Resonating Hartree-Bogoliubov Theory
for a Superconducting Fermion System with Large Quantum Fluctuations

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We develop a general theory to describe a superconducting Fermion system with large quantum fluctuations. The theory is a direct extension of the resonating Hartree-Fock (HF) theory to the Hartree-Bogoliubov case including pair correlations. We start with an exact coherent state representation of a superconducting Fermion system on a special orthogonal group. A state with large quantum fluctuations is approximated by a superposition of non-orthogonal Hartree-Bogoliubov (HB) wave functions with different correlation structures. We obtain the variational equations to determine the coefficients of configuration mixing and the orbitals in the resonating HB wave functions.

§ 1. Introduction

Fermion systems with large quantum fluctuations give us difficult many-body problems. To approach such problems, one of the authors has developed a new theory called the resonating Hartree-Fock (Res HF) and resonating HF random phase approximations (Res HF RPA). Some of such Fermion systems, however, are superconducting and the theory cannot be directly applied. In this and a following paper, we extend the theory to cover superconducting systems developing a theory called the Res Hartree-Bogoliubov (HB) and Res HB RPA approximations. A typical superconducting Fermion system to which the theory may be applied is a transitional nucleus.

In a Fermion system with small quantum fluctuations, the ground state can be well approximated by a mean field, namely the HF or HB, wave function. Quantum fluctuations are given by small amplitude harmonic oscillations of orbitals around the mean field minimum in the energy functional surface. Such fluctuations and the collective excitations due to them can be well described by the RPA. If the energy functional surface has a large anharmonicity in its low energy portion, then non-linear couplings between RPA excitation modes, so-called mode-mode couplings, become important in fluctuations. The ground state, however, may remain describable by a perturbative correction of the mean field wave function. The boson expansion theory may be suitable to describe such an anharmonicity.

If the anharmonicity in the energy functional surface is so big that the surface has multiple low energy minima, then the situation becomes essentially different. The ground state turns out to be unable to be approximated by a single mean field wave function. It becomes a superposition of multiple mean field wave functions, namely it is resonating between different correlation structures. If the ground state has such a resonating character, any perturbative approach starting from a reference mean field wave function is no more valid. The existence of the resonating ground state
was first demonstrated for a small diatomic molecule, carbon mono-oxide (CO). The ground state wave function of CO at large interatomic distances can never be approximated by a HF wave function but is well approximated by a superposition of two HF wave functions with close energies but with different correlation structures. Such a resonance may be present in transitional nuclei as suggested by the coexistence of different deformed shapes in a mean field model and the presence of superdeformations.

In this paper, we develop a new theory, the Res HB theory, to describe a superconducting Fermion system with the resonating ground state. Development of the theory can be made in a quite parallel manner to the Res HF theory. This paper is organized as follows. In § 2, we briefly describe an exact coherent state representation (CS rep) of a superconducting Fermion system on an $SO(2N)$ group (special orthogonal group of $2N$ dimensions) that is a special case of the CS rep on a Lie group. It is an integral representation of a state vector on the $SO(2N)$ group, so that it makes possible global approaches to the many-body problem. In § 3, we introduce a density matrix, called the interstate density matrix, which depends on two non-orthogonal HB wave functions. We derive in terms of it an exact expression of the Schrödinger equation in the $SO(2N)$ CS rep which shows a close connection of the exact Hamiltonian with the HB energy functional. In § 4, we approximate the integration in the $SO(2N)$ CS rep by a discrete superposition of non-orthogonal HB wave functions and derive an approximation called the Res HB approximation. We derive the variational equations for the coefficients of configuration mixing and the orbitals of each HB wave function. In § 5, we discuss the Peierls-Yoccoz projection of a Res HB wave function which is a special case of resonance for a broken symmetry Goldstone mode. In § 6, we give concluding remarks.

§ 2. $SO(2N)$ coherent state representation of a Fermion system

First, let us briefly recapitulate here the exact CS rep on an $SO(2N)$ group of a superconducting Fermion system, according to Ref. 7). We now consider a Fermion system with $N$ single particle states. Let $c_a$ and $c_a^\dagger$, $a=1, 2, \ldots, N$, be the annihilation and creation operators of the Fermion. Owing to their anticommutation relations, the pair operators

\[
\begin{align*}
E_{ab}^* &= c_a^\dagger c_b, \\
n E_{ab} &= c_a c_b, \\
n E_{\alpha\beta} &= c_\alpha^\dagger c_\beta^\dagger \nonumber
\end{align*}
\]

satisfy the commutation relations of the $SO(2N)$ Lie algebra. They generate an $SO(2N)$ canonical transformation $U(g)$, which induces the generalized Bogoliubov transformation specified by an $SO(2N)$ matrix $g$ as follows:

\[
U(g)(c, c^\dagger)U^\dagger(g)=(c, c^\dagger)g, \quad g \equiv \begin{bmatrix} a & b^* \\ b & a^* \end{bmatrix}, \quad g^\dagger g = gg^\dagger = 1.
\]
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\[ U(g)U(g') = U(gg'), \quad U(g^{-1}) = U^*(g), \quad U(1) = 1, \]  

where the \((c, c')\) is the \(2N\) dimensional row vector \((\langle c_a\rangle, \langle c'_a\rangle)\) and the \(a = (a^*_a)\) and \(b = (b_a)\) are \(N \times N\) matrices, respectively.

\(U(g)\) is an irreducible representation (irrep) of the \(SO(2N)\) group on the Hilbert space \(\mathbb{H}_e\) of even Fermion numbers. From this and the orthogonality of irrep matrices, a state vector in \(\mathbb{H}_e\) can be represented as

\[ |\Psi\rangle = 2^{N-1} \int U(g)|0\rangle \langle 0| U^*(g)|\Psi\rangle dg = 2^{N-1} \int |g\rangle \langle \Psi|U(g)dg, \]  

where the integration is the group integration on \(SO(2N)\). \(|0\rangle\) is the vacuum satisfying \(c_a|0\rangle = 0\), \(|g\rangle = U(g)|0\rangle\) is a HB wave function and \(\Psi(g) = \langle 0|U^*(g)|\Psi\rangle\). The factor \(2^{N-1}\) is the dimension of \(\mathbb{H}_e\). This is the \(SO(2N)\) CS rep of a state vector. It is an exact representation. It was first derived by Janssen et al.\(^{11}\) without noticing its group theoretical background as a generalization of the generator coordinate method (GCM).\(^{12,13}\)

We define the overlap integral \(\langle g|g'\rangle\) by

\[ \langle g|g'\rangle = \langle 0|U^*(g)U(g')|0\rangle = \langle 0|U(g^*g')|0\rangle. \]  

By using Eq. (2.4), the Schrödinger equation \((H - E)|\Psi\rangle = 0\) can be converted to an integral equation on the \(SO(2N)\) group

\[ \int \langle g|H|g'\rangle - E\langle g|g'\rangle \Psi(g')dg' = 0, \]  

\[ \langle g|H|g'\rangle = \langle 0|U^*(g)HU(g')|0\rangle. \]  

§ 3. The interstate density matrix and the Schrödinger equation in the \(SO(2N)\) CS rep

To get the explicit expression of the Schrödinger equation in the \(SO(2N)\) CS rep, we must calculate the overlap integral and the matrix element of the Hamiltonian between non-orthogonal HB wave functions. These quantities were already calculated\(^{14,13}\) in connection with the GCM. From \(\langle 0|U(g)|0\rangle = [\det a]^{1/2}\), where det is determinant, and Eqs. (2.5) and (2.2), we have

\[ \langle g|g'\rangle = [\det(a^*a' + b^*b')^{1/2} = [\det z]^{1/2}, \]  

\[ z = u^*u', \quad z = (z_{ij}), \]  

where we introduce a \(2N \times N\) isometric matrix \(u\) by

\[ u = \begin{bmatrix} b \\ a \end{bmatrix}, \quad u^*u = 1, \]  

so that \(z\) is an \(N \times N\) matrix.

Now let us introduce the following \(2N \times 2N\) matrix
\[ W(g, g') = U' z^{-1} u' \quad R(g, g') = b' z^{-1} b' \quad K(g, g') = b' z^{-1} a' \]

which obviously satisfies the idempotency condition and is hermitian as an integral operator on SO(2N)

\[ W^2(g, g') = W(g, g'), \quad \text{and} \quad W^*(g, g') = W(g', g) * W(g, g'). \]

The matrix \( W(g, g') \) is a natural extension of the interstate density matrix introduced in the \( U(N) \) CS rep to the \( SO(2N) \) CS rep. We call it the HB interstate density matrix. The submatrices \( R \) and \( K \) were called transition densities. They have the properties

\[ R^*(g, g') = R(g', g), \quad K^T(g, g') = -K(g, g'). \]

The matrix elements of the pair operators (2.1) and a two-body operator between two HB wave functions are calculated as follows:

\[ \langle g | E_{\beta \sigma} + \frac{1}{2} \delta_{\beta \sigma} | g' \rangle = R_{\beta \sigma}(g, g') \cdot [\text{det} z]^{1/2}, \quad (3.6) \]
\[ \langle g | E_{\beta \sigma} | g' \rangle = K_{\beta \sigma}(g, g') \cdot [\text{det} z]^{1/2}, \quad (3.7) \]
\[ \langle g | E_{\sigma \tau}^2 E_{\beta \sigma} | g' \rangle = \{ R_{\beta \sigma}(g, g') R_{\sigma \tau}(g, g') - R_{\beta \sigma}(g, g') R_{\tau \sigma}(g, g') \}
- K_{\sigma \tau}^*(g', g) K_{\beta \sigma}(g, g') \cdot [\text{det} z]^{1/2}. \quad (3.8) \]

New derivations of these formulas are given in the Appendix.

Let the Hamiltonian of the system be

\[ H = h_{\alpha \sigma} \left( E_{\beta \sigma} + \frac{1}{2} \delta_{\beta \sigma} \right) + \frac{1}{4} \{ a_{\beta} [\gamma \delta] E_{\tau \sigma}^* E_{\beta \sigma} \}, \quad (3.9) \]

We use the dummy index convention to take summation over the repeated indices. Using Eqs. (3.6) and (3.8), the Hamiltonian matrix element in the \( SO(2N) \) CS rep can be expressed in terms of the HB interstate density matrix and the overlap integral as

\[ \langle g | H | g' \rangle = H \left[ W(g, g') \right] \cdot [\text{det} z]^{1/2}, \quad (3.10a) \]
\[ H \left[ W(g, g') \right] = h_{\beta \sigma} R_{\beta \sigma}(g, g') \]
\[ + \frac{1}{2} \{ a_{\beta} [\gamma \delta] \left( R_{\beta \sigma}(g, g') R_{\sigma \tau}(g, g') - \frac{1}{2} K_{\sigma \tau}^*(g', g) K_{\beta \sigma}(g, g') \right) \}. \quad (3.10b) \]

We note that \( H \left[ W \right] \) has the same form as the HB energy functional except that the interstate density matrix is used instead of the HB one. Then from Eqs. (3.1) and (3.10), we get the explicit expression of the integral Schrödinger equation (2.6) in the
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SO(2N) CS rep as

$$\int [H(W(g, g') - E) \cdot [\text{det} z]^{1/2} \Psi(g') dg' = 0, \ z = u^t u'. \quad (3\cdot11)$$

We note that this is an exact integral rep of the Schrödinger equation.

We finally introduce an operator called the interstate Fock-Bogoliubov (FB) operator

$$\mathcal{F}(g, g') = \begin{pmatrix} F(g, g') & D(g, g') \\ -D^*(g', g) & -F^*(g', g) \end{pmatrix}, \quad (3\cdot12a)$$

where the matrix elements of $F(g, g')$ and $D(g, g')$ are defined as

$$F_{ab}(g, g') = \frac{\delta H(W(g, g'))}{\delta R_{ba}(g, g')} = h_{ab} + [a \beta | \gamma \delta] R_{ar}(g, g'), \quad (3\cdot12b)$$

$$D_{ab}(g, g') = \frac{\delta H(W(g, g'))}{\delta K_{ba}(g, g')} = -\frac{1}{2}[a \gamma | \beta \delta] K_{ar}(g, g').$$

§ 4. Resonating Hartree-Bogoliubov approximation

Up to the present stage, the theory has been developed exactly. We are now in the stage to introduce an approximation to solve the integral Schrödinger equation (3·11). We derive here a new approximation called the Res HB approximation in a quite parallel manner to the Res HF one.

We approximate a low energy eigenstate $|\Psi\rangle$ of $H$ by a discrete superposition of the HB wave functions which are denoted by $|g_r\rangle$, $|g_s\rangle...$. The $|g_r\rangle$'s are non-orthogonal and represent different collective correlation states. Hereafter we do not use the summation convention over the repeated Latin indices numbering the HB wave functions. Then the state $|\Psi\rangle$ is approximated as

$$|\Psi\rangle = \sum_r |g_r\rangle c_r. \quad (4\cdot1)$$

Here we consider such a situation that the HB energy functional has multiple low energy local minima. We use the HB states of the local minima as a trial of the $|g_s\rangle$'s. Then the wave function (4·1) represents a resonance of the HB states. This is a saddle points type approximation for the SO(2N) CS rep. We determine variationally not only the mixing coefficients $c_r$ but also optimize the HB wave functions $|g_r\rangle$.

The $z$ matrix and the HB interstate density matrix between $|g_r\rangle$ and $|g_s\rangle$ are, respectively, denoted as

$$z_{rs} = u^t u_s, \ W_{rs} = u_s z_{rs}^{-1} u^t. \quad (4\cdot2)$$

The $|g_r\rangle$'s are usually non-orthogonal and the mixing coefficients $c_r$ in (4·1) are normalized by

$$\langle \Psi | \Psi \rangle = \sum_r \langle g_r | g_s \rangle c_r^* c_s = \sum_r [\text{det} z_{rs}]^{1/2} c_r^* c_s = 1. \quad (4\cdot3)$$

The expectation value of the Hamiltonian $H$ by the state $|\Psi\rangle$ is given from Eq. (3·10)
In order to determine the \( |g_r\rangle \)'s and \( c_r \)'s by the variational method, we adopt the following Lagrangian with the Lagrange multiplier term to secure the normalization condition (4·3):

\[
L = \langle \Psi | H | \Psi \rangle - E \langle \Psi | H | \Psi \rangle = \sum_{rs} [H[ W_{rs} ] - E] [\det \rho_{rs}]^{1/2} c_r^* c_s .
\]

Since \( \rho_{rs} \) and \( W_{rs} \) have the same structures as those in the Res HF case except for the difference in the dimension, the variation of (4·5) can be performed in a quite parallel manner to the Res HF theory. We do not write details of derivations for such parallel cases.

From the variation of \( L \) with respect to \( c_r^* \) we get the equation to determine the mixing coefficients \( c_s \)

\[
\sum_{s} [H[ W_{rs} ] - E] [\det \rho_{rs}]^{1/2} c_s = 0 .
\]

We call the above equation the Res HB CI (configuration interaction) equation according to the usual terminology of quantum chemistry, though in that of nuclear physics it should be called the Res HB configuration mixing equation.

Next we derive the variational equation to determine the HB amplitudes \( a_r \) and \( b_r \), i.e., the matrices \( u_r \). The variations of the HB interstate density matrix \( W \) and the overlap integral \( [\det \rho]^{1/2} \) are given by

\[
\delta W = D(1-W) + (1-W) \bar{D} , \quad D = u' \rho^{-1} \delta u^* , \quad \bar{D} = \delta u' \rho^{-1} u^* .
\]

\[
\delta [\det \rho]^{1/2} = \frac{1}{2} \text{Tr} (D + \bar{D}) [\det \rho]^{1/2} .
\]

We get also

\[
\delta [H[ W(g, g')]] = \frac{1}{2} \text{Tr} [\mathcal{F}(g, g') \delta W(g, g')] .
\]

Writing \( \mathcal{L} = [H[ W ] - E] [\det \rho]^{1/2} \), then from Eqs. (4·7)~(4·9), the variation \( \delta \mathcal{L} \) is

\[
\delta \mathcal{L} = \frac{1}{2} \text{Tr} [((1-W) \mathcal{F} + H - E)D + \bar{D}(1-W) + H - E)] [\det \rho]^{1/2} .
\]

Since \( L = \sum_{rs} \mathcal{L}_{rs} c_r^* c_s \), from Eq. (4·10), we obtain the variation equation to determine the \( u_r \)'s as

\[
\sum_{s} \mathcal{K}_{rs} c_s = 0 , \quad \mathcal{K}_{rs} = [(1-W_{rs}) \mathcal{F}[ W_{rs} ] + H[ W_{rs} ] - E] W_{rs} [\det \rho_{rs}]^{1/2} .
\]

We call the above equation the Res HB equation. As shown in the Res HF theory, the Res HB CI equation (4·6) can also be derived from Eq. (4·11). So, Eq. (4·11) is
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enough to determine both the $|g_r\rangle$'s and $c_r$'s.

We can also show that Eq. (4.11) is equivalent to the following coupled eigenvalue equations:

$$
[F_r u_r] = \varepsilon_r u_r, \quad \varepsilon_r = \bar{\varepsilon}_r - 2[H[W_{rr}] - E]|c_r|^2,
$$

$$
\{F_r = F[W_{rr}]|c_r|^2 + \sum_{i} (\mathbf{K}_{rr} c_r^* c_i + \mathbf{K}_{sr} c_r^* c_i^*) = \varepsilon_r^2
$$

(4.12a)

where $\bar{\varepsilon}_r = (\delta_\varepsilon \bar{\varepsilon}_r)$ is given by

$$
u_i^* F_r u_r + 2[H[W_{rr}] - E]|c_r|^2 = \nu_i^* F[W_{rr}]|c_r|^2 u_r = \bar{\varepsilon}_r.
$$

(4.12b)

Note that from Eq. (4.12b), in the limit $|c_r|^2 \rightarrow 1$, the eigenvalues $\bar{\varepsilon}_r$ tend to the usual HB orbital energies. The coupled non-linear eigenvalue equations (4.12a) for the $u_r$'s is called the Res HB eigenvalue equation. The hermitian $2N \times 2N$ matrices $F_r$ are called the Res FB operators. The Res HB eigenvalue equation shows that every eigenfunction in a resonating state has its own orbital energies $\varepsilon_r$. This fact must be emphasized to mean that the orbital concept is still surviving in the Res HB, as well as Res HF, approximations, though orbitals of different structures are resonating. The Res HB CI equation (4.6) and the Res HB eigenvalue equation (4.12a) may in principle be solved iteratively if we can get the suitable trial $u_r$'s. Once the HB wave functions $|g_r\rangle$ in the Res HB ground state are determined, then the other solutions of the Res HB CI equation give a series of the Res HB excited states that are called resonnon excitations.

§ 5. Resonance of projected HB wave functions

If a HB wave function is of the broken symmetry, for instance, in the rotational group, then there is a set of degenerate HB wave functions which are generated by the symmetry operations from the wave functions. Such a set is called the Goldstone set for the broken symmetry. We can make resonance of the Goldstone set. The Res HB CI coefficients of the Goldstone resonance is determined only by the symmetry and given by the irrep matrix of the symmetry group. The Goldstone resonance is just identical with the Peierls-Yoccoz projection as shown in Ref. 1).

The Peierls-Yoccoz projected HB wave functions respond to the gauge and rotational symmetries operation as

$$
\{\Phi^{[\mathbf{g}_k]}(g)\} = \int e^{-i\mathbf{a} \cdot \mathbf{D}_{\mathbf{k}}}(\omega) \{\Omega g\} d\theta d\omega,
$$

$$
\Omega = \begin{bmatrix} e^{i\theta} R^+(\omega) & 0 \\
0 & e^{-i\theta} R^-(\omega) \end{bmatrix},
$$

(5.1)

where $\theta$ is a gauge phase, $n$ is a Fermion number, $\omega$ is a rotation, $R(\omega)$ is the rotation matrix to transform the HB amplitudes $a$ and $b$ and $D_{\mathbf{k}}(\omega)$ is an irrep matrix element of the rotation group, the so-called $D$ function. A Res HB wave function with the Peierls-Yoccoz projection is given by

$$
|nM\rangle = [d_{f}]^{1/2} \sum_{\mathbf{k}} \Phi^{[\mathbf{g}_k]}(g_r) c_{r\mathbf{k}}^n
$$

(5.2)
where $d_t = (2I + 1)/8\pi^2$. The Lagrangian for the projected Res HB wave function is

$$L^l = \langle nIM|H - E|nIM\rangle = \sum_{rs} \sum_{KK'} \{ H^{rl}_{kk'}(r, s) - ES^{rl}_{kk'}(r, s) \} c^r_{kk'} c^{l*}_{kk'},$$

$$H^{rl}_{kk'}(r, s) = \int e^{-i\Omega} D^{rl}_{kk'}(\omega) H[W_{rs}(\Omega)] \cdot [\det\Sigma_{rs}(\Omega)]^{1/2} d\Omega d\omega,$$

$$S^{rl}_{kk'}(r, s) = \int e^{-i\Omega} D^{rl}_{kk'}(\omega) [\det\sigma_{rs}(\Omega)]^{1/2} d\Omega d\omega.$$

(5·3)

The variation equations are

$$\sum_{lk} \{ H^{kl}_{ll'}(r, s) - ES^{kl}_{ll'}(r, s) \} c^l_{ll'} = 0,$$

$$\sum_{lk} c^l_{kl'} c^l_{ll'} \int e^{-i\Omega} D^{kl}_{ll'}(\omega) K_{rs}(\Omega) d\Omega d\omega = 0,$$

$$K_{rs}(\Omega) = \{ (1 - W_{rs}(\Omega)) \Xi[W_{rs}(\Omega)] + H[W_{rs}(\Omega)] - E \} \times W_{rs}(\Omega) [\det\Sigma_{rs}(\Omega)]^{1/2}.$$

(5·6)

In some transitional nuclei different deformed shapes may be in resonance. In such nuclei rotational excitation spectra may be much different from those in usual deformed nuclei owing to interference of rotations of different shapes. The above equations provide a means to approach such a problem.

### § 6. Concluding remarks

The Res HB theory developed in this paper may have useful applications to the problem of large amplitude collective motions in transitional nuclei. In spite of large efforts, satisfactory theory has not yet been obtained. The theories developed so far did not pay attention to the possibility of different shapes in the ground state. For instance, the boson expansion theory implicitly assumes that the ground state can be approximated by a single mean field wave function and the description of the mode-mode coupling can be made perturbatively with the single reference state. The time dependent HF (TDHF) theory is an exact theory if quantization is made by appropriate manners. However, because it is a differential theory, it is difficult to describe resonance of multiple states. The present theory starting with an integral CS rep of a state vector is naturally able to describe resonance of multiple states.

The presence of multiple shapes as local minima of the energy functional was demonstrated in Strutinsky’s macroscopic-microscopic model and a theoretical approach to them has been attempted recently by the GCM. Experiments also indicated the presence of superdeformations. Multiple shapes can be obtained in a simpler model. We found in a pairing plus quadrupole interaction model with three levels presence of two local minima of prolate and oblate shapes. The ground state of the model can be correctly described only by the resonance of the two shapes.
seems very likely that resonance of multiple shapes is taking place in transitional nuclei. Detailed description of the model and its Res HB treatment will be given elsewhere.

We finally note the relation of the Res HB theory to the GCM. In the GCM the exact CS rep (2·4) with the group integration on the \( SO(2N) \) group is approximated by an integration with several collective variables. The Schrödinger equation in the GCM is usually difficult to solve and the GCM itself does not provide algorithm how to solve it. In the Res HB theory the integration in the \( SO(2N) \) CS rep is approximated by a discrete sum. The HB wave functions in the sum and their superposition coefficients are determined variationally so as to optimize the sum.\(^{19} \) Therefore, the variational equations give an algorithm to determine the Res HB wave function. If the HB wave functions in a Res HB wave function are different only in the collective variables of the GCM, then the Res HB theory gives an approximate solution of the GCM. It depends on the appropriate choice of the initial trial to get a good Res HB wave function. The validity of the Res HB theory should be checked by applications to concrete problems.

**Appendix**

In this appendix, we give a calculation of the matrix elements of the pair operators and the two-body operators between the two non-orthogonal HB wave functions. We give a different method from that employed in the Res HF theory.\(^{1} \) First, we consider an infinitesimal \( SO(2N) \) matrix

\[
1 + \delta g = \begin{bmatrix} 1 + \delta a & \delta b^* \\ \delta b & 1 + \delta a^* \end{bmatrix}, \quad \delta a^* = -\delta a, \quad \text{Tr} \delta a = 0, \quad \delta b = -\delta b^*.
\]

(A·1)

Then we have

\[
(1 + \delta g)g = \begin{bmatrix} a + \delta aa^* + \delta b^* b & b^* + \delta ab^* + \delta b* a^* \\ b + \delta a^* b + \delta ba & a^* + \delta a^* a + \delta bb^* \end{bmatrix} + \delta g g^* + \delta g^* g + \Delta g g^*.
\]

(A·2)

\[
\begin{bmatrix} b + \delta ba + \delta a^* b \\ a + \delta aa + \delta b^* b \end{bmatrix} = (1 + \delta g^*) u .
\]

(A·3)

We can express the matrix element of an infinitesimal unitary matrix \( U(1 - \delta g) \) between the two HB wave functions \( |g\rangle \) and \( |g'\rangle \) as

\[
\langle 0 | U^*(g) U(1 - \delta g) U(g') | 0 \rangle
\]

\[
= \langle 0 | U^*(g) \left( 1 - \delta g + \frac{1}{2} \delta g^* \delta g - \frac{1}{2} [\delta g^*_r, \delta g] + \cdots \right) U(g') | 0 \rangle,
\]

(A·4)

where

\[
\delta g = -\delta a^a b^a + \frac{1}{2} \left( \delta b_{ab} E^a_{b} + \delta b_{ba} E^a_{b} \right) = \delta g^*_r + \delta g^*_l .
\]

(A·5)
\[
\delta g_r = -\frac{1}{2} \delta a^a \epsilon^a \epsilon^a = -\frac{1}{2} \delta a^a \epsilon^a \epsilon^a c_2 - \frac{1}{2} \delta a^a (c_2^* c_3 - \delta_{a b}),
\]
\[
\delta g_\lambda = -\frac{1}{2} (\delta b_{ab} \epsilon^{ab} + \delta b_{ab} \epsilon^{ab}) = -\frac{1}{2} (\delta b_{ab} c_2^* c_3 + \delta b_{ab} c_3 c_2).
\]

On the other hand, we can compute the above matrix element as

\[
\langle 0 | U^\dagger (g) U(1 - \delta g) U(g') | 0 \rangle = \langle 0 | U^\dagger ((1 + \delta g) U(g') | 0 \rangle = \langle 1 + \delta g | g') = \left[ \det(z + \delta z) \right]^{1/2},
\]

where \( z + \delta z = (1 + \delta g^*) U^\dagger U^0 \), from which the explicit form of the infinitesimal overlap matrix \( \delta z \) is given as

\[
\delta z = -a^* a - b^* b - b^* b - a^* b^* - a^* b^* b.
\]

Substituting Eq. (A·8) into

\[
\left[ \det(z + \delta z) \right]^{1/2} = \left[ \det z \right]^{1/2} \left[ 1 + \frac{1}{2} \text{Tr}(z^{-1} \delta z) + \frac{1}{8} \left[ \text{Tr}(z^{-1} \delta z) \right]^2 - \frac{1}{4} \text{Tr}((z^{-1} \delta z)^2) + \cdots \right],
\]

we can get the following equation up to the second order of the infinitesimal matrices:

\[
\left[ \det(z + \delta z) \right]^{1/2} = \left[ \det z \right]^{1/2} \times \left[ 1 - \frac{1}{2} \text{Tr}(\delta a^a z^{-1} a^a) - \frac{1}{2} \text{Tr}(\delta a^a z^{-1} \delta a^a) - \frac{1}{2} \text{Tr}(\delta b^b z^{-1} b^b) - \frac{1}{2} \text{Tr}(\delta b^b z^{-1} \delta b^b) \right] \times z^{-1}(a^a \delta a^a + b^b \delta a^a + b^b \delta b^b + a^a \delta b^b) + \cdots.
\]

Then, in the first order, we have

\[
\langle 0 | U^\dagger (g) (1 - \delta g) U(g') | 0 \rangle = [\det z]^{1/2} \times \left[ 1 - \frac{1}{2} \text{Tr}(\delta a^a z^{-1} a^a) - \frac{1}{2} \text{Tr}(\delta a^a z^{-1} \delta a^a) - \frac{1}{2} \text{Tr}(\delta b^b z^{-1} b^b) - \frac{1}{2} \text{Tr}(\delta b^b z^{-1} \delta b^b) \right] \times z^{-1}(a^a \delta a^a + b^b \delta a^a + b^b \delta b^b + a^a \delta b^b) + \cdots.
\]
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\[ + \frac{1}{2} \text{Tr}[\delta b(a'z^{-1}b')^\dagger] + \frac{1}{2} \text{Tr}[\delta b^*(b'z^{-1}a')^\dagger] \],
\]

(A·10)

from which we can obtain the result

\[ \langle 0 | U^\dagger(g)c_c^\dagger c_a U(g') | 0 \rangle = \langle b'z^{-1}b' | \delta_{ab} \cdot [\text{det} z]^{1/2} \],
\]

(A·11a)

\[ \langle 0 | U^\dagger(g)c_{\beta^c} c_a U(g') | 0 \rangle = \langle b'z^{-1}a' | \delta_{ab} \cdot [\text{det} z]^{1/2} \].
\]

(A·11b)

These equations are identical with Eqs. (3·6) and (3·7). In the second order, we need the following infinitesimal operator:

\[ \langle 0 | U^\dagger(g) \frac{1}{2!} \delta \tilde{g} \delta \tilde{g} U(g') | 0 \rangle = \frac{1}{8} \langle 0 | U^\dagger(g) \{ \delta a^\dagger c_a c_{\beta^c} c_c c_y - \delta b^\dagger a b c_{\beta^c} c_c c_y - \delta b^\dagger b c_{\beta^c} c_c c_y \} U(g') | 0 \rangle.
\]

(A·12)

In the above, for our present aim, only the last two terms are necessary. They are rewritten into the normal ordered form:

\[ \frac{1}{8} \langle 0 | U^\dagger(g) \{ \delta b_{\alpha^c} \delta b^\dagger_{\beta^c} c_{\alpha^c} c_{\beta^c} c_c c_y + \delta b_{\alpha^c} \delta b_{\beta^c} c_{\alpha^c} c_{\beta^c} c_c c_y \} U(g') | 0 \rangle
\]

(A·13)

On the other hand, from Eq. (A·9), we pick up the infinitesimal terms containing only \( \delta b b^* \). They are calculated as

\[ \frac{1}{8} \cdot 2 \cdot \text{Tr}[\delta ba'z^{-1}b'] \cdot \text{Tr}[\delta b^* b'z^{-1}a']
\]

\[ - \frac{1}{4} \text{Tr}[z^{-1}b' \delta b a'z^{-1}a' \delta b^* b'] - \frac{1}{4} \text{Tr}[z^{-1}a' \delta b^* b'z^{-1}b' \delta b a']
\]

\[ = \frac{1}{4} \delta b_{\alpha^c} \delta b^\dagger_{\beta^c} \text{Tr}[(b'z^{-1}b')_{\alpha^c}(b'z^{-1}b')_{\beta^c} - (b'z^{-1}b')_{\beta^c}(b'z^{-1}b')_{\alpha^c}]
\]

\[ - (b'z^{-1}a')_{\alpha^c} (b'z^{-1}a')_{\beta^c} \cdot \text{det} z. \quad (z' = u^\dagger u)
\]

(A·14)

By equating the terms with \( \delta b_{\alpha^c} \delta b^\dagger_{\beta^c} \) in Eqs. (A·13) and (A·14), we can get the final result

\[ \langle 0 | U^\dagger(g) c_c^\dagger c_c^\dagger c_a c_a U(g') | 0 \rangle = \{(b'z^{-1}b')_{\alpha^c}(b'z^{-1}b')_{\beta^c} - (b'z^{-1}b')_{\beta^c}(b'z^{-1}b')_{\alpha^c}]
\]

\[ - (b'z^{-1}a')_{\alpha^c} (b'z^{-1}a')_{\beta^c} \cdot [\text{det} z]^{1/2},
\]

(A·15)

which is just Eq. (3·8).
References

3) T. Holstein and H. Primakof, Phys. Rev. 58 (1940), 1098.
4) P. J. Dyson, Phys. Rev. 102 (1956), 1217, 1231.
13) F. J. Dyson, Phys. Rev. 102 (1956), 1217, 1231.