

Quantum Annealing for the Helmholtz Equation on D-Wave: QUBO Formulations and Encoding Strategies



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Abstract

Quantum annealing has emerged as a promising paradigm for solving large-scale combinatorial optimization problems. Extending this framework to the numerical solution of differential equations requires the development of suitable optimization formulations that can be efficiently implemented on current quantum hardware. In this context, this thesis investigates the application of quantum annealing to the numerical solution of differential equations, using the one-dimensional Helmholtz equation as a benchmark problem. The approximate solution is represented through spectral basis function whose coefficients are determined by formulating the problem as QUBO (Quadratic Unconstrained Binary Optimization Problem). Different encoding strategies are systematically investigated and evaluated from both algebraic and adiabatic perspectives, with their performance compared against the classical simulated annealing algorithm.

To assess the quality and reliability of the obtained solutions, several quantitative metrics are employed, including the minimum energy gap, dynamic range, and mean squared error. These measures provide insight into the adiabatic behavior of the system, numerical stability, and approximation accuracy. The results highlight the critical role of problem encoding and the resulting QUBO structure in achieving efficient quantum annealing performance. In particular, the algebraic properties of the discretized problem strongly determine the optimization landscape experienced by the quantum annealer.

Finally, the results highlight the potential of hybrid quantum–classical approaches that combine favorable algebraic properties with suitable adiabatic conditions. These findings contribute to the development of more effective QUBO formulations for differential equations and provide practical guidelines for designing quantum annealing algorithms on current and future hardware.

Аңдатпа

Кванттық күйдіру (quantum annealing) ірі көлемді комбинаторлық оңтайландыру есептерін шешуге арналған перспективалы кванттық есептеу тәсілдерінің бірі. Алайда бұл тәсілді дифференциалдық теңдеулерді сандық шешуге қолдану қазіргі кванттық құрылғыларда тиімді іске асырылатын сәйкес оңтайландыру модельдерін құруды талап етеді. Осыған байланысты, диссертациялық жұмыста бірөлшемді Гельмгольц теңдеуін модельдік есеп ретінде пайдалана отырып, оны кванттық күйдіру әдісімен сандық шешу мәселесі қарастырылады. Жуық шешім спектрлік базистік функциялар арқылы өрнектеліп, олардың коэффициенттері есепті QUBO (Quadratic Unconstrained Binary Optimization) моделіне түрлендіру арқылы анықталады. Кодтаудың әртүрлі стратегиялары алгебралық және адиабаталық тұрғыдан жүйелі түрде зерттеліп, олардың тиімділігі классикалық имитациялық күйдіру (simulated annealing) алгоритмінің нәтижелерімен салыстырылады. Алынған шешімдердің сапасы мен сенімділігін бағалау үшін минималды энергия саңылауы, динамикалық диапазон және орташа квадраттық қате сияқты сандық көрсеткіштер қолданылады. Бұл көрсеткіштер жүйенің адиабаталық қасиеттерін, сандық тұрақтылығын және жуықтау дәлдігін жан-жақты бағалауға мүмкіндік береді. Зерттеу нәтижелері есепті кодтау тәсілі мен соған сәйкес қалыптасатын QUBO моделінің құрылымы кванттық күйдірудің тиімділігіне шешуші ықпал ететінін көрсетеді. Сонымен қатар, дискреттелген есептің алгебралық қасиеттері кванттық күйдіргіштің оңтайландыру үдерісінің ерекшеліктерін айқындайтыны анықталды. Жұмыстың қорытындысында қолайлы алгебралық қасиеттер мен тиімді адиабаталық шарттарды үйлестіретін гибриді кванттық-классикалық тәсілдердің кең қолдану мүмкіндігі бар екендігі көрсетіледі. Алынған нәтижелер дифференциалдық теңдеулерді шешуге арналған тиімді QUBO модельдерін әзірлеуге үлес қосып, қазіргі және келешектегі кванттық күйдіру құрылғыларына арналған алгоритмдерді жобалауға практикалық ұсыныстар береді.

Declaration

I, **Aigerim Bazarkhanova**, certify that, with the exception of properly referenced quotations and citations, this thesis entitled [**Quantum Annealing for the Helmholtz Equation on D-Wave: QUBO Formulations and Encoding Strategies**] is entirely my own work. No part of this thesis has been submitted for any other degree at Nazarbayev University or any other institution, nor does it contain material previously submitted for a degree.

Parts of this thesis is based on my published work, which is properly cited in the relevant chapters:

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Contents

Abstract	2
Declaration	4
Acknowledgements	5
1 Introduction	1
2 Quantum Computations	6
2.1 Postulates of Quantum Mechanics	6
2.2 Hamiltonians and Time Evolution	8
2.3 Qubits as Spin Systems	9
2.4 Gate-Based and Adiabatic Quantum Computation	12
2.5 Quantum Annealing and D-Wave Implementation	13
3 Methods	16
3.1 Helmholtz equation	16
3.2 Spectral decomposition	17
3.3 Truncated Fourier Ansatz	19
3.4 Circulant Ansatz	20
3.5 QUBO formulation	21
4 Experimental Setup and Computational Framework	25
4.1 D-Wave Platform	25
4.2 Physical Realization of Quantum Annealing	26
4.3 Ocean Software Framework	27
4.4 Minor embedding	28
4.5 Sampling Procedure	29
4.6 Evaluation of Candidate Solutions	29
4.7 Software Environment and Implementation Details	30

4.8	Workflow	30
5	Experiments and Results	32
5.1	Homogeneous Helmholtz equation	34
5.2	Inhomogeneous Helmholtz equation with monochromatic driving I	35
5.3	Inhomogeneous Helmholtz equation with monochromatic driving II	40
5.4	Inhomogeneous Helmholtz equation with polichromatic driving	43
5.5	Homogeneous Helmholtz equation with irrational initial conditions	44
5.6	Alternative Ansatz: Adiabatic Prescription	46
6	Conclusion	49
	Appendix Overview	51
A	Linear system of equations	52
A.1	Linear System of Equations for TFA	53
A.2	Linear System of Equations for CA	53
B	QUBO Metrics and Spectral Reconstruction	55
B.1	Additional Numerical Results	57
B.1.1	Additional Numerical Results for Experiment 2	57
B.1.2	Additional Numerical Results for Experiment 3	58
B.1.2.1	Numerical Results with fixed N and increasing n_{spin}	58
B.1.2.2	Numerical Results with fixed number of n_{spin} and in- creasing N	59
	Bibliography	61

Chapter 1

Introduction

Solving Partial Differential Equations (PDE) is of paramount importance in modeling science and engineering due to their unparalleled capacity to describe and predict complex physical phenomena. Common examples include the behavior of fluids in aerodynamics, weather forecasting, or the spread of disease in epidemiology. Hence, the accurate and efficient numerical solution of differential equations is therefore of considerable importance across numerous disciplines. Unfortunately, these real-world problems often involve intricate models or simulations, large datasets, or sophisticated optimization procedures, that demand the building of larger parallel processing networks or bigger supercomputers to deploy a significant number of computational resources, time, and energy. Thus, addressing this challenging task will require to design advanced computational techniques as well as to develop innovative technologies with computational capabilities able to keep pace with the ever-expanding demands of science, engineering, and various applications across industries. However, exact analytical solutions are available only for a limited class of differential equations. Most practical problems involve complex geometries, nonlinearities, or boundary conditions that prevent the derivation of closed-form solutions. Consequently, numerical methods have become indispensable tools for approximating solutions. Classical approaches such as finite difference methods, finite element methods, and spectral methods transform the original continuous problem into a finite-dimensional algebraic system that can be solved computationally. While these techniques have achieved remarkable success, their computational cost often increases significantly with problem size and dimensionality, a phenomenon sometimes called the “curse of dimensionality”. These findings contribute to the development of more effective QUBO formulations for differential equations and provide practical guidelines for designing quantum annealing algorithms on current and future hardware.

One such promising direction is quantum computing. Unlike classical computers, which process information using binary bits, quantum computers exploit the principles of quantum mechanics to perform computations. Quantum bits, or qubits, can exist in superposition states, enabling the simultaneous representation of multiple computational states. Furthermore, quantum entanglement and quantum interference provide additional computational resources that have no classical counterpart. These unique features have led to the development of quantum algorithms capable of outperforming classical algorithms for certain computational tasks [67].

Several physical implementations of quantum computers have been proposed and realized, including superconducting circuits, trapped ions, neutral atoms, photonic systems, and quantum annealers [8, 44, 49, 68, 78]. Each architecture possesses its own advantages and limitations, and it remains unclear which technology will ultimately become dominant. Nevertheless, all currently available quantum devices are affected by noise and limited coherence times. Consequently, contemporary quantum hardware is commonly referred to as Noisy Intermediate-Scale Quantum (NISQ) technology. Although large-scale fault-tolerant quantum computers remain a long-term objective, substantial effort has been devoted to developing algorithms suitable for currently available devices.

The application of quantum computing to differential equations has attracted considerable attention during the last decade [6, 7, 17, 25, 56, 59, 64, 74, 85, 87]. A major motivation stems from the observation that many numerical methods reduce differential equations to systems of linear algebraic equations. Since quantum mechanics is naturally formulated in the language of linear algebra, quantum computers are naturally suited to address such problems. One of the most influential developments in this area is the Harrow - Hassidim - Lloyd (HHL) algorithm [38], which demonstrated that quantum computers can solve certain linear systems exponentially faster than the best known classical algorithms under specific assumptions. This breakthrough stimulated extensive research into quantum algorithms for the numerical solution of ordinary and partial differential equations [24].

Subsequent studies extended these ideas to a broad range of applications. Quantum algorithms have been proposed for ordinary differential equations, Poisson equations [55, 57], heat equations [23, 58, 75], and fluid dynamics [84, 92] problems. Both finite difference and finite element discretizations have been investigated, while spectral methods have also been adapted to quantum settings. More recently, variational quantum algorithms have emerged as a promising alternative for near-term quantum hardware [11, 14, 42, 55, 57, 58, 60, 76, 84, 88]. These methods combine quantum

circuits with classical optimization routines and have been successfully applied to several differential equation problems, including linear and nonlinear PDEs.

Despite these advances, gate-based quantum algorithms face significant practical challenges [77]. Many theoretical speedups rely on assumptions that are difficult to satisfy on current hardware, such as efficient state preparation, fault-tolerant quantum error correction, and large numbers of logical qubits. Moreover, deep quantum circuits are particularly sensitive to noise and decoherence, limiting their practical applicability on existing NISQ devices. These challenges have motivated researchers to explore alternative quantum computing paradigms that may be better suited for current hardware capabilities [52].

Among the proposed alternatives, quantum annealing has emerged as a promising paradigm for solving optimization problems on current quantum hardware [40]. Unlike gate-based quantum computing, quantum annealing is specifically designed for solving optimization problems [41, 62, 78, 94]. The method is based on the adiabatic theorem of quantum mechanics, which states that a quantum system remains in its ground state provided that its Hamiltonian evolves sufficiently slowly. In quantum annealing, an initial Hamiltonian with a known ground state is gradually transformed into a problem Hamiltonian whose ground state encodes the solution of the optimization problem [39, 68]. This optimization-based framework makes quantum annealing particularly well suited for numerical methods in which differential equations can be reformulated as optimization problems.

Optimization problems suitable for quantum annealing are typically formulated as Quadratic Unconstrained Binary Optimization (QUBO) problems [63]. A QUBO problem consists of minimizing a quadratic objective function defined over binary variables [4, 31, 44]. QUBO is the key ingredient that enables the methodology developed in this thesis. This formulation is particularly attractive because it can be directly transformed into an equivalent Ising Hamiltonian [8, 15, 22, 53, 63]. The ground state of the Ising Hamiltonian corresponds to the optimal solution of the original optimization problem. During the annealing process, quantum fluctuations enable the system to explore the energy landscape and potentially escape local minima through quantum tunneling. The efficiency of quantum annealing depends not only on the underlying optimization problem but also on how that problem is encoded as a QUBO model [32].

The development of quantum annealing hardware by D-Wave Systems has provided researchers with access to large-scale quantum optimization devices containing thousands of qubits. Although the extent of quantum advantage remains an active

subject of investigation, D-Wave systems have been successfully applied to a variety of optimization [90], machine learning [93], scheduling [79], and scientific computing problems [32]. Recent studies have also explored the use of quantum annealers for solving systems of algebraic equations and differential equations through QUBO formulations [46, 66, 73, 86].

Nevertheless, several important questions remain unresolved. The performance of quantum annealing depends strongly on the chosen encoding strategy, problem formulation, dynamic range of coefficients, embedding requirements, and hardware topology. Furthermore, the relationship between matrix properties and annealing performance remains insufficiently understood. In particular, there is limited understanding of how different basis representations influence the resulting optimization landscape and the probability of successfully reaching the ground state.

The present thesis aims to contribute to this area by investigating QUBO formulations and encoding strategies for the numerical solution of differential equations, using the one-dimensional Helmholtz equation as a benchmark problem. The Helmholtz equation serves as a canonical model in numerous scientific and engineering applications, including acoustics, electromagnetics, optics, and quantum mechanics [36, 43, 50, 54]. Owing to its importance and well-understood analytical properties, it provides an ideal testbed for studying quantum annealing approaches to differential equations.

The proposed methodology begins with the spectral discretization of the Helmholtz equation. The resulting algebraic system is subsequently reformulated as a least-squares optimization problem and transformed into a QUBO model suitable for quantum annealing. To investigate the influence of the QUBO formulation on quantum annealing performance, two different basis representations are considered. The first is the truncated Fourier ansatz, which represents the solution using trigonometric basis functions. The second is a circulant ansatz constructed from shifted Fourier kernels. Although both approaches yield equivalent continuous approximations, they generate significantly different algebraic structures and optimization landscapes.

The primary objective of this research is to determine how different QUBO formulations, induced by different ansatzes, affect the performance. Particular attention is devoted to the rank of the resulting matrices, dynamic range, minimum energy gaps, success rates, and mean squared error. In addition, the influence of binary encoding parameters and discretization size is systematically investigated. The performance of quantum annealing is compared with classical simulated annealing in order to evaluate the practical capabilities and limitations of current quantum annealing hardware.

The main contributions of this thesis can be summarized as follows:

1. Development of a QUBO formulation for the one-dimensional Helmholtz equation based on spectral discretization.
2. Development and comparative analysis of two spectral encoding strategies based on truncated Fourier and circulant ansatzes.
3. Identification of the influence of matrix rank, coefficient dynamic range, and minimum energy gap on quantum annealing performance.
4. Quantitative assessment of the relative performance of quantum and classical annealing methods across representative Helmholtz benchmark problems.
5. Identification of problem characteristics that influence the probability of obtaining the ground-state solution on current D-Wave hardware.
6. Development of an alternative adiabatic ansatz motivated by the observed optimization behavior.

The remainder of this thesis is organized as follows. Chapter 2 introduces the mathematical and computational background required for this work, including quantum computing, adiabatic quantum computation, quantum annealing, and spectral methods. Chapter 3 develops the spectral discretization of the Helmholtz equation and its associated QUBO formulations. Chapter 4 describes the experimental setup and the implementation on D-Wave quantum annealers. Chapter 5 presents numerical experiments and analyzes the influence of different QUBO formulations and encoding strategies on quantum annealing performance. Finally, Chapter 6 summarizes the main findings of the thesis and discusses possible directions for future research.

Chapter 2

Quantum Computations

This chapter provides the theoretical background necessary for the remainder of the thesis. It begins by introducing the fundamental principles of quantum mechanics that underpin quantum computation, followed by a discussion of the gate-based and adiabatic models of quantum computing. The section then focuses on quantum annealing and describes the physical principles underlying D-Wave quantum annealers, which solve optimization problems through the Ising model and its equivalent QUBO formulation.

2.1 Postulates of Quantum Mechanics

Quantum computation is founded on the principles of quantum mechanics. The first fundamental postulate states that the state of an isolated quantum system is represented by a vector in a complex Hilbert space [71, 81]. In principle, any physical system whose states can be described within the framework of quantum mechanics may serve as a platform for quantum computation. However, the implementation of scalable quantum processors based on higher-dimensional systems remains experimentally challenging. Consequently, most current quantum computing architectures employ two-level quantum systems, referred to as qubits.

For a two-level quantum system, the computational basis is given by

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (2.1)$$

These two basis states play a role analogous to the classical bit values 0 and 1. However, unlike a classical bit, a qubit may exist in a superposition of both basis states. A general qubit state is therefore written as

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1, \quad (2.2)$$

where $\alpha, \beta \in \mathbb{C}$ are probability amplitudes satisfying the normalization condition. This representation reflects the superposition principle, according to which any linear combination of valid quantum states is itself a valid quantum state [71].

The geometric interpretation of a single-qubit state is provided by the Bloch sphere, illustrated in Figure 2.1. Every pure qubit state corresponds to a point on the surface of the unit sphere. The north and south poles represent the computational basis states $|0\rangle$ and $|1\rangle$, respectively, while all other points correspond to superposition states with different probability amplitudes and relative phases. Using the polar angle θ and the angle ϕ , any pure qubit state can be written as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right) |1\rangle, \quad (2.3)$$

where $0 \leq \theta \leq \pi$ and $0 \leq \phi < 2\pi$.

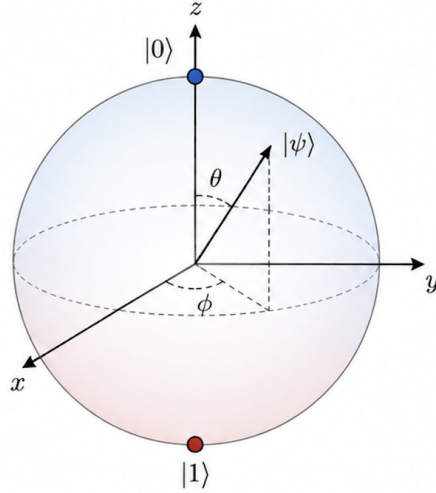


Figure 2.1: Bloch sphere representation of a qubit. The north pole corresponds to $|0\rangle$, the south pole to $|1\rangle$, and every other point on the sphere represents a pure superposition state. The angles θ and ϕ determine the probability amplitudes and relative phase of the qubit state.

The second fundamental postulate describes the time evolution of a closed quantum system. Its evolution is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle, \quad (2.4)$$

where $H(t)$ denotes the Hamiltonian of the system and $\hbar$ is the reduced Planck constant [34, 81]. Since the Hamiltonian is Hermitian, the evolution of a closed quantum system is unitary, preserving the norm of the quantum state and, consequently, the total probability. This postulate provides the mathematical foundation for all quantum-computing models, including gate-based quantum computation, adiabatic quantum computation, and quantum annealing.

The third fundamental postulate concerns quantum measurement. When the state

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

is measured in the computational basis, the outcome is $|0\rangle$ with probability $|\alpha|^2$ and $|1\rangle$ with probability $|\beta|^2$, in accordance with the Born rule [71, 81]. Consequently, quantum algorithms are designed so that the desired solution is encoded in a quantum state that can be observed with sufficiently high probability after measurement.

2.2 Hamiltonians and Time Evolution

The second postulate establishes that the evolution of a quantum system is completely determined by its Hamiltonian. In quantum computing, the Hamiltonian plays a central role because it specifies the energy landscape of the system and determines how quantum states evolve over time. While gate-based quantum computing realizes computations through sequences of quantum gates generated by suitable Hamiltonians, Hamiltonian-based models such as adiabatic quantum computation and quantum annealing encode the computational problem directly into the Hamiltonian itself.

Since the Hamiltonian is a Hermitian operator, its eigenvalues are real and its eigenvectors form a complete orthonormal basis of the Hilbert space. The corresponding eigenvalue equation is

$$H|v_j\rangle = \lambda_j|v_j\rangle, \tag{2.5}$$

where λ_j denotes the energy associated with the eigenstate $|v_j\rangle$. The eigenstate corresponding to the smallest eigenvalue is referred to as the *ground state*, whereas all remaining eigenstates are called *excited states*. In optimization-based quantum computation, the objective is to construct a Hamiltonian whose ground state represents the optimal solution of the computational problem [1, 71].

For a time-independent Hamiltonian, the Schrödinger equation admits the analytical solution

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle. \quad (2.6)$$

In many areas of quantum computing, it is convenient to adopt natural units by setting $\hbar = 1$, giving

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle. \quad (2.7)$$

The operator

$$U(t) = e^{-iHt} \quad (2.8)$$

is called the time-evolution operator and describes the unitary evolution of the quantum state. For time-dependent Hamiltonians, the evolution is generally more involved and cannot be expressed by a simple exponential operator. Such Hamiltonians arise naturally in adiabatic quantum computation and quantum annealing, where the Hamiltonian is intentionally varied throughout the computation. The following section introduces this time-dependent evolution and explains how it enables optimization through the adiabatic theorem.

2.3 Qubits as Spin Systems

As discussed in Section 2.1, quantum computation can be realized using a variety of physical systems. Depending on the hardware platform, qubits may be implemented using trapped ions, photons, neutral atoms, semiconductor devices, or superconducting circuits [51, 71]. Each hardware platform offers different advantages and is typically designed to support a particular model of quantum computation.

Among the existing quantum-computing paradigms, quantum annealing has emerged as one of the most successful approaches for solving large-scale combinatorial optimization problems. Rather than executing a sequence of quantum gates, quantum annealers exploit the continuous evolution of a quantum system toward its lowest-energy configuration. This approach has enabled the construction of quantum processors containing several thousand physical qubits and has motivated numerous applications in optimization, machine learning, scheduling, and scientific computing [40, 1].

Commercial quantum annealers developed by D-Wave Systems implement qubits as superconducting flux qubits operating at millikelvin temperatures [37, 45]. These devices are specifically engineered to realize interacting spin systems described by the

Ising Hamiltonian. Consequently, throughout the remainder of this thesis we focus on this physical realization of qubits and its mathematical formulation.

For quantum annealing, it is convenient to represent each qubit by a spin variable [40, 63]

$$s_i \in \{-1, +1\}, \quad (2.9)$$

where the two possible values correspond to the two orientations of a spin. A collection of interacting spins forms a physical system whose total energy depends both on the individual spin orientations and on the interactions between neighboring spins.

The energy of such a system is described by the Ising Hamiltonian

$$E(\mathbf{s}) = \sum_i h_i s_i + \sum_{i < j} J_{ij} s_i s_j, \quad (2.10)$$

where h_i denotes the local magnetic field acting on spin i , while J_{ij} represents the interaction strength between spins i and j [63]. Figure 2.2 illustrates the two possible spin orientations together with the most common pairwise interactions appearing in the Ising model.

The local bias terms determine whether an individual spin energetically prefers the value $+1$ or -1 , whereas the coupling coefficients determine the preferred relative orientation of neighboring spins. Ferromagnetic couplings favor aligned spins, whereas antiferromagnetic couplings favor opposite orientations. In more complex systems, competing interactions may give rise to frustration, meaning that not all pairwise interactions can be simultaneously minimized [80, 40].

The ground state of the Ising Hamiltonian corresponds to the spin configuration with the minimum total energy. In quantum annealing, optimization problems are formulated by constructing an Ising Hamiltonian whose ground state encodes the desired solution. The physical mechanism used to drive the system toward this ground state is based on adiabatic quantum evolution, which provides the theoretical foundation of quantum annealing. The next section therefore introduces the principles of adiabatic quantum computation before presenting the quantum annealing algorithm in detail.

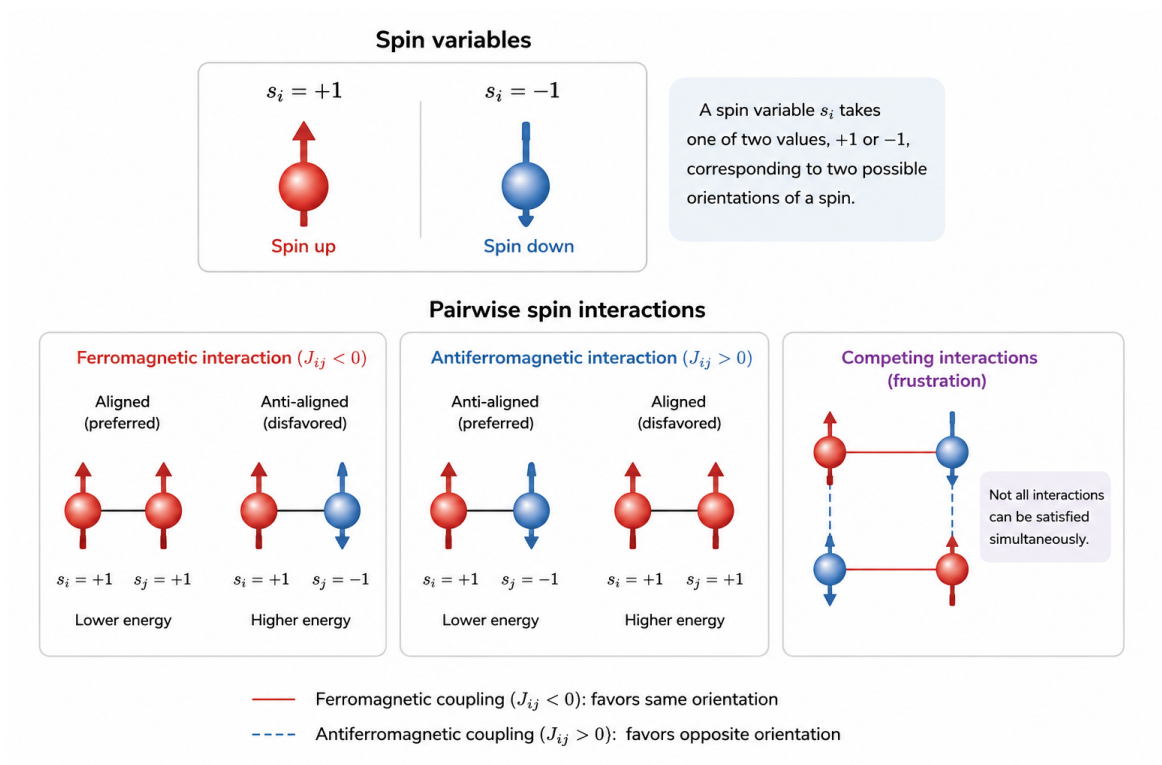


Figure 2.2: Illustration of spin variables and pairwise interactions in the Ising model. The upper panel shows the two possible spin states, $s_i = \pm 1$. The lower panels illustrate ferromagnetic interactions, antiferromagnetic interactions, and frustrated spin configurations.

2.4 Gate-Based and Adiabatic Quantum Computation

Quantum computing can be broadly divided into two major computational paradigms: the gate-based (circuit) model and Hamiltonian-based models, among which adiabatic quantum computation is one of the most prominent. Although both approaches rely on the principles of quantum mechanics, they perform computations in fundamentally different ways.

The gate-based model is the standard circuit model of quantum computation. In this framework, a computation is performed by preparing an initial quantum state and subsequently applying a sequence of quantum gates. Each quantum gate is represented by a unitary operator acting on one or more qubits, while the overall computation is described by a quantum circuit. After all gates have been applied, the final quantum state is measured to obtain classical information [71].

The gate-based model is universal, meaning that any quantum computation can be approximated by a sufficiently long sequence of elementary quantum gates. It forms the basis of many well-known quantum algorithms, including Shor’s factoring algorithm [83] and Grover’s search algorithm [35]. Despite its theoretical power, the practical implementation of large-scale gate-based algorithms remains challenging. Current hardware is limited by the number of available high-quality qubits, finite coherence times, gate errors, and the absence of large-scale quantum error correction [77].

An alternative approach is provided by adiabatic quantum computation (AQC), which belongs to the family of Hamiltonian-based computational models. Instead of performing computations through discrete gate operations, AQC solves computational problems by continuously evolving the Hamiltonian of a quantum system. The computation begins from the easily prepared ground state of an initial Hamiltonian and gradually transforms into a problem Hamiltonian whose ground state encodes the desired solution [1, 26].

The theoretical foundation of adiabatic quantum computation is the quantum adiabatic theorem. It states that if the Hamiltonian of a quantum system changes sufficiently slowly, a system initially prepared in the ground state remains close to the instantaneous ground state throughout the evolution. Consequently, after the evolution is completed, the final state approximates the ground state of the problem Hamiltonian and therefore represents the solution of the optimization problem.

Quantum annealing can be viewed as a practical implementation inspired by the principles of adiabatic quantum computation. Unlike the idealized adiabatic model, quantum annealing is specifically designed for solving optimization problems and is implemented on specialized hardware, such as the D-Wave quantum annealers considered in this thesis.

Although both computational paradigms exploit quantum-mechanical phenomena, they are designed for different classes of problems. Gate-based quantum computation provides a universal computational framework suitable for implementing a wide range of quantum algorithms. In contrast, adiabatic quantum computation and its practical realization through quantum annealing are primarily intended for solving optimization problems formulated as Hamiltonians or, equivalently, as Ising and Quadratic Unconstrained Binary Optimization (QUBO) models.

The methodology developed in this thesis follows the latter approach. Instead of solving differential equations directly on a quantum computer, the governing equation is first discretized using suitable basis functions. The unknown coefficients are then determined by minimizing the residual in the least-squares sense. This optimization problem is transformed into a QUBO formulation through binary encoding and subsequently mapped onto an equivalent Ising Hamiltonian. The D-Wave quantum annealer is employed to search for low-energy spin configurations approximating the ground state of this Hamiltonian. After decoding the resulting binary variables, the coefficients of the approximate solution are recovered.

Consequently, the D-Wave system is employed in this thesis not as a universal quantum computer but as a specialized quantum optimizer implementing interacting superconducting flux qubits described by an Ising spin system. This Hamiltonian-based computational paradigm forms the basis of the methodology developed in the following chapters. Before presenting the quantum annealing algorithm itself, the next section introduces the quantum adiabatic theorem, which provides the theoretical foundation for adiabatic evolution.

2.5 Quantum Annealing and D-Wave Implementation

Quantum annealing may be viewed as a practical implementation of adiabatic ideas for optimization problems [1, 26, 40, 47]. Instead of using a sequence of quantum gates, the quantum annealer gradually transforms a simple initial Hamiltonian into a

problem Hamiltonian. The problem Hamiltonian is constructed so that its low-energy states correspond to good solutions of the optimization problem.

D-Wave quantum annealers implement this process using superconducting flux qubits with programmable local fields and couplings [12, 37, 45]. The hardware realizes an Ising-type model of the form (2.10) [45, 65]. The user specifies the coefficients h_i and J_{ij} , and the device performs repeated annealing runs to sample low-energy spin configurations. These samples are then decoded into candidate solutions of the original optimization problem.

A practical challenge in quantum annealing arises from the limited connectivity between physical qubits on the quantum processor. Unlike the fully connected graphs often encountered in optimization problems, D-Wave quantum annealers implement a fixed hardware topology in which each qubit interacts only with a limited number of neighboring qubits. Earlier generations of D-Wave processors employed the *Chimera* architecture, whereas current Advantage processors utilize the *Pegasus* topology, which provides substantially higher qubit connectivity and consequently supports more efficient implementations of large optimization problems. Figure 2.3 compares the connectivity graphs of the Chimera and Pegasus architectures.

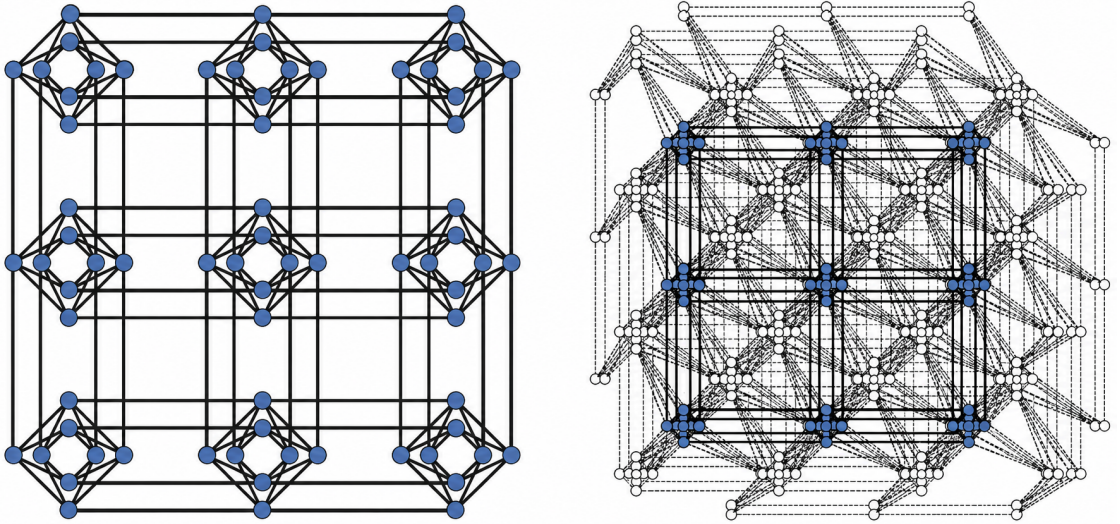


Figure 2.3: Connectivity graphs of the Chimera (left) and Pegasus (right) architectures employed in D-Wave quantum annealers. The Pegasus topology provides substantially higher qubit connectivity than the Chimera topology, enabling more efficient embeddings of optimization problems. Adapted from [33].

Since the connectivity of the logical optimization problem generally differs from that of the hardware graph, a *minor-embedding* procedure is required to map the logical graph onto the physical topology of the quantum processor [13, 18, 19]. During

this process, a single logical variable may be represented by a chain of several strongly coupled physical qubits. Consequently, the quality of the embedding directly influences the number of physical qubits required, the lengths and strengths of the chains, and ultimately the probability of obtaining the ground-state solution [9, 45].

Most optimization problems submitted to a D-Wave annealer are first formulated as Quadratic Unconstrained Binary Optimization (QUBO) problems [30, 63],

$$\min_{x \in \{0,1\}^n} x^T Q x, \quad (2.11)$$

where Q is a real matrix containing the linear and quadratic coefficients of the binary objective function. The QUBO and Ising formulations are equivalent through the change of variables [10, 30, 63]

$$s_i = 2x_i - 1, \quad x_i = \frac{s_i + 1}{2}. \quad (2.12)$$

This equivalence allows problems expressed in binary variables to be implemented on the Ising-type physical system realized by D-Wave hardware [40, 45].

Chapter 3

Methods

In this chapter, we first present the mathematical formulation of the Helmholtz equation and develop its corresponding QUBO formulation through spectral discretization. We then discuss the key challenges associated with encoding the discretized problem into a QUBO model suitable for quantum annealing and introduce the proposed ansatz, which is designed to mitigate these difficulties and improve the overall performance of the approach.

3.1 Helmholtz equation

We consider the one-dimensional Helmholtz equation

$$\begin{cases} u''(x) + \tau^2 u(x) = F(x), \\ u(0) = \alpha, \quad u'(0) = \beta, \end{cases} \quad (3.1)$$

where $u(x)$ is a real-valued function defined on the interval $x \in [0, 2\pi]$. The constants $\alpha, \beta \in \mathbb{R}$ specify the boundary conditions, while τ is a constant related to the frequency of the wave. In electromagnetic applications, τ can be interpreted as the wave number describing the propagation of an electric field in a linear, homogeneous, and isotropic medium [5, 89]. The function $F(x)$ represents an external source term, such as an electric current or potential source, allowing the model to describe a wide range of wave propagation phenomena [16]. The difficulty of solving the Helmholtz equation depends strongly on the boundary conditions and the geometry of the domain under consideration [2, 20]. Our objective is not to develop a new numerical discretization of the Helmholtz equation itself, but rather to investigate how different spectral representations affect the resulting QUBO formulation for quantum annealing.

An additional advantage of the Helmholtz equation is that it admits a closed-form solution, which enables direct validation of the numerical approximations [5]. The solution is given by

$$u(x) = u_h(x) + \frac{1}{\tau^2} \int_0^x \sin(\tau(x-s)) F(s) ds, \quad (3.2)$$

where $u_h(x)$ denotes the solution of the homogeneous problem,

$$u_h(x) = \alpha \cos(\tau x) + \frac{\beta}{\tau} \sin(\tau x). \quad (3.3)$$

In many practical applications, obtaining an exact solution of equation (3.1) can be challenging, particularly for high-frequency problems where the wave number is large relative to the size of the domain [27]. To address this difficulty, we employ a spectral approach, in which the solution is approximated by a finite expansion in terms of global basis functions $\phi_i(x)$.

3.2 Spectral decomposition

To obtain a numerical approximation of the solution, we employ a pseudospectral method, in which the unknown function is represented as a finite expansion of basis functions. Specifically, we use the pseudospectral approximation [82]

$$u_N(x) \approx \sum_{i=1}^N w_i \phi_i(x), \quad (3.4)$$

where $w_i \in \mathbb{R}$ are unknown coefficients and $\phi_i(x)$ are basis functions defined on the interval $x \in [0, 2\pi]$. For analytical convenience, these basis functions are typically chosen to be orthonormal with respect to an appropriate weight function [82]. In the present work, the choice of basis functions plays an additional role, as it directly influences the algebraic structure of the resulting QUBO formulation and, consequently, the performance of the quantum annealer.

For numerical implementation, the pseudospectral approximation is combined with a spatial discretization of the Helmholtz equation. The domain is divided into a set of discrete points x_m , known as collocation points, defined by

$$x_m = \frac{2\pi m}{N}, \quad (3.5)$$

where $m = 0, 1, \dots, N - 1$. These points are uniformly distributed over the interval $(0, 2\pi)$, resulting in a regular computational grid. Such a choice simplifies the evaluation of derivatives and interpolation procedures.

After substituting the approximation (3.4) into (3.1) and enforcing the equation at the collocation points, we obtain a system of linear equations. Including the two boundary conditions leads to an $(N+2)$ -equation system with N unknown coefficients w_i , which can be written in the compact form

$$\mathbf{a}\mathbf{w} = \mathbf{b}, \quad (3.6)$$

where $\mathbf{w} = (w_1, \dots, w_N)^T$ is the vector of unknown coefficients, $\mathbf{a}$ is an $(N+2) \times N$ real matrix, and $\mathbf{b}$ is an $(N+2)$ -dimensional vector. Both $\mathbf{a}$ and $\mathbf{b}$ are determined by the Helmholtz equation and the chosen basis functions. Solving equation (3.6) therefore provides an approximate solution of the original Helmholtz equation on the discretized domain.

The rank of the system matrix is closely related to the uniqueness of the solution. If $\mathbf{a}$ is rank-deficient, the optimization problem may exhibit degenerate minima, i.e., multiple solutions associated with the same objective value. Such degeneracy can adversely affect the performance of the annealer by increasing the likelihood of obtaining ambiguous solutions. Consequently, the choice of basis functions becomes crucial, as it influences the rank of the resulting matrix. A basis that yields a full-rank system is expected to improve the quality and accuracy of the solution to problem (3.4).

To ensure the validity of the approximate solution of equation (3.6), or equivalently equation (3.4), we seek the coefficients w_i that minimize the Euclidean norm of the residual error $|u(x) - u_N(x)|$. This can be achieved by employing the least-squares approach, which reformulates the algebraic system (3.6) as an optimization problem. Specifically, we define the following objective (cost) function:

$$\mathcal{C}(\mathbf{w}) = \sum_{m=0}^{N-1} \left| u_N''(x_m) + \tau^2 u_N(x_m) - F(x_m) \right|^2 + |u_N(0) - \alpha|^2 + |u_N'(0) - \beta|^2 =$$

$$\mathbf{w}^T \mathbf{q}\mathbf{w} + \mathbf{l}\mathbf{w} + C_0. \quad (3.7)$$

The first term measures the residual of the Helmholtz equation at the collocation points, whereas the remaining two terms penalize violations of the boundary conditions. As a result, minimizing $\mathcal{C}(\mathbf{w})$ yields an approximation that simultaneously

satisfies the differential equation and the prescribed boundary conditions in a least-squares sense. The matrices and vectors appearing in the quadratic form are given by

$$\mathbf{q} = \mathbf{a}^T \mathbf{a}, \quad \mathbf{l} = -2\mathbf{b}^T \mathbf{a}, \quad C_0 = \mathbf{b}^T \mathbf{b}. \quad (3.8)$$

As a result we obtained quadratic, linear and constant terms which means that we can formulate Ising problem as follows:

$$H_{\text{Ising}} = \sum_{i,j} q_{ij} w_i w_j + \sum_i l_i w_i + C_0, \quad (3.9)$$

where the variables $w_i \in \mathbb{R}$ denote the spin values, while the coefficients q_{ij} and l_i are determined by the matrix $\mathbf{q}$ and vector $\mathbf{l}$ defined in equation (3.8). Since the constant term C_0 does not affect the location of the minimum, it can be omitted during the optimization process. Consequently, solving the original least-squares problem is equivalent to identifying the lowest-energy configuration of the corresponding Ising Hamiltonian.

Having formulated the least-squares problem as a QUBO and mapped it to an Ising Hamiltonian, we now focus on the representation of the approximate solution. To this end, we introduce two different sets of basis functions. Since each choice leads to a different problem structure, they are presented and discussed separately in the following sections.

3.3 Truncated Fourier Ansatz

Given the periodic nature of the Helmholtz equation, a natural choice of basis functions is provided by the Fourier series, namely $\phi_n(x) = \cos(nx)$ and $\phi_n(x) = \sin(nx)$. Using these functions, the approximate solution (3.4) can be represented by a truncated Fourier expansion of the form

$$u_N^{TFA}(x) = \sum_{n=1}^{N/2} (w_n^1 \cos(nx) + w_n^2 \sin(nx)), \quad (3.10)$$

where w_n^1 and w_n^2 denote the expansion coefficients, which play the role of spin variables in the optimization problem.

Substituting the ansatz (3.10) into equation (3.4) yields the corresponding system matrix, denoted by a^{TFA} . As shown in Appendix A.1, this matrix is dense, meaning that most of its entries are nonzero. A dense matrix induces a highly connected

interaction graph in the corresponding QUBO model, increasing the complexity of the embedding on the quantum hardware. Consequently, the embedding process on the quantum hardware becomes more demanding and the computational resources required to solve the problem increase, which may ultimately restrict scalability as the problem size grows.

Fourier-based spectral methods are widely employed in the numerical treatment of differential equations [28, 61], especially when the underlying problem possesses periodic structure. By expanding the solution in terms of Fourier series, differentiation is converted into an algebraic operation in Fourier space, which substantially improves the analysis and numerical implementation. Furthermore, for smooth solutions, truncated Fourier expansions are known to exhibit spectral convergence and can achieve efficiently higher accuracy than conventional finite difference or finite element approaches [70].

3.4 Circulant Ansatz

As an alternative to the truncated Fourier expansion, we consider the circulant ansatz [3, 48, 91], defined as

$$u_N^{CA}(x) = \sum_{n=0}^{N-1} w_n h_n(x), \quad (3.11)$$

where the basis functions are given by

$$h_n(x) = \frac{1}{N} \sum_{k=-N/2}^{N/2} \frac{1}{c_k} e^{ik(x-x_n)},$$

with x_n denoting the collocation points introduced in equation (3.5) and

$$c_k = \begin{cases} 1, & |k| < N/2, \\ 2, & |k| = N/2. \end{cases}$$

Unlike the truncated Fourier expansion, the circulant ansatz is designed to induce a more structured algebraic system, which is expected to be advantageous for the subsequent QUBO formulation. Substituting the ansatz (3.11) into the pseudospectral formulation yields the matrix $\mathbf{a}^{CA}$, whose explicit form is reported in Appendix A.2. A remarkable feature of this construction is that $\mathbf{a}^{CA}$ possesses a circulant structure, meaning that each row can be obtained by a cyclic shift of the preceding one. Such matrices have been extensively studied in numerical analysis due to their favorable

algebraic properties and computational efficiency [29]. In particular, circulant matrices arise naturally in the discretization of periodic differential equations and are well suited for large-scale numerical computations because they can be manipulated efficiently using Fourier-based techniques. These properties make the circulant ansatz especially attractive in the context of quantum annealing, where matrix structure can significantly affect the complexity of the resulting optimization problem.

3.5 QUBO formulation

The QUBO formulation provides the optimization framework used to implement the proposed method on quantum annealing hardware. The key idea is to encode the continuous coefficients w_i into binary variables $\omega_i^l \in \{0, 1\}$, which can be directly represented by qubits on the quantum processor [21]. Specifically, each coefficient is approximated through the binary expansion

$$w_i = \sum_{l=0}^{n_{\text{spin}}-1} (-1)^{\alpha(l)} \frac{\omega_i^l}{2^l}, \quad (3.12)$$

where

$$\alpha(l) = \begin{cases} 1, & l = 0, \\ 0, & l \neq 0, \end{cases}$$

and n_{spin} denotes the number of binary variables used to represent each coefficient. The unknowns of the problem are therefore the binary spin variables ω_i^l , and the solution is encoded in a bitstring $\omega \in \{0, 1\}^r$ with $r = N \times n_{\text{spin}}$.

Substituting the binary representation (3.12) into the linear system (3.6) yields the equivalent formulation

$$\mathbf{A}\omega = \mathbf{b}, \quad (3.13)$$

where $\mathbf{A}$ is the $(N + 2) \times r$ block matrix

$$\mathbf{A} = \left(-\mathbf{a} \mid 2^{-1}\mathbf{a} \mid 2^{-2}\mathbf{a} \mid \dots \mid 2^{-(n_{\text{spin}}-1)}\mathbf{a} \right). \quad (3.14)$$

Following the same least-squares approach introduced in the previous section, the binary linear system (3.13) can be reformulated as a quadratic optimization problem over binary variables,

$$\min_{\omega \in \{0,1\}^r} \omega^T \mathbf{Q} \omega + \mathbf{L} \omega + C'_0, \quad (3.15)$$

which corresponds to the standard QUBO form. Since $\mathbf{Q}$ and $\mathbf{L}$ are determined by the underlying algebraic system, different basis representations produce different QUBO formulations and, consequently, different optimization landscapes. In particular,

$$\mathbf{Q} = \mathbf{A}^T \mathbf{A}, \quad \mathbf{L} = -2\mathbf{b}^T \mathbf{A}, \quad C'_0 = \mathbf{b}^T \mathbf{b}.$$

Consequently, solving the original Helmholtz problem is reduced to finding the binary vector $\boldsymbol{\omega}$ that minimizes the QUBO objective function. This formulation can then be directly embedded into the quantum annealing architecture of the D-Wave processor.

Since the constant term C'_0 does not affect the minimizer of the objective function, it can be safely disregarded during the optimization process. More importantly, the performance of the QUBO formulation strongly depends on the choice of the parameter n_{spin} . A small value of n_{spin} may lead to an insufficiently accurate representation of the coefficients w_i , whereas a large value increases the number of binary variables and, consequently, the size of the matrices $\mathbf{Q}$ and $\mathbf{L}$. This results in a more demanding optimization problem both in terms of memory requirements and computational resources. Therefore, an appropriate choice of n_{spin} is required to balance solution accuracy and computational feasibility.

Starting from the QUBO formulation (3.15), whose variables satisfy $\omega_i \in \{0, 1\}$, it is convenient to transform the problem into the equivalent Ising representation

$$\min_{\tilde{\omega} \in \{-1, 1\}^r} \tilde{\omega}^T \tilde{\mathbf{Q}} \tilde{\omega} + \tilde{\mathbf{L}} \tilde{\omega} + \tilde{C}'_0, \quad (3.16)$$

where the spin variables $\tilde{\omega}_i \in \{-1, 1\}$ are obtained through the linear transformation

$$\tilde{\omega}_i = 2\omega_i - 1.$$

The Ising formulation provides the physical model implemented by the D-Wave processor. Consequently, solving the optimization problem is equivalent to preparing the quantum system in the ground state of the corresponding Hamiltonian. In particular, the optimization problem can be encoded into the ground state of the quantum Ising Hamiltonian

$$\hat{H}_Q = \sum_{i,j} \tilde{Q}_{ij} \hat{\sigma}_i^{(z)} \hat{\sigma}_j^{(z)} + \sum_i \tilde{L}_i \hat{\sigma}_i^{(z)}, \quad (3.17)$$

where the classical spin variables are promoted to quantum spin operators. The Pauli operators acting on the i th qubit are defined as

$$\begin{aligned} \hat{\sigma}_i^{(z)} &= (\otimes_{k=1}^{i-1} \hat{I}) \otimes (\hat{\sigma}^{(z)}) \otimes (\otimes_{k=i+1}^r \hat{I}), \\ \hat{\sigma}_i^{(x)} &= (\otimes_{k=1}^{i-1} \hat{I}) \otimes (\hat{\sigma}^{(x)}) \otimes (\otimes_{k=i+1}^r \hat{I}), \end{aligned}$$

where

$$\hat{\sigma}^{(z)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \hat{\sigma}^{(x)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and $\hat{I}$ denotes the 2×2 identity matrix. Since the problem involves r qubits, the corresponding Hamiltonian acts on a Hilbert space of dimension 2^r , which rapidly becomes prohibitively large as r increases. The ground state of $\hat{H}_Q$ corresponds to the optimal binary configuration and therefore determines the approximate numerical solution of the Helmholtz equation.

To determine the ground state of $\hat{H}_Q$, D-Wave systems employ quantum annealing, where the system evolves according to the time-dependent Hamiltonian [72]

$$\hat{H}_{\text{Ising}}(t) = (1 - t/T)\hat{H}_0 + (t/T)\hat{H}_Q, \quad (3.18)$$

with the initial Hamiltonian

$$\hat{H}_0 = \sum_i \hat{\sigma}_i^{(x)},$$

and T denoting the total annealing time. The role of $\hat{H}_0$ is to prepare the system in an easily accessible ground state, which is then gradually transformed into the target Hamiltonian $\hat{H}_Q$. The objective of the annealing process is to evolve the system from the easily prepared ground state of H_0 to the ground state of H_Q , which encodes the optimal solution of the QUBO problem.

As introduced in the previous section, the quantum adiabatic theorem provides the theoretical basis for adiabatic quantum computation and quantum annealing. According to this theorem, if the Hamiltonian evolves sufficiently slowly and the quantum system is initially prepared in the ground state of the initial Hamiltonian $\hat{H}_0$, the system remains close to its instantaneous ground state throughout the evolution. Consequently, the final state approximates the ground state of the problem Hamiltonian $\hat{H}_Q$, whose measurement yields the solution of the optimization problem [1].

More quantitatively, the adiabatic theorem predicts that the required evolution time scales as

$$T = O\left(\frac{1}{g_{\min}^2}\right), \quad (3.19)$$

where $g_{\min}$ denotes the minimum spectral gap of the annealing Hamiltonian,

$$g_{\min} = \min_{t \in [0, T]} |\lambda_1(t) - \lambda_0(t)| \quad (3.20)$$

with $\lambda_0(t)$ and $\lambda_1(t)$ representing the ground-state and first-excited-state energies of $\hat{H}_{\text{Ising}}(t)$, respectively. The spectral gap plays a central role in determining the difficulty of the annealing process, since smaller gaps require longer evolution times to maintain adiabaticity. Consequently, the minimum spectral gap serves as an important indicator of the expected difficulty of the annealing process.

In practice, however, current quantum annealers operate in the presence of thermal fluctuations, environmental noise, and finite annealing times. As a consequence, the adiabatic condition is generally not satisfied exactly, and the D-Wave processor should be viewed as a heuristic quantum optimization device rather than an ideal adiabatic quantum computer. To better understand the impact of these non-ideal effects, we explicitly evaluate the spectral gap associated with equation (3.18) in several numerical experiments. Furthermore, in section 5.6 we investigate the relationship between the spectral gap and the performance of quantum annealing by considering a generic ansatz inspired by the adiabatic framework.

It should be emphasized that the computation of the spectral gap itself becomes increasingly challenging as the problem size grows. Indeed, since the dimension of the quantum Hamiltonian scales as 2^n , determining the eigenvalues required in equation (3.20) rapidly becomes computationally expensive for large QUBO matrices $\mathbf{Q}$ and $\mathbf{L}$.

Chapter 4

Experimental Setup and Computational Framework

To ensure reproducibility and facilitate the interpretation of the reported results, this chapter presents the computational framework used throughout the thesis. It describes the D-Wave quantum annealing platform, the software environment, the embedding procedure, the experimental protocol, and the performance metrics employed in the numerical investigations.

4.1 D-Wave Platform

The numerical and experimental investigations reported in this thesis were carried out using quantum annealing hardware developed by D-Wave Systems. Unlike gate-based quantum computers, which perform computations through sequences of quantum gates, D-Wave processors are designed to solve optimization problems formulated as Ising or Quadratic Unconstrained Binary Optimization (QUBO) models. In this paradigm, the optimization problem is encoded into an energy landscape specified by qubit biases and coupler interactions. The quantum annealing procedure then searches for the lowest-energy configuration of the system, which corresponds to the optimal solution of the encoded problem.

The optimization problem naturally supported by a D-Wave quantum processor is described by the Ising objective function

$$f(\mathbf{x}) = \sum_i h_i x_i + \sum_{i < j} J_{ij} x_i x_j, \quad (4.1)$$

where $x_i \in \{-1, +1\}$ represent spin variables, h_i denote local fields (biases), and J_{ij} characterize the interaction strengths between pairs of spins. The objective is to



Figure 4.1: D-Wave Advantage quantum annealing system. Source: D-Wave Systems Inc.

determine the spin configuration that minimizes the corresponding energy function.

Consequently, problems that do not naturally possess an Ising structure must first be reformulated into either an Ising or a QUBO model before they can be executed on the quantum annealer. In the framework developed in this thesis, the discretized Helmholtz equation is first recast as a least-squares optimization problem. The resulting objective function is subsequently expressed as a QUBO model and transformed into an equivalent Ising Hamiltonian, enabling its implementation on the D-Wave quantum annealing platform.

4.2 Physical Realization of Quantum Annealing

The physical implementation of quantum annealing on D-Wave processors relies on the evolution of a controllable transverse-field Ising spin system described by the time-dependent Hamiltonian

$$H(s) = -\frac{A(s)}{2} \sum_i \sigma_x^{(i)} + \frac{B(s)}{2} \left(\sum_i h_i \sigma_z^{(i)} + \sum_{i < j} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)} \right), \quad (4.2)$$

where $s \in [0, 1]$ denotes the normalized annealing parameter, h_i and J_{ij} are the local biases and coupling strengths defining the optimization problem, and σ_x and σ_z are Pauli operators. The functions $A(s)$ and $B(s)$ determine the annealing schedule.

Specifically, $A(s)$ represents the transverse-field (or tunneling) energy responsible for inducing quantum fluctuations, whereas $B(s)$ controls the strength of the problem Hamiltonian.

At the beginning of the anneal, the transverse-field term dominates the dynamics, with $A(s)$ taking a large value while $B(s)$ remains close to zero. Consequently, the qubits are initialized in a superposition of computational basis states and can explore the solution space through quantum tunneling. As the anneal progresses, the transverse-field strength is gradually reduced while the contribution of the problem Hamiltonian increases.

The quantum annealing process exploits the exponentially large configuration space available to the qubits. A system consisting of two qubits can represent $2^2 = 4$ possible states, while three qubits can represent $2^3 = 8$ states. More generally, a system containing n qubits defines an energy landscape over 2^n possible configurations. Thus, each additional qubit doubles the size of the search space, allowing increasingly complex optimization problems to be represented.

As the annealing schedule progresses, the qubit biases and couplings defining the optimization problem are gradually introduced, causing correlations and quantum entanglement to develop among the qubits. During this evolution, the quantum state simultaneously explores many candidate solutions. If the evolution is sufficiently slow, the adiabatic theorem predicts that the system remains close to its instantaneous ground state throughout the annealing process.

Near the end of the anneal, $A(s)$ approaches zero and $B(s)$ reaches its maximum value, such that the system is governed primarily by the Ising Hamiltonian encoding the optimization problem. Following measurement, the qubits collapse into classical binary states, yielding a candidate solution to the optimization problem. Ideally, this solution corresponds to the global minimum of the objective function, although near-optimal low-energy states may also be obtained in practice. Remarkably, the entire annealing procedure is completed on modern D-Wave processors within only a few microseconds.

4.3 Ocean Software Framework

All experiments were implemented using D-Wave’s Ocean Software Development Kit (SDK). The Ocean framework provides a unified interface for constructing optimization models and submitting them to a variety of computational backends, including

quantum processing units (QPUs), quantum-classical hybrid solvers, and classical samplers.

The primary experiments reported in this thesis were performed using D-Wave Advantage quantum processors accessed through the Leap cloud platform. Classical and hybrid samplers were additionally employed to validate the correctness of the formulations and benchmark the obtained results.

The QPU solver was selected through the `DWaveSampler` interface, which automatically connects to an available processor and retrieves the corresponding hardware topology and connectivity information.

4.4 Minor embedding

Modern D-Wave processors employ specialized hardware connectivity graphs. Earlier generations of D-Wave quantum annealers were based on the Chimera architecture, whereas the current Advantage processors employ the Pegasus topology, which offers substantially higher qubit connectivity and improved embedding capabilities [33].

Despite these advances, the connectivity graph associated with an optimization problem generally differs from the connectivity graph available on the physical hardware. Consequently, a direct implementation of the logical problem graph is often not possible.

To overcome this limitation, a technique known as *minor embedding* is employed. In this approach, a single logical variable may be represented by a chain of multiple physical qubits connected through strong ferromagnetic couplings. Ideally, all qubits within a chain maintain the same state throughout the annealing process and therefore behave as a single logical variable.

Following annealing, the integrity of each chain is examined. If all qubits within a chain return the same value, the chain is considered unbroken. Otherwise, a chain break occurs, requiring the application of a chain-resolution strategy such as majority voting to infer the corresponding logical state.

Although essential for mapping optimization problems onto the hardware topology, the embedding procedure introduces additional qubit overhead and often represents one of the principal limitations when solving large-scale optimization problems on current quantum annealing devices.

4.5 Sampling Procedure

Quantum annealing is inherently probabilistic. Consequently, a single annealing run does not guarantee that the global minimum will be obtained. To increase the probability of identifying optimal solutions, each problem instance is sampled multiple times.

The number of independent annealing cycles is controlled through the parameter `num_reads`. Each read corresponds to a complete annealing and measurement process and produces one candidate solution.

Throughout this work, a large number of reads was employed for every problem instance to obtain reliable statistical information regarding solution quality and success probability. The collection of returned samples was subsequently analyzed to identify the returned samples were ranked according to their energies and subsequently analyzed to evaluate both their optimization quality and the accuracy of the reconstructed numerical solution

4.6 Evaluation of Candidate Solutions

Although the quantum annealer returns solutions ordered according to their energies, the lowest-energy configuration is not necessarily the physically correct solution of the original differential equation.

In some cases, low-energy configurations may not correspond to accurate approximations of the analytical solution. Therefore, energy minimization alone cannot be used as the sole performance metric.

To verify solution quality, every candidate configuration returned by the annealer was decoded into the corresponding coefficient vector. The reconstructed solution was then substituted back into the discretized Helmholtz equation and evaluated using the mean squared error (MSE). The MSE was selected because it provides a direct quantitative comparison between the reconstructed numerical solution and the known analytical solution. This additional verification step enabled the identification of false positives and ensured that low-energy states corresponded to meaningful numerical solutions.

4.7 Software Environment and Implementation Details

The computational framework developed for this thesis was implemented in Python using the Ocean SDK and several supporting libraries for numerical computation, optimization, data processing, visualization, and quantum annealing. A summary of the software packages used and their primary functions is provided in Table 4.1.

Table 4.1: Software packages used in the experimental implementation.

Package	Purpose
NumPy	Numerical computations and matrix operations.
SciPy	Optimization routines.
dimod	Creation of Binary Quadratic Models.
dwave-system	Access to D-Wave quantum processors.
EmbeddingComposite	Automatic minor embedding onto the hardware graph.
scikit-learn	Computation of MSE and other performance metrics.
Matplotlib	Generation of plots and visualizations.
Pandas	Data storage and analysis.

The quantum annealing experiments were executed using the `DWaveSampler` class, which provides access to D-Wave quantum processing units through the Leap cloud service. To account for the connectivity constraints of the hardware graph, the sampler was wrapped within the `EmbeddingComposite` framework, which automatically performs minor embedding of the logical problem graph onto the physical qubit architecture.

For comparison purposes, the `SimulatedAnnealingSampler` provided by Ocean was employed to solve identical Ising instances on classical hardware. This enabled a direct comparison between classical and quantum annealing approaches under the same problem formulation.

The quality of the obtained solutions was evaluated through the mean squared error (MSE) between the analytical and reconstructed solutions using the `mean_squared_error()` function from `scikit-learn`.

4.8 Workflow

The overall workflow proposed in this thesis is illustrated in Figure 4.2. The methodology consists of a sequence of stages that transform the differential equation into

a form suitable for quantum annealing, beginning with the spectral discretization of the problem and concluding with the validation of the obtained solution.

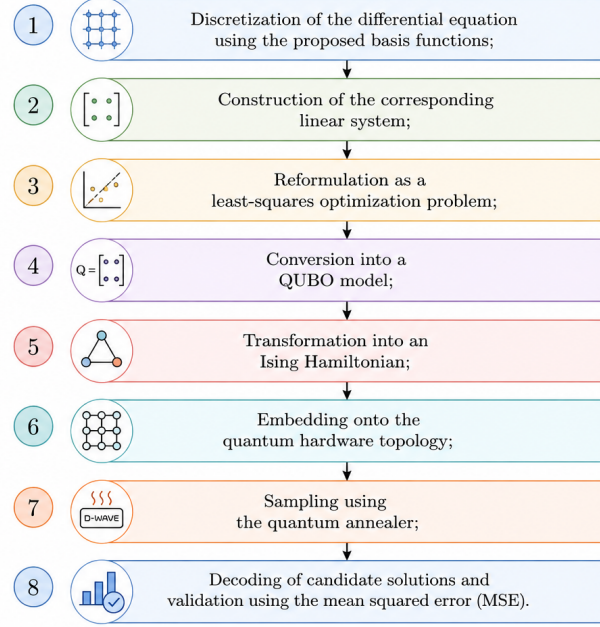


Figure 4.2: Workflow of the proposed quantum annealing framework for solving differential equations. The procedure consists of discretizing the differential equation using spectral basis functions, constructing the corresponding linear system, reformulating it as a least-squares optimization problem, converting it into a QUBO model and an equivalent Ising Hamiltonian, embedding the problem onto the quantum hardware graph, sampling candidate solutions using the D-Wave quantum annealer, and finally decoding and validating the obtained solution using the mean squared error (MSE).

To facilitate reproducibility, the complete implementation developed for this thesis has been made publicly available through the following GitHub repository. <https://github.com/aigerimhatake/QA->.

Chapter 5

Experiments and Results

The objective of this chapter is to evaluate the proposed QUBO formulations and determine how the choice of ansatz, encoding parameters, and problem characteristics influence the performance of quantum annealing. The analysis is carried out on the D-Wave quantum annealing platform, where the influence of the approximation size N and the number of spins n_{spin} spin employed in the binary encoding scheme is systematically investigated.

To assess the robustness and applicability of the proposed framework, the experiments were performed for a wide range of problem configurations. These include different values of the wave number τ , multiple combinations of the boundary condition parameters α and β , and various source functions $F(x)$. Such a comprehensive set of benchmark problems enables a detailed examination of the method under diverse physical conditions. Moreover, it provides insight into the impact of the ansatz construction and binary encoding scheme on the optimization landscape, as well as on the accuracy and success of the quantum annealing process. These benchmark problems were selected to evaluate the robustness of the proposed methodology under increasingly challenging physical and numerical conditions.

Because quantum annealing is inherently a heuristic optimization approach, approximation accuracy alone does not provide a complete characterization of its performance. To complement the error analysis, we therefore evaluate each formulation using the *success rate* (SR), defined as the percentage of annealing runs that recover the exact solution among 1000 independent executions. The success rate serves as an indicator of the robustness and consistency of the quantum annealing process, reflecting its capability to repeatedly locate the global optimum of the corresponding optimization problem.

In addition to evaluating the performance of quantum annealing independently, a comparative study with classical simulated annealing (SA) was carried out. The SA

experiments were implemented using the corresponding sampler provided within the D-Wave Ocean framework and were based on the same Ising formulations considered by the quantum annealer. This comparative analysis facilitates a direct assessment of the effectiveness of quantum and classical annealing strategies and highlights their relative capabilities in solving the optimization problems arising from the discretized Helmholtz equation.

For a more convenient analysis of the QUBO formulation, we exploit the binary nature of the variables, namely $\omega_i^2 = \omega_i$. This property allows the linear contribution $\mathbf{L}$ to be incorporated into the diagonal elements of the quadratic matrix $\mathbf{Q}$, yielding the equivalent compact representation

$$\min_{\omega \in \{0,1\}^r} \omega^T \mathbf{Q} \omega + C'_0. \quad (5.1)$$

To further assess the algebraic properties of the QUBO matrices and the performance of the proposed ansatzes, we also consider the *dynamic range* (DR), which quantifies the ratio between the largest and smallest nonzero magnitudes of the QUBO matrix entries. Originally introduced in signal processing to characterize the ratio between the smallest and largest possible values of a measurable quantity, the dynamic range is defined as

$$DR(\mathbf{Q}) = \log_2 \left(\frac{\hat{D}(\mathbf{Q})}{\check{D}(\mathbf{Q})} \right), \quad (5.2)$$

where $\mathbf{Q}$ denotes the QUBO matrix, while $\hat{D}(\mathbf{Q})$ and $\check{D}(\mathbf{Q})$ represent the absolute values of the largest and smallest nonzero entries of $\mathbf{Q}$, respectively. Notice that only nonzero entries are considered in the denominator [69]. Previous studies have shown that large dynamic ranges may adversely affect the performance of both classical and quantum annealing algorithms, making it more difficult to identify optimal solutions.

Finally, we investigate the minimum energy gap associated with the time-dependent quantum Ising Hamiltonian introduced in equation (3.20). The importance of this quantity stems from its fundamental role in adiabatic quantum evolution, as it directly affects the probability that the system remains in its ground state throughout the annealing process. Motivated by this observation, the final part of this chapter examines an alternative ansatz specifically designed to maximize the spectral gap and studies its impact on the performance of quantum annealing.

In the subsequent analysis, the *matrix rank*, *dynamic range* (DR), and *minimum energy gap* $g_{\min}$ are regarded as predictive indicators of the expected performance of a given ansatz, since they can be evaluated directly from the corresponding QUBO formulation. In contrast, the *success rate* (SR) and *mean squared error* (MSE) provide

empirical measures of performance and are used to assess the actual quality and reliability of the solutions produced by the quantum annealer.

5.1 Homogeneous Helmholtz equation

To illustrate the proposed encoding strategies based on either the truncated Fourier series ansatz (3.10) or the circulant ansatz (3.11), we first consider a simple homogeneous Helmholtz problem with prescribed initial conditions,

$$\begin{cases} u''(x) + u(x) = 0, & 0 < x < 2\pi, \\ u(0) = 0.5, & u'(0) = 0. \end{cases} \quad (5.3)$$

The analytical solution is readily obtained from (3.2) and is given by $u(x) = \frac{1}{2} \cos(x)$. This experiment serves as a baseline validation of the proposed methodology before considering more challenging inhomogeneous problems.

Since the exact solution consists of a single Fourier mode, choosing $N = 2$ together with $n_{\text{spin}} \geq 2$ is sufficient to represent it exactly within the approximation framework (3.4) for both basis constructions considered in this work. Consequently, one may expect both simulated annealing (SA) and quantum annealing (QA) implemented on the D-Wave platform to recover the exact solution of problem (5.3) with high accuracy.

Nevertheless, in practical applications the exact form of the solution is generally unknown a priori. As a result, appropriate values of the approximation order N and the number of spins n_{spin} used in the binary encoding cannot be determined beforehand. These parameters must therefore be selected through a systematic iterative procedure, in which they are progressively adjusted to achieve a suitable balance between approximation accuracy and optimization complexity.

Table 5.1: The rank, DR and energy minimum gap returned by both ansatz, TFA and CA, are shown for different values of the number of spins, while maintaining fixed the number of basis functions, i.e. $N = 2$. The last two columns show a comparison of the SR achieved by both SA and QA.

n_{spin}	$rank(\mathbf{a})$		DR		$g_{\min}$		SR SA (%)		SR QA (%)	
	TFA	CA	TFA	CA	TFA	CA	TFA	CA	TFA	CA
2	2	2	3.3	4.7	1.9×10^{-1}	9.9×10^{-2}	96.0	99.6	99.3	87.1
3	2	2	5.3	6.7	4.1×10^{-2}	2.5×10^{-2}	81.4	97.8	65.8	32.0
4	2	2	7.321	8.7	4.9×10^{-3}	7.8×10^{-3}	52.4	56.1	15.8	6.6
5	2	2	9.3	10.7	3.9×10^{-3}	1.9×10^{-3}	36.8	28.0	3.1	1.2

Since the exact solution can be represented within the considered parameter regime, the success rate (SR) serves as an appropriate metric for evaluating the performance of both ansatzes. The corresponding results, together with the remaining performance indicators, are reported in Table 5.1 for different values of n_{spin} , while keeping the number of basis functions fixed.

Overall, the truncated Fourier ansatz (TFA) exhibits slightly superior performance on both the simulated annealing (SA) and quantum annealing (QA) platforms. This observation is consistent with the theoretical considerations presented earlier, as the TFA generally yields higher success rates and larger minimum energy gaps for most values of n_{spin} . Furthermore, the results reveal a noticeable decline in the success rate of the quantum annealer as n_{spin} increases. This behavior is accompanied by a reduction in the minimum energy gap g_{min} , which becomes increasingly small as the dimension of the quantum Hamiltonian grows exponentially with $N \times n_{\text{spin}}$.

The observed degradation in QA performance can be understood in the context of the adiabatic theorem. Smaller spectral gaps require longer annealing times to ensure that the system remains in its ground state throughout the evolution. In practice, however, maintaining adiabaticity over extended time intervals becomes increasingly challenging due to hardware limitations, including thermal excitations, control errors, noise, and other non-ideal effects. As a consequence, the probability of successfully reaching the ground state decreases, leading to a lower success rate for larger problem instances.

5.2 Inhomogeneous Helmholtz equation with monochromatic driving I

We next investigate the effect of a monochromatic forcing term on the performance of both simulated annealing (SA) and quantum annealing (QA). To this end, we consider the boundary value problem

$$\begin{cases} u''(x) + u(x) = 1.5 \cos(2x), & 0 < x < 2\pi, \\ u(0) = 0, & u'(0) = 0. \end{cases} \quad (5.4)$$

The corresponding analytical solution is $u(x) = \frac{1}{2}(\cos(x) - \cos(2x))$. Since the exact solution contains two Fourier modes, it can be represented exactly by the proposed approximation (3.4) provided that $N \geq 4$ and $n_{\text{spin}} \geq 2$. Compared with the homogeneous problem studied in Section 5.1 this benchmark allows us to assess the proposed methodology for solutions with increased spectral complexity while still retaining an

exact analytical solution for validation. Consequently, this test case allows us to investigate the influence of the binary encoding on the optimization process while maintaining sufficient approximation capability to recover the exact solution.

As in the previous experiment, we analyze the impact of the approximation and encoding parameters separately. First, the number of basis functions is fixed at $N = 4$, and the number of spins n_{spin} is varied. Subsequently, the value of n_{spin} is kept fixed while the approximation order N is increased. This strategy enables us to distinguish between the effects of the approximation space and those arising from the binary encoding scheme.

The results obtained for $N = 4$ are summarized in Table 5.2. For both the truncated Fourier ansatz (TFA) and the circulant ansatz (CA), increasing the number of spins leads to a wider dynamic range and a progressive reduction of the minimum energy gap. As a consequence, the success rates of both SA and QA decrease as n_{spin} grows. The deterioration is particularly pronounced for QA, reflecting the increased difficulty of maintaining adiabatic evolution when the minimum spectral gap becomes small. These observations are consistent with the trends reported in the previous experiment and further highlight the relationship between the dynamic range, spectral gap, and annealing performance.

Table 5.2: The rank, DR and energy minimum gap returned by both ansatz, TFA and CA, are shown for different values of the number of spins, while maintaining fixed the number of basis functions, i.e. $N = 4$. The last two columns show a comparison of the SR achieved by both SA and QA.

n_{spin}	$\text{rank}(\mathbf{a})$		DR		g_{min}		SR SA (%)		SR QA (%)	
	TFA	CA	TFA	CA	TFA	CA	TFA	CA	TFA	CA
2	3	4	53.6	8.1	1.3×10^{-3}	1.5×10^{-1}	41.1	79.1	11.2	23
3	3	4	56.6	10.1	8.8×10^{-4}	3.8×10^{-2}	18.8	33	1.3	2.5

The results presented in Table 5.2 reveal notable differences between the two ansatzes. In particular, the truncated Fourier ansatz (TFA) generates a rank-deficient matrix, whereas the circulant ansatz (CA) yields a full-rank matrix. As discussed in Section 3.2, rank deficiency may introduce multiple spurious solutions, thereby increasing the likelihood of false positives and complicating the optimization process. Consequently, the optimization landscape becomes more ambiguous, making it more difficult for both SA and QA to identify the physically meaningful solution.

Another important observation concerns the dynamic range (DR), which increases with the number of spins n_{spin} for both ansatzes. However, the TFA consistently ex-

hibits a larger dynamic range than the CA. Since large dynamic ranges are generally associated with more challenging optimization landscapes, this result suggests a potential disadvantage of the TFA formulation. The consistently smaller dynamic range produced by the circulant ansatz provides further evidence that its algebraic structure is inherently better suited for optimization on current quantum annealing hardware.

Furthermore, increasing n_{spin} enlarges the dimension of the corresponding Hamiltonian, leading to a progressive reduction of the minimum energy gap g_{min} . As the spectral gap approaches zero, the performance of both simulated annealing (SA) and quantum annealing (QA) deteriorates, as reflected by the decreasing success rates. Nevertheless, the CA consistently achieves higher success rates on both platforms, indicating greater robustness and reliability as the complexity of the optimization problem increases. These findings are in agreement with the theoretical considerations presented earlier and further support the use of the circulant ansatz for constructing QUBO formulations suitable for annealing-based optimization.

Table 5.3: Comparison on TFA and CA on metrics for $n_{\text{spin}} = 2$

N	$\text{rank}(\mathbf{a})$		DR		MSE (SA)		MSE (QA)	
	TFA	CA	TFA	CA	TFA	CA	TFA	CA
4	3	4	53.609	8.189	0	0	0	0
8	7	8	63.796	56.579	0	0.011	0	0
10	9	10	65.077	57.803	0	0.026	0.124	0.044
18	17	18	69.398	59.189	0	0.065	0.5	0.241

In the second part of this experiment, summarized in Table 5.3, the number of spins is kept fixed while the approximation order N is progressively increased. This analysis allows us to investigate how enlarging the approximation space affects the properties of the resulting QUBO formulation and, consequently, the performance of the annealing algorithms.

The results show that the truncated Fourier ansatz (TFA) continues to produce rank-deficient matrices, whereas the circulant ansatz (CA) consistently yields full-rank matrices across all tested values of N . In addition, although the dynamic range (DR) increases for both formulations as the approximation order grows, it remains systematically smaller for the CA. This observation suggests that the optimization landscape associated with the circulant ansatz is generally more favorable for annealing-based optimization.

A comparison of the solution accuracy further highlights the differences between the two approaches. In the quantum annealing experiments, the CA consistently

achieves lower mean squared errors (MSE), indicating a more accurate reconstruction of the exact solution. For simulated annealing, however, the TFA exhibits slightly lower MSE values in some cases. Nevertheless, the overall QA results suggest that the combination of full-rank matrices and a reduced dynamic range contributes to improved optimization performance, ultimately leading to more accurate solutions. These findings provide additional evidence that the structural properties of the QUBO matrix play a significant role in determining the effectiveness of quantum annealing.

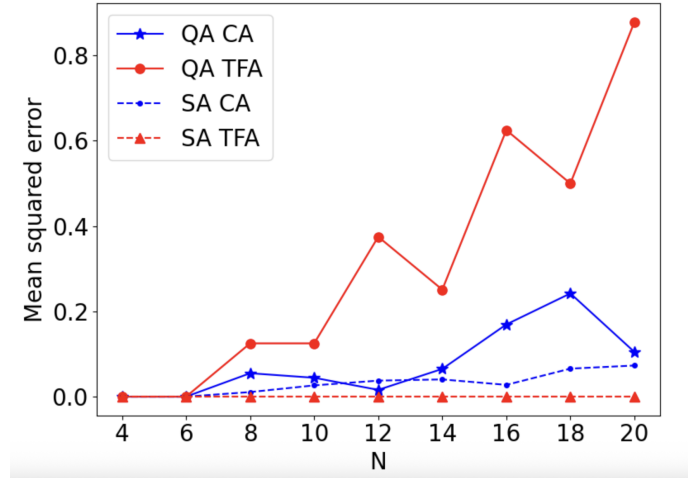


Figure 5.1: MSE, retrieved by SA and QA in the scenario of Eq. (5.4), as a function of the number N of spin functions for a fixed value of the number of spins, i.e. $n_{\text{spin}} = 2$.

As illustrated in Figure 5.1, the computational study was restricted to the range $N = 4, \dots, 20$ due to the rapid growth of the corresponding QUBO matrices with increasing approximation order. Among the configurations considered, the smallest mean squared errors (MSEs) were obtained for $N = 4$ and $N = 6$. Beyond these values, the solution accuracy gradually deteriorates as N increases.

This behavior suggests that enlarging the approximation space does not necessarily improve the performance of the annealing algorithms. On the contrary, the resulting increase in problem size makes the identification of the ground state progressively more challenging. In addition to the increased optimization complexity, several practical factors may further affect the quality of the obtained solutions. These include numerical round-off errors introduced during the construction of the QUBO and Ising formulations, as well as the finite precision with which the Ising coefficients can be represented on the quantum annealing hardware. Collectively, these effects may contribute to the observed degradation in performance for larger values of N .

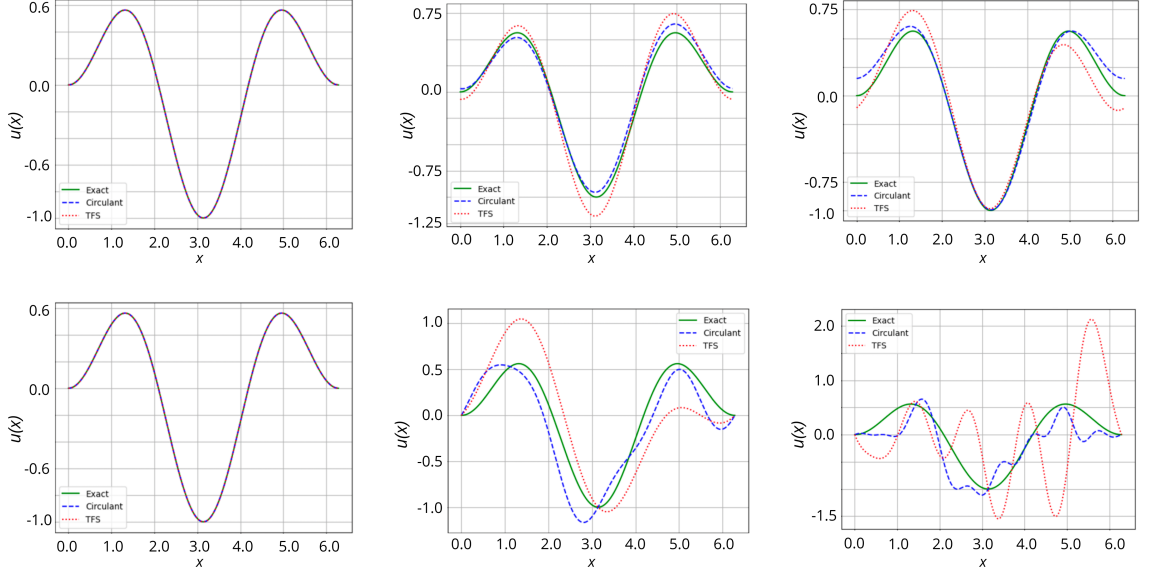


Figure 5.2: (Upper row) Exact and approximated solution returned by QA endowed with TFA and CA for increasing number of spins, $n_{\text{spin}} = 2, 8, 10$ from left to right, and fixed $N = 4$. (Lower row) Similarly, exact and approximated solution returned by QA endowed with TFA and CA for increasing number of basis functions, $N = 4, 10, 18$ from left to right, and fixed $n_{\text{spin}} = 2$.

The upper row of Figure 5.2 illustrates the effect of increasing the number of spins while keeping the approximation order N fixed. This analysis allows us to isolate the influence of the binary encoding resolution on the quality of the obtained solutions. A comparison between the two ansatzes shows that the circulant ansatz (CA) consistently provides a more accurate reconstruction of the solution than the truncated Fourier ansatz (TFA) across all considered cases. Nevertheless, both approaches achieve relatively small mean squared errors, indicating that variations in n_{spin} have only a moderate impact on the overall approximation accuracy.

The lower row of Figure 5.2 examines the complementary scenario, where the number of spins is fixed and the approximation order N is increased. This setting enables an assessment of how enlarging the approximation space affects the solution quality. For all representative cases considered $N = 4, N = 10$, and $N = 18$, the circulant ansatz again outperforms the truncated Fourier ansatz, yielding more accurate approximations of the exact solution. These results further support the conclusion that the circulant ansatz provides a more effective and robust framework for constructing QUBO formulations suitable for annealing-based optimization.

Overall, this experiment confirms that the advantages of the circulant ansatz persist beyond the simplest benchmark problem. The full-rank algebraic structure,

smaller dynamic range, and larger minimum spectral gap consistently translate into higher success rates for both simulated and quantum annealing.

5.3 Inhomogeneous Helmholtz equation with monochromatic driving II

$$\begin{cases} u''(x) + 4u(x) = -6 \cos 4x, 0 < x < 2\pi, \\ u(0) = 0.5, u'(0) = 1. \end{cases} \quad (5.5)$$

In contrast to the previous benchmark, the present experiment investigates whether the observed advantages of the circulant ansatz persist when the solution contains higher-frequency components requiring a larger approximation space. In Experiment 3, the Helmholtz equation was supplemented with a forcing term, and the primary objective was to investigate the influence of the approximation order N on the performance of the annealing algorithms. Based on the structure of the exact solution, it was anticipated that an exact representation would be achieved when $N = 8$. The numerical results confirmed this expectation, with the lowest energy state being recovered at this value of N .

The corresponding plots highlight the importance of selecting an appropriate approximation order. While increasing N enlarges the approximation space, the results indicate that the most accurate solutions are obtained when the chosen value of N matches the complexity of the underlying solution. Furthermore, the experiments demonstrate that a binary encoding with $n_{\text{spin}} = 2$ is sufficient to accurately represent the solution, suggesting that increasing the number of spins does not provide a significant advantage for this particular problem instance.

Table 5.4: Comparison of TFA and CA on metrics for nspin=2.

N	$rank(\mathbf{a})$		DR		MSE (SA)		MSE (QA)	
	TFA	CA	TFA	CA	TFA	CA	TFA	CA
4	3	4	6.882	58.064	0.374	1.251	0.125	1.054
8	6	8	61.456	59.184	0.124	0	0.124	0
10	8	10	64.511	58.201	0.124	0.008	0.125	0.041
18	16	18	68.288	59.112	0.124	0.027	0.501	0.145

In this part of the study, summarized in Table 5.4, the number of spins is kept fixed while the approximation order N is gradually increased. This allows us to examine how the size of the approximation space influences the properties of the resulting QUBO formulation and the performance of the annealing algorithms.

The rank analysis shows that the truncated Fourier ansatz (TFA) continues to produce rank-deficient matrices, whereas the circulant ansatz (CA) consistently generates full-rank matrices for all considered values of N . Although both formulations exhibit relatively large dynamic ranges (DR), the values associated with the CA remain systematically smaller than those of the TFA. In addition, the CA achieves lower mean squared error (MSE) values in the quantum annealing experiments, indicating a more accurate approximation of the exact solution.

These observations suggest that the structural properties of the QUBO matrix play an important role in determining the effectiveness of quantum annealing. In particular, maintaining a full-rank matrix while simultaneously reducing the dynamic range appears to improve the optimization process, ultimately leading to lower MSE values and enhanced solution accuracy.

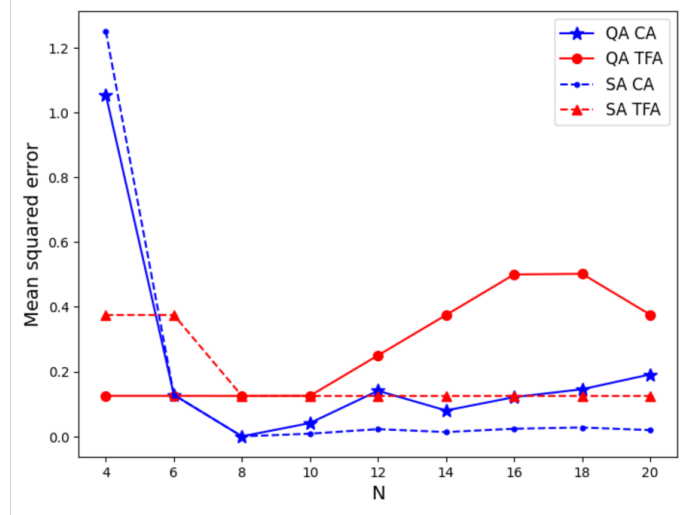


Figure 5.3: A comparison of QA and SA applied to both methods, with the number of spins fixed at 2 and varying $N = 4, 6, \dots, 20$. The corresponding MSE values are reported for each N .

As shown in Figure 5.3, the circulant ansatz (CA) successfully recovers the optimal solution when $N = 8$, whereas the truncated Fourier ansatz (TFA) does not achieve comparable performance for any of the tested values of N . This result highlights a significant difference between the two formulations and demonstrates the superior effectiveness of the CA for the problem under consideration.

The observed behavior suggests that the structural properties of the CA lead to a more favorable optimization landscape, enabling the annealing process to identify the ground state more reliably. In contrast, the TFA fails to exhibit a similar level of performance across the examined range of approximation orders. Consequently,

these results provide further evidence that the circulant ansatz offers a more robust and efficient framework for constructing QUBO formulations suitable for quantum annealing.

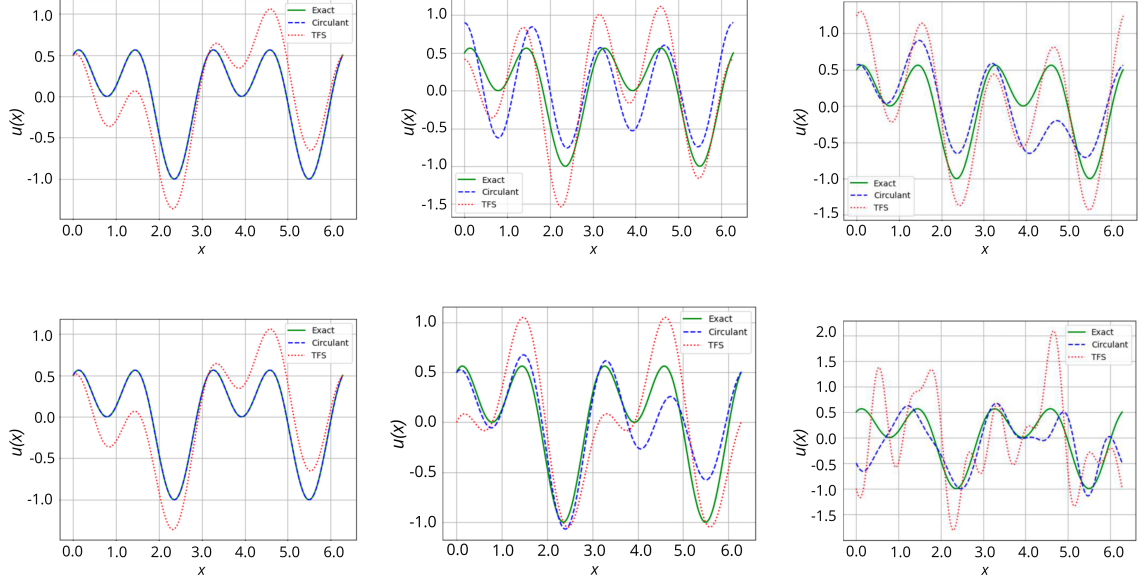


Figure 5.4: (Upper row) Exact and approximated solution returned by QA endowed with TFA and CA for a fixed number of basis functions (i.e. $N = 4$) and an increasing number of spins: $n_{\text{spin}} = 2, 8, 10$ from left to right, respectively. (Lower row) Similarly, exact and approximated solution returned by QA endowed with TFA and CA for a fixed number of spins (i.e. $n_{\text{spin}} = 2$) and an increasing number of basis functions: $N = 4, 10, 18$ from left to right, respectively.

The upper row of Figure 5.4 presents the results obtained for a fixed approximation order $N = 8$ and different values of the binary encoding parameter, namely $n_{\text{spin}} = 2, 8$, and 10 . In all cases, the circulant ansatz (CA) provides a more accurate representation of the solution than the truncated Fourier ansatz (TFA), as evidenced by its superior reconstruction of the frequency components of the exact solution.

A similar trend can be observed in the lower row of Figure 5.4, where the number of spins is fixed at $n_{\text{spin}} = 2$ and the approximation order is varied $N = 4, 10$, and 18 . Across all considered values of N , the CA consistently outperforms the TFA, yielding a closer agreement with the exact frequency spectrum. These results further confirm the superior capability of the circulant ansatz to capture the underlying spectral structure of the solution and reinforce the conclusions drawn from the quantitative performance metrics.

5.4 Inhomogeneous Helmholtz equation with polichromatic driving

This benchmark represents a substantially more demanding test of the proposed methodology, as both the forcing term and the analytical solution contain multiple interacting Fourier modes. In this part of the analysis, reported in Table 5.5, the number of spins is kept fixed while the approximation order N is progressively increased. This enables an investigation of how the size of the approximation space influences the properties of the resulting QUBO formulation and the accuracy of the obtained solutions.

$$\begin{cases} u''(x) + u(x) = 2 \cos 3x - 3.75 \cos 4x - 0.75 \sin 2x + 2 \sin 3x, 0 < x < 2\pi, \\ u(0) = -0.25, u'(0) = 0. \end{cases} \quad (5.6)$$

Table 5.5: Comparison of TFA and CA on metrics for fixed npsin=3. For fixed nspin = 3 and with an increase in N TFA encounters rank deficiency, leading to a larger dynamic range than CA. As a result, the mean squared error (MSE) of the TFA is greater than CA.

N	$rank(\mathbf{a})$		DR		MSE(SA)		MSE(QA)	
	TFA	CA	TFA	CA	TFA	CA	TFA	CA
4	3	4	58.794	9.303	0.249	1.280	0.124	0.919
8	7	8	66.212	60.261	0.031	0.015	0.125	0.054
10	9	10	67.077	60.492	0.031	0.006	0.187	0.145
18	17	18	71.398	61.270	0.031	0.035	0.688	0.236

The rank analysis indicates that the truncated Fourier ansatz (TFA) generates rank-deficient matrices, whereas the circulant ansatz (CA) consistently preserves full rank across all considered values of N . Although the dynamic range (DR) remains relatively large for both formulations, it is systematically smaller for the CA. In addition, the CA achieves lower mean squared error (MSE) values in the quantum annealing experiments, demonstrating a more accurate approximation of the exact solution.

These findings further support the hypothesis that the structural characteristics of the QUBO matrix have a significant impact on annealing performance. In particular, preserving full rank while maintaining a reduced dynamic range appears to facilitate the optimization process, resulting in improved solution quality and lower MSE values for quantum annealing.

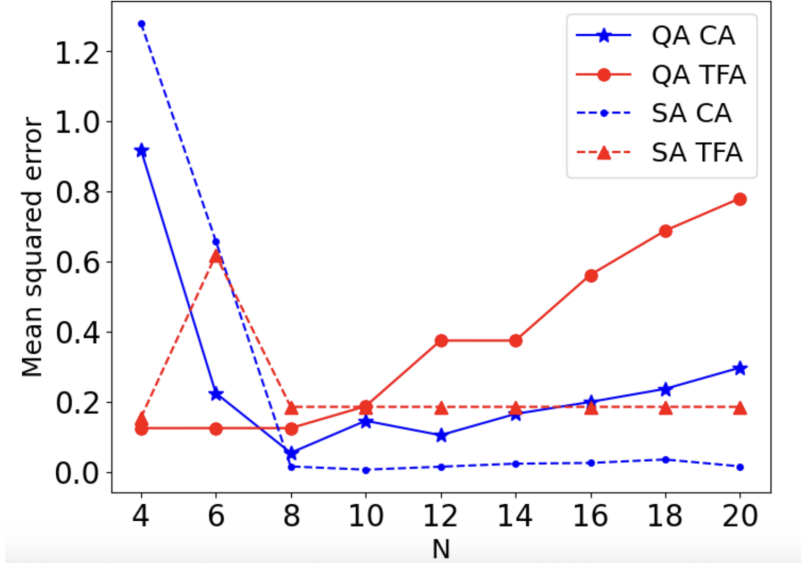


Figure 5.5: MSE, retrieved by SA and QA in the scenario of Eq. (5.6), as a function of the number N of spin functions for a fixed value of the number of spins, i.e. $n_{\text{spin}} = 3$.

The objective of this experiment, illustrated in Figure 5.5, is to examine the influence of the approximation order N and the number of spins n_{spin} on the performance of the annealing process. Based on the structure of the exact solution, we expect the minimum ground-state energy to be attained when $N = 8$. Furthermore, representing the coefficient value 0.25 in the adopted binary encoding requires at least three spins, suggesting that $n_{\text{spin}} = 3$ should be sufficient to accurately capture the solution.

The numerical results are consistent with these theoretical considerations. In particular, the circulant ansatz (CA) achieves its lowest energy at $N = 8$, indicating successful recovery of the optimal solution. This observation highlights the importance of selecting an approximation order that is well matched to the spectral content of the exact solution. It also demonstrates that increasing the number of spins beyond the minimum required for an accurate binary representation does not necessarily lead to further improvements in performance.

5.5 Homogeneous Helmholtz equation with irrational initial conditions

The previous benchmarks considered rational boundary conditions that could be represented exactly using a finite binary expansion. In practical applications, however, irrational values frequently arise and must be approximated within the binary encoding.

The purpose of this experiment is therefore to investigate how this additional approximation error affects the performance of the proposed quantum annealing framework. The final experiment was constructed such that the parameter α cannot be represented exactly using the adopted binary encoding. As a result, the corresponding QUBO formulation inherently contains approximation errors arising from the finite precision of the encoding scheme. This scenario provides a useful benchmark for assessing the robustness of the proposed methodology under non-ideal conditions.

The numerical results show that the performance of quantum annealing degrades as the approximation order N increases. The observed behavior suggests that the combined effect of encoding inaccuracies, larger QUBO matrices, and increased optimization complexity makes the recovery of the ground state progressively more difficult. Consequently, the quality of the solutions obtained by the quantum annealer decreases for larger values of N .

$$\begin{cases} u''(x) + u(x) = 0, 0 < x < 2\pi, \\ u(0) = \frac{\sqrt{2}}{2}, u'(0) = 0. \end{cases} \quad (5.7)$$

Table 5.6: Comparison of TFA and CA on metrics for $N = 2$

nspin	$rank(\mathbf{a})$		DR		g_{min}		MSE(SA)		MSE(QA)	
	TFA	CA	TFA	CA	TFA	CA	TFA	CA	TFA	CA
2	2	2	6.0	5.4	1.9×10^{-1}	1.02×10^{-1}	0.02	0.02	0.02	0.02
3	2	2	6.1	8.5	4.1×10^{-2}	2.4×10^{-2}	10^{-3}	10^{-3}	10^{-3}	10^{-3}
4	2	2	7.5	8.8	4.9×10^{-3}	4.9×10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-3}
5	2	2	9.5	10.8	1.5×10^{-3}	1.9×10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-3}

The results presented in Table 5.6 show that both the circulant ansatz (CA) and the truncated Fourier ansatz (TFA) generate full-rank matrices $\mathbf{A}$. As the number of spins increases, the dynamic range (DR) of the corresponding QUBO formulation also increases for both methods. At the same time, the minimum energy gap g_{min} decreases and gradually approaches zero as the dimension of the Hamiltonian grows. This reduction in the spectral gap is accompanied by a decline in the success rates of both simulated annealing (SA) and quantum annealing (QA).

Such behavior is consistent with the predictions of the adiabatic theorem, according to which smaller energy gaps require longer evolution times in order to maintain adiabaticity and preserve the ground state throughout the annealing process. Consequently, identifying the optimal solution becomes increasingly challenging as the

problem size increases. Despite these effects, the mean squared error (MSE) values obtained by the two ansatzes remain comparable across the tested configurations.

The principal objective of this experiment is to highlight the limitations imposed by binary encoding when representing parameters that cannot be expressed exactly in finite binary form. The results demonstrate that a larger number of spins is required to achieve a more accurate representation of such coefficients, thereby reducing encoding errors and improving the overall quality of the numerical approximation.

5.6 Alternative Ansatz: Adiabatic Prescription

In the previous experiments, we observed that ansatzes associated with larger minimum energy gaps generally achieved higher success rates. This observation motivates a more systematic investigation of the relationship between the energy spectral gap and the choice of basis functions in equation (3.4). Rather than constructing the basis from algebraic considerations, we now adopt an adiabatic perspective and seek an ansatz that directly maximizes the minimum energy spectral gap defined in Eq. (3.20).

The proposed ansatz takes the form

$$u_N(x) = \sum_{n=0}^{N-1} \omega_n G_n(x), \quad (5.8)$$

where $G_0(x), G_1(x), \dots, G_{N-1}(x)$ denotes a new set of basis functions defined as

$$G_n(x) = \sum_{k=-2}^2 g_{n,k} e^{ikx},$$

with complex coefficients $g_{n,k}$ to be determined.

It is worth noting that equation (5.8) includes the previously studied ansatzes as special cases. In particular, suitable choices of the coefficients $g_{n,k}$ recover either the truncated Fourier ansatz (TFA) or the circulant ansatz (CA). In contrast to these constructions, we now determine the coefficients by maximizing the minimum energy spectral gap (3.20). The gap is evaluated through numerical diagonalization of the corresponding quantum Ising Hamiltonian obtained from equation (5.8) following the procedure described in Section 3.5. All numerical calculations were performed using Python scientific-computing libraries.

Since the quantum Ising Hamiltonian (3.18) has dimension $2^r \times 2^r$, the optimization procedure becomes computationally demanding even for moderate values of r . For this reason, we restrict our analysis to the first experiment presented in

Section 5.1, considering the fixed parameters $N = 4$ and $n_{\text{spin}} = 2$. Although the optimization is demonstrated for a small benchmark problem, it illustrates a promising strategy for designing future encoding schemes.

To simplify the optimization problem, we impose that the basis functions are real-valued, i.e.,

$$\text{Im}[G_n(x)] = 0, \quad n = 0, 1, 2, 3,$$

for all $x \in [0, 2\pi]$. This requirement leads to the constraints

$$\begin{cases} g_{n,-2}^R = g_{n,2}^R, g_{n,-1}^R = g_{n,1}^R, \\ g_{n,-2}^I = -g_{n,2}^I, g_{n,-1}^I = -g_{n,1}^I, \\ g_{n,0}^I = 0. \end{cases}$$

Using equation (5.8), we first evaluate the minimum energy gap associated with the TFA and CA basis sets and compare their performance. Subsequently, we optimize the coefficients $g_{n,k}$ to maximize the minimum energy gap. This optimization is performed using the SciPy library, which provides efficient numerical optimization routines. The optimization requires an initial guess and a bounded search domain for the coefficients. As an illustrative example, we consider the case $N = 4$, for which the coefficient matrix $g_{n,k}$ is optimized accordingly.

Table 5.7: Comparison of TFA, CA and AA on metrics for $N = 4$ and $n_{\text{spin}}=2$ (Results on maximizing the minimum gap)

	$\text{rank}(\mathbf{a})$	DR	$g_{\min}$	SR SA (%)	SR QA (%)
TFA	3	8.228	3.977×10^{-4}	44.3	8.2
CA	4	7.169	1.229×10^{-1}	65.9	11
AA	4	16.19	1.332×10^{-1}	65.3	18

Table 5.7 summarizes the results obtained for the truncated Fourier ansatz (TFA), circulant ansatz (CA), and the adiabatic ansatz (AA).

The results indicate that increasing the minimum energy gap while maintaining a full-rank matrix generally improves the success rate of both simulated annealing (SA) and quantum annealing (QA). In particular, the proposed adiabatic ansatz achieves the largest minimum gap and yields the highest QA success rate among the three approaches considered.

Furthermore, the comparison highlights the important roles played by both the dynamic range (DR) and the minimum energy gap. Although both quantities influence the optimization performance, their effects are not equally significant. The

results suggest that the minimum energy gap has a stronger impact on the performance of quantum annealing, as expected from the adiabatic theorem. In contrast, simulated annealing does not directly depend on the spectral properties of the quantum Hamiltonian and therefore appears less sensitive to changes in the energy gap. Consequently, while both SA and QA benefit from favorable problem representations, the energy gap optimization strategy is particularly advantageous for quantum annealing.

Chapter 6

Conclusion

In this thesis, we investigated the application of quantum annealing (QA) combined with spectral methods for solving the one-dimensional Helmholtz equation on contemporary quantum hardware provided by D-Wave Systems. The study focused on two different basis-function ansatzes, namely the truncated Fourier ansatz (TFA) and the circulant ansatz (CA), under various experimental conditions characterized by different numbers of spectral components N and binary spins n_{spin} . This analysis provided a detailed assessment of the capabilities and limitations of these encoding strategies when applied to the quantum solution of differential equations.

The numerical results consistently demonstrated the advantages of the circulant ansatz. In contrast to the truncated Fourier ansatz, which frequently produced rank-deficient matrices, the circulant ansatz generated full-rank system matrices across all considered experiments. The observed behavior of the minimum energy spectral gap was also found to be consistent with the predictions of the adiabatic theorem, highlighting the critical role of ansatz design in quantum annealing applications. In particular, one of the main findings of this work is the identification of matrix rank and conditioning as key factors influencing the performance of the resulting QUBO formulation and, consequently, the effectiveness of both classical and quantum optimization methods.

A comparison with simulated annealing (SA) revealed qualitatively similar trends, providing additional validation of the obtained results. The experiments indicate that the choice of basis functions and the structural properties of the resulting matrices play a fundamental role when continuous physical problems are translated into binary optimization problems suitable for quantum hardware.

Although quantum annealing has not yet demonstrated a clear computational advantage over state-of-the-art classical methods for industrial-scale applications, this

work contributes to a deeper understanding of the challenges associated with encoding differential equations on quantum annealers. In particular, the results suggest that the development of problem-specific embedding techniques capable of preserving desirable matrix properties while respecting the connectivity constraints of D-Wave architectures may further enhance the performance of quantum annealing approaches for wave-equation problems.

Future research may extend the proposed framework in several important directions. One natural extension is the application of the proposed methodology to higher-dimensional wave and Helmholtz equations, where the increased problem size and complexity introduce additional challenges in both the QUBO formulation and the quantum annealing process. Another promising direction is the investigation of alternative basis-function constructions, such as wavelet, spline, or adaptive spectral bases, which may improve approximation accuracy while producing better-conditioned optimization problems.

Further research may also focus on the development of more efficient binary encoding schemes and embedding strategies that reduce the number of physical qubits required, improve hardware utilization, and increase the probability of obtaining the ground-state solution. In addition, hybrid quantum–classical approaches that combine quantum annealing with classical optimization algorithms, preconditioning techniques, or domain decomposition methods could provide an effective means of solving larger and more complex differential equations.

Finally, evaluating the proposed framework on future generations of quantum annealers with higher qubit counts, enhanced connectivity, improved precision, and reduced noise will provide valuable insight into its scalability and practical performance. As quantum annealing hardware and algorithms continue to mature, these developments are expected to broaden the applicability of quantum optimization techniques and contribute to the development of more efficient and scalable quantum-assisted solvers for differential equations and other challenging scientific computing problems.

Appendix Overview

The appendices provide supplementary mathematical and computational material that supports the results presented throughout this thesis. Their purpose is to supply detailed formulations of the discrete operators, forcing functions, spectral reconstruction procedures, and auxiliary quantities associated with the QUBO formulation. To maintain the flow of the main text, the emphasis in the core chapters is placed on the theoretical framework, methodology, and analysis of the results, while technical derivations and implementation details are deferred to the appendices.

Appendix A presents the explicit construction of the linear systems arising from both the truncated Fourier ansatz and the circulant ansatz. Appendix B contains the definitions of the discrete collocation grid, the benchmark forcing terms employed in the numerical experiments, and the quantitative measures used to characterize the resulting QUBO formulations. It also describes the spectral reconstruction operator used to recover approximate solutions of the Helmholtz equation from the optimized coefficients.

Appendix A

Linear system of equations

This appendix provides the explicit derivation of the linear systems associated with the two spectral ansatzes introduced in Chapter 3. While only the final matrix formulation is required for the main developments, the complete derivation is included here for completeness and reproducibility. In this appendix, we start illustrating the derivation of the QUBO problem (3.15) for a general ansatz (3.4) and in subsections A.1 and A.2 we do it for the TFA and CA ansatzes.

From the Helmholtz equation (3.1) using (3.4) and discretization over the N collocation points (3.5) we get

$$\begin{cases} \sum_{i=1}^N w_i \phi_i''(x_m) + \tau^2 \sum_{i=1}^N w_i \phi_i(x_m) = F(x_m), & m = 0, 1, \dots, N-1 \\ \sum_{i=1}^N w_i \phi_i(0) = \alpha \\ \sum_{i=1}^N w_i \phi_i'(0) = \beta. \end{cases}$$

As a result, we get $N+2$ linear equations with unknowns $\mathbf{w} = (w_1, w_2, \dots, w_N) \in \mathbb{R}^N$, which can be compactly expressed in matrix form (3.6). Using the binary encoding (3.12), we can obtain the system of equations (3.13) for unknowns

$$\boldsymbol{\omega} = (\omega_1^0, \dots, \omega_N^0, \dots, \omega_1^{n_{spin}-1}, \dots, \omega_N^{n_{spin}-1}) \in \{0, 1\}^r.$$

To reformulate our problem as QUBO we use the least squares method and get (3.15). Next we focus on obtaining the matrix $\mathbf{a}$ for each particular case.

A.1 Linear System of Equations for TFA

To obtain a compact matrix form for TFA we refer to the ansatz (3.10) introduced in Section 3.3. Following the method described in the preceding section we obtain

$$\mathbf{a}^{TFA} \mathbf{w} = \mathbf{b},$$

where

$$\mathbf{w} = (w_1^1, w_2^1, \dots, w_{N/2}^1, \dots, w_1^2, w_2^2, \dots, w_{N/2}^2) \in \mathbb{R}^N,$$

and the coefficient matrix is

$$\mathbf{a}^{TFA} = \begin{pmatrix} c_{0,1} & \cdots & c_{0,N/2} & s_{0,1} & \cdots & s_{0,N/2} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ c_{(N-1),1} & \cdots & c_{(N-1),N/2} & s_{(N-1),1} & \cdots & s_{(N-1),N/2} \\ 1 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & \cdots & N/2 \end{pmatrix}, \quad (\text{A.1})$$

for $c_{m,n} = (\tau^2 - n^2) \cos(nx_m)$ and $s_{m,n} = (\tau^2 - n^2) \sin(nx_m)$.

A.2 Linear System of Equations for CA

We proceed with the formulation of the circulant ansatz (3.11) and obtain compact matrix form as

$$\mathbf{a}^{CA} \mathbf{w} = \mathbf{b},$$

with

$$\mathbf{a}^{CA} = \begin{pmatrix} d_0 & d_\ell & \cdots & d_{(N-2)\ell} & d_{(N-1)\ell} \\ d_{-\ell} & d_0 & d_\ell & \cdots & d_{(N-2)\ell} \\ \vdots & d_{-\ell} & d_0 & \ddots & \vdots \\ d_{-(N-2)\ell} & \vdots & \ddots & \ddots & d_\ell \\ d_{-(N-1)\ell} & d_{-(N-2)\ell} & \cdots & d_{-\ell} & d_0 \\ \hline e_0 & e_\ell & \cdots & e_{(N-2)\ell} & e_{(N-1)\ell} \\ f_0 & f_\ell & \cdots & f_{(N-2)\ell} & f_{(N-1)\ell} \end{pmatrix},$$

and

$$d_{n\ell} = \sum_{k=-N/2}^{N/2} \frac{(\tau^2 - k^2)}{N c_k} e^{-ikn\ell}, \quad e_{n\ell} = \sum_{k=-N/2}^{N/2} \frac{1}{N c_k} e^{-ikn\ell}, \quad f_{n\ell} = \sum_{k=-N/2}^{N/2} \frac{ik}{N c_k} e^{-ikn\ell}$$

for $n\ell = x_n - x_0 = \frac{2\pi n}{N}$. In addition, by the periodicity

$$e^{-ik(N-j)\ell} = e^{-ikN\ell} e^{-ik(-j\ell)} = e^{-ikN\frac{2\pi}{N}} e^{-ik(-j\ell)} = e^{-ik(-j\ell)},$$

we can express

$$\mathbf{a}^{CA} = \begin{pmatrix} d_0 & d_\ell & \cdots & d_{-2\ell} & d_{-\ell} \\ d_{-\ell} & d_0 & d_\ell & \cdots & d_{-2\ell} \\ \vdots & d_{-\ell} & d_0 & \ddots & \vdots \\ d_{2\ell} & \vdots & \ddots & \ddots & d_\ell \\ d_\ell & d_{2\ell} & \cdots & d_{-\ell} & d_0 \\ \hline e_0 & e_\ell & \cdots & e_{(N-2)\ell} & e_{(N-1)\ell} \\ f_0 & f_\ell & \cdots & f_{(N-2)\ell} & f_{(N-1)\ell} \end{pmatrix}. \quad (\text{A.2})$$

Observe that the first block of the matrix provides a circulant structure which is a cyclic shift of the previous one.

Appendix B

QUBO Metrics and Spectral Reconstruction

This appendix presents the mathematical definitions of the forcing terms employed in the numerical experiments, together with the QUBO construction of the problem for each scenario under consideration.

Let us start from expression (3.6), hence the first step to formulate the problem as a QUBO model consists of converting the matrix $\mathbf{a}$ into a binary form, namely $\mathbf{A}$, such that we guarantee the solution remains unchanged. More specifically, we impose $\mathbf{a}\mathbf{w} = \mathbf{A}\boldsymbol{\omega}$ where $\mathbf{w}$ is $N - 1$ dimensional vector,

$$\boldsymbol{\omega} = (w_1^0, w_2^0, \dots, w_N^0, \dots, w_1^{n_{spin}-1}, w_2^{n_{spin}-1}, \dots, w_N^{n_{spin}-1})^T$$

As a consequence, $\mathbf{A}$ should be of size $(N + 2) \times r$ where $r = N \times n_{spin}$. After some manipulations we may observe that

$$\mathbf{A} = \begin{pmatrix} -\mathbf{a} & 2^{-1}\mathbf{a} & 2^{-2}\mathbf{a} & \dots & 2^{-(n_{spin}-1)}\mathbf{a} \end{pmatrix},$$

is a block-matrix where each block consists of $\mathbf{a}$.

Now, we will use the least squares method, which allows us to reformulate the problem by minimizing the squared differences between the given constraints and our desired solution. Concretely, we find out

$$\|\mathbf{a}\mathbf{w} - \mathbf{b}\|_2^2 = \boldsymbol{\omega}^T \mathbf{A}^T \mathbf{A} \boldsymbol{\omega} - 2\mathbf{b}^T \mathbf{A} \boldsymbol{\omega} + \mathbf{b}^T \mathbf{b}.$$

To gain further insight into the algebraic properties of the two ansatzes, we explicitly present the matrices $\mathbf{A}$ obtained for several representative values of N while keeping $n_{spin} = 2$. Examining these matrices allows us to identify structural patterns that are not immediately apparent from the analytical formulation. In particular,

we are interested in understanding how the choice of basis functions influences the matrix structure, rank properties, and the incorporation of boundary conditions. As will be shown below, the circulant ansatz leads to highly structured matrices, whereas the truncated Fourier ansatz produces matrices with a markedly different algebraic organization.

$$(N = 2, n_{\text{spin}} = 2)$$

$$\mathbf{a}^{CA} = \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \\ 1.0 & 0.0 \\ 0.0 & 0.0 \end{bmatrix}, \mathbf{a}^{TFA} = \begin{bmatrix} 0.0 & 0.0 \\ 0.0 & 0.0 \\ 1.0 & 0.0 \\ 0.0 & 1.0 \end{bmatrix}$$

$$(N = 4, n_{\text{spin}} = 2)$$

$$\mathbf{a}^{CA} = \begin{bmatrix} -0.5 & 1 & -0.5 & 1 \\ 1 & -0.5 & 1 & -0.5 \\ -0.5 & 1 & -0.5 & 1 \\ 1 & -0.5 & 1 & -0.5 \\ 1 & 2.78 \times 10^{-17} & 0 & -9.71 \times 10^{-17} \\ 0 & 0.5 & -6.12 \times 10^{-17} & -0.5 \end{bmatrix}$$

$$\mathbf{a}^{TFA} = \begin{bmatrix} 0 & -3 & 0 & 0 \\ 0 & 3 & 0 & -3.67 \times 10^{-16} \\ 0 & -3 & 0 & 7.35 \times 10^{-16} \\ 0 & 3 & 0 & -1.10 \times 10^{-15} \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 2 \end{bmatrix}$$

$$(N = 6, n_{\text{spin}} = 2)$$

$$\mathbf{a}^{CA} = \begin{bmatrix} -2.166667 & 2 & -0.6666667 & 0.5 & -0.6666667 & 2 \\ 2 & -2.166667 & 2 & -0.6666667 & 0.5 & -0.6666667 \\ -0.6666667 & 2 & -2.166667 & 2 & -0.6666667 & 0.5 \\ 0.5 & -0.6666667 & 2 & -2.166667 & 2 & -0.6666667 \\ -0.6666667 & 0.5 & -0.6666667 & 2 & -2.166667 & 2 \\ 2 & -0.6666667 & 0.5 & -0.6666667 & 2 & -2.166667 \\ 1 & 9.71 \times 10^{-17} & -5.55 \times 10^{-17} & 0 & 1.39 \times 10^{-16} & -7.36 \times 10^{-16} \\ 0 & 0.8660254 & -0.2886751 & 6.12 \times 10^{-17} & 0.2886751 & -0.8660254 \end{bmatrix}$$

$$\mathbf{a}^{TFA} = \begin{bmatrix} 0 & -3 & -8 & 0 & 0 & 0 \\ 0 & 1.5 & 8 & 0 & -2.598076 & -9.80 \times 10^{-16} \\ 0 & 1.5 & -8 & 0 & 2.598076 & 1.96 \times 10^{-15} \\ 0 & -3 & 8 & 0 & 7.35 \times 10^{-16} & -2.94 \times 10^{-15} \\ 0 & 1.5 & -8 & 0 & -2.598076 & 3.92 \times 10^{-15} \\ 0 & 1.5 & 8 & 0 & 2.598076 & -4.90 \times 10^{-15} \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 3 \end{bmatrix}$$

Taking a glance at the presented $\mathbf{A}$ matrices, we can clearly see that the matrix $\mathbf{a}^{CA}$ has a circulant structure in its main part. Each interior row is obtained by a cyclic shift of the previous one, reflecting the regular and repeating nature of the underlying discrete model. The only rows that do not follow this pattern are the last two, which arise from the imposed boundary conditions. These additional rows slightly break the perfect circulant symmetry, but they serve an important purpose: they ensure that the matrix is full rank. Without them, the purely circulant structure could introduce linear dependencies and potentially lead to spurious or false positive solutions. In contrast, the matrix $\mathbf{a}^{TFA}$ does not exhibit this circulant structure. Its rows are not generated by cyclic shifts, and the overall pattern is structurally different. This highlights a fundamental difference between the two formulations, both in their algebraic structure and in the way boundary conditions are incorporated.

B.1 Additional Numerical Results

This appendix contains additional graphical results supporting the numerical experiments presented in Chapter 5. These figures were omitted from the main text for brevity and provide a more complete visualization of the reconstructed solutions across the tested parameter ranges.. The figures provide a visual comparison between the exact solution and the numerical approximations obtained using the truncated Fourier ansatz (TFA) and the circulant ansatz (CA) for increasing values of the spectral parameter N . While the main text focuses on the quantitative measures such as the mean squared error, success rate, and energy spectral gap, the plots presented here illustrate the evolution of the reconstructed solutions and highlight the differences in oscillatory behavior exhibited by the two ansatzes. In particular, they provide additional insight into the appearance of high-frequency numerical oscillations and amplitude distortions as the number of spectral components increases.

B.1.1 Additional Numerical Results for Experiment 2

This appendix focuses on Experiment 5.2 with fixed $n_{\text{spin}} = 2$ and varying values of N . The corresponding results are shown for $N = 8, 10, 12, 14, 16, 18, 20, 22$, and 24. Similar visualizations for the remaining experiments are provided in the following appendices.

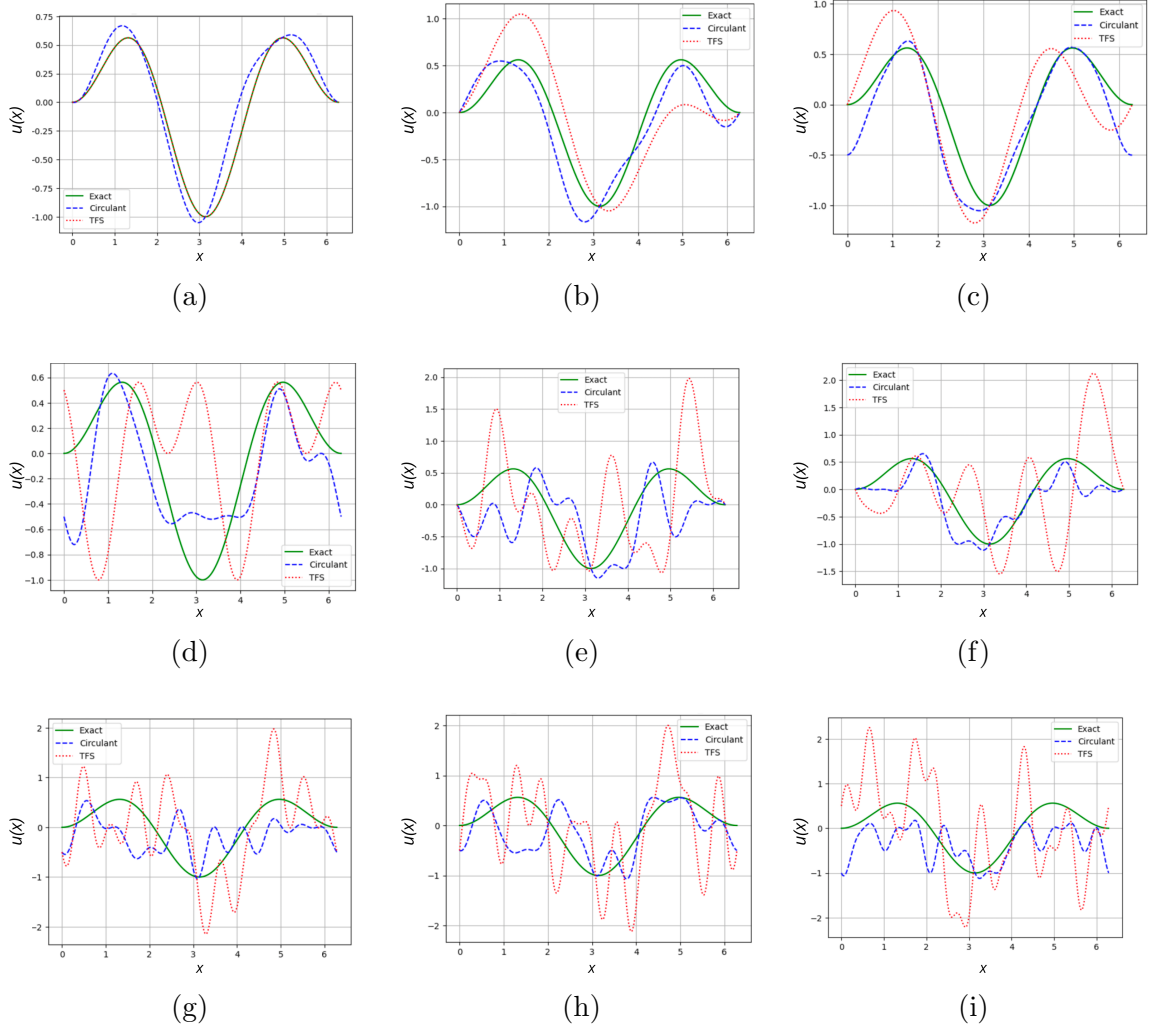


Figure B.1: Results of Experiment 2 for $N = 8, 10, 12, 14, 16, 18, 20, 22$, and 24 , with fixed $n_{\text{spin}} = 2$.

B.1.2 Additional Numerical Results for Experiment 3

B.1.2.1 Numerical Results with fixed N and increasing n_{spin}

This appendix presents additional numerical results for Experiment 5.3 obtained for increasing values of n_{spin} . The figures compare the exact solution with the approximations reconstructed using the circulant ansatz (CA) and the truncated Fourier ansatz (TFA). As n_{spin} increases, the oscillatory structure of the solution becomes progressively more complex, introducing higher-frequency components that are more challenging to approximate accurately. Throughout all considered cases, the circulant ansatz preserves the overall shape of the exact solution and maintains relatively good agreement in both amplitude and phase, although moderate discrepancies become

visible for larger values of n_{spin} . In contrast, the truncated Fourier ansatz exhibits increasingly pronounced oscillatory artifacts, including amplitude amplification, phase shifts, and overshoots near extrema. These effects become particularly evident for the largest values of n_{spin} , where high-frequency oscillations are amplified and lead to larger deviations from the exact solution. Overall, the visual comparison supports the quantitative results reported in the main text, indicating that the circulant ansatz provides a more stable and accurate reconstruction of the solution as the complexity of the encoded problem increases.

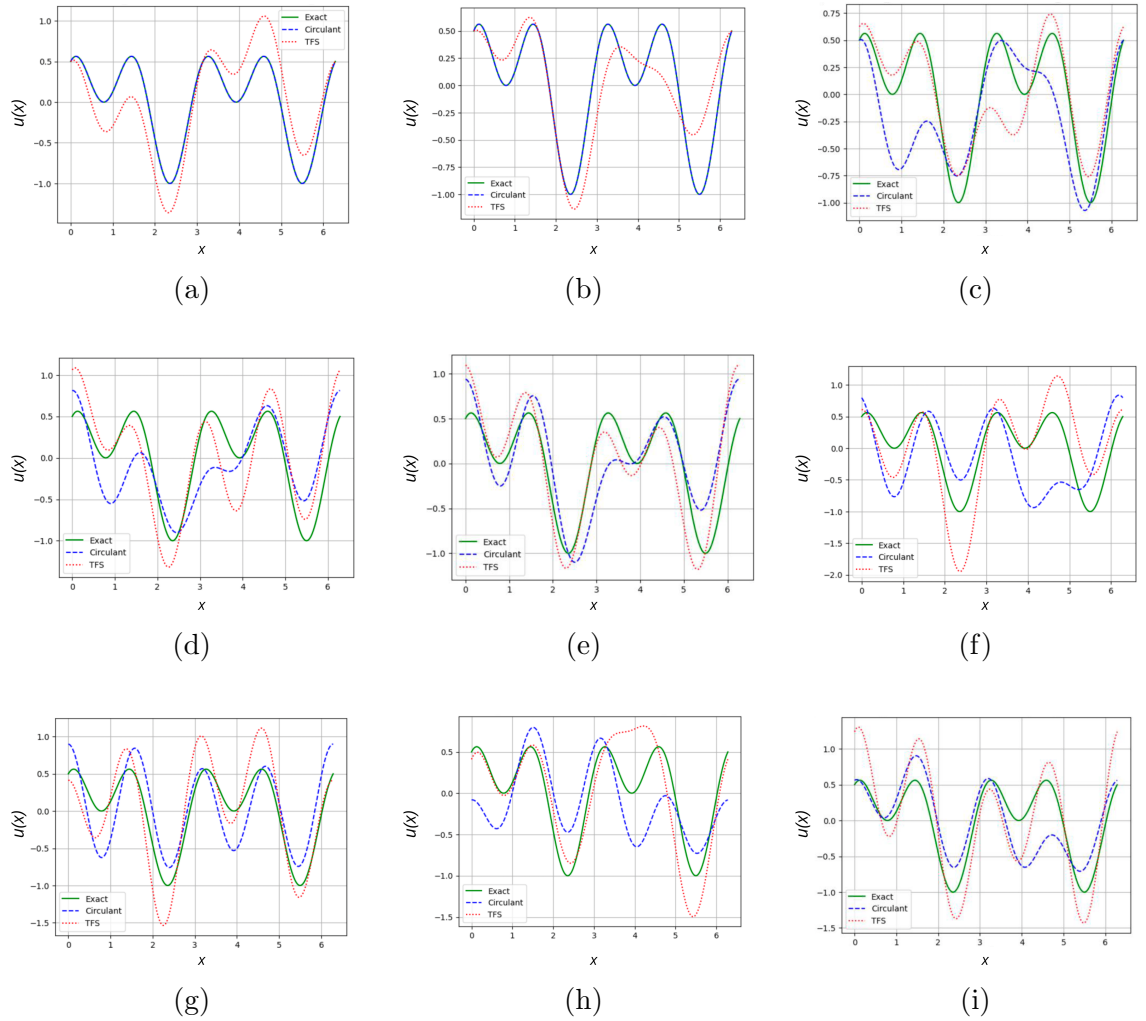


Figure B.2: Experiment 3: results obtained for n_{spin} ranging from 2 to 10.

B.1.2.2 Numerical Results with fixed number of n_{spin} and increasing N

This appendix presents additional numerical results for Experiment 5.3 obtained for increasing values of the spectral parameter N . The figures compare the exact solution

with the approximations reconstructed using the circulant ansatz (CA) and the truncated Fourier ansatz (TFA). For small values of N , both ansatzes exhibit noticeable deviations from the exact solution, reflecting the limited ability of a low-dimensional basis to represent the underlying oscillatory behavior. As N increases, the numerical approximations progressively capture the dominant frequency components of the solution, leading to improved agreement with the exact curve. In particular, the circulant ansatz demonstrates a more stable convergence behavior and generally provides a closer approximation in both amplitude and phase across the considered range of N . The truncated Fourier ansatz also benefits from the increased spectral resolution; however, larger values of N lead to increasingly pronounced oscillatory artifacts, including overshoots near extrema and localized amplitude distortions. These effects become particularly visible for the largest values of N , where the representation of higher-frequency modes introduces Gibbs-like oscillations and reduces the overall accuracy of the reconstruction. Overall, the visual results indicate that increasing N improves the representation of the solution by enabling the approximation of finer-scale oscillatory features. Nevertheless, the choice of basis functions remains crucial, as the circulant ansatz exhibits greater numerical stability and more accurately captures the behavior of the exact solution throughout the considered parameter range.

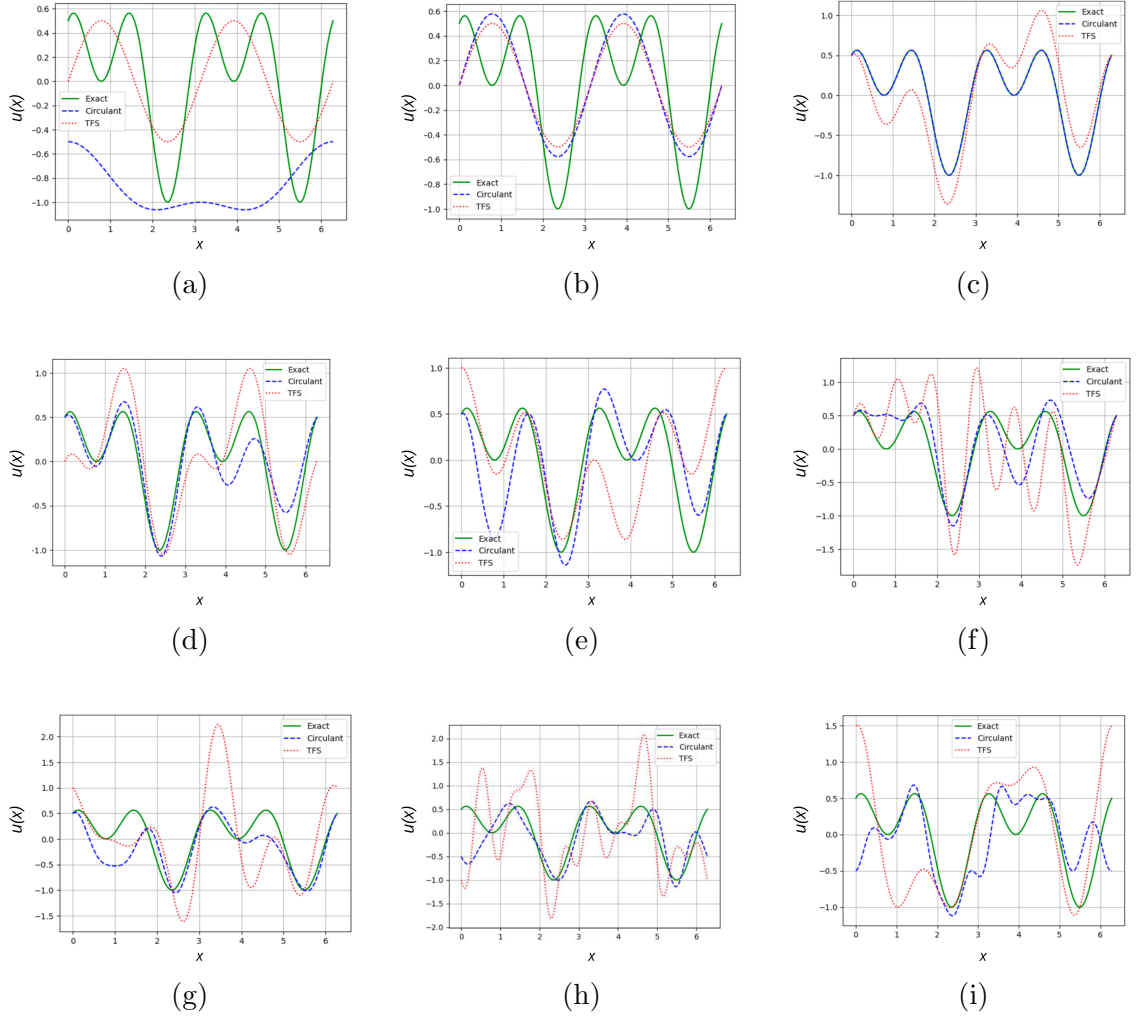


Figure B.3: Experiment 3: results obtained for $N = 4, 6, 8, 10, 12, 14, 16, 18, 20$

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