Panamerican Mathematical Journal
ISSN: 1064-9735
Vol 31 No.1 (2021)

Matrix Diagonalization: Analytical insights for Numerical implementation

Avijit k. Ganguly
MMV, Banaras Hindu University,
Varanasi 221005.
email: avijitk@hotmail.com

Article History:
Received-03.11.2020
Revised- 02.02.2021
Accepted-10.02.2021
Published -20.03.2021

Abstract

Finding the eigen-systems of a (skew)symmetric matrix M that belongs to class ∈ $C^{n\times n}$ or $R^{n\times n,}$ ana-lytically is a nontrvial task. The Estimations of numerical size of the eigen values and or the eigen vectors from the analytical estimates can be challenging depending on the differences in the order of magnitude estimates of the elements of the matrix concerned. These details turn out to be important while constructing an uniary matrix U that would diagonalize M under similarity transformation. Even the numerical routes to the solutions are subject to the mechine precision and cumulative round off errors for the roboustness of these estimates.

1. Introduction

Use of matrices is common in multiple areas of academics. In various areas of science, multiple number of fields are found to interact with each other forming a coupled interacting system. The examples of those could be found in the areas of classical physics as well as subnuclear physics where sub nuclear particle like neutrino interact in flavour space and photon interact with (axion like particles) ALP in a magnetized media. [1] -[23] during their propagation in space time. Studies of such systems require solving matrix equations to understand their space time evolution. Historically speaking, one recalls a time when the oscillation of three neutrino species was realized as the topic of urgent attention, efforts were initiated in that direction to diagonalize the neutrino mass matrix in the flavour space that involved a change from the gauge eigenstate to the mass eigenstate. A similar situation is encountered in Axion Electro Dynamics (ARD). In AED, with the inclusion of magnetic field(B), one moves from a 2x2 propagation basis to a 3x3 propagation basis- or a 4x4 basis as one incorporates the magnetized medium effects. As a result of the same, physical realisation of the three polarisation states of photon becomes possible. Two of them being transverse and one longitudinal.

In reality, depending on the discrete symmetry of the interacting ALP, one is left with either a 3x3 mixing matrix or a 4x4 one. Usually, the task of diagonalisation can be achieved if the matrix is Hermitian or real symmetric; either using Euler angles or diagonalisation by similarity transformation by unitary matrices-constructed from the eigen vectors of M. In this piece of our note we prefer to use the second, for 3x3 case. The more involved 4x4 case would be addressed later. The usual 3x3 matrix that describes ALP photon case differs from the same for neutrino oscillation in the flavour space, in the following sense. For the later, the number of nonzero elements of the matrix (M) is different from the same describing ALP photon oscillation. So, taking those additional details into consideration, the diagonalisation of such matrices would not be very different from the first one. Hence this issue will be taken up separately paying attention to the required details. Specifically our matrix under consideration would be a real symmetric (RS) one. One can convert the same into a hermitian one, with appropriate unitary transformation. We would leave out this part for a separte publication.

What makes the analysis of this paper topically appropriate, is it's ability to test the level of accuracy of the results obtained at the end of every cycle of the estimations. For real symmetric or hermitian matrices, the diagonal elements are bound to be real. However due to compunding of round off orrors and availability of limited amount of machine precision, one may find a contradicting result. In situations like this one can go back to an earlier step and consider correcting strategies to reduce the arithmathical errors. Even before relving on the results of numerical packages one should verify that they satisfy the required analytic identities. We have documented the necessary numerical checks those would be helpful to declare the results trustable and lie within desired error limit. These can be incorporated in a straight forward manner. Some of them are based on standard checks those follows from the use of the resolvents. But not the least, we have also devised some dynamical tests (based on various relations among the elements of the matrix), those the results should pass if they are to be declared trustable. Those are discussed in the appropriate sections of this article.

The organisation of this document is as follows, in the next section we will discuss diagonalization of the matrix That appears in scalar ALP photon interaction. Followed by that we would report on the same that appears for Hermitian matrices of same dimention. Our treatment will be analytical all the way from beginning to end. Further more, means for M - λi moving to efficient numerical accuracy of the results can be systematically developed using our results.

2. Constructing the orthogonal matrix for diagonalization

Here we outline diagonalization of a 3 × 3 matrix given by

$$M = \begin{bmatrix} a & b & 0 \\ b & c & d \\ 0 & d & g \end{bmatrix} . \qquad (1)$$

Generalizing it to a hermitian matrix of the kind we have is trivial, so we would concentrate on diagonalizing the type given by eqn. (1). As noted already, the Cayley-Hamilton characterictic equation for this matrix looks like, |M - λi| = 0 for the i'th eigen value. Or for that matter, for any of the three eigen values, one should have

$$\begin{vmatrix} a-\lambda_i & b & 0 \\ b & c-\lambda_i & d \\ 0 & d & g-\lambda_i \end{vmatrix} = 0 \qquad (2)$$

Which when written in algebraic form looks like,

$$\lambda^3 - \lambda^2(a+c+g) + \lambda(gc+ga+ac-d^2-b^2) + (ad^2+gb^2-gac) = 0 \qquad (3)$$

For the sake of compactness here we denote, B = −(a + c + g), C = (gc+ga+ac−d^2−b^2) and lastly D = −(ad^2+gb^2−gac). Once one employs these redfinitions the characteristic equation terns out compact in appearence. Ensuring implementaion of these in the standard prodecures.

3. Roots And The Eigen Vectors

3.1 Cardanos route to the roots

The cubic equation, that follows from the characteristic equation can be written, in terms of these newly introduced parameters B, C and D as,

$$\lambda^3+B\lambda^2+C\lambda+D=0, \qquad (4)$$

Furthermore, introducing variables P and Q , (these are functions of the coefficients of the characteristic equation) defined in the following way: $P = (\frac{3C-B^2}{9})$ and $2Q = (\frac{2B^3}{27} - \frac{BC}{3} + D)$. one can represent the root as,

$$\lambda_1 = R\cos\alpha+\sqrt{3}R\sin\alpha-b/3,$$

$$\lambda_2 = R\cos\alpha-\sqrt{3}R\sin\alpha-b/3, \text{ with } \begin{cases} \alpha = \frac{1}{3}\cos^{-1}\frac{Q}{R^3} \\ R = \sqrt{(-P)}sgn(Q) \end{cases} \qquad (5)$$

$$\lambda_3 = -2R\cos\alpha-b/3.$$

The method that is used to find the roots are called Cardano's method [29]. This method came into existence in the sixteenth century. There are many narratives associatd with the discovery of this method, those can be found in the literature.

3.2 Root Resolvants

The coefficients of the characteristic polynomial (4) satisfy some algebraic relations with the roots. And following are those relations mentioned above, that are satisfied by the roots (of (4)):

$$\lambda_1+\lambda_2+\lambda_3 = -B \qquad (6)$$

$$\lambda_1\lambda_2+\lambda_2\lambda_3+\lambda_3\lambda_1 = C \qquad (7)$$

$$\lambda_1\lambda_2\lambda_3 = -D \qquad (8)$$

These relations are also termed as resolvants.

3.3 The eigenvectors

The orthonormal eigenvectors V_j of M are to be found from the matrix relation, $[M - \lambda_j][V_j] = 0$. In terms of its elements, the normalised column vector V_j, can be denoted as,

$$V = \begin{pmatrix} u_i \\ v_i \\ w_i \end{pmatrix} \qquad (9)$$

Using the resolvants one can prove that the eigen-vectors for (i = 1 − 3)yield,

$$V_i \cdot V_j = \delta_{ij}. \qquad (10)$$

when suitably normalized. The proof that these normalized eigenvectors satisfy above the identity (10) can be established by using the relations satisfied by the components of the eigen vectors, namely:

$$(a-\lambda)u+bv = 0$$
$$bu+(c-\lambda)v+dw=0 \qquad (11)$$
$$dv+(g-\lambda)w=0$$

3.4 Orthogonality Of Eigen-Vectors

Next we check the identities those the eigen vectors satisfy analytically. To do that we start with the nontrivial solns of (11) (for any of the three eigenvalues):

$$u=-b(g-\lambda)$$
$$v=(a-\lambda)(g-\lambda) \qquad (12)$$
$$w=-d(a-\lambda).$$

and use them to show $V_1 \cdot V_2 = 0$. Other relations would follow similarly. To reach that end, we start noting that,

$$V_1 \cdot V_2 = b^2(g-\lambda_1)(g-\lambda_2)+d^2(a-\lambda_1)(a-\lambda_2)+(g-\lambda_1)(g-\lambda_2)(a-\lambda_1)\times(a-\lambda_2)] \quad (13)$$

that follows trivially. Next we start from,

$$[(g-\lambda_1)(g-\lambda_2)] = g^2-g(\lambda_1+\lambda_2)+\lambda_1\lambda_2 \qquad (14)$$

Eqn. (14) is a function of λ_1 and λ_2, and we need to convert it to a function of a single variable λ_3 to prove our point. To do that we would make use of the following tricks,

$$\lambda_1+\lambda_2=[\lambda_1+\lambda_2+\lambda_3]-\lambda_3$$
$$\lambda_1\lambda_2 = [\lambda_1\lambda_2+\lambda_2\lambda_3+\lambda_3\lambda_1]-\lambda_3(\lambda_2+\lambda_1) \qquad (15)$$

Now one can use the relations (7,8), to replace the expressions inside the square bracket in eqns. (15) to get a function of only λ_3. i.e.

$$\lambda_1+\lambda_2=a+c+g-\lambda_3$$
$$\lambda_1\lambda_2 = gc+ga+ac-d^2-b^2-\lambda_3(a+c+g-\lambda_3) \qquad (16)$$

As one uses eqns. (16) in eqn. (14) one arrives at,

$$g^2-g(\lambda_1+\lambda_2)+(\lambda_1\cdot\lambda_2) = (\lambda_3-a)(\lambda_3-c)-b^2-d^2 \qquad (17)$$

therefore,

$$b^2(g-\lambda_1)(g-\lambda_2) = b^2[(\lambda_3-a)(\lambda_3-c)-b^2-d^2] \qquad (18)$$

Similarly one can show that,

$$d^2(a-\lambda_1)(a-\lambda_2) = d^2[(\lambda_3-g)(\lambda_3-c)-b^2-d^2] \qquad (19)$$

Finally, as we substitute in eqn. (13), the results of eqns. (18) and (19), we get, after some cancellations,

$$V_1 \cdot V_2 = (c-\lambda_3)\,[(a-\lambda_3)(g-\lambda_3)(c-\lambda_3)-b^2(g-\lambda_3)-d^2(a-\lambda_3)] = 0 \qquad (20)$$

because the expression inside the square bracket of eqn. (20) after the first = sign, is zero, as can be seen by expanding the determinant (i.e., eqn. (2) after taking λ_i to be λ_3). This completes the proof. In a similar fashion it can be shown that,

$$V_1V_2 = V_2V_3 = V_3V_1 = 0 \qquad (21)$$

4. The Unitary Diagonalizing matrices

The orthonormal eigen vectors discussed in the last section can be used to write down the unitary diagonalizing matrix. Denoting the same by U, the expression for U is:

$$U = \begin{bmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{bmatrix} \qquad (22)$$

Using this metrix U and its transpose one can demonstrate the diagonalizability of X, i.e.,

$$\begin{bmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{bmatrix}^T \begin{bmatrix} a & b & 0 \\ b & c & d \\ 0 & d & g \end{bmatrix} \begin{bmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \qquad (23)$$

The essential details of diagonalization is relegated to the appendix. The process of diagonalization can be establed analytically. The same process employes the following relations,

$$U^TU = UU^T = I. \qquad (24)$$

This relation provides nine relations.

With the aid of these relations, it is possible to test the accuracy of the diagonal entries of the resulting diagonal matrix.

4.1 Testing the roots numerically

It's important to note that these roots play a crucial role, in the evaluation of the correlation function of the fields. There also exist few analytical techniques to keep track on the robustness of the magnitude of the estimated roots. One of them is using a condition that sets the angle inside the cosine to some known values like pi upon six or zero. In that case the estamates between vaious pair of the roots turn out to be very simple. One in principle can check that numerically by fixing the parameters accordingly. to provide an example, let us consider

$$A=C=G. \qquad (25)$$

As a consequence, the quantity Q of Cardan turns out to be zero. This can be verified numerically to test the goodness of the estimates. One can estimate further the difference between all possible combinations of the pair of roots– with the same condition. and verify that their difference comes in the ratio of 1 : 1 : 2 These are important quantities to keep track of because it provides the relative precision in the estimates each eigen-value.

5. Discussion

This paper discusses analytic diagonalization of 3x3 matrices without any approximation. That is to say exactly. Recalling that the field of applicability of this formalism, we realize that with the smallness of the parameters that enters the elements of the matrix, the estimations of the eigenvalue, eigenvectors and the unitary diagonalizing matrices– turns out to be challenging when precise estimates to high degree of accuracy are expected. Therefore, for a numerical prediction to be tallied with observational results, the numerical estimates need to pass the precision tests. Therefore, they should perform a precision calculation with inbuilt checks, having suitable processor and software capabilities. Hence, we have developed this method of analytical diagonalization. Incidentally the other methods of these estimates depend heavily on trigonometric functions. According to reports available in the media, the precision of the numbers generated by trigonometric operations are at times processor dependent. The same can not be said about floating point algebraic operations. Furthermore, the cpu time required for producing precise estimates using trigonometric functions often more than the same cohex one is using algebraic expressions. So using our analytic formulation of diagonalisation, one may save the cpu time (cost) and improve upon the precision. That justifies this alternative approach. We would lke to continue our investigatios for more involved situations, and would comeback to the intricacies of those in later publications.

6. Appendix

7. Proof: V's actually diagonalize the mixing matrix

The next proof involves that we are going to demonstrate is that the unitary matrix actually diagonilases the mixing matrix. To prove that we start from:

$$\begin{bmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{bmatrix}^T \begin{pmatrix} a & b & 0 \\ b & c & d \\ 0 & d & g \end{pmatrix} \begin{bmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{bmatrix} =$$

$$\begin{bmatrix} u_1 a + b v_1 & u_1 b + v_1 c + w_1 d & v_1 d + g w_1 \\ u_2 a + b v_2 & u_2 b + v_2 c + w_2 d & v_2 d + g w_2 \\ u_3 a + b v_3 & u_3 b + v_3 c + w_3 d & v_3 d + g w_3 \end{bmatrix} \begin{pmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{pmatrix} \quad (26)$$

Now if we recall (11), we see that,

$$au_1 + bv_1 = \lambda_1 u_1$$

$$bu_1 + cv_1 + dw_1 = \lambda_1 v_1 \quad (27)$$

$$dv_1 + gw_1 = \lambda_1 w_1$$

Similarly,

$$au_2 + bv_2 = \lambda_2 u_2$$

$$bu_2 + cv_2 + dw_2 = \lambda_2 v_2 \quad (28)$$

$$dv_2 + gw_2 = \lambda_2 w_2$$

And

$au_3 + bv_3 = \lambda_3 u_3$

$$bu_3 + cv_3 + dw_3 = \lambda_3 v_3 \qquad (29)$$

$dv_3 + gw_3 = \lambda_3 w_3$

So, we can substitute eqns. (27) to (29) in eqns. (27), to get:

$$\begin{bmatrix} u_1a + bv_1 & u_1v_1c + w_1dv_1 & d + gw_1 \\ u_2a + bv_2 & u_2v_2c + w_2dv_2 & d + gw_2 \\ u_3a + bv_3 & u_3v_3c + w_3dv_3 & d + gw_3 \end{bmatrix} \begin{pmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{pmatrix} = \begin{bmatrix} u_1\lambda_1 & v_1\lambda_1 & w_1\lambda_1 \\ u_2\lambda_2 & v_2\lambda_2 & w_2\lambda_2 \\ u_3\lambda_3 & v_3\lambda_3 & w_3\lambda_3 \end{bmatrix} \times$$

$$\begin{pmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{pmatrix} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \qquad (30)$$

In order to come to the last line, the orthogonality condition of the eigen vectors were are employed. So, we have checked that, the transformation matrix, constructed from the orthogonal vectors, actually diagonalize the mixing matrix. Hence the claim of diagonalization analytically is proved.

8. References

References

1] Weinberg S. (1975). The U(1) problem. Physical Review D 11, 3583. (1975)

[2] 't Hooft, G. (1976). Symmetry Breaking Through Bell-Jackiw anomalies Physical Review Letters, Vol.37, 8, (1976).

[3] 't Hooft, G. (1976). Computation of the quantum effects due to a four dimensional pseudoparticle. Physical Review D 14, 3432 (1978); (E) ibid. 18, 2199, (1978).

[4] R.J. Crewther (1978), "Effects of topological charge in gauge theories. Acta Phys. Austriaca Suppl. 19, 47.

[5] V. Baluni(1979) "CP violating effects in QCD", Physical Review D 19, 2227.

[6] R. J. Crewther, P. Di. Vecchia, G. Veneziano, E. Witten (1980) ,"Chiral estimates of the electric dipole moment of the neutron in quantum chromodynamics ", Physics Letters B, 88, 123; (E) ibid. B91, 487 (1980). 6

[7] F. Wilczek (1978), "Problem of Strong p and t Invariance in the Presence of Instantons," Physical Review Letters, Vol 40, 279.

[8] R. D. Peccei and H. R. Quinn (1977) , "CP Conservation in the Presence of Instantons," Physical Review Letters, Vol. 38, 1440. R. D. Peccei and H. R. Quinn(1977), "Constraints Imposed by CP Conservation in the Presence of Instantons," Physical Review D 16, 1791.

[9] S. Weinberg (1978) , "A New Light Boson?," Physical Review Letters, Vol 40, 223.

[10] R.D. Peccei (1996), (QCD, Strong CP and Axions). Journal of Korean Physics Society, 29, S199. [arXiv:hep-ph/9606475]. For a more extensive review of the strong CP problem, see in CP Violation, edited by C. Jarlskog (World Scientific, Singapore, 1989).

[11] M. S. Turner (1990) ,"Windows on the Axion," Physics Reports, Vol 197, 67.

[12] G. G. Raffelt (1990), "Astrophysical methods to constrain axions and other novel particle Physics Reports Vol 198, 1. G.G. Raffelt, in Proceedings of Beyond the Desert, edited by H.V. Klapder Kleingrothaus and H. Paes (Institute of Physics, Bristol, 1998), p. 808.

[13] G.G. Raffelt (1998), in Proceedings of 1997 European School of High-Energy Physics, edited by N. Ellis and M. Neubert (CERN, Geneva, 1998), p. 235. Report No. hep-ph/9712538.

[14] G.G. Raffelt (1996), Stars as Laboratories for Fundamental Physics (University of Chicago Press, Chicago, 1996).

[15] J. Preskill M. B. Wise and F. Wilczek (1983) Physics Letters,B 120, 127.

[16] M. Dine, W. Fischler and M. Srednicki (1981), "A Simple Solution to the Strong CP Problem with a Harmless Axion," Physics Letters, B104, 199.

[17] J. E. Kim (1979), "Weak Interaction Singlet and Strong CP Invariance," Physical Review Letters, Vol 43, 103.

[18] L. M. Krauss, J. Moody and F. Wilczek (1985), Physical Review. Letters, Vol.55, 1797.

[19] A. K, Ganguly (2006),"Axion Photon Mixing in Magnetized media", Annals Of Physics (N. Y.), Vol 321, 1457.

[20] G. Raffelt and D. Seckel (1988), "Bounds on Exotic Particle Interactions from SN 1987a," Physical Review Letters, Vol. 60, 1793.

[21] R. Cameron et al. (1993), "Search for nearly massless, weakly coupled particles by optical Physical Review D 47, 3707.

[22] Abe, K.; et al. (T2K Collaboration) (August 2013). "Evidence of electron neutrino appearance in a muon neutrino beam". Physical Review D. 88 (3) 032002.

[23] Avijit K. Ganguly, Pankaj Jain and Subhayan Mandal (2009): Photon and Axion Oscillation in a magnetized medium: A general treatment, Physical Review D 79, 115014.

[24] H. Goldstein, Classical Mechanics (Addison-Wesley,2002).

[25] Huber, Lindner, and Winter hep-ph/0407333,

[26] Anderson, Bai, Bischof, Blackford, Demmel, Dongarra, Du Croz, Greenbaum, Hammarling, McKenney et al. LAPACK Users' Guide, Society for Industrial and Applied Mathematics (ISBN 0-89871-447-8).

[27] M. Galassi et al., GNU Scientific Library Reference Manual, (Network Theory Ltd., 2003),

[28] W. H. Press, B. P.Flannery, S. A. Teukolsky,W. T. Vetterlin, Numerical Recipes in Fortran, (Cambridge University Press, 1990 San Francisco, CA)

[29] G. Cardano,,Ars Magna,(1545).