Pfaffian formulation for matrix elements of three-body operators in multiple quasiparticle configurations

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We present a Pfaffian formula to calculate matrix elements of three-body operators in symmetry-restoration beyond-mean-field methods, including the case of multiple quasiparticle (qp) configurations. Detailed derivation is provided and the validity of the new formula is checked numerically. The corresponding efficiency is discussed, which turns out to be about five times (one order of magnitude) higher than the conventional method when four (less than four) qp operators are considered.

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I. INTRODUCTION

Successful descriptions of nuclear structures rely heavily on the solution of the nuclear many-body problem [1], which is difficult due to two aspects: the complexity of a nucleon-nucleon interaction and the troublesome many-body techniques. On one hand, fundamental progress has been achieved during the past decades for modern understandings of nuclear forces, based on, for example, the chiral effective field theory [2,3] where three-body nuclear forces are found to play important roles in nuclear structure physics.

A lot of nuclear many-body techniques, on the other hand, employ the philosophy that reduces the nuclear many-body to effective one-body problems with the help of the concept of quasiparticles (qp) and single-particle mean-field calculations in the intrinsic frame, such as the Hartree-Fock-Bogoliubov (HFB) theory [4–6]. Residual many-body correlations could be included reasonably through beyond-mean-field methods [7–12], which provide a description of nuclear many-body wave functions in the laboratory frame.

One kind of popular nuclear model, the generator coordinate method (GCM) [1,13–25] or related angular-momentum projection (AMP) based method [26–35], usually starts from single-particle HFB calculations in the intrinsic frame where some symmetries are broken, which can be restored exactly by the projection technique from which the description of nuclear systems in the laboratory frame can be achieved. Further nucleon-nucleon correlations are then included by diagonalizing the Hamiltonian in the nonorthonormal projected basis, which leads to the solution of the Hill-Wheeler-Griffin equation. The central ingredients (kernels) of these models turn out to be different projected (or *rotated*) matrix elements generated by AMP, particle-number projection (PNP), parity projection, etc., where the AMP usually dominates analytical and numerical efforts. During the past decades, the GCM or AMP (PNP) based methods have been applied successfully to researches on nuclear low-lying states [13,16–18,36,37], high-spin physics [26,29–31,38–45], β decay [46,47], neutrinoless double-β decay [15,19,24,48–50], astrophysical weak process [51,52], nuclear fission [53–57], etc., with different effective interactions or schematic interactions.

In the above applications, collective degrees of freedom (such as shape fluctuations) [13,16,17], single-particle (such as qp excitations) degrees of freedom [26,29,38], or both of them [22] are included, according to the underlying physical problems of interests and the practical computational burden simultaneously. The computational burden concentrates on the kernels in the Hill-Wheeler-Griffin equation, i.e., the *rotated* norm overlap of HFB qp vacuum, the *rotated* norm overlap of multi-qp configuration, and the *rotated* matrix elements of Hamiltonian (including one-body, two-body, and potentially three-body operators). Historically, these kernels could be calculated by the Onishi formula [58], the generalized Wick's theorem [26], Hara's prescription (see the Appendix of Ref. [26]), etc., which, unfortunately, encountered the sign problem, the problem of combinatorial complexity and extremely computational cost, respectively.

During the past decade or so, after the pioneering work of Robledo [59] who solved the sign problem of the Onishi formula in a mathematically elegant way in terms of Pfaffian by making use of Grassmann numbers and Fermion coherent state, the Pfaffian formulations (algorithms) have been developed rapidly for all three kinds of kernels in the Hill-Wheeler-Griffin equation [59–70]. In particular, the problem of combinatorial complexity for the norm overlap of multi-qp configuration can be avoided with the help of the Pfaffian formula by Mizusaki *et al.* [66] and the calculation of *rotated* matrix elements of one-body and two-body operators can be optimized to a large extent according to the Pfaffian formula by Hu *et al.* [68]. These achievements of Pfaffian

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formulations, then, would make the GCM method one of the optimal nuclear many-body techniques from both physical (with broken symmetries restored) and numerically practical perspectives.

Recently, the GCM methods based on shell-model Hamiltonians have been developed for studies on nuclear low-lying states and neutrinoless double-β decay [21,33,71,72], and the in-medium similarity-renormalization group (IMSRG) method has been updated by employing symmetry-restored states or GCM calculations as the reference states with shell-model Hamiltonian [14] and the chiral Hamiltonian [73] to describe low-lying states of deformed light nuclei and the neutrinoless double-β decay among them. On the other hand, for many interesting nuclear-structure and decay problems such as the high-spin physics and astrophysical weak-interaction process, *ab initio* methods for both low-lying and relatively highly excited states of medium-heavy and heavy nuclei are demanded. One of the potential candidates may be a GCM method with both collective (such as shape fluctuations) and single-particle (such as multi-qp configurations) degrees of freedom by realistic nuclear forces such as the chiral forces. The evaluation of matrix elements of three-body operators is then indispensable. Besides, for neutrinoless double-β decay, the nature of neutrinos can be well understood provided that the corresponding nuclear matrix elements $M^{0\nu\beta\beta} = \langle\Psi_F|\hat{O}^{0\nu\beta\beta}|\Psi_I\rangle$ can be evaluated as precisely as possible. There are two sources of uncertainties for $M^{0\nu\beta\beta}$, the one from nuclear many-body wave functions $|\Psi_I\rangle$ and $|\Psi_F\rangle$, and the one from the decay operator $\hat{O}^{0\nu\beta\beta}$. The uncertainty in the former can be reduced to a large extent by taking into account as many correlations as possible in the nuclear wave function, such as the shape fluctuations [48,49], pairing fluctuations [19,74], qp excitation [50], etc., for which the GCM method serves as the optimal candidate model. The uncertainty from the decay operator can be reduced effectively by studying the roles of chiral two-body currents [15], which would lead to three-body and even four-body decay operators. Therefore, to provide reliable $M^{0\nu\beta\beta}$, matrix elements of three-body decay operators in GCM methods with/without qp configurations are indispensable.

In this work, we provide a Pfaffian formula for evaluation of matrix elements of general three-body operators in symmetry-restoration beyond-mean-field methods such the GCM or AMP-based methods, for cases with or without multiple qp configurations. In Sec. II we briefly introduce the basic logics of GCM or AMP (PNP) based methods. In Sec. III we provide the Pfaffian formula for evaluation of matrix elements of three-body operators, and we finally summarize our work in Sec. IV.

II. BASIC LOGIC OF GCM OR AMP-BASED METHODS

For completeness of discussion, we first give a concise introduction of the logic of GCM or AMP(PNP)-based methods [1]. The starting point of these methods is usually solutions of single-nucleon HFB mean-field equations with constraints (on quantities with respect to related coordinates $\boldsymbol{q}$, such as the total quadrupole moments, etc.) in the intrinsic frame, from which one can get different configurations based on Slater determinants with or without qp excitations, i.e.,

$$|\Phi_\kappa(\boldsymbol{q})\rangle = \{|\Phi(\boldsymbol{q})\rangle,\ \hat{\beta}_i^\dagger(\boldsymbol{q})\hat{\beta}_j^\dagger(\boldsymbol{q})|\Phi(\boldsymbol{q})\rangle,\ \cdots\}, \tag{1}$$

where $|\Phi(\boldsymbol{q})\rangle$ labels the HFB qp vacuum and the corresponding qp operators are denoted by $\{\hat{\beta}_i(\boldsymbol{q}), \hat{\beta}_i^\dagger(\boldsymbol{q})\}$. In Eq. (1) the index κ reflects the information of qp excitations.

The wave functions in Eq. (1) broke some symmetries which can be recovered by projection operators. Here, we take the AMP and PNP operators as examples since the parity projections, etc., are relatively trivial. The PNP operator is

$$\hat{P}^\tau = \frac{1}{2\pi}\int_0^{2\pi} d\phi_\tau e^{i(\hat{N}_\tau - N_\tau)\phi_\tau}, \tag{2}$$

where $\hat{N}_\tau$ is the particle-number operator for neutrons ($\tau = n$) or protons ($\tau = p$) and ϕ_τ is the gauge angle. The AMP operator reads as

$$\hat{P}^J_{MK} = \frac{2J+1}{8\pi^2}\int d\Omega D^{J*}_{MK}(\Omega)\hat{R}(\Omega) \tag{3}$$

with D^J_{MK} being the Wigner D function, $\hat{R}$ the rotation operator with respect to the Euler angle Ω.

The AMP and PNP operators can recover the broke symmetries in $|\Phi_\kappa(\boldsymbol{q})\rangle$ and provide description of nuclear many-body systems in the laboratory frame, i.e.,

$$\hat{P}^{J,NZ}_{MK}|\Phi_\kappa(\boldsymbol{q})\rangle \equiv \hat{P}^J_{MK}\hat{P}^N\hat{P}^Z|\Phi_\kappa(\boldsymbol{q})\rangle. \tag{4}$$

Besides, more nucleon-nucleon correlations could be included by diagonalizing Hamiltonian in the nonorthonormal projected basis in Eq. (4), so that one can write the nuclear many-body wave functions as

$$\left|\Psi^\sigma_{JM}\right\rangle = \int d\boldsymbol{q}\sum_{K\kappa} f^{J\sigma}_{K\kappa}(\boldsymbol{q})\hat{P}^{J,NZ}_{MK}|\Phi_\kappa(\boldsymbol{q})\rangle, \tag{5}$$

where σ denotes the σth eigenstate for angular momentum J. This corresponds to the solution of the Hill-Wheeler-Griffin equation,

$$\sum_{K'\kappa'\boldsymbol{q}'}\left[\mathcal{H}^J_{K\kappa K'\kappa'}(\boldsymbol{q},\boldsymbol{q}') - E^\sigma_J\mathcal{N}^J_{K\kappa K'\kappa'}(\boldsymbol{q},\boldsymbol{q}')\right]f^{J\sigma}_{K'\kappa'}(\boldsymbol{q}') = 0, \tag{6}$$

from which the coefficient $f^{J\sigma}_{K\kappa}(\boldsymbol{q})$ in Eq. (5) can be obtained and the nuclear many-body wave functions $|\Psi^\sigma_{JM}\rangle$ can be well defined.

Then, physical quantities in the laboratory frame can be calculated and compared with measurements. Let us take typical transitions and decays as examples. With the corresponding operator $\mathcal{T}^{\lambda\mu}$, the (reduced) transition strengths could be obtained by means of

$$\left\langle\Psi^{(\mathcal{S})\sigma}_{JM}\middle|\mathcal{T}^{\lambda\mu}\middle|\Psi^{(\mathcal{S}')\sigma'}_{J'M'}\right\rangle, \tag{7}$$

where $(\mathcal{S})$ and $(\mathcal{S}')$ can represent the same nuclear system (such as, for electromagnetic transitions) or two different nuclear systems (such as, for β decay and double β decay, etc.).

In Eq. (6) $\mathcal{H}$ and $\mathcal{N}$ read as

$$\mathcal{H}^J_{K\kappa K'\kappa'}(\boldsymbol{q},\boldsymbol{q}') = \langle\Phi_\kappa(\boldsymbol{q})|\hat{H}\hat{P}^{J,NZ}_{KK'}|\Phi_{\kappa'}(\boldsymbol{q}')\rangle, \tag{8a}$$

$$\mathcal{N}^J_{K\kappa K'\kappa'}(\boldsymbol{q},\boldsymbol{q}') = \langle\Phi_\kappa(\boldsymbol{q})|\hat{P}^{J,NZ}_{KK'}|\Phi_{\kappa'}(\boldsymbol{q}')\rangle. \tag{8b}$$

As mentioned in the Introduction, the central ingredients (kernels) of the GCM methods are three kinds of *rotated* matrix elements generated by projection techniques. From Eqs. (2), (3), (5), (7), 8(a), 8(b) it is seen that the three kinds of (kernels) *rotated* matrix elements are

$$\langle\Phi^a|\quad \hat{\mathcal{R}}\quad |\Phi^b\rangle, \tag{9a}$$

$$\langle\Phi^a|\hat{\alpha}_1\cdots\hat{\alpha}_m\quad \hat{\mathcal{R}}\quad \hat{\beta}_1^\dagger\cdots\hat{\beta}_{m'}^\dagger|\Phi^b\rangle, \tag{9b}$$

$$\langle\Phi^a|\hat{\alpha}_1\cdots\hat{\alpha}_m\ \hat{\mathcal{O}}\hat{\mathcal{R}}\ \hat{\beta}_1^\dagger\cdots\hat{\beta}_{m'}^\dagger|\Phi^b\rangle, \tag{9c}$$

i.e., the norm overlap of HFB qp vacuum, the norm overlap of multi-qp configuration, and the *rotated* matrix elements of operators, respectively. In Eq. (9), the indices $a \equiv \{\mathcal{S}, \boldsymbol{q}\}$ and $b \equiv \{\mathcal{S}', \boldsymbol{q}'\}$ can represent the same or different nuclear systems with corresponding qp operators $\hat{\alpha}_i$ and $\hat{\beta}_j$, and $\hat{\mathcal{R}}$ labels the total unitary (*rotation*) operator, i.e., $\hat{\mathcal{R}} \equiv \hat{R}(\Omega)e^{i\hat{N}_\tau\phi_\tau}$ in the AMP + PNP case considered here. The operator $\hat{\mathcal{O}}$ can be the Hamiltonian (one-body, two-body, and even three-body scalar operators) and the transition or decay operators (one-body, two-body, and even three-body tensor operators).

Fortunately, the norm overlap of HFB qp vacuum in Eq. 9(a) can be calculated by the Pfaffian formula in Refs. [59,60,62,63,65,67,69,70] avoiding the notorious sign problem in the Onishi formula, the norm overlap among multi-qp configurations in Eq. 9(b) can be evaluated with the help of the Pfaffian formula in Refs. [62,64,66,68] which do not suffer from the problem of combinatorial complexity in the generalized Wick's theorem any more, and the Pfaffian formula for evaluation of *rotated* matrix elements of one-body and two-body operators are provided in Ref. [68]. In the next section, we follows the techniques in Refs. [64,68] to provide the Pfaffian formula for *rotated* matrix elements of three-body operators.

III. THE PFAFFIAN FORMULATION FOR THREE-BODY OPERATORS

As mentioned previously, the Pfaffian formula for *rotated* matrix elements of one-body and two-body operators are derived by Hu *et al.* [68]. The derivations are achieved in a much mathematical way by adopting the expansion properties of the Pfaffian with respect to rows and columns. In the following we adopt the similar techniques to derive the Pfaffian formula for *rotated* matrix elements of three-body operators, and discuss the underlying physics and treatments in potential applications in nuclear structure physics. In the second quantization representation we can write three-body operators as

$$\hat{V}^{(3)} = \sum_{\mu\nu\delta\omega\rho\gamma}^{M} W_{\mu\nu\delta\omega\rho\gamma}\ \hat{c}_\mu^\dagger\hat{c}_\nu^\dagger\hat{c}_\delta^\dagger\ \hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega, \tag{10}$$

where the factor 1/36 is absorbed to the antisymmetric matrix W, $\hat{c}^\dagger$, and $\hat{c}$ denote the particle creation and annihilation operators in the spherical harmonic oscillator basis and M labels the dimension of the single-particle model space.

To derive and better understand the Pfaffian formula for physical operator, we need to rely on the following generalized Pfaffian formula of norm overlaps which is derived in Ref. [68] and which actually corresponds to the generalized Wick's theorem, i.e.,

$$\langle\Phi|\hat{z}_1\cdots\hat{z}_{2N}|\Phi'\rangle = \mathrm{Pf}(\mathbb{S})\langle\Phi|\Phi'\rangle, \tag{11}$$

where $\mathbb{S}$ is a $2N\times 2N$ skew-symmetric matrix with the elements

$$\mathbb{S}_{ij} \equiv \frac{\langle\Phi|\hat{z}_i\hat{z}_j|\Phi'\rangle}{\langle\Phi|\Phi'\rangle} \qquad (i<j). \tag{12}$$

Note that in Eq. (11) $\langle\Phi|\Phi'\rangle \neq 0$ is assumed [68] and can be calculated by the Pfaffian formulas in the literatures [59,60,62,63,65,67,69,70]. $|\Phi\rangle$ and $|\Phi'\rangle$ can be the same or different HFB vacua [as in Eqs. (1), (9)], or some unitary transformation of HFB vacua (see below), or even the true vacuum $|-\rangle$. Besides, the single-fermion operators $\hat{z}_i$ could be the qp creation (annihilation) operators for either $|\Phi\rangle$ or $|\Phi'\rangle$, or any unitary transformation between them (such as the particle operators $\hat{c}^\dagger$ and $\hat{c}$, etc.). Equation (11) is equivalent to the generalized Wick's theorem that considers all possible contractions among $\hat{z}_i$ [with $(2N-1)!!$ contractions in total]. The norm overlap of multi-qp configuration in Eq. 9(b) represents a simple example of Eq. (11).

As illustrated by Eqs. (6), (7), (8), (9) we now treat the *rotated* matrix elements of three-body operators

$$I_3 = \sum_{\mu\nu\delta\omega\rho\gamma}^{M} W_{\mu\nu\delta\omega\rho\gamma} \times \langle\Phi^a|\hat{\alpha}_1\cdots\hat{\alpha}_L\hat{c}_\mu^\dagger\hat{c}_\nu^\dagger\hat{c}_\delta^\dagger\ \hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\hat{\mathcal{R}}\hat{\beta}_{L+1}^\dagger\cdots\hat{\beta}_{2N}^\dagger|\Phi^b\rangle \tag{13}$$

which can be written as

$$I_3 = \sum_{\mu\nu\delta\omega\rho\gamma}^{M} W_{\mu\nu\delta\omega\rho\gamma} \times \langle\Phi|\hat{z}_1\cdots\hat{z}_L\hat{c}_\mu^\dagger\hat{c}_\nu^\dagger\hat{c}_\delta^\dagger\ \hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\hat{z}_{L+1}\cdots\hat{z}_{2N}|\Phi'\rangle \tag{14}$$

by defining

$$\hat{z}_k = \begin{cases}\hat{\alpha}_k, & 1\leqslant k\leqslant L\\ \hat{\mathcal{R}}\hat{\beta}_k^\dagger\hat{\mathcal{R}}^{-1}, & L+1\leqslant k\leqslant 2N,\end{cases} \tag{15a}$$

$$|\Phi\rangle = |\Phi^a\rangle, \tag{15b}$$

$$|\Phi'\rangle = \hat{\mathcal{R}}|\Phi^b\rangle. \tag{15c}$$

Now the evaluation of *rotated* matrix elements for physical operators is much more straightforward actually. Taking the three-body operator case I_3 as an example, one can calculate each $\langle\Phi|\hat{z}_1\cdots\hat{z}_L\hat{c}_\mu^\dagger\hat{c}_\nu^\dagger\hat{c}_\delta^\dagger\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\hat{z}_{L+1}\cdots\hat{z}_{2N}|\Phi'\rangle$, multiplied by corresponding $W_{\mu\nu\delta\omega\rho\gamma}$ and finally consider the six-fold loops (summations) for indices $\{\mu\nu\delta\omega\rho\gamma\}$ in Eq. (14). The $\langle\Phi|\hat{z}_1\cdots\hat{z}_L\hat{c}_\mu^\dagger\hat{c}_\nu^\dagger\hat{c}_\delta^\dagger\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\hat{z}_{L+1}\cdots\hat{z}_{2N}|\Phi'\rangle$ can be calculated by the generalized Wick's theorem, or equivalently by the Pfaffian formula in Eq. (11) for which a $(2N+6)\times(2N+6)$ skew-symmetric matrix (say $\mathbb{M}$) should be defined first. In either of the two ways, basic contractions among $\{\hat{z}_i, \hat{c}_\mu^\dagger, \hat{c}_\nu\}$ (the

matrix elements of $\mathbb{M}$) should be calculated in advance. The basic contractions among $\{\hat{z}_i\}$ themselves have been defined in Eq. (12). For the basic contractions involving $\hat{c}^\dagger$ and/or $\hat{c}$ we define them in the following:

$$\mathbb{S}^{(+)}_{\mu k} = \begin{cases} -\frac{\langle\Phi|\hat{z}_k\hat{c}^\dagger_\mu|\Phi'\rangle}{\langle\Phi|\Phi'\rangle} & 1 \leqslant k \leqslant L \\ \frac{\langle\Phi|\hat{c}^\dagger_\mu\hat{z}_k|\Phi'\rangle}{\langle\Phi|\Phi'\rangle} & L+1 \leqslant k \leqslant 2N \end{cases}, \tag{16a}$$

$$\mathbb{S}^{(-)}_{\mu k} = \begin{cases} -\frac{\langle\Phi|\hat{z}_k\hat{c}_\mu|\Phi'\rangle}{\langle\Phi|\Phi'\rangle} & 1 \leqslant k \leqslant L \\ \frac{\langle\Phi|\hat{c}_\mu\hat{z}_k|\Phi'\rangle}{\langle\Phi|\Phi'\rangle} & L+1 \leqslant k \leqslant 2N \end{cases}, \tag{16b}$$

$$\mathbb{C}^{(+)}_{\mu\nu} = \frac{\langle\Phi|\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu|\Phi'\rangle}{\langle\Phi|\Phi'\rangle}, \tag{16c}$$

$$\mathbb{C}^{(0)}_{\mu\nu} = \frac{\langle\Phi|\hat{c}^\dagger_\mu\hat{c}_\nu|\Phi'\rangle}{\langle\Phi|\Phi'\rangle}, \tag{16d}$$

$$\mathbb{C}^{(-)}_{\mu\nu} = \frac{\langle\Phi|\hat{c}_\mu\hat{c}_\nu|\Phi'\rangle}{\langle\Phi|\Phi'\rangle}. \tag{16e}$$

Although one can calculate I_3 in the above straightforward way, it should be much time-consuming due to the six-fold loops in large model space and the non-negligible CPU time for computation of the Pfaffian of $(2N+6)\times(2N+6)$ matrix [61] for each loop. In the following we derive a compact form for the evaluation of I_3 in terms of Pfaffians. The derivation can be done by either Hara's prescription or the expansion properties of Pfaffian with respect to six neighboring rows. We would adopt the former way and leave the equivalent latter way in the Appendix.

For the $\langle\Phi|\hat{z}_1\cdots\hat{z}_L\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu\hat{c}^\dagger_\delta\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\hat{z}_{L+1}\cdots\hat{z}_{2N}|\Phi'\rangle$ in the calculations of I_3 in Eq. (14), by either the generalized Wick's theorem or the Pfaffian formula in Eq. (11) we need to consider $(2N+6-1)!!$ terms, each of the terms corresponds to a possible contraction way for $\{\hat{z},\hat{c}^\dagger,\hat{c}\}$. From Hara's prescription one can classify these $(2N+6-1)!!$ terms into four classes, and get

$$\frac{I_3}{\langle\Phi|\Phi'\rangle} = O^{(0)} + O^{(1)} + O^{(2)} + O^{(3)}. \tag{17}$$

The first class $O^{(0)}$ corresponds to contractions among $\{\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu\hat{c}^\dagger_\delta\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\}$ themselves multiplied by contractions among $\{\hat{z}_i,\ 1\leqslant i\leqslant 2N\}$, i.e.,

$$O^{(0)} = W_0\mathrm{Pf}(\mathbb{S}), \tag{18}$$

where

$$W_0 = \sum_{\mu\nu\delta\omega\rho\gamma} W_{\mu\nu\delta\omega\rho\gamma}\mathbb{C}_{\mu\nu\delta\gamma\rho\omega}, \tag{19}$$

$$\begin{aligned}\mathbb{C}_{\mu\nu\delta\gamma\rho\omega} = {}& \mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(0)}_{\delta\gamma}\mathbb{C}^{(-)}_{\rho\omega} - \mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(0)}_{\delta\rho}\mathbb{C}^{(-)}_{\gamma\omega} + \mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(0)}_{\delta\omega}\mathbb{C}^{(-)}_{\gamma\rho} \\ & - \mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(0)}_{\nu\gamma}\mathbb{C}^{(-)}_{\rho\omega} + \mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(0)}_{\nu\rho}\mathbb{C}^{(-)}_{\gamma\omega} - \mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(0)}_{\nu\omega}\mathbb{C}^{(-)}_{\gamma\rho} \\ & + \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(+)}_{\nu\delta}\mathbb{C}^{(-)}_{\rho\omega} - \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(0)}_{\nu\rho}\mathbb{C}^{(0)}_{\delta\omega} + \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(0)}_{\nu\omega}\mathbb{C}^{(0)}_{\delta\rho} \\ & - \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(+)}_{\nu\delta}\mathbb{C}^{(-)}_{\gamma\omega} + \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(0)}_{\nu\gamma}\mathbb{C}^{(0)}_{\delta\omega} - \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(0)}_{\nu\omega}\mathbb{C}^{(0)}_{\delta\gamma} \\ & + \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(+)}_{\nu\delta}\mathbb{C}^{(-)}_{\gamma\rho} - \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(0)}_{\nu\gamma}\mathbb{C}^{(0)}_{\delta\rho} + \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(0)}_{\nu\rho}\mathbb{C}^{(0)}_{\delta\gamma}.\end{aligned} \tag{20}$$

The second class $O^{(1)}$ corresponds to contractions between one pair of operators in $\{\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu\hat{c}^\dagger_\delta\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\}$ and one pair of operators in $\{\hat{z}_i,\ 1\leqslant i\leqslant 2N\}$, multiplied by contractions among the remaining two pairs in $\{\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu\hat{c}^\dagger_\delta\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\}$ then multiplied by contractions among the remaining $N-1$ pairs in $\{\hat{z}_i,\ 1\leqslant i\leqslant 2N\}$, i.e.,

$$O^{(1)} = \sum_{ij}^{2N}\mathbb{W}^{(1)}_{ij}(-1)^{i+j}\alpha_{ij}\mathrm{Pf}(\mathbb{S}\{i,j\}), \tag{21}$$

where

$$\mathbb{W}^{(1)}_{ij} = \sum_{\mu\nu\delta\omega\rho\gamma} W_{\mu\nu\delta\omega\rho\gamma}\mathbb{D}^{ij}_{\mu\nu\delta\gamma\rho\omega}, \tag{22}$$

$$\begin{aligned}\mathbb{D}^{ij}_{\mu\nu\delta\gamma\rho\omega} = {}& \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\big(\mathbb{C}^{(0)}_{\delta\gamma}\mathbb{C}^{(-)}_{\rho\omega} - \mathbb{C}^{(0)}_{\delta\rho}\mathbb{C}^{(-)}_{\gamma\omega} + \mathbb{C}^{(0)}_{\delta\omega}\mathbb{C}^{(-)}_{\gamma\rho}\big) \\ & + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\delta j}\big(-\mathbb{C}^{(0)}_{\nu\gamma}\mathbb{C}^{(-)}_{\rho\omega} + \mathbb{C}^{(0)}_{\nu\rho}\mathbb{C}^{(-)}_{\gamma\omega} - \mathbb{C}^{(0)}_{\nu\omega}\mathbb{C}^{(-)}_{\gamma\rho}\big) \\ & + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(-)}_{\gamma j}\big(\mathbb{C}^{(+)}_{\nu\delta}\mathbb{C}^{(-)}_{\rho\omega} - \mathbb{C}^{(0)}_{\nu\rho}\mathbb{C}^{(0)}_{\delta\omega} + \mathbb{C}^{(0)}_{\nu\omega}\mathbb{C}^{(0)}_{\delta\rho}\big) \\ & + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(-)}_{\rho j}\big(-\mathbb{C}^{(+)}_{\nu\delta}\mathbb{C}^{(-)}_{\gamma\omega} + \mathbb{C}^{(0)}_{\nu\gamma}\mathbb{C}^{(0)}_{\delta\omega} - \mathbb{C}^{(0)}_{\nu\omega}\mathbb{C}^{(0)}_{\delta\gamma}\big) \\ & + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(-)}_{\omega j}\big(\mathbb{C}^{(+)}_{\nu\delta}\mathbb{C}^{(-)}_{\gamma\rho} - \mathbb{C}^{(0)}_{\nu\gamma}\mathbb{C}^{(0)}_{\delta\rho} + \mathbb{C}^{(0)}_{\nu\rho}\mathbb{C}^{(0)}_{\delta\gamma}\big) \\ & + \mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(+)}_{\delta j}\big(\mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(-)}_{\rho\omega} - \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(-)}_{\gamma\omega} + \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(-)}_{\gamma\rho}\big) \\ & + \mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(-)}_{\gamma j}\big(-\mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(-)}_{\rho\omega} + \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(0)}_{\delta\omega} - \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(0)}_{\delta\rho}\big) \\ & + \mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(-)}_{\rho j}\big(\mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(-)}_{\gamma\omega} - \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(0)}_{\delta\omega} + \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(0)}_{\delta\gamma}\big) \\ & + \mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(-)}_{\omega j}\big(-\mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(-)}_{\gamma\rho} + \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(0)}_{\delta\rho} - \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(0)}_{\delta\gamma}\big) \\ & + \mathbb{S}^{(+)}_{\delta i}\mathbb{S}^{(-)}_{\gamma j}\big(\mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(-)}_{\rho\omega} - \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(0)}_{\nu\omega} + \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(0)}_{\nu\rho}\big) \\ & + \mathbb{S}^{(+)}_{\delta i}\mathbb{S}^{(-)}_{\rho j}\big(-\mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(-)}_{\gamma\omega} + \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(0)}_{\nu\omega} - \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(0)}_{\nu\gamma}\big) \\ & + \mathbb{S}^{(+)}_{\delta i}\mathbb{S}^{(-)}_{\omega j}\big(\mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(-)}_{\gamma\rho} - \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(0)}_{\nu\rho} + \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(0)}_{\nu\gamma}\big) \\ & + \mathbb{S}^{(-)}_{\gamma i}\mathbb{S}^{(-)}_{\rho j}\big(\mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(0)}_{\delta\omega} - \mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(0)}_{\nu\omega} + \mathbb{C}^{(0)}_{\mu\omega}\mathbb{C}^{(+)}_{\nu\delta}\big) \\ & + \mathbb{S}^{(-)}_{\gamma i}\mathbb{S}^{(-)}_{\omega j}\big(-\mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(0)}_{\delta\rho} + \mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(0)}_{\nu\rho} - \mathbb{C}^{(0)}_{\mu\rho}\mathbb{C}^{(+)}_{\nu\delta}\big) \\ & + \mathbb{S}^{(-)}_{\rho i}\mathbb{S}^{(-)}_{\omega j}\big(\mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(0)}_{\delta\gamma} - \mathbb{C}^{(+)}_{\mu\delta}\mathbb{C}^{(0)}_{\nu\gamma} + \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(+)}_{\nu\delta}\big).\end{aligned} \tag{23}$$

In Eq. (21) $\mathbb{S}\{i,j\}$ is defined as a submatrix of $\mathbb{S}$ with its ith and jth rows and columns removed, the phase $(-1)^{i+j}$ and the permutation phase α_{ij} come from the contractions regarding $\hat{z}_i$ and $\hat{z}_j$, in which $\alpha_{ij}=1$ when $i<j$ and $\alpha_{ij}=-1$ when $i>j$.

Similarly, the third class $O^{(2)}$ corresponds to contractions between two pairs of operators in $\{\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu\hat{c}^\dagger_\delta\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\}$ and two pairs of operators in $\{\hat{z}_i,\ 1\leqslant i\leqslant 2N\}$, multiplied by contractions among the remaining one pair in $\{\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu\hat{c}^\dagger_\delta\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\}$ then multiplied by contractions among the remaining $N-2$ pairs in $\{\hat{z}_i,\ 1\leqslant i\leqslant 2N\}$, i.e.,

$$O^{(2)} = \sum_{ijkl}^{2N}\mathbb{W}^{(2)}_{ijkl}(-1)^{i+j+k+l}\alpha_{ijkl}\mathrm{Pf}(\mathbb{S}\{i,j,k,l\}), \tag{24}$$

where

$$\mathbb{W}^{(2)}_{ijkl} = \sum_{\mu\nu\delta\omega\rho\gamma} W_{\mu\nu\delta\omega\rho\gamma}\mathbb{E}^{ijkl}_{\mu\nu\delta\gamma\rho\omega}, \tag{25}$$

$$\begin{aligned}\mathbb{E}^{ijkl}_{\mu\nu\delta\gamma\rho\omega} = {} & \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\mathbb{S}^{(+)}_{\delta k}\mathbb{S}^{(-)}_{\gamma l}\mathbb{C}^{(-)}_{\rho\omega} - \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\mathbb{S}^{(+)}_{\delta k}\mathbb{S}^{(-)}_{\rho l}\mathbb{C}^{(-)}_{\gamma\omega} \\ & + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\mathbb{S}^{(+)}_{\delta k}\mathbb{S}^{(-)}_{\omega l}\mathbb{C}^{(-)}_{\gamma\rho} + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\mathbb{S}^{(-)}_{\gamma k}\mathbb{S}^{(-)}_{\rho l}\mathbb{C}^{(0)}_{\delta\omega} \\ & - \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\mathbb{S}^{(-)}_{\gamma k}\mathbb{S}^{(-)}_{\omega l}\mathbb{C}^{(0)}_{\delta\rho} + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\mathbb{S}^{(-)}_{\rho k}\mathbb{S}^{(-)}_{\omega l}\mathbb{C}^{(0)}_{\delta\gamma} \\ & - \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\delta j}\mathbb{S}^{(-)}_{\gamma k}\mathbb{S}^{(-)}_{\rho l}\mathbb{C}^{(0)}_{\nu\omega} + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(-)}_{\omega j}\mathbb{S}^{(+)}_{\delta k}\mathbb{S}^{(-)}_{\gamma l}\mathbb{C}^{(0)}_{\nu\rho} \\ & - \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\delta j}\mathbb{S}^{(-)}_{\rho k}\mathbb{S}^{(-)}_{\omega l}\mathbb{C}^{(0)}_{\nu\gamma} + \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(-)}_{\gamma j}\mathbb{S}^{(-)}_{\rho k}\mathbb{S}^{(-)}_{\omega l}\mathbb{C}^{(+)}_{\nu\delta} \\ & + \mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(+)}_{\delta j}\mathbb{S}^{(-)}_{\gamma k}\mathbb{S}^{(-)}_{\rho l}\mathbb{C}^{(0)}_{\mu\omega} - \mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(-)}_{\omega j}\mathbb{S}^{(+)}_{\delta k}\mathbb{S}^{(-)}_{\gamma l}\mathbb{C}^{(0)}_{\mu\rho} \\ & + \mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(+)}_{\delta j}\mathbb{S}^{(-)}_{\rho k}\mathbb{S}^{(-)}_{\omega l}\mathbb{C}^{(0)}_{\mu\gamma} - \mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(-)}_{\gamma j}\mathbb{S}^{(-)}_{\rho k}\mathbb{S}^{(-)}_{\omega l}\mathbb{C}^{(+)}_{\mu\delta} \\ & + \mathbb{S}^{(+)}_{\delta i}\mathbb{S}^{(-)}_{\gamma j}\mathbb{S}^{(-)}_{\rho k}\mathbb{S}^{(-)}_{\omega l}\mathbb{C}^{(+)}_{\mu\nu}. \end{aligned} \tag{26}$$

In Eq. (24) $\mathbb{S}\{i, j, k, l\}$ is defined as a submatrix of $\mathbb{S}$ with its ith, jth, kth, and lth rows and columns removed, the phase $(-1)^{i+j+k+l}$ and the permutation phase α_{ijkl} come from the contractions regarding $\hat{z}_i$, $\hat{z}_j$, $\hat{z}_k$, and $\hat{z}_l$, where $\alpha_{ijkl} = 1$ when $i < j < k < l$ and changes its sign one time for each permutation among the indices i, j, k, l.

The last class $O^{(3)}$ reflects the last possible contraction way, i.e., each of the (all) three pairs of operators in $\{\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu\hat{c}^\dagger_\delta\hat{c}_\gamma\hat{c}_\rho\hat{c}_\omega\}$ are contracted with each of the three pairs of operators in $\{\hat{z}_i,\ 1 \leqslant i \leqslant 2N\}$, multiplied by contractions among the remaining $N-3$ pairs in $\{\hat{z}_i,\ 1 \leqslant i \leqslant 2N\}$, for this way one has

$$\begin{aligned} O^{(3)} = {} & \sum_{ijklmn}^{2N} \mathbb{W}^{(3)}_{ijklmn}(-1)^{i+j+k+l+m+n}\alpha_{ijklmn} \\ & \times \mathrm{Pf}(\mathbb{S}\{i, j, k, l, m, n\}), \end{aligned} \tag{27}$$

where

$$\mathbb{W}^{(3)}_{ijklmn} = \sum_{\mu\nu\delta\omega\rho\gamma} W_{\mu\nu\delta\omega\rho\gamma}\mathbb{F}^{ijklmn}_{\mu\nu\delta\gamma\rho\omega}, \tag{28}$$

$$\mathbb{F}^{ijklmn}_{\mu\nu\delta\gamma\rho\omega} = \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\mathbb{S}^{(+)}_{\delta k}\mathbb{S}^{(-)}_{\gamma l}\mathbb{S}^{(-)}_{\rho m}\mathbb{S}^{(-)}_{\omega n}. \tag{29}$$

Here, the matrix $\mathbb{S}\{i, j, k, l, m, n\}$ and the phases $(-1)^{i+j+k+l+m+n}$, α_{ijklmn} are defined in a similar way as the $O^{(2)}$ case.

From Eqs. (17), (18), (21), (24), (27) we can get a Pfaffian formula for the three-body operator matrix elements as

$$\begin{aligned} \frac{I_3}{\langle\Phi|\Phi'\rangle} &= O^{(0)} + O^{(1)} + O^{(2)} + O^{(3)} \\ &= W_0\mathrm{Pf}(\mathbb{S}) + \sum_{ij}^{2N}\mathbb{W}^{(1)}_{ij}(-1)^{i+j}\alpha_{ij}\mathrm{Pf}(\mathbb{S}\{i, j\}) + \sum_{ijkl}^{2N}\mathbb{W}^{(2)}_{ijkl}(-1)^{i+j+k+l}\alpha_{ijkl}\mathrm{Pf}(\mathbb{S}\{i, j, k, l\}) \\ &\quad + \sum_{ijklmn}^{2N}\mathbb{W}^{(3)}_{ijklmn}(-1)^{i+j+k+l+m+n}\alpha_{ijklmn}\mathrm{Pf}(\mathbb{S}\{i, j, k, l, m, n\}). \end{aligned} \tag{30}$$

Such an algorithm in Eq. (30) can also be obtained by adopting the expansion property of Pfaffian with respect to six neighboring rows (see Appendix).

In most cases of practical applications, the norm overlaps are nonzero, so that we have $\mathrm{Pf}(\mathbb{S}) \neq 0$ from Eqs. (9), (11). For these cases the inverse of the matrix $\mathbb{S}$ would exist and we can then get a more compact and efficient expression for I_3 by applying the following Pfaffian identity (the Pfaffian version of the Lewis Carroll formula) which is derived by Mizusaki and Oi (see Eq. 49 of Ref. [64]):

$$\mathrm{Pf}(\mathbb{X})\mathrm{Pf}[(\mathbb{X}^{-1})_I] = (-1)^{|I|}\mathrm{Pf}(\mathbb{X}_{\bar{I}}), \tag{31}$$

which holds for any skew-symmetric matrix $\mathbb{X}$. Let the matrix $\mathbb{X}$ has $2N \times 2N$ elements as the matrix $\mathbb{S}$ in the above discussions, and employ $[2N] \equiv \{1, 2, 3, \ldots, 2N\}$ to denote a set of integers which correspond to the numbers of rows and columns of the matrix $\mathbb{X}$. We divide $[2N]$ in two groups, with $I \equiv \{i_1, i_2, i_3, \ldots, i_{2n}\}$ denote a set of indices which corresponds to a subset of $[2N]$ with $1 \leqslant \{i_1, i_2, i_3, \ldots, i_{2n}\} \leqslant 2N$, the rest of the indices are denoted as $\bar{I} = [2N] - I$ meaning the complementary group of I in $[2N]$. In Eq. (31) $|I| = \sum_{k=1}^{2n} i_k$, $\mathbb{X}^{-1}$ labels the inverse matrix of $\mathbb{X}$ and $\mathbb{X}_I$ represents a $2n \times 2n$ skew matrix with its matrix elements being expressed as $(\mathbb{X}_I)_{k,l} = \mathbb{X}_{i_k,i_l}$. The notation $\mathbb{X}_{\bar{I}}$ labels a $2(N-n) \times 2(N-n)$ submatrix of the matrix $\mathbb{X}$ by removing the rows and columns of $\{i_1, i_2, i_3, \ldots, i_{2n}\}$ from the original matrix $\mathbb{X}$.

From the Pfaffian identity shown in Eq. (31), the Pfaffians of submatrix in Eq. (30) can be avoided and the expression of I_3 in Eq. (30) can by further written as (see Appendix)

$$\begin{aligned} \frac{I_3}{\langle\Phi|\Phi'\rangle} = {} & W_0\mathrm{Pf}(\mathbb{S}) - \mathrm{Tr}(\mathbb{W}^{(1)}\mathbb{S}^{-1})\mathrm{Pf}(\mathbb{S}) \\ & + \sum_{ijkl}^{2N}\mathbb{W}^{(2)}_{ijkl}\big(\mathbb{S}^{-1}_{ij}\mathbb{S}^{-1}_{kl} - \mathbb{S}^{-1}_{ik}\mathbb{S}^{-1}_{jl} + \mathbb{S}^{-1}_{il}\mathbb{S}^{-1}_{jk}\big)\mathrm{Pf}(\mathbb{S}) \\ & + \sum_{ijklmn}^{2N}\mathbb{W}^{(3)}_{ijklmn}\mathbb{S}^{-1}_{ijklmn}\mathrm{Pf}(\mathbb{S}), \end{aligned} \tag{32}$$

where

$$\begin{aligned} \mathbb{S}^{-1}_{ijklmn} = {} & \mathbb{S}^{-1}_{ij}\mathbb{S}^{-1}_{kl}\mathbb{S}^{-1}_{mn} - \mathbb{S}^{-1}_{ij}\mathbb{S}^{-1}_{km}\mathbb{S}^{-1}_{ln} + \mathbb{S}^{-1}_{ij}\mathbb{S}^{-1}_{kn}\mathbb{S}^{-1}_{lm} \\ & - \mathbb{S}^{-1}_{ik}\mathbb{S}^{-1}_{jl}\mathbb{S}^{-1}_{mn} + \mathbb{S}^{-1}_{ik}\mathbb{S}^{-1}_{jm}\mathbb{S}^{-1}_{ln} - \mathbb{S}^{-1}_{ik}\mathbb{S}^{-1}_{jn}\mathbb{S}^{-1}_{lm} \\ & + \mathbb{S}^{-1}_{il}\mathbb{S}^{-1}_{jk}\mathbb{S}^{-1}_{mn} - \mathbb{S}^{-1}_{il}\mathbb{S}^{-1}_{jm}\mathbb{S}^{-1}_{kn} + \mathbb{S}^{-1}_{il}\mathbb{S}^{-1}_{jn}\mathbb{S}^{-1}_{km} \end{aligned}$$

$$- \mathbb{S}^{-1}_{im}\mathbb{S}^{-1}_{jk}\mathbb{S}^{-1}_{ln} + \mathbb{S}^{-1}_{im}\mathbb{S}^{-1}_{jl}\mathbb{S}^{-1}_{kn} - \mathbb{S}^{-1}_{im}\mathbb{S}^{-1}_{jn}\mathbb{S}^{-1}_{kl}$$
$$+ \mathbb{S}^{-1}_{in}\mathbb{S}^{-1}_{jk}\mathbb{S}^{-1}_{lm} - \mathbb{S}^{-1}_{in}\mathbb{S}^{-1}_{jl}\mathbb{S}^{-1}_{km} + \mathbb{S}^{-1}_{in}\mathbb{S}^{-1}_{jm}\mathbb{S}^{-1}_{kl}. \quad (33)$$

Now let us remark the differences between the calculation of three-body operator matrix elements I_3 by Eq. (14) directly and the evaluation of I_3 by the Pfaffian formula in Eq. (32). For the former way, due to the six-fold loops of $\{\mu\nu\delta\omega\rho\gamma\}$ in large model space (with dimension M), as many as M^6 Pfaffians of $(2N+6)\times(2N+6)$ matrices need to be calculated numerically, which would turn out to be too time-consuming for large model space as the calculation time of Pfaffian is non-negligible [61]. On the other hand, we note the fact that for either the spectroscopy or the transition and/or decay problems, the norm overlaps in Eqs. 9(a), 9(b) should be calculated first before the evaluation of matrix elements of physical operators in Eq. 9(c) (or I_3 in the above discussions). This indicates that, as seen from Eq. (11), the matrix $\mathbb{S}$, its Pfaffian $\mathrm{Pf}(\mathbb{S})$ and its reverse $\mathbb{S}^{-1}$ have already been prepared and stored to the memory before the evaluation of I_3, which means that the Pfaffian formula in Eq. (32) should be much efficient than Eq. (14) since taking data from memory and then making manipulation is usually much faster than preparing matrices and then calculating their Pfaffians.

More interestingly, one can further reduce the Pfaffian formula in Eq. (32) according to the underlying physics in practical applications. As discussed in Eqs. (17), (18), (21), (24), (27), the four terms in Eq. (32) correspond to contractions of the three-body operator with no pair, one pair, two pairs, and three pairs of operators in the configurations $\{\hat{z}_i,\ 1\leqslant i\leqslant 2N\}$, respectively. Therefore, for even-even nuclei, if only the collective degrees of freedom are of interest for studies of low-lying states so that only qp vacua are included in the configuration space (as for most of the current GCM methods [13,16,17]), we would have $2N=0$ and only the first term $W_0\mathrm{Pf}(\mathbb{S})$ survives in Eq. (32). Similarly, for low-lying states of odd-mass nuclei, when only the 1-qp configurations [70] are considered we then have $2N=2$ and only the first two terms in Eq. (32) would survive. For an ambitious GCM method that considers both collective and single-particle degrees of freedom taking into account up to 2-qp configurations as in Ref. [22], one has $2N\leqslant 4$ and does not need to worry about the last term in Eq. (32).

Finally, we discuss a rare case in which $\mathbb{S}^{-1}$ does not exist so that Eq. (32) is no longer valid. For such case we can get another expression for I_3 readily in the similar way as in Ref. [68] (see Eqs. (38, 39, 53) of Ref. [68] for details):

$$\begin{aligned}\frac{I_3}{\langle\Phi|\Phi'\rangle} &= W_0\mathrm{Pf}(\mathbb{S}) - \sum_{ij}^{2N}(-1)^{i+j+1}\alpha_{ij}\tilde{\mathbb{S}}^{i}_{ij}\mathrm{Pf}(\tilde{\mathbb{S}}^{i}\{i,j\}) + \sum_{ij}^{2N}(-1)^{i+j+1}\alpha_{ij}\sum_{kl}^{2N}(-1)^{k+l+1}\alpha_{kl}\tilde{\mathbb{S}}^{ijk}_{ijkl}\mathrm{Pf}(\tilde{\mathbb{S}}^{ijk}\{i,j,k,l\}) \\ &\quad + \sum_{ijklmn}^{2N}\mathbb{W}^{(3)}_{ijklmn}(-1)^{i+j+k+l+m+n}\alpha_{ijklmn}\mathrm{Pf}(\mathbb{S}\{i,j,k,l,m,n\}) \\ &= W_0\mathrm{Pf}(\mathbb{S}) - \sum_{i}^{2N}\mathrm{Pf}(\tilde{\mathbb{S}}^{i}) + \sum_{ij}^{2N}(-1)^{i+j+1}\alpha_{ij}\sum_{k}^{2N}\mathrm{Pf}(\tilde{\mathbb{S}}^{ijk}\{i,j\}) \\ &\quad + \sum_{ijklmn}^{2N}\mathbb{W}^{(3)}_{ijklmn}(-1)^{i+j+k+l+m+n}\alpha_{ijklmn}\mathrm{Pf}(\mathbb{S}\{i,j,k,l,m,n\}),\end{aligned} \quad (34)$$

where we have adopted the relation $\mathrm{Pf}(\mathbb{X}) = \sum_j(-1)^{i+j+1}\alpha_{ij}\mathbb{X}_{ij}\mathrm{Pf}(\mathbb{X}\{i,j\})$ [68] so that the matrix $\tilde{\mathbb{S}}^{i}$ is constructed in the way that only replacing the ith row and column of matrix $\mathbb{S}$ by the ith row of $\mathbb{W}^{(1)}$, i.e., $\tilde{\mathbb{S}}^{i}_{ij} = \mathbb{W}^{(1)}_{ij}$ and keep the skew symmetry. The matrix $\tilde{\mathbb{S}}^{ijk}$ is the same as $\mathbb{S}$ except for replacing the kth row and column by the matrix elements of $\mathbb{W}^{(2)}$, i.e., $\tilde{\mathbb{S}}^{ijk}_{ijkl} = \mathbb{W}^{(2)}_{ijkl}$ and keep the skew symmetry of $\tilde{\mathbb{S}}^{ijk}$.

The validity of the new Pfaffian formula in Eq. (32) can be checked numerically, for which we constructed a testing FORTRAN90 code which can calculate one matrix element I_3 by both the conventional method in Eq. (14) and the new Pfaffian formula in Eq. (32), where the matrix elements for $W, \mathbb{S}, \mathbb{C}$ in Eqs. (10), (12), (16) are adopted as random numbers. The above two methods are found to give exactly the same values for I_3 and the validity of the new Pfaffian formula in Eq. (32) is then confirmed.

Besides, the efficiency of the Pfaffian algorithm in Eq. (32) can also be evaluated roughly by the testing code. In Fig. 1 we show the elapsed CPU time for the conventional method in Eq. (14) t_1, and for the new Pfaffian formula in Eqs. (19), (22), (25), (28), (32) t_2 which includes both the calculations of W_0, $\mathbb{W}^{(1)}$, $\mathbb{W}^{(2)}$, $\mathbb{W}^{(3)}$ and the calculation of I_3 by Eq. (32), as a function of the number of qp $2N$ and the dimension of model space M, where the calculations are performed on an Intel CPU with 2.6GHz. For the results shown in Fig. 1, which correspond to calculations of only one matrix element I_3 each time, the calculation time for I_3 by Eq. (32) is negligible (less than 3×10^{-4} s) so that the calculation time for W_0, $\mathbb{W}^{(1)}$, $\mathbb{W}^{(2)}$, $\mathbb{W}^{(3)}$ dominates completely t_2. In this case, as seen from Fig. 1(a), the new algorithm (t_2) is more efficient than the conventional one (t_1) by about one order of magnitude when $2N=0$ where no qp configuration is considered. One can see that the new algorithm (t_2) is about 20 times faster than the conventional one (t_1) when $2N=2$, and about 5

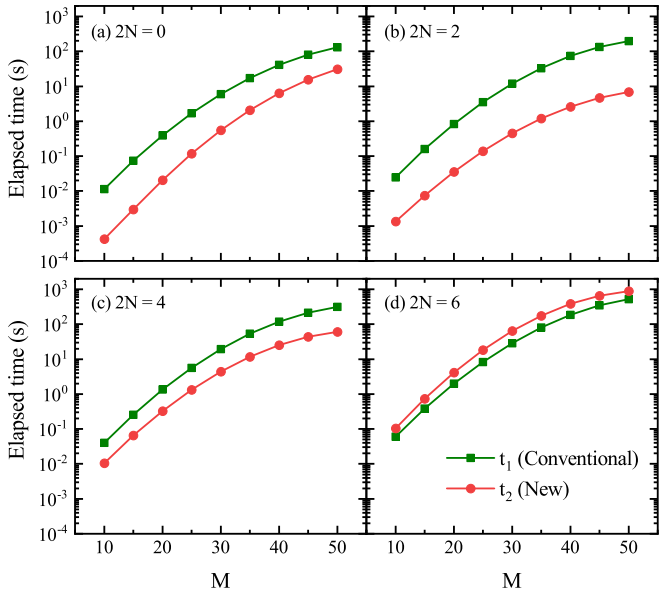

FIG. 1. The elapsed CPU time for the conventional method in Eq. (14) t_1 and the new Pfaffian formula in Eqs. (19), (22), (25), (28), (32) t_2 which includes the calculations for W_0, $\mathbb{W}^{(1)}$, $\mathbb{W}^{(2)}$, and $\mathbb{W}^{(3)}$, as a function of $2N$ and M.

times faster than the conventional one (t_1) when $2N = 4$, as seen from Figs. 1(b) and 1(c) which correspond to including 1-qp and 2-qp configurations, respectively. Including further higher-order qp configurations is unpractical for three-body-operator problems, since the elapsed CPU time for even one matrix element I_3 is as time-consuming as 1000 s when $2N = 6$ and $M = 50$ as seen from Fig. 1(d), for which the new algorithm is a little bit slower than the conventional one.

On the other hand, different from the cases of calculating only one matrix element I_3 each time in Fig. 1, in practical nuclear-structure applications, fortunately, a lot of matrix elements with different qp configurations need to be calculated. Many of them would then share the common W_0, $\mathbb{W}^{(1)}$, $\mathbb{W}^{(2)}$, $\mathbb{W}^{(3)}$ which then need to be evaluated just one time for given $|\Phi\rangle$ and $|\Phi'\rangle$ [26,68]. As the calculation time for W_0, $\mathbb{W}^{(1)}$, $\mathbb{W}^{(2)}$, $\mathbb{W}^{(3)}$ dominates completely t_2, this then implies that the new Pfaffian formula in Eq. (32) should be much more efficient than the effects shown in Fig. 1.

IV. SUMMARY

To summarize, we present a compact and efficient Pfaffian algorithm for evaluation of matrix elements of general three-body operators in beyond-mean-field nuclear models such as the generator coordinate method (GCM) or angular-momentum-projection (AMP) based methods, for cases with or without qp configurations. Further optimization of the Pfaffian algorithm in practical nuclear-structure problems is discussed for cases such as the low-lying states of even-even or odd-mass nuclei. The validity of the new Pfaffian algorithm is confirmed numerically by a testing code, from which the efficiency of the new Pfaffian algorithm is tentatively explored in different cases. The new Pfaffian algorithm turns out to be about five times (one order of magnitude) faster than the conventional method when four qp operators (less than four qp operators) are considered, and much higher efficiency of the Pfaffian algorithm in practical nuclear-structure models is expected.

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APPENDIX

First, we show that the Eq. (30) can be obtained equivalently by the expansion property of the Pfaffian with respect to six neighboring rows or columns which can be derived in the similar way as in Refs. [68] based on Lemma 2.3 of Ref. [75]. The derivation is complicated and tedious so that we only provide the conclusion in the following.

The expansion property of the Pfaffian for a matrix X with respect to the neighboring i_0th, j_0th, k_0th, l_0th, m_0th, and n_0th rows reads as

$$\begin{aligned}\mathrm{Pf}(X) &= Y_{i_0j_0k_0l_0m_0n_0}\mathrm{Pf}(X\{i_0,j_0,k_0,l_0,m_0,n_0\})\\ &+\sum_{ij}(-1)^{i+j}\alpha_{ij}Z^{ij}_{i_0j_0k_0l_0m_0n_0}\mathrm{Pf}(X\{i_0,j_0,k_0,l_0,m_0,n_0,i,j\})\\ &+\sum_{ijkl}(-1)^{i+j+k+l}\alpha_{ijkl}W^{ijkl}_{i_0j_0k_0l_0m_0n_0}\mathrm{Pf}(X\{i_0,j_0,k_0,l_0,m_0,n_0,i,j,k,l\})\\ &+\sum_{ijklmn}(-1)^{i+j+k+l+m+n}\alpha_{ijklmn}U^{ijklmn}_{i_0j_0k_0l_0m_0n_0}\mathrm{Pf}(X\{i_0,j_0,k_0,l_0,m_0,n_0,i,j,k,l,m,n\}),\end{aligned}\tag{A1}$$

where

$$\begin{aligned}Y_{i_0j_0k_0l_0m_0n_0} &= X_{i_0j_0}X_{k_0l_0}X_{m_0n_0}-X_{i_0j_0}X_{k_0m_0}X_{l_0n_0}+X_{i_0j_0}X_{k_0n_0}X_{l_0m_0}-X_{i_0k_0}X_{j_0l_0}X_{m_0n_0}+X_{i_0k_0}X_{j_0m_0}X_{l_0n_0}-X_{i_0k_0}X_{j_0n_0}X_{l_0m_0}\\ &+X_{i_0l_0}X_{j_0k_0}X_{m_0n_0}-X_{i_0l_0}X_{j_0m_0}X_{k_0n_0}+X_{i_0l_0}X_{j_0n_0}X_{k_0m_0}-X_{i_0m_0}X_{j_0k_0}X_{l_0n_0}+X_{i_0m_0}X_{j_0l_0}X_{k_0n_0}-X_{i_0m_0}X_{j_0n_0}X_{k_0l_0}\\ &+X_{i_0n_0}X_{j_0k_0}X_{l_0m_0}-X_{i_0n_0}X_{j_0l_0}X_{k_0m_0}+X_{i_0n_0}X_{j_0m_0}X_{k_0l_0},\end{aligned}\tag{A2}$$

$$
\begin{aligned}
Z^{ij}_{i_0j_0k_0l_0m_0n_0} = {} & X_{i_0i}X_{j_0j}X_{k_0l_0}X_{m_0n_0} - X_{i_0i}X_{j_0j}X_{k_0m_0}X_{l_0n_0} + X_{i_0i}X_{j_0j}X_{k_0n_0}X_{l_0m_0} - X_{i_0i}X_{k_0j}X_{j_0l_0}X_{m_0n_0} + X_{i_0i}X_{k_0j}X_{j_0m_0}X_{l_0n_0} \\
& - X_{i_0i}X_{k_0j}X_{j_0n_0}X_{l_0m_0} + X_{i_0i}X_{l_0j}X_{j_0k_0}X_{m_0n_0} - X_{i_0i}X_{l_0j}X_{j_0m_0}X_{k_0n_0} + X_{i_0i}X_{l_0j}X_{j_0n_0}X_{k_0m_0} \\
& - X_{i_0i}X_{m_0j}X_{j_0k_0}X_{l_0n_0} + X_{i_0i}X_{m_0j}X_{j_0l_0}X_{k_0n_0} - X_{i_0i}X_{m_0j}X_{j_0n_0}X_{k_0l_0} + X_{i_0i}X_{n_0j}X_{j_0k_0}X_{l_0m_0} - X_{i_0i}X_{n_0j}X_{j_0l_0}X_{k_0m_0} \\
& + X_{i_0i}X_{n_0j}X_{j_0m_0}X_{k_0l_0} + X_{j_0i}X_{k_0j}X_{i_0l_0}X_{m_0n_0} - X_{j_0i}X_{k_0j}X_{i_0m_0}X_{l_0n_0} + X_{j_0i}X_{k_0j}X_{i_0n_0}X_{l_0m_0} \\
& - X_{j_0i}X_{l_0j}X_{i_0k_0}X_{m_0n_0} + X_{j_0i}X_{l_0j}X_{i_0m_0}X_{k_0n_0} - X_{j_0i}X_{l_0j}X_{i_0n_0}X_{k_0m_0} + X_{j_0i}X_{m_0j}X_{i_0k_0}X_{l_0n_0} - X_{j_0i}X_{m_0j}X_{i_0l_0}X_{k_0n_0} \\
& + X_{j_0i}X_{m_0j}X_{i_0n_0}X_{k_0l_0} - X_{j_0i}X_{n_0j}X_{i_0k_0}X_{l_0m_0} + X_{j_0i}X_{n_0j}X_{i_0l_0}X_{k_0m_0} - X_{j_0i}X_{n_0j}X_{i_0m_0}X_{k_0l_0} \\
& + X_{k_0i}X_{l_0j}X_{i_0j_0}X_{m_0n_0} - X_{k_0i}X_{l_0j}X_{i_0m_0}X_{j_0n_0} + X_{k_0i}X_{l_0j}X_{i_0n_0}X_{j_0m_0} - X_{k_0i}X_{m_0j}X_{i_0j_0}X_{l_0n_0} + X_{k_0i}X_{m_0j}X_{i_0l_0}X_{j_0n_0} \\
& - X_{k_0i}X_{m_0j}X_{i_0n_0}X_{j_0l_0} + X_{k_0i}X_{n_0j}X_{i_0j_0}X_{l_0m_0} - X_{k_0i}X_{n_0j}X_{i_0l_0}X_{j_0m_0} + X_{k_0i}X_{n_0j}X_{i_0m_0}X_{j_0l_0} \\
& + X_{l_0i}X_{m_0j}X_{i_0j_0}X_{k_0n_0} - X_{l_0i}X_{m_0j}X_{i_0k_0}X_{j_0n_0} + X_{l_0i}X_{m_0j}X_{i_0n_0}X_{j_0k_0} - X_{l_0i}X_{n_0j}X_{i_0j_0}X_{k_0m_0} + X_{l_0i}X_{n_0j}X_{i_0k_0}X_{j_0m_0} \\
& - X_{l_0i}X_{n_0j}X_{i_0m_0}X_{j_0k_0} + X_{m_0i}X_{n_0j}X_{i_0j_0}X_{k_0l_0} - X_{m_0i}X_{n_0j}X_{i_0k_0}X_{j_0l_0} + X_{m_0i}X_{n_0j}X_{i_0l_0}X_{j_0k_0}, \qquad \text{(A3)}
\end{aligned}
$$

$$
\begin{aligned}
W^{ijkl}_{i_0j_0k_0l_0m_0n_0} = {} & X_{i_0i}X_{j_0j}X_{k_0k}X_{l_0l}X_{m_0n_0} - X_{i_0i}X_{j_0j}X_{k_0k}X_{m_0l}X_{l_0n_0} + X_{i_0i}X_{j_0j}X_{k_0k}X_{n_0l}X_{l_0m_0} + X_{i_0i}X_{j_0j}X_{l_0k}X_{m_0l}X_{k_0n_0} \\
& - X_{i_0i}X_{j_0j}X_{l_0k}X_{n_0l}X_{k_0m_0} + X_{i_0i}X_{j_0j}X_{m_0k}X_{n_0l}X_{k_0l_0} - X_{i_0i}X_{k_0j}X_{l_0k}X_{m_0l}X_{j_0n_0} + X_{i_0i}X_{n_0j}X_{k_0k}X_{l_0l}X_{j_0m_0} \\
& - X_{i_0i}X_{k_0j}X_{m_0k}X_{n_0l}X_{j_0l_0} + X_{i_0i}X_{l_0j}X_{m_0k}X_{n_0l}X_{j_0k_0} + X_{j_0i}X_{k_0j}X_{l_0k}X_{m_0l}X_{i_0n_0} - X_{j_0i}X_{n_0j}X_{k_0k}X_{l_0l}X_{i_0m_0} \\
& + X_{j_0i}X_{k_0j}X_{m_0k}X_{n_0l}X_{i_0l_0} - X_{j_0i}X_{l_0j}X_{m_0k}X_{n_0l}X_{i_0k_0} + X_{k_0i}X_{l_0j}X_{m_0k}X_{n_0l}X_{i_0j_0}, \qquad \text{(A4)}
\end{aligned}
$$

$$
U^{ijklmn}_{i_0j_0k_0l_0m_0n_0} = X_{i_0i}X_{j_0j}X_{k_0k}X_{l_0l}X_{m_0m}X_{n_0n}. \qquad \text{(A5)}
$$

from Eqs. (14), (A1) one can then obtain Eq. (30) readily.

Secondly we show that from Eq. (31) we get

$$
\mathrm{Pf}(\mathbb{S}\{i,j\}) = (-1)^{i+j}\alpha_{ij}\mathbb{S}^{-1}_{ij}\mathrm{Pf}(\mathbb{S}), \qquad \text{(A6a)}
$$

$$
\mathrm{Pf}(\mathbb{S}\{i,j,k,l\}) = (-1)^{i+j+k+l}\alpha_{ijkl}\big(\mathbb{S}^{-1}_{ij}\mathbb{S}^{-1}_{kl} - \mathbb{S}^{-1}_{ik}\mathbb{S}^{-1}_{jl} + \mathbb{S}^{-1}_{il}\mathbb{S}^{-1}_{jk}\big)\mathrm{Pf}(\mathbb{S}), \qquad \text{(A6b)}
$$

$$
\begin{aligned}
\mathrm{Pf}(\mathbb{S}\{i,j,k,l,m,n\}) = {} & (-1)^{i+j+k+l+m+n}\alpha_{ijklmn}\big(\mathbb{S}^{-1}_{ij}\mathbb{S}^{-1}_{kl}\mathbb{S}^{-1}_{mn} - \mathbb{S}^{-1}_{ij}\mathbb{S}^{-1}_{km}\mathbb{S}^{-1}_{ln} + \mathbb{S}^{-1}_{ij}\mathbb{S}^{-1}_{kn}\mathbb{S}^{-1}_{lm} - \mathbb{S}^{-1}_{ik}\mathbb{S}^{-1}_{jl}\mathbb{S}^{-1}_{mn} \\
& + \mathbb{S}^{-1}_{ik}\mathbb{S}^{-1}_{jm}\mathbb{S}^{-1}_{ln} - \mathbb{S}^{-1}_{ik}\mathbb{S}^{-1}_{jn}\mathbb{S}^{-1}_{lm} + \mathbb{S}^{-1}_{il}\mathbb{S}^{-1}_{jk}\mathbb{S}^{-1}_{mn} - \mathbb{S}^{-1}_{il}\mathbb{S}^{-1}_{jm}\mathbb{S}^{-1}_{kn} + \mathbb{S}^{-1}_{il}\mathbb{S}^{-1}_{jn}\mathbb{S}^{-1}_{km} - \mathbb{S}^{-1}_{im}\mathbb{S}^{-1}_{jk}\mathbb{S}^{-1}_{ln} \\
& + \mathbb{S}^{-1}_{im}\mathbb{S}^{-1}_{jl}\mathbb{S}^{-1}_{kn} - \mathbb{S}^{-1}_{im}\mathbb{S}^{-1}_{jn}\mathbb{S}^{-1}_{kl} + \mathbb{S}^{-1}_{in}\mathbb{S}^{-1}_{jk}\mathbb{S}^{-1}_{lm} - \mathbb{S}^{-1}_{in}\mathbb{S}^{-1}_{jl}\mathbb{S}^{-1}_{km} + \mathbb{S}^{-1}_{in}\mathbb{S}^{-1}_{jm}\mathbb{S}^{-1}_{kl}\big)\mathrm{Pf}(\mathbb{S}) \qquad \text{(A6c)}
\end{aligned}
$$

with the help of which we can obtain Eq. (32) from Eq. (30).

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