Pfaffian Notes

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1 Introduction

The Pfaffian is

$$\mathrm{Pf}A = \mathcal{A}[a_{12}a_{34}a_{45}...a_{N-1,N}] \tag{1}$$

where $\mathcal{A}$ is the antisymmetrization operator, the result is normalized such that every equivalent term occurs only once, and $a_{ij} = -a_{ji}$. For the case where $N = 4$ this becomes

$$\mathrm{Pf}A = [a_{12}a_{34} - a_{13}a_{24} + a_{14}a_{23}] \tag{2}$$

The Pfaffian is zero if N is odd and has $(N-1)!!$ terms otherwise.

The Pfaffian can be constructed recursively as

$$\begin{aligned}\mathrm{Pf}A &= \sum_{N-1 \text{ cyclic permutations of } 2-N} a_{12}\mathcal{A}[a_{34}a_{56}...a_{N-1,N}] \\ &\equiv \sum_{j=2}^{N} a_{1j}P_c(a_{1j})\end{aligned} \tag{3}$$

Since there are an odd number of indices in the cyclic exchange, the sign is positive. Here $P_c(a_{1j})$ is defined to be the Pfaffian cofactor of a_{1j}. For $N = 2$ it becomes

$$a_{12}a_{34} + a_{13}a_{42} + a_{14}a_{23} \tag{4}$$

and using $a_{42} = -a_{24}$ gives Eq. (2). $N = 6$ gives a slightly more complicated example with the pfaffian written as

$$a_{12}\mathcal{A}[a_{34}a_{56}] + a_{13}\mathcal{A}[a_{45}a_{62}] + a_{14}\mathcal{A}[a_{56}a_{23}] + a_{15}\mathcal{A}[a_{62}a_{34}] + a_{16}\mathcal{A}[a_{23}a_{45}]\,. \tag{5}$$

Applying Eq. (2) gives all 15 terms.

In general a skew-symmetric matrix A

$$A = \begin{pmatrix} 0 & a_{12} & a_{13} & a_{14} \\ -a_{12} & 0 & a_{23} & a_{24} \\ -a_{13} & -a_{23} & 0 & a_{34} \\ -a_{14} & -a_{24} & -a_{34} & 0 \end{pmatrix}, \tag{6}$$

is written and the pfaffian of this matrix is defined to be Eq.1. As seen below, the determinant of A is the square of the Pfaffian.

2 Computation of the Pfaffian

Let's try elmination on the 4x4 Skew-symmetric matrix. First note that we can pivot rows and columns of the matrix. For example interchanging rows and columns 1 and 3 gives the matrix with all $1 \leftrightarrow 3$ and the Pfaffian changes sign, but the determinant is invariant. This particular permutation moves the a_{23} element into the 12 position. Similar pivoting can be used to move a large element into the next position for a division.

Next notice that adding a multiple of row j to row k while adding the same multiple of column j to column k keeps the matrix in skew-symmetric form. Substituting this change into Eq. (3) shows that, just as in the calculation of a determinant, these add terms that are not antisymmetric and cancel. They therefore leave the pfaffian invariant.

Gauss elimination can start by using the column containing a_{12} to eliminate a_{13} and a_{14}. Exactly the same operations are used with the row containing $-a_{12}$ to eliminate $-a_{13}$ and $-a_{14}$. The matrix becomes

$$A' = \begin{pmatrix} 0 & a_{12} & 0 & 0 \\ -a_{12} & 0 & a_{23} & a_{24} \\ 0 & -a_{23} & 0 & a_{34} + \frac{a_{14}a_{23}}{a_{12}} - \frac{a_{13}a_{24}}{a_{12}} \\ 0 & -a_{24} & -a_{34} - \frac{a_{14}a_{23}}{a_{12}} + \frac{a_{13}a_{24}}{a_{12}} & 0 \end{pmatrix}. \tag{7}$$

Since the first row and first column only contain a_{12}, they can now be used to eliminate the other elements in the second row and column to give

$$A'' = \begin{pmatrix} 0 & a_{12} & 0 & 0 \\ -a_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & a_{34} + \frac{a_{14}a_{23}}{a_{12}} - \frac{a_{13}a_{24}}{a_{12}} \\ 0 & 0 & -a_{34} - \frac{a_{14}a_{23}}{a_{12}} + \frac{a_{13}a_{24}}{a_{12}} & 0 \end{pmatrix}. \tag{8}$$

Which immediately allows us to calculate the Pfaffian as the product of the nonzeo elements of the first subdiagonal. In general, the elimination step above gives the result a_{12} term times an (N-2)x(N-2) Pfaffian. Repeating will give the complete Pfaffian.

The matrix operation that goes from A to A' is

$$A' = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -\frac{a_{13}}{a_{12}} & 1 & 0 \\ 0 & -\frac{a_{14}}{a_{12}} & 0 & 1 \end{pmatrix} \underbrace{\begin{pmatrix} 0 & a_{12} & a_{13} & a_{14} \\ -a_{12} & 0 & a_{23} & a_{24} \\ -a_{13} & -a_{23} & 0 & a_{34} \\ -a_{14} & -a_{24} & -a_{34} & 0 \end{pmatrix}}_{A} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -\frac{a_{13}}{a_{12}} & -\frac{a_{14}}{a_{12}} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{9}$$

and including the terms to go to A'' gives

$$A'' = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{a_{23}}{a_{12}} & -\frac{a_{13}}{a_{12}} & 1 & 0 \\ \frac{a_{24}}{a_{12}} & -\frac{a_{14}}{a_{12}} & 0 & 1 \end{pmatrix} \underbrace{\begin{pmatrix} 0 & a_{12} & a_{13} & a_{14} \\ -a_{12} & 0 & a_{23} & a_{24} \\ -a_{13} & -a_{23} & 0 & a_{34} \\ -a_{14} & -a_{24} & -a_{34} & 0 \end{pmatrix}}_{A} \begin{pmatrix} 1 & 0 & \frac{a_{23}}{a_{12}} & \frac{a_{24}}{a_{12}} \\ 0 & 1 & -\frac{a_{13}}{a_{12}} & -\frac{a_{14}}{a_{12}} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{10}$$

We see that the Pfaffian can be calculated by the same factorization used to find the inverse. Here is a Fortran code to calculate the Pfaffian of a given complex skew symmetric matrix. No pivoting is used for clarity, but a production code must pivot for stability. In the i loop below, searching for the largest magnitude element a_{in} with $n > i$ and pivoting this row and column to the $i+1$ position gives good results.

```
   subroutine pfafnopivot(a,n,p)
!
! no pivoting, destroys a, pfaffian returned in p
!
   integer(kind=4) :: n,i,j
   complex(kind=8) :: a(n,n),p,fac
   if (mod(n,2).ne.0) then
      p=(0.0d0,0.0d0)
      return
   endif
   p=(1.0d0,0.0d0)
   do i=1,n,2
      do j=i+2,n
         fac=-a(i,j)/a(i,i+1)
         a(i+1:n,j)=a(i+1:n,j)+fac*a(i+1:n,i+1)
         a(j,i+1:n)=a(j,i+1:n)+fac*a(i+1,i+1:n)
      enddo
      p=p*a(i,i+1)
   enddo
   return
   end subroutine pfafnopivot
```

Returning to the pfaffian calculation, the Gaussian transformation matrices used have determinant 1. Taking the determinant of both sides of Eq. 10, the determinant of A'' is trivially calculated to be the square of the Pfaffian. The determinant of the right hand side is the product of the determinants and since the Gaussian elmination matrices have determinant one, we see that the determinant of a skew-symmetric matrix is the square of its Pfaffian. While Eq. 10 is written for a 4x4 matrix, it should be obvious that the result holds by Gaussian elimination of a general skew-symmetric matrix. Notice that a matrix with N odd will necessarily have a zero determinant and Pfaffian.

Cayley showed[**?**] (according to Knuth[**?**])

$$
\mathrm{Det}\begin{pmatrix}
0 & b_{12} & b_{13} & \ldots & b_{1,N} \\
-a_{12} & 0 & a_{23} & \ldots & a_{2,N} \\
. & . & . & . & . \\
. & . & . & . & . \\
. & . & . & . & . \\
-a_{1N} & -a_{2N} & -a_{3N} & \ldots & 0
\end{pmatrix} =
$$

$$
\mathrm{Pf}\begin{pmatrix} 0 & a_{12} & a_{13} & \ldots & a_{1,N} \\ -a_{12} & 0 & a_{23} & \ldots & a_{2,N} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ -a_{1N} & -a_{2N} & -a_{3N} & \ldots & 0 \end{pmatrix} \qquad \mathrm{Pf}\begin{pmatrix} 0 & b_{12} & b_{13} & \ldots & b_{1,N} \\ -b_{12} & 0 & a_{23} & \ldots & a_{2,N} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ -b_{1N} & -a_{2N} & -a_{3N} & \ldots & 0 \end{pmatrix}. \tag{11}
$$

This shows that the Pfaffian obtained by changing the space or spin coordinates of one particle can be calculated from the inverse, determinant and Pfaffian of A in order N operations. That is calling B the matrix with the first row and column changed, its Pfaffian is

$$
\mathrm{Pf}B = \frac{\mathrm{Det}A \sum_j b_{1j} A^{-1}_{j1}}{\mathrm{Pf}A} \tag{12}
$$

or since the square of the Pfaffian is the determinant,

$$
\mathrm{Pf}B = \mathrm{Pf}A \sum_j b_{1j} A^{-1}_{j1} \tag{13}
$$

which shows that the inverse transpose times the Pfaffian is the Pfaffian cofactor.

We can derive Cayley's result by using Eq. (3) and the result that the square of the Pfaffian is the determinant to write

$$
\mathrm{Det}A = \sum_k a_{1k} P_c(a_{1k}) \sum_j a_{1j} P_c(a_{1j}) \tag{14}
$$

Notice that the only way that both elements a_{1k} and a_{1j} can appear in the determinant is if one is from row 1 and the other from column 1. We can therefore replace one of the a_{1k} or a_{1j} with b. Since they enter in a symmetric manner we get the determinant of the left hand matrix of Eq. 11 as

$$
\sum_k a_{1k} P_c(a_{1k}) \sum_j b_{1j} P_c(a_{1j}) \tag{15}
$$

which demonstrates his result.

For efficient algorithms with spin-dependent potentials we want to be able to change two particles. A straightforward implementation would first change 1 row of the matrix as above and calculate the new Pfaffian, and update the inverse. Then change the corresponding column to obtain the skew-symmetric matrix and its inverse (its determinant is the square of the Pfaffian obtained before). This will require $O(N^2)$ operations. For each of the N second particles we will require $O(N)$ operations to calculate the new Pfaffian if the first column is different for each pair. Unfortunately the result is $O(N^4)$ to calculate pairwise potentials.

However, for our case, the operation needed on a column or row is independent of the other column or row (except for the common element). We can therefore imagine doing a single update for particle 1 and using this for all the terms where the pair contains particle 1. The common element does not require an update and can be done separately.

It is most efficient to write this as a set of matrix multiplies. We define the new column j of the matrix to be C_{ij}, corresponding to a spin or derivative operator on particle j. Defining

$$
P_{ij} = \sum_k A^{-1}_{ik} C_{kj}
$$

$$G_{ij} = \sum_{mk} C^T_{im} A^{-1}_{mk} C_{kj} = \sum_m C_{mi} P_{mj} = -G_{ji} \tag{16}$$

we find that the ratio of the new to old Pfaffians with the two rows and columns denoted by α and β changed is

$$\frac{\mathrm{Pf(new)}}{\mathrm{Pf(old)}} = A^{-1}_{\beta\alpha}[A^{new}_{\alpha\beta} + G_{\alpha\beta}] + P_{\alpha\alpha}P_{\beta\beta} - P_{\alpha\beta}P_{\beta\alpha} \tag{17}$$

The expression is independent of the value of the $C_{\alpha\beta}$ or $C_{\beta\alpha}$ terms, i.e. they have already been subtracted off. The first term is the single element piece.

The inverse update of a skew-symmetric matrix when changing a single row and column of the matrix keeping it skew symmetric can be done with a Fortran routine like:

```
   subroutine updateinv(a,row,i,n)
   complex(kind=8) :: a(n,n),row(n),prod(n)
   integer(kind=4) :: i,j,n
!
! update row and column using skew-symmetry of matrix
!
    call zgemv('n',n,n,(1.0d0,0.0d0),a,n,row,1,(0.0d0,0.0d0),prod,1)
    a(i,:)=-a(i,:)/prod(i)
    a(:,i)=-a(:,i)/prod(i)
    do j=1,n
       if (j.ne.i) then
          a(j,:)=a(j,:)+prod(j)*a(i,:)
          a(:,j)=a(:,j)+prod(j)*a(:,i)
       endif
    enddo
   return
   end subroutine updateinv
```

where *a(n,n)* is the inverse matrix, *row* is the new row *i*, and *zgemv* is the BLAS complex matrix vector multiply. The ratio of the new to old pfaffians can be returned as the value of *prod(i)* if desired.

3 The determinant as bipartite Pfaffian

If the skew symmetric matrix is bipartite in the sense that if $a_{ij} \neq 0$ and $a_{i'j'} \neq 0$, then $a_{ii'} = a_{j,j'} = 0$, and we can pivot the matrix into the form

$$\begin{pmatrix} 0 & B \\ -B^T & 0 \end{pmatrix} . \tag{18}$$

Here B is the matrix of nonzero elements of A, B^T is the transpose of B, and 0 is the zero matrix. The Pfaffian of this matrix is the deteminant of B.

4 Pairing Wave Functions

A pairing wave function can be written in the form

$$a_{12} = \phi(\vec{r}_1, s_1; \vec{r}_2 s_2)\,. \tag{19}$$

Often better coordinates would be the relative and center of mass positions along with the spin singlet and triplet state amplitudes. Notice that with spin singlet pairing, evaluating the Pfaffian with particles 1 through $N/2$ up and $N/2+1$ through N down gives a bipartite matrix as in Eq. 18, and the singlet pairing function can be written as a determinant.

5 Combinations of paired and unpaired orbitals

A general state with n paired and o unpaired orbitals for a total of $N = 2n + o$ particles can be written as

$$\mathcal{A}[\phi_{12}\phi_{34}...\phi_{2n-1,2n}...\psi_1(2n+1)...\psi_o(N)] \tag{20}$$

which is the pfaffian of the $(N+o)\times(N+o)$ matrix

$$A = \begin{pmatrix} 0 & \phi_{12} & \phi_{13} & ... & \phi_{1N} & \psi_1(1) & ... & \psi_o(1) \\ -\phi_{12} & 0 & \phi_{23} & ... & \phi_{2N} & \psi_1(2) & ... & \psi_o(2) \\ -\phi_{13} & \phi_{23} & 0 & ... & \phi_{3N} & \psi_1(3) & ... & \psi_o(3) \\ \vdots & \vdots & \vdots & \vdots\vdots\vdots & \vdots & \vdots & \vdots\vdots\vdots & \vdots \\ -\phi_{1N} & -\phi_{2N} & -\phi_{3N} & ... & 0 & \psi_1(N) & ... & \psi_o(N) \\ -\psi_1(1) & -\psi_1(2) & -\psi_1(3) & ... & -\psi_1(N) & 0 & ... & 0 \\ \vdots & \vdots & \vdots & \vdots\vdots\vdots & \vdots & \vdots & \vdots\vdots\vdots & \vdots \\ -\psi_o(1) & -\psi_o(2) & -\psi_o(3) & ... & -\psi_o(N) & 0 & ... & 0 \end{pmatrix}, \tag{21}$$

where the lower $o\times o$ section is all zeroes.