1 Motivation

In a project of finding analytical solutions to the problem of energy levels of electron filled orbital in the crystal field, we construct a Hamiltonian, with certain symmetries originating from the symmetry of the crystal.

With ideas of quantum mechanics the Hamiltonian can be represented as a matrix $\mathcal{H} \in \mathbb{C}_n^n$, where n denotes the dimensionality of the problem. The eigenvalues of $\mathcal{H}$ correspond to the energy levels, for which we desire to have analytical solutions. Physical symmetries of the problem will imply certain symmetries of $\mathcal{H}$ matrix. For example, see the following matrix corresponds to energy levels of $J = 2$ orbital in an 222 point group symmetry:

$$\mathcal{H}_1 = \begin{bmatrix} 6B_{20} + 12B_{40} & 0 & \sqrt{6}B_{22} + 3\sqrt{6}B_{42} & 0 & 12B_{44} \\ 0 & -3B_{20} - 48B_{40} & 0 & 3B_{22} - 12B_{42} & 0 \\ \sqrt{6}B_{22} + 3\sqrt{6}B_{42} & 0 & -6B_{20} + 72B_{40} & 0 & \sqrt{6}B_{22} + 3\sqrt{6}B_{42} \\ 0 & 3B_{22} - 12B_{42} & 0 & -3B_{20} - 48B_{40} & 0 \\ 12B_{44} & 0 & \sqrt{6}B_{22} + 3\sqrt{6}B_{42} & 0 & 6B_{20} + 12B_{40} \end{bmatrix},$$

$B_{ij} \in \mathbb{R}$.

As a fundamental postulate of quantum mechanics $\mathcal{H}$ is hermitian. In many cases some diagonals of the $\mathcal{H}$ will contain 0. In addition, some matrices, as the one in the example, are *persymmetric*.

Finding the eigenvalues of $\mathcal{H}$ corresponds to finding roots of its characteristic polynomial, $p_\lambda(\mathcal{H}) = det(\mathcal{H} - \lambda\mathbb{I})$. Analytical formulas of polynomial roots exist only for irreducible polynomials of degree three, as Cardano formulas. Given the symmetry of the Hamiltonian, even though $p_\lambda(\mathcal{H})$ is mostly of degree higher than three, it can be reduced to a form containing polynomials of degree 3 or lower.

2 Introduction

Definition 1 (Persymmetric matrix)**.** *Following Wikipedia*

A persymmetric matrix is a square matrix which is symmetric with respect to the northeast-to-southwest diagonal.

Let $A = (a_{ij}) \in \mathbb{C}_n^n$. A is persymmetric $\Leftrightarrow \forall i, j, a_{ij} = a_{n-j+1,n-i+1}$.

Definition 2 (m-diagonal matrix)**.** *Let $A = (a_{ij}) \in \mathbb{C}_n^n$. A is m-diagonal $\Leftrightarrow$ m diagonals of A contain nonzero elemnts.*

Example, matrix 1 is hermitian, persymmetric, 5-diagonal.

3 Problem

Problem 1. *For a hermitian, persymmetric, m-diagonal matrix $A \in \mathbb{C}_n^n$, for which m and n the characteristic polynomial of A can be reduced to polynomials of degree two?*

Problem 2. *For a hermitian, m-diagonal matrix $A \in \mathbb{C}_n^n$, for which m and n the characteristic polynomial of A can be reduced to polynomials of degree two?*