integral equation (BIE):

$$c(P)\psi(P) = \int_\Gamma \Big[G(P,Q)\,\psi_{,n}(Q) - G_{,n}(P,Q)\,\psi(Q)\Big]\,\mathrm{d}Q \tag{V.2}$$

where $P$ and $Q$ are source and field points, respectively, $c(P)$ is the solid angle coefficient, the subscript $()_{,n}$ denotes the derivative with respect to the unit outward normal $\boldsymbol{n} = \boldsymbol{n}(Q)$ to $\Gamma$, *i.e.*, $\psi_{,n} = \dfrac{\partial\psi}{\partial\boldsymbol{n}}$, $\mathrm{d}Q$ is an infinitesimal boundary length, and the fundamental solution $G(P,Q)$ is given by

$$G(P,Q) = \frac{i}{4}H_0^{(1)}(kr) = -\frac{1}{4}\Big(Y_0(kr) - iJ_0(kr)\Big) \tag{V.3}$$

In this equation, $H_0^{(1)}$ is the zero-order Hankel function of the first kind, $J_0$ and $Y_0$ are the zero-order Bessel functions of the first and second kinds, respectively, $i$ is the imaginary unit, and $r$ is the distance between $P$ and $Q$.

An equivalent version of Eq. (V.2) is written for a source point $P_e$ exterior to the domain and approaching the boundary,

$$\lim_{P_e \to P} \int_\Gamma \Big[ G(P_e, Q)\, \psi_{,n}(Q) - G_{,n}(P_e, Q)\, \psi(Q) \Big]\, \mathrm{d}Q = 0 \tag{V.4}$$

Note that as $P_e$ crosses the boundary $\Gamma$, there is a jump in the Cauchy Principal Value integral which accounts for the free term $c(P)\psi(P)$. Thus, Eqs. (V.2) and (V.4) are exactly the same.

In Eq. (V.4),

$$G(P_e, Q) = -\frac{1}{4}\Big( Y_0(kr) - iJ_0(kr) \Big) \tag{V.5}$$

where $r$ is the distance between $P_e$ and $Q$, *i.e.*, $r = \|Q - (P + \varepsilon \boldsymbol{n}(P))\|$.

Use of Eq. (V.5) in Eq. (V.4) results in

$$-\frac{1}{4} \lim_{\varepsilon \to 0} \int_\Gamma \Big[ (Y_0 - iJ_0)\, \psi_{,n}(Q) - (Y_{0,n} - iJ_{0,n})\, \psi(Q) \Big]\, \mathrm{d}Q = 0 \tag{V.6}$$

or,

$$-\frac{1}{4} \lim_{\varepsilon \to 0} \int_\Gamma \left\{ Y_0\, \psi_{,n}(Q) - Y_{0,n}\, \psi(Q) - i\Big[ J_0\, \psi_{,n}(Q) - J_{0,n}\, \psi(Q) \Big] \right\} \mathrm{d}Q = 0 \tag{V.7}$$

This equation implies that

$$-\frac{1}{4} \lim_{\varepsilon \to 0} \int_\Gamma \Big[ Y_0(kr)\, \psi_{,n}(Q) - Y_{0,n}(kr)\, \psi(Q) \Big]\, \mathrm{d}Q = 0 \tag{V.8}$$

and

$$-\frac{1}{4}\lim_{\varepsilon\to 0}\int_{\Gamma}\Big[J_0(kr)\,\psi_{,n}(Q)-J_{0,n}(kr)\,\psi(Q)\Big]\,\mathrm{d}Q=0 \tag{V.9}$$

At this point, consider the series expansions of $Y_0$ and $J_0$ given by

$$Y_0(kr)=\frac{2}{\pi}\left[M(k)\,J_0(kr)+\sum_{j=0}^{\infty}F_j(k)\,\Lambda_j(r)\right] \tag{V.10}$$

and

$$J_0(kr)=\sum_{j=0}^{\infty}F_j(k)\,\Omega_j(r) \tag{V.11}$$

where

$$\begin{aligned}
M(k) &= \gamma+\ln\frac{k}{2} && \text{(V.12)}\\
F_j(k) &= \frac{k^{2j}}{(-4)^j(j!)^2} && \text{(V.13)}\\
\Lambda_j(r) &= (\ln r-S_j)r^{2j} && \text{(V.14)}\\
S_j &= \sum_{\ell=1}^{j}\frac{1}{\ell} && \text{(V.15)}\\
\Omega_j(r) &= r^{2j} && \text{(V.16)}
\end{aligned}$$

where $\gamma$ is the Euler-Mascheroni constant.

By using the series expansion (V.10) in Eq. (V.8), one obtains

$$-\frac{1}{2\pi}\lim_{\varepsilon\to 0}\int_{\Gamma}\Big[\Big(M\,J_0+\sum_{j=0}^{\infty}F_j\,\Lambda_j\Big)\psi_{,n}(Q)-\Big(M\,J_{0,n}+\sum_{j=0}^{\infty}F_j\,\Lambda_{j,n}\Big)\,\psi(Q)\Big]\,\mathrm{d}Q=0 \tag{V.17}$$

which, by taking Eq. (V.9) into account, becomes

$$-\frac{1}{2\pi}\sum_{j=0}^{\infty}F_j(k)\lim_{\varepsilon\to 0}\int_{\Gamma}\Big[\Lambda_j(r)\,\psi_{,n}(Q)-\Lambda_{j,n}(r)\,\psi(Q)\Big]\,\mathrm{d}Q=0 \tag{V.18}$$

Substitution of the series expansion (V.11) into Eq. (V.9) results in

$$-\frac{1}{4}\sum_{j=0}^{\infty} F_j(k) \lim_{\varepsilon\to 0}\int_{\Gamma}\Big[\Omega_j(r)\,\psi_{,n}(Q) - \Omega_{j,n}(r)\,\psi(Q)\Big]\,\mathrm{d}Q = 0 \tag{V.19}$$

Now, by placing the series-expansion format of Eqs. (V.8) and (V.9), *i.e.* Eqs. (V.18) and (V.19), respectively, back into Eq. (V.7), we have

$$\sum_{j=0}^{\infty} F_j(k) \lim_{\varepsilon\to 0}\int_{\Gamma}\Big\{\Big[\frac{-\Lambda_j(r)}{2\pi} + i\frac{\Omega_j(r)}{4}\Big]\psi_{,n}(Q) - \Big[\frac{-\Lambda_{j,n}(r)}{2\pi} + i\frac{\Omega_{j,n}(r)}{4}\Big]\,\psi(Q)\Big\}\,\mathrm{d}Q = 0 \tag{V.20}$$

or

$$\sum_{j=0}^{\infty} \lambda^j \lim_{P_e\to P}\int_{\Gamma}\Big[\bar{G}_j(P_e,Q)\,\psi_{,n}(Q) - \bar{G}_{j,n}(P_e,Q)\,\psi(Q)\Big]\,\mathrm{d}Q = 0 \tag{V.21}$$

where $\lambda = k^2$ and

$$\bar{G}_j(P,Q) = \frac{1}{(-4)^j(j!)^2}\left[\frac{-\Lambda_j(r)}{2\pi} + i\frac{\Omega_j(r)}{4}\right] = \frac{r^{2j}\Big[2(S_j - \ln r) + i\pi\Big]}{4\pi(-4)^j(j!)^2} \tag{V.22}$$

$$\bar{G}_{j,n}(P,Q) = \frac{r^{2j-1}\Big[2j(S_j - \ln r) - 1 + ij\pi\Big]}{2\pi(-4)^j(j!)^2}\,\frac{\partial r}{\partial \boldsymbol{n}} \tag{V.23}$$

Unlike the original fundamental solution $G(P,Q)$, $\bar{G}_j(P,Q)$ in Eq. (V.22) is independent of the wave number $k$.

By taking the limit as $P_e \to P$, Eq. (V.21) becomes

$$c(P)\psi(P) = \sum_{j=0}^{\infty} \lambda^j \int_{\Gamma}\Big[\bar{G}_j(P,Q)\,\psi_{,n}(Q) - \bar{G}_{j,n}(P,Q)\,\psi(Q)\Big]\,\mathrm{d}Q \tag{V.24}$$

where the free term $c(P)\psi(P)$ appears in case $j = 0$ due to the $1/r$ singularity of $\bar{G}_{0,n}$ in Eq. (V.23).

In Eq. (V.22), as $r$ is finite and $\lim_{j\to\infty} \bar{G}_j(P,Q) = 0$, $\bar{G}_j$ represents a convergent alternating series. Thus, it is sufficient to use the first $(m+1)$ terms in the series for numerical analysis if the truncation error is small enough for the eigenvalues to be obtained with a desired accuracy.

By discretizing Eq. (V.24) with $N$ boundary elements and using the first $(m+1)$ terms of the series expansion on the right hand side of this equation, the following system of equation is obtained:

$$\sum_{j=0}^{m} \lambda^j \sum_{i=1}^{N} G_{ji\ell}\psi_{,n\ell} = \sum_{j=0}^{m} \lambda^j \sum_{i=1}^{N} H_{ji\ell}\psi_{\ell} \tag{V.25}$$

By applying the homogeneous boundary conditions, one gets

$$\sum_{j=0}^{m} \lambda^j \, \boldsymbol{A}_j \boldsymbol{u}_0 = \boldsymbol{0} \tag{V.26}$$

where $\boldsymbol{u}_0$ is the vector of unknown nodal degrees of freedom $\psi$ and $\psi_{,n}$ on the boundary $\Gamma$.

By rewriting Eq. (V.26) as

$$\bar{\boldsymbol{A}}(k)\boldsymbol{u}_0 = \boldsymbol{0} \tag{V.27}$$

where

$$\bar{\boldsymbol{A}}(k) = \sum_{j=0}^{m} \lambda^j \, \boldsymbol{A}_j = \sum_{j=0}^{m} k^{2j} \, \boldsymbol{A}_j \tag{V.28}$$

it can be seen that the contribution of the remaining terms $(j > m)$ in the polynomial to $\bar{\boldsymbol{A}}(k)$ is negligible if

$$k_{\max}^{2(m+1)} \cdot ||\boldsymbol{A}_{m+1}|| < \bar{\varepsilon} \tag{V.29}$$

where $k_{\max}$ is the largest eigenvalue sought, $||\boldsymbol{A}_{m+1}||$ denotes the 2-norm (maximum singular value) of matrix $\boldsymbol{A}_{m+1}$ and $\bar{\varepsilon}$ is a small number. The condition in Eq. (V.29) can be used as a guide for selecting a suitable value for $m$.

### 5.3.1 Search for the eigenvalues by scanning $k$ (Conventional method vs proposed method I)

By numerically implementing Eq. (V.4) with boundary elements, one gets the following system of equations:

$$\boldsymbol{B}(k)\boldsymbol{u}_0 = \boldsymbol{0} \tag{V.30}$$

Non-trivial solutions for $\boldsymbol{u}_0$ in Eq. (V.30) may be determined from the following condition:

$$\det[\boldsymbol{B}(k)] = 0 \tag{V.31}$$

It should be noted that, while the roots of Eq. (V.31) can be a complex number due to the use of numerical analysis, the eigenvalues in terms of $k$ are only the real roots of this equation.

The simplest technique (conventional method) for finding the real roots of Eq. (V.31) is to locate the local minima of $|\det[\boldsymbol{B}(k)]|$ by scanning $k$ within intervals $k_{\min} \leq k \leq k_{\max}$ using a small step size $\Delta k$. In this case, the number of search iterations is $N_k = (k_{\max} - k_{\min})/\Delta k$. As $\boldsymbol{B}(k)$ is dependent of $k$ and as it is a common practice to choose a very small value for $\Delta k$, corresponding to very large $N_k$, to avoid missing any eigenvalues during the scan, this conventional method is known to be extremely expensive as it requires the re-evaluation of the boundary integrals in Eq. (V.4) as well as the determinant in Eq. (V.31) at each iteration for a total of $N_k$ times.

In case of the proposed technique outlined in Section 2, the condition for having non-trivial solutions for $\boldsymbol{u}_0$ is (see Eq. (V.28))

$$\det[\bar{\boldsymbol{A}}(k)] = 0 \tag{V.32}$$

As indicated by Eq. (V.28), $\bar{\boldsymbol{A}}$ is a polynomial whose coefficients $\boldsymbol{A}_j$ are independent of $k$ because the integrals in Eq. (V.24) are not functions of $k$. This means that, for a given problem, these boundary integrals only need to be evaluated $(m+1)$ times to determine $(m+1)$ coefficients $\boldsymbol{A}_0, \boldsymbol{A}_1, \ldots, \boldsymbol{A}_m$. Then, as a polynomial (see Eq. (V.28)), $\bar{\boldsymbol{A}}$ can be quickly calculated for every value of $k$ within the interval $k_{\min} \leq k \leq k_{\max}$, even with a very small value of $\Delta k$. Since $m$ is typically much smaller than $N_k$, the proposed technique makes the search for the local minima of $|\det[\bar{\boldsymbol{A}}(k)]|$ (called method I in this paper) much more computationally effective than that for the local minima of $|\det[\boldsymbol{B}(k)]|$. A trade-off here is that method I requires more computer memory to store $(m+1)$ matrices $\boldsymbol{A}_j$. In case of very large scale analyses, a number of matrices $\boldsymbol{A}_j$ may need to be temporarily stored and accessed from a hard drive. However, the resulting increase in computing time should not be significant. The computational cost in this case is still a small fraction of that from using the conventional method to solve these very large scale problems.

### 5.3.2 Formulation of the standard and generalized eigenvalue problems (Proposed method II)

Equation (V.26) can also be rewritten as

$$\sum_{j=0}^{m} \boldsymbol{A}_j \boldsymbol{u}_j = \boldsymbol{0} \tag{V.33}$$

or

$$\sum_{j=0}^{m-1} \boldsymbol{A}_j \boldsymbol{u}_j = -\boldsymbol{A}_m \boldsymbol{u}_m \tag{V.34}$$

where $\boldsymbol{u}_j = \lambda \boldsymbol{u}_{j-1}$, thus $\boldsymbol{u}_j = \lambda^j \boldsymbol{u}_0$.

Premultiplying the left and right hand sides of Eq. (V.34) by $-\boldsymbol{A}_m^{-1}$ results in

$$-\boldsymbol{A}_m^{-1} \sum_{j=0}^{m-1} \boldsymbol{A}_j \boldsymbol{u}_j = \boldsymbol{A}_m^{-1} \boldsymbol{A}_m \boldsymbol{u}_m = \boldsymbol{I} \boldsymbol{u}_m = \lambda \boldsymbol{u}_{m-1} \tag{V.35}$$

where $\boldsymbol{I}$ is the identity matrix.

As $\boldsymbol{u}_i = \lambda \boldsymbol{u}_{i-1}$, one can write

$$\begin{array}{ccc} \boldsymbol{I}\boldsymbol{u}_{m-1} + \boldsymbol{0}\boldsymbol{u}_{m-2} + & \cdots + \boldsymbol{0}\boldsymbol{u}_1 + \boldsymbol{0}\boldsymbol{u}_0 & = \lambda \boldsymbol{u}_{m-2} \\ \vdots & \ddots & \vdots \\ \boldsymbol{0}\boldsymbol{u}_{m-1} + \boldsymbol{0}\boldsymbol{u}_{m-2} + & \cdots + \boldsymbol{I}\boldsymbol{u}_1 + \boldsymbol{0}\boldsymbol{u}_0 & = \lambda \boldsymbol{u}_0 \end{array} \tag{V.36}$$

Equations (V.35) and (V.36) form the following system:

$$\begin{bmatrix} -\boldsymbol{A}_m^{-1}\boldsymbol{A}_{m-1} & -\boldsymbol{A}_m^{-1}\boldsymbol{A}_{m-2} & \cdots & -\boldsymbol{A}_m^{-1}\boldsymbol{A}_1 & -\boldsymbol{A}_m^{-1}\boldsymbol{A}_0 \\ \boldsymbol{I} & \boldsymbol{0} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \vdots & & \ddots & & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{I} & \boldsymbol{0} \end{bmatrix} \begin{Bmatrix} \boldsymbol{u}_{m-1} \\ \boldsymbol{u}_{m-2} \\ \boldsymbol{u}_{m-3} \\ \vdots \\ \boldsymbol{u}_0 \end{Bmatrix} = \lambda \begin{Bmatrix} \boldsymbol{u}_{m-1} \\ \boldsymbol{u}_{m-2} \\ \boldsymbol{u}_{m-3} \\ \vdots \\ \boldsymbol{u}_0 \end{Bmatrix} \tag{V.37}$$

which represents an eigenvalue problem of the standard form $\boldsymbol{D}\boldsymbol{u} = \lambda \boldsymbol{u}$. Numerical techniques for large scale eigenvalue problems with sparse matrices can be employed to directly find the energy eigenvalues in terms of $\lambda = k^2$.

If matrix $\boldsymbol{A}_m$ in Eq. (V.37) is ill-conditioned, the standard eigenvalue problem (V.37) can be rewritten in the form of the generalized eigenvalue problem

$$\boldsymbol{V}\boldsymbol{u} = \lambda \boldsymbol{W}\boldsymbol{u} \tag{V.38}$$

where

$$\boldsymbol{V} = \begin{bmatrix} \boldsymbol{A}_{m-1} & \boldsymbol{A}_{m-2} & \cdots & \boldsymbol{A}_1 & \boldsymbol{A}_0 \\ \boldsymbol{I} & \boldsymbol{0} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \vdots & & \ddots & & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{I} & \boldsymbol{0} \end{bmatrix} \tag{V.39}$$

and

$$\boldsymbol{W} = \begin{bmatrix} -\boldsymbol{A}_m & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} & \cdots & \boldsymbol{0} \\ \vdots & & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{I} \end{bmatrix} \tag{V.40}$$

## 5.4 Numerical Examples

In this work, four various cases, including circular and rectangular domains under Dirichlet and/or Neumann boundary conditions, were investigated to verify the effectiveness and accuracy of the proposed methods I and II. The first 20 distinct eigenvalues were sought for each of the four examples considered herein. In order to implement the BEA formulations for the evaluation of the eigenvalues of the Helmholtz equation, MATLAB codes were developed. The MATLAB built-in function `eig` based on the LAPACK routine `ZGEEV` [24] was utilized to compute the eigenvalues from either the standard eigenvalue problem (Eq. (V.37)) or the generalized eigenvalue problem (Eq. (V.38)). The domain boundary was discretized

using quadratic elements. The condition in Eq. (V.29) where $\bar{\varepsilon} = 1.5 \times 10^{-3}$ was employed to select $m$ for each of the four numerical examples considered in this work.

While the eigenvalues of the Helmholtz equation are real numbers, the resulting eigenvalues obtained from using method II contain imaginary parts due to the use of numerical analysis. Therefore, only values with negligible imaginary parts are selected as the eigenvalues sought. It should be noted that, if the boundary of the domain is discretized into $N_n$ nodes, then solving the eigenvalue problems of Eqs. (V.37) or (V.38) would result in $(N_n \cdot m)$ potential eigenvalues and the majority of the resulting eigenvalues have large imaginary parts. For the proposed technique, they should be eliminated and not be regarded as spurious eigenvalues. Spurious eigenvalues are supposed to also have negligible imaginary parts but they are simply not the true eigenvalues of the problem. In addition, the number of the same eigenvalues found (with negligible imaginary parts) indicates the multiplicity of those eigenvalues. If needed, the eigenvectors can be determined by using MATLAB function `eig` or by solving for non-trivial solutions $\boldsymbol{u}$ to the equation $(\boldsymbol{D} - \lambda \boldsymbol{I})\boldsymbol{u} = \boldsymbol{0}$ (see Eq. (V.37)) after the eigenvalues $k$, thus $\lambda$, have been found.

### 5.4.1 Circular domain under Dirichlet boundary condition

Consider a circular domain of unit radius subjected to Dirichet boundary conditions ($\psi = 0$ along its boundary). The analytical solution for the eigenvalues $k$ for this problem is the roots of equation $J_\nu(k) = 0$ where $\nu = 0, 1, 2, \ldots$. Additionally, the circular boundary was discretized using 24 uniform quadratic elements ($N_e = 24$).

To assess the accuracy of the proposed methods I and II, a wave number increment $\Delta k = 10^{-4}$ was chosen for method I to search for the local minima of

Table 4. The first 20 distinct eigenvalues $k$ for the circular domain under Dirichlet boundary conditions ($m = 35, N_e = 24$).

| Analytical Solution | Method I | % error | Method II | % error | Analytical Solution | Method I | % error | Method II | % error |
|---|---|---|---|---|---|---|---|---|---|
| 2.4048 | 2.4048 | 0.000 | 2.4048 | 0.000 | 9.7610 | 9.7610 | 0.000 | 9.7610 | 0.000 |
| 3.8317 | 3.8317 | 0.000 | 3.8317 | 0.000 | 9.9346 | 9.9355 | 0.006 | 9.9355 | 0.006 |
| 5.1356 | 5.1356 | 0.000 | 5.1356 | 0.000 | 10.1735 | 10.1735 | 0.000 | 10.1735 | 0.000 |
| 5.5201 | 5.5201 | 0.000 | 5.5201 | 0.000 | 11.0647 | 11.0646 | 0.001 | 11.0646 | 0.001 |
| 6.3802 | 6.3801 | 0.002 | 6.3801 | 0.002 | 11.0864 | 11.0851 | 0.012 | 11.0851 | 0.012 |
| 7.0156 | 7.0156 | 0.000 | 7.0156 | 0.000 | 11.6198 | 11.6199 | 0.001 | 11.6199 | 0.001 |
| 7.5883 | 7.5883 | 0.000 | 7.5883 | 0.000 | 11.7915 | 11.7916 | 0.001 | 11.7916 | 0.001 |
| 8.4172 | 8.4173 | 0.001 | 8.4173 | 0.001 | 12.2251 | 12.2227 | 0.020 | 12.2227 | 0.020 |
| 8.6537 | 8.6537 | 0.000 | 8.6537 | 0.000 | 12.3386 | 12.3382 | 0.003 | 12.3382 | 0.003 |
| 8.7715 | 8.7712 | 0.003 | 8.7712 | 0.003 | 13.0152 | 13.0115 | 0.028 | 13.0115 | 0.028 |

$|\det[\bar{\boldsymbol{A}}(k)]|$ in the interval $2 \leq k \leq 13.2$ which contains the first 20 distinct eigenvalues. This $\Delta k$ allows the numerical results obtained from method I to be accurate up to four decimal places and it was also employed for the remaining examples considered in this work. By using Eq. (V.29) where $k_{\max} = 13.2$, the value $m = 35$ was suggested to be selected. The resulting minima are depicted in Fig. 17. The distinct eigenvalues obtained from both methods are compared in Table 4. As is shown, there is a perfect agreement between two groups of numerical results with a maximum percentage error less than 0.03 %. The CPU time used by MATLAB to run method I on the computer employed for this work was 453.71 seconds (for 112,000 iterations) while that used to run method II was 59.07 seconds.

### 5.4.2 Circular domain under Neumann boundary conditions

The circular domain of unit radius is again considered, but the domain is now subjected to Neumann boundary conditions ($\psi_{,n} = 0$ along its boundary). The

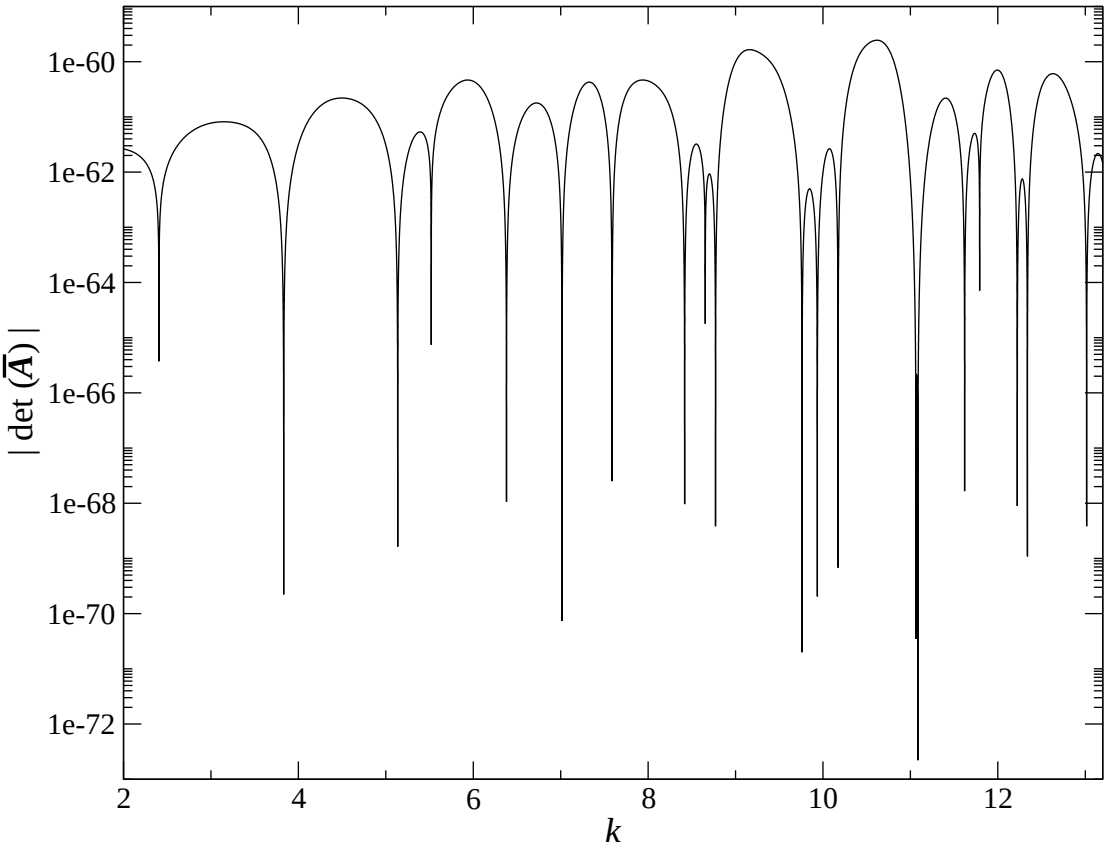


Figure 17. Plot of $|\det[\bar{\boldsymbol{A}}(k)]|$ for the circular domain under Dirichlet boundary condition.

exact solution for the eigenvalues $k$ of this problem is the roots of equation $\dfrac{\partial J_\nu(k)}{\partial k} = 0$ where $\nu = 0, 1, 2, \ldots$. For the BEA, the same discretization ($N_e = 24$) and choice of $m$ ($m = 35$) as in the previous example were used to find the eigenvalues in the interval $0 \leq k \leq 11.5$ which encompasses the first 20 distinct eigenvalues for this problem. It should be noted that the suggested value for $m$ is 34 according to the condition in Eq. (V.29) where $k_{\max} = 11.5$.

Figure 18 depicts the local minima of $|\det[\bar{\boldsymbol{A}}(k)]|$ in the aforementioned interval. All the first 20 eigenvalues obtained from methods I and II are represented in Table 5. Again, the numerical results from the two proposed methods are identical when those obtained from method II are rounded to the nearest ten

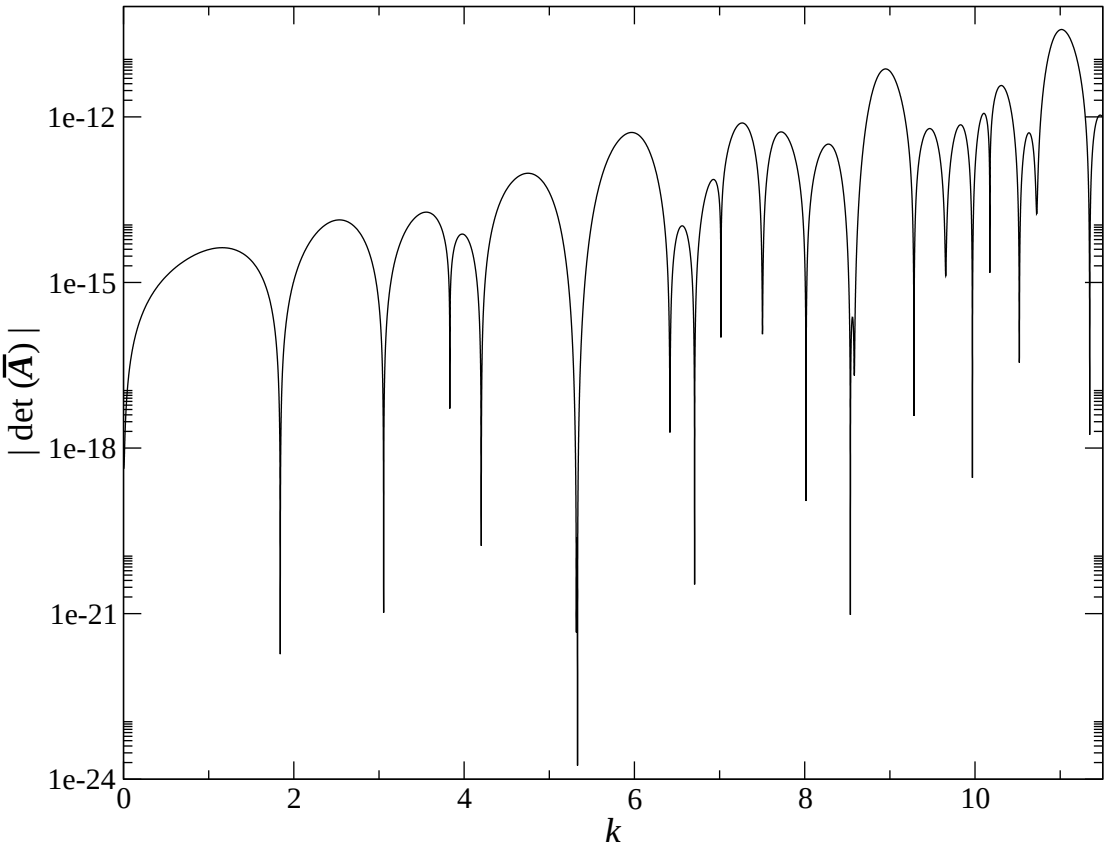


Figure 18. Plot of $|\det[\bar{\boldsymbol{A}}(k)]|$ for the circular domain under Neumann boundary condition.

thousandth. The percentage errors are less than 0.13% which show an excellent agreement with the analytical results. The CPU times for methods I and II were 458.24 seconds (115,000 iterations) and 56.13 seconds, respectively.

### 5.4.3 Rectangular domain under Neumann boundary conditions

In this example, a rectangular domain under Neumann boundary conditions was studied. The domain is defined by $0 \leq x \leq a$, $0 \leq y \leq b$ where $a = 1$ and $b = 0.8$. The analytical solution for the eigenvalues for this problem is given by [25],

$$k = \pi \sqrt{\left(\frac{p}{a}\right)^2 + \left(\frac{q}{b}\right)^2} \tag{V.41}$$

Table 5. The first 20 distinct eigenvalues $k$ for the circular domain under Neumann boundary conditions ($m = 35, N_e = 24$).

| Analytical Solution | Method I | % error | Method II | % error | Analytical Solution | Method I | % error | Method II | % error |
|---|---|---|---|---|---|---|---|---|---|
| 1.8412 | 1.8412 | 0.000 | 1.8412 | 0.000 | 8.0152 | 8.0154 | 0.002 | 8.0154 | 0.002 |
| 3.0542 | 3.0543 | 0.003 | 3.0543 | 0.003 | 8.5363 | 8.5364 | 0.001 | 8.5364 | 0.001 |
| 3.8317 | 3.8318 | 0.003 | 3.8318 | 0.003 | 8.5778 | 8.5826 | 0.056 | 8.5828 | 0.058 |
| 4.2012 | 4.2014 | 0.005 | 4.2014 | 0.005 | 9.2824 | 9.2828 | 0.004 | 9.2828 | 0.004 |
| 5.3176 | 5.3182 | 0.011 | 5.3181 | 0.009 | 9.6474 | 9.6558 | 0.087 | 9.6558 | 0.087 |
| 5.3314 | 5.3315 | 0.002 | 5.3315 | 0.002 | 9.9695 | 9.9696 | 0.001 | 9.9696 | 0.001 |
| 6.4156 | 6.4170 | 0.022 | 6.4170 | 0.022 | 10.1735 | 10.1735 | 0.000 | 10.1735 | 0.000 |
| 6.7061 | 6.7062 | 0.001 | 6.7062 | 0.001 | 10.5199 | 10.5207 | 0.008 | 10.5207 | 0.008 |
| 7.0156 | 7.0156 | 0.000 | 7.0156 | 0.000 | 10.7114 | 10.7245 | 0.122 | 10.7249 | 0.126 |
| 7.5013 | 7.5040 | 0.036 | 7.5040 | 0.036 | 11.3459 | 11.3461 | 0.002 | 11.3461 | 0.002 |

where $p, q = 0, 1, 2, \ldots$ are the zero points for the eigenmodes in the longitudinal and transverse directions, respectively.

Each side of the rectangular domain was discretized with 6 quadratic elements of equal lengths ($N_x = N_y = 6$). To find the first 20 distinct eigenvalues for this problem which are in the interval $0 \leq k \leq 15.8$, a value of $m = 28$ was suggested by Eq. (V.29) where $k_{\max} = 15.8$. However, a further analysis indicated that a choice of $m = 25$ is sufficient. The result from the search for the local minima of $|\det[\bar{\boldsymbol{A}}(k)]|$ obtained from method I is depicted in Fig. 19. The numerical results obtained from methods I and II are shown in Table 6 together with the analytical solution. Method I produces a maximum relative error of 0.08% while that number for method II is 0.04%. The CPU times needed by methods I and II were 453.78 seconds (for 158,000 iterations) and 35.97 seconds, respectively.

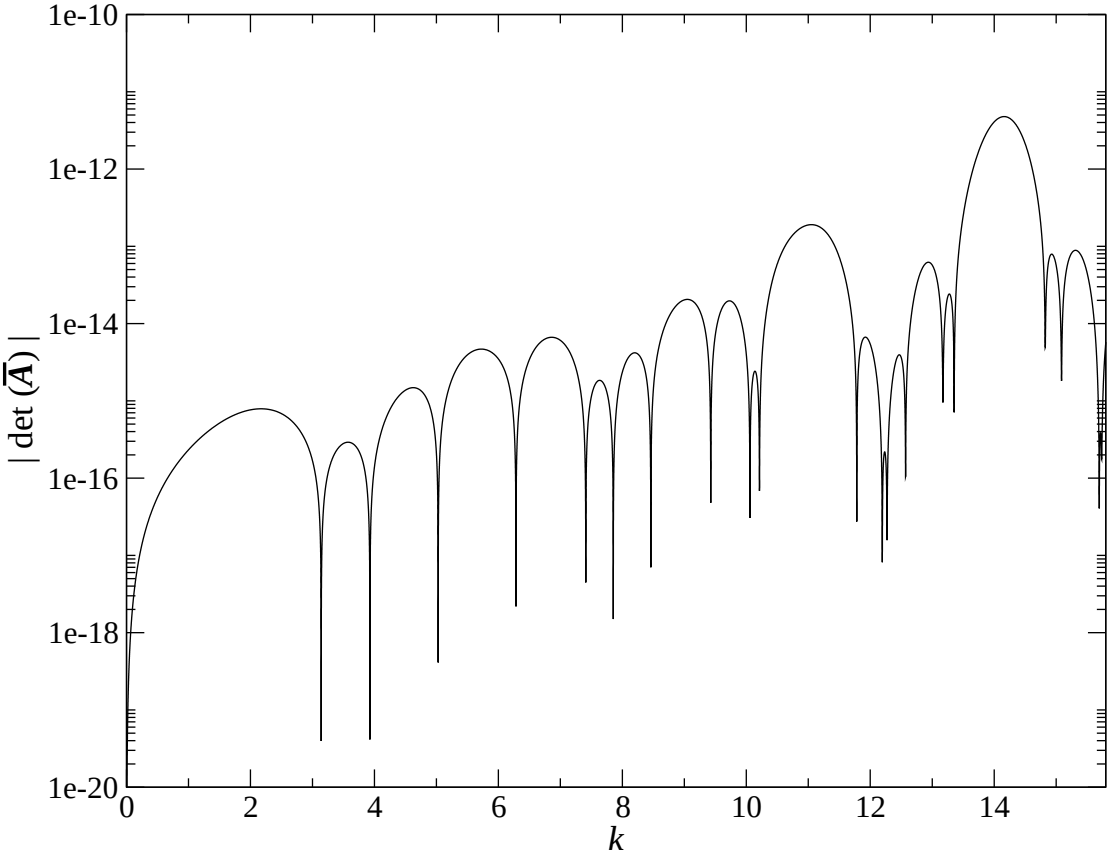


Figure 19. Plot of $|\det[\bar{\boldsymbol{A}}(k)]|$ for the rectangular domain under Neumann boundary condition.

### 5.4.4 Rectangular domain under both Dirichlet and Neumann boundary conditions

The last example involves a rectangular domain under mixed boundary conditions. The domain is defined by $0 \leq x \leq a$, $0 \leq y \leq b$ where $a = 0.9$ and $b = 0.4$. The side $x = 0$ is under Dirichlet boundary conditions while the other sides are under Neumann boundary conditions. For this problem, the analytical solution for the eigenvalues can be obtained from [25] as,

$$k = \pi \sqrt{\left(\frac{p - 0.5}{a}\right)^2 + \left(\frac{q}{b}\right)^2} \tag{V.42}$$

Table 6. The first 20 distinct eigenvalues $k$ for the rectangular domain under Neumann boundary conditions ($m = 25, N_x = N_y = 6$).

| p,q | Anal. Sol. | Method I | % error | Method II | % error | p,q | Anal. Sol. | Method I | % error | Method II | % error |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0,0 | 0.0000 | 0.0000 | – | 0.0055 | – | 3,1 | 10.2102 | 10.2128 | 0.026 | 10.2132 | 0.029 |
| 1,0 | 3.1416 | 3.1416 | 0.000 | 3.1416 | 0.000 | 0,3 | 11.7810 | 11.7822 | 0.010 | 11.7819 | 0.008 |
| 0,1 | 3.9270 | 3.9270 | 0.000 | 3.9270 | 0.000 | 1,3 | 12.1927 | 12.1948 | 0.018 | 12.1976 | 0.040 |
| 1,1 | 5.0290 | 5.0291 | 0.002 | 5.0291 | 0.002 | 3,2 | 12.2683 | 12.2710 | 0.022 | 12.2693 | 0.008 |
| 2,0 | 6.2832 | 6.2836 | 0.007 | 6.2836 | 0.007 | 4,0 | 12.5664 | 12.5702 | 0.031 | 12.5687 | 0.018 |
| 2,1 | 7.4094 | 7.4100 | 0.008 | 7.4101 | 0.009 | 4,1 | 13.1657 | 13.1729 | 0.055 | 13.1694 | 0.028 |
| 0,2 | 7.8540 | 7.8543 | 0.004 | 7.8543 | 0.004 | 2,3 | 13.3518 | 13.3541 | 0.018 | 13.3544 | 0.020 |
| 1,2 | 8.4590 | 8.4595 | 0.006 | 8.4596 | 0.007 | 4,2 | 14.8189 | 14.8241 | 0.035 | 14.8235 | 0.031 |
| 3,0 | 9.4248 | 9.4263 | 0.016 | 9.4263 | 0.016 | 3,3 | 15.0870 | 15.0864 | 0.004 | 15.0903 | 0.022 |
| 2,2 | 10.0580 | 10.0589 | 0.009 | 10.0584 | 0.004 | 0,4 | 15.7080 | 15.6956 | 0.079 | 15.7075 | 0.003 |

Five quadratic elements were employed to discretize each side of the rectangular domain ($N_x = N_y = 5$). The interval of interest for the wave number is $0 \leq k \leq 24.5$ as it holds the first 20 distinct eigenvalues for this problem. According to Eq. (V.29), a minimum value of 33 should be chosen for $m$. However, matrix $\boldsymbol{A}_m$ in the standard eigenvalue problem of Eq. (V.37) becomes ill-conditioned in double precision if $m \geq 20$. Hence, the generalized eigenvalue problem of Eq. (V.38) with $m = 35$ was used for method II instead. However, while method I was able to accurately produce the first 20 distinct eigenvalues within the interval $0 \leq k \leq 24.5$ (see Fig. 20 and Table 7), solving the generalized eigenvalue problem resulted in only the first 13 distinct eigenvalues with acceptable accuracy. To overcome this issue, a characteristic length $L_c = 0.07$ was employed to make the normalized size of the domain ($\bar{a} = a/L_c, \bar{b} = b/L_c$) large. In this case, per Eq. (V.1), the dimensionless wavenumber $\bar{k}$ is related to $k$ by $\bar{k} = L_c k$. The method using normalized coordinates for solving the generalized eigenvalue problem of Eq. (V.38)

is called method II(a) in this section. Twenty accurate eigenvalues produced by method II(a) can be found in Table 7 as they are compared to the analytical solution. The maximum percentage error for method II(a) is 0.54%.

To be able to solve the standard eigenvalue problem for this example, higher precision than the built-in double precision in MATLAB needs to be used to make the matrix in Eq. (V.37) well-conditioned. To demonstrate this, a precision using 34 decimal digits was also employed to find the first 20 distinct eigenvalues for this example. This number of digits is in accordance with IEEE 174-2008 standard for the quadruple precision and supported by the ADVANPIX multiprecision toolbox for MATLAB [26]. The method using quadruple precision for solving the standard eigenvalue problem of Eq. (V.37) is called method II(b) in this section.

As illustrated in Table 7, excellent agreement between the numerical results obtained from methods I and II(b) can be observed even though the results from method I were produced using double precision. The maximum percentage errors for methods I and II(b) were 0.53% and 0.44%, respectively.

In terms of computational effectiveness, the CPU times required for methods I and II(a) were 717.82 seconds (for 245,000 iterations) and 84.21 seconds, respectively. The computational cost of method II(b) was much higher due to the use of quadruple precision. As the accuracies of the resulting eigenvalues produced by all three methods I, II(a) and II(b) are comparable (see Table 7), it is suggested to use methods I or II(a) if the matrix of the standard eigenvalue problem in Eq. (V.37) is ill-conditioned.

## 5.5 Conclusion

By employing the series expansions of zero-order Bessel functions for the fundamental solution to the 2-D Helmholtz equation, a series of new fundamental

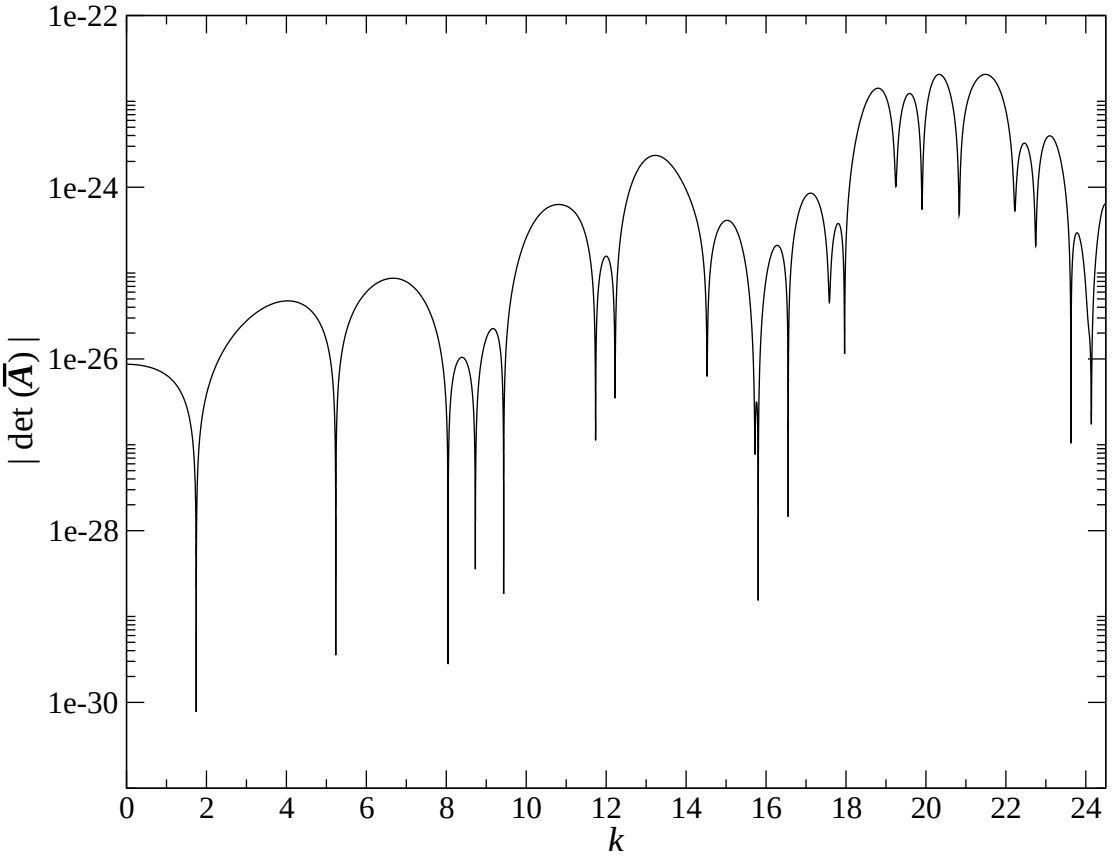


Figure 20. Plot of $|\det[\bar{\boldsymbol{A}}(k)]|$ for the rectangular domain under mixed boundary conditions.

solutions independent of the wave number $k$ was derived. As a result, the coefficient matrix of the Helmholtz BEA homogeneous system of equations can be represented as a polynomial in wavenumber $k$. This development resulted in (a) a much faster search for the Helmholtz eigenvalues by scanning $k$ over an interval of interest to find the local minima of the determinant of the aforementioned coefficient matrix, and (b) a formulation of the standard or generalized eigenvalue problems which can be used to directly solve for the eigenvalues without resort to any iterative method. By using the complex-valued fundamental solution of the Helmholtz operator, the proposed technique avoids producing any fictitious eigenvalues for simply connected domains [21] (Figs. 17, 18, 19 and 20 show no fictitious eigenvalues within the

Table 7. The first 20 distinct eigenvalues $k$ for the rectangular domain under mixed boundary conditions ($m = 35, N_x = N_y = 5$).

| p,q | Analytical Solution | Method I | % error | Method II(a) | % error | Method II(b) | % error |
|---|---|---|---|---|---|---|---|
| 0,0 or 1,0 | 1.7453 | 1.7445 | 0.046 | 1.7429 | 0.138 | 1.7445 | 0.046 |
| 2,0 | 5.2360 | 5.2349 | 0.021 | 5.2329 | 0.059 | 5.2349 | 0.021 |
| 0,1 or 1,1 | 8.0456 | 8.0451 | 0.006 | 8.0443 | 0.016 | 8.0451 | 0.006 |
| 3,0 | 8.7266 | 8.7277 | 0.013 | 8.7229 | 0.042 | 8.7277 | 0.013 |
| 2,1 | 9.4393 | 9.4356 | 0.039 | 9.4343 | 0.053 | 9.4356 | 0.039 |
| 3,1 | 11.7405 | 11.7359 | 0.039 | 11.7300 | 0.089 | 11.7359 | 0.039 |
| 4,0 | 12.2173 | 12.2236 | 0.052 | 12.2171 | 0.002 | 12.2236 | 0.052 |
| 4,1 | 14.5240 | 14.5263 | 0.016 | 14.5129 | 0.076 | 14.5263 | 0.016 |
| 5,0 | 15.7080 | 15.7230 | 0.096 | 15.7157 | 0.049 | 15.7227 | 0.094 |
| 0,2 or 1,2 | 15.8046 | 15.8049 | 0.002 | 15.8043 | 0.002 | 15.8049 | 0.002 |
| 2,2 | 16.5576 | 16.5552 | 0.015 | 16.5543 | 0.020 | 16.5552 | 0.015 |
| 5,1 | 17.5620 | 17.5854 | 0.133 | 17.5586 | 0.019 | 17.5853 | 0.133 |
| 3,2 | 17.9693 | 17.9653 | 0.022 | 17.9600 | 0.052 | 17.9653 | 0.022 |
| 6,0 | 19.1986 | 19.2487 | 0.261 | 19.2186 | 0.104 | 19.2488 | 0.262 |
| 4,2 | 19.8998 | 19.9037 | 0.020 | 19.8886 | 0.056 | 19.9038 | 0.020 |
| 6,1 | 20.7430 | 20.8349 | 0.443 | 20.7571 | 0.068 | 20.8348 | 0.443 |
| 5,2 | 22.2144 | 22.2262 | 0.053 | 22.2129 | 0.007 | 22.2255 | 0.050 |
| 7,0 | 22.6893 | 22.7468 | 0.253 | 22.7314 | 0.186 | 22.7468 | 0.253 |
| 0,3 or 1,3 | 23.6265 | 23.6283 | 0.008 | 23.6286 | 0.009 | 23.6283 | 0.008 |
| 7,1 | 24.0102 | 24.1362 | 0.525 | 24.1386 | 0.535 | 24.0861 | 0.316 |

interval of $k$ under consideration). For exterior and multiply connected domains, the Burton-Miller method can be employed in conjunction with the proposed technique to eliminate the fictitious eigenvalues. By considering various geometries under

different boundary conditions, the proposed technique shows that it can accurately and effectively produce a large number of the lowest eigenvalues. A hybrid (numerical and analytical) evaluation of the weakly singular boundary integrals in Eq. (V.24) and a more effective algorithm for finding the eigenvalues for the sparse matrix in Eq. (V.37) would result in a larger number of accurate eigenvalues that can be produced by the proposed method II. Finally, the proposed technique is readily extended to three dimensions and this investigation is currently being pursued by the authors.

## 5.6 Acknowledgements

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## 5.7 Conflict of Interest:

The authors declare that they have no conflict of interest.

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# CHAPTER VI

# CONCLUSIONS AND FUTURE WORK

In this dissertation, a model-based systems engineering methodology has been developed in order to cope with the complexities of quantum systems. This approach is applied to the four main phases of system analysis, system design, system manufacturing, and system verification, validation and testing during the system lifecycle. Quantum dot solar cells are selected as an exemplar quantum system during this system development procedure. It is shown that using appropriate models in the system development procedure can help to obtain a better understanding of these complex systems, and perform the system design and evaluation more accurately. All of the models used in the analysis stage are prepared by employing SysML in Cameo Systems Modeler software package.

In particular, the main focus of current research is on the analysis and design stages of the development of quantum dot solar cells. This system development procedure is associated with several important steps. One of these main steps is to identify the governing equation of the quantum system. Since the time-independent Schrödinger equation is the governing equation of most quantum systems, the key element in the analysis and design of these systems is to solve this governing equation under various boundary conditions, such as Dirichlet and Neumann boundary conditions, for finding energy eigenvalues of the quantum systems. It is worthwhile to mention that by solving this eigenvalue problem, the important features of the quantum system like its energy levels can be obtained which are

required for the design stage. As the BEM has several key advantages in solving the time-independent Schrödinger equation, novel boundary integral formulations were presented in Chapters IV and V to effectively and accurately solve this equation under various boundary conditions. Several examples representing quantum billiards with different geometries were shown to demonstrate the accuracy and effectiveness of the proposed technique. The reason for considering quantum billiards is that the behavior of particles in the quantum billiards is similar to the movement of electrons in the quantum systems. This process is feasible by making the BEM integrand independent of the wave number.

After performing the system analysis stage using SysML and the system design using MATLAB, these two parts were integrated in Cameo Systems Modeler. The integration process for all these steps can be carried out using parametric diagrams to show the impact of each system parameter on the overall system performance. After providing models for system manufacturing and testing, it is illustrated that the system integration can also be performed for verification, validation, and testing process to confirm that the system design stage is accomplished successfully.

Future works are recommended as follows:

- Develop a boundary integral formulation for directly solving the standard and generalized eigenvalue problems for the 3-D time-independent Schrödinger equation under both Dirichlet and Neumann boundary conditions.
- Extend the current framework to develop a complete MBSE framework for quantum systems.
- Apply the proposed boundary integral formulation to optimize the technical parameters of quantum dot solar cells including inter-dot spacing, quantum dot shape, size, etc.

- Apply the proposed numerical method to other problems governed by the time-independent Schrödinger or Helmholtz equation, such as acoustics.

# APPENDICES

# Appendix A

## Modeling Details Supplementing Article 1

In this part, the additional information that is required to accomplish the development of quantum dot solar cells is provided. According to the system lifecycle processes indicated in systems engineering Vee diagram[1] (Fig. A.1), there are several steps in each product development. These steps are categorized into four main groups: systems analysis, system design, system manufacturing, and system testing. Most of the information reported here is for the system analysis phase, and the remaining parts are related to the system design and verification, validation, and testing (VV&T).

### A.1 Supplementary Information for System Analysis

Modeling quantum systems can be performed based on statistical data taken from experiments. In other words, one should establish a model for quantum devices

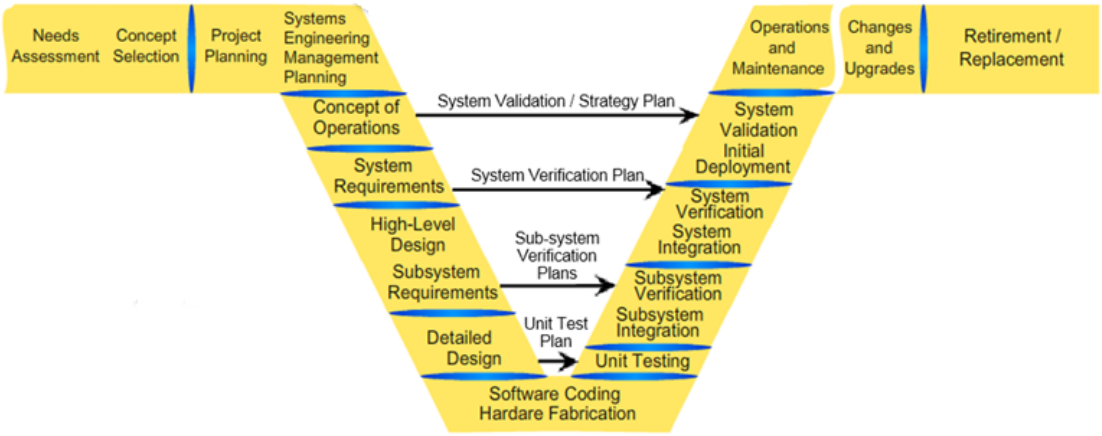


Figure A.1. Systems engineering Vee diagram.

[1]https://connected-corridors.berkeley.edu/planning-system/planning-system-development-semp

that is in agreement with experimental results as well as the quantum theories. This model may not be in complete consistency with the actual physical system. In this regard, the quantum system should be assumed as a black box, and then an approximate model is created according to the experimental data based on quantum mechanics. The first step in developing a quantum system using MBSE is the system analysis. The main stages of the system analysis using MBSE are as below:

- Derive stakeholder requirements
- Prepare the concept of operation (ConOp), including the system context
- Define quantum system domain (domain diagram)
- Identify systems uses (Use Case diagram)
- Define system requirements
- Decompose uses to tasks
- Define system architecture
- Engineering analysis

The system modeling language (SysML) is employed here as an intuitive tool to perform the previously-mentioned analysis. Despite the fact that this procedure may not include every detail in the analysis of the quantum systems, it gives a better understanding of quantum systems and the complexity in their architecture. As mentioned before, quantum dot solar cells are the new generation of the solar cells which represent an attempt to improve the performance of current solar cells available in the market. The influence of multiple parameters on the behavior of such systems has made it difficult to predict the behavior of these complex systems. Therefore, the MBSE method is applied to these systems to model such quantum

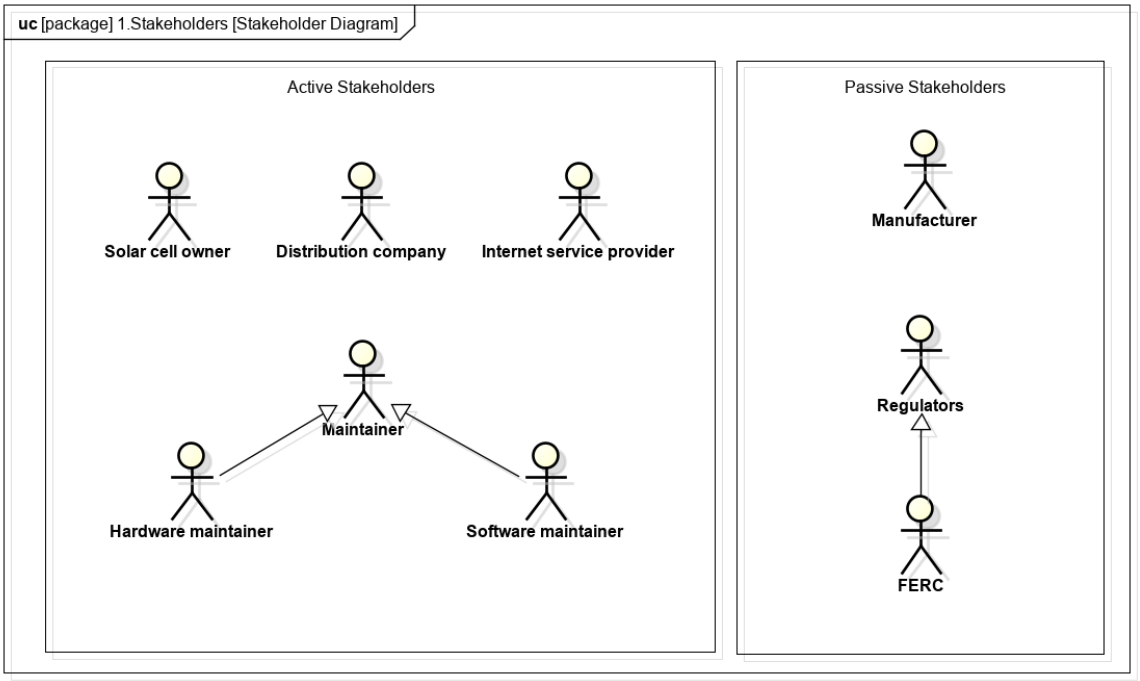


Figure A.2. Solar cells stakeholder diagram.

systems more easily. The stages of system context definition, system decomposition to the relevant tasks, and design of system logical and physical architecture, which have not been described in Article 1, are discussed here.

**A.1.1 Stakeholders:**

Quantum systems like any other system which is going to be developed, has active stakeholders who will be the main system users, or the people who interact with the system directly. There are also passive stakeholders that affect the system indirectly. These stakeholders should be identified for each quantum system at the initial steps of the product development, because it is crucial to identify their desirements in an appropriate way. These stakeholders for the quantum dot solar cells, as a representative quantum system, are depicted in Fig. A.2. The interaction of these stakeholders with the solar cell system is demonstrated in the form of a context diagram, as demonstrated by Fig. A.3.

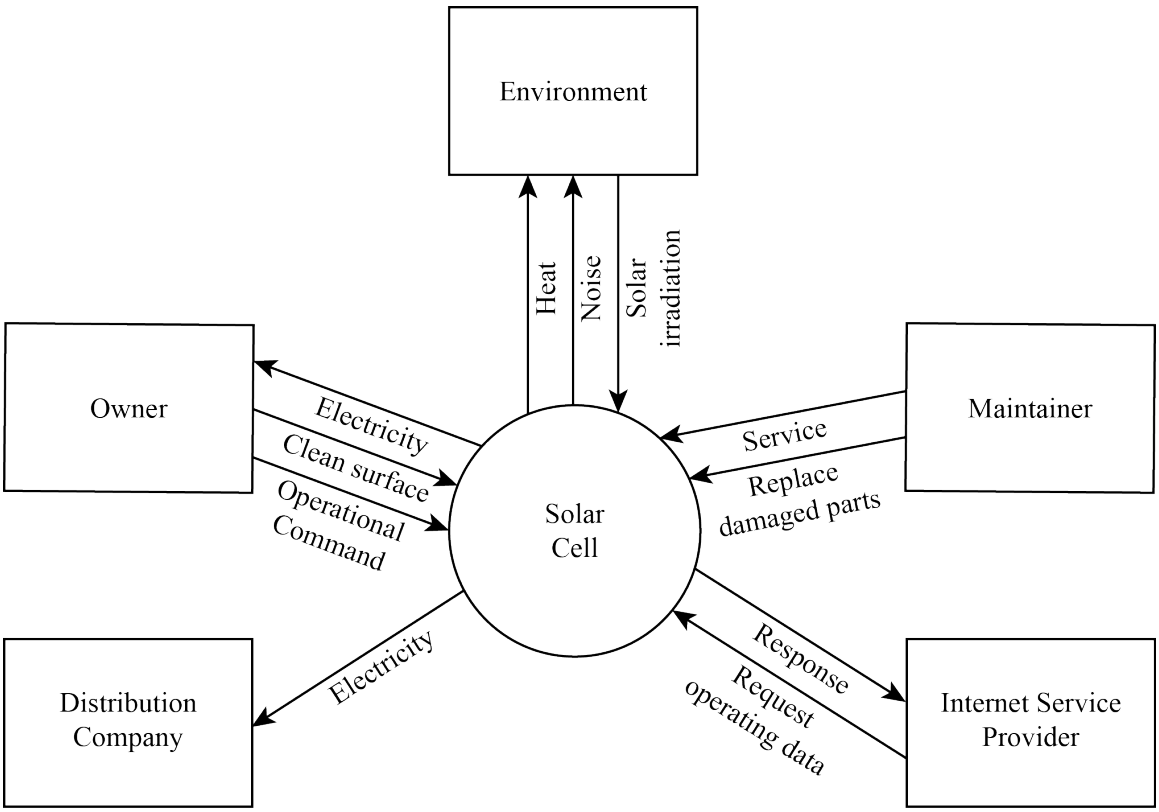


Figure A.3. The context diagram of the solar cell system.

### A.1.2 System Decomposition

In this stage, the quantum system uses and functionalities are decomposed into relevant tasks and activities. The activity diagram prepared for a quantum dot solar cell as the selected system of interest is indicated in Fig. A.4. According to this diagram, the solar cell should be exposed to solar irradiation to absorb solar photons. Then if the photon energy is high enough, the electron will be excited and move to the higher energy levels. This excited electron can relax and move to a lower energy level, and release a photon. Consequently, the released photon can create a new electron-hole pair. With this procedure, up to three excitons may be created by each solar photon, which increase the system efficiency accordingly.

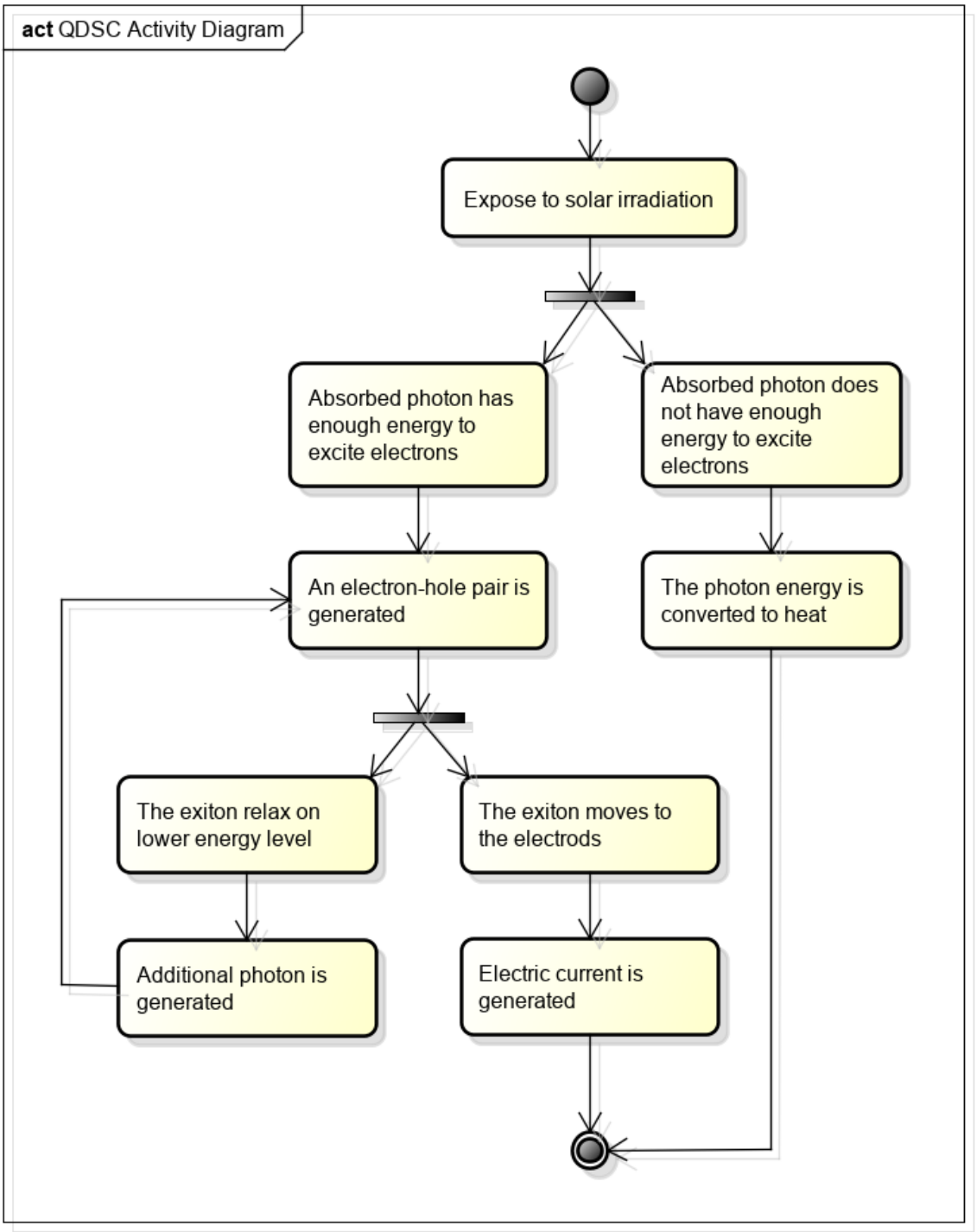


Figure A.4. Activity diagram for the top level use case of the solar cell.

### A.1.3 System Architecture

In the next step, the quantum system logical architecture design is performed based on the stakeholders and also the derived system requirements. The system requirements to logical architecture allocation diagram is illustrated in Fig. A.5. According to this diagram, logical subsystems are considered to enable electricity generation with high efficiency, and also remote monitoring of the amount of the generated electrical power. So, both main stakeholder requirements are met. Moreover, a logical architecture diagram can be used to show the newly designed architecture in a better way (Fig. A.6). To have a better understanding of this concept, the external interfaces of the solar cell, including the inputs and outputs of this system, can be indicated using ports in a block definition diagram (Fig. A.7). Additionally, internal block diagrams (IBD) can be employed to represent each logical subsystem with more details (Fig. A.8).

A physical architecture can also be considered for the new system according to the designed logical architecture. The logical to physical allocation diagram demonstrates all the required physical modules based on the defined logical aspects. The allocation diagram showing the relevant allocations between the logical and physical architectures is depicted in Fig. A.9. Six main modules are defined in the physical architecture to meet all the requirements (Fig. A.10).

## A.2 Supplementary Information for System Manufacturing

In order to employ model-based systems engineering to model the quantum systems manufacturing procedure, three main models should be prepared:

- Product model
- Process model
- Resources/Facility models

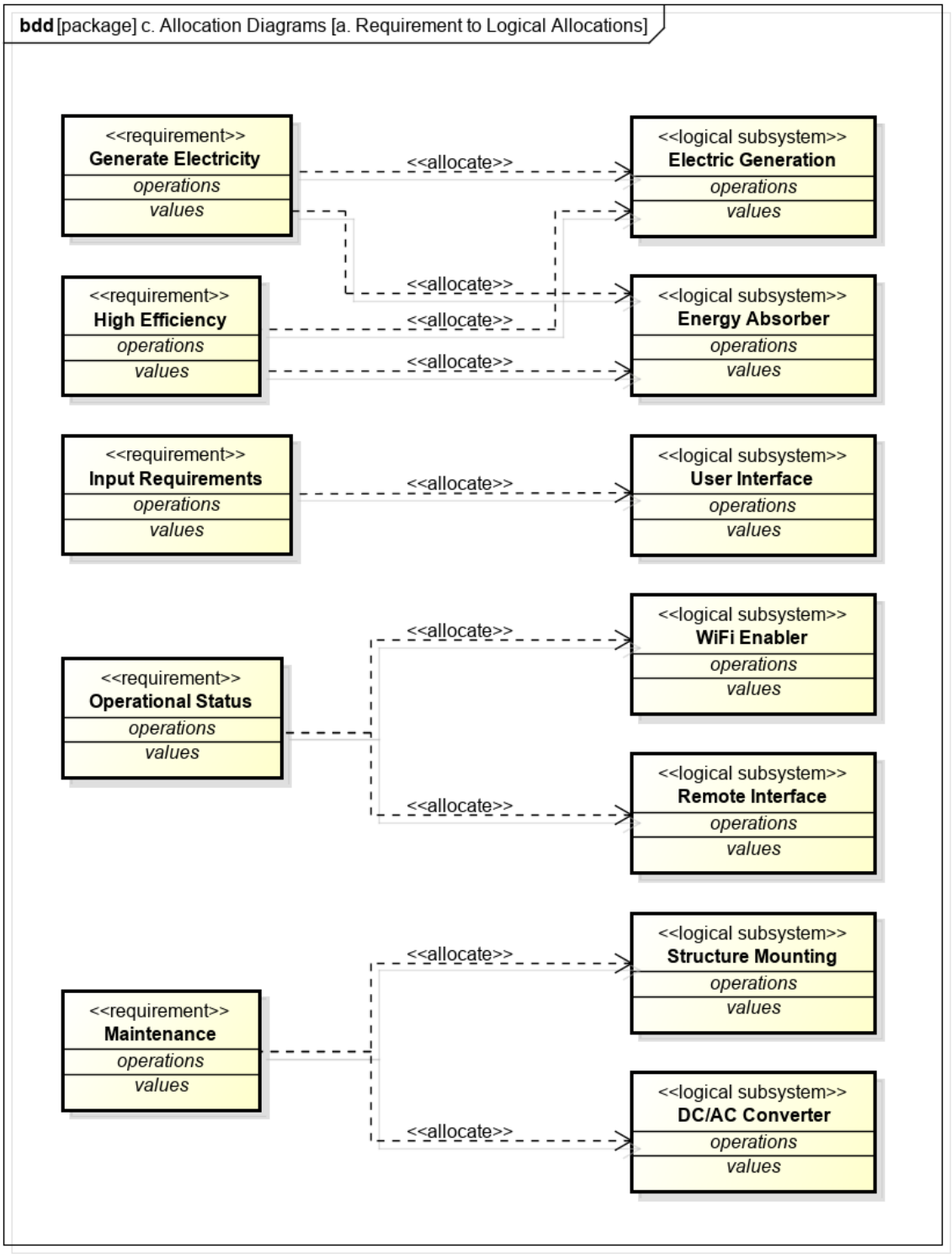


Figure A.5. Requirements to logical architecture allocations of the solar cell.

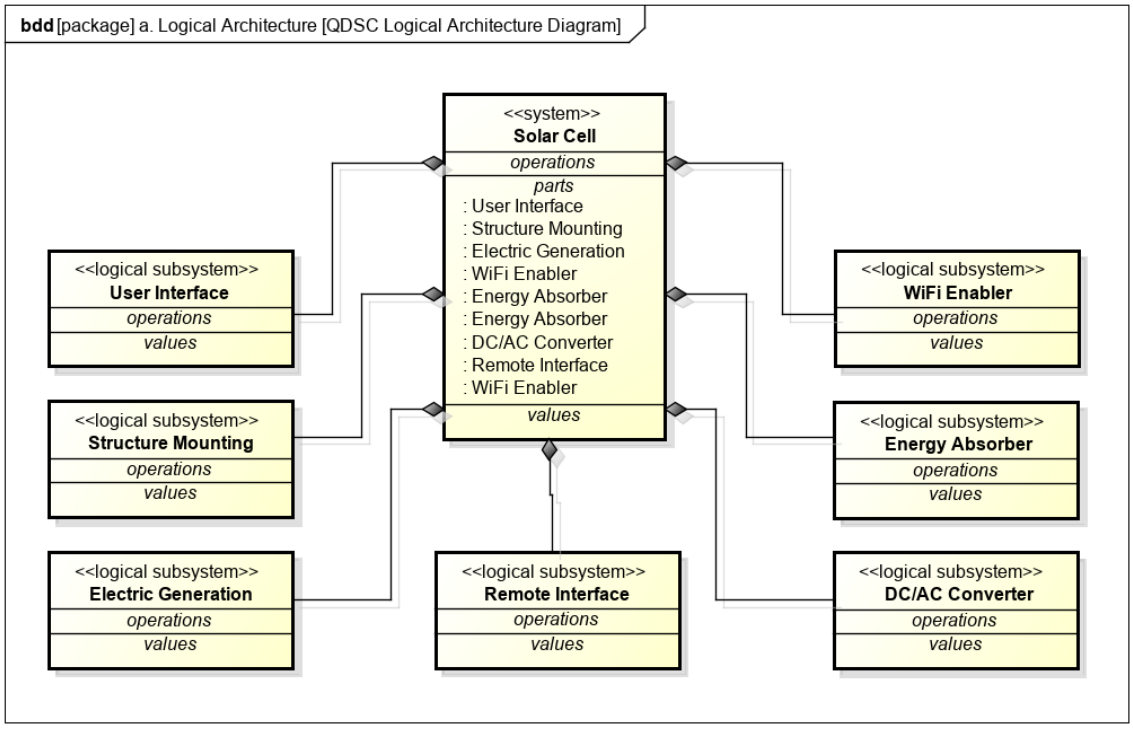


Figure A.6. Logical architecture diagram of the solar cell.

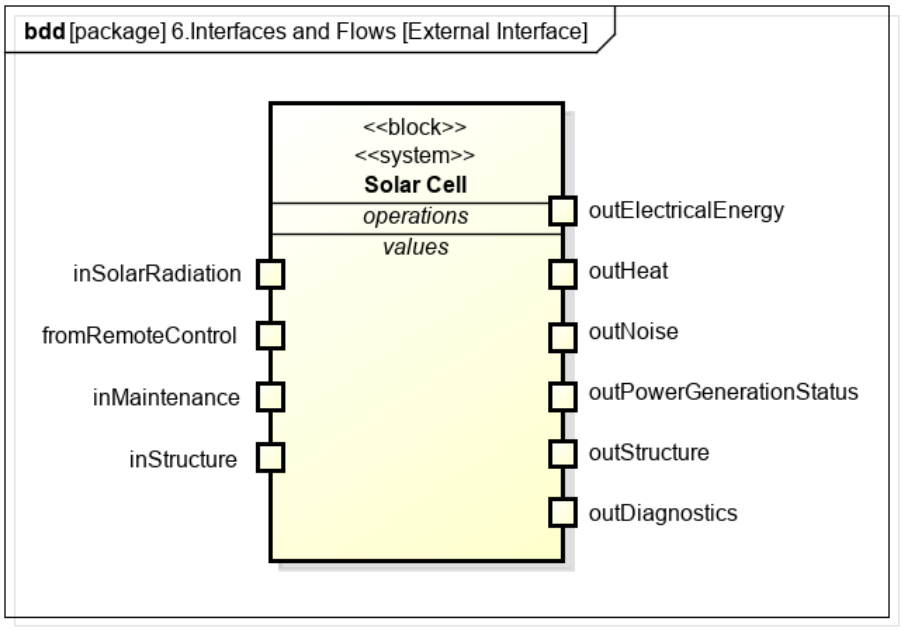


Figure A.7. External interfaces of the solar cell.

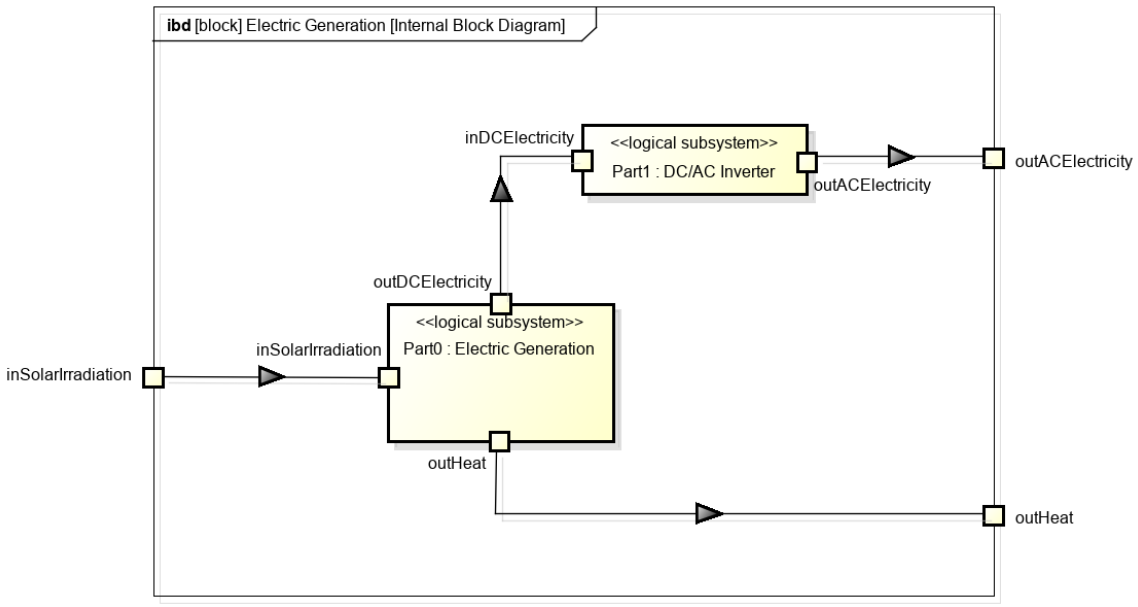


Figure A.8. Internal block diagram for the electricity generation.

The process model has been described completely in the first article. Here, the product model is prepared for the quantum dot solar cells as a typical quantum system selected in this research. Various systems and subsystems used in the quantum dot solar cell systems are illustrated in Fig. A.11. In addition, Fig. A.12 represents a facility model prepared by National Institute of Standards and Technology (NIST), which can be employed for the purpose of this research as well[2].

### A.3 Application of the Proposed Numerical Method in the Analysis, Design, and VV&T of Quantum Dot Solar Cells

In this section, the application of the proposed technique in the analysis, design, and VV&T of quantum dot solar cells as a typical quantum system is represented. As previously mentioned, one of the most important aspects of the process of analyzing and designing quantum systems and developing new devices is to solve the energy eigenvalue problem of the Helmholtz or time-independent

[2]https://www.nist.gov/document/16dmbisevalueproposition2019aprv2-timothysprockpdf

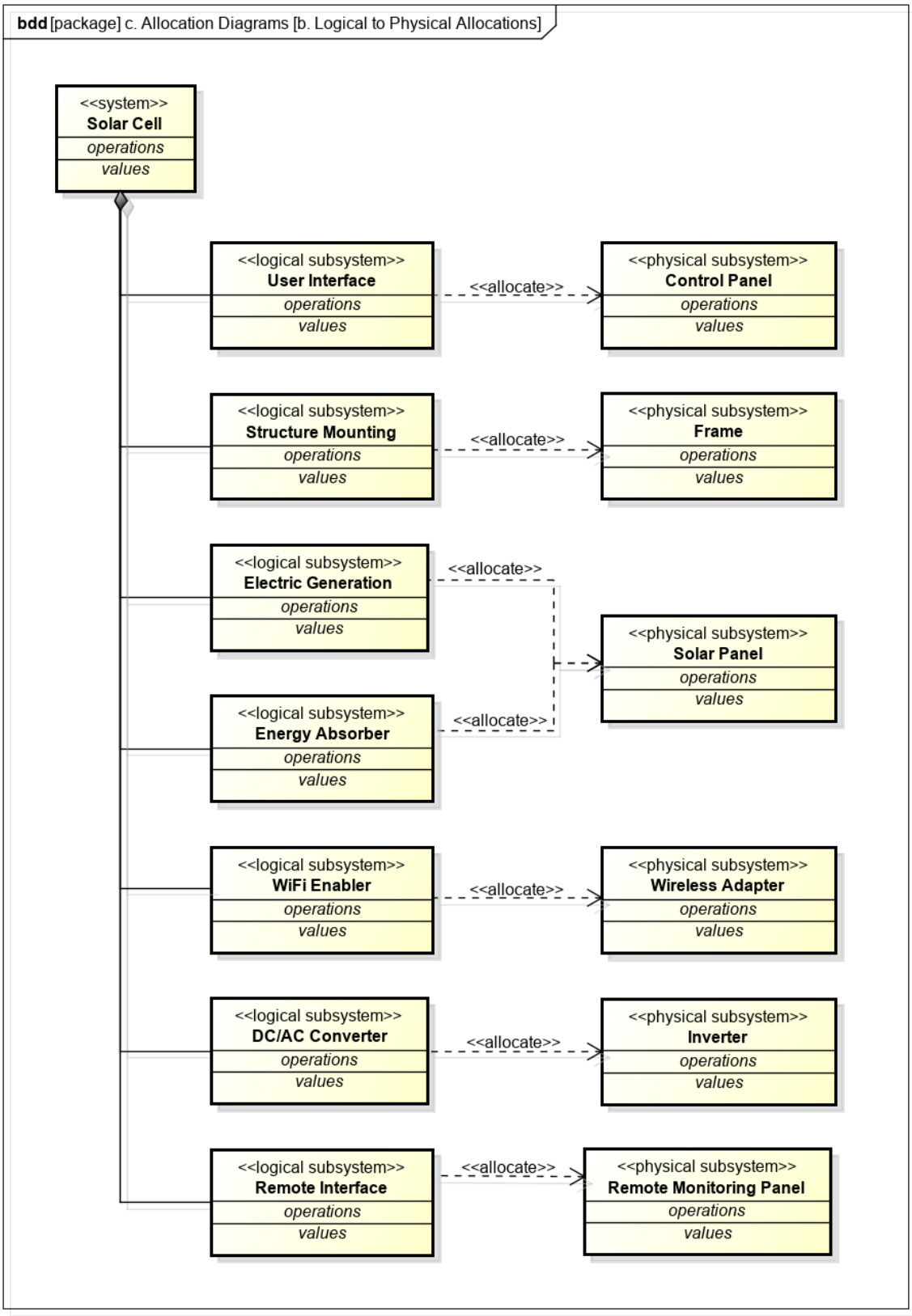


Figure A.9. Logical to physical architecture allocations.

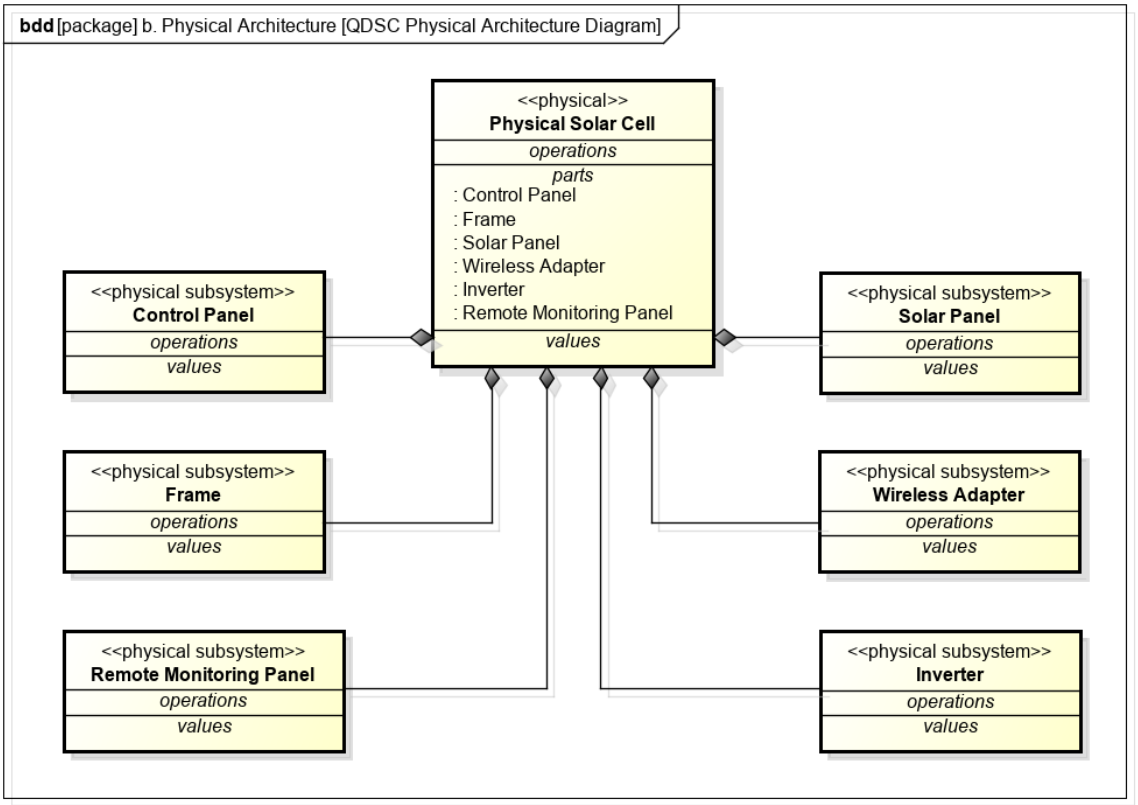


Figure A.10. Physical architecture diagram of the solar cell.

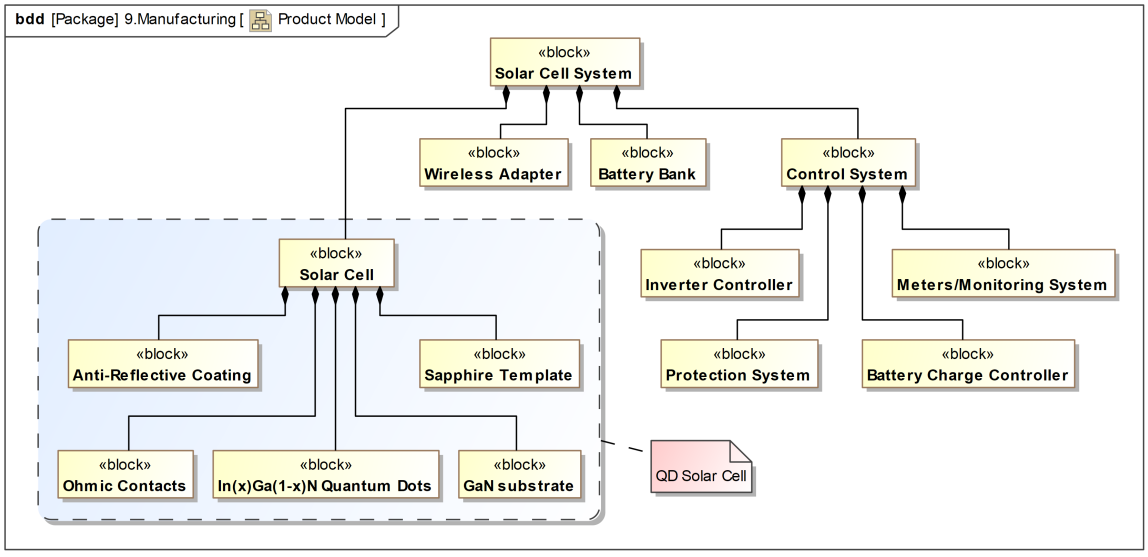


Figure A.11. Manufacturing product model.

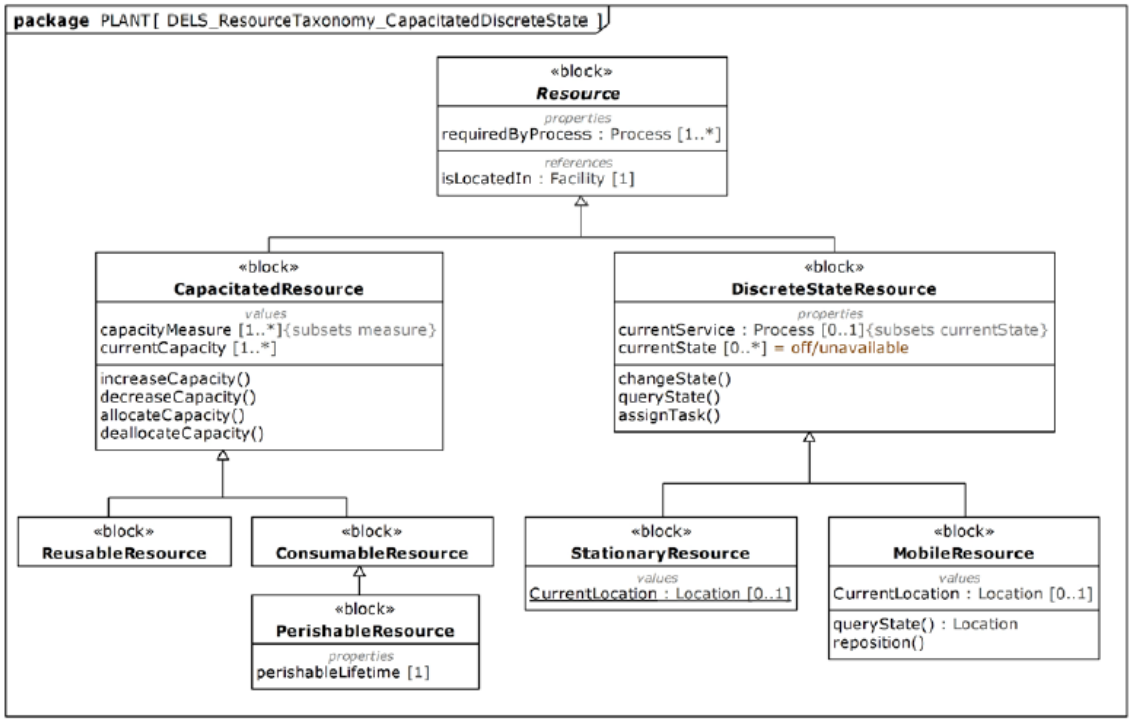


Figure A.12. Manufacturing facility model.

Schrödinger equation, which is the governing equation of such systems. This is one of the main steps in quantum systems design, as is shown in the system design model in Fig. 8. The remainder of this section describes how these systems can be designed more effectively and also accurately using MBSE and a novel BEM approach.

As mentioned previously, the performance of quantum dot solar cells and their efficiency are in direct relationship with the layout of quantum dots in the semiconductors, including their size, shape, and inter-dot spacing. In this regard, obtaining the energy eigenvalues will help in the determination of the particles state energy, and evaluating the efficiency of the quantum dot solar cells for each specific geometry. Furthermore, as it is described in Article 1, it is important to manufacture quantum dot solar cells uniformly. Therefore, a uniform arrangement

of the quantum dots is crucial during system design stage. Several researches have been performed recently to find an optimal quantum dot layout in this regard. As one of the main goals of our research, the proposed technique can help researchers to carry out the required computations more efficiently. Figure A.13 depicts the models that can be employed for this study. The experimental results can be used to find the appropriate boundary conditions while modeling and simulating such systems. Therefore, having knowledge of both theoretical and experimental aspects of the system will contribute to an appropriate design and accurate results.

The Helmholtz or time-independent Schrödinger equation for quantum dot solar cells can be solved more conveniently using numerical methods like the BEM instead of analytical approaches. As a matter of fact, the problem can be solved on the boundary of the quantum dots as the domain boundary (instead of the entire domain), while the substrate is assumed as the exterior part of the region. As indicated in Fig. A.13, the Ben-Daniel-Duke boundary condition is an appropriate selection for this case based on the experimental and operational conditions of these devices. According to this boundary condition, the amount of the wave function on the quantum dot boundary should be equal for both the interior and exterior regions (the quantum dot is known as the interior, and the substrate is known as the exterior):

$$\left[\Psi_{QD}(x)\right]_{x=\pm\frac{L}{2}} = \left[\Psi_{Substrate}(x)\right]_{x=\pm\frac{L}{2}} \tag{A.1}$$

Furthermore, the relationship between the derivative of the wave function for these two regions is expressed as below for a rectangular quantum dot[3]:

$$\frac{1}{m^*(\mathrm{In_xGa_{(1-x)}N})}\left[\frac{d\Psi_{QD}(x)}{dx}\right]_{x=\pm\frac{L}{2}} = \frac{1}{m^*(\mathrm{GaN})}\left[\frac{d\Psi_{Substrate}(x)}{dx}\right]_{x=\pm\frac{L}{2}} \tag{A.2}$$

[3]A. El Aouami, E. Feddi, A. Talbi, F. Dujardin, and C. A. Duque, "Electronic state and photoionization cross section of a single dopant in GaN/InGaN core/shell quantum dot under magnetic field and hydrostatic pressure," *Applied Physics A*, vol. 124, no. 6, pp. 1–11, 2018.

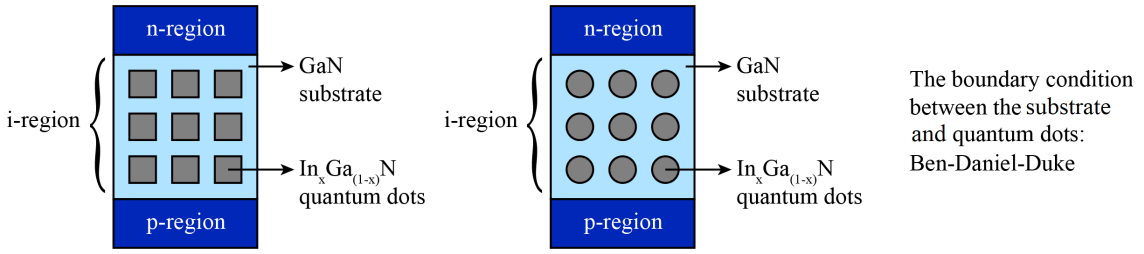


Figure A.13. Schematic diagram of the proposed model for the quantum dot solar cells.

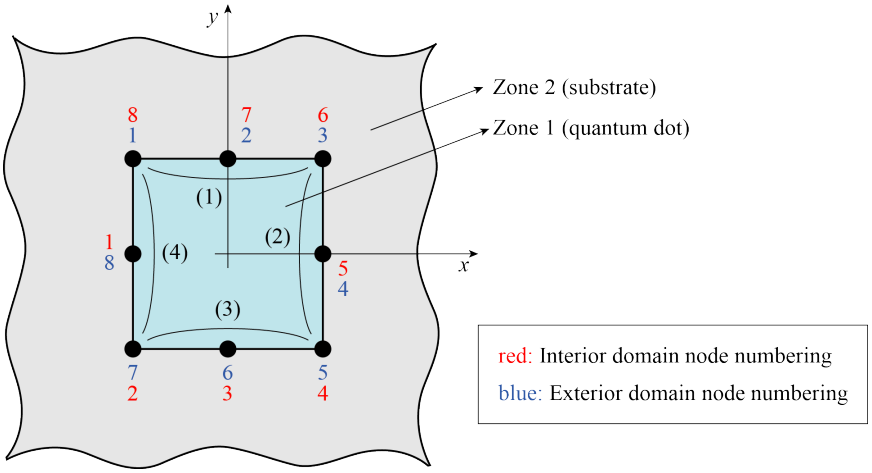


Figure A.14. BEM model for a typical square quantum dot.

where $L$ is the quantum dot length, $\Psi$ is the wave function, and $m^*$ is the particle effective mass. It should be noted that Eq. A.2 can similarly be written for the $y$-axis. By considering the boundary integral equation for each element on the quantum dot boundary, the BEM system of equations will be achieved. For this purpose, Fig. A.14 illustrates the two-dimensional BEM model for a typical square quantum dot. The time-independent Schrödinger equation for this case can be represented as,

$$\mathcal{H}\Psi(X,Y) = E\Psi(X,Y) \tag{A.3}$$

where $\Psi$ is the wave function, $E$ is the particle energy level, and $\mathcal{H}$ is the Hamiltonian of the system which is given as,

$$\mathcal{H} = \mathcal{H}(X) + \mathcal{H}(Y) \tag{A.4}$$

where,

$$\mathcal{H}(p) = -\frac{\hbar^2}{2m}\triangle_p + V_p \ , \quad p \in \{X, Y\} \tag{A.5}$$

In this equation, $V$ is the potential energy, $\hbar$ is the reduced Planck's constant, and $m$ is the particle mass. Equation A.3 is an implicit equation for $E$ and $\Psi$, so this differential equation can be replaced by the following implicit integral equation[4],

$$\psi(\mathbf{r}') = \frac{\hbar^2}{2m}\oint_\Gamma \left[\psi_n(\mathbf{r})\partial_\upsilon G(\mathbf{r}, \mathbf{r}'; E_n) - G(\mathbf{r}, \mathbf{r}'; E_n)\partial_\upsilon \psi_n(\mathbf{r})\right] \mathrm{d}s(\mathbf{r}) \tag{A.6}$$

where $\partial_\upsilon \equiv \upsilon(\mathbf{r}) \cdot \nabla_r$ in which $\upsilon$ denotes the exterior normal unit vector to the boundary $\Gamma$. Moreover, $\mathrm{d}s$ is an infinitesimal length on the boundary, $\mathbf{r}$ and $\mathbf{r}'$ are functions of $X$ and $Y$, and $G$ can be defined as,

$$G(\mathbf{r}, \mathbf{r}') = -\frac{m}{\pi\hbar^2} K_0\left(-ik|\mathbf{r} - \mathbf{r}'|\right) \tag{A.7}$$

where $K_0$ is the second kind modified Bessel of order zero, $i$ is the imaginary unit, and $k$ is the wave number of the particle. By solving Eq. A.6 for each element in Fig. A.14, a system of equations like $\mathbf{Bx} = \mathbf{0}$ can be derived in which $\mathbf{B}$ is the matrix of coefficients and $\mathbf{x}$ is the vector of unknowns. If we consider the BEM

[4] I. Kosztin and K. Schulten, "Boundary integral method for stationary states of two-dimensional quantum systems," *International Journal of Modern Physics C*, vol. 8, no. 02, pp. 293–325, 1997.

system of equations for zone (1) and (2) as follows,

$$\begin{bmatrix} \mathbf{A_1} & \mathbf{A_2} \end{bmatrix} \begin{Bmatrix} \mathbf{u}^{(1)} \\ \mathbf{q}^{(1)} \end{Bmatrix} = \mathbf{0} \ , \quad \text{for zone (1)} \tag{A.8}$$

$$\begin{bmatrix} \mathbf{B_1} & \mathbf{B_2} \end{bmatrix} \begin{Bmatrix} \mathbf{u}^{(2)} \\ \mathbf{q}^{(2)} \end{Bmatrix} = \mathbf{0} \ , \quad \text{for zone (2)} \tag{A.9}$$

where $\mathbf{u}^{(1)}$ and $\mathbf{q}^{(1)}$ are the unknown variables of zone (1), while $\mathbf{u}^{(2)}$ and $\mathbf{q}^{(2)}$ are the unknown variables of zone (2), then matrix $\mathbf{B}$ can be derived by,

$$\mathbf{B} = \begin{bmatrix} \mathbf{A_1} & \mathbf{A_2} \\ \mathbf{B_1} & c\mathbf{B_2} \end{bmatrix} \tag{A.10}$$

where,

$$c = \frac{m^*(\text{quantum dot material})}{m^*(\text{substrate material})} \tag{A.11}$$

The eigenvalues of Eq. A.10, which can be obtained by solving $det(\mathbf{B}) = 0$, are identical to the energy eigenvalues of the quantum dot solar cell governing equation. The novel BEM procedure proposed in Articles 2 and 3 can be employed to solve this energy eigenvalue problem more effectively.

## Appendix B

## Mathematical Details Supplementing Articles 2 and 3

The energy eigenvalues of Helmholtz or time-independent Schrödinger equation should be identified in order to study the behaviour of quantum billiards. The time-independent Schrödinger equation can be expressed as follows:

$$\hat{H}\psi_n(\mathbf{r}) \equiv \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r}) \tag{B.1}$$

where $V$ is the potential, $H$ is the Hamiltonian, and $E_n$ and $\psi_n$ are the energy eigenvalue and its relevant eigenfunction, respectively. According to this equation, the Hamiltonian for a quantum billiard including a particle with mass $m$ moving in a simply connected region $D$ can be written as:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \tag{B.2}$$

By using the Green's function $G(\mathbf{r}, \mathbf{r}'; E)$ for the differential operator $E - \hat{H}$, we have:

$$\left[E - \hat{H}(\mathbf{r})\right] G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}') \tag{B.3}$$

where $\mathbf{r}$ and $\mathbf{r}'$ are the source and field points in $D$, and $\delta(\mathbf{r} - \mathbf{r}')$ is the 2-D $\delta$-function. By multiplying Eq. B.3 by $\psi_n$ and Eq. B.2 by $G(\mathbf{r}, \mathbf{r}'; E)$, the potential term can be eliminated as below:

$$\psi_n(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') = \frac{\hbar^2}{2m}\left[\psi_n(\mathbf{r})\nabla^2 G(\mathbf{r}, \mathbf{r}'; E_n) - G(\mathbf{r}, \mathbf{r}'; E_n)\nabla^2\psi_n(\mathbf{r})\right] \tag{B.4}$$

In addition, for the differentiable functions, $v$ and $u$, we have:

$$u\nabla^2 v = \nabla(u\nabla v) - \nabla u \nabla v \tag{B.5}$$

So, Eq. B.4 can be rewritten as:

$$\psi_n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') = \frac{\hbar^2}{2m}\nabla\cdot[\psi_n(\mathbf{r})\nabla G(\mathbf{r},\mathbf{r}';E_n) - G(\mathbf{r},\mathbf{r}';E_n)\nabla\psi_n(\mathbf{r})] \tag{B.6}$$

By applying the Green's formula and integrating with respect to $\mathbf{r}$ over the domain $D$, the above equation becomes:

$$\psi_n(\mathbf{r}') = \frac{\hbar^2}{2m}\oint_\Gamma [\psi_n(\mathbf{r})G_{,\nu}(\mathbf{r},\mathbf{r}';E_n) - G(\mathbf{r},\mathbf{r}';E_n)\psi_{n,\nu}(\mathbf{r})]\,\mathrm{d}s(\mathbf{r}) \tag{B.7}$$

In this equation, $\mathrm{d}s(\mathbf{r})$ is an infinitesimal length considered along boundary $\Gamma$. For evaluation of the boundary integral formulation in the singular points, where $\varepsilon \equiv \mathbf{r}-\mathbf{r}' \longrightarrow 0$ based on Fig. B.1, the Green's function can be given as:

$$G(\mathbf{r},\mathbf{r}';E_n) \sim -\frac{m}{\pi\hbar^2}\ln(k\varepsilon), \quad \varepsilon \to 0 \tag{B.8}$$

The Green's function for a billiard with a particle moving freely inside it is defined as:

$$G(\mathbf{r},\mathbf{r}';E) = -\frac{im}{2\hbar^2}H_0^{(1)}(k|\mathbf{r}-\mathbf{r}'|) \tag{B.9}$$

where $k = \sqrt{2mE}/\hbar$. So, it can be expressed by:

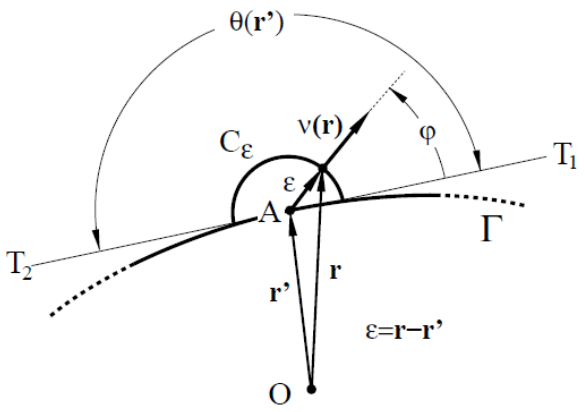


Figure B.1. Geometry of the billiard boundary near the singularity point.

$$G_{,\nu}(\mathbf{r},\mathbf{r}';E_n)=\nu(\mathbf{r})\cdot\nabla_r\left[-\frac{im}{2\hbar^2}H_0^{(1)}(k|\mathbf{r}-\mathbf{r}'|)\right]=\frac{imk}{2\hbar^2}\left[\nu(\mathbf{r})\cdot\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\right]H_1^{(1)}(k|\mathbf{r}-\mathbf{r}'|) \tag{B.10}$$

Here, it has been considered that $\mathrm{d}H_0^{(1)}(z)/\mathrm{d}z=-H_1^{(1)}(z)$. According to Fig. B.1, the following equation can be obtained:

$$\begin{aligned}\lim_{\varepsilon\to0}\frac{\hbar^2}{2m}\int_{C_\varepsilon}\psi_n(\mathbf{r})G_{,\nu}(\mathbf{r},\mathbf{r}';E_n)\mathrm{d}s(\mathbf{r})&=\frac{\hbar^2}{2m}\psi_n(\mathbf{r}')\lim_{\varepsilon\to0}\int_0^{\theta(\mathbf{r}')}\left(\frac{imk}{2\hbar^2}\right)\left(-\frac{2i}{\pi k\varepsilon}\right)\varepsilon\mathrm{d}\varphi\\&=\frac{\theta(\mathbf{r}')}{2\pi}\psi_n(\mathbf{r}')\end{aligned} \tag{B.11}$$

in which $\theta(\mathbf{r}')=\pi$ for a smooth boundary.

# BIOGRAPHICAL SKETCH

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