Progress of Theoretical Physics, Vol. 77, No. 5, May 1987

Non-Unitary Realization of the Selfconsistent Collective-Coordinate Method

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(Received January 7, 1987)

Recently we reformulated the selfconsistent collective-coordinate (SCC) method of Marumori, Maskawa, Sakata and Kuriyama. In this reformulation, biunitary forms of state vectors are used and the resultant representation corresponds to a c-number image of the Dyson-type boson expansion theory. This non-unitary version of the SCC method is rederived from a general point of view in order to clarify the relation to the original unitary version. Moreover, it is shown that the expansion technique to solve the basic equations is as applicable to this new version as to the unitary one, so that applications to realistic problems are easily done.

§ 1. Introduction

Recently it has become increasingly important to determine the collective subspace selfconsistently for understanding the anharmonicity or non-linearity of the large amplitude nuclear collective motion. The selfconsistent collective-coordinate (SCC) method,*) originally proposed by Marumori, Maskawa, Sakata and Kuriyama,[1] is promising for this purpose because it can properly take into account the effect of coupling to non-collective degrees of freedom. It is known that, if the coupling effect or the dynamical anharmonicity effect is neglected, this theory turns to the well-known boson expansion theory for only the collective phonons under a suitable quantization procedure. Then, it enables us to construct a new type of "dynamical boson expansion theory" which incorporates the dynamical anharmonicity as well as the kinematical one originating from the Pauli principle. This new dynamical boson theory is expected to provide us a powerful method for investigating the nuclear structure problems full-microscopically.

The original version of the SCC method corresponds, roughly speaking, to the Holstein-Primakoff type boson theory.[6),7)] Quite recently we have shown in Ref. 2) (from now on referred to as I) that there exists another version corresponding to the Dyson-type boson theory; namely, a "non-unitary realization" of the SCC method, so to speak. Although both the types of boson theory are strictly equivalent to each other, the Dyson theory is more convenient for realistic applications, since a method of hermitian treatment of the theory is established.[3)] Therefore the newly proposed Dyson version of the SCC method can be superior for the purpose of investigating the dynamical coupling effect, because the kinematical anharmonicity is evaluated without any approximation such as truncation of the expansion. In other words, the "zero-th order collective subspace" is constructed without any ambiguities.

*) The SCC method itself has a wide range of applicabilities, e.g., to heavy ion reactions, spontaneous fissions and rotational motions.[10)] However, we are mainly concerned, in this paper, with an application to the boson description of low-lying collective states.

However, the formulation of I seems somewhat different in its appearance from the original SCC method and the relation between the two is not clear. This is mainly because the "biunitary" Thouless form of state vectors are used in I, whereas not in the original version. This seems to spoil the usefulness of the (η, η^*)-expansion technique[1),8)] which is very powerful to solve the basic equations in the original version.

In this paper, the Dyson-type non-unitary realization of the SCC method is rederived from a general point of view, i.e., the theory of the canonical coordinate system for the TDHF manifold formulated by Kuriyama and Yamamura[4)] for the original version. In the course of the rederivation, the relation between the non-unitary and unitary realizations is clarified. Moreover, it is shown that the (η, η^*)-expansion technique suitable for the unitary realization can be applied to the non-unitary one with slight modifications.

In § 2, we introduce a general expression of non-unitary form of Slater determinants, which is a starting point of the SCC method. After presenting basic elements needed for later developments, the canonical-coordinate system and the TDHF equation for the non-unitary realization are investigated in § 3. Section 4 deals with the basic equations in the non-unitary case. Section 5 is devoted to concluding remarks.

§ 2. Non-unitary expression of Slater determinantal state vector

The SCC method is based on the time-dependent Hartree-Fock (TDHF) theory generated from a static HF solution $|\phi_0\rangle$. Let us denote the particle (hole) creation operator $a_\mu{}^\dagger$, $\mu=1, 2, \cdots N_p$ ($b_i{}^\dagger$, $i=1, 2, \cdots N_h$) with respect to $|\phi_0\rangle$. Then a general Slater determinant, which is not necessarily normalized to unity, can be represented by

$$|\phi\rangle=\hat{U}|\phi_0\rangle\,, \qquad \hat{U}=e^{\hat{S}} \tag{2·1}$$

with

$$\hat{S}=\sum_{\mu i}\{\Gamma_1(i\mu)a_\mu{}^\dagger b_i{}^\dagger-\Gamma_2(\mu i)b_i a_\mu\}\,. \tag{2·2}$$

Since $\hat{U}$ is not necessarily unitary transformation, we need to introduce another state vector which is not hermitian conjugate of $|\phi\rangle$,

$$\langle\varphi|=\langle\phi_0|\hat{U}^{-1}\,, \tag{2·3}$$

together with which the normalization condition

$$\langle\varphi|\phi\rangle=1 \tag{2·4}$$

is fulfilled. With the aid of Eq. (2·2), the transformation of the particle and hole fermion operators is obtained:

$$\hat{U}^{-1}\begin{pmatrix} a \\ b^\dagger \end{pmatrix}\hat{U}=\begin{pmatrix} D_p{}^T, & C_1{}^T \\ -C_2{}^T, & D_h{}^T \end{pmatrix}\begin{pmatrix} a \\ b^\dagger \end{pmatrix},$$

$$\hat{U}^{-1}\begin{pmatrix} a^\dagger \\ b \end{pmatrix}\hat{U}=\begin{pmatrix} D_p, & C_2 \\ -C_1, & D_h \end{pmatrix}\begin{pmatrix} a^\dagger \\ b \end{pmatrix}, \qquad (2\cdot5)$$

where the matrices D_p, D_h, C_1 and C_2 are given by

$$D_p(\mu\nu)=[\cos\sqrt{\Gamma_2\Gamma_1}]_{\mu\nu},$$

$$D_h(ij)=[\cos\sqrt{\Gamma_1\Gamma_2}]_{ij},$$

$$C_1(i\mu)=[\Gamma_1\cdot\sin\sqrt{\Gamma_2\Gamma_1}/\sqrt{\Gamma_2\Gamma_1}]_{i\mu},$$

$$C_2(\mu i)=[\Gamma_2\cdot\sin\sqrt{\Gamma_1\Gamma_2}/\sqrt{\Gamma_1\Gamma_2}]_{\mu i}. \qquad (2\cdot6)$$

Here and hereafter, the obvious matrix notations are used. It is clear from Eq. (2·6) that not all of these matrices are independent but they satisfy the following identities:

$$D_p{}^2+C_2C_1=1_p, \qquad D_h{}^2+C_1C_2=1_h,$$

$$C_1D_p=D_hC_1, \qquad D_pC_2=C_2D_h. \qquad (2\cdot7)$$

Here $1_p(1_h)$ means the unit matrix of dimension $N_p(N_h)$ and is simply denoted by 1, hereafter.

As stated in § 1, the Thouless form of the Slater determinant is used in Ref. 2) rather than the exponential form of Eqs. (2·1) and (2·2). It is easy to convert the latter into the former representation:

$$|\phi\rangle=N^{1/2}e^{\hat{Z}_1}|\phi_0\rangle, \qquad \hat{Z}_1=\sum_{\mu i}Z_1(i\mu)a_\mu{}^\dagger b_i{}^\dagger,$$

$$\langle\varphi|=N^{1/2}\langle\phi_0|e^{\hat{Z}_2}, \qquad \hat{Z}_2=\sum_{\mu i}Z_2(\mu i)b_i a_\mu \qquad (2\cdot8)$$

with

$$N^{1/2}=\det D_p=\det D_h \qquad (2\cdot9)$$

and

$$Z_1=C_1D_p{}^{-1}=D_h{}^{-1}C_1,$$

$$Z_2=D_p{}^{-1}C_2=C_2D_h{}^{-1}. \qquad (2\cdot10)$$

Now it has been clarified that there are, at least, three sets of variables, i.e., C_i, Z_i and $\Gamma_i(i=1,2)$, which characterize a Slater determinant being not necessarily normalized. We summarize here the relations between them, which are easily derived from Eqs. (2·6), (2·7) and (2·10):

$$C_1=Z_1\cdot(1+Z_2Z_1)^{-1/2}, \qquad Z_1=C_1\cdot(1-C_2C_1)^{-1/2}, \qquad (2\cdot11)$$

$$Z_1=\Gamma_1\cdot\tan\sqrt{\Gamma_2\Gamma_1}/\sqrt{\Gamma_2\Gamma_1}, \qquad \Gamma_1=Z_1\cdot\arctan\sqrt{Z_2Z_1}/\sqrt{Z_2Z_1}, \qquad (2\cdot12)$$

$$\Gamma_1=C_1\cdot\arcsin\sqrt{C_2C_1}/\sqrt{C_2C_1}, \qquad C_1=\Gamma_1\cdot\sin\sqrt{\Gamma_2\Gamma_1}/\sqrt{\Gamma_2\Gamma_1}. \qquad (2\cdot13)$$

The corresponding relations between C_2, Z_2 and Γ_2 are obtained by interchanging indices 1 and 2 in Eqs. (2·11)~(2·13). The c-number images of the fermion pair operators are represented by these sets of variables. With the aid of Eq. (2·5), they are given by

$$\begin{aligned}\langle\varphi|a_\mu{}^\dagger b_i{}^\dagger|\phi\rangle &= [C_2\cdot\sqrt{1-C_1C_2}\,]_{\mu i}\\ &= [Z_2\cdot(1+Z_1Z_2)^{-1}]_{\mu i}\\ &= [\Gamma_2\cdot\sin 2\sqrt{\Gamma_1\Gamma_2}/2\sqrt{\Gamma_1\Gamma_2}\,]_{\mu i}\,,\end{aligned} \tag{2·14}$$

$$\begin{aligned}\langle\varphi|b_i a_\mu|\phi\rangle &= [\sqrt{1-C_1C_2}\cdot C_1]_{i\mu}\\ &= [(1+Z_1Z_2)^{-1}\cdot Z_1]_{i\mu}\\ &= [\sin 2\sqrt{\Gamma_1\Gamma_2}/2\sqrt{\Gamma_1\Gamma_2}\cdot\Gamma_1]_{i\mu}\,,\end{aligned} \tag{2·15}$$

$$\begin{aligned}\langle\varphi|a_\mu{}^\dagger a_\nu|\phi\rangle &= [C_2C_1]_{\mu\nu}\\ &= [Z_2Z_1\cdot(1+Z_2Z_1)^{-1}]_{\mu\nu}\\ &= [\sin^2\sqrt{\Gamma_2\Gamma_1}\,]_{\mu\nu}\,,\end{aligned} \tag{2·16}$$

$$\begin{aligned}\langle\varphi|b_i{}^\dagger b_j|\phi\rangle &= [C_1C_2]_{ji}\\ &= [Z_1Z_2\cdot(1+Z_1Z_2)^{-1}]_{ji}\\ &= [\sin^2\sqrt{\Gamma_1\Gamma_2}\,]_{ji}\,.\end{aligned} \tag{2·17}$$

Needless to say, all the formulae turn into those in the unitary realization by setting $C_2=C_1{}^\dagger$, $Z_2=Z_1{}^\dagger$ and $\Gamma_2=\Gamma_1{}^\dagger$.

§ 3. Canonical-variable description of full TDHF theory in the non-unitary realization

The introduction of the canonical-variable condition (CVC) was a crucial step toward developing the SCC method.[1] It was moreover shown[5] that this condition combining with the "analyticity requirement", which will be explained below, *uniquely* determines the canonical-coordinate system (CCS) which parametrizes the TDHF submanifold corresponding to the collective subspace in the full shell model space.

In order to extract the collective subspace, it is better to formulate first the CCS within the full TDHF framework. Then the SCC method is derived naturally by restricting the degrees of freedom to the collective one.[4),6)] For this purpose, we modify the general theory of the CCS formulated in Ref. 4) so as to make it suitable for the non-unitary realization.

3.1. *Canonical-coordinate system*

It is known[4),6),13)] that the TDHF theory is strictly equivalent to the Hamiltonian dynamical system on the symplectic manifold, called TDHF manifold, which is parametrized by the canonical coordinates q_K and momenta p_K, $K=1, 2, \cdots N_p\times N_h$. This may also be the case even when the non-unitary representation of the Slater determinantal states is used. In place of (q_K, p_K), the complex variables $(\eta_K{}^*, \eta_K)$ defined by

$$\eta_K^* = \frac{1}{\sqrt{2}}(q_K - ip_K)\,, \qquad \eta_k = \frac{1}{\sqrt{2}}(q_K + ip_K)\,, \tag{3·1}$$

which are suitable for the boson description, are introduced in the usual unitary case. However, the variables (3·1) cannot be used in our case because of non-unitarity of the representation. Instead, we introduce a new type of complex variables (ξ_K, η_K) which may, in principle, be obtained by a coordinate transformation,

$$\xi_K = g_K(q, p)\,, \qquad \eta_K = f_K(q, p)\,. \tag{3·2}$$

The introduction of pairs of complex variables seems to make the number of degrees of freedom double. This causes no problem because (ξ_K, η_K) and their complex conjugate variables (η_K^*, ξ_K^*) are not mixed in the state vectors (2·1) and (2·3). Namely one has two kinds of parametrization, which are "conjugate" of each other, and they are completely decoupled. Actually, the "conjugate representation" in terms of (η_K^*, ξ_K^*) is obtained by taking

$$|\varphi\rangle = (\hat{U}^{-1})^\dagger |\phi_0\rangle \quad \text{and} \quad \langle\psi| = \langle\phi_0|\hat{U}^\dagger\,, \tag{3·3}$$

in place of $|\psi\rangle$ and $\langle\varphi|$, respectively, or equivalently by replacing $\Gamma_1(\Gamma_2)$ by $\Gamma_2^\dagger(\Gamma_1^\dagger)$ in all equations in § 2 (see also the Appendix).

From now on, we call the variables (ξ_K, η_K) *canonical coordinates* since the weak CVC equation, Eq. (3·6) below, should hold. It is worth noticing that the use of these variables enlarges the class of canonical transformations compared with the variables (η_K^*, η_K) because unitarity of the theory is abandoned. This is actually the reason why the Dyson-type formulation of the SCC method is possible.

3.2. *Full TDHF theory and canonical-variable condition*

The TDHF variational equation for non-unitary realization is

$$\delta\langle\varphi|\left(i\frac{d}{dt} - \hat{H}\right)|\psi\rangle = 0 \tag{3·4}$$

or equivalently,

$$i\frac{d}{dt}\langle\varphi|\hat{F}|\psi\rangle = \langle\varphi|[\hat{F}, \hat{H}]|\psi\rangle \tag{3·5}$$

for an arbitrary one-body operator $\hat{F}$. The parameters (ξ_K, η_K) introduced in § 3.1 are canonical coordinates if and only if the following weak CVC holds:

$$\langle\varphi|[\hat{O}_\eta(K), \hat{O}_\xi(L)]|\psi\rangle = \delta_{KL}\,,$$
$$\langle\varphi|[\hat{O}_\eta(K), \hat{O}_\eta(L)]|\psi\rangle = \langle\varphi|[\hat{O}_\xi(K), \hat{O}_\xi(L)]|\psi\rangle = 0\,, \tag{3·6}$$

where the generators with respect to ξ_K and η_K are defined by

$$\hat{O}_\xi(K) = \frac{\partial\hat{U}}{\partial\eta_K}\cdot\hat{U}^{-1}\,, \qquad \hat{O}_\eta(K) = -\frac{\partial\hat{U}}{\partial\xi_K}\cdot\hat{U}^{-1}\,. \tag{3·7}$$

Thus the time development of an arbitrary one-body operator $\hat{F}$ is converted to that of the classical mechanics:

$$i\dot{F}=\{F, \mathcal{H}_D\}_{\rm PB} \tag{3·8}$$

with the definitions

$$F=\langle\varphi|\hat{F}|\psi\rangle\,, \tag{3·9}$$

$$\mathcal{H}_D=\langle\varphi|\hat{H}|\psi\rangle-\langle\phi_0|\hat{H}|\phi_0\rangle \tag{3·10}$$

and the Poisson bracket given by

$$\{A, B\}_{\rm PB}=\sum_K\left(\frac{\partial A}{\partial\eta_K}\frac{\partial B}{\partial\xi_K}-\frac{\partial B}{\partial\eta_K}\frac{\partial A}{\partial\xi_K}\right). \tag{3·11}$$

Equation (3·8) is a direct consequence of Hamilton's equations of motion:

$$i\dot{\eta}_K=\frac{\partial\mathcal{H}_D}{\partial\xi_K}\,,\qquad i\dot{\xi}_K=-\frac{\partial\mathcal{H}_D}{\partial\eta_K}\,, \tag{3·12}$$

which is equivalent to the TDHF variational principle Eq. (3·4). Notice that the TDHF equation for the density matrix,

$$(\rho_D)_{\beta\alpha}\equiv\langle\varphi|c_\alpha{}^\dagger c_\beta|\psi\rangle \tag{3·13}$$

with respect to an arbitrary fixed creation (annihilation) operators $c_\alpha{}^\dagger(c_\beta)$, takes the usual form:

$$i\dot{\rho}_D=[h(\rho_D), \rho_D]\,, \tag{3·14}$$

where the mean-field hamiltonian,

$$[h(\rho_D)]_{\alpha\beta}\equiv\frac{\partial\mathcal{H}_D}{\partial(\rho_D)_{\beta\alpha}} \tag{3·15}$$

has exactly the same functional dependence on the density matrix as that in the unitary case, though $h(\rho_D)^\dagger\neq h(\rho_D)$ since $\rho_D{}^\dagger\neq\rho_D$.

It is clear[4] that the whole theory is invariant under general canonical transformations of the coordinates (ξ_K, η_K). Therefore, in order to fix the canonical-coordinate system, we should impose, from outside of the TDHF framework, some condition which explicitly breaks the invariance. This is done through the canonical-variable condition.

By introducing the one-form ω which is defined on the full TDHF manifold as

$$\omega=\langle\varphi|d\psi\rangle\,, \tag{3·16}$$

the general form of the CVC is expressed[4]

$$\omega+dS=\omega_c\,, \tag{3·17}$$

where ω_c is the canonical one-form characterizing the symplectic structure of the TDHF manifold, and is given by

$$\omega_c=\frac{1}{2}\sum_K(\xi_K\cdot d\eta_K-d\xi_K\cdot\eta_K)\,. \tag{3·18}$$

Here S is an arbitrary function of (ξ_K, η_K) and represents the freedom of choice of the

CCS resulting from the invariance mentioned above. In other words, this choice of S is nothing but a kind of "gauge-fixing". To speak in terms of the TDHF framework, this freedom corresponds to that of (ξ_K, η_K)-dependent phase factor. Namely by changing the state vectors as

$$|\psi\rangle \longrightarrow |\psi_S\rangle = \hat{U}_S|\phi_0\rangle\,,$$
$$\langle\varphi| \longrightarrow \langle\varphi_S| = \langle\phi_0|\hat{U}_S^{-1} \qquad (3\cdot19)$$

with

$$\hat{U}_S \equiv e^S \hat{U}\,,$$

dS in Eq. (3·17) is eliminated:

$$\omega_S = \omega_c\,, \qquad \omega_S = \langle\varphi_S|d\psi_S\rangle\,. \qquad (3\cdot20)$$

3.3. *Solutions of the CVC equation*

The ambiguity of the CCS can be removed partially by a suitable choice of the function S and completely*),[5] by requiring, in addition, the analyticity of ω_S at the point $(\xi_K, \eta_K)=0$ which represents the static HF state $|\phi_0\rangle$. In the following, we denote the canonical coordinates by $(\xi_{\mu i}, \eta_{i\mu})$, explicitly using the particle-hole indices. We shall discuss three possibilities corresponding to the three kinds of descriptions in terms of the variables C_i, Z_i and $\Gamma_i (i=1, 2)$ defined in § 2. It is easy to calculate Eq. (3·16) in each description:

$$\omega[C] = \frac{1}{2}\mathrm{Tr}[C_2\cdot dC_1 - dC_2\cdot C_1]\,, \qquad (3\cdot21)$$

$$\omega[Z] = \frac{1}{2}\mathrm{Tr}[(1+Z_2Z_1)^{-1}\cdot(Z_2\cdot dZ_1 - dZ_2\cdot Z_1)]\,, \qquad (3\cdot22)$$

$$\omega[\Gamma] = \frac{1}{2}\mathrm{Tr}[(\sin\sqrt{\Gamma_2\Gamma_1}/\sqrt{\Gamma_2\Gamma_1})^2\cdot(\Gamma_2\cdot d\Gamma_1 - d\Gamma_2\cdot\Gamma_1)]\,, \qquad (3\cdot23)$$

where C_i, Z_i and Γ_i are considered to be functions of $(\xi_{\mu i}, \eta_{i\mu})$.

Case (i): C-form

The result of this case is well-known.[7] With the choice of

$$S = S_1 \equiv \mathrm{const}\,, \qquad (3\cdot24)$$

the unique solution is determined as

$$C_2(\mu i) = \xi_{\mu i}\,, \qquad C_1(i\mu) = \eta_{i\mu}\,. \qquad (3\cdot25)$$

This case allows the interpretation of $\xi_{\mu i}$ as the complex conjugate of $\eta_{i\mu}$, i.e., $C_2 = C_1{}^\dagger$, since it makes the representation coincide with its "conjugate" one defined in § 3.1. Therefore, the result is reduced to the unitary realization and leads to the generalized

*) Strictly speaking, there remains a freedom associated with the linear canonical (symplectic) transformation of (ξ_K, η_K) which preserves the form of ω_c. Here we leave it free, because it brings up no physical importance at the classical level. However, this freedom becomes of importance in quantizing the classical version (see Ref. 9)).

Holstein-Primakoff representation of the pair operators, as is clear from Eqs. (2·14) ~(2·17).

Case (ii): Z-form

This case exactly reproduces the formulation of I. By simple manipulation, $\omega[Z]$ in Eq. (3·22) can be transformed into the "standard form" (see the Appendix),

$$\omega[Z]=\frac{1}{2}\mathrm{Tr}[G\cdot dF-dG\cdot F]-dS_{\mathrm{II}} \qquad (3\cdot 26)$$

with the definitions

$$G=Z_2\,,\qquad F=(1+Z_1Z_2)^{-1}Z_1 \qquad (3\cdot 27)$$

and

$$S_{\mathrm{II}}=\frac{1}{2}\mathrm{Tr}[GF]-\frac{1}{2}\mathrm{Tr}[\log(1+Z_2Z_1)]-\frac{1}{2}\mathrm{Tr}[1_p]\,. \qquad (3\cdot 28)$$

Thus the solution of Eq. (3·20) is uniquely determined with choosing $S=S_{\mathrm{II}}$ as

$$G(\mu i)=\xi_{\mu i}\,,\qquad F(i\mu)=\eta_{i\mu}\,. \qquad (3\cdot 29)$$

The c-number images of the pair operators in Eqs. (2·14)~(2·17) are reduced to the generalized Dyson representation[11]

$$\langle\varphi|a_\mu{}^\dagger b_i{}^\dagger|\psi\rangle=(\xi-\xi\eta\xi)_{\mu i}\,,\qquad \langle\varphi|b_i a_\mu|\psi\rangle=\eta_{i\mu}\,,$$
$$\langle\varphi|a_\mu{}^\dagger a_\nu|\psi\rangle=(\xi\eta)_{\mu\nu}\,,\qquad \langle\varphi|b_i{}^\dagger b_j|\psi\rangle=(\eta\xi)_{ji}\,, \qquad (3\cdot 30)$$

because $\xi_{\mu i}$ and $\eta_{i\mu}$ are interpreted as boson creation and annihilation operators $\boldsymbol{b}_{\mu i}^\dagger$ and $\boldsymbol{b}_{\mu i}$. The choice of $S=S_{\mathrm{II}}$, which is quite natural in this derivation, leads to the Thouless form,

$$|\psi_{S_{\mathrm{II}}}\rangle=e^{S_{\mathrm{II}}}N^{1/2}e^{\hat{Z}_1}|\phi_0\rangle=e^{(1/2)\mathrm{Tr}[GF]}Ne^{\hat{Z}_1}|\phi_0\rangle\,,$$
$$\langle\varphi_{S_{\mathrm{II}}}|=e^{-S_{\mathrm{II}}}N^{1/2}\langle\phi_0|e^{\hat{Z}_2}=e^{(-1/2)\mathrm{Tr}[GF]}\langle\phi_0|e^{\hat{Z}_2}\,, \qquad (3\cdot 31)$$

which is exactly the form assumed from the beginning in I for the Dyson-type realization, being set $k=\alpha=1$ in the notations of I. Here we omitted the irrelevant constant term $-(1/2)\mathrm{Tr}[1_p]$ and used the identity,

$$\exp(-\mathrm{Tr}[\log(1+Z_2Z_1)])=(\det D_p)^2=N\,.$$

Case (iii): Γ-form

This representation is very new. Similar to Eq. (3·26), $\omega[\Gamma]$ in Eq. (3·23) is rewritten,

$$\omega[\Gamma]=\frac{1}{2}\mathrm{Tr}[\Gamma_2\cdot d((\sin\sqrt{\Gamma_1\Gamma_2}/\sqrt{\Gamma_1\Gamma_2})^2\cdot\Gamma_1)$$
$$-d\Gamma_2\cdot((\sin\sqrt{\Gamma_1\Gamma_2}/\sqrt{\Gamma_1\Gamma_2})^2\cdot\Gamma_1)]-dS_{\mathrm{III}} \qquad (3\cdot 32)$$

with

$$S_{\rm III}={\rm Tr}\left[\int_0^{\sqrt{\Gamma_2\Gamma_1}}dx(\sin x\cdot\cos x-\sin^2 x/x)\right], \tag{3·33}$$

so that the unique solution in this case is found to be

$$\Gamma_2(\mu i)=\xi_{\mu i}, \quad [(\sin\sqrt{\Gamma_1\Gamma_2}/\sqrt{\Gamma_1\Gamma_2})^2\cdot\Gamma_1]_{i\mu}=\eta_{i\mu}. \tag{3·34}$$

The pair operators are represented by

$$\langle\varphi|a_\mu{}^\dagger b_i{}^\dagger|\psi\rangle=[\xi\cdot\sqrt{1-\eta\xi}\cdot(\arcsin\sqrt{\eta\xi}/\sqrt{\eta\xi})^{-1}]_{\mu i},$$

$$\langle\varphi|b_i a_\mu|\psi\rangle=[(\arcsin\sqrt{\eta\xi}/\sqrt{\eta\xi})\cdot\sqrt{1-\eta\xi}\cdot\eta]_{i\mu},$$

$$\langle\varphi|a_\mu{}^\dagger a_\nu|\psi\rangle=(\xi\eta)_{\mu\nu}, \qquad \langle\varphi|b_i{}^\dagger b_j|\psi\rangle=(\eta\xi)_{ji}. \tag{3·35}$$

Namely, the boson images of the particle-hole pair operators in this case become neither hermitian nor finitely expanded form. Therefore this case seems not so useful for applications.

It should be mentioned that the c-number images of particle-particle and hole-hole pair operators are simple bilinear forms of $\xi_{\mu i}$ and $\eta_{i\mu}$ in all three cases. This point as well as the proof of the uniqueness of the solutions is discussed in the Appendix.

§ 4. Dyson-type realization of the SCC method

In the previous section, we have clarified how to fix the CCS suitable for the non-unitary realization. We shall here proceed to investigating a feasible method to extract the collective submanifold by restricting the number of degrees of freedom to one pair; i.e., (ξ, η).

Among the three possibilities considered in § 3, Case (i) is already known. Case (iii) seems to have little merit to be developed further. Then we concentrate here on Case (ii).

First, the effect of the phase factor in Eq. (3·19), which depends on (ξ, η) in the non-unitary realization, is considered. The state vectors $|\psi_S\rangle$ and $\langle\varphi_S|$ with $S=S_{\rm II}$ are simply denoted by $|\psi\rangle$ and $\langle\varphi|$ in this section. The infinitesimal generators in the "collective direction" are defined by

$$\hat{O}_\xi|\psi\rangle=\frac{\partial}{\partial\eta}|\psi\rangle, \qquad \hat{O}_\eta|\psi\rangle=-\frac{\partial}{\partial\xi}|\psi\rangle, \tag{4·1}$$

so that

$$\hat{O}_\xi=\frac{\partial S}{\partial\eta}+\frac{\partial\hat{U}}{\partial\eta}\cdot\hat{U}^{-1}, \qquad \hat{O}_\eta=-\frac{\partial S}{\partial\xi}-\frac{\partial\hat{U}}{\partial\xi}\hat{U}^{-1}. \tag{4·2}$$

Since the first terms in Eq. (4·2) do not change $|\psi\rangle$ and $\langle\varphi|$ by their action, they play no role in the variational principle

$$\delta\langle\varphi|(\hat{H}-i\dot{\eta}\hat{O}_\xi+i\dot{\xi}\hat{O}_\eta)|\psi\rangle=0 \tag{4·3}$$

and in the weak CVC

$$\langle\varphi|[\hat{O}_\eta, \hat{O}_\xi]|\psi\rangle=1\,. \tag{4·4}$$

As is usual, the equations of motion for the collective coordinates (ξ, η) are derived from Eqs. (4·3) and (4·4):

$$i\dot{\eta}=\frac{\partial\mathcal{H}_D}{\partial\xi}\,,\qquad i\dot{\xi}=-\frac{\partial\mathcal{H}_D}{\partial\eta}\,. \tag{4·5}$$

Here the c-number image of a collective hamiltonian $\mathcal{H}_D$, which is not real, is defined by Eq. (3·10). The fact that the extra terms resulting from the phase-factor S have no effect on Eqs. (4·3) and (4·4) is just the invariance property of the CCS under the canonical transformation.

Thus, the basic equations of the SCC method turn into

$$\delta\langle\phi_0|e^{-\hat{S}}\left(\hat{H}-\frac{\partial\mathcal{H}_D}{\partial\xi}\cdot\frac{\partial}{\partial\eta}+\frac{\partial\mathcal{H}_D}{\partial\eta}\cdot\frac{\partial}{\partial\xi}\right)e^{\hat{S}}|\phi_0\rangle=0\,, \tag{4·6}$$

$$\langle\phi_0|\left[\frac{\partial\hat{Z}}{\partial\eta},\hat{Z}\right]|\phi_0\rangle=\xi\,,$$

$$\langle\phi_0|\left[\frac{\partial\hat{Z}}{\partial\xi},\hat{Z}\right]|\phi_0\rangle=-\eta\,, \tag{4·7}$$

where Eq. (4·5) is used, and the operator $\hat{S}$ is defined by Eq. (2·2) and $\hat{Z}$ by

$$\hat{Z}=\sum_{\mu i}\{F(i\mu)a_\mu{}^\dagger b_i{}^\dagger-G(\mu i)b_i a_\mu\} \tag{4·8}$$

with the definitions (3·27) of matrices F and G. The second equation (4·7) comes from the CVC equation (3·20) and Eq. (3·26) with ω_c replaced by

$$\omega_c=\frac{1}{2}(\xi\cdot d\eta-d\xi\cdot\eta)\,. \tag{4·9}$$

By using Eqs. (2·12) and (3·27), the matrices Γ_1 and Γ_2 appearing in the operator $\hat{S}$ can be represented to be

$$\Gamma_1=(1-GF)^{-1/2}\cdot\Gamma=F+\frac{2}{3}FGF+\frac{8}{15}FGFGF+\cdots\,,$$

$$\Gamma_2=\tilde{\Gamma}\cdot(1-GF)^{1/2}=G-\frac{1}{3}GFG-\frac{2}{15}GFGFG-\cdots \tag{4·10a}$$

with

$$\Gamma=F\cdot\arcsin\sqrt{GF}/\sqrt{GF}\,,\qquad \tilde{\Gamma}=\arcsin\sqrt{GF}/\sqrt{GF}\cdot G\,. \tag{4·10b}$$

Note that Γ in Eq. (4·10b) has the same form as in the unitary case ($\tilde{\Gamma}=\Gamma^\dagger$) if $C_1=C$ and $C_2=C^\dagger$ are used in place of F and G, respectively. The equations (4·6) and (4·7) are solved perturbatively for the unknown F and G by expanding them in the forms

$$F=\sum_{n=1}^{\infty}F^{(n)}\,,\qquad F^{(n)}(i\mu)=\sum_{r+s=n}f^{(r,s)}(i\mu)\cdot(\eta)^r(\xi)^s\,,$$

$$G=\sum_{n=1}^{\infty}G^{(n)}, \qquad G^{(n)}(\mu i)=\sum_{r+s=n}g^{(r,s)}(\mu i)\cdot(\eta)^r(\xi)^s \tag{4·11}$$

and correspondingly the operators $\hat{S}$ and $\hat{Z}$ are expanded in a similar way. Actually, the solutions $F^{(n)}$ and $G^{(n)}$ can be obtained in quite a way similar to in the case of the original SCC method.[1] In order to show this explicitly, we shall follow Ref. 8), where the method to solve the basic equations in the unitary realization is presented transparently.

The lowest order treatment is exactly the same as in the unitary case because of $\hat{S}^{(1)}=\hat{Z}^{(1)}$, leading to the RPA equation for the amplitudes $F^{(1)}(i\mu)$ and $G^{(1)}(\mu i)$. Therefore, the RPA eigenmode representation is more convenient than the particle-hole pair operator representation; we write

$$\hat{Z}=\sum_{\lambda}(F_\lambda\cdot\hat{X}_\lambda^\dagger-G_\lambda\cdot\hat{X}_\lambda), \tag{4·12}$$

where F_λ and G_λ are given by

$$F_\lambda=\mathrm{Tr}[x_\lambda^\dagger\cdot F-G\cdot y_\lambda^\dagger],$$
$$G_\lambda=\mathrm{Tr}[G\cdot x_\lambda-y_\lambda\cdot F] \tag{4·13}$$

with the definition of the RPA eigenmode operator

$$\hat{X}_\lambda^\dagger=\sum_{\mu i}\{x_\lambda(i\mu)a_\mu^\dagger b_i^\dagger-y_\lambda(\mu i)b_i a_\mu\}. \tag{4·14}$$

The higher orders of Eqs. (4·6) and (4·7) ($n\geqq 2$) can be written

$$\delta\langle\phi_0|\Big\{[\hat{H},\hat{Z}^{(n)}]-\Big(\frac{\partial\mathcal{H}_D{}^{(2)}}{\partial\xi}\frac{\partial}{\partial\eta}-\frac{\partial\mathcal{H}_D{}^{(2)}}{\partial\eta}\frac{\partial}{\partial\xi}\Big)\hat{Z}^{(n)}$$
$$-\Big(\frac{\partial\mathcal{H}_D{}^{(n+1)}}{\partial\xi}\frac{\partial}{\partial\eta}-\frac{\partial\mathcal{H}_D{}^{(n+1)}}{\partial\eta}\frac{\partial}{\partial\xi}\Big)Z^{(1)}\Big\}|\phi_0\rangle=\delta\langle\phi_0|\hat{D}^{(n)}|\phi_0\rangle, \tag{4·15}$$

$$\langle\phi_0|\Big\{\Big[\frac{\partial\hat{Z}^{(n)}}{\partial\eta},\hat{Z}^{(1)}\Big]+\Big[\frac{\partial\hat{Z}^{(1)}}{\partial\eta},\hat{Z}^{(n)}\Big]\Big\}|\phi_0\rangle=2C_\xi{}^{(n)},$$
$$\langle\phi_0|\Big\{\Big[\frac{\partial\hat{Z}^{(n)}}{\partial\xi},\hat{Z}^{(1)}\Big]+\Big[\frac{\partial\hat{Z}^{(1)}}{\partial\xi},\hat{Z}^{(n)}\Big]\Big\}|\phi_0\rangle=-2C_\eta{}^{(n)} \tag{4·16}$$

with

$$\hat{D}^{(n)}=\hat{B}^{(n)}-[\hat{H},(\hat{S}^{(n)}-\hat{Z}^{(n)})]$$
$$+\Big(\frac{\partial\mathcal{H}_D{}^{(2)}}{\partial\xi}\frac{\partial}{\partial\eta}-\frac{\partial\mathcal{H}_D{}^{(2)}}{\partial\eta}\frac{\partial}{\partial\xi}\Big)(\hat{S}^{(n)}-\hat{Z}^{(n)}), \tag{4·17}$$

$$C_\eta{}^{(n)}=\frac{1}{2}\sum_{k=2}^{n-1}\langle\phi_0|\Big[\frac{\partial\hat{Z}^{(n+1-k)}}{\partial\xi},\hat{Z}^{(k)}\Big]|\phi_0\rangle, \qquad C_\eta{}^{(2)}=0,$$
$$C_\xi{}^{(n)}=-\frac{1}{2}\sum_{k=2}^{n-1}\langle\phi_0|\Big[\frac{\partial\hat{Z}^{(n+1-k)}}{\partial\eta},\hat{Z}^{(k)}\Big]|\phi_0\rangle, \qquad C_\xi{}^{(2)}=0. \tag{4·18}$$

The explicit form of $\hat{B}^{(n)}$ is not given here,[8] but it is easily calculated by the well-known formula

$$e^{-\hat{S}}\hat{A}e^{\hat{S}}=\sum_{n=0}^{\infty}\frac{1}{n!}[\cdots[\hat{A},\hat{S}],\cdots\hat{S}],$$

and expressed only by $\mathcal{H}_D{}^{(m)}$ and $\hat{S}^{(m)}$ with $m\leqq n-1$. It should be noticed from Eq. (4·10) that the quantity $\hat{S}^{(n)}-\hat{Z}^{(n)}$ contains only $\hat{Z}^{(m)}$ with $m\leqq n-2$. Therefore $C_\eta{}^{(n)}$, $C_\xi{}^{(n)}$ and $\hat{D}^{(n)}$ in Eqs. (4·15) and (4·16) can be calculated by using quantities known already in the lower order of iterations.

Thus, by choosing the simple boundary condition*)

$$F_\lambda{}^{(1)}=\delta_{\lambda\lambda_0}\cdot\eta\,,\qquad G_\lambda{}^{(1)}=\delta_{\lambda\lambda_0}\cdot\xi \tag{4·19}$$

and

$$\mathcal{H}_D{}^{(2)}=\omega_{\lambda_0}\cdot\xi\eta\,, \tag{4·20}$$

the n-th order solutions are obtained explicitly[8] to be

$$F_{\lambda_0}^{(n)}=C_\eta{}^{(n)}-\frac{1}{n-1}\frac{\partial}{\partial\xi}(\xi C_\eta{}^{(n)}-\eta C_\xi{}^{(n)})\,,$$

$$G_{\lambda_0}^{(n)}=C_\xi{}^{(n)}+\frac{1}{n-1}\frac{\partial}{\partial\eta}(\xi C_\eta{}^{(n)}-\eta C_\xi{}^{(n)}) \tag{4·21}$$

and

$$F_\lambda{}^{(n)}=(\omega_{\lambda_0}-\mathring{D})^{-1}\cdot B_\lambda{}^{(n)}\,,$$

$$G_\lambda{}^{(n)}=(\omega_{\lambda_0}+\mathring{D})^{-1}\cdot A_\lambda{}^{(n)}\,,\qquad (\lambda\neq\lambda_0) \tag{4·22}$$

where the operator $\mathring{D}$ acting on the polynomials of ξ and η is defined by

$$\mathring{D}=\frac{\partial\mathcal{H}_D{}^{(2)}}{\partial\xi}\frac{\partial}{\partial\eta}-\frac{\partial\mathcal{H}_D{}^{(2)}}{\partial\eta}\frac{\partial}{\partial\xi}=\omega_{\lambda_0}\left(\eta\frac{\partial}{\partial\eta}-\xi\frac{\partial}{\partial\xi}\right) \tag{4·23}$$

and

$$B_\lambda{}^{(n)}=\langle\phi_0|[\hat{X}_\lambda,\hat{D}^{(n)}]|\phi_0\rangle\,,$$

$$A_\lambda{}^{(n)}=\langle\phi_0|[\hat{D}^{(n)},\hat{X}_\lambda{}^\dagger]|\phi_0\rangle\,. \tag{4·24}$$

Once $\hat{Z}$ is obtained, the c-number images of an arbitrary one-body operator can be calculated by those of pair operators which is given in Eq. (3·30) with replacing $\xi_{\mu i}$ and $\eta_{i\mu}$ by $G(\mu i)$ and $F(i\mu)$, respectively. It is worth mentioning that the solution is reduced to $\hat{Z}=\hat{Z}^{(1)}$, i.e., $\hat{Z}^{(n)}=0$ $(n\geqq2)$, if the mode-mode coupling is neglected, as it is shown from Eq. (4·18) (see also the Appendix). Consequently, as has been pointed out in I, the collective hamiltonian ends up with a finitely expanded form. This is the merit of the Dyson-type realization.

Finally, let us summarize how to modify the (η,η^*)-expansion technique established in the original version to be suitable for the Dyson-type realization:
1) Attach the extra terms (the second and third terms in Eq. (4·17)) to the imhomogeneous term on the right-hand side of the equation of collective path, Eq. (4·15).
2) Use the simplified $C^{(n)}$'s given by Eq. (4·18) in the CVC equation (4·16).

*) As for the general boundary condition suitable for quantization, see Refs. 8) and 9).

3) Make good use of Eq. (4·10) for calculating $\hat{S}^{(m)}$ with $m \leqq n-1$; i.e., for expressing Γ_1 and Γ_2 in terms of F and G.

At the end of this section, it should be pointed out that the method to solve the basic equations and all the formulae derived above can equally be applied to those in the unitary realization by setting

$$\xi = \eta^*, \quad F = C(=C_1), \quad G = C^\dagger(=C_2), \tag{4·25}$$

$$\Gamma_1 = \Gamma, \quad \Gamma_2 = \Gamma^\dagger(=\hat{\Gamma}) \tag{4·26}$$

and expanding the matrix C by (η, η^*) like Eq. (4·11). Correspondingly, the following identities hold:

$$\mathcal{H}_D = \mathcal{H}_D^*, \quad C_\xi^{(n)} = C_\eta^{(n)*},$$
$$\hat{D}^{(n)} = \hat{D}^{(n)\dagger}, \quad A_\lambda^{(n)} = B_\lambda^{(n)*}. \tag{4·27}$$

If the mode-mode coupling is neglected, this method to solve the basic equations for the unitary realization leads to $C = C^{(1)} = \delta_{\lambda\lambda_0} \cdot \eta$ and the c-number hamiltonian of the Holstein-Primakoff type. Notice that this result of the "truncated approximation" does not necessarily coincide with that of Refs. 1) and 8) in which the matrix Γ is expanded rather than C, especially when the closed-algebra approximation is not used and/or the single-particle energies are not degenerate.[9]

§ 5. Concluding remarks

Based on the exponential form of a Slater determinant, the non-unitary realization of the selfconsistent collective-coordinate method has been investigated. In order to describe a state vector which is not normalized to unity, a pair of matrices Γ_1 and Γ_2, and consequently the canonical variables (ξ, η), have been introduced. At first sight, the introduction of two complex variables seems to make the number of degrees of freedom for parametrizing the TDHF manifold double. This is not the case, however. As has been shown in § 3, the classical image of an arbitrary observable is expressed only by $\xi_{i\mu}$ and $\eta_{\mu i}$: The representations in terms of (ξ, η) and of (η^*, ξ^*) are decoupled and equivalent to each other. Actually, the weak CVC tells us that $(\xi_{\mu i}, \eta_{i\mu})$ or $(\eta^*_{i\mu}, \xi^*_{\mu i})$ in the "conjugate representation", are the classical image of boson operators $(\boldsymbol{b}^\dagger_{\mu i}, \boldsymbol{b}_{\mu i})$ in the non-unitary realization. A similar situation, i.e., operators corresponding to $\boldsymbol{b}^\dagger_{\mu i}$ and $\boldsymbol{b}_{\mu i}$ are not hermite conjugate of each other, also occurs in the formulation of the Dyson-type boson expansion theory with the use of the generator coordinate method[11] or the generalized coherent state.[12] We have shown that the canonical description of the TDHF theory can straightforwardly be extended to the non-unitary realization. It is clarified, furthermore, that different types of realizations, including the original one of the Holstein-Primakoff type [1),6),7)] and the newly proposed one of the Dyson type,[2] correspond to different choices of the arbitrary "gauge-fixing" function S appearing in the general form of the CVC.[4]

Moreover, it has been shown that the (η, η^*)-expansion technique,[1),8)] which is a powerful method to solve the equation of collective path, can also be applied for the non-unitary version with slight modifications. It should be stressed that the collective hamiltonian obtained in the Dyson-type realization results in a finite order polynomial with respect to the collective parameters if the mode-mode coupling is neglected. Therefore the dynamical-coupling effect can be examined in a more transparent manner.

Recently, Matsuo extended the SCC method so as to restore the number conservation in the quasiparticle description of superconducting nuclei.[8] This number conserving-treatment is important in realistic applications. Although not explicitly shown in this paper, it is apparent that the Dyson type version can be formulated in terms of the quasiparticle representation and the method of Ref. 8) can be equally incorporated. Thus, we can say that the non-unitary realization of the SCC method has been brought up to the same level of applicability to realistic problems as the unitary version.[9]

Acknowledgements

Helpful and stimulating discussions with Dr. M. Matsuo are greatly acknowledged.

Appendix

In this appendix, we discuss the uniqueness of the solution of the canonical-variable condition.

First let us prove the uniqueness for the "standard form" defined by

$$\omega_{\mathrm{STD}}=\frac{1}{2}\mathrm{Tr}[A\cdot dB-dA\cdot B]\,, \qquad (\mathrm{A}\cdot 1)$$

where $A(\mu i)$ and $B(i\mu)$ are matrix-functions of $(\xi_{\mu i},\ \eta_{i\mu})$. Substituting Eq. (A·1) into Eq. (3·20), we have partial differential equations:

$$\mathrm{Tr}\left[A\cdot\frac{\partial B}{\partial\eta_{i\mu}}-\frac{\partial A}{\partial\eta_{i\mu}}\cdot B\right]=\xi_{\mu i}\,,$$

$$\mathrm{Tr}\left[A\cdot\frac{\partial B}{\partial\xi_{\mu i}}-\frac{\partial A}{\partial\xi_{\mu i}}\cdot B\right]=-\eta_{i\mu}\,. \qquad (\mathrm{A}\cdot 2)$$

What should be shown is that the solution of Eq. (A·2) is unique and is given by

$$A(\mu i)=\xi_{\mu i}\,,\qquad B(i\mu)=\eta_{i\mu}\,, \qquad (\mathrm{A}\cdot 3)$$

under the condition that A and B are the *analytic* functions of $(\xi_{\mu i},\ \eta_{i\mu})$ at $\xi_{\mu i}=\eta_{i\mu}=0$.

The proof is given by expanding A and B as

$$A=\sum_n A^{(n)}\,,\qquad B=\sum_n B^{(n)}\,, \qquad (\mathrm{A}\cdot 4)$$

where $A^{(n)}$ and $B^{(n)}$ are the n-th order homogeneous polynomials with respect to their arguments $(\xi_{\mu i},\ \eta_{i\mu})$. Notice that the expansion starts from $n=0$ due to the analyticity requirement. Moreover, using the freedom of the linear symplectic transformation, we can assume, without loss of generality that $A^{(0)}=B^{(0)}=0$, and $A^{(1)}$ and $B^{(1)}$ are functions of only $\xi_{\mu i}$ and of $\eta_{i\mu}$, respectively. Thus we obtain

$$A^{(1)}(\mu i)=\xi_{\mu i}\,, \qquad B^{(1)}(i\mu)=\eta_{i\mu}\,. \tag{A·5}$$

Substitution of Eq. (A·5) into Eq. (A·2) leads to

$$A^{(n)}(\mu i)+\mathrm{Tr}\left[\xi\cdot\frac{\partial B^{(n)}}{\partial\eta_{i\mu}}-\frac{\partial A^{(n)}}{\partial\eta_{i\mu}}\cdot\eta\right]=2\cdot C_{\xi}{}^{(n)}(\mu i)\,,$$

$$B^{(n)}(i\mu)-\mathrm{Tr}\left[\xi\cdot\frac{\partial B^{(n)}}{\partial\xi_{\mu i}}-\frac{\partial A^{(n)}}{\partial\xi_{\mu i}}\cdot\eta\right]=2\cdot C_{\eta}{}^{(n)}(i\mu) \tag{A·6}$$

for the higher order equations ($n\geqq 2$). Here $C_{\xi}{}^{(n)}$ and $C_{\eta}{}^{(n)}$ are defined by

$$C_{\eta}{}^{(n)}(i\mu)=\frac{1}{2}\sum_{k=2}^{n-1}\mathrm{Tr}\left[A^{(k)}\cdot\frac{\partial B^{(n+1-k)}}{\partial\xi_{\mu i}}-\frac{\partial A^{(n+1-k)}}{\partial\xi_{\mu i}}\cdot B^{(k)}\right],$$

$$C_{\xi}{}^{(n)}(\mu i)=-\frac{1}{2}\sum_{k=2}^{n-1}\mathrm{Tr}\left[A^{(k)}\cdot\frac{\partial B^{(n+1-k)}}{\partial\eta_{i\mu}}-\frac{\partial A^{(n+1-k)}}{\partial\eta_{i\mu}}\cdot B^{(k)}\right]. \tag{A·7}$$

By using the identity[8)]

$$2\cdot\mathrm{Tr}[\xi\cdot C_{\eta}{}^{(n)}-C_{\xi}{}^{(n)}\cdot\eta]=(n-1)\cdot\mathrm{Tr}[A^{(n)}\cdot\eta-\xi\cdot B^{(n)}]\,, \tag{A·8}$$

which is obtained from Eq. (A·6) by the Euler theorem for homogeneous polynomials, the solution of Eq. (A·6) is given by

$$A^{(n)}(\mu i)=C_{\xi}{}^{(n)}(\mu i)+\frac{1}{n-1}\frac{\partial}{\partial\eta_{i\mu}}\mathrm{Tr}[\xi\cdot C_{\eta}{}^{(n)}-C_{\xi}{}^{(n)}\cdot\eta]\,,$$

$$B^{(n)}(i\mu)=C_{\eta}{}^{(n)}(i\mu)-\frac{1}{n-1}\frac{\partial}{\partial\xi_{\mu i}}\mathrm{Tr}[\xi\cdot C_{\eta}{}^{(n)}-C_{\xi}{}^{(n)}\cdot\eta]\,. \tag{A·9}$$

Noticing that $C_{\eta}{}^{(2)}=C_{\xi}{}^{(2)}=0$, and $C_{\eta}{}^{(n)}$ and $C_{\xi}{}^{(n)}$ are expressed only by $A^{(m)}$ and $B^{(m)}$ with $2\leqq m\leqq n-1$, we obtain

$$A^{(n)}(\mu i)=B^{(n)}(i\mu)=0\,. \qquad (n\geqq 2) \tag{A·10}$$

This completes the proof. The uniqueness of the solutions for Cases (i)~(iii) considered in § 3 is deduced by setting

$$A=C_2\,, \qquad B=C_1 \qquad \text{for Case (i)}\,,$$

$$A=G=Z_2\,, \qquad B=F=(1+Z_1Z_2)^{-1}\cdot Z_1 \qquad \text{for Case (ii)}\,,$$

$$A=\Gamma_2\,, \qquad B=(\sin\sqrt{\Gamma_1\Gamma_2}/\sqrt{\Gamma_1\Gamma_2})^2\cdot\Gamma_1 \qquad \text{for Case (iii)}\,. \tag{A·11}$$

Now, the reason why the c-number images of the particle-particle and hole-hole pair operators take simple forms in all three cases is clear, because they are expressed by using Eqs. (2·16) and (2·17) as

$$\langle\varphi|a_{\mu}{}^{\dagger}a_{\nu}|\psi\rangle=(A\cdot B)_{\mu\nu}\,, \qquad \langle\varphi|b_i{}^{\dagger}b_j|\psi\rangle=(B\cdot A)_{ji}\,. \tag{A·12}$$

Here let us add a remark: The "conjugate representation", referred to in § 3, of the c-number image of pair operators is obtained by taking complex conjugate of all equations in § 3. For example in Case (ii),

$$\langle\psi|a_\mu{}^\dagger b_i{}^\dagger|\varphi\rangle=\eta^*_{i\mu}\,,\qquad \langle\psi|b_i a_\mu|\varphi\rangle=(\xi^*-\xi^*\eta^*\xi^*)_{\mu i}\,,$$
$$\langle\psi|a_\mu{}^\dagger a_\nu|\varphi\rangle=(\xi^*\cdot\eta^*)_{\nu\mu}\,,\qquad \langle\psi|b_i{}^\dagger b_j|\varphi\rangle=(\eta^*\cdot\xi^*)_{ij} \tag{A·13}$$

and now $\eta^*_{i\mu}$ and $\xi^*_{\mu i}$ are identified with the bosons $\boldsymbol{b}^\dagger_{\mu i}$ and $\boldsymbol{b}_{i\mu}$, respectively.

Next, it is instructive to consider the simple case of $SU(2)$ algebra ($\hat{J}_+$, $\hat{J}_-$, $\hat{J}_z$) because, in this case, a general solution is known.[2] Choosing the Thouless form and a rather wide class of S with arbitrary parameters a and $\boldsymbol{k}$

$$S=\frac{1}{2}a\xi\eta+(k-1)\log N\,,\qquad N=\langle\phi_0|e^{\hat{Z}_2}e^{\hat{Z}_1}|\phi_0\rangle\,, \tag{A·14}$$

it is shown in I that a complete solution parametrized by complex numbers (separation constants) λ and K is given by

$$Z_1=K\cdot(\eta)^{\lambda(1-a)}\cdot(\xi)^{-\lambda(1+a)}(\xi\eta/(2\lambda-c\cdot\xi\eta))^k\,,$$
$$Z_2=\frac{1}{K}\cdot(\eta)^{-\lambda(1-a)}\cdot(\xi)^{\lambda(1+a)}(\xi\eta/(2\lambda-c\cdot\xi\eta))^{1-k}\,. \tag{A·15}$$

Here c is related to the rank of the representation of $SU(2)$ algebra, and is fixed by the starting state $|\phi_0\rangle$, $c=\pm1/2J$. It is easy to see that the analyticity requirement restricts the values of parameters λ, k and a such as

$$\lambda=\pm\frac{1}{2}\,,\qquad 1+a=\pm2k\qquad \text{for } c=\pm1/2J\,. \tag{A·16}$$

Thus the solution allowed by the analyticity requirement leads*) to

$$\langle\varphi|\hat{J}_+|\psi\rangle=\xi\cdot(2J-\xi\eta)^k\,,$$
$$\langle\varphi|\hat{J}_-|\psi\rangle=(2J-\xi\eta)^{1-k}\cdot\eta\qquad \text{for } \lambda=+1/2 \tag{A·17}$$

with only one free parameter k, and for $\lambda=-1/2$, it leads to the same result but ξ and η interchanged. Although this example is very simple, it gives us a feeling of how the choice of S and the analyticity requirement restrict the possible representation of the pair operators in terms of the canonical coordinates.

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*) Here the physically irrelevant parameter K is set $c^{k-1/2}$. This choice corresponds to the special linear canonical transformation of scaling type,

$$\eta\to K\cdot\eta\,,\qquad \xi\to K^{-1}\cdot\xi\,.$$

A similar treatment has been done in Eq. (A·5).

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