FYS3150 Computational Physics - Project 2

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This is an abstract

INTRODUCTION

THEORY, ALGORITHMS AND METHODS

Preservation of scalar product & orthogonality in unitary transformations

Consider an orthonormal set of basis vectors $\mathbf{v}_i$ such that $\mathbf{v}_j^T\mathbf{v}_i = \delta_{ij}$. Let unitary matrix U where $U^TU = I_N$, where I_N denotes the $N \times N$ identity matrix, operate on $\mathbf{v}_i$ to get $\mathbf{w}_i$

$$\mathbf{w}_i = U\mathbf{v}_i \tag{1}$$

Then

$$\mathbf{w}_j^T\mathbf{w}_i = (U\mathbf{v}_j)^TU\mathbf{v}_i = \mathbf{v}_j^TU^TU\mathbf{v}_i = \mathbf{v}_j^T\mathbf{v}_i = \delta_{ij} \tag{2}$$

In the unitary transformation of $\mathbf{v}_i$ both the scalar product and orthogonality has been preserved.

Givens rotation

A Givens rotation is a unitary transformation which performs a rotation in the plane spanned by two coordinate axes, represented by the matrix in Eqn. 3.

$$G(i,j,\theta) = \begin{bmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \dots & \cos\theta & \dots & -\sin\theta & \dots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \dots & \sin\theta & \dots & \cos\theta & \dots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{bmatrix} \tag{3}$$

where nonzero entries $g_{kk} = 1$ for $k \neq i, j$, $g_{kk} = cos\theta$ for $k = i, j$ and $g_{ji} = -g_{ij} = -\sin\theta$ [2]

As the Givens transformation it unitary, it also follows that it preserves both the scalar product and orthogonality, as shown in the section prior.

Jacobi Eigenvalue Algorithm

The jacobi eigenvalue algorithm finds the eigenpairs of real, symmetric matrices by diagonalization with Givens rotation matrix.

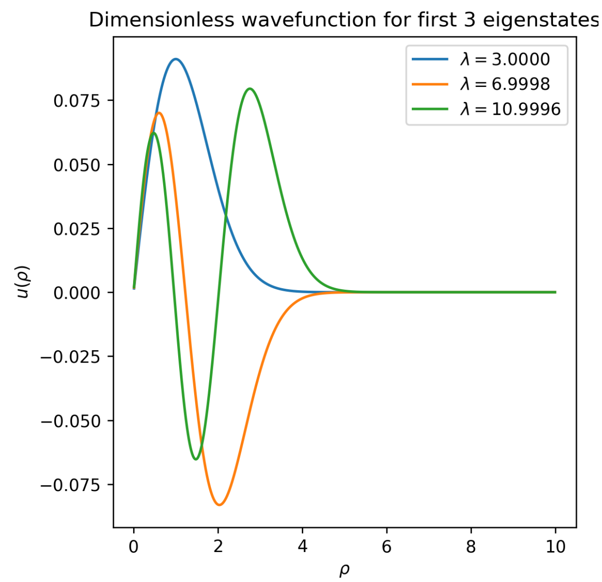

FIG. 1. First 3 eigenpairs in the solution of the harmonic oscillator potential for $N = 1000$

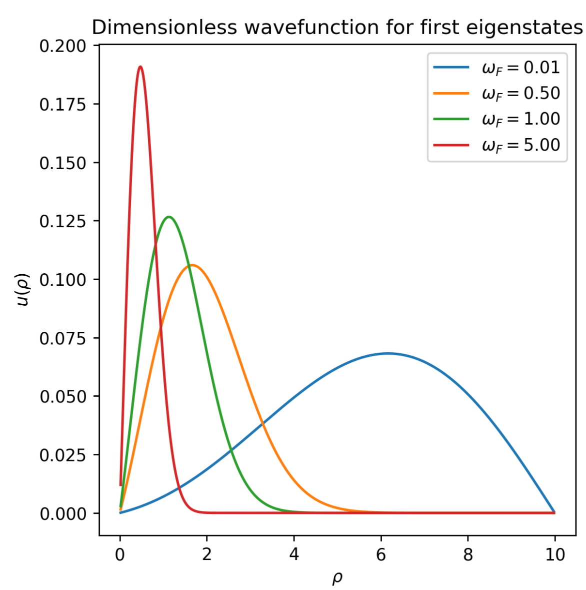

FIG. 2. ...

RESULTS AND DISCUSSIONS

CONCLUSIONS

[1] M. Hjorth-Jensen, Computational Physics - Lecture Notes 2015, (2015).

[2] Wikipedia contributors, Givens rotation — Wikipedia, The Free Encyclopedia, [Online; accessed 1-October-2018]

Jacobi Eigenvalue Algorithm

$\tau = \frac{a_{ll}-a_{kk}}{2a_{kl}}$

if $\tau \geq 0$:
 $t = \frac{1}{\tau+\sqrt{1+\tau^2}}$
else:
 $t = \frac{-1}{-\tau+\sqrt{1+\tau^2}}$

$c = \frac{1}{\sqrt{1+t^2}}$
$s = tc$

$a'_{kk} = a_{kk}$
$a'_{ll} = a_{ll}$

$a_{kk} = c^2 * a'_{kk} - 2cs * a_{kl} + s^2 * a'_{ll}$
$a_{ll} = s^2 * a'_{kk} + 2cs * a_{kl} + c^2 * a'_{ll}$
$a_{kl} = 0.0$
$a_{lk} = 0.0$

for $i = 1, 2, \ldots N$:
 if $i \neq k$ **and** $i \neq l$:
  $a_{ik} = a_{ik}$
  $a_{il} = a_{il}$
  $a_{ik} = c * a_{ik} - s * a_{il}$
  $a_{ki} = a_{ik}$
  $a_{il} = c * a_{il} + s * a_{ik}$
  $a_{li} = a_{il}$