

Methods of solving eigenvalue problems

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Abstract

We implement Jacobi's method for solving eigenvalue problems on the form $A\mathbf{v} = \lambda\mathbf{v}$, where A is a symmetric matrix. By scaling the equations, we can use our algorithm to solve the buckling beam, single electron in an harmonic oscillator potential, and two electrons in an harmonic oscillator potential problems. By looking at the buckling beam problem, we find that the number of iterations needed to diagonalize the matrix is proportional to n^2 , while the CPU-time is proportional to n^4 . The relative error in the eigenvalues converges to $\sim 10^{-5.77}$ for n larger than 25. For n larger than 20, the Armadillo function `eig_sym` is faster than Jacobi's method. We therefore conclude that Jacobi's method gives a good approximation, even though it is slow for large n . We also studied the case of the two electrons in more detail, and found that a stronger potential results in a narrower wave function and higher energy eigenvalues. Furthermore, we found that the Coloumb interaction acts to increase the distance between the two electrons, but not necessarily increase the spread in the wave function. This is because of the new equilibrium obtained between the harmonic oscillator potential and the Coloumb interaction, and we also see this in the increasing increase of the energy eigenvalues as a function of ω_r .

1 Introduction

value problem

A great variety of problems in the physical sciences can be represented as eigenvalue problems, which generally takes the form:

$$O\mathbf{v} = \lambda\mathbf{v}, \quad (1)$$

where O is an operator, λ is an eigenvalue, and \mathbf{v} is an eigenvector. Such problems can easily be solved in terms of linear algebra, and is therefore of great use in simplifying complicated problems, as well as providing a framework for creating efficient algorithms. In particular, we will look at the motion of a fixed buckling beam, and show that this is numerically identical to the motion of quantum dots. Specifically, we will solve the following eigen-

$$\left(\frac{d^2}{dx^2} + f(x)\right)u(x) = \lambda u(x). \quad (2)$$

Starting with the methods section, we will present the buckling beam problem, as well as the quantum dot problem, scaling and generalising them to the form of eq. 1. Using different numerical methods, we will use unit testing to make sure that each algorithm is implemented correctly. Moving on to the results section, we will present the efficiency and error of each algorithm in terms of CPU-time and relative error respectively. Then finally, in the discussion section, we will compare the different methods, and look at more possibilities for problems that can be solved using the same general algorithms.

2 Methods

We will solve three different problems and develop one algorithm

2.1 The buckling beam

Considering first the buckling beam problem, we have

$$\gamma \frac{d^2 u}{dx^2} = -Fu(x), \quad x \in [0, L] \quad (3)$$

where γ is a property constant, $u(x)$ the vertical displacement, and F the force applied at $(L, 0)$ towards the origin. We can scale this equation by defining a parameter $\rho = \frac{x}{L}$. Inserting, we get

$$-\frac{d^2}{d\rho^2} u(\rho) = \lambda u(\rho), \quad \rho \in [0, 1] \quad (4)$$

where $\lambda = \frac{FL^2}{\gamma}$. Now we see that this equation is on the form of eq. 2. However, enforcing Dirichlet boundary conditions $u(0) = u(1) = 0$ and using a 2nd order central approximation for n integration steps we obtain

$$-\frac{v_{i+1} - 2v_i + v_{i-1}}{h^2} + \mathcal{O}(h^2) = \lambda_i v_i, \quad (5)$$

where $h = \frac{\rho_n - r_{ho0}}{n}$. Disregarding the boundaries (which are set to 0) we obtain the eigenvalue equation

$$A\mathbf{v} = \lambda\mathbf{v}. \quad (6)$$

Here

$$A = \begin{bmatrix} d & a & 0 & \dots & \dots & 0 \\ a & d & a & 0 & \dots & 0 \\ 0 & a & d & a & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \ddots & a & d & a \\ 0 & \dots & \dots & 0 & a & d \end{bmatrix}, \quad (7)$$

is an tridiagonal matrix where $d = \frac{2}{h^2}$ and $a = -\frac{1}{h^2}$, λ is an eigenvalue, and $\mathbf{v} \in (0, n)$

is an eigenvector. The analytical eigenvalues are given by

$$\lambda_j = d + 2a \cos\left(\frac{j\pi}{n+1}\right), \quad (8)$$

$$j = 1, 2, \dots, n-1.$$

2.2 Single electron in an harmonic oscillator potential

We want to model an electron in a three dimensional harmonic oscillator potential

$$V(r) = \frac{1}{2}m\omega^2 r^2, \quad r = \sqrt{x^2 + y^2 + z^2} \quad (9)$$

$r \in (0, \infty)$ FLAGG, m is the mass, and ω is the frequency. The quantum state can then be represented as the wavefunction

$$|\Psi\rangle \simeq \Psi(r, \phi, \theta) = R(r)Y_l^m(\phi, \theta), \quad (10)$$

where $R(r)$ is the radial part, and $Y_l^m(\theta, \phi)$ are the spherical harmonics. What we need to solve then is the radial equation

$$\left(\frac{-\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) + \frac{l(l+1)}{r^2}\right)u(r) = Eu(r). \quad (11)$$

(See the appendix for more details on the wavefunction and the radial eq.) Here l is the orbital momentum, $u(r) = rR(r)$, and E are the eigenvalues of $\Psi(r, \theta, \phi)$. We will assume our electron has no orbital momentum ($l = 0$), and scale eq. 11 by substituting $\rho = \frac{r}{\alpha}$ and $\lambda = \frac{E}{\epsilon}$, inserting $V(r)$, and get

$$-\frac{\hbar^2}{2m\alpha^2} \left(\frac{d^2}{d\rho^2} - \frac{m^2\omega^2\alpha^4}{\hbar^2}\rho^2\right)u(\rho) = \epsilon\lambda u(\rho), \quad (12)$$

where we can define a natural energy scale $\epsilon = \frac{\hbar^2}{2m\alpha^2}$, and a natural length scale $\alpha = \sqrt{\frac{\hbar}{m\omega}}$, yielding the dimensionless equation

$$\left(-\frac{d^2}{d\rho^2} + \rho^2\right)u(\rho) = \lambda u(\rho). \quad (13)$$

Discretising as in eq. 5, the equation becomes

$$-\frac{v_{i+1} - 2v_i + v_{i-1}}{h^2} + V_i v_i = \lambda v_i, \quad (14)$$

where $V_i = \rho_i^2 = (\rho_0 + ih)^2$. Enforcing the Dirichlet boundary conditions, we see that 14 can be written on matrix form as

$$A\mathbf{v} = \lambda\mathbf{v}. \quad (15)$$

Here

$$A = \begin{bmatrix} d_1^e & a & 0 & \dots & \dots & 0 \\ a & d_2^e & a & 0 & \dots & 0 \\ 0 & a & d_3^e & a & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \ddots & a & d_{n-1}^e & a \\ 0 & \dots & \dots & 0 & a & d_n^e \end{bmatrix}, \quad (16)$$

where $d_i^e = \frac{2}{h^2} + V_i$ and a is as before. The analytical eigenvalues are here given by:

2.3 Two electrons in an harmonic oscillator potential

We will now consider the problem of two electrons in the aforementioned potential. As the electrons are interacting, we will have to modify the radial equation by adding the Coloumb interaction term

$$V(r_1, r_2) = \frac{\beta e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (17)$$

where $\beta e^2 = 1.44eVnm$, e is the electron charge, and \mathbf{r}_1 and \mathbf{r}_2 are the positions of electron 1 and 2 respectively. To get the modified radial equation on the form of eq. 2, we use the relative distance $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$, center of mass $\mathbf{R} \equiv \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ reference system. Furthermore, we will only consider the radial solution of the relative distance, and not the center of mass. Using the same scaling parameters α , ϵ , as before, we obtain the equation:

$$\left(-\frac{d^2}{d\rho^2} + \omega_r^2 \rho^2 + \frac{1}{\rho}\right)\psi(r) = \lambda\psi(r). \quad (18)$$

Here $\rho = \frac{r}{\alpha}$, $\omega_r^2 = \frac{1}{4} \frac{m^2 \omega^2}{\hbar^2} \alpha^4$, and $\psi(r)$ is the relative distance part of the radial solution. Discretising as usual, and enforcing the Dirichlet conditions, we get our equation on matrix form

$$A\mathbf{v} = \lambda\mathbf{v},$$

where the diagonal elements are now given by $d_i^{2e} = \frac{2}{h^2} + \omega_r^2 \rho^2 + \frac{1}{\rho}$. When we look at the eigenfunction corresponding to the ground state of this equation, we will refer to it as the "wavefunction". For our case, where $l = 0$, this is not entirely untrue, since the spherical harmonic Y_0^0 corresponds to a constant. We can therefore just imagine we have scaled the eigenfunction with this constant as well.

2.4 Algorithm: Jacobi's method

Let U be a unitary matrix, and

$$\mathbf{w}_i = U\mathbf{v}_i,$$

a unitary transformation. Then we have that

$$\mathbf{w}_j^\dagger \mathbf{w}_i = \mathbf{v}_j^\dagger U^\dagger U \mathbf{v}_i = \mathbf{v}_j^\dagger \mathbf{v}_i = \delta_{ij},$$

and the orthogonality is conserved. The strategy of Jacobi's method is then to perform a series of similarity transformations on the matrix A in order to diagonalize the matrix. See for example D.C. Lay [1] for a derivation of the matrix properties. We say that matrix B is similar to A if

$$B = S^{-1}AS, \quad (19)$$

and that the transformation from A to B is a similarity transformation. If S is a real orthogonal matrix we have that

$$S^{-1} = S^T \quad \text{and} \quad B = S^T A S. \quad (20)$$

Since A is a real symmetric matrix there exists a real orthogonal matrix P such that

$$D = P^T A P \quad (21)$$

is a diagonal matrix. Furthermore, the entries along the diagonal of D is the eigenvalues of A , and the column vectors of P are the corresponding eigenvectors. Since the matrix product of two orthogonal matrices is another orthogonal matrix, we can perform a series of similarity transformations until we (ideally) get a diagonal matrix. That is

$$S_j^T S_{j-1}^T \cdots S_1^T A S_1 \cdots S_{j-1} S_j = D \quad (22)$$

where S_i , $i = 1, \dots, j$ are real orthogonal matrices. In Jacobi's method, the matrix S_i is on the form

$$S = \begin{bmatrix} s_{11} & \cdots & s_{1n} \\ \vdots & \ddots & \vdots \\ s_{n1} & \cdots & s_{nn} \end{bmatrix}, \quad (23)$$

where

$$\begin{aligned} s_{kk} &= s_{ll} = \cos \theta \\ s_{lk} &= -s_{kl} = \sin \theta \\ s_{ii} &= 1, \quad i \neq k, l \end{aligned} \quad (24)$$

and elsewhere zero. The matrix S_i is a rotational matrix, which performs a plane rotation around an angle θ in the n -dimensional Euclidean space. For the full transformation expressions, see the appendix.

The idea now is to set k and l such that $a_{kl} = a_{lk}$ is the largest (not considering the sign) non-diagonal element in A , and choose θ so that $b_{kl} = 0$. See the appendix for the expression for θ . Notice that when rotating A such that a_{kl} is set to zero, other matrix elements previously equal to zero may change. However, the frobenius norm of an orthogonal transformation is always preserved, so no elements will blow up. Using the same procedure on the new matrix, we repeat until all non-diagonal elements are essentially zero. Since we want the eigenvectors as well, we need to compute $S_1 \cdots S_{j-1} S_j$ continuously. This gives us the following algorithm

```

initialise  $A, S$ ;
while  $max > tol$  do
    find  $max, k, l$ ;
    compute  $\tau, \sin \theta, \cos \theta$ ;
    rotate  $A$ ;
    update  $S$ ;

```

Now, the diagonal elements of A and the column vectors of S are the eigenvalues and the corresponding eigenvectors, respectively.

2.5 Error

When the analytical solution is known, we define the error in the eigenvalue as

$$\epsilon_i = \left(\left| \frac{\lambda_i - \lambda_i^{comp}}{\lambda_i} \right| \right) \quad (25)$$

where λ_i is the analytical value and λ_i^{comp} is the computed value.

2.6 Comparing CPU time

To get an idea how the algorithm performs we compare the CPU time for our implementation of Jacobi's method and Armadillo's `eig_sym` function applied at the buckling beam problem. In both cases we time the computation of both the eigenvalues and the eigenvectors, not including the initialisation of the program. The mean time of ten runs is recorded for each n , and we measure the standard deviation for each sample.

2.7 Programming technicalities

All our programs are written in C++, using python3.6 to produce figures and tables. We use armadillo with LAPACK to define matrices and vectors, as well as comparing LAPACK's eigenvalue solver with the Jacobi algorithm.

All our code can be found in a github repository "FYS3150" by janadr¹.

3 Results

The first thing we measured was the convergence rate of Jacobi's algorithm, see Figure 1. We see that after some fluctuations for low n , the curve becomes linear as n increases, with a slope of approximately 2. As this is in logspace, we have that the number of iterations increases as $\sim n^2$.

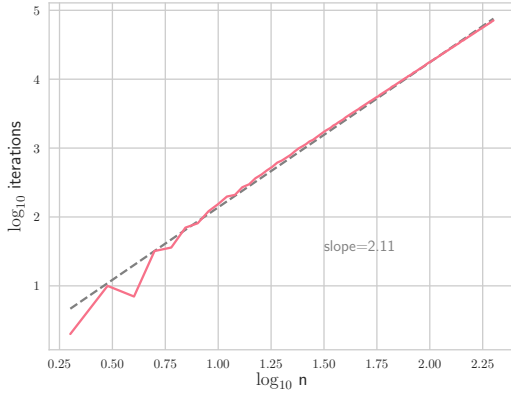


Figure 1: Number of iterations used for solving the buckling beam problem as a function of the matrix dimension n with a logarithmic scale. The slope of the linear fit is 2.11.

In Figure 2 we compare the CPU time between Jacobi's method and armadillo's built-in eigenvalue solver, where we see that the CPU time of Jacobi's method has a similar shape as in Figure 1. Looking at the graph for the armadillo function we see that the slope is rising slower, but have a similar shape, except for the fluctuations occurring after the $\log_{10} n = 1.25$ mark.

In Figure 3, we show the maximum relative error of the Jacobi algorithm when computing

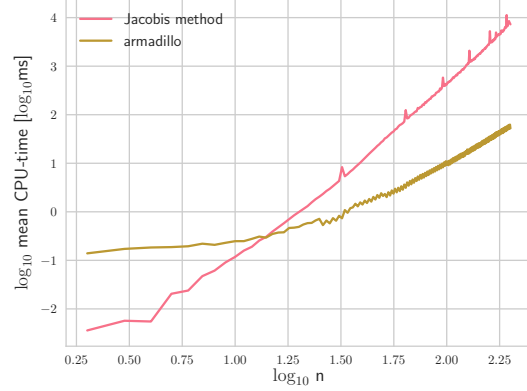


Figure 2: CPU time in ms for solving the buckling beam as a function of the matrix dimension n . Both Jacobi's method (red) and armadillo's `eig_sym` function (yellow) is shown. The scale is logarithmic.

the eigenvalues in the buckling beam problem. We see that the error increases with a steep slope for low n , before converging towards a constant error for increasing n .

Having benchmarked our implementation of Jacobi's algorithm, we then study the case of electrons in an harmonic oscillator potential. In particular, in Figure 4, we looked at the effects of varying ω_r in the ground state. We see that for increasing ω_r , the wavefunction becomes narrower and closer to the origin. The energy eigenvalues also increases as a function of ω_r .

Finally, studying the effects of the Coloumb interaction, we compare the same case as in Figure 4 with and without the Coloumb interaction. In Figure 5 then, we see that the wavefunctions are all shifted out from the origin. For the energy eigenvalues, we see that for every ω_r the value increases more and more for increasing ω_r , comparing to the non-

¹<https://github.com/janadr/FYS3150/tree/master/projects/interacting>

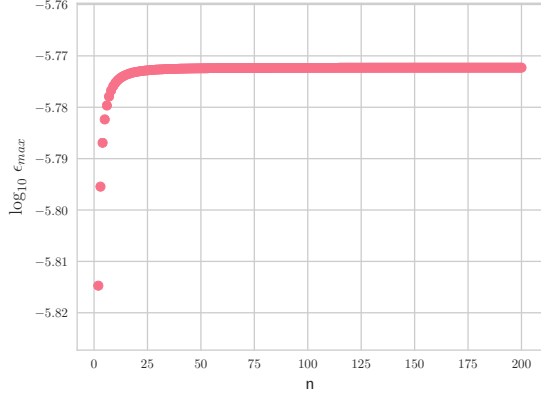


Figure 3: Maximum relative error, ϵ_{max} of Jacobi's algorithm applied on the buckling beam problem. Here n is the matrix dimension, and the scale is logarithmic.

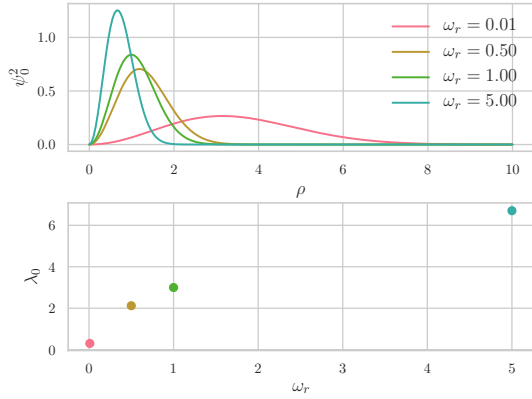


Figure 4: The "wavefunction" for the ground state for different values of ω_r with $n = 200$ and no Coloumb interaction. Underneath is the energy eigenvalue λ_0 as a function of ω_r .

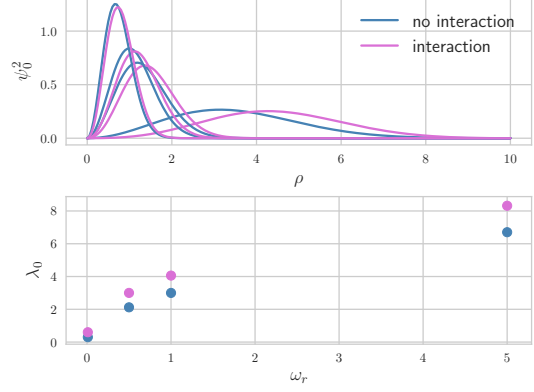


Figure 5: Here we have the same parameters as in Figure 4. We compare the case of no interaction between the electrons (blue) and the case of interaction between the electrons (pink).

4 Discussion

As we have seen in Figure 2, Jacobi's method is quite time consuming for large n , compared to Armadillo's function `eig_sym`. Our implementation of Jacobi's method is more efficient than Armadillo's function for n smaller than about 20, but for larger n the roles change. Estimating the slope, we get that the CPU-time is proportional to approx. n^4 . The number of iterations is proportional to approx. n^2 , so CPU-time per iteration must increase as n^2 . In our case, n is the resolution in the discretization of the displacement function for the buckling beam, and of the wave function for the electron(s). So large n is usually preferred, and therefore Armadillo may be a better choice.

The relative error, on the other hand, converges quickly, as shown in Figure 3. The relative error is smallest for small n , and stabilises quickly to $\sim 10^{-5.77}$ for n larger than 25.

So Jacobi's method gives a good approximation, even though it can be slow for large n .

Looking back at Figure 4, the effects of increasing ω_r can be understood in the perspec-

tive that ω_r alters the strength of the potential. So for larger ω_r , the potential is stronger, and the electrons are more likely to be measured closer to each other. As for the narrowing of the wave function, we see that the energy eigenvalues increase because of the greater potential energy of the electrons. We see then that as ω_r increases, the electrons become more and more trapped, and they are therefore less likely to be spread out.

Comparing the case of no Coloumb interaction, and the case with, we see that the wave function is shifted to the right for all ω_r , but at the greatest for the lowest ω_r . This means that the effect is most prominent for weaker potentials. At close range, the Coloumb force $\frac{1}{\rho}$ will dominate, and the electrons will repel each other heavily. The spread in ψ_0^2 will thus increase until there is a new equilibrium between the two. This makes it so that it is more likely to measure the electrons further away from each other. The fact that the energy eigenvalues increase more and more for increasing ω_r is because the stronger harmonic oscillator potential makes the Coloumb interaction store more potential energy, as ρ must be smaller to stay in equilibrium.

In conclusion, we have implemented and benchmarked Jacobi's algorithm for solving eigenvalue problems. Here, we find that our implementation is generally slow compared to armadillo's built-in function *eigsym()*, but that the error stabilises for increasing n very quickly. We applied the algorithm on three different physical systems, where we used the case of the buckling beam for benchmarking, and the case of the single electron for showing similarity between the two. Our analysis was therefore focused on the problem of two interacting electrons, where we find that a greater harmonic oscillator potential results in a narrower wave function as well as higher energy eigenvalues. Including the Coloumb interac-

tion between the electrons, we find that they are more likely to be found further apart, and that the interaction amplifies the effect of increasing the potential energy of the electrons.

References

- [1] D.C. Lay. *Linear Algebra and Its Applications*. Pearson Education, 2002.

A

Derivation of the radial equation

Considering the case of a particle in a three dimensional harmonic oscillator potential, we have the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r), \quad r = \sqrt{x^2 + y^2 + z^2} \quad (\text{A.1})$$

which in spherical coordinates is given by

$$H = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + V(r) + \frac{L^2}{2mr^2}, \quad (\text{A.2})$$

where

$$L^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right], \quad (\text{A.3})$$

is the squared angular momentum operator. Since L^2 does not act on r , we have that H and L^2 commute, and neglecting spin, a quantum state can then be represented as a wavefunction

$$|\Psi\rangle \simeq \Psi(r, \phi, \theta) = R(r)Y_l^m(\phi, \theta), \quad (\text{A.4})$$

where $R(r)$ is the radial solution, and $Y_l^m(\theta, \phi)$ are the eigenfunctions of L^2 (spherical harmonics). The Schrodinger equation is then

$$HR(r)Y_l^m(\phi, \theta) = ER(r)Y_l^m(\phi, \theta). \quad (\text{A.5})$$

Here E are the eigenvalues of $\Psi(r, \theta, \phi)$. Letting L^2 act on $Y_m^l(\theta, \phi)$ we obtain its eigenvalues $\hbar^2 l(l+1)$. Substituting $R(r) = \frac{u(r)}{r}$, we see that

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \frac{u(r)}{r} = \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \left(\frac{\partial u}{\partial r} \frac{1}{r} - \frac{u(r)}{r^2} \right) \right] = \frac{1}{r^2} \left(\frac{\partial u}{\partial r} + r \frac{\partial^2 u}{\partial r^2} - \frac{\partial u}{\partial r} \right) = \frac{1}{r} \frac{\partial^2 u}{\partial r^2}.$$

Multiplying by r on both sides, the problem then reduces to the radial equation

$$-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} - V(r) - \frac{l(l+1)}{r^2} \right) u(r) = Eu(r). \quad (\text{A.6})$$

Expressions for computing the Jacobi rotation

The resulting matrix from the transformation in eq. 20, written on the same form as eq. 23, is

$$\begin{aligned} b_{ii} &= a_{ii}, \quad i \neq k, l \\ b_{ik} &= a_{ik} \cos \theta - a_{il} \sin \theta, \quad i \neq k, l \\ b_{il} &= a_{il} \cos \theta + a_{ik} \sin \theta, \quad i \neq k, l \\ b_{kk} &= a_{ll} \cos^2 \theta - 2a_{kl} \cos \theta \sin \theta + a_{kk} \sin^2 \theta \\ b_{ll} &= a_{kk} \cos^2 \theta + 2a_{kl} \cos \theta \sin \theta + a_{ll} \sin^2 \theta \\ b_{kl} &= (a_{kk} - a_{ll}) \cos \theta \sin \theta + a_{kl} (\cos^2 \theta - \sin^2 \theta) \end{aligned} \quad (\text{A.7})$$

Using eq. A.7, and letting $\tau = \cot 2\theta$, we get that to satisfy $b_{kl} = 0$, we must have

$$\tau = \frac{a_{ll} - a_{kk}}{2a_{kl}} \quad (\text{A.8})$$

By using the trigonometric identity $\cot 2\theta = \frac{1}{2}(\cot \theta - \tan \theta)$, we get the quadratic equation

$$\tan^2 \theta + 2\tau \tan \theta - 1 = 0 \quad (\text{A.9})$$

with the solution

$$\begin{aligned} \tan \theta &= -\tau \pm \sqrt{1 + \tau^2} \\ \cos \theta &= \frac{1}{\sqrt{1 + \tan^2 \theta}} \\ \sin \theta &= \tan \theta \cos \theta \end{aligned} \quad (\text{A.10})$$