Hartee-Fock-Bogoliubov Eigenvalue Problem with Applications in Computational Physics

Bjelčić, Antonio

UNIVERSITY OF ZAGREB
FACULTY OF SCIENCE
DEPARTMENT OF MATHEMATICS

Antonio Bjelčić

HARTREE-FOCK-BOGOLIUBOV EIGENVALUE PROBLEM WITH APPLICATIONS IN COMPUTATIONAL PHYSICS

Diploma thesis

Thesis supervisor:

prof. dr. sc. Zlatko Drmač

Zagreb, 2020.

Ovaj diplomski rad obranjen je dana _____ pred ispitnim povjerenstvom u sastavu:

1. _____, predsjednik
2. _____, član
3. _____, član

Povjerenstvo je rad ocijenilo ocjenom _____.

Potpisi članova povjerenstva:

1. _____
2. _____
3. _____

”Yeah, yeah, yeah, yeah, I’d like to thank my fans, my momma and my dealer.”

P.B.

Contents

Introduction

In practical implementations of numerical simulations arising in quantum mechanic, one often has to find stationary states of the quantum system under investigation. Mathematically speaking, when the infinite dimensional space in which the solution of the quantum system (the *wave function*) resides is approximated by a finite dimensional space (so called *variational approximation*), one has to simply find the spectral decomposition of a certain Hermitian matrix. That matrix is called the ***Hamiltonian*** of the (approximated) quantum system and it defines the interaction forces which determine the behavior of the quantum system. **Eigenvalues** of the spectral decomposition correspond to the stationary **energies** in which the quantum system can be found while the associated eigenvectors usually carry information on the stationary wave function describing the quantum mechanical stationary states. An elementary textbook example is hydrogen atom having electron trapped in orbitals with energies: $E_n = -13.6/n^2$ eV, $n \in \mathbb{N}$, while its Hamiltonian is constructed purely from Coulomb interaction of electron and the nucleus of the hydrogen atom.

Virtually all modern subbranches in physics use quantum mechanics as its framework, from molecular and atomic, to nuclear and elementary particle physics. While each one of the subbranches has some special features, all of them require some form of spectral eigensolver when it comes to practical calculations. In some subbranches, such as theoretical nuclear physics and quantum chemistry, Hermitian Hamiltonian matrix $\mathbf{H}$ of the quantum systems shows additional symmetries due to the inherent peculiarity. Time-reversal symmetry for example, renders the additional substructure of the Hamiltonian $\mathbf{H}$:

$$\mathbf{H} = \begin{bmatrix} \mathbf{h} & \mathbf{\Delta} \\ \mathbf{\Delta} & -\mathbf{h} \end{bmatrix}, \tag{1}$$

where $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{n \times n}$ are symmetric matrices. Therefore, is is suboptimal to find the spectral decomposition of $\mathbf{H}$ by using a generic eigensolver for symmetric real matrices. Even though the currently available eigensolvers for symmetric real matrices are *state-of-the-art* and extremely well optimised, they still ignore the mentioned substructure. In this thesis, we propose and analyse new methods for finding the spectral decomposition of such symmetric matrices taking advantage of the additional substructure.

Chapter 1

Physical background

1.1 Constrained Hartree-Fock-Bogoliubov equation

In theoretical nuclear physics, one can describe a quantum interaction between protons and neutrons confined in a nucleus using a well established framework called *Quantum Chromodynamics* (QCD). However, practical calculations in QCD are far from doable. Therefore, physicists in many branches which involve quantum many body problem use *Energy Density Functional Theory* (EDF) as a framework of choice.

The solution of a quantum system (*wave function*) usually resides in some form of Cartesian product of Sobolev space $\left(H_0^1\left(\mathbb{R}^3\right)\right)^d$, where $d = 2$ in classical quantum mechanics and $d = 4$ in relativistic environment. In practical calculations, one chooses an orthonormal basis $(e_k)_{k\in\mathbb{N}}$ for $\left(H_0^1(\mathbb{R}^3)\right)^d$ (which is usually chosen as a basis such that for some convenient injective compact Hermitian operator A one has: $\left(H_0^1(\mathbb{R}^3)\right)^d = \bigotimes_{\lambda\in\sigma_p(A)} \mathrm{Ker}(A - \lambda I)$), and truncates it: $(e_k)_{k=1}^n$. In other words, $\mathrm{span}(e_k)_{k=1}^n$ is used as a variational approximation of the full space $\left(H_0^1(\mathbb{R}^3)\right)^d$. Popular choice in the past few decades is the truncated quantum harmonic oscillator (QHO) basis [1] or various finite-elements approximations which are favoured for weakly bounded systems.

Suppose we are dealing with a nucleus having Z protons and N neutrons with Z and N even. Since EDF is no longer *ab initio* theory, one has to come up with a model which describes the interaction felt by nucleons in a nucleus. In the so called **Hartree-Fock-Bogoliubov** theory [2], an interaction model generates a Hermitian operator h and antisymmetric operator Δ. Physically, operator h is the effective single-particle mean-field Hamiltonian of the independently-moving quasiparticles, while Δ sums up the short-range pairing correlations that lead to a superfluid state [3]. When operators h and Δ are represented in the truncated

basis $(e_k)_{k=1}^n$, we obtain the corresponding matrices: $\mathbf{h} \in \mathbb{C}^{n\times n}$ and $\mathbf{\Delta} \in \mathbb{C}^{n\times n}$, where $\mathbf{h}$ is Hermitian[1] $\mathbf{h} = \mathbf{h}^\dagger$ and $\mathbf{\Delta}$ is antisymmetric $\mathbf{\Delta}^T = -\mathbf{\Delta}$. Suppose we are given a fixed predetermined value $f_0 \in \mathbb{R}$. In the rest of the thesis, we refer to f_0 as the *target value*. In our case, f_0 is equal to the number of protons $Z \in \mathbb{N}$ or the number of neutrons $N \in \mathbb{N}$ in the nucleus under consideration.

We define the Hartree-Fock-Bogoliubov (HFB) Hamiltonian:

$$\mathbf{H} := \begin{bmatrix} \mathbf{h} & \mathbf{\Delta} \\ -\mathbf{\Delta}^* & -\mathbf{h}^* \end{bmatrix}, \tag{1.1}$$

which is a Hermitian matrix $\mathbf{H} \in \mathbb{C}^{2n\times 2n}$. For any $\lambda \in \mathbb{R}$, we define the corresponding constrained HFB Hamiltonian (CHFB):

$$\mathbf{H}_\lambda := \mathbf{H} - \lambda \begin{bmatrix} I_{n\times n} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -I_{n\times n} \end{bmatrix} = \begin{bmatrix} \mathbf{h} - \lambda I_{n\times n} & \mathbf{\Delta} \\ -\mathbf{\Delta}^* & -\mathbf{h}^* + \lambda I_{n\times n} \end{bmatrix}, \tag{1.2}$$

also called a *Routhian*.

Remark 1.1.1. *Notice that if* $\begin{bmatrix} u_E^{(\lambda)} \\ v_E^{(\lambda)} \end{bmatrix} \in \mathbb{C}^{2n}$ *is an eigenvector of* $\mathbf{H}_\lambda$ *for an eigenvalue* $E > 0$, *then* $\begin{bmatrix} \left(v_E^{(\lambda)}\right)^* \\ \left(u_E^{(\lambda)}\right)^* \end{bmatrix} \in \mathbb{C}^{2n}$ *is also an eigenvector of* $\mathbf{H}_\lambda$ *but for eigenvalue* $-E$. *This justifies the search of Routhian's unitary eigenvectors matrix in special form:*

$$\begin{bmatrix} U^{(\lambda)} & \left(V^{(\lambda)}\right)^* \\ V^{(\lambda)} & \left(U^{(\lambda)}\right)^* \end{bmatrix} \in \mathbb{C}^{2n\times 2n}. \tag{1.3}$$

Therefore, one can find a diagonal matrix $E_{(+)}^{(\lambda)} \in \mathbb{R}^n$ *with non-negative diagonal elements, such that:*

$$\begin{bmatrix} U^{(\lambda)} & \left(V^{(\lambda)}\right)^* \\ V^{(\lambda)} & \left(U^{(\lambda)}\right)^* \end{bmatrix}^\dagger \mathbf{H}_\lambda \begin{bmatrix} U^{(\lambda)} & \left(V^{(\lambda)}\right)^* \\ V^{(\lambda)} & \left(U^{(\lambda)}\right)^* \end{bmatrix} = \begin{bmatrix} E_{(+)}^{(\lambda)} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -E_{(+)}^{(\lambda)} \end{bmatrix}. \tag{1.4}$$

In nuclear structure calculations, one has to find $\lambda_0 \in \mathbb{R}$ (in the rest of the thesis referred to as the *target value*) such that when one calculated the spectral decomposition of a Routhian matrix $\mathbf{H}_{\lambda_0}$:

$$\begin{bmatrix} U^{(\lambda_0)} & \left(V^{(\lambda_0)}\right)^* \\ V^{(\lambda_0)} & \left(U^{(\lambda_0)}\right)^* \end{bmatrix}^\dagger \begin{bmatrix} \mathbf{h} - \lambda_0 I_{n\times n} & \mathbf{\Delta} \\ -\mathbf{\Delta}^* & -\mathbf{h}^* + \lambda_0 I_{n\times n} \end{bmatrix} \begin{bmatrix} U^{(\lambda_0)} & \left(V^{(\lambda_0)}\right)^* \\ V^{(\lambda_0)} & \left(U^{(\lambda_0)}\right)^* \end{bmatrix} = \begin{bmatrix} E_{(+)}^{(\lambda_0)} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -E_{(+)}^{(\lambda_0)} \end{bmatrix}, \tag{1.5}$$

[1] In this thesis, we use $A^\dagger$ for Hermitian conjugate, A^T for transposition and A^* for complex conjugation.

assuming that $\mathbf{H}_{\lambda_0}$ is regular matrix, and $E^{(\lambda_0)}_{(+)}$ being a diagonal matrix with positive diagonal, one also has the following equation satisfied:

$$\text{Trace}\left[V^{(\lambda_0)}\left(V^{(\lambda_0)}\right)^{\dagger}\right] = f_0. \tag{1.6}$$

In that case, $U^{(\lambda_0)}$ and $V^{(\lambda_0)}$ are called *Bogoliubov matrices* and the target value λ_0 is called the *Fermi energy*. Equation (1.5) is called the *constrained Hartree-Fock-Bogoliubov* equation.

Physically, $\lambda \in \mathbb{R}$ is a chemical potential [2] (Lagrange multiplier) used to constrain the expected value of the number of particles: Trace $\left[V^{(\lambda)}, \left(V^{(\lambda)}\right)^{\dagger}\right]$ to the given value f_0, where $f_0 = Z, N \in \mathbb{N}$. Operator which corresponds to the number of particles has its matrix representation simply as $I_{n\times n} \in \mathbb{R}^{n\times n}$ and thus the Lagrange multiplier is imposed on matrix $\mathbf{h}$ by a simple substitution with $\mathbf{h} - \lambda I_{n\times n}$. The Bogoliubov matrices $U^{(\lambda_0)}$ and $V^{(\lambda_0)}$ represent the coefficients of Bogoliubov transformation [3] used for transformation from configuration basis to the *quasiparticle basis*. In this thesis, we focus only on the zero-temperature case, otherwise the expected number of particles formula (1.6) looks different (see e.g. [4]).

1.2 CHFB with time-reversal symmetry

In many nuclear structure calculations [5], one deals with systems preserving time-reversal symmetry, e.g. when calculating ground state properties of even-even nuclei. In short, if we denote the time-reversal antiunitary operator [6] with $\mathcal{T}$, one can carefully choose a truncated orthonormal basis $(e_k)_{k=1}^n$ such that it can be arranged into two blocks:

$$(e_k)_{k=1}^n = \left[\left(\phi_k\right)_{k=1}^p, \left(\overline{\phi}_k\right)_{k=1}^p\right], \tag{1.7}$$

where $\overline{\phi}_k = \mathcal{T}\phi_k$ is time-reversed vector of ϕ_k, and $n = 2p$. Classical widely used example of such basis is the quantum harmonic oscillator (QHO) basis [1] .

If the nuclear system preserves time-reversal symmetry [6], then the Hermitian operator h and the antisymmetric operator Δ have the following matrix representations in the basis (1.7):

$$h = \begin{bmatrix} \mathbf{h} & \mathbf{0}_{p\times p} \\ \mathbf{0}_{p\times p} & \mathbf{h}^* \end{bmatrix} \text{ and } \Delta = \begin{bmatrix} \mathbf{0}_{p\times p} & \mathbf{\Delta} \\ -\mathbf{\Delta} & \mathbf{0}_{p\times p} \end{bmatrix}, \tag{1.8}$$

where $\mathbf{h} \in \mathbb{C}^{p\times p}$ is Hermitian matrix ($\mathbf{h}^\dagger = \mathbf{h}$) and $\mathbf{\Delta} \in \mathbb{C}^{p\times p}$ is symmetric matrix ($\mathbf{\Delta}^T = \mathbf{\Delta}$). In that case, the original CHFB eigenvalue problem (1.5):

$$\begin{bmatrix} \mathbf{h} - \lambda I_{p\times p} & \mathbf{0}_{p\times p} & \mathbf{0}_{p\times p} & \mathbf{\Delta} \\ \mathbf{0}_{p\times p} & \mathbf{h}^* - \lambda I_{p\times p} & -\mathbf{\Delta} & \mathbf{0}_{p\times p} \\ \mathbf{0}_{p\times p} & -\mathbf{\Delta}^* & -\mathbf{h}^* + \lambda I_{p\times p} & \mathbf{0}_{p\times p} \\ \mathbf{\Delta}^* & \mathbf{0}_{p\times p} & \mathbf{0}_{p\times p} & -\mathbf{h} + \lambda I_{p\times p} \end{bmatrix} \begin{bmatrix} \mathbf{u}_1^{(\lambda)} \\ \mathbf{u}_2^{(\lambda)} \\ \mathbf{v}_1^{(\lambda)} \\ \mathbf{v}_2^{(\lambda)} \end{bmatrix} = E \begin{bmatrix} \mathbf{u}_1^{(\lambda)} \\ \mathbf{u}_2^{(\lambda)} \\ \mathbf{v}_1^{(\lambda)} \\ \mathbf{v}_2^{(\lambda)} \end{bmatrix}, \tag{1.9}$$

one can easily recast as two eigenvalue problems:

$$\begin{bmatrix} \mathbf{h} - \lambda I & \mathbf{\Delta} \\ \mathbf{\Delta}^* & -\mathbf{h} + \lambda I \end{bmatrix} \begin{bmatrix} \mathbf{u}_1^{(\lambda)} \\ \mathbf{v}_2^{(\lambda)} \end{bmatrix} = +E \begin{bmatrix} \mathbf{u}_1^{(\lambda)} \\ \mathbf{v}_2^{(\lambda)} \end{bmatrix} \text{ and } \begin{bmatrix} \mathbf{h} - \lambda I & \mathbf{\Delta} \\ \mathbf{\Delta}^* & -\mathbf{h} + \lambda I \end{bmatrix} \begin{bmatrix} \left(\mathbf{v}_1^{(\lambda)}\right)^* \\ \left(\mathbf{u}_2^{(\lambda)}\right)^* \end{bmatrix} = -E \begin{bmatrix} \left(\mathbf{v}_1^{(\lambda)}\right)^* \\ \left(\mathbf{u}_2^{(\lambda)}\right)^* \end{bmatrix}, \tag{1.10}$$

which are said to be Kramers degenerated, where $\mathbf{u}_1^{(\lambda)}, \mathbf{u}_2^{(\lambda)}, \mathbf{v}_1^{(\lambda)}, \mathbf{v}_2^{(\lambda)} \in \mathbb{C}^p$. The choice of a nuclear interaction together with the choice of a basis usually [8, 9] lead to real matrices $\mathbf{h} \in \mathbb{R}^{p\times p}$ and $\mathbf{\Delta} \in \mathbb{R}^{p\times p}$. Therefore, in the rest of the thesis we will assume $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{p\times p}$ being real symmetric matrices and focus on the reduced CHFB eigenvalue equation (1.10). In the next section, a formal mathematical statement of the problem we are dealing with in this thesis is given.

1.3 Problem statement

Suppose that we are given two real symmetric matrices $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{n\times n}$, together with the fixed real target value $f_0 \in \mathbb{R}$. We define the corresponding Hamiltonian:

$$\mathbf{H} = \begin{bmatrix} \mathbf{h} & \mathbf{\Delta} \\ \mathbf{\Delta} & -\mathbf{h} \end{bmatrix} \in \mathbb{R}^{2n\times 2n}, \tag{1.11}$$

and for any $\lambda \in \mathbb{R}$, a Routhian as:

$$\mathbf{H}_\lambda = \mathbf{H} - \lambda \begin{bmatrix} I_{n\times n} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -I_{n\times n} \end{bmatrix} \in \mathbb{R}^{2n\times 2n}. \tag{1.12}$$

The task is to find $\lambda \in \mathbb{R}$, such that in the spectral decomposition of the Routhian:

$$\begin{bmatrix} Q_1^{(\lambda)} & -Q_2^{(\lambda)} \\ Q_2^{(\lambda)} & Q_1^{(\lambda)} \end{bmatrix}^T \begin{bmatrix} \mathbf{h} - \lambda I_{n\times n} & \mathbf{\Delta} \\ \mathbf{\Delta} & -(\mathbf{h} - \lambda I_{n\times n}) \end{bmatrix} \begin{bmatrix} Q_1^{(\lambda)} & -Q_2^{(\lambda)} \\ Q_2^{(\lambda)} & Q_1^{(\lambda)} \end{bmatrix} = \begin{bmatrix} E_{(+)}^{(\lambda)} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -E_{(+)}^{(\lambda)} \end{bmatrix}, \tag{1.13}$$

where $Q_1^{(\lambda)}, Q_1^{(\lambda)} \in \mathbb{R}^{n\times n}$ and $E_{(+)}^{(\lambda)} \in \mathbb{R}^{n\times n}$ is diagonal with non-negative diagonal elements, the spectral subspace corresponding to the non-negative eigenvalues $E_{(+)}^{(\lambda)}$ has certain properties. In particular, if we define a function of $\lambda \in \mathbb{R}$ as:

$$f(\lambda) := \left\| Q_2^{(\lambda)} \right\|_F^2, \tag{1.14}$$

where $\|\cdot\|_F$ denotes the Frobenius norm, we seek $\lambda_0 \in \mathbb{R}$ such that $f(\lambda_0) = f_0$. Function $f(\lambda)$ will be referred to as the *target function*.

Remark 1.3.1. *Notice that if* $\begin{bmatrix} q_1^{(\lambda)} \\ q_2^{(\lambda)} \end{bmatrix} \in \mathbb{R}^{2n}$ *is an eigenvector of* $\mathbf{H}_\lambda$ *for an eigenvalue* $E > 0$*, then* $\begin{bmatrix} -q_2^{(\lambda)} \\ q_1^{(\lambda)} \end{bmatrix} \in \mathbb{R}^{2n}$ *is also an eigenvector but for the eigenvalue* $-E$*. This justifies the search of the Routhian's eigenvectors in the special form* $\begin{bmatrix} Q_1^{(\lambda)} & -Q_2^{(\lambda)} \\ Q_2^{(\lambda)} & Q_1^{(\lambda)} \end{bmatrix}$*, which is known in the literature as an orthogonal symplectic form [10].*

Remark 1.3.2. *In terms of concepts from the control theory, Routhian matrix* $\mathbf{H}_\lambda$ *has a Hamiltonian structure and the spectral decomposition (1.13) can be written as a special type of the continuous algebraic Riccati equation (CARE) [10]. In CARE equation, for given* $A, B, Q, R \in \mathbb{R}^{n\times n}$*, one seeks symmetric* $P \in \mathbb{R}^{n\times n}$ *such that:*

$$A^T P + PA - PBR^{-1}B^T P + Q = 0. \tag{1.15}$$

It is possible to find the solution by finding the Schur decomposition of a larger system, the associated Hamiltonian matrix:

$$\begin{bmatrix} A & -BR^{-1}B^T \\ -Q & -A^T \end{bmatrix}, \tag{1.16}$$

thus our problem (1.13) can be seen as a special type of the CARE equation. Therefore, already in this early phase we notice a strong link with the control theory which is present throughout this thesis.

Remark 1.3.3. *Notice that the target function* $f(\lambda)$ *is not well defined in case of* $\lambda \in \mathbb{R}$*, for which the Routhian* $\mathbf{H}_\lambda$ *is singular. In that case, one can not uniquely decompose the spectrum on positive* $E_{(+)}^{(\lambda)}$ *and negative* $-E_{(+)}^{(\lambda)}$ *part as in (1.13) since we have zero in the spectrum of* $\mathbf{H}_\lambda$*. This apparent flaw of the CHFB theory is addressed in the following chapter.*

In nuclear physics scientific community, there are many software packages available based on the Hartree-Fock-Bogoliubov theory which have been used by researches for more than 30 years. To name a few, very popular and widely used classical code called HFBTHO [9] or a relativistic one called DIRHB [8], use constrained HFB as a framework of choice and numerically solve the stated CHFB problem. To the author's best knowledge, all available solvers construct the Routhian matrix (1.12) explicitly, and calculate the spectral decomposition ignoring the regular substructure. Our main goal is to provide a method which

utilizes that regular substructure and thus speeds up the calculation of spectral decomposition, rendering it useful in real applications.

Thesis is organised as follows. In Chapter 2 we give preliminar theoretical results regarding the properties of the CHFB equation and show that the CHFB problem (1.13) is well defined. In Chapter 3 we propose a method for numerical computation of the spectral decomposition of Routhian matrix $\mathbf{H}_\lambda$, together with the results of numerical experiments. The proposed method works well for Routhians with relatively small degenerate eigenvalue blocks and shows approximately 2.5 times faster execution compared to the currently available *state-of-the-art* eigenvalue solvers such as `eig` function from MATLAB [11] or LAPACK subroutines for symmetric matrices [12] such as `dsyevr`, `dsyevd` and `dsyevx`, when one ignores the substructure of (1.13). Since the Routhians that arise in practice in nuclear structure calculations have the size of the largest degenerated eigenvalue block always less than $\approx 1\%$ of the size n of the matrices $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{n\times n}$, the proposed method performs well on test matrices coming from real applications. In Chapter 4 we briefly present a method together with an efficient *cache-aware* implementation based on the Paige-Van Loan algorithm for spectral decomposition of matrices with quaternionic substructure. Numerical experiments show approximately two times better performance compared to the naive approach. Paige-Van Loan algorithm [13] was originally designed for calculation of the Schur decomposition of the CARE's associated Hamiltonian matrix. In the final chapter, we give a quick overview with plans for further investigations.

Chapter 2

Properties of the CHFB equation

2.1 Well-posedness

In this chapter, we consider purely the matrix theoretical aspects of the problem. We first note that for $\lambda \in \mathcal{I}$, where $\mathcal{I} \subseteq \mathbb{R}$ is any suitably chosen interval, we expect (in a generic situation) that $\mathbf{H}_\lambda$ is nonsingular. Indeed, if, for some λ_0, zero was an eigenvalue of $\mathbf{H}_{\lambda_0}$, it would have to be multiple. That is unlikely, however. Recall that the eigenvalues of the Routhian $\mathbf{H}_\lambda$ always come in pairs e_λ and $-e_\lambda$. By continuity theorem of the eigenvalues with varying the λ parameter, and the Hamiltonian structure, as λ approaches λ_0 two eigenvalues of $\mathbf{H}_\lambda$, with opposite signs $e_\lambda > 0$ and $-e_\lambda < 0$, would be on the collision course and the collision should happen at zero. However, this is unlikely, as the symmetric matrices with multiple eigenvalues are a subvariety of codimension two. This is the well known *avoidance of crossing phenomenon*, first described by Wigner and von Neumann in [14]. We first give the simplest possible example illustrating the avoidance of crossing phenomenon.

Example 2.1.1. *Study of a two-level system [15] is of vital importance in quantum mechanics because it embodies simplification of many of physically realizable systems. The effect of perturbation on a two-state system Hamiltonian is manifested through avoided crossings in the plot of individual energy vs. the perturbation strength. Suppose we are given a simple symmetric matrix $H_\Delta \in \mathbb{R}^{2\times 2}$:*

$$H_\Delta = \begin{bmatrix} E_1 & \Delta \\ \Delta & E_2 \end{bmatrix}. \tag{2.1}$$

The parameter $\Delta \in \mathbb{R}$ is considered as a perturbation imposed on top of the unperturbed

Hamiltonian $H_0 = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}$. *Trivial calculation yields two eigenvalues* $E^\Delta_\pm \in \mathbb{R}$ *of* H_Δ*:*

$$E^\Delta_\pm = \frac{E_1 + E_1}{2} \pm \sqrt{\left(\frac{E_1 + E_1}{2}\right)^2 + \Delta^2}. \tag{2.2}$$

Figure 2.1 depicts graphically previous equation when one varies symmetrically E_1 *and* E_2*. One easily sees that even if we have originally degenerated eigenvalues* $E_1 = E_2$*, the slightest perturbation* $\Delta \neq 0$ *will make* H_Δ *matrix have non-degenerate eigenvalues* $E^\Delta_\pm$*. In practice, we always encounter some perturbations (numerical if nothing else), and thus even in this trivial example, we can say that the probability of having degenerated eigenvalues is zero. Therefore, assumption on having a matrix* H_Δ *regular is not a great demand.*

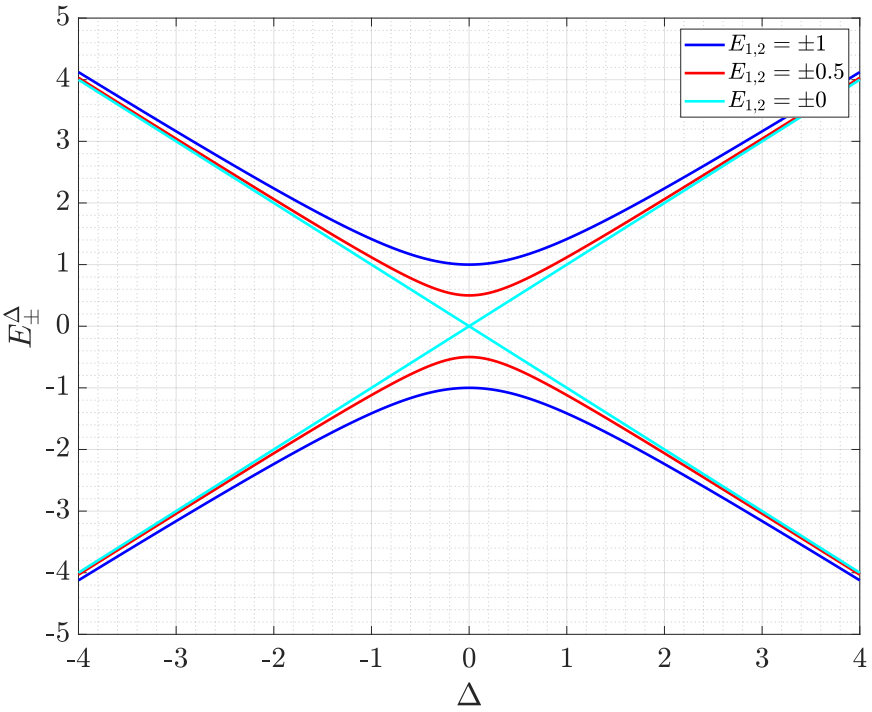


Figure 2.1: Depiction of the crossing avoidance phenomenon on the simplest possible Hermitian matrix H_Δ having the spectrum $\sigma(H_\Delta) = \{E^\Delta_+, E^\Delta_-\}$.

Example 2.1.2. *To illustrate the avoidance of crossing on matrices from real application, we take the Hamiltonian* $\mathbf{H}$ *as in equation (1.11) of dimension* $2n = 4048$ *which, in physics terminology, corresponds to the Hamiltonian obtained from publicly available DIRHBT program package [16] of the very heavy nucleus* ^{240}Pu *in deformed configuration with Hill-Wheeler deformation parameters:* $(\beta, \gamma) = (0.6, 6^o)$*, where 20 QHO shells are used and only simplex (+) block is taken for neutrons.*

We construct Routhians $\mathbf{H}_\lambda$ *as in equation (1.12) and compute the eigenvalues* $\sigma(\mathbf{H}_\lambda)$ *for* $\lambda \in \mathbb{R}$ *ranging from* $\lambda_{\min} = -10$ MeV *to* $\lambda_{\max} = 5$ MeV *with very dense step* $\delta\lambda = 0.001$ MeV. *The selected interval* $\lambda \in [\lambda_{min}, \lambda_{max}]$*, reflects the fact that the target value* λ_0 *is typically located in that region and we used standard unit of measurements of energy* MeV. *We plot the spectrum* $\sigma(\mathbf{H}_\lambda)$ *for* $\lambda \in [\lambda_{min}, \lambda_{max}]$ *in Figure 2.2, or in other words, we take samples from the line segment* $\{\mathbf{H}_{\lambda_{\min}} + t(\mathbf{H}_{\lambda_{\max}} - \mathbf{H}_{\lambda_{\min}}) : t \in [0, 1]\}$ *and plot the spectrum. Since n is rather large, we show only the part of the spectrum near zero, and plot the evolution of different eigenvalues as* λ *is changed in different colors. One immediately sees that eigenvalues are repelled from zero similarly as they do in the simplest possible case explained in Example 2.1.1. If we zoom in as shown in figures 2.3 and 2.4, one observes the same crossing avoidance pattern already seen in Figure 2.1 in Example 2.1.1.*

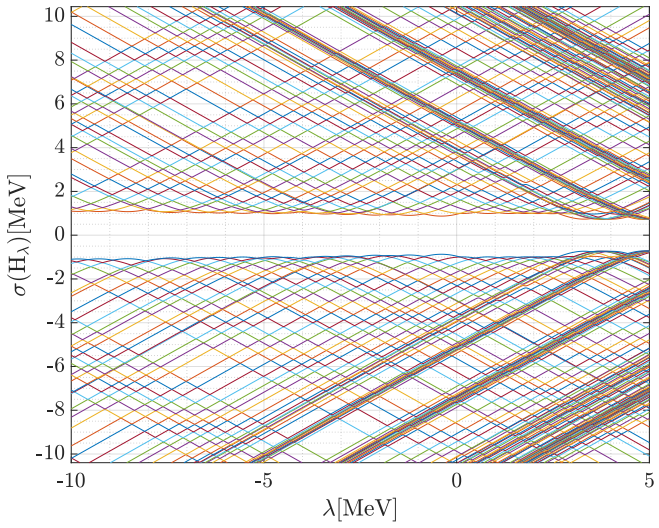


Figure 2.2: Spectrum $\sigma(\mathbf{H}_\lambda)$ near zero when λ is chosen from the interval $\lambda \in [-10, 5]$. Evolution of eigenvalues when λ changes is depicted by curves with different colors.

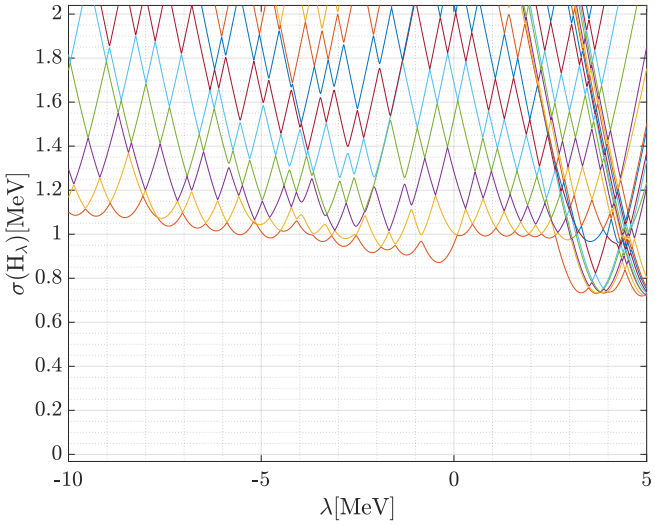


Figure 2.3: Same as Figure 2.2 only zoomed in. Closer inspection suggest that distinct eigenvalues indeed do not cross each other as they evolve with changing the parameter λ.

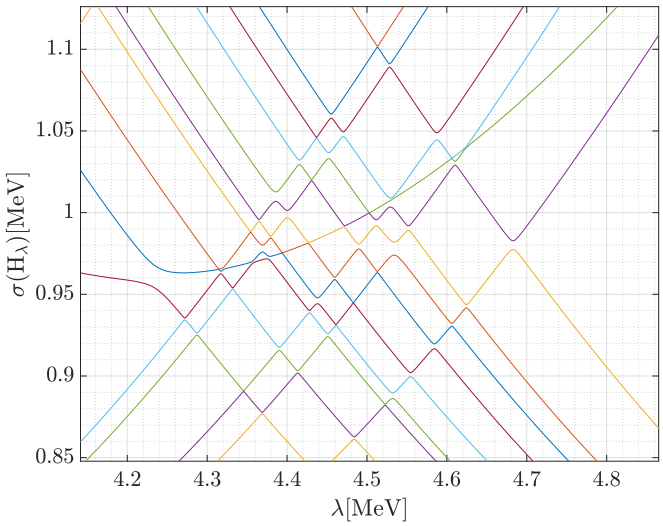


Figure 2.4: Same as Figure 2.3 only zoomed in even more. Locally, one observes the crossing avoidance pattern similar to the one demonstrated in Figure 2.1 in Example 2.1.1.

In conclusion, the crossing avoidance phenomenon first noted by Wigner and von Neumann, prevent non-zero pair $e_\lambda, -e_\lambda \in \sigma(\mathbf{H}_\lambda)$ of eigenvalues $e_\lambda > 0$ and $-e_\lambda < 0$ to cross at zero, thus rendering $\mathbf{H}_\lambda$ regular matrix. Even if the crossing occurs, it happens on a zero-measure set in $\mathbb{R}$ and therefore in the rest of the thesis we will assume $\mathbf{H}_\lambda$ being a regular matrix for all $\lambda \in \mathcal{I} \subseteq \mathbb{R}$.

In order to prove well-posedness of the CHFB problem, we first give a lemma regarding the solvability of the *Sylvester equation*, which is well known and can be found in many textbooks. In the field of control theory, a Sylvester equation is a matrix equation of the form:

$$AX + XB = C, \tag{2.3}$$

where $A, B, C \in \mathbb{C}^{n\times n}$, and the problem is to find all possible matrices $X \in \mathbb{C}^{n\times n}$ that obey this equation. A Sylvester equation has a unique solution for X exactly when there are no common eigenvalues of A and $-B$. The proof of that statement (taken from [17]) follows.

Lemma 2.1.3. *Let $A, B \in \mathbb{C}^{n\times n}$. There exists unique $X \in \mathbb{C}^{n\times n}$ such that $AX + XB = C$ for all $C \in \mathbb{C}^{n\times n}$ if and only if A and $-B$ have no common eigenvalues: $\sigma(A) \cap \sigma(-B) = \emptyset$.*

Proof: Let us define the linear transformation $\mathcal{S} : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$, given by $\mathcal{S}(X) := AX+XB$.

Suppose A and $-B$ have no common eigenvalues. Then their characteristic polynomials $p_A(z)$ and $p_{-B}(z)$ have highest common factor 1, and therefore Bézout's Theorem gives the existence of polynomials $q_1(z)$ and $q_2(z)$ such that: $p_A(z)q_1(z) + p_{-B}(z)q_2(z) = 1$. By the Hamilton-Cayley theorem: $p_A(A) = p_{-B}(-B) = 0$, hence $q_2(A)p_{-B}(A) = I$. Let $X_0 \in \operatorname{Ker}\mathcal{S}$, that is: $AX_0 = X_0(-B)$. Iterating previous identity, one obtains: $A^kX_0 = X_0(-B)^k$ for any $k \in \mathbb{N}$, and therefore $p(A)X_0 = X_0p(-B)$ for any polynomial p. From $I = q_2(A)p_{-B}(A)$, we have $X_0 = q_2(A)p_{-B}(A)X_0 = q_2(A)X_0p_{-B}(-B) = 0$, rendering $\operatorname{Ker}\mathcal{S} = \{\mathbf{0}_{n\times n}\}$. Hence by the rank–nullity theorem, $\mathcal{S}$ is invertible, so for any $C \in \mathbb{C}^{n\times n}$ there exists a unique solution X.

Conversely, suppose that $\lambda \in \sigma(A) \cap \sigma(-B)$ is a common eigenvalue of A and $-B$. Note that also $\lambda \in \sigma(A^T)$. Therefore, there exist $v, w \neq 0$, such that $A^Tw = \lambda w$ and $Bv = -\lambda v$. One can easily construct C such that $Cv = w^*$. If we had $X \in \mathbb{C}^{n\times n}$ such that $AX + XB = C$, then there would also hold: $\langle (AX + XB)v, w\rangle = \langle Cv, w\rangle = \langle w^*, w\rangle = \|w\|^2 > 0$, where we denoted $\langle x, y\rangle = \sum_{i=1}^n x_iy_i$. On the other hand:

$$0 < \|w\|^2 = \langle (AX + XB)v, w\rangle = \langle Xv, A^Tw\rangle + \langle XBv, w\rangle = \langle Xv, \lambda w\rangle + \langle X(-\lambda v), w\rangle = 0,$$

yielding a contradiction. ⊠

Now when we have necessary and sufficient condition for the solvability of Sylvester equation, we are ready to prove that the target function $f(\lambda)$, given in eq. (1.14), is well defined.

Proposition 2.1.4. *Assume that $\mathbf{H}_\lambda \in \mathbb{R}^{2n\times 2n}$ given in eq. (1.12) is nonsingular for $\lambda \in \mathcal{I} \subseteq \mathbb{R}$. Then, the function $\lambda \mapsto \left\|Q_2^{(\lambda)}\right\|$, $\lambda \in \mathcal{I}$, is well defined for any unitarily invariant norm $\|\cdot\|$, i.e. it is independent of the concrete choice of the eigenvector matrix:*

$$Q^{(\lambda)} = \begin{bmatrix} Q_1^{(\lambda)} & -Q_2^{(\lambda)} \\ Q_2^{(\lambda)} & Q_1^{(\lambda)} \end{bmatrix}, \tag{2.4}$$

in the diagonalization (1.13). In fact, $Q_2^{(\lambda)}\left(Q_2^{(\lambda)}\right)^T$, $Q_2^{(\lambda)}\left(Q_1^{(\lambda)}\right)^T$ and $\left\|Q_2^{(\lambda)}\right\|$ are functions of the spectral subspace defined by the positive eigenvalues. Instead of the matrix of the eigenvectors, we can use any orthonormal basis of the sum of the eigenspaces of the positive eigenvalues. In other words, the matrix $E_{(+)}^{(\lambda)}$ in (1.13) does not have to be diagonal, it suffices if it is positive definite and we will still obtain the same target function $f(\lambda)$.

Proof: Consider another diagonalization with an orthogonal matrix $\widetilde{Q}^{(\lambda)} \in \mathbb{R}^{2n\times 2n}$, with the corresponding blocks $\widetilde{Q}_1^{(\lambda)}$, $\widetilde{Q}_2^{(\lambda)} \in \mathbb{R}^{n\times n}$:

$$\begin{bmatrix} \widetilde{Q}_1^{(\lambda)} & -\widetilde{Q}_2^{(\lambda)} \\ \widetilde{Q}_2^{(\lambda)} & \widetilde{Q}_1^{(\lambda)} \end{bmatrix}^T \begin{bmatrix} \mathbf{h} - \lambda I_{n\times n} & \mathbf{\Delta} \\ \mathbf{\Delta} & -\mathbf{h} + \lambda I_{n\times n} \end{bmatrix} \begin{bmatrix} \widetilde{Q}_1^{(\lambda)} & -\widetilde{Q}_2^{(\lambda)} \\ \widetilde{Q}_2^{(\lambda)} & \widetilde{Q}_1^{(\lambda)} \end{bmatrix} = \begin{bmatrix} \widetilde{E}_{(+)}^{(\lambda)} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -\widetilde{E}_{(+)}^{(\lambda)} \end{bmatrix} =: \widetilde{\mathcal{E}}^{(\lambda)},$$

where $\widetilde{E}_{(+)}^{(\lambda)}$ contains positive eigenvalues and equals $E_{(+)}^{(\lambda)}$ up to a permutation of diagonal entries. From $\mathbf{H}_\lambda Q^{(\lambda)} = Q^{(\lambda)}\mathcal{E}^{(\lambda)}$ and $\mathbf{H}_\lambda \widetilde{Q}^{(\lambda)} = \widetilde{Q}^{(\lambda)}\widetilde{\mathcal{E}}^{(\lambda)}$ it follows that:

$$\mathcal{E}^{(\lambda)}\left(Q^{(\lambda)}\right)^T \widetilde{Q}^{(\lambda)} = \left(Q^{(\lambda)}\right)^T \widetilde{Q}^{(\lambda)}\widetilde{\mathcal{E}}^{(\lambda)}. \tag{2.5}$$

If we set $\Psi := \left(Q^{(\lambda)}\right)^T \widetilde{Q}^{(\lambda)} = \left(\begin{smallmatrix} \Psi_{11} & \Psi_{12} \\ \Psi_{21} & \Psi_{22} \end{smallmatrix}\right) \in \mathbb{R}^{2n\times 2n}$, then the previous equation yields:

$$E_{(+)}^{(\lambda)}\Psi_{12} + \Psi_{12}\widetilde{E}_{(+)}^{(\lambda)} = \mathbf{0}_{n\times n}. \tag{2.6}$$

This is the Sylvester equation and since $E_{(+)}^{(\lambda)}$ and $\widetilde{E}_{(+)}^{(\lambda)}$ contain on diagonal the same elements of $\sigma(\mathbf{H}_\lambda)$ up to a permutation, and since $\mathbf{H}_\lambda$ is regular: $0 \notin \operatorname{diag} E_{(+)}^{(\lambda)}, \operatorname{diag} \widetilde{E}_{(+)}^{(\lambda)}$, we have that $\sigma\left(E_{(+)}^{(\lambda)}\right) \cap \sigma\left(-\widetilde{E}_{(+)}^{(\lambda)}\right) = \emptyset$. Thus, $\Psi_{12} = \mathbf{0}_{n\times n}$ is the only solution of the eq. (2.6) according to Lemma 2.1.3. Analogously, $\Psi_{21} = \mathbf{0}_{n\times n}$. Since $\Psi = \left(Q^{(\lambda)}\right)^T \widetilde{Q}^{(\lambda)}$ is obtained as a product of two orthogonal matrices, Ψ itself is orthogonal, and thus Ψ_{11} and Ψ_{22} are orthogonal as well. From $\widetilde{Q}^{(\lambda)} = Q^{(\lambda)}\Psi$ we have:

$$\begin{bmatrix} \widetilde{Q}_1^{(\lambda)} \\ \widetilde{Q}_2^{(\lambda)} \end{bmatrix} = \begin{bmatrix} Q_1^{(\lambda)} \\ Q_2^{(\lambda)} \end{bmatrix} \Psi_{11}, \quad \Psi_{11}^{-1} = \Psi_{11}^T. \tag{2.7}$$

In particular, $\widetilde{Q}_1^{(\lambda)} = Q_1^{(\lambda)}\Psi_{11}$ and $\widetilde{Q}_2^{(\lambda)} = Q_2^{(\lambda)}\Psi_{11}$, which gives: $\widetilde{Q}_2^{(\lambda)}\left(\widetilde{Q}_2^{(\lambda)}\right)^T = Q_2^{(\lambda)}\left(Q_2^{(\lambda)}\right)^T$, $\widetilde{Q}_2^{(\lambda)}\left(\widetilde{Q}_1^{(\lambda)}\right)^T = Q_2^{(\lambda)}\left(Q_1^{(\lambda)}\right)^T$ and $\left\|\widetilde{Q}_2^{(\lambda)}\right\| = \left\|Q_2^{(\lambda)}\right\|$ for any unitarily invariant norm $\|\cdot\|$. Of course, same result holds if we change $Q_2^{(\lambda)}$ with $Q_1^{(\lambda)}$. ⊠

In Hartree-Fock-Bogoliubov theory [3], two matrices play a key role: the *density matrix* $\rho = \left(V^{(\lambda_0)}\right)^* \left(V^{(\lambda_0)}\right)^T$, and the *pairing tensor* $\kappa = \left(V^{(\lambda_0)}\right)^* \left(U^{(\lambda_0)}\right)^T$. When time-reversal symmetry is taken into account as in eq. (1.9), density matrix and pairing tensor are reduced, and are equal to:

$$\boldsymbol{\rho} := Q_2^{(\lambda_0)} \left(Q_2^{(\lambda_0)}\right)^T \text{ and } \boldsymbol{\kappa} := Q_1^{(\lambda_0)} \left(Q_2^{(\lambda_0)}\right)^T, \tag{2.8}$$

up to a multiplicative factor which we ignore in our analysis. Proposition 2.1.4 shows that $\boldsymbol{\rho}$ and $\boldsymbol{\kappa}$ are well defined together with the target function $f(\lambda) = \left\|Q_2^{(\lambda)}\right\|_F^2 = \text{Trace}\,[\boldsymbol{\rho}]$, in a sense that the final result for $\boldsymbol{\rho}$, $\boldsymbol{\kappa}$ and $f(\lambda)$ is independent of the concrete choice of the eigenvector matrix $Q^{(\lambda_0)}$ in eq. (1.13).

2.2 Explicit formulas for density matrix and pairing tensor

In this section, we characterize the density matrix and the pairing tensor as the Cauchy contour integral of a Schur complement in the resolvent of the Routhian $\mathbf{H}_\lambda$. First we will need one lemma regarding the inverse of 2×2 block matrix which is well known and can be found in any text dealing with Schur complement.

Lemma 2.2.1. *Suppose we are given matrices $A, B, C, D \in \mathbb{C}^{n\times n}$, such that the matrix A and that the supermatrix:*

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \in \mathbb{C}^{2n\times 2n}, \tag{2.9}$$

are both regular. Then the corresponding Schur complement: $D - CA^{-1}B$, is also regular. Furthermore there holds:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \left[\begin{array}{c|c} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ \hline -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{array}\right]. \tag{2.10}$$

Proof: The proof follows from the block LU decomposition:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} I_{n\times n} & \mathbf{0}_{n\times n} \\ CA^{-1} & I_{n\times n} \end{bmatrix} \begin{bmatrix} A & B \\ \mathbf{0}_{n\times n} & D - CA^{-1}B \end{bmatrix}, \tag{2.11}$$

which is trivially checked. Next, since matrices $\begin{bmatrix} A & B \\ C & D \end{bmatrix}$ and $\begin{bmatrix} I_{n\times n} & \mathbf{0}_{n\times n} \\ CA^{-1} & I_{n\times n} \end{bmatrix}$ are nonsingular, matrix $\begin{bmatrix} A & B \\ \mathbf{0}_{n\times n} & D - CA^{-1}B \end{bmatrix}$ is also nonsingular. From Schur decomposition of matrices: $A = UT_AU^\dagger$ and $D - CA^{-1}B = VT_{D-CA^{-1}B}V^\dagger$, where $U, V \in \mathbb{C}^{n\times n}$ are unitary and

$T_A, T_{D-CA^{-1}B} \in \mathbb{C}^{n\times n}$ are upper triangular, one sees that the following two matrices are unitarily similar:

$$\begin{bmatrix} A & B \\ \mathbf{0}_{n\times n} & D - CA^{-1}B \end{bmatrix} \sim \begin{bmatrix} T_A & UBV^\dagger \\ \mathbf{0}_{n\times n} & T_{D-CA^{-1}B} \end{bmatrix}. \tag{2.12}$$

Therefore, zero can not be on the diagonal of the upper triangular matrix $T_{D-CA^{-1}B}$, otherwise the matrix $\begin{bmatrix} A & B \\ \mathbf{0}_{n\times n} & D - CA^{-1}B \end{bmatrix}$ would be singular. Since $T_{D-CA^{-1}B}$ on its diagonal contains the spectrum $\sigma\left(D - CA^{-1}B\right)$, we conclude that the Schur complement $D - CA^{-1}B$ is indeed nonsignular matrix. Formula (2.10) is directly checked. ⊠

Remark 2.2.2. *We can obtain dual (but equivalent) formulas by using:*

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \left[\begin{array}{c|c} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ \hline -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{array}\right], \tag{2.13}$$

provided that D is nonsingular.

Next we recall the Cauchy integral representation of a spectral projector corresponding to a given subset of the eigenvalues by means of matrix resolvent formalism.

Lemma 2.2.3. *Suppose we are given a Hermitian matrix $A \in \mathbb{C}^{n\times n}$ with a k-element subset of its spectrum $\Lambda \subseteq \sigma(A) \subseteq \mathbb{R}$, counted with multiplicity. Let $Q_\Lambda \in \mathbb{C}^{n\times k}$ be a matrix of its eigenvectors such that $Q_\Lambda^\dagger Q_\Lambda = I_{k\times k}$ and $AQ_\Lambda = Q_\Lambda D_\Lambda$, for $D_\Lambda \in \mathbb{R}^{k\times k}$ diagonal with* $\operatorname{diag} D_\Lambda = \Lambda$*, corresponding to a given subset of the eigenvalues Λ. Let $\Gamma \subseteq \mathbb{C}$ be a positively oriented closed contour containing the given eigenvalues in its interior $\Lambda \subseteq \operatorname{Int}\Gamma$, not intersection any eigenvalue: $\Gamma \cap \sigma(A) = \emptyset$. Then the spectral projector $P_\Lambda = Q_\Lambda Q_\Lambda^\dagger$, can be written as:*

$$P_\Lambda = Q_\Lambda Q_\Lambda^\dagger = \frac{1}{2\pi \mathrm{i}} \int_\Gamma (\zeta I_{n\times n} - A)^{-1} d\zeta. \tag{2.14}$$

Proof: First note that due to $\Gamma \cap \sigma(A) = \emptyset$, matrix $\zeta I_{n\times n} - A$ can not be singular for $\zeta \in \Gamma$. Hence, the integral $\int_\Gamma (\zeta I_{n\times n} - A)^{-1} d\zeta$ is well defined. Let $Q_{\sigma(A)\setminus\Lambda} \in \mathbb{C}^{n\times(n-k)}$ be an eigenvector matrix $Q_{\sigma(A)\setminus\Lambda}^\dagger Q_{\sigma(A)\setminus\Lambda} = I_{(n-k)\times(n-k)}$ for the rest of the spectrum $\sigma(A) \setminus \Lambda$, such that the spectral decomposition of A can be written as:

$$A = [Q_\Lambda, Q_{\sigma(A)\setminus\Lambda}] \left[\begin{array}{c|c} D_\Lambda & \mathbf{0}_{k\times(n-k)} \\ \hline \mathbf{0}_{(n-k)\times k} & D_{\sigma(A)\setminus\Lambda} \end{array}\right] [Q_\Lambda, Q_{\sigma(A)\setminus\Lambda}]^\dagger. \tag{2.15}$$

Then there holds:

$$(\zeta I_{n\times n} - A)^{-1} = [Q_\Lambda, Q_{\sigma(A)\setminus\Lambda}] \left[\begin{array}{c|c} (\zeta I_{k\times k} - D_\Lambda)^{-1} & \mathbf{0}_{k\times(n-k)} \\ \hline \mathbf{0}_{(n-k)\times k} & \left(\zeta I_{(n-k)\times(n-k)} - D_{\sigma(A)\setminus\Lambda}\right)^{-1} \end{array}\right] [Q_\Lambda, Q_{\sigma(A)\setminus\Lambda}]^\dagger . \tag{2.16}$$

Due to the Cauchy integral formula, there holds:

$$\int_\Gamma (\zeta I_{k\times k} - D_\Lambda)^{-1} d\zeta = 2\pi i I_{k\times k} \quad \text{and} \quad \int_\Gamma (\zeta I_{(n-k)\times(n-k)} - D_{\sigma(A)\setminus\Lambda})^{-1} d\zeta = \mathbf{0}_{(n-k)\times(n-k)}, \tag{2.17}$$

which implies:

$$\frac{1}{2\pi i}\int_\Gamma (\zeta I_{n\times n} - A)^{-1} d\zeta = [Q_\Lambda, Q_{\sigma(A)\setminus\Lambda}] \left[\begin{array}{c|c} I_{k\times k} & \mathbf{0}_{k\times(n-k)} \\ \hline \mathbf{0}_{(n-k)\times k} & \mathbf{0}_{(n-k)\times(n-k)} \end{array}\right] [Q_\Lambda, Q_{\sigma(A)\setminus\Lambda}]^\dagger . \tag{2.18}$$

Finally, formula (2.14) follows immediately. ⊠

In the following proposition, we give explicit formulas in integral representation of density matrix $\boldsymbol{\rho}$ and pairing tensor $\boldsymbol{\kappa}$ defined in equation (2.8). To author's knowledge, no such formula ever appear in any research papers or textbooks dealing with theoretical nuclear physics and Hartree-Fock-Bogoliubov theory specifically.

Proposition 2.2.4. *Let $\Gamma_{(+)} \subseteq \mathbb{C}$ be a positively oriented closed contour in complex plane that encloses, in its interior, the positive eigenvalues of the nonsingular Routhian $\mathbf{H}_\lambda$, for some $\lambda \in \mathcal{I} \subseteq \mathbb{R}$, and such that it does not intersect the spectrum of $\mathbf{H}_\lambda$ and $\mathbf{h} - \lambda I_{n\times n}$. Then the following formula holds:*

$$Q_2^{(\lambda)} \left(Q_2^{(\lambda)}\right)^T = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{(+)}} \left\{(\zeta - \lambda) I_{n\times n} + \mathbf{h} - \boldsymbol{\Delta} \left[(\zeta + \lambda) I_{n\times n} - \mathbf{h}\right]^{-1} \boldsymbol{\Delta}\right\}^{-1} d\zeta. \tag{2.19}$$

For the norm $\left\|Q_2^{(\lambda)}\right\|_F^2 = \mathrm{Trace}\left[Q_2^{(\lambda)} \left(Q_2^{(\lambda)}\right)^T\right]$, only the diagonal of the above integral is needed:

$$\left\|Q_2^{(\lambda)}\right\|_F^2 = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{(+)}} \mathrm{Trace}\left[\left\{(\zeta - \lambda) I_{n\times n} + \mathbf{h} - \boldsymbol{\Delta}[(\zeta + \lambda) I_{n\times n} - \mathbf{h}]^{-1} \boldsymbol{\Delta}\right\}^{-1}\right] d\zeta. \tag{2.20}$$

Also, there holds:

$$Q_1^{(\lambda)} \left(Q_2^{(\lambda)}\right)^T = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{(+)}} [(\zeta + \lambda) I_{n\times n} - \mathbf{h}]^{-1} \boldsymbol{\Delta} \left\{(\zeta - \lambda) I_{n\times n} + \mathbf{h} - \boldsymbol{\Delta}[(\zeta + \lambda) I_{n\times n} - \mathbf{h}]^{-1} \boldsymbol{\Delta}\right\}^{-1} d\zeta. \tag{2.21}$$

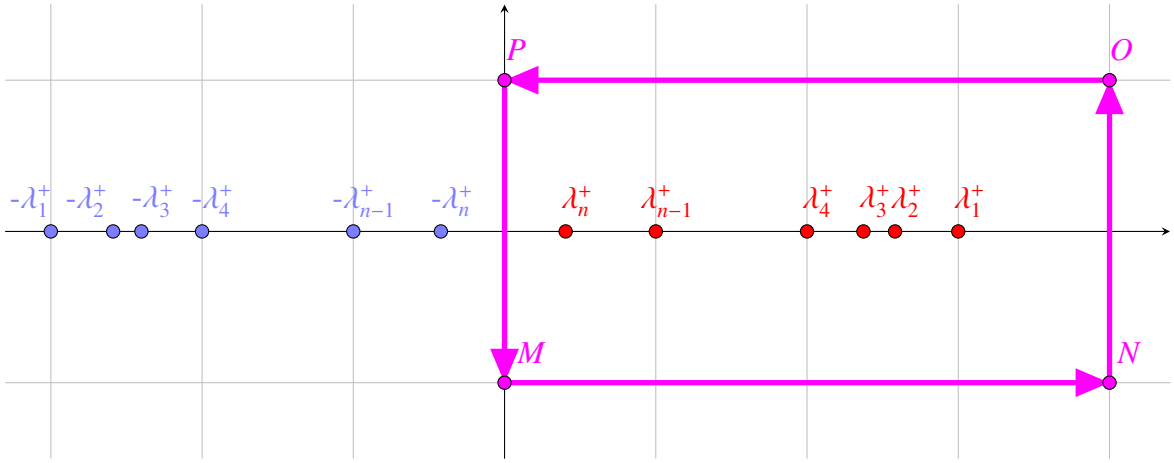


Figure 2.5: An example of the contour $\Gamma_{(+)}$ that encloses the positive eigenvalues of the nonsingular Routhian $\mathbf{H}_{\lambda_0}$. If $\Gamma_{(+)}$ does not intersect the spectrum of $\mathbf{H}_{\lambda_0}$ and $\mathbf{h} - \lambda_0 I_{n\times n}$, then the density matrix $\boldsymbol{\rho}$ and the pairing tensor $\boldsymbol{\kappa}$ can be written as a Cauchy integral over the contour $\Gamma_{(+)}$. (See Proposition 2.2.4)

Proof: The proof has three main ingredients. First, the orthogonal projector $P_{(+)}^{(\lambda)}$ to the spectral subspace of $\mathbf{H}_\lambda$ that corresponds to the positive eigenvalues is given as:

$$P_{(+)}^{(\lambda)} = \begin{bmatrix} Q_1^{(\lambda)} \\ Q_2^{(\lambda)} \end{bmatrix} \begin{bmatrix} \left(Q_1^{(\lambda)}\right)^T & \left(Q_2^{(\lambda)}\right)^T \end{bmatrix} = \left[\begin{array}{c|c} Q_1^{(\lambda)}\left(Q_1^{(\lambda)}\right)^T & Q_1^{(\lambda)}\left(Q_2^{(\lambda)}\right)^T \\ \hline Q_2^{(\lambda)}\left(Q_1^{(\lambda)}\right)^T & Q_2^{(\lambda)}\left(Q_2^{(\lambda)}\right)^T \end{array}\right], \tag{2.22}$$

where $Q_1^{(\lambda)}$ and $Q_2^{(\lambda)}$ are defined as in eq. (1.13). Then, our matrices of interest are in the second block of columns of $P_{(+)}^{(\lambda)}$. Second, recall the Cauchy integral representation of a spectral projector corresponding to a given subset of the eigenvalues: since $\Gamma_{(+)}$ is a contour containing the given positive eigenvalues in its interior, then according to the Lemma 2.2.3:

$$P_{(+)}^{(\lambda)} = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{(+)}} (\zeta I_{2n\times 2n} - \mathbf{H}_\lambda)^{-1} d\zeta. \tag{2.23}$$

Since the second block columns of $P_{(+)}^{(\lambda)}$ are obtainable from expression: $P_{(+)}^{(\lambda)} \begin{bmatrix} \mathbf{0}_{n\times n} \\ I_{n\times n} \end{bmatrix}$, we can

further calculate:

$$
\begin{aligned}
P^{(\lambda)}_{(+)}\begin{bmatrix}\mathbf{0}_{n\times n}\\ I_{n\times n}\end{bmatrix} &= \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_{(+)}} (\zeta I_{2n\times 2n} - \mathbf{H}_\lambda)^{-1} d\zeta \begin{bmatrix}\mathbf{0}_{n\times n}\\ I_{n\times n}\end{bmatrix} && (2.24)\\
&= \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_{(+)}} (\zeta I_{2n\times 2n} - \mathbf{H}_\lambda)^{-1} \begin{bmatrix}\mathbf{0}_{n\times n}\\ I_{n\times n}\end{bmatrix} d\zeta && (2.25)\\
&= \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_{(+)}} \left(\zeta I_{2n\times 2n} - \begin{bmatrix} \mathbf{h} - \lambda I_{n\times n} & \mathbf{\Delta} \\ \mathbf{\Delta} & -\mathbf{h} + \lambda I_{n\times n}\end{bmatrix}\right)^{-1} \begin{bmatrix}\mathbf{0}_{n\times n}\\ I_{n\times n}\end{bmatrix} d\zeta && (2.26)\\
&= \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_{(+)}} \begin{bmatrix} (\zeta+\lambda) I_{n\times n} - \mathbf{h} & -\mathbf{\Delta} \\ -\mathbf{\Delta} & (\zeta-\lambda) I_{n\times n} + \mathbf{h}\end{bmatrix}^{-1} \begin{bmatrix}\mathbf{0}_{n\times n}\\ I_{n\times n}\end{bmatrix} d\zeta. && (2.27)
\end{aligned}
$$

Third, we recall an explicit formula from Lemma 2.2.1 for the inverse of a certain block partitioned matrices. Namely, if an invertible matrix is partitioned into a 2×2 block partition, with square diagonal blocks, then it holds that:

$$
\begin{bmatrix} A & B \\ C & D\end{bmatrix}^{-1} = \left[\begin{array}{c|c} A^{-1} + A^{-1}B(D-CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D-CA^{-1}B)^{-1} \\ \hline -(D-CA^{-1}B)^{-1}CA^{-1} & (D-CA^{-1}B)^{-1}\end{array}\right], \qquad (2.28)
$$

provided that A is nonsingular. Lemma 2.2.1 gives that the Schur complement $D - CA^{-1}B$ must be nonsingular.

In our case, nonsingularity of $\begin{bmatrix} A & B \\ C & D\end{bmatrix}$ means that $\zeta I_{2n\times 2n} - \mathbf{H}_\lambda$ is nonsingular along $\zeta \in \Gamma_{(+)}$, which is true because of the assumption that the contour $\Gamma_{(+)}$ does not intersect the spectrum of $\mathbf{H}_\lambda$. Furthermore, nonsingularity of A means that: $(\zeta+\lambda)I_{n\times n} - \mathbf{h} = -(\mathbf{h} - \lambda I_{n\times n}) + \zeta I_{n\times n}$ must be nonsingular along $\zeta \in \Gamma_{(+)}$. That is equivalent to the condition that $\Gamma_{(+)}$ does not pass through any eigenvalue of $\mathbf{h} - \lambda I_{n\times n}$ which is also fulfilled by the assumption. Since $\mathbf{h}$ is symmetric and λ is real, all those critical points of possible intersections are real, hence we can take $\Gamma_{(+)}$ to cross the real line only twice and we can use many computationally cheap methods to localise the spectrum of $\mathbf{h} - \lambda I_{n\times n}$ for the purpose of avoiding it, see Figure 2.5.

Therefore, all assumptions of the Lemma 2.2.1 are fulfilled, and simply plugging in matrices: $A = (\zeta+\lambda)I_{n\times n} - \mathbf{h}$, $B = -\mathbf{\Delta}$, $C = -\mathbf{\Delta}$, $D = (\zeta-\lambda)I_{n\times n} + \mathbf{h}$ into equation (2.28), together with the expression (2.27), one finally obtains the desired equations (2.19), (2.20) and (2.21). ⊠

The above formulas (2.19), (2.20) and (2.21), when evaluated for $\lambda = \lambda_0$, under the assumptions given in Proposition (2.2.4), will give a closed form expressions for the density matrix $\boldsymbol{\rho} = Q_2^{(\lambda_0)} \left(Q_2^{(\lambda_0)}\right)^T$ and the pairing tensor $\boldsymbol{\kappa} = Q_1^{(\lambda_0)} \left(Q_2^{(\lambda_0)}\right)^T$. They can be used to gain an insight in terms of physical intepretation, and also for deriving perturbation bounds to study the sensitivity of the density matrix to changes in λ, $\mathbf{h}$ and $\boldsymbol{\Delta}$. Furthermore, they can be used as a starting point for a numerical scheme based on numerical integration.

Remark 2.2.5. *In matrices coming from real applications, it turns out that matrix $\boldsymbol{\Delta} \in \mathbb{R}^{n\times n}$ is much "*weaker*" than $\mathbf{h} \in \mathbb{R}^{n\times n}$, in a sense that $\|\boldsymbol{\Delta}\|_F$ is much less than $\|\mathbf{h}\|_F$. Then the formula (2.19):*

$$Q_2^{(\lambda)} \left(Q_2^{(\lambda)}\right)^T = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{(+)}} \left\{(\zeta - \lambda) I_{n\times n} + \mathbf{h} - \boldsymbol{\Delta} \left[(\zeta + \lambda) I_{n\times n} - \mathbf{h}\right]^{-1} \boldsymbol{\Delta}\right\}^{-1} d\zeta, \tag{2.29}$$

can be used as a starting point for deriving an approximate expression of the target function $f(\lambda)$. For example, if we initially diagonalize the matrix $\mathbf{h}$, and work in a basis where $\mathbf{h}$ is diagonal, then the second term $\boldsymbol{\Delta} \left[(\zeta + \lambda) I_{n\times n} - \mathbf{h}\right]^{-1} \boldsymbol{\Delta}$ in eq. (2.29) can be treated as a weak perturbation when compared to the first term $(\zeta - \lambda) I_{n\times n} + \mathbf{h}$ which is a diagonal matrix.

Therefore, we seek approximate formula for an inverse of a diagonal matrix plus small perturbation, where one can invoke Neumann series expansion and obtain an approximate expression in terms of a truncated infinite series, where the contour integral in each term can be exactly caclulated. The series would rapidly converge since $\|\boldsymbol{\Delta}\|_F$ is small compared to $\|\mathbf{h}\|_F$. Further investigation is in progress.

2.3 Target function

Careful reader might noticed that Proposition 2.1.4 only proves that the target function $f(\lambda)$ is well defined, but does not prove that there exists any $\lambda_0 \in \mathcal{I} \subseteq \mathbb{R}$ such that $f(\lambda_0) = f_0$. Also, the uniqueness of $\lambda_0 \in \mathcal{I} \subseteq \mathbb{R}$ such that $f(\lambda_0) = f_0$ is an open question. In nuclear physics scientific community, CHFB theory has been used for a long time and it appears that if the size $n \in \mathbb{N}$ of a truncated basis, which approximates full space $\left(H_0^1(\mathbb{R}^3)\right)^d$, is selected large enough (often reaching $n \geq 3000$ and more), there always exists such $\lambda_0 \in \mathcal{I} \subseteq \mathbb{R}$ which satisfies $f(\lambda_0) = f_0$, where f_0 is never larger than ≈ 200 in applications. Also, only in degenerated case: $\boldsymbol{\Delta} = \mathbf{0}_{n\times n}$, which is know as the Hartree-Fock theory [3], one encounters nonuniqueness of such λ_0, but that case is trivial to solve since the Routhian's blocks $\mathbf{h} - \lambda I_{n\times n}$ and $\boldsymbol{\Delta} = \mathbf{0}_{n\times n}$ are decoupled.

In the following example, we illustrate the behaviour of the target function $f(\lambda)$ on a simple toy-example matrices $\mathbf{h}$ and $\mathbf{\Delta}$.

Example 2.3.1. *Suppose we take* $n = 9$ *and define* $\mathbf{h} \in \mathbb{R}^{n\times n}$ *as:*

$$\mathbf{h} = q\,\mathrm{diag}\,[-10,-8,-5,-4,-1,-1,6,7,12]\,q^T, \tag{2.30}$$

where $q \in \mathbb{R}^{n\times n}$ *is taken as a random orthogonal matrix. Take another random symmetric matrix* $\mathbf{\Delta}_0 \in \mathbb{R}^{n\times n}$ *from standard normal distribution. We define* $\mathbf{\Delta}^{(G)} := G\mathbf{\Delta}_0$*, for* $G \in \mathbb{R}$ *determining the strength parameter. Next, we build the corresponding Hamiltonian:* $\mathbf{H}^{(G)} = \begin{bmatrix} \mathbf{h} & \mathbf{\Delta}^{(G)} \\ \mathbf{\Delta}^{(G)} & -\mathbf{h} \end{bmatrix} \in \mathbb{R}^{2n\times 2n}$*, and for any* $\lambda \in \mathbb{R}$*, Routhian as:* $\mathbf{H}^{(G)}_{\lambda} = \mathbf{H}^{(G)} - \lambda \begin{bmatrix} I_{n\times n} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -I_{n\times n} \end{bmatrix} \in \mathbb{R}^{2n\times 2n}$*, all parameterized with strength parameter* G*. Then, from the spectral decomposition of the Routhian:*

$$\begin{bmatrix} Q_1^{(\lambda,G)} & -Q_2^{(\lambda,G)} \\ Q_2^{(\lambda,G)} & Q_1^{(\lambda,G)} \end{bmatrix}^T \begin{bmatrix} \mathbf{h} - \lambda I_{n\times n} & \mathbf{\Delta}^{(G)} \\ \mathbf{\Delta}^{(G)} & -(\mathbf{h} - \lambda I_{n\times n}) \end{bmatrix} \begin{bmatrix} Q_1^{(\lambda,G)} & -Q_2^{(\lambda,G)} \\ Q_2^{(\lambda,G)} & Q_1^{(\lambda,G)} \end{bmatrix} = \begin{bmatrix} E_{(+)}^{(\lambda,G)} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -E_{(+)}^{(\lambda,G)} \end{bmatrix}, \tag{2.31}$$

we simply calculate the target function $f^{(G)}(\lambda) = \left\|Q_2^{(\lambda,G)}\right\|^2$*. By varying the parameter* $\lambda \in \mathbb{R}$*, we can plot the family of target functions* $f^{(G)}(\lambda)$ *parameterized by strength* $G \in \mathbb{R}$*.*

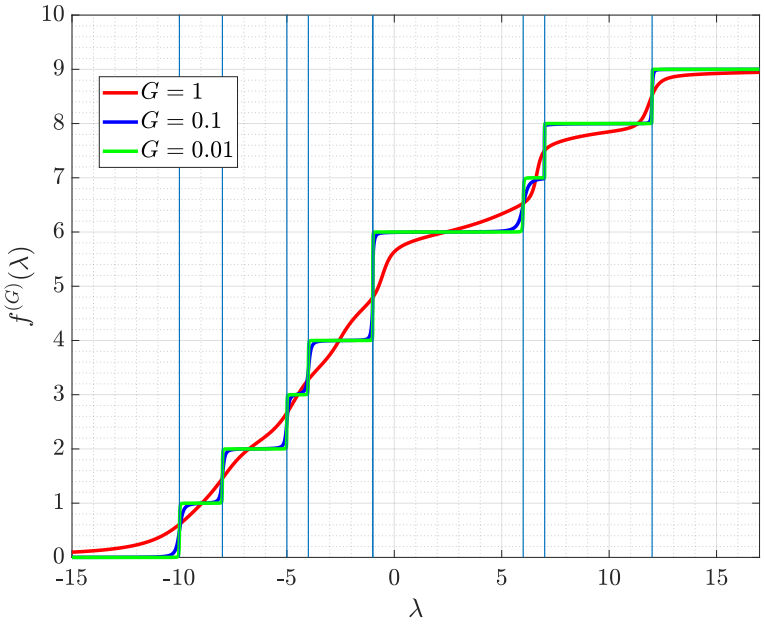


Figure 2.6: Illustration of target function $f^{(G)}(\lambda)$ when one varies the strength parameter G.

Figure 2.6 illustrates the family of target functions $f^{(G)}(\lambda)$ when one varies the strength parameter G. Eigenvalues of matrix $\mathbf{h}$ *are shown as vertical lines. We notice that when G approaches zero, one obtains a step function with discontinuities precisely at positions where* $\mathbf{h}$ *has eigenvalues, with jumps equal to the multiplicity of the given eigenvalue. As G is increased, the step function smears out near eigenvalues of* $\mathbf{h}$ *and saturates as λ overpasses the maximum eigenvalue of* $\mathbf{h}$*. The target function values $f^{(G)}(\lambda)$ appear to reside in a strip $[0, n]$, which means that if the target value $f_0 \in \mathbb{R}$ is located in $[0, n]$, we would have a unique solution of equation $f^{(G)}(\lambda_0) = f_0$, unless one encounters a degenerate case where G parameter is precisely zero.*

Previous example suggests that the target function $f(\lambda)$ appears to be strictly increasing function (unless $\mathbf{\Delta} = \mathbf{0}_{n\times n}$, which is trivial case) with values in $[0, n]$. Proof that this is indeed true, authors of [18] of hope to obtain from derived closed expression (2.20) of $f(\lambda)$ by showing that it is increasing function when $\mathbf{\Delta} \neq \mathbf{0}_{n\times n}$. That, together with $\lim_{\lambda\to-\infty} f(\lambda) = 0$, and $\lim_{\lambda\to+\infty} f(\lambda) = n$, would completely answer the well-posedness question. Work is still in progress and that proof would demonstrate the internal consistency of the CHFB theory.

2.4 Other properties

In this section, we give some remarks regarding the CHFB theory with time-reversal symmetry which will probably be more interesting in future investigations.

CS decomposition

The blocks of an orthogonal matrix partitioned into 2-by-2 form have highly related singular value decompositions. This is the gist of the so called *CS decomposition*. Proof of the following very useful theorem can be found in many textbooks dealing with matrix theory, such as [19].

Theorem 2.4.1. (The CS decomposition) *Consider the matrix:*

$$Q = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}, \; Q_1 \in \mathbb{R}^{m_1\times n_1}, Q_2 \in \mathbb{R}^{m_2\times n_1}, \tag{2.32}$$

where $m_1 \geq n_1$ and $m_2 \geq n_1$. If the columns of Q are orthonormal: $Q^T Q = I_{n_1\times n_1}$, then there exist orthogonal matrices $U_1 \in \mathbb{R}^{m_1\times m_1}$, $U_2 \in \mathbb{R}^{m_2\times m_2}$ and $V_1 \in \mathbb{R}^{n_1\times n_1}$ such that:

$$\begin{bmatrix} U_1 & \mathbf{0}_{m_1\times m_2} \\ \mathbf{0}_{m_2\times m_1} & U_2 \end{bmatrix}^T \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} V_1 = \begin{bmatrix} C \\ S \end{bmatrix}, \tag{2.33}$$

where:

$$C = \operatorname{diag}(\cos\theta_1, \cos\theta_2, \ldots, \cos\theta_{n_1}) \in \mathbb{R}^{m_1 \times n_1}\ ,\ S = \operatorname{diag}(\sin\theta_1, \sin\theta_2, \ldots, \sin\theta_{n_1}) \in \mathbb{R}^{m_2 \times n_1}, \tag{2.34}$$

and:

$$0 \leq \theta_1 \leq \theta_2 \leq \cdots \leq \theta_{n_1} \leq \frac{\pi}{2}. \tag{2.35}$$

Proof: See [19]. ⊠

Next, we show that matrices U_1 and U_2 from CS decomposition are essentially the same when one has additional orthogonal symplectic structure of Q_1 and Q_2.

Proposition 2.4.2. *Suppose we are given matrices $Q_1, Q_2 \in \mathbb{R}^{n\times n}$ such that the matrix:*

$$Q = \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix} \in \mathbb{R}^{2n\times 2n}, \tag{2.36}$$

is orthogonal. Then there exist orthogonal matrices $U, V \in \mathbb{R}^{n\times n}$ and real numbers $(c_i)_{i=1}^n, (s_i)_{i=1}^n$, satisfying $c_i^2 + s_i^2 = 1$ and $s_i \geq 0$, for $i = 1, \ldots, n$, such that $Q_1 = UCV^T$ and $Q_2 = USV^T$, where $C = \operatorname{diag}(c_i)_{i=1}^n$ and $S = \operatorname{diag}(s_i)_{i=1}^n$.

Proof: From orthogonality of Q matrix, we easily see that there holds:

$$Q_1^T Q_1 + Q_2^T Q_2 = I_{n\times n}, \tag{2.37}$$

$$Q_1 Q_1^T + Q_2 Q_2^T = I_{n\times n}, \tag{2.38}$$

$$Q_1 Q_2^T = Q_2 Q_1^T. \tag{2.39}$$

Thus, the columns of matrix $\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$ are orthonormal, and therefore Theorem 2.4.1 gives $U_1, U_2, V_1 \in \mathbb{R}^{n\times n}$ orthogonal, and $(c_i)_{i=1}^n, (s_i)_{i=1}^n$ such that $c_i^2 + s_i^2 = 1$, and $c_i, s_i \geq 0$, for $i = 1, \ldots, n$, giving: $Q_1 = U_1 C V_1^T$ and $Q_2 = U_2 S V_1^T$, where $C = \operatorname{diag}(c_i)_{i=1}^n$ and $S = \operatorname{diag}(s_i)_{i=1}^n$. Equation (2.38) gives: $U_1 C^2 U_1^T + U_2 S^2 U_2^T = I_{n\times n}$, which if we define orthogonal matrix: $Q := U_1^T U_2 \in \mathbb{R}^{n\times n}$, can be equivalently written as: $C^2 Q = Q C^2$, and thus for all $i, j \in 1 \ldots n$, there holds $(c_i^2 - c_j^2) Q_{ij} = 0$. Therefore, if we write: $C = \bigoplus_{i=1}^p c_i I_{n_i \times n_i}$ and $S = \bigoplus_{i=1}^p s_i I_{n_i \times n_i}$, where $n_1 + \cdots + n_p = n$, then since $c_i \geq 0$, we have that Q can be written as block matrix: $Q = \bigoplus_{i=1}^p q_i$, where $q_i \in \mathbb{R}^{n_i \times n_i}$ are orthogonal for every $i = 1 \ldots p$. From equation (2.39) we obtain: $U_1 C S U_2^T = U_2 C S U_1^T$, which can be equivalently written as: $CS = QCSQ$. Using block partition, we have $c_i s_i I_{n_i\times n_i} = c_i s_i q_i^2$, for every $i = 1, \ldots, p$, rendering that for all $i = 1, \ldots, p$, such that $c_i \notin \{0, 1\}$, orthogonal matrices $q_i \in \mathbb{R}^{n_i \times n_i}$ also satisfy $q_i^2 = I_{n_i \times n_i}$. Using $U_1 = U_2 Q^T$, we can write:

$$Q_1 = U_2 Q^T C V_1^T \text{ and } Q_2 = U_2 S V_1^T. \tag{2.40}$$

In conclusion, we can say that there exists orthogonal matrix $Z = \bigoplus_{i=1}^{p} z_i$ for $z_i \in \mathbb{R}^{n_i \times n_i}$ for all $i = 1, \ldots, p$, where $z_i^2 = I_{n_i \times n_i}$ for all blocks $i = 1, \ldots, p$, where $c_i \notin \{0, 1\}$, such that there holds:

$$Q_1 = U_2 Z C V_1^T \text{ and } Q_2 = U_2 S V_1^T. \tag{2.41}$$

Notice that if we take any block $i_0 = 1, \ldots, p$, such that $c_{i_0} = 0$, we can select $z_{i_0} = I_{n_{i_0} \times n_{i_0}}$ and still have previous statement satisfied, with only difference that $z_i^2 = I_{n_i \times n_i}$ will hold for all blocks $i = 1, \ldots, p$, where $c_i \neq 1$. Next, for blocks where $c_i = 1$, we also have $s_i = 0$, and thus one can see that there holds:

$$Q_1 = U_2 W Y C V_1^T \text{ and } Q_2 = U_2 W S V_1^T, \tag{2.42}$$

where $W = \bigoplus_{i=1}^{p} w_i$, $w_i = I_{n_i \times n_i}$ for blocks i having $c_i \neq 1$ and $w_i = z_i$ for blocks having $c_i = 1$, while $Y = \bigoplus_{i=1}^{p} y_i$, $y_i = I_{n_i \times n_i}$ for blocks i having $c_i = 1$ and $y_i = z_i$ for blocks having $c_i \neq 1$. Notice that now all blocks $y_i \in \mathbb{R}^{n_i \times n_i}$, are orthogonal matrices $y_i^T y_i = I_{n_i \times n_i}$ also satisfying $y_i^2 = I_{n_i \times n_i}$, for all $i = 1, \ldots, p$. Thus for all $i = 1, \ldots, p$, $y_i \in \mathbb{R}^{n_i \times n_i}$ are orthogonal symmetric matrices, and therefore we have spectral decompositions: $y_i = x_i d_i x_i^T$, for $x_i \in \mathbb{R}^{n_i \times n_i}$ orthogonal and $d_i \in \mathbb{R}^{n_i \times n_i}$ diagonal matrix with diagonal elements $+1$ or -1. If we define orthogonal matrix $X = \bigoplus_{i=1}^{p} x_i \in \mathbb{R}^{n \times n}$, and diagonal matrix $D = \bigoplus_{i=1}^{p} d_i$ with entries $+1$ or -1, one can easily verify:

$$Q_1 = U_2 W X D C X^T V_1^T \text{ and } Q_2 = U_2 W X S X^T V_1^T. \tag{2.43}$$

If we define orthogonal matrices $U := U_2 W X \in \mathbb{R}^{n \times n}$ and $V := V_1 X \in \mathbb{R}^{n \times n}$, then there finally holds:

$$Q_1 = U D C V^T \text{ and } Q_2 = U S V^T, \tag{2.44}$$

which proves the desired statement because $D \in \mathbb{R}^{n \times n}$ is diagonal with entries ± 1. ⊠

Suppose we have density matrix $\boldsymbol{\rho} = Q_2^{(\lambda_0)} \left(Q_2^{(\lambda_0)}\right)^T$ and pairing tensor $\boldsymbol{\kappa} = Q_1^{(\lambda_0)} \left(Q_2^{(\lambda_0)}\right)^T$. Proposition 2.4.2 shows the existence of $P^{(\lambda_0)}, R^{(\lambda_0)} \in \mathbb{R}^{n \times n}$ orthogonal matrices such that $Q_1^{(\lambda_0)} = P^{(\lambda_0)} C^{(\lambda_0)} \left(R^{(\lambda_0)}\right)^T$ and $Q_2^{(\lambda_0)} = P^{(\lambda_0)} S^{(\lambda_0)} \left(R^{(\lambda_0)}\right)^T$, where $C^{(\lambda_0)}, S^{(\lambda_0)} \in \mathbb{R}^{n \times n}$ are diagonal matrices satisfying $\left(C^{(\lambda_0)}\right)^2 + \left(S^{(\lambda_0)}\right)^2 = I_{n \times n}$. Then we have:

$$\boldsymbol{\rho} = P^{(\lambda_0)} \left(S^{(\lambda_0)}\right)^2 \left(P^{(\lambda_0)}\right)^T, \tag{2.45}$$

$$\boldsymbol{\kappa} = P^{(\lambda_0)} C^{(\lambda_0)} S^{(\lambda_0)} \left(P^{(\lambda_0)}\right)^T. \tag{2.46}$$

Notice that $|C^{(\lambda_0)}|$ and $|S^{(\lambda_0)}|$ do not depend on the concrete choice of $Q_1^{(\lambda_0)}$ and $Q_1^{(\lambda_0)}$ in eq. (1.13) because according to Proposition 2.1.4, they all have the same singular values.

Since $|C^{(\lambda_0)}|$ are singular values of $Q_1^{(\lambda_0)}$ while $|S^{(\lambda_0)}|$ are singular values of $Q_2^{(\lambda_0)}$, they do not depend on the concrete choice of $Q_1^{(\lambda_0)}$ and $Q_2^{(\lambda_0)}$. In nuclear physics, values $\left(c_i^2\right)_{i=1}^n$ and $\left(s_i^2\right)_{i=1}^n$ are known as the *BCS occupation probabilities*. Result given in Proposition 2.4.2, adapted to HFB theory with time-reversal symmetry, is known in nuclear physics as the *Bloch-Messiah Theorem* [3].

Now we would like to consider a practical application of Proposition 2.4.2. In practice, CHFB theory is often used as a starting point which calculates the ground state properties of a nuclei under consideration. The obtained matrices $Q_1^{(\lambda_0)}$ and $Q_2^{(\lambda_0)}$ are then used as a building blocks for further calculations beyond ground state. For example, in nuclear structure physics, CHFB theory results are used for investigation of excited states of nuclei in a framework called *Quasiparticle Random Phase Approximation* (QRPA). In the past decade, a method for solving the QRPA equation, known as the *Finite Amplitude Method* (FAM), has received significant popularity. One recent example of a software package for solving the QRPA equation using FAM method is [20].

In practical implementations of iterative FAM method, one has to calculate many matrix products of type $X^T\mathcal{F}_iY$, where $\mathcal{F}_i \in \mathbb{C}^{n\times n}$ is a certain matrix obtained in the i-th iteration, while matrices $X \in \mathbb{R}^{n\times n}$ and $Y \in \mathbb{R}^{n\times n}$ are constant during iterations and are equal to: $X, Y \in \left\{Q_1^{(\lambda_0)}, Q_2^{(\lambda_0)}\right\}$. In usual applications, one notices that the large majority of singular values from CS decomposition: $\left(c_i^2\right)_{i=1}^n, \left(s_i^2\right)_{i=1}^n$, are very close to 0 or 1. Thus if we want to calculate for example: $\left(Q_1^{(\lambda_0)}\right)^T \mathcal{F}_i Q_2^{(\lambda_0)}$, from Proposition 2.4.2 we obtain:

$$\left(Q_1^{(\lambda_0)}\right)^T \mathcal{F}_i Q_2^{(\lambda_0)} = R^{(\lambda_0)} C^{(\lambda_0)} \left[\left(P^{(\lambda_0)}\right)^T \mathcal{F}_i P^{(\lambda_0)}\right] S^{(\lambda_0)} \left(R^{(\lambda_0)}\right)^T, \tag{2.47}$$

for $P^{(\lambda_0)}, R^{(\lambda_0)} \in \mathbb{R}^{n\times n}$ orthogonal matrices which are precalculated and stored. Since only a small fraction of diagonal elements in matrices $C^{(\lambda_0)}$ and $S^{(\lambda_0)}$ are not well approximated by 0 or 1, we need to calculate only a smaller submatrix of a matrix: $\left[\left(P^{(\lambda_0)}\right)^T \mathcal{F}_i P^{(\lambda_0)}\right]$, and thus obtain $\left(Q_1^{(\lambda_0)}\right)^T \mathcal{F}_i Q_2^{(\lambda_0)}$ with controllable error much more efficient. As we approach the final solution during iterative procedure in FAM, we can increase the precision of the approximation and overall obtain the same result faster.

Non-zero temperature case

The presented CHFB theory with time-reversal symmetry only applies for nuclei at zero temperature. In future investigations, authors of [18] plan to address the problem for non-zero temperature also, but for now, we only state some remarks which might be useful.

Remark 2.4.3. *Suppose we are given $Q_1^{(\lambda)}, Q_2^{(\lambda)} \in \mathbb{R}^{n\times n}$ and $\widetilde{Q}_1^{(\lambda)}, \widetilde{Q}_2^{(\lambda)} \in \mathbb{R}^{n\times n}$ as in the proof of Proposition 2.1.4. By a von Neumann theory, a unitarily invariant norm on matrices is necessarily a symmetric gauge function of its singular values, see e.g. [21, II.3]. So, if $\boldsymbol{\sigma}_1^{(\lambda)} \geq \cdots \geq \boldsymbol{\sigma}_n^{(\lambda)}$ are the singular values of $Q_2^{(\lambda)}$ (and thus also of $\widetilde{Q}_2^{(\lambda)}$), then the target function is: $f(\lambda) = \left\|Q_2^{(\lambda)}\right\|_F^2 = \sum_{i=1}^n \left(\boldsymbol{\sigma}_i^{(\lambda)}\right)^2$. But, for example, the nuclear norm $g(\lambda) = \sum_{i=1}^n \sigma_i^{(\lambda)}$ of $Q_2^{(\lambda)}$ is well defined as well. The choice of a particular gauge function is then motivated by its interpretation in a concrete application.*

Remark 2.4.4. *From the proof of Proposition 2.1.4 it follows that the ℓ_2 norms of the rows of $Q_1^{(\lambda)}$ and $Q_2^{(\lambda)}$ are also independent of a particular choice of the decomposition (1.13). Denote the rows of $Q_2^{(\lambda)}$ by $q_j^{(\lambda)}$, $j = 1, \ldots, n$. If we define $\wp_j^{(\lambda)} := \frac{\left\|q_j^{(\lambda)}\right\|_2^2}{\left\|Q_2^{(\lambda)}\right\|_F^2}$ then we have $\sum_{j=1}^n \wp_j^{(\lambda)} = 1$, i.e. $(\wp_1^{(\lambda)}, \ldots, \wp_n^{(\lambda)})$ is a probability distribution, and we can use its (Shannon) entropy: $S(\lambda) = -\sum_{j=1}^n \wp_j^{(\lambda)} \log \wp_j^{(\lambda)}$, as a function of λ. $S(\lambda)$ is maximal if $Q_2^{(\lambda)}$ is orthogonal (i.e. $\wp_1^{(\lambda)} = \ldots = \wp_n^{(\lambda)} = 1/n$ and in that case $Q_1^{(\lambda)} = \mathbf{0}_{n\times n}$). In that case $f(\lambda) = n$ also attains its maximum. Note that:*

$$G^{(\lambda)} = \frac{1}{\left\|Q_2^{(\lambda)}\right\|_F^2} Q_2^{(\lambda)} \left(Q_2^{(\lambda)}\right)^T,$$

is semidefinite of trace one (it is essentially a density matrix) and that also the von Neumann entropy: $N(\lambda) = -\mathrm{Trace}\left(G^{(\lambda)} \log G^{(\lambda)}\right)$ is well defined. Since the eigenvalues of $G^{(\lambda)}$ are $\alpha_j^{(\lambda)} = \left(\sigma_j^{(\lambda)}\right)^2 / \left\|Q_2^{(\lambda)}\right\|_F^2$, we have $N(\lambda) = -\sum_{j=1}^n \alpha_j^{(\lambda)} \log \alpha_j^{(\lambda)}$. It is well known fact that $S(\lambda) \geq N(\lambda)$.

Symmetric quasi-definite matrices

Definition 2.4.5. *We say that a symmetric matrix $K \in \mathbb{R}^{(m+n)\times(m+n)}$ with real entries is* symmetric quasi-definite *(SQD) if:*

$$K = \begin{bmatrix} H & A^T \\ A & -G \end{bmatrix}, \tag{2.48}$$

where $H \in \mathbb{R}^{n\times n}$ and $G \in \mathbb{R}^{m\times m}$ are symmetric positive definite matrices, and $A \in \mathbb{R}^{m\times n}$.

Symmetric quasi-definite matrices arise in numerous applications, notably in interior point methods in mathematical programming. Several authors have derived various properties of these matrices.

Definition 2.4.6. *For two symmetric matrices $H_1, H_2 \in \mathbb{R}^{n\times n}$, we define the* Loewner partial order $\succ$ *as:*

$$H_1 \succ H_2 \;\; (H_1 \succeq H_2) \;\; \text{if } H_1 - H_2 \text{ is positive definite (positive semidefinite).} \tag{2.49}$$

Suppose we have $H_1 \succ H_2$. Since $H_1 = H_2 + (H_1 - H_2)$, then the Courant–Fischer–Weyl min-max principle for symmetric matrices implies that the eigenvalues of H_1 dominate the eigenvalues of H_2. More precisely, if $\boldsymbol{\varepsilon}_1(H_1) \geq \ldots \geq \boldsymbol{\varepsilon}_n(H_1)$, and $\boldsymbol{\varepsilon}_1(H_2) \geq \ldots \geq \boldsymbol{\varepsilon}_n(H_2)$, are their respective eigenvalues, then: $\boldsymbol{\varepsilon}_i(H_1) \geq \boldsymbol{\varepsilon}_i(H_2)$, for all $i = 1, \ldots, n$.

We now state one interesting property of SQD matrices.

Proposition 2.4.7. *Suppose we are given a SQD matrix K as in definition 2.4.5. Assume that $\lambda_1, \ldots, \lambda_k$ are positive eigenvalues with corresponding eigenvectors $\begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$, for $U_1 \in \mathbb{R}^{n\times k}$ and $U_2 \in \mathbb{R}^{m\times k}$. Then there holds:*

$$U_1^T U_1 \succ U_2^T U_2. \tag{2.50}$$

In particular, one also has: $\|U_1\|_F > \|U_2\|_F$ and $\|U_1\|_2 > \|U_2\|_2$.

Proof: See [22, Property 7]. ⊠

We are now ready to state a corollary dealing with Routhian as a SQD matrix.

Corollary 2.4.8. *Let $\lambda \in \mathcal{I} \subseteq \mathbb{R}$ be such that $\mathbf{h} - \lambda I_{n\times n} \in \mathbb{R}^{n\times n}$ from equation (1.13) is positive definite, i.e. we have: $\lambda < \boldsymbol{\varepsilon}_{\min}(\mathbf{h})$, where $\boldsymbol{\varepsilon}_{\min}(\mathbf{h})$ denotes the smallest eigenvalue of $\mathbf{h}$. Then $\left(Q_1^{(\lambda)}\right)^T Q_1^{(\lambda)} \succ \left(Q_2^{(\lambda)}\right)^T Q_2^{(\lambda)}$ in the Loewner partial order $\succ$. In particular:*

$$\boldsymbol{\varepsilon}_i\left(Q_1^{(\lambda)}\left(Q_1^{(\lambda)}\right)^T\right) = \boldsymbol{\varepsilon}_i\left(\left(Q_1^{(\lambda)}\right)^T Q_1^{(\lambda)}\right) \geq \boldsymbol{\varepsilon}_i\left(\left(Q_2^{(\lambda)}\right)^T Q_2^{(\lambda)}\right) = \boldsymbol{\varepsilon}_i\left(Q_2^{(\lambda)}\left(Q_2^{(\lambda)}\right)^T\right), \quad i = 1, \ldots, n, \tag{2.51}$$

and $\left\|Q_1^{(\lambda)}\left(Q_1^{(\lambda)}\right)^T\right\|_F \geq \left\|Q_2^{(\lambda)}\left(Q_2^{(\lambda)}\right)^T\right\|_F$. If $\lambda > \boldsymbol{\varepsilon}_{\max}(\mathbf{h})$, all above inequalities are reversed.

Proof: Note that the assumption on λ implies that the Routhian $\mathbf{H}_\lambda$ is a symmetric quasi-definite (SQD) matrix, and then Proposition 2.4.7 yields the desired result. ⊠

Chapter 3

Numerical method for CHFB eigenvalue problem

Once we have established that the target function $f(\lambda)$ is well defined, we address the numerical aspects of its computation in finite precision arithmetic. In particular, we would like to find an efficient algorithm for spectral decomposition of a symmetric Routhian matrix $\mathbf{H}_\lambda \in \mathbb{R}^{2n\times 2n}$ which utilizes the internal substructure:

$$\mathbf{H}_\lambda = \begin{bmatrix} \mathbf{h} - \lambda I_{n\times n} & \mathbf{\Delta} \\ \mathbf{\Delta} & -\mathbf{h} + \lambda I_{n\times n} \end{bmatrix}, \tag{3.1}$$

for given symmetric matrices $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{n\times n}$ and $\lambda \in \mathbb{R}$. Roughly, out of $4n^2$ matrix elements of Routhian, we only need to know $\approx n^2$ to completely determine it. On the other hand, ignoring the internal substructure, and using only the fact that $\mathbf{H}_\lambda$ is symmetric, we would need roughly $\approx 2n^2$ elements. Also, if we knew only the positive part of the spectrum with the corresponding eigenvectors of $\mathbf{H}_\lambda$, we could easily reconstruct the full spectral decomposition of $\mathbf{H}_\lambda$ as easily seen in eq. (1.13). Therefore, this naive reasoning suggests that there should exist a method which utilizes the substructure (3.1) and is at least twice as fast than currently most advanced eigensolver for generic symmetric matrices when the internal substructure is ignored.

To author's knowledge, all available software packages dealing with practical implementation of the CHFB theory with time reversal symmetry, explicitly construct the full symmetric matrix $\mathbf{H}_\lambda$ in computer memory, simply followed by a call of one of the well established and highly efficient methods for spectral decomposition of generic symmetric matrix (usually from LAPACK [12] library). In this chapter, we propose a new method and show that when deployed on matrices coming from real applications, it is at least twice as fast than the described naive approach usually encountered in nuclear physics calculations.

3.1 Method description

The fact that knowing only the positive part of Routhian's spectrum, one can easily reconstruct its full spectral decomposition, motivates us to look at the squared Routhian $\mathbf{H}_\lambda^2$, or equivalently $\mathbf{H}_\lambda\mathbf{H}_\lambda^T$, since $\sigma\left(\mathbf{H}_\lambda\mathbf{H}_\lambda^T\right) = \sigma(\mathbf{H}_\lambda)^2$. Of course, problem may arise when explicitly squaring a matrix $\mathbf{H}_\lambda\mathbf{H}_\lambda^T$ in computer memory using finite precision arithmetic. In particular, eigenvalues of $\mathbf{H}_\lambda$ with small absolute value can be very poorly reproduced if one calculates the roots of small eigenvalues of a squared matrix $\mathbf{H}_\lambda\mathbf{H}_\lambda^T$.

For example, if we take the following matrix: $A = Q\,\mathrm{diag}\left[10^0, 10^{-1}, 10^{-2}, \ldots, 10^{-15}\right] Q^T$, for $Q \in \mathbb{R}^{16\times 16}$ random orthogonal matrix, and if we use MATLAB's function `eig` and compare outputs of two commands: `eig(A)` and `sqrt(eig(A*A))`, we will see that even though in theory we should have $\sigma(A) = \sqrt{\sigma(A^2)}$, eigenvalues less than 10^{-8} could not be reproduced. More precisely, if Routhian $\mathbf{H}_\lambda$ in eq. (1.13) has a small eigenvalue $e \in \mathrm{diag}\, E_{(+)}^{(\lambda)}$, such that $|e| \leq \sqrt{\varepsilon}\,\|\mathbf{H}_\lambda\|_2$, where ε is machine epsilon, and it is necessary to compute this eigenvalue as accurately as possible, squaring a matrix is not the right approach (see [13] for further details). Luckily enough, in Routhians coming from real applications, there seems to be a distinct gap between zero and the smallest eigenvalue $e \in \mathrm{diag}\, E_{(+)}^{(\lambda)}$ (see Figure 2.2 for illustration). Actually, nuclear structure physicists, when going beyond ground state calculations, often use the inverse of a matrix $E_{(+)}^{(\lambda_0)}$ in perturbation series (more precisely, terms $\left(\left(E_{(+)}^{(\lambda_0)}\right)_{ii} + \left(E_{(+)}^{(\lambda_0)}\right)_{jj}\right)^{-1}$, for $i, j = 1, \ldots, n$, often appear). Therefore, it is a common knowledge that such eigenvalues of Routhian, small in absolute value, are unlikely to appear in real applications. In future, authors of [18] will further investigate a true mathematical reason for that phenomenon which creates the mentioned gap in the spectrum. For now, we will only take for granted that we can carelessly explicitly calculate the squared Routhian $\mathbf{H}_\lambda\mathbf{H}_\lambda^T$ without worrying too much about losing precision.

Next, we introduce a concept of a quaternionic substructure of a matrix, which is the key observation for the method we propose. First, one well known but instructive example is worth recalling.

Example 3.1.1. (Matrix representation of complex numbers)
Complex number $a + b\mathrm{i} \in \mathbb{C}$ can also be represented by 2×2 matrix that has the following form:

$$\begin{bmatrix} a & -b \\ b & a \end{bmatrix} \in \mathbb{R}^{2\times 2}. \tag{3.2}$$

The sum and product of two such matrices is again of this form, and the sum and product of complex numbers correspond to the sum and product of such matrices, e.g. the product

being:

$$\begin{bmatrix} a & -b \\ b & a \end{bmatrix}\begin{bmatrix} c & -d \\ d & c \end{bmatrix} = \begin{bmatrix} ac - bd & -(ad + bc) \\ ad + bc & ac - bd \end{bmatrix}. \tag{3.3}$$

Moreover, the square of the absolute value of a complex number expressed as a matrix is equal to the determinant of that matrix:

$$|a + b\mathrm{i}|^2 = \begin{vmatrix} a & -b \\ b & a \end{vmatrix} = a^2 + b^2. \tag{3.4}$$

Therefore, orthogonal matrices correspond to complex numbers on unit circle in $\mathbb{C}$. The conjugate $a - b\mathrm{i}$ corresponds to the transpose of the matrix representative.

Motivated by previous example, one notices that complex matrices of form: $A + B\mathrm{i} \in \mathbb{C}^{n\times n}$, where $A \in \mathbb{R}^{n\times n}$ is symmetric, and $B \in \mathbb{R}^{n\times n}$ is antisymmetric, can be represented by symmetric $2n \times 2n$ supermatrices that has the following form:

$$\begin{bmatrix} A & -B \\ B & A \end{bmatrix} \in \mathbb{R}^{2n\times 2n}, \tag{3.5}$$

where again the sum and product of two such complex matrices in $\mathbb{C}^{n\times n}$ correspond to the sum and product of the corresponding supermatrices in $\mathbb{R}^{2n\times 2n}$. In applied mathematics literature [23], Hermitian matrices of type:

$$\begin{bmatrix} D & -E^* \\ E & D^* \end{bmatrix} \in \mathbb{C}^{2n\times 2n}, \tag{3.6}$$

where $D \in \mathbb{C}^{n\times n}$ is Hermitian $D^\dagger = D$, and $E \in \mathbb{C}^{n\times n}$ is antisymmetric $E^T = -E$, are refered to as Hermitian plus skew-Hamiltonian matrices. Some authors, quantum chemists in particular (e.g. [7, 24]), refer to this matrices as ***quaternionic*** *matrices*, because the matrix in eq. (3.6) can also be represented by an $n \times n$ matrix of quaternions. Even though we are currently interested in the situation where D and E are real matrices, in which case quaternions degenerate to ordinary complex numbers, we will still refer to matrices of form given in eq. (3.5) as quaternionic matrices.

In the following, we will use abbreviation: $\mathbf{h}_\lambda = \mathbf{h} - \lambda I_{n\times n}$. Let us calculate a square a of Routhian matrix:

$$\mathbf{H}_\lambda^2 = \begin{bmatrix} \mathbf{h}_\lambda^2 + \mathbf{\Delta}^2 & -(\mathbf{\Delta}\mathbf{h}_\lambda - \mathbf{h}_\lambda\mathbf{\Delta}) \\ \mathbf{\Delta}\mathbf{h}_\lambda - \mathbf{h}_\lambda\mathbf{\Delta} & \mathbf{h}_\lambda^2 + \mathbf{\Delta}^2 \end{bmatrix} \in \mathbb{R}^{2n\times 2n}. \tag{3.7}$$

First, notice that due to the fact that $\mathbf{h}_\lambda, \mathbf{\Delta} \in \mathbb{R}^{n\times n}$ are symmetric, square of Routhian matrix: $\mathbf{H}_\lambda^2$, has the quaternionic form given in eq. (3.5). Also, notice that complex Hermitian matrix:

$$(\mathbf{h}_\lambda + \mathbf{\Delta}\mathrm{i})(\mathbf{h}_\lambda + \mathbf{\Delta}\mathrm{i})^\dagger = \left(\mathbf{h}_\lambda^2 + \mathbf{\Delta}^2\right) + (\mathbf{\Delta}\mathbf{h}_\lambda - \mathbf{h}_\lambda\mathbf{\Delta})\,\mathrm{i} \in \mathbb{C}^{n\times n}, \tag{3.8}$$

has its corresponding quaternionic supermatrix given by $\mathbf{H}_\lambda^2$ in eq. (3.7). Since complex matrix $(\mathbf{h}_\lambda + \mathbf{\Delta}\mathfrak{i})(\mathbf{h}_\lambda + \mathbf{\Delta}\mathfrak{i})^\dagger$ is Hermitian and positive semidefinite, we can find its spectral decomposition :

$$(\mathbf{h}_\lambda + \mathbf{\Delta}\mathfrak{i})(\mathbf{h}_\lambda + \mathbf{\Delta}\mathfrak{i})^\dagger = Q^{(\lambda)} \operatorname{diag}\left(\boldsymbol{\varepsilon}_i^{(\lambda)}\right)_{i=1}^n \left(Q^{(\lambda)}\right)^\dagger, \tag{3.9}$$

for some unitary matrix $Q^{(\lambda)} \in \mathbb{C}^{n\times n}$, and nonnegative eigenvalues $\left(\boldsymbol{\varepsilon}_i^{(\lambda)}\right)_{i=1}^n$. It turns out that real and imaginary parts of matrix $Q^{(\lambda)}$ can be used to calculate the spectral decomposition of Routhian $\mathbf{H}_\lambda$ itself. On the other hand, computation of spectral decomposition of a complex $n \times n$ Hermitian matrix is at least two times faster than computation of spectral decomposition of a real $2n \times 2n$ matrix.

We can now state and prove the capital result of the thesis as follows.

Theorem 3.1.2. *Let $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{n\times n}$ be symmetric matrices, and let $Q \in \mathbb{C}^{n\times n}$ be a unitary matrix such that for nonnegative eigenvalues $(\boldsymbol{\varepsilon}_i)_{i=1}^n$ in non-decreasing order, there holds:*

$$Q^\dagger(\mathbf{h} + \mathbf{\Delta}\mathfrak{i})(\mathbf{h} + \mathbf{\Delta}\mathfrak{i})^\dagger Q = \operatorname{diag}(\boldsymbol{\varepsilon}_i)_{i=1}^n. \tag{3.10}$$

If $Q_1, Q_2 \in \mathbb{R}^{n\times n}$ are, respectively, the real and the imaginary part of Q, i.e. $Q = Q_1 + Q_2\mathfrak{i}$, then there holds:

$$\begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix}^T \underbrace{\begin{bmatrix} \mathbf{h} & \mathbf{\Delta} \\ \mathbf{\Delta} & -\mathbf{h} \end{bmatrix}}_{\mathbf{H}} \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix} = \begin{bmatrix} \boldsymbol{e} & \boldsymbol{d} \\ \boldsymbol{d} & -\boldsymbol{e} \end{bmatrix}, \tag{3.11}$$

where $\boldsymbol{e}, \boldsymbol{d} \in \mathbb{R}^{n\times n}$ are block diagonal symmetric matrices with square blocks along their diagonals, and matrix $\boldsymbol{Q} = \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix} \in \mathbb{R}^{2n\times 2n}$ is orthogonal. A j-th block in $\boldsymbol{e}$ (with its paired j-th block in $\boldsymbol{d}$) corresponds to an eigenvalue of (3.10), and its size is determined by the eigenvalue multiplicity. In addition, there holds:

$$\sigma(\mathbf{H}) = \sigma\left(\begin{bmatrix} \mathbf{h} & \mathbf{\Delta} \\ \mathbf{\Delta} & -\mathbf{h} \end{bmatrix}\right) = \left\{\left(\sqrt{\boldsymbol{\varepsilon}_i}\right)_{i=1}^n, \left(-\sqrt{\boldsymbol{\varepsilon}_i}\right)_{i=1}^n\right\}. \tag{3.12}$$

Proof: For the sake of completeness and for the reader's convenience, we first recall again an elementary fact from matrix algebra. Suppose that $M = A + B\mathfrak{i} \in \mathbb{C}^{n\times n}$ is Hermitian, with real $A = A^T$ and $B = -B^T$, and that it is diagonalized by a unitary $W \in \mathbb{C}^{n\times n}$ as: $W^\dagger M W = \Lambda = \operatorname{diag}(\lambda_i)_{i=1}^n$, where $W = U + V\mathfrak{i}$ with real U, V. Then there holds:

$$\begin{bmatrix} U & -V \\ V & U \end{bmatrix}^T \begin{bmatrix} U & -V \\ V & U \end{bmatrix} = \begin{bmatrix} I_{n\times n} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & I_{n\times n} \end{bmatrix} \text{ and } \begin{bmatrix} U & -V \\ V & U \end{bmatrix}^T \begin{bmatrix} A & -B \\ B & A \end{bmatrix} \begin{bmatrix} U & -V \\ V & U \end{bmatrix} = \begin{bmatrix} \Lambda & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & \Lambda \end{bmatrix}. \tag{3.13}$$

In our case, $M = (\mathbf{h} + \mathbf{\Delta}\mathrm{i})(\mathbf{h} + \mathbf{\Delta}\mathrm{i})^\dagger = \left(\mathbf{h}^2 + \mathbf{\Delta}^2\right) + (\mathbf{\Delta h} - \mathbf{h\Delta})\mathrm{i}$, and we immediately have:

$$\begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix}^T \underbrace{\begin{bmatrix} \mathbf{h}^2 + \mathbf{\Delta}^2 & \mathbf{h\Delta} - \mathbf{\Delta h} \\ \mathbf{\Delta h} - \mathbf{h\Delta} & \mathbf{h}^2 + \mathbf{\Delta}^2 \end{bmatrix}}_{=\mathbf{H}^2} \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix} = \begin{bmatrix} \mathrm{diag}(\boldsymbol{\varepsilon}_i)_{i=1}^n & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & \mathrm{diag}(\boldsymbol{\varepsilon}_i)_{i=1}^n \end{bmatrix} = \widehat{E}, \quad (3.14)$$

which means that $Q = \left[\begin{smallmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{smallmatrix}\right] \in \mathbb{R}^{2n\times 2n}$ diagonalizes $\mathbf{H}^2$. Hence, $Q^T\mathbf{H}^2Q = \widehat{E}$, and we conclude that $\left(Q^T\mathbf{H}Q\right)^2 = \widehat{E}$. This further implies that $\left(Q^T\mathbf{H}Q\right)\widehat{E} = \widehat{E}\left(Q^T\mathbf{H}Q\right)$. Additionally, one can easily check that the product $Q^T\mathbf{H}Q$ will have the structure given in eq. (3.11), i.e. there exist $\boldsymbol{e}, \boldsymbol{d} \in \mathbb{R}^{n\times n}$ such that eq. (3.11) holds.

Let us first consider the generic case: the nonegative eigenvalues $(\boldsymbol{\varepsilon}_i)_{i=1}^n$ are all simple. Then for all $i \neq j \in \{1, \ldots, n\}$, there holds:

$$\left(Q^T\mathbf{H}Q\right)_{i,j}\boldsymbol{\varepsilon}_j = \boldsymbol{\varepsilon}_i\left(Q^T\mathbf{H}Q\right)_{i,j} \Longrightarrow \left(Q^T\mathbf{H}Q\right)_{i,j} = 0. \quad (3.15)$$

Similarly, for all $i \neq j \in \{1, \ldots, n\}$, there also holds:

$$\left(Q^T\mathbf{H}Q\right)_{i,j+n} = \left(Q^T\mathbf{H}Q\right)_{i+n,j} = \left(Q^T\mathbf{H}Q\right)_{i+n,j+n} = 0. \quad (3.16)$$

Equations (3.15) and (3.16) show that matrices $\boldsymbol{e}$ and $\boldsymbol{d}$ from (3.11) are indeed diagonal matrices.

Now consider the general case, where the eigenvalues $(\boldsymbol{\varepsilon}_i)_{i=1}^n$ have arbitrary multiplicities. It is convenient to list them on the diagonal of $\mathrm{diag}\,(\boldsymbol{\varepsilon}_i)_{i=1}^n$ so that all copies of a multiple eigenvalue occupy consecutive positions along the diagonal. If p is the total number of distinct eigenvalues and if m_i is the multiplicity of $\boldsymbol{\varepsilon}_i$, $i = 1, \ldots, p$, then there holds: $\mathrm{diag}\,(\boldsymbol{\varepsilon}_i)_{i=1}^n = \boldsymbol{\varepsilon}_1 I_{m_1\times m_1} \oplus \boldsymbol{\varepsilon}_2 I_{m_2\times m_2} \oplus \cdots \oplus \boldsymbol{\varepsilon}_p I_{m_p\times m_p}$. Now, the multiplicities $(m_1, \ldots, m_p, m_1, \ldots, m_p)$ induce a $2p \times 2p$ block partition of $Q^T\mathbf{H}Q$, and the above argumentation now applies to the block submatrices, denoted by: $\left(Q^T\mathbf{H}Q\right)_{[i,j]}$. More precisely, analogously to (3.15), we have for $i \neq j \in \{1, \ldots, p\}$:

$$\left(Q^T\mathbf{H}Q\right)_{[i,j]}[\boldsymbol{\varepsilon}_j I_{m_j\times m_j}] = [\boldsymbol{\varepsilon}_i I_{m_i\times m_i}]\left(Q^T\mathbf{H}Q\right)_{[i,j]} \Longrightarrow \left(Q^T\mathbf{H}Q\right)_{[i,j]} = \mathbf{0}_{m_i\times m_j}. \quad (3.17)$$

Similar to eq. (3.16), for all $i \neq j \in \{1, \ldots, p\}$, there also holds:

$$\left(Q^T\mathbf{H}Q\right)_{[i,j+n]} = \left(Q^T\mathbf{H}Q\right)_{[i+n,j]} = \left(Q^T\mathbf{H}Q\right)_{[i+n,j+n]} = \mathbf{0}_{m_i\times m_j}. \quad (3.18)$$

Therefore, equations (3.17) and (3.18) show that matrices $\boldsymbol{e}$ and $\boldsymbol{d}$ from (3.11) are indeed block diagonal matrices: $\boldsymbol{e} = \bigoplus_{i=1}^p \boldsymbol{e}_i$ and $\boldsymbol{d} = \bigoplus_{i=1}^p \boldsymbol{d}_i$, for $\boldsymbol{e}_i, \boldsymbol{d}_i \in \mathbb{R}^{m_i\times m_i}$, $i = 1, \ldots, p$.

Hence, for e.g. a 10×10 matrix $\mathbf{H}$ (case where $n = 5$), in the cases of simple and multiple eigenvalues with $p = 3$, $m_1 = 1$, $m_2 = m_3 = 2$, the structure of $Q^T\mathbf{H}Q$ is, respectively:

$$Q^T\mathbf{H}Q = \left[\begin{array}{c|c} \ddots & \ddots \\ \hline \ddots & \ddots \end{array}\right], \tag{3.19}$$

$$Q^T\mathbf{H}Q = \left[\begin{array}{cc|cc} \ddots & & \ddots & \\ & \ddots & & \ddots \\ \hline \ddots & & \ddots & \\ & \ddots & & \ddots \end{array}\right] = \left[\begin{array}{ccc|ccc} \boldsymbol{e}_1 & & & \boldsymbol{d}_1 & & \\ & \boldsymbol{e}_2 & & & \boldsymbol{d}_2 & \\ & & \boldsymbol{e}_p & & & \boldsymbol{d}_p \\ \hline \boldsymbol{d}_1 & & & -\boldsymbol{e}_1 & & \\ & \boldsymbol{d}_2 & & & -\boldsymbol{e}_2 & \\ & & \boldsymbol{d}_p & & & -\boldsymbol{e}_p \end{array}\right]. \tag{3.20}$$

One can easily check that $\boldsymbol{e}, \boldsymbol{d} \in \mathbb{R}^{n\times n}$ are symmetric, rendering submatrices $\boldsymbol{e}_i, \boldsymbol{d}_i \in \mathbb{R}^{m_i\times m_i}$ also symmetric. Equation (3.14) gives $\sigma\left(\mathbf{H}^2\right) = \left\{(\boldsymbol{\varepsilon}_i)_{i=1}^n\right\}$, and therefore equation (3.12) follows from the fact that for every eigenvalue $\lambda \in \sigma(\mathbf{H})$, we have the corresponding negative eigenvalue: $-\lambda \in \sigma(\mathbf{H})$.

To complete the digonalization of $\mathbf{H}$, we first independently diagonalize the block matrices: $\begin{bmatrix} \boldsymbol{e}_i & \boldsymbol{d}_i \\ \boldsymbol{d}_i & -\boldsymbol{e}_i \end{bmatrix} \in \mathbb{R}^{2m_i\times 2m_i}$, with orthogonal matrices $\begin{bmatrix} C_i & -S_i \\ S_i & C_i \end{bmatrix} \in \mathbb{R}^{2m_i\times 2m_i}$, for $i = 1, \ldots, p$, as follows:

$$\begin{bmatrix} C_i & -S_i \\ S_i & C_i \end{bmatrix}^T \begin{bmatrix} \boldsymbol{e}_i & \boldsymbol{d}_i \\ \boldsymbol{d}_i & -\boldsymbol{e}_i \end{bmatrix} \begin{bmatrix} C_i & -S_i \\ S_i & C_i \end{bmatrix} = \begin{bmatrix} E_i^{(+)} & \mathbf{0}_{m_i\times m_i} \\ \mathbf{0}_{m_i\times m_i} & -E_i^{(+)} \end{bmatrix}, \tag{3.21}$$

where $E_i^{(+)} \in \mathbb{R}^{m_i\times m_i}$ are diagonal matrices with nonnegative diagonal. Then, if we introduce a column partition: $Q = \left[Q_1, \ldots, Q_{2p}\right]$, where $Q_i, Q_{p+i} \in \mathbb{R}^{2n\times m_i}$, for $i = 1, \ldots, n$, the Q is updated as: $\widetilde{Q} = Q\begin{bmatrix} C & -S \\ S & C \end{bmatrix}$, where $C = \bigoplus_{i=1}^p C_i$ and $S = \bigoplus_{i=1}^p S_i \in \mathbb{R}^{n\times n}$, by p concurrent structure preserving multiplications:

$$\left[\widetilde{Q}_i, \widetilde{Q}_{p+i}\right] = \left[Q_i, Q_{p+i}\right] \begin{bmatrix} C_i & -S_i \\ S_i & C_i \end{bmatrix}, \quad i = 1, \ldots, p. \tag{3.22}$$

As a result, we finally obtain the spectral decomposition of matrix $\mathbf{H}$:

$$\widetilde{Q}^T\mathbf{H}\widetilde{Q} = \begin{bmatrix} E^{(+)} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -E^{(+)} \end{bmatrix}, \quad E^{(+)} = \bigoplus_{i=1}^p E_i^{(+)}, \quad \widetilde{Q} = \begin{bmatrix} \widetilde{Q}_1 & -\widetilde{Q}_2 \\ \widetilde{Q}_2 & \widetilde{Q}_1 \end{bmatrix}. \tag{3.23}$$

⊠

Remark 3.1.3. *Notice that updates* $\left[\widetilde{Q}_i, \widetilde{Q}_{p+i}\right]$ *in eq. (3.22):*

$$\widetilde{Q} = \begin{bmatrix} \widetilde{Q_1} & -\widetilde{Q_2} \\ \widetilde{Q_2} & \widetilde{Q_1} \end{bmatrix} = Q \begin{bmatrix} C & -S \\ S & C \end{bmatrix} = \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix} \begin{bmatrix} C & -S \\ S & C \end{bmatrix}, \tag{3.24}$$

can be efficiently calculated in complex arithmetic:

$$\widetilde{Q}_1 = \mathrm{Re}\left[(Q_1 + Q_2\mathrm{i})(C + S\,\mathrm{i})\right] \quad \textit{and} \quad \widetilde{Q}_2 = \mathrm{Im}\left[(Q_1 + Q_2\mathrm{i})(C + S\,\mathrm{i})\right], \tag{3.25}$$

where $C + S\,\mathrm{i} = \bigoplus_{i=1}^{p}(C_i + S_i\mathrm{i})$ *is block diagonal complex matrix.*

Remark 3.1.4. *One can easily derive the following expressions for matrices* $\boldsymbol{e}, \boldsymbol{d} \in \mathbb{R}^{n\times n}$*:*

$$\boldsymbol{e} = Q_1^T \mathbf{h} Q_1 - Q_2^T \mathbf{h} Q_2 + Q_1^T \boldsymbol{\Delta} Q_2 + Q_2^T \boldsymbol{\Delta} Q_1, \tag{3.26}$$

$$\boldsymbol{d} = Q_1^T \boldsymbol{\Delta} Q_1 - Q_2^T \boldsymbol{\Delta} Q_2 - Q_1^T \mathbf{h} Q_2 - Q_2^T \mathbf{h} Q_1. \tag{3.27}$$

According to the Theorem 3.1.2, we know that $\boldsymbol{e} = \bigoplus_{i=1}^{p} \boldsymbol{e}_i$ *and* $\boldsymbol{d} = \bigoplus_{i=1}^{p} \boldsymbol{d}_i$ *are block diagonal. These blocks can be calculated as follows. First calculate and store products:* $\mathbf{h}Q_1$*,* $\mathbf{h}Q_2$*,* $\boldsymbol{\Delta}Q_1$ *and* $\boldsymbol{\Delta}Q_2$*, using BLAS [25] routine* `dsymm` *for example. Introduce a partition of any matrix* $A \in \mathbb{R}^{n\times n}$ *denoted as:* $A = \left[A^{(1)}, \ldots, A^{(p)}\right]$*, for* $A^{(i)} \in \mathbb{R}^{n\times m_i}$*. Then blocks* $\boldsymbol{e}_i, \boldsymbol{d}_i \in \mathbb{R}^{m_i\times m_i}$ *can be efficiently calculated from:*

$$\boldsymbol{e}_i = \left(Q_1^{(i)}\right)^T [\mathbf{h}Q_1]^{(i)} - \left(Q_2^{(i)}\right)^T [\mathbf{h}Q_2]^{(i)} + \left(\left(Q_1^{(i)}\right)^T [\boldsymbol{\Delta}Q_2]^{(i)} + \left([\boldsymbol{\Delta}Q_2]^{(i)}\right)^T Q_1^{(i)}\right), \tag{3.28}$$

$$\boldsymbol{d}_i = \left(Q_1^{(i)}\right)^T [\boldsymbol{\Delta}Q_1]^{(i)} - \left(Q_2^{(i)}\right)^T [\boldsymbol{\Delta}Q_2]^{(i)} - \left(\left(Q_1^{(i)}\right)^T [\mathbf{h}Q_2]^{(i)} + \left([\mathbf{h}Q_2]^{(i)}\right)^T Q_1^{(i)}\right), \tag{3.29}$$

for $i = 1, \ldots, p$*, where one can use convenient BLAS subroutine* `dsyr2k` *for calculation of last terms in previous equations.*

Remark 3.1.5. *If* $m_i = 1$*, for some* $i = 1, \ldots, p$*, then the corresponding diagonal blocks* $\boldsymbol{e}_i, \boldsymbol{d}_i$ *generate a* 2×2 *matrix* $\begin{bmatrix} \boldsymbol{e}_i & \boldsymbol{d}_i \\ \boldsymbol{d}_i & -\boldsymbol{e}_i \end{bmatrix}$ *which can be explicitly diagonalized using a Jacobi rotation [19]. In that case* $\boldsymbol{e}_i, \boldsymbol{d}_i, C_i, S_i \in \mathbb{R}^{1\times 1}$ *are degenerated to real numbers.*

On the other hand, if $m_i > 1$*, for some* $i = 1, \ldots, p$*, the computation is technically more involved, and (3.21) is obtained numerically. If we collect all these local transformations, then the global transformation* $\mathcal{T} \in \mathbb{R}^{2n\times 2n}$ *reads, e.g. in the example (3.20):*

$$\mathcal{T} = \left[\begin{array}{ccc|ccc} C_1 & & & -S_1 & & \\ & C_2 & & & -S_2 & \\ & & C_p & & & -S_p \\ \hline S_1 & & & C_1 & & \\ & S_2 & & & C_2 & \\ & & S_p & & & C_p \end{array}\right], \quad \mathcal{T}^T\left(Q^T \mathbf{H} Q\right)\mathcal{T} = \begin{bmatrix} E_1^{(+)} & & & & & \\ & E_2^{(+)} & & & & \\ & & E_p^{(+)} & & & \\ & & & -E_1^{(+)} & & \\ & & & & -E_2^{(+)} & \\ & & & & & -E_p^{(+)} \end{bmatrix}. \tag{3.30}$$

Remark 3.1.6. *When calculating the spectral decomposition of a Hermitian matrix in eq. (3.10), one can use any of the well established LAPACK subroutines such as:* `zheevd`*,* `zheevx` *or* `zheevr`*.*

Now we are ready to propose an algorithm for solving the equation $f(\lambda_0) = f_0$ described in the section 1.3. Algorithm starts with an initial guess for $\lambda_0 \in \mathbb{R}$, namely $\lambda^{(0)} \in \mathbb{R}$, and generates a sequence of successive approximations: $\lambda^{(i)} \in \mathbb{R}$, $i \geq 1$, using any root finding method. Since we do not have an easy access to the derivative $f'(\lambda)$, one usually uses a combination of secant and bisection method which proved to perform well in real applications [8, 9]. Apart from supplying the initial value $\lambda^{(0)}$, one also has to supply the stopping criterion tolerance $\epsilon_{tol} > 0$ for stopping criterion of the root finder: $\left| f\left(\lambda^{(i)}\right) - f_0 \right| < \epsilon_{tol}$, and also one has to supply the tolerance $\epsilon_{deg} > 0$, under which eigenvalues $(\boldsymbol{\varepsilon}_i)_{i=1}^n$ from eq. (3.10) are considered degenerated: $\boldsymbol{\varepsilon}_i$ and $\boldsymbol{\varepsilon}_j$ are degenerated if: $\left| \boldsymbol{\varepsilon}_i - \boldsymbol{\varepsilon}_j \right| < \epsilon_{deg}$.

Algorithm 1: CHFB eigenvalue problem

Input : $\mathbf{h}, \boldsymbol{\Delta} \in \mathbb{R}^{n\times n}$ symmetric, $f_0 \in \mathbb{R}$, $\lambda^{(0)} \in \mathbb{R}$, $\epsilon_{tol} > 0$, $\epsilon_{deg} > 0$.
Output: $\lambda^{(i)} \in \mathbb{R}$ such that $\left| f\left(\lambda^{(i)}\right) - f_0 \right| < \epsilon_{tol}$.

- Calculate and store matrix: $(\mathbf{h} + \boldsymbol{\Delta}\mathrm{i})\,(\mathbf{h} + \boldsymbol{\Delta}\mathrm{i})^\dagger = \left(\mathbf{h}^2 + \boldsymbol{\Delta}^2\right) + (\boldsymbol{\Delta}\mathbf{h} - \mathbf{h}\boldsymbol{\Delta})\,\mathrm{i}$;
- Set $i = 0$;

while $\left| f\left(\lambda^{(i)}\right) - f_0 \right| \geq \epsilon_{tol}$ **do**

- Calculate: $(\mathbf{h}_{\lambda^{(i)}} + \boldsymbol{\Delta}\mathrm{i})\,(\mathbf{h}_{\lambda^{(i)}} + \boldsymbol{\Delta}\mathrm{i})^\dagger = \left(\mathbf{h}^2 + \boldsymbol{\Delta}^2 - 2\lambda^{(i)}\mathbf{h} + \left(\lambda^{(i)}\right)^2 I_{n\times n}\right) + (\boldsymbol{\Delta}\mathbf{h} - \mathbf{h}\boldsymbol{\Delta})\,\mathrm{i}$;
- Find the spectral decomposition of $(\mathbf{h}_{\lambda^{(i)}} + \boldsymbol{\Delta}\mathrm{i})\,(\mathbf{h}_{\lambda^{(i)}} + \boldsymbol{\Delta}\mathrm{i})^\dagger$ (see Remark 3.1.6), i.e. find $Q = Q_1 + Q_2\mathrm{i} \in \mathbb{C}^{n\times n}$ unitary and nonnegative $(\boldsymbol{\varepsilon}_i)_{i=1}^n$ as in eq. (3.10);
- Using eigenvalues $(\boldsymbol{\varepsilon}_i)_{i=1}^n$ and ϵ_{deg}, generate block partition of degenerated eigenvalues: $\operatorname{diag}(\boldsymbol{\varepsilon}_i)_{i=1}^n = \boldsymbol{\varepsilon}_1 I_{m_1\times m_1} \oplus \boldsymbol{\varepsilon}_2 I_{m_2\times m_2} \oplus \cdots \oplus \boldsymbol{\varepsilon}_p I_{m_p\times m_p}$;
- Find block diagonal matrices $\boldsymbol{e} = \bigoplus_{i=1}^p \boldsymbol{e}_i$ and $\boldsymbol{d} = \bigoplus_{i=1}^p \boldsymbol{d}_i$ (see Remark 3.1.4);
- Find $C = \bigoplus_{i=1}^p C_i$ and $S = \bigoplus_{i=1}^p S_i$, as in eq. (3.21) (see Remark 3.1.5).
- Update matrices Q_1, Q_2 as in eq. (3.22) and obtain $\widetilde{Q}_1, \widetilde{Q}_2$ (See Remark 3.1.3);
- Calculate $f\left(\lambda^{(i)}\right) = \left\|\widetilde{Q}_2\right\|_F^2$;
- Using root finding method, generate new approximation $\lambda^{(i+1)}$;
- Set $i = i + 1$;

end

First, we immediately see that since the matrix $(\mathbf{h}_{\lambda^{(i)}} + \mathbf{\Delta i})(\mathbf{h}_{\lambda^{(i)}} + \mathbf{\Delta i})^{\dagger}$ is explicitly calculated in finite precision arithmetic, there should not be eigenvalues of Routhian $\mathbf{H}_{\lambda^{(i)}}$ which are small in absolute value. As we already discussed, it appears that such scenario never happens in practice.

Second important observation is that if there are very large degenerated blocks in eigenvalues: $\operatorname{diag}(\boldsymbol{\varepsilon}_i)_{i=1}^{n} = \boldsymbol{\varepsilon}_1 I_{m_1 \times m_1} \oplus \boldsymbol{\varepsilon}_2 I_{m_2 \times m_2} \oplus \cdots \oplus \boldsymbol{\varepsilon}_p I_{m_p \times m_p}$, blocks in block diagonal matrices $\boldsymbol{e} = \bigoplus_{i=1}^{p} \boldsymbol{e}_i$ and $\boldsymbol{d} = \bigoplus_{i=1}^{p} \boldsymbol{d}_i$ will also be rather large, rendering diagonalization in eq. (3.21) expensive i.e. rendering the calculation of matrices : $C = \bigoplus_{i=1}^{p} C_i$ and $S = \bigoplus_{i=1}^{p} S_i$, expensive. Luckily, in real applications [8, 9], one can show that large degenerated blocks never appear. This is owed to the fact that the QHO basis is used as a basis for variational approximation (see section 1.1). More technically, the QHO basis is characterized by a number $N_{sh} \in \mathbb{N}$, also known as the *number of oscillator shells*, which determines the size of truncated basis n. One can show that if N_{sh} shells are used, the size n of a QHO basis is given by: $n = \frac{(N_{sh}+1)(N_{sh}+2)(N_{sh}+3)}{6}$, while on the other hand for the maximum size of degenerate block there holds: $\max_{i=1,\ldots,p} m_i \leq N_{sh}$. Maximum $\max_{i=1,\ldots,p} m_i = N_{sh}$ can be reached for example if one studies a nucleus which belongs to a set of so called *magic nuclei*, which are known to be perfectly spherical in shape and thus eigenvalues are strongly degenerated. Even then, if for example we take $N_{sh} = 24$ shells, one obtains $n = 2925$, while degenerated blocks have size less than $\max_{i=1,\ldots,p} m_i = 24$, which is below 1% compared to n.

Third, in practice, root finding algorithm terminates rather quickly. Root finder typically requires 3 to 10 evaluations of the target function $f(\lambda)$ to reach λ_0 such that $f(\lambda_0) = f_0$. On average, there seems to be ≈ 5 iterations, also called *the lambda iterations* [8, 9].

Therefore, even though the proposed Algorithm 1 has its flaws, in real applications it can perform well. In the following section we show the results of numerical tests on matrices coming from real application, but before we state a remark showing a connection to the so called *Takagi decomposition*.

Remark 3.1.7. *Note that in eq. (3.10), the matrix Q is the matrix of the left singular vectors of $\mathbf{h} + \mathbf{\Delta i}$, while the eigenvalues $(\boldsymbol{\varepsilon}_i)_{i=1}^{n}$ are the squared singular values $(\boldsymbol{\sigma}_i)_{i=1}^{n}$, i.e. $(\boldsymbol{\varepsilon}_i)_{i=1}^{n} = \left(\boldsymbol{\sigma}_i^2\right)_{i=1}^{n}$. Now, the key observation is that here we have the SVD of the complex symmetric matrix: $\mathbf{h} + \mathbf{\Delta i}$. The complex symmetry implies certain symmetry in the SVD, which is then known as the Takagi decomposition. Hence, in Theorem 3.1.2, we can define Q as the complex unitary matrix such that: $\mathbf{h} + \mathbf{\Delta i} = Q \operatorname{diag}(\boldsymbol{\sigma}_i)_{i=1}^{n} Q^T$ is the Takagi decomposition. Further, since $\left(Q^T\right)^{-1} = Q^*$, we have $(\mathbf{h} + \mathbf{\Delta i})Q^* = Q \operatorname{diag}(\boldsymbol{\sigma}_i)_{i=1}^{n}$, i.e. for a j-th column q_j of Q we have $(\mathbf{h} + \mathbf{\Delta i})q_j^* = \boldsymbol{\sigma}_j q_j$. This means that we can characterize Q and $\operatorname{diag}(\boldsymbol{\sigma}_i)_{i=1}^{n}$ as the solution of the con-eigenvalue problem for $\mathbf{h} + \mathbf{\Delta i}$.*

3.2 Numerical experiments

For numerical tests in this thesis, we used Intel® NUC Kit NUC8i7HVK (32GB of RAM) machine with MATLAB R2018a installed on it. Since the machine has 4 physical cores, we used 4 threads in MATLAB simulations (command `maxNumCompThreads('automatic')` enables it) described in this section. A very naive and direct implementation of Algorithm 1 is used, with only difference that, for the purpose of simulation, we did not actually had the stopping condition as in Algorithm 1, rather we simply predefined a number of lambda iterations N_λ and stopped when the iteration index i reached N_λ. Also, the root finding step is omitted and we simply generate a random $\lambda^{(i)}$ from standard normal distribution in each lambda iteration to simulate the root finding step.

We conducted four numerical experiments. First two tests are entirely synthetic. First test uses a random symmetric matrix $\mathbf{H}$ with given non-degenerated spectrum, while the in the other test, the Hamiltonian matrix $\mathbf{H}$ is determined by prescribing its eigenvalues which are highly degenerated and taking $\mathbf{\Delta} = \mathbf{0}_{n\times n}$. Third and fourth tests use Hamiltonian matrix $\mathbf{H}$ from real application. More precisely, third test uses $\mathbf{H}$ for which the spectrum is non-degenerated - very heavy deformed nucleus ^{240}Pu, while fourth test uses the most degenerated case possible - spherical doubly magic nucleus ^{16}O. All four conducted tests are available at the following *GitHub* repository:

`https://github.com/abjelcic/Method-for-solving-CHFB-eigenvalue-problem`.

Corresponding MATLAB code can be found in files `Test1.m`, `Test2.m`, `Test3.m` and `Test4.m`. In all conducted tests, $N_\lambda = 5$ lambda iterations are simulated using $\epsilon_{deg} = 10^{-6}$.

Test 1 (Non-degenerated case)

In this test, we generate a random Hamiltonian matrix $\mathbf{H} \in \mathbb{R}^{2n\times 2n}$ with its positive spectrum being: $\sigma(\mathbf{H}) \cap \langle 0, +\infty\rangle = \left\{1 + \frac{10i}{n} : i = 1, \ldots, n\right\} := \Lambda_n$. To generate $\mathbf{H}$, we first generate two random orthogonal matrices $U, V \in \mathbb{R}^{n\times n}$, followed by a generation of random diagonal matrices $C, S \in \mathbb{R}^{n\times n}$ such that $C^2 + S^2 = I_{n\times n}$. Then we take $Q_1 = UCV^T$ and $Q_2 = USV^T$, and finally define $\mathbf{H}$ as:

$$\mathbf{H} := \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix}^T \begin{bmatrix} \Lambda_n & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -\Lambda_n \end{bmatrix} \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix}. \tag{3.31}$$

The size n of the problem is taken $n = 3000$ which approximately corresponds to the size of matrices $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{n\times n}$, which appear when $N_{sh} = 24$ shells are being used in the triaxial version of the code [8]. When compared to the naive approach, which explicitly constructs full Routhian $\mathbf{H}_{\lambda^{(i)}}$ in each one of the $N_\lambda = 5$ lambda iterations, Algorithm 1

shows ≈ 2.5 times faster execution. More precisely, naive approach took ≈ 78.0 seconds, while approach using Algorithm 1 took ≈ 30.6 seconds to execute. One can easily convince himself by executing the `Test1.m` script.

Test 2 (Highly-degenerated case)

In this test, $n = 3000$ is also taken, and $\mathbf{H} \in \mathbb{R}^{2n\times 2n}$ is generated as follows. First, $\mathbf{\Delta} = \mathbf{0}_{n\times n}$ is taken, while $\mathbf{h} \in \mathbb{R}^{n\times n}$ is taken as a random symmetric matrix $\mathbf{h} = q\Lambda_n q^T$, for $q \in \mathbb{R}^{n\times n}$ random orthogonal matrix, and $\Lambda_n = -2I_{1000\times 1000} \oplus -1I_{1000\times 1000} \oplus 3I_{1000\times 1000}$, i.e. the spectrum $\sigma(\mathbf{h}) = \{-2, -1, 3\}$ is selected such that each eigenvalue has geometric multiplicity equal to 1000. Then, the Hamiltonian matrix $\mathbf{H} \in \mathbb{R}^{2n\times 2n}$, which is taken as:

$$\mathbf{H} := \begin{bmatrix} \mathbf{h} & \mathbf{\Delta} \\ \mathbf{\Delta} & -\mathbf{h} \end{bmatrix} = \begin{bmatrix} \mathbf{h} & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & -\mathbf{h} \end{bmatrix}, \tag{3.32}$$

ensures that each Routhian $\mathbf{H}_\lambda$ for any $\lambda \in \mathbb{R}$, has highly-degenerated spectrum:

$$\sigma\left(\mathbf{H}_\lambda\right) = \{\pm(-2-\lambda), \pm(-1-\lambda), \pm(3-\lambda)\}. \tag{3.33}$$

To be fully precise, $\mathbf{\Delta} \in \mathbb{R}^{n\times n}$ is not taken exactly as zero matrix, but such that $\mathbf{\Delta}_{i,j} = 10^{-12}$, with intention of preventing the eigensolver's automatic deduction that matrix which is diagonalized: $(\mathbf{h} + \mathbf{\Delta}\mathrm{i})(\mathbf{h} + \mathbf{\Delta}\mathrm{i})^\dagger$, ends up having real entries. With such large degenerated blocks, Algorithm 1 outperforms the naive approach only by a factor of ≈ 1.7, or to be precise, naive approach took ≈ 72.6 seconds, while the approach using Algorithm 1 took ≈ 41.4 seconds to execute. Therefore, as expected, the proposed method does not perform very well when one encounters large degenerated blocks in the spectrum of $\mathbf{H}_\lambda$, but luckily, this scenario can never happen in real applications, as we will see in the next two test cases.

Test 3 (Non-degenerated case - deformed ^{240}Pu nucleus)

In this test case, we take $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{n\times n}$ for $n = 2024$, which in physics terminology corresponds to the matrices obtained from publicly available DIRHBT program package [16] of the very heavy nucleus ^{240}Pu in deformed configuration with Hill-Wheeler deformation parameters: $(\beta, \gamma) = (0.6, 6^o)$, where $N_{sh} = 20$ QHO shells are used and only simplex (+) block is taken for neutrons. The proposed method in Algorithm 1 outperforms the naive approach currently used in e.g. [8, 9] by a factor of ≈ 2.5, with execution time of ≈ 9.45 seconds, while the naive approach took ≈ 23.8 seconds.

Test 4 (Highly-degenerated case - spherical ^{16}O nucleus)

Matrices $\mathbf{h}, \mathbf{\Delta} \in \mathbb{R}^{n\times n}$ in this test case are generated in the same way as in Test 3, with only exception that now non-deformed spherical nucleus ^{16}O is taken. As discussed earlier,

degenerated blocks do appear in this case, but the maximum size of degenerated block is less than $\approx 1\%$ compared to n, and therefore the proposed method is expected to perform well in this case too. Still, for spherical nucleus, the proposed method in Algorithm 1 outperforms the naive approach by a factor of ≈ 2.5, with execution time of ≈ 9.55 seconds, while the naive approach took ≈ 24.1 seconds.

Conclusion

Based on the conducted numerical experiments of directly implemented Algorithm 1 using MATLAB, the proposed method is worth of a more careful implementation using lower-level language such as FORTRAN77. The proposed method has already been incorporated in the DIRHB software package [8], implemented using LAPACK coupled to OpenBLAS [26] library - an open-source efficient implementation of BLAS, fine-tuned for many modern architectures, comparable to Intel MKL. The DIRHB code has been significantly improved and the improved version is available at the following *GitHub* repository:

`https://github.com/abjelcic/DIRHBspeedup`.

Many other calculations are improved in the original DIRHB code, making the improved version much faster, while still reproducing the relevant quantum observables with agreement of 7-8 most significant digits compared to the original code.

Chapter 4

Numerical method for quaternionic matrices

As shown in the previous chapter, generic matrix with quaternionic substructure:

$$\begin{bmatrix} D & -E^* \\ E & D^* \end{bmatrix} \in \mathbb{C}^{2n\times 2n}, \tag{4.1}$$

for $D \in \mathbb{C}^{n\times n}$ Hermitian $D^\dagger = D$, and $E \in \mathbb{C}^{n\times n}$ antisymmetric $E^T = -E$, when degenerated to having real entries: $D, E \in \mathbb{R}^{n\times n}$, has the structure:

$$\begin{bmatrix} A & -B \\ B & A \end{bmatrix} \in \mathbb{R}^{2n\times 2n}, \tag{4.2}$$

for $A \in \mathbb{R}^{n\times n}$ symmetric and $B \in \mathbb{R}^{n\times n}$ antisymmetric. The proposed method in previous chapter is based on a simple trick: the supermatrix in (4.2) can be identified with Hermitian matrix $A + B\mathrm{i}$. If we try and follow the same logic for generic quaternionic matrix, we would end up having the identification of (4.1), with a $n \times n$ matrix having quaternion as entries. Since quaternionic algebra is not supported by modern hardware, we seek an algorithm which could diagonalize generic quaternionic matrix while preserving and utilizing the substructure (4.1). Such an algorithm exist and is known as the Paige-Van Loan algorithm which was developed in landmark papers [13, 27] in the context of finding the Schur decomposition of Hamiltonian matrices coming from CARE equation (see eq. (1.16)). In this thesis, as a proof of concept, we only focus on real quaternionic case in eq. (4.2) and briefly present an efficient *cache-aware* implementation. In future development, authors of [18] plan to upgrade the existing implementation for generic quaternionic matrices (4.1).

Matrices of type (4.1) are often encountered in relativistic quantum chemistry [7]. More precisely, every Hermitian operator that is symmetric under time reversal symmetry, when represented in a matrix form using a Kramers restricted basis, has the shape as in eq. (4.1).

4.1 Paige-Van Loan algorithm

In this section we follow a brief description of Paige-Van Loan algorithm taken from [24]. For a more detailed discussion, see the original papers [13, 27].

The Householder transformation is often used in tridiagonalization of a symmetric matrix. It transforms a symmetric matrix $A \in \mathbb{R}^{n\times n}$ as:

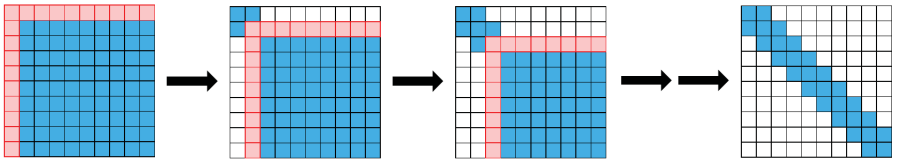
$$A_1 \leftarrow H_1 A H_1^T, \quad H_1 = 1 - \tau_1 v_1 v_1^T, \tag{4.3}$$

such that the first column and row of $A_1 \in \mathbb{R}^{n\times n}$ is zero except for the first two elements. The transformation matrix can be computed using the first column of the input matrix $A \in \mathbb{R}^{n\times n}$ as:

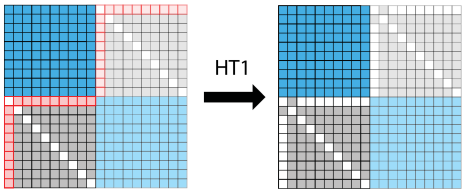
$$v_1 = \left[0, 1, \frac{A_{3,1}}{\alpha}, \frac{A_{4,1}}{\alpha}, \ldots, \frac{A_{n,1}}{\alpha}\right]^T \in \mathbb{R}^n, \tag{4.4}$$

$$\tau_1 = \alpha/\gamma, \quad \alpha = A_{2,1} + \gamma, \quad \gamma^2 = \sum_{i=2}^{n} \left|A_{i,1}\right|^2 . \tag{4.5}$$

The transformation matrix $H_1 \in \mathbb{R}^{n\times n}$ satisfies: $H_1^T H_1 = H_1^2 = I_{n\times n}$. By performing this procedure recursively, one obtains a tridiagonal matrix:



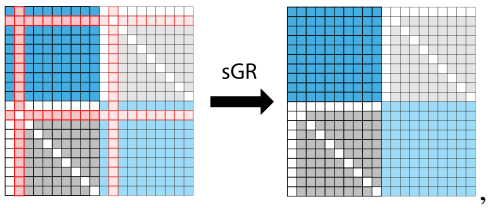
When a matrix is antisymmetric $A^T = -A$, a similar procedure can be used, i.e. we note that the transformed matrix has the same symmetry as the original matrix. The Paige-Van Loan algorithm applies similar transformations to quaternionic matrices (4.2). First, a Householder transformation $H_1 \in \mathbb{R}^{n\times n}$ is applied to the off-diagonal blocks as:



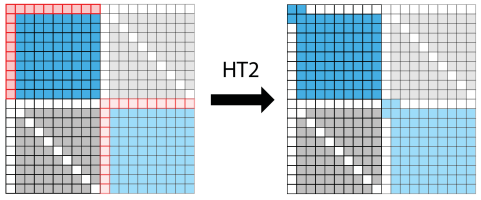
Since the symmetry is preserved, the right half of the matrix does not have to be stored and transformed. The transformation can be written as:

$$\begin{bmatrix} A & -B \\ B & A \end{bmatrix} \leftarrow \begin{bmatrix} H_1^T & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & H_1^T \end{bmatrix} \begin{bmatrix} A & -B \\ B & A \end{bmatrix} \begin{bmatrix} H_1 & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & H_1 \end{bmatrix}. \tag{4.6}$$

We then use a Givens rotation $G \in \mathbb{R}^{2n\times 2n}$ to clear out the remaining elements in the first column and row in submatrix $B \in \mathbb{R}^{n\times n}$:



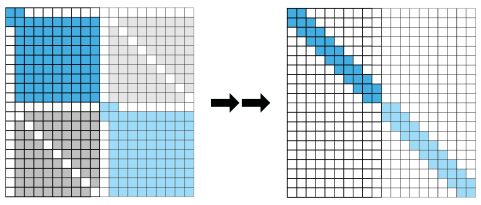
where the Givens rotation can be selected to have quaternionic structure: $G = \begin{bmatrix} C & -S \\ S & C \end{bmatrix}$, for $C, S \in \mathbb{R}^{n\times n}$ diagonal such that $C^2 + S^2 = I_{n\times n}$, with intention of preserving the quaternionic structure we have so far. Finally, we perform another Householder transformation $H_2 \in \mathbb{R}^{n\times n}$ on the submatrix $A \in \mathbb{R}^{n\times n}$, yielding:



The transformation reads:

$$\begin{bmatrix} A & -B \\ B & A \end{bmatrix} \leftarrow \begin{bmatrix} H_2^T & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & H_2^T \end{bmatrix} \begin{bmatrix} A & -B \\ B & A \end{bmatrix} \begin{bmatrix} H_2 & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & H_2 \end{bmatrix}. \tag{4.7}$$

It can be show [13] that repeating this procedure yields a block-diagonal matrix, whose block diagonal blocks are symmetric and tridiagonal:



The tridiagonal symmetric matrix can be efficiently diagonalized using LAPACK. In essence, Paige-Van Loan algorithm takes advantage of the quaternionic structure and clears out the off-diagonal blocks via successive applications of the Householder reflectors and Givens rotations. It is observed [13] that the operations count of this algorithm is roughly two times less compared to the operations count for diagonalization of $2n \times 2n$ symmetric matrix.

4.2 Cache-aware implementation

Even though the described Paige-Van Loan algorithm has to do less operations when diagonalizing a quaternionic matrix than naive approach, if implemented directly it is no match for current *state-of-the-art* eigensolvers for generic symmetric matrix such as the function `eig` from MATLAB or subroutines `dsyevd`, `dsyevr` and `dsyevx` from LAPACK. The reason for that is the memory hierarchy in modern computer architecture which strongly benefits when an algorithm is implemented *cache-friendly* fashion.

A cache-aware algorithm is designed to minimize the movement of memory pages in and out of the processor's on-chip memory cache. The idea is to avoid what's called "cache misses," which cause the processor to stall while it loads data from RAM into the processor cache. A cache-aware algorithm that is less than optimum on paper can outperform a traditional algorithm that is in theory "faster," because the cache-aware algorithm uses memory more efficiently. A cache-aware algorithm is explicitly coded to take advantage of the processor's cache behavior. Intimate details about the processor's memory page size and "cache lines" are coded into the algorithm. As such, a cache-aware algorithm will be highly processor specific. However, in numerical linear algebra, one usually uses single parameter n_b called the block size which is machine specific and is usually chosen as $n_b = 32$ on many modern architectures.

To give an idea how blocked algorithms work, suppose one wants to calculate an orthogonal transformation $Q \in \mathbb{R}^{n\times n}$ obtained as an accumulation of Householder reflectors: $Q = H_1 H_2 \cdots H_n$ used for reduction of symmetric matrix to tridiagonal form. One can naively start with $Q = I_{n\times n}$ and iterate through $i = n, n-1, \ldots, 2, 1$, updating $Q \leftarrow H_i Q$. However, since matrices H_i have simple rank-1 representation (see eq. (4.4)), such simple accumulation will use only Level 2 BLAS subroutines, while one can make use of cache-friendly Level 3 BLAS subroutines as follows. One can easily see that the product of n_b Householder reflectors $H_1 H_2 \cdots H_{n_b}$ can be represented as:

$$H_1 H_2 \cdots H_{n_b} = I_{n\times n} - WTW^T, \tag{4.8}$$

where $W \in \mathbb{R}^{n\times n_b}$ and $T \in \mathbb{R}^{n_b \times n_b}$ is upper triangular. Thus, if the product of n Householder reflectors $Q = H_1 H_2 \cdots H_n$ is divided into $\approx n/n_b$ blocks, with each block consisting of n_b products as in eq. (4.8), one can utilize Level 3 BLAS subroutines and have superior performance compared to the naive sequential accumulation.

Generalization of previous idea on CARE Hamiltonian matrices was done by D. Kressner, and is known as Kressner's compact WY-like representation. The reader is referred to [28] for a detailed description of the blocked method which is rather complicated and thus

not included here. Adaptation of Kressner's compact WY-like representation on quaternionic matrices was done by a relativistic quantum chemist, T. Shiozaki in [24]. Although Shiozaki's code shows two times better performance compared to the routine `zheev` from LAPACK, it is well known that diagonalization of tridiagonal matrix part in `zheev` is many times slower than it is in for example `zheevd`, `zheevx` or `zheevr`, thus hiding the poor implementation of structured tridiagonal reduction using Paige-Van Loan algorithm. The main reason why efficient implementation of Paige-Van Loan algorithm is difficult is the lack of BLAS support for antisymmetric/skew-Hermitian matrices. For example, subroutines analogous to `dsymv` and `dsyr2k` for symmetric matrices, but generalized to antisymmetric would come in handy.

With this motivation in mind, authors of [18] have created a *GitHub* repository:

`https://github.com/abjelcic/zquatev`,

which contains programs for calculating the spectral decomposition:

$$\begin{bmatrix} U & -V \\ V & U \end{bmatrix}^T \begin{bmatrix} A & -B \\ B & A \end{bmatrix} \begin{bmatrix} U & -V \\ V & U \end{bmatrix} = \begin{bmatrix} D & \mathbf{0}_{n\times n} \\ \mathbf{0}_{n\times n} & D \end{bmatrix}, \tag{4.9}$$

for given $A \in \mathbb{R}^{n\times n}$ symmetric and $B \in \mathbb{R}^{n\times n}$ antisymmetric, where $D \in \mathbb{R}^{n\times n}$ is diagonal and $U, V \in \mathbb{R}^{n\times n}$ are such that $\begin{bmatrix} U & -V \\ V & U \end{bmatrix} \in \mathbb{R}^{2n\times 2n}$ is orthogonal. In further development, authors of [18] plan to implement the same algorithm but for general quaternionic matrices as in eq. (4.1). Current implementation uses OpenBLAS [26] for implementation of BLAS library. In the following section, numerical results of current implementation is shown, which motivates further development of implementation for generic quaternionic matrices.

4.3 Numerical experiments

A random symmetric matrix $A \in \mathbb{R}^{n\times n}$ with entries coming from uniform distribution on $[0, 1]$ is generated, together with a random antisymmetric matrix $B \in \mathbb{R}^{n\times n}$ generated in the same manner. Since the current implementation is still not parallelized, we used only single thread (achievable by exporting a constant `OPENBLAS_NUM_THREADS=1` in local environment, or using a command `maxNumCompThreads(1)` in MATLAB). The described Paige-Van Loan algorithm was used to find the spectral decomposition as in eq. (4.9) and the results were compared to the ones obtained by the *state-of-the-art* subroutine `dsyevd` from LAPACK, called on explicitly built symmetric Hamiltonian matrix: $\begin{bmatrix} A & -B \\ B & A \end{bmatrix}$. In our first test, size n of the generated matrices A and B is taken to be $n = 6000$, producing the

corresponding $2n \times 2n = 12000 \times 12000$ Hamiltonian matrix. Blocked implementation of Paige-Van Loan algorithm took $\approx$ 115 seconds to execute, while the naive approach took $\approx$ 216 seconds. If we repeat the same naive approach using single-threaded MATLAB, function `eig` executes in 294 seconds when diagonalizing $2n \times 2n$ symmetric Hamiltonian matrix. On the other hand, if MATLAB is allowed to use optimum number of threads (4 on our machine), it executes in $\approx$ 95 seconds.

In the second test case, we repeated the procedure as in the first test, with only difference in increasing the size n to $n = 8000$. Now, blocked implementation of Paige-Van Loan algorithm took $\approx$ 274 seconds to execute, while the naive approach took $\approx$ 500 seconds. When MATLAB is used in single-thread mode, it took $\approx$ 677 seconds, while if the optimum number of threads are used (4 on our machine), it took $\approx$ 223 seconds.

Thus, authors of [18] feel compelled to continue further development and implement the parallelized eigensolver for generic quaternionic matrix as in eq. (4.1), since they are needed in relativistic quantum chemistry simulations - [29] for example.

Chapter 5

Conclusion

In this thesis, we have shown some interesting properties of the CHFB eigenvalue problem, some of which are completely new even though the field has been active for three decades. The proposed method in Chapter 3 for solving the central equation: $f(\lambda_0) = f_0$, shows at least two times better performance compared to the naive straightforward approach that is currently used in the field.

There are still many open questions and problems that will be addressed by the authors of [18] in future investigations. Namely, answer the question on the true mathematical reason why there appears to be a distinct gap near zero when family of spectra $\sigma(\mathbf{H}_\lambda)$ for $\lambda \in \mathbb{R}$ is plotted as in Figure 2.2, rendering the Routhian $\mathbf{H}_\lambda$ nonsingular. Second very important problem is to prove that the target function $f(\lambda)$ is indeed increasing and that there holds: $\lim_{\lambda\to-\infty} f(\lambda) = 0$ and $\lim_{\lambda\to+\infty} f(\lambda) = n$, demonstrating that the equation $f(\lambda_0) = f_0$ always has the unique solution λ_0 (in $\mathbf{\Delta} \neq \mathbf{0}_{n\times n}$ case). One should also continue on implementing the eigensolver for generic quaternionic matrices as in eq. (4.1), since preliminar results for matrices with real entries showed promising results.

In a more distant future, authors of [18] plan to address the problem of generic CHFB theory without time-reversal symmetry assumed. Also, the non-zero temperature case is worth studying, where the target function looks different than in the zero-temperature case.

Bibliography

[1] Y.K. Ghambhir, P. Ring, A. Thimet, Ann Phys. (NY) **198**, 132 (1990)

[2] J.-P. Blaizot, G. Ripka, *Quantum Theory of Finite Systems*, MIT, Cambridge, MA (1986)

[3] P. Ring, P. Schuck, *The Nuclear Many-Body Problem*, Springer-Verlag, Heidelberg, (1980)

[4] N. Schunck, L.M. Robledo, Rep. Prog. Phys. **79**, 116301 (2016)

[5] T. Nikšić, D. Vretenar, P. Ring, Prog. Part. Nucl. Phys. **66**, 512 (2011)

[6] A. Goodman, Nucl. Phys. A **230**, 446 (1974)

[7] T. Saue, PhD thesis, Department of Chemistry, University of Oslo (1996)

[8] T. Nikšić, N. Paar, D. Vretenar, P. Ring, Comp. Phys. Comm. **185**, 1808 (2014)

[9] R.N. Perez, N. Schunck, R.D. Lasseri, C. Zhang, J. Sarich, Comp. Phys. Comm. **220**, 363 (2017)

[10] V. Mehrmann, *The Autonomous Linear Quadratic Control Problem, Theory and Numerical Solution*, Springer-Verlag, Heidelberg (1991)

[11] MATLAB documentation of `eig` function,
`https://www.mathworks.com/help/matlab/ref/eig.html`

[12] LAPACK documentation, `http://www.netlib.org/lapack`

[13] C.F. Van Loan, Lin. Alg. Appl. **61**, 233 (1984)

[14] J. von Neumann, E. Wigner, Physikalische Zeitschrift **30**, 467 (1929)

[15] Wikipedia article on avoided crossing phenomenon,
`https://en.wikipedia.org/wiki/Avoided_crossing`

[16] T. Nikšić, N. Paar, D. Vretenar, DIRHB program package, https://data.mendeley.com/datasets/cx55fkbjy6/1

[17] Wikipedia article on Sylvester equation, https://en.wikipedia.org/wiki/Sylvester_equation

[18] A. Bjelčić, Z. Drmač, T. Nikšić, Technical report, University of Zagreb, Faculty of Science, Department of Mathematics, (2020)

[19] G.H. Golub, C.F. Van Loan, *Matrix Computations*, The Johns Hopkins University Press (1996)

[20] A. Bjelčić, T. Nikšić, Comp. Phys. Comm. **253**, 107184 (2020)

[21] G.W. Stewart, Ji-guang Sun, *Matrix Perturbation Theory*, Academic Press (1990)

[22] A. George, Kh.D. Ikramov, A.B. Kucherov, SIAM Journal on Matrix Analysis and Applications **21**, 1318 (2000)

[23] D. Kressner, *Numerical Methods for General and Structured Eigenvalue Problems*, Springer-Verlag, Berlin (2005)

[24] T. Shiozaki, Molecular Physics, (2015)

[25] BLAS documentation, http://www.netlib.org/blas

[26] OpenBLAS - an optimized BLAS library based on GotoBLAS2, https://www.openblas.net

[27] C. Paige, C.F. Van Loan, Lin. Alg. Appl. **41**, 11 (1981)

[28] D. Kressner, BIT Numerical Mathematics **43**, 775 (2003)

[29] DIRAC, a relativistic *ab initio* quantum chemistry program, http://www.diracprogram.org/doku.php

Sažetak

Constrained Hartree-Fock-Bogoliubov (CHFB) teorija se danas smatra jednom od najuspješnijih metoda za teorijska istraživanja nuklearne strukture. U numeričkim simulacijama, javlja se potreba za efikasnim računanjem spektralne dekompozicije matrice Routhiana. Unatoč tome što matrica Routhiana posjeduje dodatnu podstrukturu, ona nije iskorištena u trenutno dostupnim programskim paketima za numeričke simulacije u okviru CHFB teorije. U ovom radu predložen je algoritam za računanje spektralne dekompozicije matrice Routhiana, koji efikasno iskorištava dodatnu tzv. kvaternionsku podstrukturu. Provedeni numerički testovi demonstriraju da je predložena metoda 2.5 puta efikasnija od trenutno korištenog pristupa. Dodatno, dokazana su i neka zanimljiva svojstva CHFB teorije, te je dana i efikasna implementacija Paige-Van Loan algoritma za dijagonalizaciju kvaternionskih matrica.

Summary

Constrained Hartree-Fock-Bogoliubov (CHFB) theory is considered to be one of the most successful methods for theoretical studies of nuclear structure. In numerical simulations, one often has to find the spectral decomposition of Routhian matrix. Even though the Routhian matrix exhibits a certain substructure, currently used software packages for numerical simulations in the CHFB framework do not utilize it. In this thesis, a new method for diagonalization of the Routhian matrix, which exploits the additional quaternionic substructure, is proposed and tested. Numerical experiments show that the proposed method outperforms, by a factor of 2.5, currently used naive and straightforward approach. Additionally, in this thesis some interesting properties of the CHFB theory are provided, together with an efficient implementation of the Paige-Van Loan algorithm for diagonalization of quaternionic matrices.