Project 2

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Abstract

The goal of this project is to explore a model of quantum dots. We will be investigating the behavior of two electron in a 3-D simple harmonic potential while comparing the models with and without the particles interacting. To do this we will be solving the Schrdinger equation using the Jacobi method.

1 Introduction

2 Jacobi Method

The procedure is as follows:

1. Search for the largest matrix element $|a_{pq}|$, where indices p and q denote the row and column of the max non-diagonal element of the matrix.
2. Given p and q, we performed the Jacobi rotation. We defined the quantities s, c, t as $\sin\theta$, $\cos\theta$, and $\tan\theta$ respectively, and $\tau = \frac{a_{qq}-a_{pp}}{a_{pq}}$ where $t^2 + 2\tau\ t - 1 = 0$

$$f(a,b) = \begin{cases} \text{open}, & \text{if } \mathrm{RMSD}_{\text{s-open}} \geq 6, \mathrm{RMSD}_{\text{closed}} \geq 6 \text{ closed}, \\ \quad \text{if } \mathrm{RMSD}_{\text{closed}} \leq 2 \text{ semiopen}, & \text{if } \mathrm{RMSD}_{\text{s-open}} \leq 2 \text{ transition}, \\ \quad \text{otherwise.} \end{cases}$$

3 References