

Hyper-Pfaffian for quartet wave function

Takahiro Mizusaki

Institute of Natural Sciences, Senshu University, 101-8425, Japan

Peter Schuck

Institut de Physique Nucléaire, F-91406 Orsay CEDEX, France

We found that the overlap matrix element between M -scheme state and quartet wave function, which plays an essential role in the variational Monte Carlo method, can be represented by the hyper-Pfaffian with $k = 4$. The hyper-Pfaffian is not well-known and seems not to have many useful mathematical properties, and is difficult for numerical computation. To overcome this difficulty, we found that the hyper-Pfaffian with $k = 4$ for the alpha-like quartet wave function can be reduced into the sum of usual Pfaffians, by which its numerical evaluation becomes faster and feasible. We present its formula up to $n = 3$, which corresponds to a 12-particle system.

I. INTRODUCTION

In the long history of the quantum many-body problem, the pairing correlation has been one of the central and most interesting issues. As its microscopic theory, Bardeen-Cooper-Schrieffer (BCS) theory[1], Hartree-Fock Bogolyubov (HFB) theory, projected HFB theories [2] and so on have been developed and various phenomena, which are manifestations of the pairing correlation, have been clarified.

Very recently it turned out that the number conserved or number projected BCS and HFB wave functions can be shown by the Pfaffian. One successful application is to solve the minus-sign problem of the Onishi formula[3–5]. The Pfaffian is also turned out to be very useful to express Wick's theorem [6–9] and it is useful to extend the multi quasi-particle calculation with the projection technique[10, 11]. Another successful application is the variational Monte Carlo method with the Pfaffian wave function[12–15].

In some cases of the quantum systems, quartet correlation is also essential. The alpha particle, which consists of two protons and two neutrons, is a good example. For nuclei, the alpha correlation often plays a decisive role. A mathematical expression for such four particle correlation is, however, unknown, unlike the Pfaffian for the pairing correlation. We could successfully extend the Pfaffian idea for four particle correlation, but we also found that such expression is also known as hyper-Pfaffian for mathematicians, by searching mathematical papers[16–23], where there are several definitions of the hyper-Pfaffian. What we found is exactly the same as one of the definitions. Unlike the Pfaffian, the

hyper-Pfaffian, unfortunately, seems to have no good mathematical relations. It is quite inconvenient for physicists to use it. In this paper, we found out some relations to compute the hyper-Pfaffian for alpha-like quartet wave functions.

II. PFAFFIAN

First we discuss the definition of the Pfaffian. Although there are several ways to define the Pfaffian, here we define the Pfaffian for a skew-symmetric matrix $A = (a_{ij})$ with dimension $2n \times 2n$ as follows:

$$Pf(A) \equiv \sum_{\sigma} \text{sgn}(\sigma) \prod_{i=1}^n a_{\sigma(2i-1)\sigma(2i)}, \quad (1)$$

where the σ is a permutation of $\{1, 2, 3, \dots, 2n\}$ with the condition of

$$\begin{aligned} \sigma(2i-1) < \sigma(2i) \text{ for } 1 \leq i \leq n \\ \sigma(1) < \sigma(3) < \dots < \sigma(2n-1). \end{aligned} \quad (2)$$

The Pfaffian has many mathematical relations. Among them, the following as

$$Pf(A)^2 = Det(A) \quad (3)$$

represents a fundamental relation between well-known determinant and the Pfaffian. However, in the following hyper-Pfaffian, this extension is not valid. Moreover, various relations for the Pfaffian cannot also be unfortunately extended.

III. DEFINITIONS OF HYPER-PFAFFIAN

Historically the generalization of the determinant concerning a higher order tensor (multi-dimensional array, hypermatrix) was discovered by Arthur Cayley in 1845 [24] and is called the hyper-Determinant. On the other hand, the generalization of the Pfaffian was recently and first introduced by Alexander I. Barvinok[16].

According to the Barvinok paper[16], the hyper-Pfaffian is defined by

$$Pf^{[k]}(M) \equiv \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_r} \text{sgn}(\sigma) \prod_{i=1}^n M_{\sigma(k(i-1)+1), \sigma(k(i-1)+2), \dots, \sigma(ki)} \quad (4)$$

with $r = kn$ for some $n \in \mathfrak{N}$ and a k -dimensional tensor with order r ,

$$M = \{M_{i_1, \dots, i_k} : 1 \leq i_1, \dots, i_k \leq r\}. \quad (5)$$

Product part of Eq.(4) is an n -product of M components as

$$M_{\sigma(1), \dots, \sigma(k)} \cdots M_{\sigma((k(n-1)+1), \dots, \sigma(kn))}. \quad (6)$$

We call it the Barvinok hyper-Pfaffian. In the case of $k = 2$, the Barvinok hyper-Pfaffian is not reduced to the usual Pfaffian.

Next, we consider the definition of the hyper-Pfaffian by Jean-Gabriel Luque and Jean-Yves Thibon [17], who generalize the Pfaffian defined in Eqs. (1) and (2) in a natural way. For the tensor M_{i_1, \dots, i_k} , which has a property as

$$M_{i_{\sigma(1)}, \dots, i_{\sigma(k)}} = \text{sgn}(\sigma) M_{i_1, \dots, i_k}, \quad (7)$$

the hyper-Pfaffian is defined as

$$Pf^{[k]}(M) \equiv \sum_{\sigma \in \mathfrak{S}_{kn, k}} \text{sgn}(\sigma) \prod_{i=1}^n M_{\sigma(k(i-1)+1), \sigma(k(i-1)+2), \dots, \sigma(ki)} \quad (8)$$

where summation is taken over

$$\begin{aligned} \mathfrak{S}_{kn, k} \equiv \{ \sigma \in \mathfrak{S}_{kn} \mid & \sigma(k(i-1)+1) < \cdots < \sigma(ki), \\ & \sigma(k(p-1)+1) < \sigma(kp+1), \\ & 1 \leq i \leq n, 1 \leq p \leq n-1 \}. \end{aligned} \quad (9)$$

The second condition means $\sigma(1) < \sigma(k+1) < \cdots < \sigma(kn-k+1)$. We call this definition the Luque-Thibon hyper-Pfaffian. In the case of $k = 2$, the Luque-Thibon hyper-Pfaffian reduces to the same as the usual Pfaffian. What we discovered in the quantum many-body problem was just the same as the Luque-Thibon hyper-Pfaffian. Note that, in the thesis of Daniel Redelmeier[19], there is a brief comment on these two definitions of the hyper-Pfaffian.

There is an alternative definition of the hyper-Pfaffian, which is defined by Sho Matsumoto [21]. For a tensor M with

$$M_{i_{\tau(1)}, \dots, i_{\tau(2k)}} = \text{sgn}(\tau_1) \cdots \text{sgn}(\tau_k) M_{i_1, \dots, i_{2k}}, \quad (10)$$

for any permutations $(\tau_1, \dots, \tau_k) \in (\mathfrak{S}_2)^k$, the hyper-Pfaffian is defined as

$$Pf^{[2k]}(M) \equiv \frac{1}{n!} \sum_{\sigma_1, \dots, \sigma_m \in \mathfrak{E}_{2n}} \text{sgn}(\sigma_1 \cdots \sigma_m) \prod_{i=1}^n M_{\sigma_1(2i-1), \sigma_1(2i), \dots, \sigma_m(2i-1), \sigma_m(2i)}, \quad (11)$$

where

$$\mathfrak{E}_{2n} \equiv \{ \sigma \in \mathfrak{S}_{2n} \mid \sigma(2i-1) < \sigma(2i), 0 \leq i \leq n \}. \quad (12)$$

We call it the Matsumoto hyper-Pfaffian. Hereafter, we consider the Luque-Thibon hyper-Pfaffian.

IV. HYPER-PFAFFIAN AND QUARTET CORRELATION

In the quantum many-body problem[12–15], the following simplified matrix element plays an important role for the pairing correlation, as

$$\langle c_{2n} \cdots c_1 | e^{\sum_{i<j}^{2n} z_{ij} c_i^\dagger c_j^\dagger} \rangle \quad (13)$$

where $z_{ij} = -z_{ji}$ and $c_1^\dagger, \dots, c_{2n}^\dagger$ are fermion creation operators. Note that we only consider the particular case, but we easily generalize it[5].

The expansion of this exponent is given by

$$e^Z |-\rangle = \left(1 + Z + \frac{1}{2!} Z^2 + \frac{1}{3!} Z^3 + \cdots + \frac{1}{n!} Z^n\right) |-\rangle \quad (14)$$

where $Z = \sum_{i<j}^{2n} z_{ij} c_i^\dagger c_j^\dagger$. This expansion series terminates at n because of the Pauli's exclusion principle. Therefore, the above matrix element is given by

$$\langle c_{2n} \cdots c_1 | e^{\sum_{i<j}^{2n} z_{ij} c_i^\dagger c_j^\dagger} \rangle = \frac{1}{n!} \langle - | c_{2n} \cdots c_1 Z^n | - \rangle. \quad (15)$$

For $n = 1$,

$$\langle - | c_2 c_1 \sum_{i,j=1}^2 z_{ij} c_i^\dagger c_j^\dagger | - \rangle = \langle - | c_2 c_1 z_{12} c_1^\dagger c_2^\dagger | - \rangle = z_{12} = Pf \begin{pmatrix} 0 & z_{12} \\ & 0 \end{pmatrix}, \quad (16)$$

where the lower matrix elements are suppressed due to the anti-symmetry of the matrix. This suppression is used hereafter. For $n = 2$,

$$\begin{aligned} \frac{1}{2!} \langle - | c_4 c_3 c_2 c_1 \sum_{i<j}^4 z_{ij} c_i^\dagger c_j^\dagger \sum_{p<q}^4 z_{pq} c_p^\dagger c_q^\dagger | - \rangle &= z_{12} z_{34} - z_{13} z_{24} + z_{14} z_{23} \\ &= Pf \begin{pmatrix} 0 & z_{12} & z_{13} & z_{14} \\ & 0 & z_{23} & z_{24} \\ & & 0 & z_{34} \\ & & & 0 \end{pmatrix}. \end{aligned} \quad (17)$$

In general, by noting the following relation as

$$\begin{aligned} \frac{1}{n!} Z^n &= \frac{1}{n!} \sum_{i_1 < j_1}^{2n} \cdots \sum_{i_n < j_n}^{2n} z_{i_1 j_1} c_{i_1}^\dagger c_{j_1}^\dagger \cdots z_{i_n j_n} c_{i_n}^\dagger c_{j_n}^\dagger \\ &= \sum_{i_1 < j_1, \dots, i_n < j_n \text{ and } i_1 < \dots < i_n}^{2n} z_{i_1 j_1} \cdots z_{i_n j_n} c_{i_1}^\dagger c_{j_1}^\dagger \cdots c_{i_n}^\dagger c_{j_n}^\dagger, \end{aligned} \quad (18)$$

we can obtain the general overlap as

$$\langle c_{2n} \cdots c_1 | e^{\sum_{i < j}^{2n} z_{ij} c_i^\dagger c_j^\dagger} \rangle = \sum_{\sigma \in \mathfrak{S}_n} \text{sgn}(\sigma) z_{\sigma(1)\sigma(2)} \cdots z_{\sigma(2n-1)\sigma(2n)}, \quad (19)$$

where the permutation σ runs under the condition, $i_1 < j_1, \dots, i_n < j_n$ and $i_1 < \dots < i_n$. Therefore, this overlap matrix element is shown by the Pfaffian as

$$\langle c_{2n} \cdots c_1 | e^{\sum_{i < j}^{2n} z_{ij} c_i^\dagger c_j^\dagger} \rangle = Pf \begin{pmatrix} 0 & z_{1,2} & \cdots & z_{1,2n} \\ & 0 & & \vdots \\ & & \ddots & z_{2n-1,2n} \\ & & & 0 \end{pmatrix}. \quad (20)$$

More complete explanation is given in [5, 13].

Next, we consider the exponential operator of quartet correlation,

$$\langle c_{4n} \cdots c_1 | e^{\sum_{i < j < l < m}^{4n} z_{ijlm} c_i^\dagger c_j^\dagger c_l^\dagger c_m^\dagger} \rangle \quad (21)$$

where $z_{\sigma(i)\sigma(j)\sigma(l)\sigma(m)} = \text{sgn}(\sigma) z_{ijlm}$ for any permutations σ . This form is a straightforward generalization of the pairing correlation Eq.(13). In the same way as the above derivation of the pairing correlation, we can obtain the closed form as

$$\begin{aligned} & \langle c_{4n} \cdots c_1 | e^{\sum_{i < j < l < m}^{4n} z_{ijlm} c_i^\dagger c_j^\dagger c_l^\dagger c_m^\dagger} \rangle \\ &= \sum_{\sigma \in \mathfrak{S}_{4n,4}} \text{sgn}(\sigma) z_{\sigma(1)\sigma(2)\sigma(3)\sigma(4)} \cdots z_{\sigma(4n-3)\sigma(4n-2)\sigma(4n-1)\sigma(4n)} \\ &= \sum_{\sigma \in \mathfrak{S}_{4n,4}} \text{sgn}(\sigma) \prod_{i=1}^n z_{\sigma(4i-3),\sigma(4i-2),\dots,\sigma(4i)} \end{aligned} \quad (22)$$

with

$$\begin{aligned} \mathfrak{S}_{4n,4} \equiv \{ \sigma \in \mathfrak{S}_{4n} \mid & \sigma(4i-3) < \cdots < \sigma(4i), \\ & \sigma(1) < \sigma(5) < \cdots < \sigma(4n-3), \\ & 1 \leq i \leq n \}. \end{aligned} \quad (23)$$

Therefore, this overlap matrix element can be expressed by the Luque-Thibon hyper-Pfaffian Eqs.(8,9) with $k = 4$ as

$$\langle c_{4n} \cdots c_1 | e^{\sum_{i < j < l < m}^{4n} z_{ijlm} c_i^\dagger c_j^\dagger c_l^\dagger c_m^\dagger} \rangle = Pf_{Luque-Thibon}^{[4]}(Z). \quad (24)$$

V. HYPER-PFAFFIAN WITH $k = 4$

According to the definition of the Pfaffian Eqs.(1) and (2), the number of terms satisfying the condition (2) is $\frac{(2n)!}{(2!)^{n!}} = (2n - 1)!!$ where $2n$ is a dimension of matrix of the Pfaffian, namely, 1, 3, 15, 105, 945, 10395, 135135, \dots . In the numerical evaluation of the Pfaffian, it is, however, unnecessary to use such terms explicitly. We can use fast computational methods [25].

Next, we consider the hyper-Pfaffian. According to Eq. (9) with $k = 4$, the number of terms is $\frac{(4n)!}{(4!)^{n!}}$, that is, 1, 35, 5775, 2627625, 2546168625, 4509264634875, \dots . It increases explosively, but a fast computational method has not been known yet.

For example, we consider the $n = 1$.

$$Pf^{[4]} [Z] = z_{1234}, \quad (25)$$

For $n = 2$,

$$\begin{aligned} Pf^{[4]} (Z) = & z_{1234}z_{5678} - z_{1235}z_{4678} + z_{1236}z_{4578} - z_{1237}z_{4568} + z_{1238}z_{4567} + z_{1245}z_{3678} \\ & - z_{1246}z_{3578} + z_{1247}z_{3568} - z_{1248}z_{3567} + z_{1256}z_{3478} - z_{1257}z_{3468} + z_{1258}z_{3467} \\ & + z_{1267}z_{3458} - z_{1268}z_{3457} + z_{1278}z_{3456} - z_{1345}z_{2678} + z_{1346}z_{2578} - z_{1347}z_{2568} \\ & + z_{1348}z_{2567} - z_{1356}z_{2478} + z_{1357}z_{2468} - z_{1358}z_{2467} - z_{1367}z_{2458} + z_{1368}z_{2457} \\ & - z_{1378}z_{2456} + z_{1456}z_{2378} - z_{1457}z_{2368} + z_{1458}z_{2367} + z_{1467}z_{2358} - z_{1468}z_{2357} \\ & + z_{1478}z_{2356} - z_{1567}z_{2348} + z_{1568}z_{2347} - z_{1578}z_{2346} + z_{1678}z_{2345}. \end{aligned} \quad (26)$$

For $n \geq 3$, a computer calculation is needed to enumerate all terms.

For some quantum systems, the alpha-like correlation plays a decisive role. Therefore we consider a special case for the Z tensor, which obeys the condition as $z_{ijkl} = 0$ for $i > m$ or $j > m$ or $k \leq m$ or $l \leq m$ where $2m = n$. For $n = 2$, the hyper-Pfaffian is composed of

$$\begin{aligned} Pf^{[4]} (Z) = & z_{1256}z_{3478} - z_{1257}z_{3468} + z_{1258}z_{3467} + z_{1267}z_{3458} - z_{1268}z_{3457} + z_{1278}z_{3456} \\ & - z_{1356}z_{2478} + z_{1357}z_{2468} - z_{1358}z_{2467} - z_{1367}z_{2458} + z_{1368}z_{2457} - z_{1378}z_{2456} \\ & + z_{1456}z_{2378} - z_{1457}z_{2368} + z_{1458}z_{2367} + z_{1467}z_{2358} - z_{1468}z_{2357} + z_{1478}z_{2356}. \end{aligned} \quad (27)$$

The number of terms is $(\frac{4!}{2!2!})^2 \times 2 = 18$. At the first line of Eq.(27), the index (1, 2), (3, 4) is fixed and is recasted by the Pfaffian as

$$Pf \begin{pmatrix} 0 & z_{1256} & z_{1257} & z_{1258} \\ & 0 & z_{3467} & z_{3468} \\ & & 0 & z_{3478} \\ & & & 0 \end{pmatrix} + Pf \begin{pmatrix} 0 & z_{3456} & z_{3457} & z_{3458} \\ & 0 & z_{1267} & z_{1268} \\ & & 0 & z_{1278} \\ & & & 0 \end{pmatrix} \quad (28)$$

where the second term is again obtained from the first term by changing $(1, 2) \leftrightarrow (3, 4)$. At the second line of Eq.(27), the index $(1, 3), (2, 4)$ is fixed and is recasted by the Pfaffian as

$$-Pf \begin{pmatrix} 0 & z_{1356} & z_{1357} & z_{1358} \\ & 0 & z_{2467} & z_{2468} \\ & & 0 & z_{2478} \\ & & & 0 \end{pmatrix} - Pf \begin{pmatrix} 0 & z_{2456} & z_{2457} & z_{2458} \\ & 0 & z_{1367} & z_{1368} \\ & & 0 & z_{1378} \\ & & & 0 \end{pmatrix} \quad (29)$$

where the second term is obtained from the first term by changing $(1, 3) \leftrightarrow (2, 4)$. In the same way, the third line of Eq.(27) is recasted by the Pfaffian as

$$Pf \begin{pmatrix} 0 & z_{1456} & z_{1457} & z_{1458} \\ & 0 & z_{2367} & z_{2368} \\ & & 0 & z_{2378} \\ & & & 0 \end{pmatrix} + Pf \begin{pmatrix} 0 & z_{2356} & z_{2357} & z_{2358} \\ & 0 & z_{1467} & z_{1468} \\ & & 0 & z_{1478} \\ & & & 0 \end{pmatrix} \quad (30)$$

where the second term is obtained from the first term by changing $(2, 3) \leftrightarrow (1, 4)$.

By defining the following matrix as

$$Z_{ab,cd} \equiv \begin{pmatrix} 0 & z_{ab56} & z_{ab57} & z_{ab58} \\ & 0 & z_{cd67} & z_{cd68} \\ & & 0 & z_{cd78} \\ & & & 0 \end{pmatrix}, \quad (31)$$

we can express the hyper-Pfaffian with alpha-like correlation as

$$\begin{aligned} Pf^{[4]}(Z) &= Pf(Z_{12,34}) - Pf(Z_{13,24}) + Pf(Z_{14,23}) \\ &\quad + Pf(Z_{34,12}) - Pf(Z_{24,13}) + Pf(Z_{23,14}) \\ &= \sum_{\sigma \in \mathfrak{S}_4} \text{sgn}(\sigma) Pf(Z_{\sigma(1)\sigma(2),\sigma(3)\sigma(4)}), \end{aligned} \quad (32)$$

where

$$\sigma(1) < \sigma(2), \quad \sigma(3) < \sigma(4). \quad (33)$$

In general, the number of terms can be shown by $\frac{(2n)!}{(2!)^n n!} 2n!$, that is, 1, 18, 1350, 264600, 107163000, \dots . The increase as a function of n is somewhat moderate compared to general quartet correlation but is still hard to direct numerical computation based on the definition if n increases. Therefore, we investigate the case of $n = 3$ in detail. As the number of terms of this case is 1350, we only show 15 terms, satisfying with

$z_{1,2,a,b}z_{3,4,c,d}z_{5,6,e,f}$, ($a < c < e$) below,

$$\begin{aligned}
& z_{1,2,7,8}z_{3,4,9,10}z_{5,6,11,12} - z_{1,2,7,8}z_{3,4,9,11}z_{5,6,10,12} + z_{1,2,7,8}z_{3,4,9,12}z_{5,6,10,11} \\
& - z_{1,2,7,9}z_{3,4,8,10}z_{5,6,11,12} + z_{1,2,7,9}z_{3,4,8,11}z_{5,6,10,12} - z_{1,2,7,9}z_{3,4,8,12}z_{5,6,10,11} \\
& + z_{1,2,7,10}z_{3,4,8,9}z_{5,6,11,12} - z_{1,2,7,10}z_{3,4,8,11}z_{5,6,9,12} + z_{1,2,7,10}z_{3,4,8,12}z_{5,6,9,11} \\
& - z_{1,2,7,11}z_{3,4,8,9}z_{5,6,10,12} + z_{1,2,7,11}z_{3,4,8,10}z_{5,6,9,12} - z_{1,2,7,11}z_{3,4,8,12}z_{5,6,9,10} \\
& + z_{1,2,7,12}z_{3,4,8,9}z_{5,6,10,11} - z_{1,2,7,12}z_{3,4,8,10}z_{5,6,9,11} + z_{1,2,7,12}z_{3,4,8,11}z_{5,6,9,10}.
\end{aligned} \tag{34}$$

These 15 terms can be shown by two Pfaffians and lower matrix element is again omitted due to anti-symmetry as

$$\begin{aligned}
& z_{1,2,7,8}z_{3,4,9,10}z_{5,6,11,12} - z_{1,2,7,8}z_{3,4,9,11}z_{5,6,10,12} + z_{1,2,7,8}z_{3,4,9,12}z_{5,6,10,11} \\
& = z_{1,2,7,8} Pf \begin{pmatrix} 0 & z_{3,4,9,10} & z_{3,4,9,11} & z_{3,4,9,12} \\ & 0 & z_{5,6,10,11} & z_{5,6,10,12} \\ & & 0 & z_{5,6,11,12} \\ & & & 0 \end{pmatrix},
\end{aligned} \tag{35}$$

and

$$\begin{aligned}
& - z_{1,2,7,9}z_{3,4,8,10}z_{5,6,11,12} + z_{1,2,7,9}z_{3,4,8,11}z_{5,6,10,12} - z_{1,2,7,9}z_{3,4,8,12}z_{5,6,10,11} \\
& + z_{1,2,7,10}z_{3,4,8,9}z_{5,6,11,12} - z_{1,2,7,10}z_{3,4,8,11}z_{5,6,9,12} + z_{1,2,7,10}z_{3,4,8,12}z_{5,6,9,11} \\
& - z_{1,2,7,11}z_{3,4,8,9}z_{5,6,10,12} + z_{1,2,7,11}z_{3,4,8,10}z_{5,6,9,12} - z_{1,2,7,11}z_{3,4,8,12}z_{5,6,9,10} \\
& + z_{1,2,7,12}z_{3,4,8,9}z_{5,6,10,11} - z_{1,2,7,12}z_{3,4,8,10}z_{5,6,9,11} + z_{1,2,7,12}z_{3,4,8,11}z_{5,6,9,10} \\
& = Pf \begin{pmatrix} 0 & 0 & z_{1,2,7,9} & z_{1,2,7,10} & z_{1,2,7,11} & z_{1,2,7,12} \\ & 0 & z_{3,4,8,9} & z_{3,4,8,10} & z_{3,4,8,11} & z_{3,4,8,12} \\ & & 0 & z_{5,6,9,10} & z_{5,6,9,11} & z_{5,6,9,12} \\ & & & 0 & z_{5,6,10,11} & z_{5,6,10,12} \\ & & & & 0 & z_{5,6,11,12} \\ & & & & & 0 \end{pmatrix}.
\end{aligned} \tag{36}$$

Thus, we define the following matrices as

$$Z_{cd,ef}^2 \equiv \begin{pmatrix} 0 & z_{cd9,10} & z_{ef9,11} & z_{ef9,12} \\ & 0 & z_{ef10,11} & z_{ef10,12} \\ & & 0 & z_{ef11,12} \\ & & & 0 \end{pmatrix}, \tag{37}$$

and

$$Z_{ab,cd,ef}^3 \equiv \begin{pmatrix} 0 & 0 & z_{ab79} & z_{ab7,10} & z_{ab7,11} & z_{ab7,12} \\ 0 & z_{cd89} & z_{cd8,10} & z_{cd8,11} & z_{cd8,12} & \\ & 0 & z_{ef9,10} & z_{ef9,11} & z_{ef9,12} & \\ & & 0 & z_{ef10,11} & z_{ef10,12} & \\ & & & 0 & z_{ef11,12} & \\ & & & & 0 & \end{pmatrix}. \quad (38)$$

Then, we can express the hyper-Pfaffian with $n = 3$ with alpha-like correlation as

$$\begin{aligned} Pf^{[4]}(Z) = & \sum_{\sigma \in \mathfrak{S}_6} \text{sgn}(\sigma) [Pf(Z_{\sigma(1),\sigma(2),\sigma(3),\sigma(4),\sigma(5),\sigma(6)}^3) \\ & + z_{\sigma(1),\sigma(2),9,10} Pf(Z_{\sigma(3),\sigma(4),\sigma(5),\sigma(6)}^2)] \end{aligned} \quad (39)$$

where

$$\sigma(1) < \sigma(2), \quad \sigma(3) < \sigma(4), \quad \sigma(5) < \sigma(6). \quad (40)$$

For $n = 2$ and $n = 3$, we compared the numerical values of the hyper-Pfaffians, and we confirmed that our Pfaffian formula for the hyper-Pfaffian give the correct numerical values.

VI. CONCLUSION

The quartet correlation is significant for some quantum many-body systems similar to the pairing correlation. To handle the quartet correlation, we extended the overlap matrix element in the variational Monte Carlo straightforwardly. We successfully obtained a new formula, and we found that it can also be expressed by the hyper-Pfaffian, which is known in the mathematical field.

The hyper-Pfaffian is recently developed, and it seems to have no good mathematical relations, compared to the Pfaffian. Therefore we tried to find out some relations to use it for numerical computations. We found out to express the hyper-Pfaffian with $k = 4$ by the sum of the usual Pfaffians. The obtained formulae are currently for $n = 2, 3$. Its general expression and more suitable computation method are now in progress.

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