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2004 J. Phys. A: Math. Gen. 37 10585

(http://iopscience.iop.org/0305-4470/37/44/009)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 10585–10607 PII: S0305-4470(04)77770-7

Group-theoretical deduction of a dyadic Tamm–Dancoff equation by using a matrix-valued generator coordinate*

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Received 12 March 2004
Published 20 October 2004
Online at stacks.iop.org/JPhysA/37/10585
doi:10.1088/0305-4470/37/44/009

Abstract

The traditional Tamm–Dancoff (TD) method is one of the standard procedures for solving the Schrödinger equation of fermion many-body systems. However, it meets a serious difficulty when an instability occurs in the symmetry-adapted ground state of the independent particle approximation (IPA) and when the stable IPA ground state becomes of broken symmetry. If one uses the stable but broken symmetry IPA ground state as the starting approximation, TD wave functions also become of broken symmetry. On the contrary, if we start from a symmetry-adapted but unstable wave function, the convergence of the TD expansion becomes bad. Thus, the requirements of symmetry and rapid convergence are not in general compatible in the conventional TD expansion of the systems with strong collective correlations. Along the same line as Fukutome's, we give a group-theoretical deduction of a $U(n)$ dyadic TD equation by using a matrix-valued generator coordinate.

PACS numbers: 21.60.Fw, 05.30.Fk

1. Introduction

One of the most challenging problems of nuclear physics and molecular physics is to give a theory suitable for description of collective motions with large amplitudes in soft nuclei and molecules with strong collective correlations. A conventional standard description of

* A preliminary version of this work was first presented by S Nishiyama at the *Workshop on Quantum Field Theory and its Application* held at the Yukawa Institute for Theoretical Physics, Kyoto, Japan, 24–26 December 2003.

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fermion many-body systems starts with the most basic approximation that is based on an independent-particle picture, i.e., a self consistent field (SCF) for motion of the fermions. The Hartree–Fock (HF) theory is typically one such approximation for ground states of the fermion systems. Excited states are treated with the well-known random phase approximation (RPA). As is well known, the HF theory is formulated by a variational method to optimize an energy expectation value by a Slater determinant (S-det) and to obtain a variational equation for orbitals in the S-det [1]. A set of particle–hole pair operators of the fermions with n single-particle states is closed under a Lie multiplication and forms a basis of a Lie algebra u_n [2]. The u_n Lie algebra of the fermion pair operators generates a Thouless transformation [3], which induces a representation of the corresponding $U(n)$ Lie group. The $U(n)$ canonical transformation transforms a S-det with m particles to another S-det. This means that any S-det is obtained by a $U(n)$ canonical transformation of a reference S-det. The Thouless transformation provides an exact wave function of fermion state vector, which is the generalized coherent state representation (CS rep) on $U(n)$ Lie group of the fermion state [4].

Meanwhile, the traditional Tamm–Dancoff (TD) method has been one of the standard procedures of solving the Schrödinger equation for such problems mentioned above. As we have often experienced, the TD method meets with the following serious problems: they occur when an independent particle ground state, of an independent particle approximation (IPA) affiliated with some symmetry, becomes unstable and when the stable IPA ground state becomes of broken symmetry. If the stable but broken symmetry IPA wave function is used as the starting approximation, the symmetry is also broken by the approximate TD wave functions and the identification of the wave functions with eigenstates of the Hamiltonian may become ambiguous or even impossible. In contrast, if we start from a symmetry-adapted but unstable wave function, the convergence of the TD expansion becomes truly bad and a cutoff of the expansion may lead to a qualitatively incorrect result because the effect of the collective correlation incorporated into the broken symmetry IPA wave function extends up to higher-order terms of such an expansion. The requirements of both symmetry and rapid convergence are not in general compatible with each other and can never be realized simultaneously, if we try to describe fermion systems with strong collective correlations by the conventional TD expansion method. Such correlations may be really anticipated to occur in highly deformed and superconducting nuclei and also in superconducting molecular systems.

For providing a general microscopic means for unified description of collective excitations in strongly correlated fermion systems and for eliminating the above-mentioned dilemma, Fukutome has proposed the new TD method based on the $SO(2n)$ and the $SO(2n+1)$ (the special orthogonal groups of $2n$ and $2n+1$ dimensions) fundamental spinor representations (n being the number of the single-particle states) [5, 6]. The Hartree–Bogoliubov (HB) wave function is generated by the $SO(2n)$ canonical transformation. The symmetry-projected TD expansion method gives good wave functions for the ground and excited states up to any higher-order approximation if we start from the HB wave function and use its non-Euclidean property of transformation by a matrix-valued generator coordinate. However, a fermion number nonconserving treatment is known to be unsatisfactory. One of the present authors (SN) has developed the first-order approximation of the number-projected (NP) $SO(2n)$ TD equation to describe ground and excited states. This equation is expressed as a higher-order differential equation with respect to geminal coset variables. As was done in [7], it can be reduced to a simpler form by the Schur function of group characters, which has a close connection with the soliton theory on the group manifold.

Along the same way as above, we give a group-theoretical deduction of a $U(n)$ dyadic TD equation by using a matrix-valued generator coordinate. In section 2, we introduce a matrix-valued generator coordinate and derive a non-Euclidean transformation rule of the coset variables. In section 3, we make a $U(n)$ dyadic TD expansion of a state in a particle–hole frame. In section 4, we deduct a $U(n)$ dyadic TD equation group theoretically and give an expression for the Hamiltonian matrix element between two $U(n)$ dyadic TD wave functions. In section 5, we approximate the $U(n)$ dyadic TD equation up to the first order. Finally, in section 6, we give the summary and discussions on *the generalized Brillouin theorem* and *the weak killer condition* [8]. In the appendices, we first recapitulate algebraic relations between the coset coordinates and the Plücker coordinates, which play crucial roles in the SCF and the soliton theories. We also give differential formulae needed for variational calculations and explicit forms of the Schur functions.

2. Generator coordinate and non-Euclidean transformation

We consider a finite many-fermion system with n single-particle states. Let c_α and $c_\alpha^\dagger$ ($\alpha = 1, \ldots, n$) be the annihilation and creation operators of the fermion. Owing to the anti-commutation relations

$$\{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha\beta}, \qquad \{c_\alpha, c_\beta\} = \{c_\alpha^\dagger, c_\beta^\dagger\} = 0, \tag{2.1}$$

fermion pair operators $e_{\alpha\beta} \equiv c_\alpha^\dagger c_\beta$ satisfy a Lie commutation relation

$$[e_{\alpha\beta}, e_{\gamma\delta}] = \delta_{\beta\gamma} e_{\alpha\delta} - \delta_{\alpha\delta} e_{\gamma\beta}, \tag{2.2}$$

and span a Lie algebra u_n. The brackets $\{\cdot, \cdot\}$ and $[\cdot, \cdot]$ denote the anti-commutator and the commutator, respectively. A canonical transformation $U(g) = e^{\gamma_{\alpha\beta} c_\alpha^\dagger c_\beta} (\gamma^\dagger = -\gamma)$, which is specified by a $U(n)$ matrix g ($=e^\gamma$), generates a transformation such that

$$\begin{aligned} &U(g) c_\alpha^\dagger U^{-1}(g) = c_\beta^\dagger g_{\beta\alpha}, \qquad U(g) c_\alpha U^{-1}(g) = c_\beta g_{\beta\alpha}^*, \\ &U^{-1}(g) = U(g^{-1}) = U(g^\dagger), \qquad U(gg') = U(g)U(g'), \qquad g^\dagger g = g g^\dagger = 1_n, \end{aligned} \tag{2.3}$$

where 1_n is an n-dimensional unit matrix. We use the dummy index convention to sum up repeated indices unless there is scope for misunderstanding. Symbols $\dagger$, $*$ and T mean hermitian conjugation, complex conjugation and transposition, respectively. Let $|0\rangle$ be a free vacuum and $|\phi_m\rangle$ be an m particle S-det

$$\begin{aligned} &c_\alpha |0\rangle = 0, \quad (\alpha = 1, \ldots, n), \qquad |\phi_m\rangle = c_m^\dagger \cdots c_1^\dagger |0\rangle, \\ &U(g)|\phi_m\rangle = (c^\dagger g)_m \cdots (c^\dagger g)_1 |0\rangle \overset{d}{=} |g\rangle, \qquad U(g)|0\rangle = |0\rangle, \end{aligned} \tag{2.4}$$

where $c^\dagger$ means an n-dimensional row vector $c^\dagger = (c_1^\dagger, \ldots, c_n^\dagger)$. Equation (2.4) shows that m particle S-det is an exterior product of m single-particle states and that $U(g)$ transforms $|\phi_m\rangle$ to another S-det (Thouless transformation) [3] under (2.3). Such states are called 'simple' states. The set of all simple states of unit modulus together with the equivalence relation, identifying distinct states only in phases with the same state, constitutes a manifold known as a Grassmannian Gr_m. The Gr_m is an orbit of the group given through (2.4). Any simple state $|\phi_m\rangle \in Gr_m$ defines a decomposition of single-particle Hilbert space into sub-Hilbert spaces of occupied and unoccupied states [9]. Thus, the Gr_m corresponds to a coset space

$$Gr_m \sim U(n)/(U(m) \times U(n-m)). \tag{2.5}$$

Following Fukutome [10], let us introduce triangular matrix functions $S(\zeta)$, $C(\zeta)$ and $\tilde{C}(\zeta)$ defined as

$$
\begin{aligned}
S(\zeta) &= (S_{ia}(\zeta)) = \sum_{k=0}^{\infty}(-1)^k \frac{1}{(2k+1)!}\zeta(\zeta^\dagger\zeta)^k, \\
C(\zeta) &= (C_{ab}(\zeta)) = 1_m + \sum_{k=1}^{\infty}(-1)^k \frac{1}{(2k)!}(\zeta^\dagger\zeta)^k = C^\dagger(\zeta), \\
\tilde{C}(\zeta) &= (\tilde{C}_{ij}(\zeta)) = 1_{n-m} + \sum_{k=1}^{\infty}(-1)^k \frac{1}{(2k)!}(\zeta\zeta^\dagger)^k = \tilde{C}^\dagger(\zeta),
\end{aligned}
\tag{2.6}
$$

which have the properties analogous to the usual triangular functions

$$
C^2(\zeta) + S^\dagger(\zeta)S(\zeta) = 1_m, \qquad \tilde{C}^2(\zeta) + S(\zeta)S^\dagger(\zeta) = 1_{n-m}, \qquad S(\zeta)C(\zeta) = \tilde{C}(\zeta)S(\zeta).
\tag{2.7}
$$

The indices i and a denote unoccupied states $(m+1,\ldots,n)$ and occupied states $(1,\ldots,m)$, respectively. The matrix p is defined as $p = (p_{ia}) = S(\zeta)C^{-1}(\zeta) = \tilde{C}^{-1}(\zeta)S(\zeta)$. Using equations (2.6) and (2.7), we have relations $\det C = [\det(1 + p^\dagger p)]^{-\frac{1}{2}}$ and $\det\tilde{C} = [\det(1 + pp^\dagger)]^{-\frac{1}{2}}$, where $\det C$ and $\det\tilde{C}$ are determinants of matrices C and $\tilde{C}$, respectively. The matrix g in (2.3) is decomposed as $g = g_\zeta g_w$ using the matrices given by

$$
\begin{aligned}
&g_\zeta = e^{\gamma'} = \begin{bmatrix} C(\zeta) & -S(\zeta)^\dagger \\ S(\zeta) & \bar{C}(\zeta) \end{bmatrix}, \qquad \gamma' = \begin{bmatrix} 0 & -\zeta^\dagger \\ \zeta & 0 \end{bmatrix}, \\
&g_w = e^{\gamma''} = \begin{bmatrix} w & 0 \\ 0 & \bar{w} \end{bmatrix}, \qquad \gamma'' = \begin{bmatrix} \eta & 0 \\ 0 & \bar{\eta} \end{bmatrix}, \qquad \eta^\dagger = -\eta, \qquad \bar{\eta}^\dagger = -\bar{\eta},
\end{aligned}
\tag{2.8}
$$

where ζ is an $(n-m)\times m$ matrix (ζ_{ia}) and η and $\bar{\eta}$ are $m\times m$ and $(n-m)\times(n-m)$ anti-hermitian matrices (η_{ab}) and $(\bar{\eta}_{ij})$, respectively.

Let us start with a state $|f\rangle$, an exact representaion on the $U(n)$ group

$$
\begin{aligned}
|f\rangle &= {}_nC_m \int U(g')|\phi_m\rangle\langle\phi_m|U^\dagger(g')|f\rangle dg' \\
&= {}_nC_m \int |g'\rangle\Phi_{0f}(g')dg' \quad \left({}_nC_m = \frac{n!}{m!(n-m)!}\right),
\end{aligned}
\tag{2.9}
$$

where dg' is an invariant group integration over the $U(n)$ group. Using the invariance of the group measure of the transformation of the variable g by any group element, from (2.9) we have

$$
U(g)|f\rangle = {}_nC_m \int |g'\rangle\Phi_{0f}(g^\dagger g')dg',
\tag{2.10}
$$

which means that the canonical transformation $U(g)$ to the state $|f\rangle$ corresponds to a left coordinate tranformation by $g^\dagger$ of the matrix-valued generator coordinate g'. Instead of g', let us introduce the matrix-valued generator coordinate $\mathring{g}$ in the g particle–hole frame by $\mathring{g} = g^\dagger g'$. Then, conversely, the g' is represented as

$$
\begin{aligned}
g' &= \begin{bmatrix} C'w' & -S'^\dagger\bar{w}' \\ S'w' & \tilde{C}'\bar{w}' \end{bmatrix} = g\mathring{g} = \begin{bmatrix} Cw & -S^\dagger\bar{w} \\ Sw & \tilde{C}\bar{w} \end{bmatrix} \begin{bmatrix} \mathring{C}\mathring{w} & -\mathring{S}^\dagger\mathring{\bar{w}} \\ \mathring{S}\mathring{w} & \mathring{\tilde{C}}\mathring{\bar{w}} \end{bmatrix} \\
&= \begin{bmatrix} Cw\mathring{C}\mathring{w} - S^\dagger\bar{w}\mathring{S}\mathring{w} & -Cw\mathring{S}^\dagger\mathring{\bar{w}} - S^\dagger\bar{w}\mathring{\tilde{C}}\mathring{\bar{w}} \\ Sw\mathring{C}\mathring{w} + \tilde{C}\bar{w}\mathring{S}\mathring{w} & -Sw\mathring{S}^\dagger\mathring{\bar{w}} + \tilde{C}\bar{w}\mathring{\tilde{C}}\mathring{\bar{w}} \end{bmatrix}.
\end{aligned}
\tag{2.11}
$$

From (2.11) and the definition of a coset variable $\mathring{p} \equiv \mathring{S}\mathring{C}^{-1}$ in the coordinate $\mathring{g}$, we obtain the relations

$$\begin{aligned} C'w' &= Cw\mathring{C}\mathring{w} - S^\dagger\bar{w}\mathring{S}\mathring{w} = [Cw - S^\dagger\bar{w}\mathring{S}\mathring{w}(\mathring{C}\mathring{w})^{-1}]\mathring{C}\mathring{w} \\ &= [Cw - S^\dagger\bar{w}\mathring{p}]\mathring{C}\mathring{w} = Cw[1-(Cw)^{-1}S^\dagger\bar{w}\mathring{p}]\mathring{C}\mathring{w}, \\ S'w' &= Sw\mathring{C}\mathring{w} + \tilde{C}\bar{w}\,\mathring{S}\mathring{w} = [Sw + \tilde{C}\bar{w}\mathring{S}\mathring{w}(\mathring{C}\mathring{w})^{-1}]\mathring{C}\mathring{w} = [Sw + \tilde{C}\bar{w}\mathring{p}]\mathring{C}\mathring{w}\,. \end{aligned} \tag{2.12}$$

On the other hand, from $g^\dagger g = 1$, i.e. $\bar{w}^\dagger\tilde{C}^\dagger\tilde{C}\bar{w} + \bar{w}^\dagger SS^\dagger\bar{w} = 1$, we also have

$$\tilde{C}\bar{w} + (\bar{w}^\dagger\tilde{C}^\dagger)^{-1}\bar{w}^\dagger SS^\dagger\bar{w} = \tilde{C}\bar{w} + pS^\dagger\bar{w} = (\bar{w}^\dagger\tilde{C}^\dagger)^{-1}. \tag{2.13}$$

We further define a coset variable $p' \equiv S'C'^{-1}$ in the g' frame. A $U(n)$ wave function generated by a canonical transformation to a g' particle–hole frame is regarded as a function of the generator coordinate $\mathring{g}: |g'\rangle = U(g\mathring{g})|g\mathring{g}\rangle$. With the aid of (2.12) and (2.13), the coset variable p' is written as

$$\begin{aligned} p' &= S'w'(C'w')^{-1} = [Sw + \tilde{C}\bar{w}\mathring{p}][1-(Cw)^{-1}S^\dagger\bar{w}\mathring{p}]^{-1}(Cw)^{-1} \\ &= [Sw\{1-(Cw)^{-1}S^\dagger\bar{w}\mathring{p}\} + \{pS^\dagger\bar{w} + \tilde{C}\bar{w}\}\mathring{p}][1-(Cw)^{-1}S^\dagger\bar{w}\mathring{p}]^{-1}(Cw)^{-1} \\ &= p + (\bar{w}^\dagger\tilde{C}^\dagger)^{-1}\mathring{p}[1-(Cw)^{-1}S^\dagger\bar{w}\mathring{p}]^{-1}(Cw)^{-1}. \end{aligned} \tag{2.14}$$

Let us introduce following matrices r, q and e:

$$\begin{aligned} r &\equiv (Cw)^{-1}S^\dagger\bar{w} = w^{-1}p^\dagger\bar{w}, \\ q &\equiv (\bar{w}^\dagger\tilde{C}^\dagger)^{-1}\mathring{p}(Cw)^{-1} = (\bar{w}^\dagger\tilde{C})^{-1}\mathring{p}(Cw)^{-1}, \\ e &\equiv -(Cw)^* r^* (\bar{w}^\dagger\tilde{C}^\dagger)^* = -S^{\mathrm{T}}\tilde{C}^{\mathrm{T}} = -p^{\mathrm{T}}(1+p^*p^{\mathrm{T}})^{-1}. \end{aligned} \tag{2.15}$$

Then, the p' is rewritten as

$$p' = p + q[1-(Cw)r\mathring{p}(Cw)^{-1}]^{-1} = p + q[1-(Cw)r(\bar{w}^\dagger\tilde{C}^\dagger)q]^{-1} = p + q(1+e^*q)^{-1}, \tag{2.16}$$

whose transformation rule causes the non-Euclidean properties of the coset variables because the coset variables (the geminals) are quantities defined on the non-commutative $U(n)$ group, which belong to the Grassmann manifold $U(n)/(U(m) \times U(n-m))$ [11].

Finally, we define the overlap integral of $U(n)$ wave functions

$$S(g, g') = \Phi_{00}^*(g^\dagger g') = \langle\phi_m|U^\dagger(g)U(g')|\phi_m\rangle. \tag{2.17}$$

Multiplying equation (2.9) by $\langle\phi_m|U^\dagger(g)$, we have

$$\Phi_{0f}(g) = {}_nC_m \int \langle\phi_m|U^\dagger(g)U(g')|\phi_m\rangle\phi_{0f}(g')dg' = {}_nC_m \int S(g, g')\Phi_{0f}(g')dg', \tag{2.18}$$

in which it is easily verified that the overlap integral $S(g, g')$ satisfies

$$S(g, g') = {}_nC_m \int S(g, g'')S(g'', g')dg''. \tag{2.19}$$

This property shows that the ${}_nC_m S(g, g')$ is just the projection operator to the $U(n)$ S-det. Putting $\mathring{g} = g^\dagger g'$ in (2.17) and using the same type of representaion as that of (2.11), we have

$$\Phi_{00}^*(g^\dagger g') = \Phi_{00}^*(\mathring{g}) = \det(\mathring{C}\mathring{w}), \tag{2.20}$$

$$\begin{aligned} \mathring{g} = g^\dagger g' &= \begin{bmatrix} w^\dagger C^\dagger & w^\dagger S^\dagger \\ -\bar{w}^\dagger S & \bar{w}^\dagger\tilde{C}^\dagger \end{bmatrix} \begin{bmatrix} C'w' & -S'^\dagger\bar{w}' \\ S'w' & \tilde{C}'\bar{w}' \end{bmatrix} \\ &= \begin{bmatrix} w^\dagger(C^\dagger C' + S^\dagger S')w' & -w^\dagger(C^\dagger S'^\dagger - S^\dagger\tilde{C}')\bar{w}' \\ -\bar{w}^\dagger(SC' - \tilde{C}^\dagger S')w' & \bar{w}^\dagger(\tilde{C}^\dagger\tilde{C}' + SS'^\dagger)\bar{w}' \end{bmatrix}. \end{aligned} \tag{2.21}$$

Then, an explicit expression for the overlap integral is obtained as

$$S(g,g') = \det(C''w'') = \det\{C^{\dagger}(1 + C^{\dagger -1}S^{\dagger}S'C'^{-1})C'\}\det(w^{\dagger})\det(w')$$
$$= D(p'^{\mathrm{T}}p^{*})\Phi_{00}(g)\Phi_{00}^{*}(g'), \tag{2.22}$$

where the function $D(p'^{\mathrm{T}}p^{*})$, expressing its other form in appendix D, is defined by

$$D(p'^{\mathrm{T}}p^{*}) \equiv \det(1 + p'^{\mathrm{T}}p^{*}) = \det(1 + p^{\dagger}p'). \tag{2.23}$$

3. TD expansion of a state in a particle–hole frame

Taking the coordinate g' instead of the generator coordinate $\overset{\circ}{g}$ in (2.20), we have

$$\Phi_{00}(g') = \langle\phi_m|U^{\dagger}(g')|\phi_m\rangle = \det(C'w'), \qquad g' = g\overset{\circ}{g}\,. \tag{3.1}$$

Through (2.12) and (2.15), computation of a determinant of $C'w'$ is carried out as

$$\det(C'w') = \det(Cw)\det(\overset{\circ}{C}\overset{\circ}{w})\det[1 - (Cw)^{-1}S^{\dagger}\tilde{C}q(Cw)]$$
$$= \det(Cw)\det(\overset{\circ}{C}\overset{\circ}{w})\det[(Cw)^{-1}(1 - S^{\dagger}\tilde{C}q)(Cw)]$$
$$= \det(Cw)\det(\overset{\circ}{C}\overset{\circ}{w})\det(1 + eq^{*}). \tag{3.2}$$

On the other hand, by using equations (A.1) and (2.9), the $U(N)$ spinor function $\Phi_{0f}(g')$ is shown to be in the following form:

$$\langle\phi_m|U^{\dagger}(g')|f\rangle = \phi_{0f}(g') = [\Phi_{00}^{*}(g')e^{p'_{ia}c_i^{\dagger}c_a}|\phi_m\rangle]^{\dagger}|f\rangle = \mathcal{X}_f(p'^{*})\Phi_{00}(g')$$
$$= \mathcal{X}_f\{p^{*} + q^{*}(1 + eq^{*})^{-1}\}D(eq^{*})\Phi_{00}(g)\Phi_{00}(\overset{\circ}{g}), \tag{3.3}$$

where the functions $\mathcal{X}_f(p'^{*})$ and $D(eq^{*})$ are defined as

$$\mathcal{X}_f(p'^{*}) \equiv \langle\phi_m|e^{p'^{*}_{ia}c_a^{\dagger}c_i}|f\rangle, \qquad D(eq^{*}) \equiv \det(1 + eq^{*}). \tag{3.4}$$

We also have used the non-Euclidean transformation (2.16) and the above equations (3.1) and (3.2). From (3.3) we have

$$\Phi_{0f}(g') = \mathcal{X}_f(p^{*} + K^{*})D(eq^{*})\Phi_{00}(g)\phi_{00}(\overset{\circ}{g}), \qquad K^{*} \equiv q^{*}(1 + eq^{*})^{-1}. \tag{3.5}$$

Applying the differential formulae of $D(ep^{*})$ with respect to e_{ai} in appendix E

$$\frac{\partial^{\rho}D(eq^{*})}{\partial e_{a_1i_1}\partial e_{a_2i_2}\cdots\partial e_{a_{\rho}i_{\rho}}} = \mathcal{A}(K^{*}_{i_1a_1}K^{*}_{i_2a_2}\cdots K^{*}_{i_{\rho}a_{\rho}})D(eq^{*}) \quad (\rho = 1,\ldots,\min(m,n-m)) \tag{3.6}$$

to the Tayler expansion made below and using the anti-symmetric property of the differentials of $\mathcal{X}_f(p^{*})$

$$\frac{\partial^2\mathcal{X}_f(p^{*})}{\partial p^{*}_{jb}\partial p^{*}_{ia}} = -\frac{\partial^2\mathcal{X}_f(p^{*})}{\partial p^{*}_{ib}\partial p^{*}_{ja}},\ldots, \tag{3.7}$$

we can make a Tayler expansion of $\mathcal{X}_f(p^{*} + K^{*})$ in (3.5) with respect to K^{*}. A matrix element p^{*}_{ia} appears only once in $\mathcal{X}_f(p^{*})$, because the $\mathcal{X}_f(p^{*})$ is an anti-symmetric function of p^{*}, which is proved with the use of equations (B.21) and (B.22). Then, the Tayler series leads to

$$\mathcal{X}_f(p^{*} + K^{*})D(eq^{*}) = \mathcal{X}_f(p^{*})D(eq^{*}) + \sum_{\rho=1}^{M}\sum_{\substack{1\leqslant a_1<\cdots<a_{\rho}\leqslant m;\\ m+1\leqslant i_1<\cdots<i_{\rho}\leqslant n}}\frac{\partial^{\rho}\mathcal{X}_f(p^{*})}{\partial p^{*}_{i_1a_1}\partial p^{*}_{i_2a_2}\cdots\partial p^{*}_{i_{\rho}a_{\rho}}}$$
$$\times\mathcal{A}(K^{*}_{i_1a_1}K^{*}_{i_2a_2}\cdots K^{*}_{i_{\rho}a_{\rho}})D(eq^{*}). \tag{3.8}$$

Furthermore, with the help of the expression for the $D(p'^{\mathrm{T}} p^*)$ in appendix D, the explicit expression for the $D(eq^*)$ is calculated to be

$$D(eq^*) = \sum_{\rho=0}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \mathcal{A}(e_{a_1 i_1}\cdots e_{a_\rho i_\rho})\mathcal{A}(q^*_{i_1 a_1}\cdots q^*_{i_\rho a_\rho}). \tag{3.9}$$

Let $\mathcal{D}^\rho = 1$ for $\rho = 0$. Substituting (3.9) into (3.8), we have

$$\begin{aligned}\Phi_{0f}(g') &= \mathcal{X}_f(p^* + K^*)D(eq^*)\Phi_{00}(g)\Phi_{00}(\mathring{g})\\ &= \Phi_{00}(g)\sum_{\rho=0}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \mathcal{A}(q^*_{i_1 a_1}\cdots q^*_{i_\rho a_\rho})\mathcal{D}^\rho_{a_1 i_1\cdots a_\rho i_\rho}\mathcal{X}_f(p^*)\Phi_{00}(\mathring{g}),\end{aligned} \tag{3.10}$$

where the ρth-order covariant differential operator $\mathcal{D}^\rho_{a_1 i_1\cdots a_\rho i_\rho}$ is defined as

$$\mathcal{D}^\rho_{a_1 i_1\cdots a_\rho i_\rho} \equiv \mathcal{A}(e_{a_1 i_1}\cdots e_{a_\rho i_\rho}) + \mathcal{A}\left(e_{a_2 i_2}\cdots e_{a_\rho i_\rho}\frac{\partial}{\partial p^\dagger_{a_1 i_1}}\right) + \cdots + \mathcal{A}\left(\frac{\partial}{\partial p^\dagger_{a_1 i_1}}\cdots\frac{\partial}{\partial p^\dagger_{a_\rho i_\rho}}\right). \tag{3.11}$$

From the second equation of (2.15), we have an explicit form of q^* as $q^*_{ia} = \{(\tilde{C}\bar{w})^{\mathrm{T}-1}\}_{ij}\mathring{p}^*_{jb} \times\{(Cw)^{*-1}\}_{ba}$, in which we have used again the dummy index convention to sum up repeated indices j and b. Substituting this into (3.10) and defining the differential operator $\Delta^\rho_{b_1 j_1\cdots b_\rho j_\rho}$ ($\Delta^\rho = 1$ for $\rho = 0$) as

$$\begin{aligned}\Delta^\rho_{b_1 j_1\cdots b_\rho j_\rho} \equiv \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} &\{(Cw)^{*-1}\}_{b_1 a_1}\{(\tilde{C}\bar{w})^{-1}\}_{j_1 i_1}\cdots\{(Cw)^{*-1}\}_{b_\rho a_\rho}\\ &\times\{(\tilde{C}\bar{w})^{-1}\}_{j_\rho i_\rho}\mathcal{D}^\rho_{a_1 i_1\cdots a_\rho i_\rho},\end{aligned} \tag{3.12}$$

we finally get

$$\Phi_{0f}(g') = \phi_{0f}(g\mathring{g}) = \phi_{00}(g)\sum_{\rho=0}^{M}\mathcal{A}(\mathring{p}^*_{j_1 b_1}\cdots\mathring{p}^*_{j_\rho b_\rho})\Delta^\rho_{b_1 j_1\cdots b_\rho j_\rho}\mathcal{X}_f(p^*)\Phi_{00}(\mathring{g}), \tag{3.13}$$

which is the dyadic TD expansion of a state function $\Phi_{0f}(g')$ in the g particle–hole frame.

Fermion many-body systems always have a symmetry group s which is a subgroup of the $U(n)$ group. An eigenstate of a Hamiltonian H belongs to an irreducible representation of the symmetry group. We denote the irreducible representation by I, the quantum number to specify its orthogonal bases by M and the other quantum numbers by ω. The symmetry group s is an element of the $U(n)$ group and there is a $U(n)$ canonical transformation $U(s)$ corresponding to s. Following [2], we give a generator coordinate representation of a symmetry adapted state vector $|IM\omega\rangle$ in terms of the projected $U(n)$ wave function. The state vector $|f\rangle = |IM\omega\rangle$ is transformed by $U(s)$ as

$$U(s)|IM\omega\rangle = \sum_K |IK\omega\rangle D^I_{KM}(s), \qquad s = \begin{bmatrix} s_h & 0\\ 0 & s_p\end{bmatrix}, \qquad s^\dagger s = ss^\dagger = 1_n, \tag{3.14}$$

where $D^I_{KM}(s)$'s are the so-called D functions, which are the matrix elements of the representation matrix of the irreducible representation I of the group s. From (2.9), we have

$$U(s)|IM\omega\rangle = {}_nC_m\int U(sg)|\phi_m\rangle\langle\phi_m|U^\dagger(g)|IM\omega\rangle dg. \tag{3.15}$$

Multiplying equation (3.15) by $D^{I*}_{KM}(s)$, integrating over the group s, and using (3.14) and the orthogonality relation for the D functions

$$\int D^{I*}_{KM}(s) D^{I'}_{K'M'}(s) ds = [d(I)]^{-1} \delta_{II'} \delta_{KK'} \delta_{MM'}, \tag{3.16}$$

we obtain a generator coordinate representation of the symmetry adapted state vector

$$|IK\omega\rangle = d(I)\,{}_nC_m \int |\Phi^I_{KM}(g)\rangle \langle \phi_m | U^\dagger(g) | IM\omega\rangle dg, \tag{3.17}$$

where $d(I)$ is the dimension of the representation I and the volume of the symmetry group s. The state vector $|\Phi^I_{KM}(g)\rangle$ is defined as

$$\begin{aligned} |\Phi^I_{KM}(g)\rangle &\equiv \int D^{I*}_{KM}(s) U(sg) |\phi_m\rangle ds, \\ \langle \Phi^I_{KM}(g) | \Phi^{I'}_{K'M'}(g')\rangle &= [d(I)]^{-1} \delta_{II'} \delta_{KK'} S^I_{MM'}(g, g'), \\ S^I_{MM'}(g, g') &\equiv \int D^{I*}_{MM'}(s') S(g, s'g') ds', \end{aligned} \tag{3.18}$$

which is just the Peierls–Yoccoz symmetry projected HF wave function [2, 5, 10, 12].

4. $U(n)$ dyadic TD equation

Multiplying equation (2.9) by $\langle \phi_m | U^\dagger(g) X$, we have

$$\begin{aligned} \langle \phi_m | U^\dagger(g) X | f\rangle &= {}_nC_m \int X(g, g') \Phi_{00}(g') dg', \\ X(g, g') &\equiv \langle \phi_m | U^\dagger(g) X U(g') | \phi_m\rangle. \end{aligned} \tag{4.1}$$

On the other hand, from the definition (4.1) and equation (A.1), the integral operator $X(g, g')$ becomes

$$\begin{aligned} X(g, g') &= [\phi^*_{00}(g) e^{p_{ia} c^\dagger_i c_a} |\phi_m\rangle]^\dagger X \Phi^*_{00}(g') e^{p'_{jb} c^\dagger_j c_b} |\phi_m\rangle \\ &= \langle \phi_m | e^{p^*_{ia} c^\dagger_a c_i} X e^{p'_{jb} c^\dagger_j c_b} |\phi_m\rangle \Phi_{00}(g) \Phi^*_{00}(g'), \end{aligned} \tag{4.2}$$

from which the integral operator is expressed with p^* and p' as

$$X(g, g') = X(p^*, p') \Phi_{00}(g) \Phi^*_{00}(g'), \qquad X(p^*, p') \equiv \langle \phi_m | e^{p^*_{ia} c^\dagger_a c_i} X e^{p'_{jb} c^\dagger_j c_b} |\phi_m\rangle. \tag{4.3}$$

Applying equation (3.13) to equation (4.3), then, the dyadic TD expansion of an operator X in the two particle–hole frames $\hat{g}$ and $\check{g}$

$$X(\hat{g}\,\mathring{\hat{g}}, \check{g}\,\mathring{\check{g}}) = \langle \phi_m | U^\dagger(\hat{g}\,\mathring{\hat{g}}) X U(\check{g}\,\mathring{\check{g}}) |\phi_m\rangle, \tag{4.4}$$

can be obtained in the following way: putting $\hat{g}' = \hat{g}\,\mathring{\hat{g}}$, the integral operator $X(g, g')$ is written as

$$\begin{aligned} X(\hat{g}\,\mathring{\hat{g}}, \check{g}\,\mathring{\check{g}}) &= \langle \phi_m | U^\dagger(\hat{g}') X U(\check{g}') |\phi_m\rangle = [\Phi^*_{00}(\hat{g}') e^{\hat{p}'_{ia} c^\dagger_i c_a} |\phi_m\rangle]^\dagger X \Phi^*_{00}(\check{g}') e^{\check{p}'_{jb} c^\dagger_j c_b} |\phi_m\rangle \\ &= \langle \phi_m | e^{\hat{p}'^*_{ia} c^\dagger_a c_i} X e^{\check{p}'_{jb} c^\dagger_j c_b} |\phi_m\rangle \Phi_{00}(\hat{g}') \Phi^*_{00}(\check{g}') \\ &= \mathcal{X}_{\mathrm{X}}(\hat{p}'^*, \check{p}') \Phi_{00}(\hat{g}') \Phi^*_{00}(\check{g}') \\ &= \mathcal{X}_{\mathrm{X}}(\hat{p}^* + \hat{K}^*, \check{p} + \check{K}) D(\hat{e}\hat{q}^*) D(\check{e}^*\check{q}) \Phi_{00}(\hat{g}) \Phi_{00}(\mathring{\hat{g}}) \Phi^*_{00}(\check{g}) \Phi^*_{00}(\mathring{\check{g}}), \end{aligned} \tag{4.5}$$

where the $\mathcal{X}_{\mathrm{X}}(\hat{p}'^*, \check{p}')$ is defined as

$$\mathcal{X}_{\mathrm{X}}(\hat{p}'^*, \check{p}') \equiv \langle \phi_m | e^{\hat{p}'^*_{ia} c^\dagger_a c_i} X e^{\check{p}'_{jb} c^\dagger_j c_b} |\phi_m\rangle = X(\hat{p}'^*, \check{p}'), \tag{4.6}$$

and where we have used the relation $\hat{p}' = \hat{p} + \hat{q}(1 + \hat{e}^*\hat{q})^{-1} = \hat{p} + \hat{K}$, derived from the relation (2.16) and the definition in (3.5). The function $\mathcal{X}_{\mathrm{X}}(\hat{p}'^*, \check{p}')$ satisfies the anti-symmetric properties of the differentials with respects to $\hat{p}^*$ and $\check{p}$ each of which is quite similar to that in (3.7). According to equation (3.8), the $\mathcal{X}_{\mathrm{X}}$ can also be cast to

$$\mathcal{X}_{\mathrm{X}}(\hat{p}^* + \hat{K}^*, \check{p} + \check{K}) = \mathcal{X}_{\mathrm{X}}(\hat{p}^*, \check{p} + \check{K}) + \sum_{\rho=1}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \frac{\partial^\rho \mathcal{X}_X(\hat{p}^*, \check{p} + \check{K})}{\partial \hat{p}^*{}_{i_1 a_1} \cdots \partial \hat{p}^*{}_{i_\rho a_\rho}} \times \mathcal{A}(\hat{K}^*{}_{i_1 a_1} \cdots \hat{K}^*{}_{i_\rho a_\rho}). \tag{4.7}$$

From the above equation, we have

$$\mathcal{X}_{\mathrm{X}}(\hat{p}^* + \hat{K}^*, \check{p} + \check{K}) D(\hat{e}\hat{q}^*) = \sum_{\rho=0}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \mathcal{A}(\hat{q}^*_{i_1 a_1} \cdots \hat{q}^*_{i_\rho a_\rho}) \hat{\mathcal{D}}^\rho_{a_1 i_1 \cdots a_\rho i_\rho} X(\hat{p}^*, \check{p} + \check{K}). \tag{4.8}$$

Similarly, we get

$$\mathcal{X}_{\mathrm{X}}(\hat{p}^*, \check{p} + \check{K}) D(\check{e}^*\check{q}) = \sum_{\rho=0}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \mathcal{A}(\check{q}_{i_1 a_1} \cdots \check{q}_{i_\rho a_\rho}) \check{\mathcal{D}}^{\rho *}_{a_1 i_1 \cdots a_\rho i_\rho} X(\hat{p}^*, \check{p}). \tag{4.9}$$

Combining (4.8) with (4.9), we obtain

$$X(\hat{g}\,\mathring{\hat{g}}, \check{g}\,\mathring{\check{g}}) = \sum_{\rho'=0}^{M} \sum_{\substack{1\leqslant a'_1<\cdots<a'_{\rho'}\leqslant m;\\ m+1\leqslant i'_1<\cdots<i'_{\rho'}\leqslant n}} \mathcal{A}(\hat{q}^*_{i'_1 a'_1} \cdots \hat{q}^*_{i'_{\rho'} a'_{\rho'}}) \hat{\mathcal{D}}^{\rho'}_{a'_1 i'_1 \cdots a'_{\rho'} i'_{\rho'}} \sum_{\rho=0}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \times \mathcal{A}(\check{q}_{i_1 a_1} \cdots \check{q}_{i_\rho a_\rho}) \check{\mathcal{D}}^{\rho *}_{a_1 i_1 \cdots a_\rho i_\rho} X(\hat{p}^*, \check{p}) \Phi_{00}(\hat{g}) \Phi_{00}(\mathring{\hat{g}}) \Phi^*_{00}(\check{g}) \Phi^*_{00}(\mathring{\check{g}}). \tag{4.10}$$

Introducing again the differential operator $\Delta^\rho_{b_1 j_1 \cdots b_\rho j_\rho}$ ($\Delta^\rho = 1$ for $\rho = 0$) defined in (3.12), we can get the $U(n)$ dyadic TD expansion of any operator X in the two particle–hole frames $\hat{g}$ and $\check{g}$

$$X(\hat{g}\,\mathring{\hat{g}}, \check{g}\,\mathring{\check{g}}) = \Phi_{00}(\hat{g}) \Phi^*_{00}(\check{g}) \sum_{\rho'=0}^{M} \sum_{\substack{1\leqslant b'_1<\cdots<b'_{\rho'}\leqslant m;\\ m+1\leqslant j'_1<\cdots<j'_{\rho'}\leqslant n}} \mathcal{A}(\mathring{\hat{p}}^*{}_{j'_1 b'_1} \cdots \mathring{\hat{p}}^*{}_{j'_{\rho'} b'_{\rho'}}) \hat{\Delta}^{\rho'}_{b'_1 j'_1 \cdots b'_{\rho'} j'_{\rho'}} \times \sum_{\rho=0}^{M} \sum_{\substack{1\leqslant b_1<\cdots<b_\rho\leqslant m;\\ m+1\leqslant j_1<\cdots<j_\rho\leqslant n}} \mathcal{A}(\mathring{\check{p}}_{j_1 b_1} \cdots \mathring{\check{p}}_{j_\rho b_\rho}) \check{\Delta}^{\rho *}_{b_1 j_1 \cdots b_\rho j_\rho} X(\hat{p}^*, \check{p}) \Phi_{00}(\mathring{\hat{g}}) \Phi^*_{00}(\mathring{\check{g}}). \tag{4.11}$$

Let $|\Phi^\rho_{b_1 j_1 \cdots b_\rho j_\rho}(\check{g})\rangle = d^\dagger_{b_1}(\check{g}) d^\dagger_{j_1}(\check{g}) \cdots d^\dagger_{b_\rho}(\check{g}) d^\dagger_{j_\rho}(\check{g}) U(\check{g})|\phi_m\rangle$ be the TD basis with ρ particle–hole pairs in a physical fermion space and $d^\dagger_j(\check{g}) \equiv U(\check{g}) c^\dagger_j U^{-1}(\check{g})$ and $d^\dagger_b(\check{g}) \equiv U(\check{g}) c_b U^{-1}(\check{g})$ be the creation operators of a $\check{g}$ particle and hole frame. The dyadic TD matrix elements of X are therefore given as

$$\langle \Phi^{\rho'}_{b'_1 j'_1 \cdots b'_{\rho'} j'_{\rho'}}(\hat{g}) | X | \Phi^\rho_{b_1 j_1 \cdots b_\rho j_\rho}(\check{g}) \rangle = \Phi_{00}(\hat{g}) \Phi^*_{00}(\check{g}) \hat{\Delta}^{\rho'}_{b'_1 j'_1 \cdots b'_{\rho'} j'_{\rho'}} \check{\Delta}^{\rho *}_{b_1 j_1 \cdots b_\rho j_\rho} X(\hat{p}'^*, \check{p}). \tag{4.12}$$

We expand the state $|IK\omega\rangle$ in terms of the states $|\Phi^{\rho}_{b_1 j_1 \cdots b_\rho j_\rho}(\check{g})\rangle$ as

$$|IK\omega\rangle = \sum_{\rho} \sum_{(b_1 j_1)<\cdots<(b_\rho j_\rho)} \Gamma^{I}_{K\omega, b_1 j_1 \cdots b_\rho j_\rho} |\Phi^{\rho}_{b_1 j_1 \cdots b_\rho j_\rho}(\check{g})\rangle, \tag{4.13}$$

which is just the dyadic TD expansion of the eigenstate of the Hamiltonian H. The summation convention over the indices in (4.13), but simply abbreviated, means the one appeared in (4.11). After making the variation of the energy $E^{I}_{\omega} = \langle IK\omega|H|IK\omega\rangle/\langle IK\omega|IK\omega\rangle$, we apply equation (4.12) to the operator $H^{I}_{KK} - E^{I}_{\omega} S^{I}_{KK}$ and put $\hat{g} = \check{g} = g$. Then, we finally get the $U(n)$ dyadic TD equation to determine the expansion coefficients $\Gamma^{I}_{K\omega, b_1 j_1 \cdots b_\rho j_\rho}$:

$$\sum_{\rho'} \sum_{(b_1 j_1)<\cdots<(b_{\rho'} j_{\rho'})} \Delta^{\rho}{}_{a_1 i_1 \cdots a_\rho i_\rho} \delta^{\rho' *}{}_{b_1 j_1 \cdots b_{\rho'} j_{\rho'}} \{H^{I}_{KK}(p^*, p) - E^{I}_{\omega} S^{I}_{KK}(p^*, p)\} \Gamma^{I}_{K\omega, b_1 j_1 \cdots b_{\rho'} j_{\rho'}} = 0, \tag{4.14}$$

where the quantities $H^{I}_{KK}(p^*, p)$ and $S^{I}_{KK}(p^*, p)$ are given through the following relations:

$$\begin{aligned} H^{I}_{KK}(g, g) &= \langle \phi_m | U^\dagger(g) H | \Phi^{I}_{KK}(g)\rangle = \int D^{I*}_{KK}(s) H(g, sg) ds = H^{I}_{KK}(p^*, p) |\Phi_{00}(g)|^2, \\ S^{I}_{KK}(g, g) &= \langle \phi_m | U^\dagger(g) | \Phi^{I}_{KK}(g)\rangle = \int D^{I*}_{KK}(s) S(g, sg) ds = S^{I}_{KK}(p^*, p) |\Phi_{00}(g)|^2. \end{aligned} \tag{4.15}$$

Let us introduce the modified dyadic TD coefficients

$$\begin{aligned} \mathcal{C}^{I}_{K\omega, b_1 j_1 \cdots b_\rho j_\rho} \equiv & \sum_{(a_1 i_1)<\cdots<(a_\rho i_\rho)} \{(Cw)^{*-1}\}_{b_1 a_1} \{(\tilde{C}\bar{w})^{-1}\}_{j_1 i_1} \cdots \{(Cw)^{*-1}\}_{b_\rho a_\rho} \\ & \times \{(\tilde{C}\bar{w})^{-1}\}_{j_\rho i_\rho} \Gamma^{I}_{K\omega, a_1 i_1 \cdots a_\rho i_\rho}. \end{aligned} \tag{4.16}$$

Then, equation (4.14) is converted to the projected $U(n)$ dyadic TD equation,

$$\sum_{\rho'} \sum_{(b_1 j_1)<\cdots<(b_{\rho'} j_{\rho'})} \mathcal{D}^{\rho}{}_{a_1 i_1 \cdots a_\rho i_\rho} \mathcal{D}^{\rho' *}{}_{b_1 j_1 \cdots b_{\rho'} j_{\rho'}} \{H^{I}_{KK}(p^*, p) - E^{I}_{\omega} S^{I}_{KK}(p^*, p)\} \mathcal{C}^{I}_{K\omega, b_1 j_1 \cdots b_{\rho'} j_{\rho'}} = 0. \tag{4.17}$$

The modified coefficients $\mathcal{C}^{I}_{K\omega, b_1 j_1 \cdots b_{\rho'} j_{\rho'}}$ have to satisfy the normalization condition

$$\begin{aligned} \sum_{\rho, \rho'} \sum_{(a_1 i_1)<\cdots<(a_\rho i_\rho), (b_1 j_1)<\cdots<(b_{\rho'} j_{\rho'})} & \mathcal{D}^{\rho}{}_{a_1 i_1 \cdots a_\rho i_\rho} \mathcal{D}^{\rho' *}{}_{b_1 j_1 \cdots b_{\rho'} j_{\rho'}} S^{I}_{KK}(p^*, p) \mathcal{C}^{I*}_{K\omega, a_1 i_1 \cdots a_\rho i_\rho} \mathcal{C}^{I}_{K\omega, b_1 j_1 \cdots b_{\rho'} j_{\rho'}} \\ & = d(I) \cdot |\Phi_{00}(g)|^{-2}, \end{aligned} \tag{4.18}$$

which is obtained from (3.17) and $\langle IK\omega|IK\omega\rangle = 1$.

5. First-order approximation to projected $U(n)$ TD equation

We make an approximation to the projected $U(n)$ TD expansion of the state $|IK\omega\rangle$, (4.13) up to the first order and determine simultaneously both the expansion coefficients and the coset variable p in equation (4.17). With this approximation, it is possible to get easily the best p in determining them variationally, by using the same state vector. To look for the best p, both the projected $U(n)$ TD equation (4.17) and the equation for p must be treated as a set of equations, which should be solved self-consistently. However, in order to make our calculations manageable, we decouple the equation for p from the projected $U(n)$ TD equation.

We adopt the following first-order approximation of the projected $U(n)$ TD expansion of the state $|IK\omega\rangle$:

$$|IK\omega\rangle_{\mathrm{ap}} = |IK\omega\rangle^{(0)} + |IK\omega\rangle^{(1)} = \sum_M \left\{ \mathcal{C}^I_{M\omega} |\Phi^I_{MK}(p)\rangle + \sum_{ai} \mathcal{C}^I_{M\omega,ai} \mathcal{D}^{1*}_{ai} |\Phi^I_{MK}(p)\rangle \right\} \Phi^*_{00}(g), \tag{5.1}$$

which gives the first-order projected $U(n)$ TD basis elements within the approximation ignoring two or more particle–hole pair excitations. We have used the relation $|\Phi^I_{MK}(g)\rangle = |\Phi^I_{MK}(p)\rangle \Phi^*_{00}(g)$. The norm of the $|IK\omega\rangle_{\mathrm{ap}}$ is given by

$$N^{IK\omega}_{\mathrm{approx}}(g, g) = N^{IK\omega}_{\mathrm{approx}}(p^*, p) \cdot |\Phi^*_{00}(g)|^2,$$

$$N^{IK\omega}_{\mathrm{approx}}(p^*, p) = [d(I)]^{-1} \cdot \sum_M \left\{ \mathcal{C}^{I*}_{M\omega} \mathcal{C}^I_{M\omega} + \sum_{ai} (\mathcal{C}^{I*}_{M\omega} \mathcal{C}^I_{M\omega,ai} \mathcal{D}^{1*}_{ai} + \mathcal{C}^{I*}_{M\omega,ai} \mathcal{C}^I_{M\omega} \mathcal{D}^1_{ai}) \right. \tag{5.2}$$

$$\left. + \sum_{ai} \sum_{bj} \mathcal{C}^{I*}_{M\omega,ai} \mathcal{C}^I_{M\omega,bj} \mathcal{D}^1_{ai} \mathcal{D}^{1*}_{bj} \right\} \cdot S^I_{KK}(p^*, p).$$

Let $W^I_{K\omega}$ be an approximate value of the energy E^I_ω in the approximate eigenstate $|IK\omega\rangle_{\mathrm{ap}}$. Along the same line as the above, the projected $U(n)$ TD equation (4.17) is also approximated up to first order as follows:

$$H^I_{KK}(p^*, p) \mathcal{C}^I_{K\omega} + \sum_{bj} \mathcal{D}^{1*}_{bj} H^I_{KK}(p^*, p) \mathcal{C}^I_{K\omega,bj}$$
$$- W^I_{K\omega} \left\{ S^I_{KK}(p^*, p) \mathcal{C}^I_{K\omega} + \sum_{bj} \mathcal{D}^{1*}_{bj} S^I_{KK}(p^*, p) \mathcal{C}^I_{K\omega,bj} \right\} = 0,$$
$$\mathcal{D}^1_{ai} H^I_{KK}(p^*, p) \mathcal{C}^I_{K\omega} + \sum_{bj} \mathcal{D}^1_{ai} \mathcal{D}^{1*}_{bj} H^I_{KK}(p^*, p) \mathcal{C}^I_{K\omega,bj} \tag{5.3}$$
$$- W^I_{K\omega} \left\{ \mathcal{D}^1_{ai} S^I_{KK}(p^*, p) \mathcal{C}^I_{K\omega} + \sum_{bj} \mathcal{D}^1_{ai} \mathcal{D}^{1*}_{bj} S^I_{KK}(p^*, p) \mathcal{C}^I_{K\omega,bj} \right\} = 0,$$

a set of which is an eigenvalue equation containing an unknown coset variable p. We can determine it by the variational equation for p, $\delta_p W^I_{K\omega} = \delta_p\{\langle IK\omega|H|IK\omega\rangle_{\mathrm{ap}} / \langle IK\omega|IK\omega\rangle_{\mathrm{ap}}\} = 0$, from which the equation for p is given as

$$\left\{ \frac{\partial H^I_{KK}(p^*, p)}{\partial p^\dagger_{ai}} - W^I_{K\omega} \frac{\partial S^I_{KK}(p^*, p)}{\partial p^\dagger_{ai}} \right\} \mathcal{C}^{I*}_{K\omega} \mathcal{C}^I_{K\omega}$$
$$+ \left\{ \frac{\partial}{\partial p^\dagger_{ai}} \sum_{bj} \mathcal{D}^{1*}_{bj} H^I_{KK}(p^*, p) - W^I_{K\omega} \frac{\partial}{\partial p^\dagger_{ai}} \sum_{bj} \mathcal{D}^{1*}_{bj} S^I_{KK}(p^*, p) \right\} \mathcal{C}^{I*}_{K\omega} \mathcal{C}^I_{K\omega,bj}$$
$$+ \left\{ \frac{\partial}{\partial p^\dagger_{ai}} \sum_{bj} \mathcal{D}^1_{bj} H^I_{KK}(p^*, p) - W^I_{K\omega} \frac{\partial}{\partial p^\dagger_{ai}} \sum_{bj} \mathcal{D}^1_{bj} S^I_{KK}(p^*, p) \right\} \mathcal{C}^{I*}_{K\omega,bj} \mathcal{C}^I_{K\omega}$$
$$+ \left\{ \frac{\partial}{\partial p^\dagger_{ai}} \sum_{bj} \sum_{ck} \mathcal{D}^1_{bj} \mathcal{D}^{1*}_{ck} H^I_{KK}(p^*, p) - W^I_{K\omega} \frac{\partial}{\partial p^\dagger_{ai}} \sum_{bj} \sum_{ck} \mathcal{D}^1_{bj} \mathcal{D}^{1*}_{ck} S^I_{KK}(p^*, p) \right\}$$
$$\times \mathcal{C}^{I*}_{K\omega,bj} \mathcal{C}^I_{K\omega,ck} = 0, \tag{5.4}$$

to which substitution of the lowest energy solution of the eigenvalue equation (5.3) determines the $p^\dagger$. Equation (5.4) is also derived by differentiations of (5.3) with respect to $p^\dagger_{ai}$. Then, the eigenvalue equation (5.3) should be solved keeping the solved eigenvalue to be compatible with the $p^\dagger$ determined variationally.

To get a self-consistent optimal solution of the set of equations (5.3) and (5.4), it may be powerful to adopt the optimization algorithm consisting of some iteration steps [5, 7]. Under the change of the particle–hole frame, $g \to g\overset{\circ}{g}$ and $p \to p'$, we calculate the differential of $W^I_{K\omega}(p')$ up to the same order as the one in (5.4). Let us start to solve the eigenvalue equation (5.3) with a trial $p^\dagger$. Substitute its lowest energy solution and the trial $p^\dagger$ into the approximate differential formula for $W^I_{K\omega}(p')$. Our desired $q^\dagger$ is determined so as to satisfy $\partial W^I_{K\omega}(p')/\partial q^\dagger_{ai} = 0$, though we omit its derivative formula which is very complicated. Assuming the $q^\dagger$ to be small and using the dyadic TD expansion of any operator X (4.10), we can compute the derivative formula up to second order in q and q^*. Then, the iteration steps proceed a way quite parallel to the one taken in [5, 7]. In each step, we can calculate the $p'^\dagger$ in the left-hand side of equation (2.16) from $p^\dagger$ and $q^\dagger$ and use it as the new $p^\dagger$ of the next iteration cycle.

6. Summary and discussions

The $U(n)$ TD method discards the IPA as the starting approximation but its first-order approximation describes stationary states of Bose condensed particle–hole pairs. The pairs are in a coherent motion affiliated with a certain symmetry of a system since the state of particle–hole pairs is changing under an operation of the symmetry. The Peierls–Yoccoz projection selects out the stationary states of the coherent motion because the representation matrices of the symmetry group s are the eigenstates of the motion. To go beyond the zeroth-order approximation, we have developed the first-order approximation of the symmetry-projected $U(n)$ TD equation keeping the non-Euclidean transformation rule (2.16). We can reduce the first-order equation to simpler forms, though we omit the details here. A manipulation is based on both the character theory of group and the recursion relation associated with the Schur function, i.e. the character polynomials corresponding to the completely anti-symmetric Young diagram. Our theory has been constructed by a group-theoretical deduction and hence has a universal applicability. Due to its physical aspects, it is expected to work better in nuclear and molecular systems with strong collective correlations, where ground states are well approximated by Bose condensates. It provides a general microscopic tool for a unified understanding of collective excitations in such fermion systems.

The first-order approximation (5.1) is expected to work better than the IPA to describe ground and excited states of the fermion systems with strong collective correlations. The reason for the expectation is mainly due to the following points: (i) easier diagonalization of the eigenvalue equation and faster convergence may be achieved simultaneously compared with the diagonalization and convergence of the original eigenvalue equation, because we make no use of an unstable IPA wave function from the outset; (ii) through all the iteration steps for the optimization, we adopt the first-order covariant differential operator instead of the usual first derivative, to evaluate derivatives of the Hamiltonian matrix element and the overlap integral in the particle–hole pair excitation states. The covarint derivative yields important different results compared with the use of the usual derivative, e.g. the trivially identical equation $\mathcal{D}^{1*}_{ai} S(p^*, p) = 0$. If the condition $\mathcal{D}^{1*}_{ai} S^I_{KK}(p^*, p) = 0$ is satisfied for any particle–hole pair ia, *the generalized Brillouin theorem* $\mathcal{D}^{1*}_{ai} H^I_{KK}(p^*, p) = 0$ holds exactly. An action of the $\mathcal{D}^{1*}_{ai}$ brings no essential difference in the results obtained by the usual derivatives [6]. In the symmetry-projected $U(n)$ case, the condition is hardly satisfied and *the generalized Brillouin theorem* is not established exactly. To satisfy the condition, another one called the killer condition must be fulfilled. See the details in [6, 8]. To see this, diagonalize ζ as $\zeta_{ia} = \sum_{A=1}^{M} \tilde{v}_{iA}\zeta_A v_{aA}^*$, where $\tilde{v} = (\tilde{v}_{iA})$ and $v = (v_{aA})$ are $(n-m)\times M$ and $m \times M$ matrices. Then, we have $p_{ia} = \sum_{A=1}^{M} \tilde{v}_{iA} p_A v_{aA}^* (p_A = \tan\zeta_A)$ and $e_{ai} = -\sum_{A=1}^{M} v_{aA}^* p_A (1+p_A^2)^{-1}\tilde{v}_{iA}$ [2]. In (3.14), for simplicity putting $s_h = 1_m$ and $\tilde{s} = s_p$, from these relations and $\sum_{i=m+1}^{n} \tilde{v}_{iA}^*(\tilde{s}\tilde{v})_{iB} = z_A(\tilde{s})\delta_{AB}$, we get the killer condition

$$\sum_{A=1}^{M} v_{aA}^* \frac{p_A}{1+p_A^2} \int D_{KK}^{I*}(\tilde{s}) \left[\tilde{v}_{iA} - \frac{1+p_A^2}{1+z_A(\tilde{s})p_A^2}(\tilde{s}\tilde{v})_{iA}\right] \det\{1+p^\dagger(\tilde{s}p)\} d\tilde{s} = 0. \tag{6.1}$$

Rowe *et al* have decoupled the variational equation for ground state and the IPA equation for excited states from each other [13]. On the other hand, due to the above reason, we have matrix elements between the zeroth-order component of the $U(n)$ TD wave function and the first-order one which includes contributions from all pairwise excitations. Then, our eigenvalue equation (5.3) becomes suitable for the description of such a strong coupling between the ground state and the excited state of soft nuclei with strong collective correlations. Nevertheless, suppose a slightly loose condition called *the weak killer condition*

$$\int D_{KK}^{I*}(\tilde{s}) \left[1 - \frac{z_A(\tilde{s})(1+p_A^2)}{1+z_A(\tilde{s})p_A^2}\right] \det\{1+p^\dagger(\tilde{s}p)\} d\tilde{s} = 0, \tag{6.2}$$

which is derived by multiplying (6.1) with $\tilde{v}_{iA}^*$ for any A and summing up over i and whose original form has appeared first in [7]. Employing this instead of the original strong killer condition, we are able to ensure *the generalized Brillouin theorem* $\mathcal{D}_{ai}^{1*} H_{KK}^{I}(p^*, p) = 0$, which in turn resolves the eigenvalue equation (5.3) into two secular equations and determines the ground state and the excited states, separately. Furthermore, using the mathematical technique in appendix D and adopting the same method as the one in [7], this eigenvalue equation is expressed in terms of the Schur function. Then, the handling of the eigenvalue equation (5.3) becomes very easy. It is solved self-consistently keeping the non-Euclidean property of transformation. Adding these, we have another advantage that the $U(n)$ TD approximation can be extended up to any higher order if necessary. Throughout this paper emphasis has been put on explaining the rather basic idea which is developed from the previous attempt [7]. The present discussions have been made in the general form as much as possible.

In a forthcoming paper, we shall illustrate a practical usefulness of the first-order $U(n)$ TD approximation. This approximation is tractable by calculation of equations (5.3) and (5.4) for the simplest schematic models of nuclei, e.g. the famous two-level $SU(2)$ Lipkin–Meshkov–Glick (LMG) Hamiltonian [14, 15] and the three-level $SU(3)$ LMG Hamiltonian [16]; both of them have non-degenerate single-particle energies. The $SU(3)$ model poses a non-trivial problem for finding the solution but still simple enough to allow the calculation of equations (5.3) and (5.4) and comparisons with the solution by the ordinary TD approximation and the exact solution, though the $SU(2)$ is a too simple toy model to compare with them. Furthermore, it is very interesing to investigate whether the weak killer condition may hold with good accuracy or not for the $SU(2)$ and $SU(3)$ LMG model Hamiltonians, respectively.

In conclusion, we have developed the first-order approximation to the projected $U(n)$ dyadic TD equation keeping the non-Euclidean property of transformation by the generator coordinate. The approximate equation can be reduced to simpler forms by the Schur function of group characters which makes possible to connect the present theory with the soliton theory on the group manifold [17–19].

Appendix A. Slater determinant and Plücker relation

Using the representation of g and the variable p of the coset space defined in section 2, following Fukutome [10], we express the third equation of (2.4), m particle S-det as

$$U(g)|\phi_m\rangle = \langle\phi_m|U(g_\zeta g_w)|\phi_m\rangle e^{p_{ia}c_i^\dagger c_a}|\phi_m\rangle, \quad (g = g_\zeta g_w) \tag{A.1}$$

where we have used the relations

$$1 + \sum_{\rho=1}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m,\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \mathcal{A}(p_{i_1a_1}\cdots p_{i_\rho a_\rho})c_{i_1}^\dagger c_{a_1}\cdots c_{i_\rho}^\dagger c_{a_\rho} = e^{p_{ia}c_i^\dagger c_a},$$
$$\langle\phi_m|U(g_\zeta g_w)|\phi_m\rangle = [\det(1+p^\dagger p)]^{-\frac{1}{2}}\cdot\det w, \tag{A.2}$$

and the definition

$$\mathcal{A}(p_{i_1a_1}\cdots p_{i_\rho a_\rho}) \stackrel{d}{=} \det\begin{bmatrix} p_{i_1a_1} & \cdots & p_{i_1a_\rho}\\ \vdots & & \vdots\\ p_{i_\rho a_1} & \cdots & p_{i_\rho a_\rho}\end{bmatrix}. \tag{A.3}$$

In equation (A.2) the maximum value M is given by $M = \min(n-m, m)$ and $\mathcal{A}$ is an anti-symmetrizer.

On the other hand, in the Gr_m (2.5) we can introduce an expression called the Plücker coordinate, which has played important roles for an algebraic construction of soliton theory in its early stage [20],

$$U(g)|\phi_m\rangle = \sum_{1\leqslant\alpha_1,\ldots,\alpha_m\leqslant n} v^{1,\ldots,m}_{\alpha_1,\ldots,\alpha_m}(g)c^\dagger_{\alpha_m}\cdots c^\dagger_{\alpha_1}|0\rangle,$$
$$v^{1,\ldots,m}_{\alpha_1,\ldots,\alpha_m}(g) = \det\begin{bmatrix} g_{\alpha_1,1} & \cdots & g_{\alpha_1,m}\\ \vdots & & \vdots\\ g_{\alpha_m,1} & \cdots & g_{\alpha_m,m}\end{bmatrix} \quad \text{(Plücker coordinate).} \tag{A.4}$$

From an elementary determinantal calculus, we prove easily that the Plücker coordinate has a relation

$$\sum_{i=1}^{m+1}(-1)^{i-1}v^{1,\ldots,m}_{\alpha_1,\ldots,\alpha_{m-1},\beta_i}\cdot v^{1,\ldots,m}_{\beta_1,\ldots,\beta_{i-1},\beta_{i+1},\ldots,\beta_{m+1}} = 0 \quad \text{(Plücker relation),} \tag{A.5}$$

where the indices denote the distinct sets $1\leqslant\alpha_1,\ldots,\alpha_{m-1}\leqslant n$ and $1\leqslant\beta_1,\ldots,\beta_{m+1}\leqslant n$.

Now we study a relation between coset coordinates appearing in (A.2) and Plücker coordinates in (A.4). Each coordinate makes a crucial role to construct the time-dependent HF theory [1] and the soliton theory [18] on the Gr_m. Using expressions for unoccupied and occupied states in (A.2), we can rewrite (A.4) as

$$\begin{aligned} U(g)|\phi_m\rangle &= |\phi_m\rangle + \sum_{\rho=1}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m,\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} v^{1,\ldots,m}_{1,\ldots,a_1-1,a_1+1,\cdots,a_\rho-1,a_\rho+1,\cdots,m,i_1,\ldots,i_\rho}(g_\zeta g_w)\\ &\quad\cdot c^\dagger_{i_\rho}\cdots c^\dagger_{i_1}c^\dagger_m\cdots c^\dagger_{a_\rho+1}c^\dagger_{a_\rho-1}\cdots c^\dagger_{a_1+1}c^\dagger_{a_1-1}\cdots c^\dagger_1|0\rangle\\ &= |\phi_m\rangle + v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta g_w)\sum_{\rho=1}^{M} \sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m,\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \frac{v^{1,\ldots,a_1,\ldots,a_\rho,\ldots,m}_{1,\ldots,i_1,\ldots,i_\rho,\ldots,m}(g_\zeta g_w)}{v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta g_w)}\\ &\quad\cdot c^\dagger_{i_1}c_{a_1}\cdots c^\dagger_{i_\rho}c_{a_\rho}|\phi_m\rangle. \end{aligned} \tag{A.6}$$

The last line of the above is recast again into the form of (A.4) after many time exchanges between $c_{a_1} \cdots c_{a_\rho}$ and all creation operators so that all the annihilation operators are ordered in such a way that they are to the right of all the creation operators including the ones in $|\phi_m\rangle$. Then we have the relation

$$v^{1,\cdots,m}_{1,\ldots,a_1-1,a_1+1,\cdots,a_\rho-1,a_\rho+1,\cdots,m,i_1,\ldots,i_\rho}(g_\zeta g_w) = (-1)^{\sum_{j=0}^{\rho-1}(m-j-a_{\rho-j})} v^{1,\ldots,a_1,\ldots,a_\rho,\ldots,m}_{1,\ldots,i_1,\ldots,i_\rho,\ldots,m}(g_\zeta g_w), \tag{A.7}$$

and the following decompositions:

$$\begin{aligned} &v^{1,\ldots,a_1,\ldots,a_\rho,\ldots,m}_{1,\ldots,i_1,\ldots,i_\rho,\ldots,m}(g_\zeta g_w) = v^{1,\ldots,a_1,\ldots,a_\rho,\ldots,m}_{1,\ldots,i_1,\ldots,i_\rho,\ldots,m}(g_\zeta) v^{1,\ldots,m}_{1,\ldots,m}(g_w), \\ &v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta g_w) = v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta) v^{1,\ldots,m}_{1,\ldots,m}(g_w), \quad v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta) = \det C(\zeta) = [\det(1 + p^\dagger p)]^{-\frac{1}{2}}, \end{aligned} \tag{A.8}$$

where

$$v^{1,\ldots,a_1,\ldots,a_\rho,\ldots,m}_{1,\ldots,i_1,\ldots,i_\rho,\ldots,m}(g_\zeta) = \det \begin{bmatrix} C(\zeta)_{1,1} & \cdots & C(\zeta)_{1,m} \\ \vdots & & \vdots \\ C(\zeta)_{a_1-1,1} & \cdots & C(\zeta)_{a_1-1,m} \\ S(\zeta)_{i_1,1} & \cdots & S(\zeta)_{i_1,m} \\ C(\zeta)_{a_1+1,1} & \cdots & C(\zeta)_{a_1+1,m} \\ \vdots & & \vdots \\ C(\zeta)_{a_\rho-1,1} & \cdots & C(\zeta)_{a_\rho-1,m} \\ S(\zeta)_{i_\rho,1} & \cdots & S(\zeta)_{i_\rho,m} \\ C(\zeta)_{a_\rho+1,1} & \cdots & C(\zeta)_{a_\rho+1,m} \\ \vdots & & \vdots \\ C(\zeta)_{m,1} & \cdots & C(\zeta)_{m,m} \end{bmatrix}, \qquad v^{1,\ldots,m}_{1,\ldots,m}(g_w) = \det w. \tag{A.9}$$

Here matrix elements in the a_1-th, ... and a_ρ-th rows, $C(\zeta)_{a_1,1\sim m}, \ldots$ and $C(\zeta)_{a_\rho,1\sim m}$ are replaced with $S(\zeta)_{i_1,1\sim m}, \ldots$ and $S(\zeta)_{i_\rho,1\sim m}$ to describe $\rho\,(1 < \rho < m)$ times particle–hole excitations from hole state a_1 to particle state $i_1, \ldots$ and those of hole state a_ρ to particle state i_ρ, respectively.

Equating (A.2) and (A.4) with (A.6) and (A.9), respectively, we obtain the anti-symmetrized $\mathcal{A}(\cdots)$ and the coset variable expressed in terms of Plücker coordinates as

$$\mathcal{A}(p_{i_1a_1} \cdots p_{i_\rho a_\rho}) = \frac{v^{1,\ldots,a_1,\ldots,a_\rho,\ldots,m}_{1,\ldots,i_1,\ldots,i_\rho,\ldots,m}(g_\zeta)}{v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta)}, \qquad p_{ia} = [S(\zeta)C^{-1}(\zeta)]_{ia} = \frac{v^{1,\ldots,a,\ldots,m}_{1,\ldots,i,\ldots,m}(g_\zeta)}{v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta)}, \tag{A.10}$$

in the second Plücker coordinate of which, only one row matrix elements of its determinantal form (A.9) $C(\zeta)_{a,1\sim m}$ are replaced with $S(\zeta)_{i,1\sim m}$. Expanding the anti-symmetrized $\mathcal{A}(\cdots)$ in the left-hand side of the first equation of (A.10) with respect to, for example, the first column, we have a decomposition rule

$$\begin{aligned} \frac{v^{1,\ldots,a_1,\ldots,a_\rho,\ldots,m}_{1,\ldots,i_1,\ldots,i_\rho,\ldots,m}(g_\zeta)}{v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta)} &= \sum_{j=1}^{\rho} (-1)^{j+1} p_{i_j a_1} \mathcal{A}(p_{i_1 a_2} \cdots p_{i_{j-1},a_j} p_{i_{j+1}a_{j+1}} \cdots p_{i_\rho a_\rho}) \\ &= \sum_{j=1}^{\rho} (-1)^{j+1} \frac{v^{1,\ldots a_1,\ldots,m}_{1,\ldots,i_j,\ldots,m}(g_\zeta)}{v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta)} \frac{v^{1,\ldots,a_1,\ldots,a_2,\ldots,a_j,\ldots,a_{j+1},\ldots,a_\rho,\ldots,m}_{1,\ldots,a_1,\ldots,i_1,\ldots,i_{j-1},\ldots,i_{j+1},\ldots,i_\rho,\ldots,m}(g_\zeta)}{v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta)}, \end{aligned} \tag{A.11}$$

which is rewritten to another form (the second Plücker relation)

$$v^{1,\ldots,m}_{1,\ldots,m}(g_\zeta)v^{1,\ldots,a_1,\ldots,a_\rho,\ldots,m}_{1,\ldots,i_1,\ldots,i_\rho,\ldots,m}(g_\zeta)+\sum_{j=1}^{\rho}(-1)^j v^{1,\ldots a_1,\ldots,m}_{1,\ldots,i_j,\ldots,m}(g_\zeta)v^{1,\ldots,a_1,\ldots,a_2,\ldots,a_j,\ldots,a_{j+1},\ldots,a_\rho,\ldots,m}_{1,\ldots,a_1,\ldots,i_1,\ldots,i_{j-1},\ldots,i_{j+1},\ldots,i_\rho,\ldots,m}(g_\zeta)=0, \tag{A.12}$$

in which a hole state a_1 in the last Plücker coordinate make no changes ($a_1 \to a_1$) since in the second one a particle–hole excitation already occurred from the hole state a_1 to the particle state i_j [19].

It is well-known that the Plücker relation (A.5) is equivalent to a bilinear identity equation

$$\sum_{\alpha=1}^{n} c_\alpha^\dagger U(g)|\phi_m\rangle \otimes c_\alpha U(g)|\phi_m\rangle = \sum_{\alpha=1}^{n} U(g)c_\alpha^\dagger|\phi_m\rangle \otimes U(g)c_\alpha|\phi_m\rangle = 0, \tag{A.13}$$

which have made an important role to construct many kinds of solitons on various group manifolds by using the corresponding τ-functions [18].

Appendix B. Derivation of particle–hole operators and vacuum function

Consider a function $\Psi(g)$ on the $U(n)$ group corresponding to a state vector $|\Psi\rangle$ in the fermion space

$$|\Psi\rangle = \int U(g)|0\rangle\langle 0|U^\dagger(g)|\Psi\rangle dg = \int U(g)|0\rangle\Psi(g)dg, \tag{B.1}$$

where dg is an invariant group integration over the $U(n)$ group. The explicit representation of g is given by (2.8). When an infinitesimal operator $1+\delta\hat{g}$ and a corresponding infinitesimal unitary transformation $U(1+\delta g)$ is operated on $|\Psi\rangle$, using $U^{-1}(1+\delta g) \simeq U(1-\delta g)$, it transforms $|\Psi\rangle$ as

$$\begin{aligned} U(1-\delta g)|\Psi\rangle &\equiv (1-\delta\hat{g})|\Psi\rangle = \int U(g)|0\rangle\langle 0|U^\dagger((1+\delta g)g)|\Psi\rangle dg \\ &= \int U(g)|0\rangle\Psi((1+\delta g)g)dg = \int U(g)|0\rangle(1+\delta\boldsymbol{g})\Psi(g)dg, \end{aligned} \tag{B.2}$$

where

$$\delta g \equiv \begin{bmatrix} \delta_{Cw} & -\delta_{S^\dagger\bar{w}} \\ \delta_{Sw} & \delta_{\tilde{C}\bar{w}} \end{bmatrix}, \qquad \begin{aligned} \delta\hat{g} &= (\delta_{Cw})_{ab}e_{ab} + (\delta_{\tilde{C}\bar{w}})_{ij}e_{ij} + (\delta_{Sw})_{ia}e^{ia} + (\delta_{S^\dagger\bar{w}})_{ai}e_{ai}, \\ \delta\boldsymbol{g} &= (\delta_{Cw})_{ab}\boldsymbol{e}_{ab} + (\delta_{\tilde{C}\bar{w}})_{ij}\boldsymbol{e}_{ij} + (\delta_{Sw})_{ia}\boldsymbol{e}^{ia} + (\delta_{S^\dagger\bar{w}})_{ai}\boldsymbol{e}_{ai}. \end{aligned} \tag{B.3}$$

Equation (B.2) shows that the operation of $1-\delta\hat{g}$ on the $|\Psi\rangle$ in the fermion space corresponds to the left multiplication by $1+\delta g$ for the variable of g of the function $\Psi(g)$. For a small parameter ε, we obtain a representaion on $\Psi(g)$ as

$$\rho(e^{\varepsilon\delta g})\Psi(g) = \Psi(e^{-\varepsilon\delta g}g) = \Psi(g-\varepsilon\delta g g) = \Psi(g+dg), \tag{B.4}$$

which leads us to a relation $dg = -\varepsilon\delta g g$. From this, we express it explicitly as

$$\begin{bmatrix} dg_{ab} & dg_{ai} \\ dg_{ia} & dg_{ij} \end{bmatrix} = -\varepsilon \begin{bmatrix} \{(\delta_{Cw})\cdot(Cw) - (\delta_{S^\dagger\bar{w}})\cdot(Sw)\}_{ab} & -\{(\delta_{Cw})\cdot(S^\dagger\bar{w}) + (\delta_{S^\dagger\bar{w}})\cdot(\tilde{C}\bar{w})\}_{ai} \\ \{(\delta_{Sw})\cdot(Cw) + (\delta_{\tilde{C}\bar{w}})\cdot(Sw)\}_{ia} & \{(\delta_{\tilde{C}\bar{w}})\cdot(\tilde{C}\bar{w}) - (\delta_{Sw})\cdot(S^\dagger\bar{w})\}_{ij} \end{bmatrix}, \tag{B.5}$$

$$
\begin{aligned}
dg_{ab} &= \varepsilon \frac{\partial g_{ab}}{\partial g_{cd}} \frac{\partial g_{cd}}{\partial \varepsilon} = \varepsilon \frac{\partial g_{ab}}{\partial \varepsilon} = -\varepsilon\{(\delta_{Cw})\cdot(Cw) - (\delta_{S^\dagger \bar{w}})\cdot(Sw)\}_{ab}, \\
dg_{ia} &= \varepsilon \frac{\partial g_{ia}}{\partial g_{jb}} \frac{\partial g_{jb}}{\partial \varepsilon} = \varepsilon \frac{\partial g_{ia}}{\partial \varepsilon} = -\varepsilon\{(\delta_{Sw})\cdot(Cw) + (\delta_{\tilde{C}\bar{w}})\cdot(Sw)\}_{ia}, \\
dg_{ai} &= \varepsilon \frac{\partial g_{ai}}{\partial g_{bj}} \frac{\partial g_{bj}}{\partial \varepsilon} = \varepsilon \frac{\partial g_{ai}}{\partial \varepsilon} = \varepsilon\{(\delta_{Cw})\cdot(S^\dagger \bar{w}) + (\delta_{S^\dagger \bar{w}})\cdot(\tilde{C}\bar{w})\}_{ai}, \\
dg_{ij} &= \varepsilon \frac{\partial g_{ij}}{\partial g_{kl}} \frac{\partial g_{kl}}{\partial \varepsilon} = \varepsilon \frac{\partial g_{ij}}{\partial \varepsilon} = -\varepsilon\{(\delta_{\tilde{C}\bar{w}})\cdot(\tilde{C}\bar{w}) - (\delta_{Sw})\cdot(S^\dagger \bar{w})\}_{ij}.
\end{aligned} \tag{B.6}
$$

A differential representaion of $\rho(\delta g)$, $d\rho(\delta g)$, is given as

$$
d\rho(\delta g)\Psi(g) = \left[\frac{\partial g_{ab}}{\partial \varepsilon}\frac{\partial}{\partial g_{ab}} + \frac{\partial g_{ij}}{\partial \varepsilon}\frac{\partial}{\partial g_{ij}} + \frac{\partial g_{ia}}{\partial \varepsilon}\frac{\partial}{\partial g_{ia}} + \frac{\partial g_{ai}}{\partial \varepsilon}\frac{\partial}{\partial g_{ai}}\right]\Psi(g). \tag{B.7}
$$

Substituting (B.6) into (B.7), we can get explicit forms of the differential representaion

$$
d\rho(\delta g)\Psi(g) = [(\delta_{Cw})_{ab}\boldsymbol{e}_{ab} + (\delta_{\tilde{C}\bar{w}})_{ij}\boldsymbol{e}_{ij} + (\delta_{Sw})_{ia}\boldsymbol{e}^{ia} + (\delta_{S^\dagger\bar{w}})_{ai}\boldsymbol{e}_{ai}]\Psi(g) = \delta\boldsymbol{g}\Psi(g), \tag{B.8}
$$

where each operator in $\delta\boldsymbol{g}$ is expressed in a differential form as

$$
\begin{aligned}
\boldsymbol{e}_{ab} &= -(Cw)_{bc}\frac{\partial}{\partial g_{ac}} + (S^\dagger\bar{w})_{bi}\frac{\partial}{\partial g_{ai}}, \qquad \boldsymbol{e}_{ij} = -(\tilde{C}\bar{w})_{jk}\frac{\partial}{\partial g_{ik}} - (Sw)_{ja}\frac{\partial}{\partial g_{ia}}, \\
\boldsymbol{e}^{ia} &= -(Cw)_{ab}\frac{\partial}{\partial g_{ib}} + (S^\dagger\bar{w})_{aj}\frac{\partial}{\partial g_{ij}}, \qquad \boldsymbol{e}_{ai} = (\tilde{C}\bar{w})_{ij}\frac{\partial}{\partial g_{aj}} + (Sw)_{ib}\frac{\partial}{\partial g_{ab}}.
\end{aligned} \tag{B.9}
$$

Then, partial derivative formulae for group variables can be derived in the following forms:

$$
\begin{aligned}
\frac{\partial}{\partial g_{ac}} &= \frac{\partial p_{ie}}{\partial C_{ad}}(w^{-1})_{cd}\frac{\partial}{\partial p_{ie}} + \frac{\partial \tau}{\partial (Cw)_{ac}}\frac{\partial}{\partial \tau} \\
&= -p_{ia}((Cw)^{-1})_{ce}\frac{\partial}{\partial p_{ie}} - \frac{\mathrm{i}}{2}[(Cw)^{-1}\{1 + (1 + p^\dagger p)^{-1}\}]_{ca}\frac{\partial}{\partial \tau}, \\
\frac{\partial}{\partial g_{ik}} &= \frac{\partial p^*_{ga}}{\partial \tilde{C}^*{}_{li}}(\bar{w}^{-1})_{kl}\frac{\partial}{\partial p^*_{ga}} + \frac{\partial \tau}{\partial (\tilde{C}\bar{w})_{ik}}\frac{\partial}{\partial \tau} \\
&= -p^*_{ia}((\tilde{C}\bar{w})^{-1})_{kg}\frac{\partial}{\partial p^*_{ga}} + \frac{\mathrm{i}}{2}[(\tilde{C}\bar{w})^{-1}p(1 + p^\dagger p)^{-1}p^\dagger]_{ki}\frac{\partial}{\partial \tau}, \\
\frac{\partial}{\partial g_{ib}} &= \frac{\partial p_{jd}}{\partial S_{ic}}(w^{-1})_{bc}\frac{\partial}{\partial p_{jd}} + \frac{\partial \tau}{\partial (Sw)_{ib}}\frac{\partial}{\partial \tau} \\
&= ((Cw)^{-1})_{bd}\frac{\partial}{\partial p_{id}} - \frac{\mathrm{i}}{2}[(Cw)^{-1}(1 + p^\dagger p)^{-1}p^\dagger]_{bi}\frac{\partial}{\partial \tau}, \\
\frac{\partial}{\partial g_{ai}} &= \frac{\partial p^*_{kb}}{\partial (-S^\dagger)_{aj}}(\bar{w}^{-1})_{ij}\frac{\partial}{\partial p^*_{kb}} + \frac{\partial \tau}{\partial (-S^\dagger\bar{w})_{ai}}\frac{\partial}{\partial \tau}, \\
&= -((\tilde{C}\bar{w})^{-1})_{ik}\frac{\partial}{\partial p^*_{ka}} + \frac{\mathrm{i}}{2}[(\tilde{C}\bar{w})^{-1}p(1 + p^\dagger p)^{-1}]_{ia}\frac{\partial}{\partial \tau},
\end{aligned} \tag{B.10}
$$

where we have introduced a variable $\tau = -\mathrm{i}\ln\det w$ which is, by means of $p = SC^{-1} = C^{-1}S$, cast to

$$
\begin{aligned}
\tau &= -\mathrm{i}\ln\left(\frac{\det(Cw)}{\det C}\right) = -\mathrm{i}\ln\,\det(Cw) - \frac{\mathrm{i}}{2}\ln[\det(1 + p^\dagger p)] \\
&= -\mathrm{i}\ln\det(Cw) - \frac{\mathrm{i}}{2}\ln[\det\{1 + (S^\dagger\bar{w})(\tilde{C}\bar{w})^{-1}(Sw)(Cw)^{-1}\}],
\end{aligned} \tag{B.11}
$$

which includes the group variables $Cw, \tilde{C}\bar{w}, Sw$ and $S^\dagger\bar{w}$ only in the first order and their inverse $(Cw)^{-1}$ and $(\tilde{C}\bar{w})^{-1}$. This expression makes a crucial role to get the correct form of τ-differential. Substituting (B.10) into (B.9), we can get the explicit expressions for the differential operators for particle–hole pairs in the following forms:

$$\boldsymbol{e}^{ia} \stackrel{d}{=} -\left(p^*_{ja}p^*_{ib}\frac{\partial}{\partial p^*_{jb}} + \frac{\partial}{\partial p_{ia}} - \frac{\mathrm{i}}{2}p^*_{ia}\frac{\partial}{\partial\tau}\right), \qquad \boldsymbol{e}_{ai} \stackrel{d}{=} -\left(p_{ja}p_{ib}\frac{\partial}{\partial p_{jb}} + \frac{\partial}{\partial p^*_{ia}} + \frac{\mathrm{i}}{2}p_{ia}\frac{\partial}{\partial\tau}\right),$$
$$\boldsymbol{e}_{ab} \stackrel{d}{=} p_{ia}\frac{\partial}{\partial p_{ib}} - p^*_{ib}\frac{\partial}{\partial p^*_{ia}} + \mathrm{i}\delta_{ab}\frac{\partial}{\partial\tau}, \qquad \boldsymbol{e}_{ij} \stackrel{d}{=} p^*_{ia}\frac{\partial}{\partial p^*_{ja}} - p_{ja}\frac{\partial}{\partial p_{ia}}, \tag{B.12}$$

by which we can prove that the Lie commutation relation (2.2) is also satisfied. Then from equations (B.2) and (B.3), it can easily be shown that the infinitesimal left transformation of the variable g is equivalent to operate the differential operators (B.12) on $\Psi(g)$.

To construct a free particle–hole vacuum function, using the second equation of (A.2), we put

$$\Psi_{m,m}(p, p^*, \tau) = \langle\phi_m|U(g)|\phi_m\rangle = [\det(1 + p^\dagger p)]^{-\frac{1}{2}} \cdot \det w. \tag{B.13}$$

Let us introduce a function $\Phi_{m,m}(p, p^*, \tau)$ defined as

$$\Phi_{m,m}(p, p^*, \tau) = \Psi^*_{m,m}(p, p^*, \tau) = [\det(1 + p^\dagger p)]^{-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}\tau}. \tag{B.14}$$

By using the famous formula for differential of a determinant, we can easily calculate differentials of $\det(1 + p^\dagger p)$ as

$$\begin{aligned}\frac{\partial}{\partial p_{jb}}[\det(1 + p^\dagger p)]^{-\frac{1}{2}} &= -\tfrac{1}{2}p^*_{jc}[(1 + p^\dagger p)^{-1}]^{\mathrm{T}}_{cb}[\det(1 + p^\dagger p)]^{-\frac{1}{2}},\\ \frac{\partial}{\partial p^*_{ia}}[\det(1 + p^\dagger p)]^{-\frac{1}{2}} &= -\tfrac{1}{2}p_{id}[(1 + p^\dagger p)^{-1}]_{da}[\det(1 + p^\dagger p)]^{-\frac{1}{2}}.\end{aligned} \tag{B.15}$$

Then, from equations (B.14) and (B.15) we get

$$\begin{aligned}\boldsymbol{e}^{ia}\Phi_{m,m}(p, p^*, \tau) &= \{\tfrac{1}{2}p^*_{ib}p^*_{ja} \cdot p_{jc}[(1 + p^\dagger p)^{-1}]_{cb} + \tfrac{1}{2}[p^*(1 + p^\dagger p)^{\mathrm{T}-1}]_{ia} + \tfrac{1}{2}p^*_{ia}\}\\ &\quad \times \Phi_{m,m}(p, p^*, \tau)\\ &= \{\tfrac{1}{2}[p^*(1 + p^{\mathrm{T}}p^*)^{-1}(1 + p^{\mathrm{T}}p^*)]_{ia} + \tfrac{1}{2}p^*_{ia}\}\Phi_{m,m}(p, p^*, \tau)\\ &= p^*_{ia}\Phi_{m,m}(p, p^*, \tau),\end{aligned} \tag{B.16}$$

$$\begin{aligned}\boldsymbol{e}_{ai}\Phi_{m,m}(p, p^*, \tau) &= \{\tfrac{1}{2}p_{ib}p_{ja} \cdot p^*_{jc}[(1 + p^\dagger p)^{-1}]^{\mathrm{T}}_{cb}\\ &\quad + \tfrac{1}{2}p_{id}[(1 + p^\dagger p)^{-1}]_{da} - \tfrac{1}{2}p_{ia}\}\Phi_{m,m}(p, p^*, \tau)\\ &= \{\tfrac{1}{2}[p(1 + p^\dagger p)^{-1}(1 + p^\dagger p)]_{ia} - \tfrac{1}{2}p_{ia}\}\Phi_{m,m}(p, p^*, \tau) = 0,\end{aligned} \tag{B.17}$$

$$\boldsymbol{e}_{ab}\Phi_{m,m}(p, p^*, \tau) = \delta_{ab}\Phi_{m,m}(p, p^*, \tau), \tag{B.18}$$

$$\boldsymbol{e}_{ij}\Phi_{m,m}(p, p^*, \tau) = 0, \tag{B.19}$$

and finally we obtain a relation

$$\boldsymbol{e}^{ia}p^*_{jb} = -p^*_{ib}p^*_{ja} + p^*_{jb}\boldsymbol{e}^{ia}. \tag{B.20}$$

Thus, we have proved that on the function $\Phi_{m,m}(p, p^*, \tau)$ the particle–hole differential operators (B.12) satisfy the relations (B.21) and the commutation relation $[\boldsymbol{e}^{ia}, p^*_{jb}] = -p^*_{ib}p^*_{ja}$. Therefore, it turns out that the function $\Phi_{m,m}(p, p^*, \tau)$ should be regarded as a free particle–hole vacuum in the physical fermion space.

From the above calculations, these differential operators are also proved to satisfy the relations

$$e^{ia}\Phi_{m,m}(p,p^*,\tau) = p^*_{ia}\phi_{m,m}(p,p^*,\tau), \qquad e_{ai}\Phi_{m,m}(p,p^*,\tau) = 0,$$
$$e_{ab}\Phi_{m,m}(p,p^*,\tau) = \delta_{ab}\Phi_{m,m}(p,p^*,\tau), \qquad e_{ij}\Phi_{m,m}(p,p^*,\tau) = 0, \tag{B.21}$$

for the free particle–hole vacuum function $\Phi_{m,m}(p,p^*,\tau)$. Furthermore, we can introduce higher-order differential operators obeying the relation

$$D^{1,\ldots,a_1,\cdots,a_\mu,\cdots,m}_{1,\ldots,i_1,\cdots,i_\mu,\cdots,m}(p,\partial_p,\partial_{p^*},\partial_\tau) \stackrel{d}{=} e^{i_1a_1}\cdots e^{i_\mu a_\mu},$$
$$D^{1,\ldots,a_1,\cdots,a_\mu,\cdots,m}_{1,\ldots,i_1,\cdots,i_\mu,\cdots,m}(p,\partial_p,\partial_{p^*},\partial_\tau)\Phi_{m,m}(p,p^*,\tau) = \mathcal{A}(p^*_{i_1a_1}\cdots p^*_{i_\mu a_\mu})\Phi_{m,m}(p,p^*,\tau), \tag{B.22}$$

which show that by operating the differential operator D on the vacuum function Φ we obtain the Plücker coordinate $\mathcal{A}$. The Plücker relation (A.12) becomes a finite set of partial differential equations satisfying

$$\Phi_{m,m}(p,p^*,\tau)D^{1,\ldots,a_1,\cdots,a_\rho,\cdots,m}_{1,\ldots,i_1,\cdots,i_\rho,\cdots,m}\phi_{m,m}(p,p^*,\tau) + \sum_{j=1}^{\rho}(-1)^j D^{1,\ldots,a_1,\ldots,m}_{1,\ldots,i_1,\ldots,m}\Phi_{m,m}(p,p^*,\tau)$$
$$\times D^{1,\ldots,a_1,\ldots,a_2,\ldots,a_j,\ldots,a_{j+1},\ldots,a_\rho,\ldots,m}_{1,\ldots,a_1,\ldots,i_1,\ldots,i_{j-1},\ldots,i_{j+1},\ldots,i_\rho,\ldots,m}\Phi_{m,m}(p,p^*,\tau) = 0, \tag{B.23}$$
$$(v^{1,\ldots,a_1,\cdots,a_\mu,\cdots,m}_{1,\ldots,i_1,\cdots,i_\mu,\cdots,m}(g_\zeta g_w))^* = (v^{1,\ldots,a_1,\cdots,a_\mu,\cdots,m}_{1,\ldots,i_1,\cdots,i_\mu,\cdots,m}(g_\zeta)\det w)^* = D^{1,\ldots,a_1,\cdots,a_\mu,\cdots,m}_{1,\ldots,i_1,\cdots,i_\mu,\cdots,m}\Phi_{m,m}(p,p^*,\tau).$$

Thus, in both the SCF theory and the soliton theory on a group, we can find the common features that the Grassmannian is just identical with the solution space of the bilinear differential equation. The solution space of each differential equation becomes an integral surface [19, 21, 22]. The free particle–hole vacuum function $\Phi_{m,m}(p,p^*,\tau)$ can be also expressed in terms of the Schur polynomials given in the next appendix.

Appendix C. Schur polynomials

Let us introduce Schur polynomials $S_l(\chi)$ belonging to $\mathbb{C}(\chi_1,\chi_2,\ldots)$ through a generating function

$$\exp\left(\sum_{l=1}^{\infty}\chi_l t^l\right) = \sum_{l=0}^{\infty} S_l(\chi)t^l. \tag{C.1}$$

For an element of an $\mathcal{N}$-dimensional linear group $GL(\mathcal{N})$, the Schur polynomial is related to a symmetric function h_l, $\sum_{l\geqslant 0} h_l t^l = \prod_{i=1}^{\mathcal{N}}(1-\epsilon_i t)^{-1}$. Then, the Schur polynomial $S_l(\chi)$ is written as

$$S_l(\chi) = h_l(\epsilon_1,\epsilon_2,\ldots,\epsilon_{\mathcal{N}}), \qquad \chi_l = \frac{1}{l}(\epsilon_1^l + \epsilon_2^l + \cdots + \epsilon_{\mathcal{N}}^l). \tag{C.2}$$

The Schur polynomial $S_\lambda(\chi)$ is given as

$$S_\lambda(\chi) = S_{\lambda_1,\lambda_2,\lambda_3,\ldots,\lambda_l}(\chi) = \begin{vmatrix} S_{\lambda_1} & S_{\lambda_1+1} & S_{\lambda_1+2} & \cdots & S_{\lambda_1+l-1} \\ S_{\lambda_2-1} & S_{\lambda_2} & S_{\lambda_2+1} & \cdots & S_{\lambda_2+l-2} \\ S_{\lambda_3-2} & S_{\lambda_3-1} & S_{\lambda_3} & \cdots & S_{\lambda_3+l-3} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ S_{\lambda_l+1-l} & S_{\lambda_l+2-l} & S_{\lambda_l+3-l} & \cdots & S_{\lambda_l} \end{vmatrix} = \det\{(S_{\lambda_i+j-i}(\chi))_{i,j}\}, \tag{C.3}$$

where the λ denotes a partition $\lambda = \{\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_l > 0\}$ [17].

For the special partition $\lambda = 1^m \equiv \{\lambda_1 = 1, \lambda_2 = 1, \lambda_3 = 1, \lambda_4 = 1, \ldots, \lambda_m = 1\}$, i.e. the completely anti-symmetric Young diagram,

$$S_{1^m}(\chi) = \begin{vmatrix} S_1(\chi) & S_2(\chi) & S_3(\chi) & S_4(\chi) & \cdots & S_m(\chi) \\ 1 & S_1(\chi) & S_2(\chi) & S_3(\chi) & \cdots & S_{m-1}(\chi) \\ 0 & 1 & S_1 & S_2(\chi) & \cdots & S_{m-2}(\chi) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & S_1(\chi) \end{vmatrix} = (-1)^m S_m(-\chi), \tag{C.4}$$

where we have used the explicit forms of the Schur polynomials (D.6) given in the next appendix.

Appendix D. Other expressions for $D(p'^T p^*)$

Inserting the completeness relation, we can express the overlap integral (2.17) in the form

$$\begin{aligned} S(g,g') &= \langle\phi_m|U^\dagger(g) \sum_{\substack{1\leqslant a<b<\cdots\leqslant m;\\ m+1\leqslant i<j<\cdots\leqslant n}} |S^m_{ij\cdots ab\cdots}\rangle\langle S^m_{ij\cdots ab\cdots}|U(g')|\phi_m\rangle = [\langle\phi_m|U(g)|\phi_m\rangle e^{p_{ia}c_i^\dagger c_a}|\phi_m\rangle]^\dagger \\ &\quad\times\left[\sum_{\rho=0}^{M}\sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m,\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} |S^m_{1,\ldots,m \text{ without }\{a_1,\ldots,a_\rho\};i_1,\ldots,i_\rho}\rangle\langle S^m_{1,\ldots,m \text{ without }\{a_1,\ldots,a_\rho\};i_1,\ldots,i_\rho}|\right] \\ &\quad\times[\langle\phi_m|U(g')|\phi_m\rangle e^{p'_{ia}c_i^\dagger c_a}|\phi_m\rangle] = [e^{p_{ia}c_i^\dagger c_a}|\phi_m]^\dagger \\ &\quad\times\left[\sum_{\rho=0}^{M}\sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m,\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} |S^m_{1,\ldots,m \text{ without }\{a_1,\cdots,a_\rho\};i_1,\ldots,i_\rho}\rangle\langle S^m_{1,\ldots,m \text{ without }\{a_1,\ldots,a_\rho\};i_1,\ldots,i_\rho}|\right] \\ &\quad\times[e^{p'_{ia}c_i^\dagger c_a}|\phi_m\rangle]\Phi_{00}(g)\Phi^*_{00}(g') \\ &= \sum_{\rho=0}^{M}\sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m,\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} [\langle S^m_{1,\ldots,m \text{ without }\{a_1,\ldots,a_\rho\};i_1,\ldots,i_\rho}|e^{p_{ia}c_i^\dagger c_a}|\phi_m\rangle]^* \\ &\quad\times[\langle S^m_{1,\ldots,m \text{ without }\{a_1,\cdots,a_\rho\};i_1,\ldots,i_\rho}|e^{p'_{ia}c_i^\dagger c_a}|\phi_m\rangle]\Phi_{00}(g)\Phi^*_{00}(g'), \end{aligned} \tag{D.1}$$

where $|S^m_{ij\cdots ab\cdots}\rangle = c_i^\dagger c_a c_j^\dagger c_b\cdots|S^m\rangle$ and $|S^m\rangle = |\phi_m\rangle$. In the above equation, we have used the first relation of (A.2). Let $\mathcal{A} = 1$ for $\rho = 0$. Then, we have

$$\begin{aligned} S(g,g') &= \sum_{\rho=0}^{M}\sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \mathcal{A}(p^*_{i_1a_1}\cdots p^*_{i_\rho a_\rho})\mathcal{A}(p'_{i_1a_1}\cdots p'_{i_\rho a_\rho})\Phi_{00}(g)\Phi^*_{00}(g') \\ &= S(p^*,p')\Phi_{00}(g)\Phi^*_{00}(g'), \end{aligned} \tag{D.2}$$

from which we can obtain one of the other expressions for $D(p'^{\mathrm{T}}p^*)$ $(= S(p^*, p'))$ as

$$D(p'^{\mathrm{T}}p^*) = \sum_{\rho=0}^{M}\sum_{\substack{1\leqslant a_1<\cdots<a_\rho\leqslant m;\\ m+1\leqslant i_1<\cdots<i_\rho\leqslant n}} \mathcal{A}(p'_{i_1a_1}\cdots p'_{i_\rho a_\rho})\mathcal{A}(p^*_{i_1a_1}\cdots p^*_{i_\rho a_\rho}). \tag{D.3}$$

Of course, the above equation is exactly identical with (2.23).

Using the famous formula and the Schur polynomials $S_l(\chi)(\chi = (\chi_1, \chi_2, \chi_3, \ldots)$, $S_0(\chi) = 1)$ (C.1)

$$\det(1 + X) = \exp\{\mathrm{Tr}\ \ln(1 + X)\} = \exp\left\{\sum_{l=1}^{\infty}(-1)^{l-1}\frac{1}{l}\mathrm{Tr}(X^l)\right\}, \tag{D.4}$$

and denoting $z = p^\dagger p'$, we have another expression for $D(p'^{\mathrm{T}} p^*)$ as

$$D(p'^{\mathrm{T}} p^*) = \det(1 + p^\dagger p') = \sum_{l=0}^{\infty} S_l(\chi), \qquad \begin{cases} \chi_l \equiv (-1)^{l-1}\dfrac{1}{l}\mathrm{Tr}(z^l), \\ \chi_l = S_l(\chi) = 0, \quad (l \geqslant M + 1), \end{cases} \tag{D.5}$$

where the first few Schur polynomials $S_l(\chi)$ read

$$\begin{aligned} &S_1(\chi) = \chi_1, \qquad S_2(\chi) = \chi_2 + \tfrac{1}{2}\chi_1^2, \qquad S_3(\chi) = \chi_3 + \chi_1\chi_2 + \tfrac{1}{6}\chi_1^3, \\ &S_4(\chi) = \chi_4 + \chi_1\chi_3 + \tfrac{1}{2}\chi_2^2 + \tfrac{1}{2}\chi_1^2\chi_2 + \tfrac{1}{24}\chi_1^4, \ldots . \end{aligned} \tag{D.6}$$

With the aid of the formula

$$[\det(1 + X)]^{-\frac{1}{2}} = \exp\{\mathrm{Tr}\ln(1 + X)^{-\frac{1}{2}}\} = \exp\left\{\sum_{l=1}^{\infty}(-1)^l\frac{1}{2l}\mathrm{Tr}(X^l)\right\}, \tag{D.7}$$

to our great surprise, the free particle–hole vacuum function $\Phi_{m,m}(p, p^*, \tau)$ (B.14) can be also expressed in terms of the Schur polynomials $S_l(\xi)$ as

$$\Phi_{m,m}(p, p^*, \tau) = \sum_{l=0}^{\infty} S_l(\xi) \cdot e^{-\mathrm{i}\tau}, \qquad \begin{cases} \xi_l \equiv (-1)^l\dfrac{1}{2l}\mathrm{Tr}([p^\dagger p]^l), \\ \xi_l = S_l(\xi) = 0. \quad (l \geqslant M + 1). \end{cases} \tag{D.8}$$

Rowe *et al* showed that the NP $SO(2n)$ wave function satisfies recursion relations and were able to express it with the aid of the relations in a form of determinant which is well known as the completely anti-symmetric Schur function in the theory of group characters [13, 23]. In the present $U(n)$ case, equation (D.5) is also given by a determinant form

$$\varphi_l(z) = \frac{1}{l!}\begin{vmatrix} \chi_1 & 1 & 0 & 0 & \cdots & 0 \\ 2\chi_2 & \chi_1 & 2 & 0 & \cdots & 0 \\ 3\chi_3 & 2\chi_2 & \chi_1 & 3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \cdots & \cdots & l-1 \\ l\chi_l & (l-1)\chi_{l-1} & (l-2)\chi_{n-2} & (l-3)\chi_{l-3} & \cdots & \chi_1 \end{vmatrix} = (-1)^l S_l(-\chi), \tag{D.9}$$

which is exactly the same form as that given in [7]. The Schur function $\varphi_l(z)$ satisfies the recursion relation and the differential formula

$$\varphi_l(z) = \frac{1}{l}\left\{\chi_1 - \sum_{l'=1}^{l-1}(l' + 1)\chi_{l'+1}\frac{\partial}{\partial\chi_{l'}}\right\}\varphi_{l-1}(z), \qquad \frac{\partial}{\partial\chi_{l'}}\varphi_l(z) = (-1)^{l'+1}\varphi_{l-l'}(z). \tag{D.10}$$

By using the second equation of (D.10), we can rewrite the above recursion relation as

$$\varphi_l(z) = \frac{1}{l}\sum_{l'=1}^{l}(-1)^{l'+1}l'\chi_{l'}\varphi_{l-l'}(z) \quad (\varphi_0 = 1). \tag{D.11}$$

Appendix E. Differential formulae for $D(ep^*)$ with respect to e_{ai}

A differential formula for $D(ep^*)$ with respect to e_{ai} is easily given as

$$\frac{\partial D(eq^*)}{\partial e_{ai}} = \frac{\partial \det(1+eq^*)}{\partial(1+eq^*)_{bc}} \frac{\partial(1+eq^*)_{bc}}{\partial e_{ai}} = K^*_{ia} D(eq^*), \quad (K^* \equiv q^*(1+eq^*)^{-1}), \tag{E.1}$$

and we have used the famous differential formulas for a regular matrix $A = (A_{ab})$

$$\frac{\partial \det A}{\partial A_{ab}} = (A^{-1})_{ba} \det A, \qquad \frac{\partial (A^{-1})_{dc}}{\partial A_{ab}} = -(A^{-1})_{bc}(A^{-1})_{da}. \tag{E.2}$$

As for the second differential for the $D(ep^*)$, it is easily carried out as follows:

$$\begin{aligned} \frac{\partial^2 D(eq^*)}{\partial e_{bj}\partial e_{ai}} &= \frac{\partial K^*_{ia}}{\partial e_{bj}} D(eq^*) + K^*_{jb}K^*_{ia} D(eq^*) \\ &= \left[q^*_{ia'} \frac{\partial\{(1+eq^*)^{-1}\}_{a'a}}{\partial\{(1+eq^*)\}_{cd}} \frac{\partial\{(1+eq^*)\}_{cd}}{\partial e_{bj}} + K^*_{jb}K^*_{ia} \right] D(eq^*) \\ &= [K^*_{ia}K^*_{jb} - K^*_{ib}K^*_{ja}] D(eq^*) \\ &= \mathcal{A}(K^*_{ia}K^*_{jb}) D(eq^*). \end{aligned} \tag{E.3}$$

Then, succesive differential calculi to higher orders lead to a general differential formula

$$\frac{\partial^\rho D(eq^*)}{\partial e_{a_1 i_1}\partial e_{a_2 i_2}\cdots\partial e_{a_\rho i_\rho}} = \mathcal{A}(K^*_{i_1 a_1}K^*_{i_2 a_2}\ldots K^*_{i_\rho a_\rho}) D(eq^*) \quad (\rho = 1, \ldots, \min(m, n-m)). \tag{E.4}$$

A similar differential formula to equation (E.4) was derived by Fukutome on the $SO(2n+1)$ Lie algebra for superconducting fermion systems [5].

Acknowledgments

One of the authors (SN) would like to express his sincere thanks to Professor J da Providência for kind and warm hospitality extended to him at the Centro de Física Teórica, Universidade de Coimbra. This work was supported by the Portuguese Project POCTI/FIS/451/94. He was supported by the Portuguese program POCTI/FIS/451/94. The authors are greatly indebted to Professor J da Providência for his careful reading of the original manuscript and critical comments. Finally, the authors thank Yukawa Institute for Theoretical Physics at Kyoto University, where discussions held during the YITP workshop (YITP-W-04-03) *Quantum Field Theory 2004* were useful to complete this work.

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