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Canonical Coordinate System Suitable for Adiabatic Treatment of Collective Motion

—— General Case ——

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For the general case of particle-pair correlation or particle-hole correlation, we define a canonical coordinate system of TDHF symplectic manifold which may be suitable for the adiabatic description of collective motion. Following the prescription of Baranger and Veneroni, we adopt a Slater determinantal state generated by two-step unitary transformation. In this case, the canonicity condition plays an important role.

§ 1. Introduction

A canonical form of full time-dependent Hartree-Fock (TDHF) method, where we introduce a necessary and sufficient set of parameters to specify a time-dependent Slater determinantal state, easily leads us to a canonical formulation of TDHF method for a classical description of large amplitude collective motion.[1] The choice of canonical coordinate system (CCS) of collective submanifold is arbitrary, since the collective submanifold and the collective motion on it are independent of it. In general, however, the collective submanifold and the collective Hamiltonian are determined in an approximate form, by solving the equation of collective submanifold with certain conditions, such as the RPA boundary condition. In this sense, we must choose a proper CCS which is suitable for the description of characteristic of collective motion to be treated.[2]

On the other hand, all of the basic equations and conditions can be formulated in invariant forms under any canonical transformation of CCS of TDHF symplectic manifold.[1] For the practical aim, however, its proper choice gives rise to a transparent formulation of the basic equations of collective submanifold and its CCS.[3] In this sense, we are not insensible in the choice of CCS of TDHF symplectic manifold.

In this paper, we introduce a new type of CCS of TDHF symplectic manifold, which may provide a base suitable for the adiabatic description of collective motion. The basic idea has been given in the previous paper with the use of $SU(2)$-product model,[4] in which the coordinates and momenta are specified with the prescription of Baranger and Veneroni.[5] We extend this prescription to more general cases, for the aim of applying adiabatic TDHF to the description of realistic nuclear collective motion and also of studying non-adiabatic effect in a systematic manner.

In §2, we give a Slater determinantal state generated by a two-step unitary transformation, following the prescription of Baranger and Veneroni. Section 3 is devoted to the introduction of CCS of TDHF symplectic manifold with the aid of the canonicity condition. In §4, the classical image of every type of one-body operators is expressed with the aid of the CCS defined in §3. In the text, we treat only a case of general particle-pair correlation for fixing the notations. In the Appendix, we give also the result for a case of general particle-hole correlation.

§ 2. Two-step transformation

In order to introduce a CCS of TDHF symplectic manifold, we start with the following Slater determinantal state generated by a two-step unitary transformation:

$$|c\rangle = W|0\rangle; \tag{2·1}$$

$$\hat{c}_\alpha|0\rangle = 0\,, \tag{2·2}$$

where $\hat{c}_\alpha$ denotes an annihilation operator of fermion in the state α which is specified a set of quantum numbers $(n_\alpha,\ l_\alpha,\ j_\alpha,\ m_\alpha,\ \tau_\alpha)$. The unitary operator W is defined as follows:

$$W = \mathring{U}U\,; \tag{2·3}$$

$$U = \exp[\tfrac{1}{2}S]; \qquad S = \sum_{\alpha\beta}(\hat{c}_\alpha{}^*\hat{c}_\beta{}^*\Gamma_{\alpha\beta} - \Gamma^*_{\alpha\beta}\hat{c}_\beta\hat{c}_\alpha), \tag{2·4a}$$

$$\mathring{U} = \exp[\tfrac{1}{2}\mathring{S}]; \qquad \mathring{S} = \sum_{\alpha\beta}(\hat{\mathring{a}}_\alpha{}^*\hat{\mathring{a}}_\beta{}^*\mathring{\Gamma}_{\alpha\beta} - \mathring{\Gamma}^*_{\alpha\beta}\hat{\mathring{a}}_\beta\hat{\mathring{a}}_\alpha). \tag{2·4b}$$

In the above, we have used the definition of quasi-particle operators

$$\hat{\mathring{a}}_\alpha{}^* = U\hat{c}_\alpha{}^*U^\dagger\,, \qquad \hat{\mathring{a}}_\alpha = U\hat{c}_\alpha U^\dagger\,. \tag{2·5}$$

The explicit form of Eq. (2·5) can be given as

$$\begin{bmatrix}\hat{\mathring{a}}^*\\ \hat{\mathring{a}}\end{bmatrix} = \begin{bmatrix}A^\dagger & B^\dagger\\ B^T & A^T\end{bmatrix}\begin{bmatrix}\hat{c}^*\\ \hat{c}\end{bmatrix}; \tag{2·6a}$$

$$A_{\alpha\beta} = [\cos\sqrt{\Gamma^\dagger\Gamma}\,]_{\alpha\beta}\,, \qquad B_{\alpha\beta} = [\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\sqrt{\Gamma^\dagger\Gamma}\,]_{\alpha\beta}\,. \tag{2·6b}$$

The superscripts $*$, T and $\dagger$ express respectively complex-conjugate, transposed and hermite-conjugate matrix. We also use the following quasi-particle operators:

$$\hat{a}_\alpha{}^* = W\hat{c}_\alpha{}^*W^\dagger, \qquad \hat{a}_\alpha = W\hat{c}_\alpha W^\dagger\,, \tag{2·7}$$

i.e.,

$$\begin{bmatrix}\hat{a}^*\\ \hat{a}\end{bmatrix} = \begin{bmatrix}\mathring{A}^\dagger & \mathring{B}^\dagger\\ \mathring{B}^T & \mathring{A}^T\end{bmatrix}\begin{bmatrix}A^\dagger & B^\dagger\\ B^T & A^T\end{bmatrix}\begin{bmatrix}\hat{c}^*\\ \hat{c}\end{bmatrix}; \tag{2·8a}$$

$$\mathring{A}_{\alpha\beta} = [\cos\sqrt{\mathring{\Gamma}^\dagger\mathring{\Gamma}}\,]_{\alpha\beta}, \qquad \mathring{B}_{\alpha\beta} = [\mathring{\Gamma}(\mathring{\Gamma}^\dagger\mathring{\Gamma})^{-1/2}\sin\sqrt{\mathring{\Gamma}^\dagger\mathring{\Gamma}}\,]_{\alpha\beta}\,. \tag{2·8b}$$

The parameters $(\Gamma_{\alpha\beta},\ \Gamma^*_{\alpha\beta})$ and $(\mathring{\Gamma}_{\alpha\beta},\ \mathring{\Gamma}^*_{\alpha\beta})$ satisfy the antisymmetry relation

$$\Gamma^T = -\Gamma\,, \qquad \mathring{\Gamma}^T = -\mathring{\Gamma}. \tag{2·9}$$

Following the prescription of Baranger and Veneroni, we further require the following relation, i.e, time-reversal relation:

$$\Gamma_{\bar{\alpha}\bar{\beta}} = \Gamma^*_{\alpha\beta}\,, \qquad \mathring{\Gamma}_{\bar{\alpha}\bar{\beta}} = -\mathring{\Gamma}^*_{\alpha\beta}\,. \tag{2·10}$$

Then matrices A, B, $\mathring{A}$ and $\mathring{B}$ satisfy the following relations:

$$A^{\dagger}A+B^{\dagger}B=1, \quad A^{T}B=BA\,; \quad A^{\dagger}=A\,, \quad B^{T}=-B\,, \tag{2·11a}$$

$$\mathring{A}^{\dagger}\mathring{A}+\mathring{B}^{\dagger}\mathring{B}=1\,, \quad \mathring{A}^{T}\mathring{B}=\mathring{B}\mathring{A}; \quad \mathring{A}^{\dagger}=\mathring{A}\,, \quad \mathring{B}^{T}=-\mathring{B}\,. \tag{2·11b}$$

$$B_{\tilde{\alpha}\tilde{\beta}}=[B^{*}]_{\alpha\beta}, \qquad A_{\tilde{\alpha}\tilde{\beta}}=[A^{*}]_{\alpha\beta}\,, \tag{2·12a}$$

$$\mathring{B}_{\tilde{\alpha}\tilde{\beta}}=-[\mathring{B}^{*}]_{\alpha\beta}\,, \quad \mathring{A}_{\tilde{\alpha}\tilde{\beta}}=[\mathring{A}^{*}]_{\alpha\beta}\,. \tag{2·12b}$$

The classical image of one-body operator can be given as its expectation with respect to $|c\rangle$:

$$\langle c|\hat{c}_{\alpha}{}^{*}\hat{c}_{\beta}{}^{*}-\hat{c}_{\tilde{\beta}}\hat{c}_{\tilde{\alpha}}|c\rangle=2[A^{\dagger}\mathring{B}^{*}\mathring{A}^{T}A^{*}+B^{\dagger}\mathring{A}^{*}\mathring{B}^{T}B^{*}]_{\alpha\beta}\,, \tag{2·13a}$$

$$\langle c|\hat{c}_{\alpha}{}^{*}\hat{c}_{\beta}{}^{*}+\hat{c}_{\tilde{\beta}}\hat{c}_{\tilde{\alpha}}|c\rangle=-2[A^{\dagger}\mathring{B}^{*}\mathring{B}^{T}B^{*}+B^{\dagger}\mathring{A}^{*}\mathring{A}^{T}A^{*}]_{\alpha\beta}\,, \tag{2·13b}$$

$$\langle c|\hat{c}_{\alpha}{}^{*}\hat{c}_{\tilde{\beta}}+\hat{c}_{\beta}{}^{*}\hat{c}_{\tilde{\alpha}}|c\rangle=2[A\mathring{B}^{\dagger}\mathring{A}^{T}B+B^{\dagger}\mathring{A}^{T}\mathring{B}A]_{\alpha\tilde{\beta}}\,, \tag{2·13c}$$

$$\langle c|\hat{c}_{\alpha}{}^{*}\hat{c}_{\tilde{\beta}}-\hat{c}_{\beta}{}^{*}\hat{c}_{\tilde{\alpha}}|c\rangle=2[A\mathring{B}^{*}\mathring{B}^{T}A+B^{\dagger}\mathring{A}^{*}\mathring{A}^{T}B]_{\alpha\tilde{\beta}}\,. \tag{2·13d}$$

§ 3. Canonical coordinate system

Up to now, the independent variables are given by $\Gamma_{\alpha\beta}$ and $\mathring{\Gamma}_{\alpha\beta}$. In this section, we introduce a possible CCS of TDHF symplectic manifold specified by the Slater determinantal state (2·1).

3. 1. *Infinitesimal generator*

For this aim, we first consider the following infinitesimal generator:

$$\hat{O}_{X}=i\partial_{X}W\cdot W^{\dagger}\,. \tag{3·1}$$

After some calculations, we obtain the following explicit form of $\hat{O}_{X}$:

$$\hat{O}_{X}=i\Big\{\frac{1}{2}A^{0}+\sum_{\alpha\beta}A^{11}_{\beta\alpha}\hat{\mathring{a}}_{\alpha}{}^{*}\hat{\mathring{a}}_{\beta}+\frac{1}{2}\sum_{\alpha\beta}(A^{20}_{\alpha\beta}\hat{\mathring{a}}_{\alpha}{}^{*}\hat{\mathring{a}}_{\beta}{}^{*}-A^{02}_{\beta\alpha}\hat{\mathring{a}}_{\beta}\hat{\mathring{a}}_{\alpha})\Big\}$$
$$+i\Big\{\frac{1}{2}\mathring{A}^{0}+\sum_{\alpha\beta}\mathring{A}^{11}_{\beta\alpha}\hat{a}_{\alpha}{}^{*}\hat{a}_{\beta}+\frac{1}{2}\sum_{\alpha\beta}(\mathring{A}^{20}_{\alpha\beta}\hat{a}_{\alpha}{}^{*}\hat{a}_{\beta}{}^{*}-\mathring{A}^{02}_{\beta\alpha}\hat{a}_{\beta}\hat{a}_{\alpha})\Big\}, \tag{3·2}$$

where we have used the notations A^{0}, $A^{11}_{\beta\alpha}$, $A^{20}_{\alpha\beta}$ and $A^{02}_{\beta\alpha}$ defined by

$$A^{0}=\frac{1}{2}\mathrm{Tr}[B^{\dagger}B_{,X}-B^{\dagger}_{,X}B], \tag{3·3a}$$

$$A^{11}_{\beta\alpha}=\frac{1}{2}[A_{,X}A-AA_{,X}+B^{\dagger}_{,X}B-B^{\dagger}B_{,X}]_{\beta\alpha}\,, \tag{3·3b}$$

$$A^{20}_{\alpha\beta}=\frac{1}{2}[A^{T}B_{,X}-A^{T}_{,X}B+B^{T}A_{,X}-B^{T}_{,X}A]_{\alpha\beta}\,, \tag{3·3c}$$

$$A^{02}_{\beta\alpha}=\frac{1}{2}[A_{,X}B^{*}-AB^{*}_{,X}+B^{\dagger}_{,X}A^{T}-B^{\dagger}A^{T}_{,X}]_{\beta\alpha}\,, \tag{3·3d}$$

and $\mathring{A}^{0}$, $\mathring{A}^{11}_{\beta\alpha}$, $\mathring{A}^{20}_{\alpha\beta}$ and $\mathring{A}^{02}_{\beta\alpha}$ defined in the same way as the above with the use of $\mathring{A}$ and $\mathring{B}$ in place of A and B. The detail of the derivation is given in the Appendix. In the above definition, we have also used the abbreviations such as

$$[A_{,X}]_{\alpha\beta}=A_{\alpha\beta,X}=\partial_X A_{\alpha\beta}\,,$$
$$[B_{,X}]_{\alpha\beta}=B_{\alpha\beta,X}=\partial_X B_{\alpha\beta}\,. \qquad (3\cdot4)$$

Such abbreviations as the above are frequently used in succeeding discussion.

3. 2. *Classical image of infinitesimal generator*

Now we consider the classical image of the above infinitesimal generator, which is given as the expectation with respect to $|c\rangle$:

$$O_X=\langle c|\hat{O}_X|c\rangle. \qquad (3\cdot5)$$

With the use of time-reversal relation (2·12), we can rewrite RHS of Eq. (3·5) as follows:

$$O_X=\frac{i}{2}\mathrm{Tr}[(AB^*_{,X}-A_{,X}B^*+B^\dagger A^T_{,X}-B^\dagger_{,X}A^T)(\mathring{B}\mathring{A})]. \qquad (3\cdot6)$$

With the use of the relation (2·11a) and the identity*)

$$A^{-1}A_{,X}+(A^{-1})_{,X}A=0\,, \qquad (3\cdot7)$$

RHS of Eq. (3·6) can be rewritten as

$$\mathrm{RHS}=\mathrm{Tr}[\{B^*(A^T)^{-1}+A^{-1}B^*\}_{,X}(A^T\mathring{B}\mathring{A}A)]. \qquad (3\cdot8)$$

Then, we obtain the expression of O_X

$$O_X=-i\mathrm{Tr}[(A^{-1}B^\dagger)_{,X}(A^T\mathring{B}\mathring{A}A)]. \qquad (3\cdot9)$$

At the end of this subsection, we list up the relations satisfied by matrices, such as $A^{-1}B^\dagger$.

(1) Anti-symmetry relation:

$$A^T\mathring{B}\mathring{A}A=-(A^T\mathring{B}\mathring{A}A)^T\,, \qquad B^T\mathring{A}\mathring{B}^\dagger B=-(B^T\mathring{A}\mathring{B}^\dagger B)^T\,,$$
$$A^{-1}B^\dagger=-(A^{-1}B^\dagger)^T\,. \qquad (3\cdot10\mathrm{a})$$

(2) Time-reversal relation:

$$[A^T\mathring{B}\mathring{A}A]_{\bar{\alpha}\bar{\beta}}=-[(A^T\mathring{B}\mathring{A}A)^*]_{\alpha\beta}\,,\quad [B^T\mathring{A}\mathring{B}^\dagger B]_{\bar{\alpha}\bar{\beta}}=-[(B^T\mathring{A}\mathring{B}^\dagger B)^*]_{\alpha\beta}\,,$$
$$[A^{-1}B^\dagger]_{\bar{\alpha}\bar{\beta}}=[(A^{-1}B^\dagger)^*]_{\alpha\beta}\,. \qquad (3\cdot10\mathrm{b})$$

3. 3. *Canonicity condition*

Now we are in a position to introduce the canonicity condition which selects a proper CCS suitable for the adiabatic description of collective motion. First we define the following infinitesimal generators:

$$\hat{p}_{\alpha\beta}=i\partial_{q^*_{\alpha\beta}}W\cdot W^\dagger\,, \qquad \hat{q}^*_{\alpha\beta}=-i\partial_{p_{\alpha\beta}}W\cdot W^\dagger\,. \qquad (3\cdot11)$$

Following the previous discussion,[2] we adopt the following form of canonicity condition:

$$\langle c|\hat{p}_{\alpha\beta}|c\rangle=p_{\alpha\beta}\,, \qquad \langle c|\hat{q}^*_{\alpha\beta}|c\rangle=0\,. \qquad (3\cdot12)$$

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*) As long as the overlap $\langle c|0\rangle$ does not vanish, A and $\mathring{A}$ are made to be positive definite.

With the aid of Eq. (3·9), we can easily obtain the following solution satisfying the canonicity condition (3·12):

$$q^*_{\alpha\beta}=[A^{-1}B^\dagger]_{\alpha\beta}\,,\qquad p_{\alpha\beta}=2i[A^T\mathring{B}\mathring{A}A]_{\alpha\beta}\,, \tag{3·13}$$

i.e.,

$$q^*=A^{-1}B^\dagger\,,\qquad p=2iA^T\mathring{B}\mathring{A}A\,. \tag{3·14}$$

By the relations (3·10a) and (3·10b), q^* and p also satisfy the relations

$$(q^*)^T=-q^*\,,\qquad p^T=-p\,, \tag{3·15a}$$

$$q^*_{\bar{\alpha}\bar{\beta}}=q_{\alpha\beta}\,,\qquad p_{\bar{\alpha}\bar{\beta}}=p^*_{\alpha\beta}\,. \tag{3·15b}$$

Further it is easily ascertained that the infinitesimal generators $\hat{q}^*$ and $\hat{p}$ satisfy the weak canonicity condition

$$\langle c|[\hat{q}^*_{\alpha\beta},\ \hat{p}_{\gamma\delta}]|c\rangle=i\delta_{[\alpha\beta,\gamma\delta]}\,,$$

$$\langle c|[\hat{q}^*_{\alpha\beta},\ \hat{q}^*_{\gamma\delta}]|c\rangle=\langle c|[\hat{p}_{\alpha\beta},\ \hat{p}_{\gamma\delta}]|c\rangle=0\,; \tag{3·16}$$

$$\delta_{[\alpha\beta,\gamma\delta]}=\delta_{\alpha\gamma}\delta_{\beta\delta}-\delta_{\alpha\delta}\delta_{\beta\gamma}\,. \tag{3·17}$$

The geometry of the present TDHF symplectic manifold is specified by the Poisson bracket

$$\{F,\ G\}_{(q^*,p)}=\sum\nolimits_{(\alpha\beta)}(\partial_{q^*_{\alpha\beta}}F\cdot\partial_{p_{\alpha\beta}}G-\partial_{p_{\alpha\beta}}F\cdot\partial_{q^*_{\alpha\beta}}G), \tag{3·18}$$

where the summation runs over all independent pair states $(\alpha\beta)$. By properly ordering the pair states, they are specified by single Greek letter μ. For instance, the Poisson bracket is written as

$$\{F,\ G\}_{(q^*,p)}=\sum_\mu(\partial_{q^*_\mu}F\cdot\partial_{p_\mu}G-\partial_{p_\mu}F\cdot\partial_{q^*_\mu}G). \tag{3·19}$$

§ 4. Classical image in canonical form

Now we express the classical image of one-body operator of fermion system given by Eq. (2·13), in terms of canonical variables q^* and p.

4.1. *Canonical form of one-body operator in classical image*

First we express matrices A, B, $\mathring{A}$ and $\mathring{B}$ in terms of q^* and p. Using the definition (3·14), we obtain

$$BA^{-1}=-q\,. \tag{4·1}$$

With the aid of Eq. (2·11a) and the positive-definite and hermite property of A, we obtain the expressions of A and $B^\dagger$:

$$A=(1+q^\dagger q)^{-1/2}\,,\qquad B^\dagger=-(1+q^\dagger q)^{-1/2}q^\dagger\,. \tag{4·2}$$

Using these expressions, we can get those of $\mathring{A}$ and $\mathring{B}$ with the use of relations (2·11a) and (2·11b):

$$\mathring{A}=\frac{1}{\sqrt{2}}[1+\{1-(1+q^\dagger q)^{1/2}p^\dagger(1+qq^\dagger)p(1+q^\dagger q)^{1/2}\}^{1/2}]^{1/2},$$

$$\mathring{B}=-\frac{i}{2}(1+qq^\dagger)^{1/2}p(1+q^\dagger q)^{1/2}\mathring{A}^{-1}. \qquad (4\cdot3)$$

In the above derivation, we have used the positive-definite and hermite property of $\mathring{A}$ and also the boundary condition

$$\mathring{A}\xrightarrow[p\to 0]{}1. \qquad (4\cdot4)$$

Then we can easily obtain the expressions of classical image of one-body operator in terms of q^* and p:

$$\langle c|\hat{c}_\alpha{}^*\hat{c}_\beta{}^*-\hat{c}_{\bar\beta}\hat{c}_{\bar\alpha}|c\rangle=-i[p^\dagger+q^\dagger pq^\dagger]_{\alpha\beta}, \qquad (4\cdot5\text{a})$$

$$\begin{aligned}\langle c|\hat{c}_\alpha{}^*\hat{c}_\beta{}^*+\hat{c}_{\bar\beta}\hat{c}_{\bar\alpha}|c\rangle=&[(1+q^\dagger q)^{-1/2}\{1-(1+q^\dagger q)^{1/2}p^\dagger(1+qq^\dagger)p(1+q^\dagger q)^{1/2}\}^{1/2}\\&\times(1+q^\dagger q)^{-1/2}q^\dagger\\&+q^\dagger(1+qq^\dagger)^{-1/2}\{1-(1+qq^\dagger)^{1/2}p(1+q^\dagger q)p^\dagger(1+qq^\dagger)^{1/2}\}^{1/2}\\&\times(1+qq^\dagger)^{-1/2}]_{\alpha\beta},\end{aligned} \qquad (4\cdot5\text{b})$$

$$\langle c|\hat{c}_\alpha{}^*\hat{c}_{\bar\beta}+\hat{c}_\beta{}^*\hat{c}_{\bar\alpha}|c\rangle=-i[p^\dagger q-q^\dagger p]_{\alpha\bar\beta}, \qquad (4\cdot5\text{c})$$

$$\begin{aligned}\langle c|\hat{c}_\alpha{}^*\hat{c}_{\bar\beta}-\hat{c}_\beta{}^*\hat{c}_{\bar\alpha}|c\rangle=&[1+(1+q^\dagger q)^{-1/2}q^\dagger\{1-(1+qq^\dagger)^{1/2}p(1+q^\dagger q)p^\dagger(1+qq^\dagger)^{1/2}\}^{1/2}\\&\times q(1+q^\dagger q)^{-1/2}\\&-(1+q^\dagger q)^{-1/2}\{1-(1+q^\dagger q)^{1/2}p^\dagger(1+qq^\dagger)p(1+q^\dagger q)^{1/2}\}^{1/2}\\&\times(1+q^\dagger q)^{-1/2}]_{\alpha\bar\beta}.\end{aligned} \qquad (4\cdot5\text{d})$$

4. 2. *Poisson bracket for classical image of one-body operator*

We show that the quantal commutation relation among one-body operators can be transcribed into the Poisson bracket among their classical images. For this aim, we adopt the following abbreviations of notations:

$$\{\text{the set of one-body operators}\}=\{\hat{O}_i\}, \qquad (4\cdot6)$$

and their quantal commutation relations are written as

$$[\hat{O}_i,\ \hat{O}_j]=\sum_k C_{ijk}\hat{O}_k, \qquad (4\cdot7)$$

where C_{ijk} denotes the structure constant. Then their classical images can be given as

$$O_i=\langle|\hat{O}_i|c\rangle, \qquad (4\cdot8)$$

$$\langle c|[\hat{O}_i,\ \hat{O}_j]|c\rangle=\sum_k C_{ijk}O_k. \qquad (4\cdot9)$$

Now we show that Eq. (4·9) can be written as follows:

$$i\{O_i,\ O_j\}_{(q*,p)}=\sum_k C_{ijk}O_k. \qquad (4\cdot10)$$

In order to show the above relation, it is not necessary to derive the derivatives with respect to q^* and p. We use only the facts that *all* $\hat{O}_i$*'s are one-body operators and* $(\hat{q}_\mu{}^*, \hat{p}_\mu)$ *satisfy the weak canonicity condition* (3·16). Considering that the $\hat{O}_i$'s are one-body operators, we can express them in terms of $\hat{q}_\mu{}^*$ and $\hat{p}_\mu$ as follows:

$$\hat{O}_i = \sum_\mu (O_{i\mu}^{(q^*)} \hat{q}_\mu{}^* + O_{i\mu}^{(p)} \hat{p}_\mu) + (C\text{-number} + \text{terms of } \hat{a}^* \hat{a}). \tag{4·11}$$

Then, we obtain the following expression for Eq. (4·9) using the weak canonicity condition (3·16):

$$\sum_k C_{ijk} O_k = i \sum_\mu (O_{i\mu}^{(q^*)} O_{j\mu}^{(p)} - O_{i\mu}^{(p)} O_{j\mu}^{(q^*)}). \tag{4·12}$$

On the other hand, the Poisson bracket, i.e., LHS of Eq. (4·10), can be written as follows:

$$\begin{aligned} i\{O_i, O_j\}_{(q*,p)} &= i\sum_\mu (\partial_{q_\mu^*} O_i \cdot \partial_{p_\mu} O_j - \partial_{p_\mu} O_i \cdot \partial_{q_\mu^*} O_j) \\ &= i\sum_\mu (\langle c|[\hat{O}_i, \hat{p}_\mu]|c\rangle\langle c|[\hat{O}_j, \hat{q}_\mu{}^*]|c\rangle - \langle c|[\hat{O}_i, \hat{q}_\mu{}^*]|c\rangle\langle c|[\hat{O}_j, \hat{p}_\mu]|c\rangle) \\ &= i\sum_\mu (O_{i\mu}^{(q^*)} O_{j\mu}^{(p)} - O_{i\mu}^{(p)} O_{j\mu}^{(q^*)}) \\ &= \sum_k C_{ijk} O_k . \end{aligned} \tag{4·13}$$

In this way, we can show that the quantal commutation relation among one-body operators can be transcribed into the Poisson bracket among their classical images.

From the above general discussion, the following facts become clear:

(1) The quantal algebra can be transcribed into the corresponding classical algebra specified by the Poisson bracket, only for those of one-body operators, within the TDHF method.

(2) The correspondence between Eqs. (4·7) and (4·10) does not depend on the choice of CCS of TDHF symplectic manifold.

(3) The quantization of the classical system obtained by full TDHF method can be performed by requiring that, after the quantization, the classical algebra of one-body operators, not of general operators, returns to the original quantal algebra. This procedure is widely adopted by many authors in order to get the quantized TDHF representation, i.e., the boson representation.[6),7)]

§ 5. Conclusion

In this paper, we have introduced a canonical coordinate system of TDHF symplectic manifold which may be suitable for the adiabatic treatment of collective motion. The basic idea exists in the adoption of the Baranger-Veneroni type of Slater determinantal state and the proper form of canonicity condition.

The resultant canonical form of one-body operators in their classical images is clearly different from that obtained from the boson representation of the Holstein-Primakoff type. But it is somewhat similar to that obtained by Nishiyama as the coherent state representation of the coset space of $SU(2n)/U(n)$.[8)] It is interesting to clarify the relation to these representations and also to quantize the present classical image.

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Appendix A

—— Derivation of Explicit Form of Infinitesimal Generator ——

In this appendix, we give the derivation procedure of the explicit form of infinitesimal generator

$$\hat{O}_X = i\partial_X W \cdot W^\dagger . \qquad \text{(A1·1)}$$

First we recall that Eq. (A1·1) can be rewritten in the following form:

$$\hat{O}_X = i\partial_X U \cdot U^\dagger + U \cdot i\partial_X(U^\dagger \mathring{U} U)\cdot(U^\dagger \mathring{U} U)^\dagger U^\dagger . \qquad \text{(A1·2)}$$

Considering the relation

$$U^\dagger \mathring{U} U = \exp[\frac{1}{2}\sum_{\alpha\beta}(\hat{c}_\alpha{}^* \hat{c}_\beta{}^* \mathring{\Gamma}_{\alpha\beta} - \mathring{\Gamma}^*_{\alpha\beta}\hat{c}_\beta \hat{c}_\alpha)], \qquad \text{(A1·3)}$$

we need to estimate explicitly only the first term on RHS of Eq. (A1·2).

In order to estimate the first term, we use the formula

$$U^\dagger \partial_X U = \frac{1}{2}\int_0^1 d\,\beta U(-\beta)\sum_{\alpha\beta}(\hat{c}_\alpha{}^* \hat{c}_\beta{}^* \Gamma_{\alpha\beta,X} - \Gamma^*_{\alpha\beta,X}\hat{c}_\beta \hat{c}_\alpha)U(\beta), \qquad \text{(A1·4)}$$

where $U(\beta)$ is defined by

$$U(\beta) = \exp\left[\frac{1}{2}\beta S\right]. \qquad \text{(A1·5)}$$

Using the transformation of fermion under the unitary transformation U given by Eq. (2·6), Eq. (A1·4) can be written as follows:

$$U^\dagger \partial_X U = \frac{1}{2}A^0 + \Sigma_{\alpha\beta} A^{11}_{\beta\alpha} \hat{c}_\alpha{}^* \hat{c}_\beta + \frac{1}{2}\sum_{\alpha\beta}(A^{20}_{\alpha\beta}\hat{c}_\alpha{}^* \hat{c}_\beta{}^* - A^{02}_{\beta\alpha}\hat{c}_\beta \hat{c}_\alpha), \qquad \text{(A1·6)}$$

where A^0, $A^{11}_{\beta\alpha}$, $A^{20}_{\alpha\beta}$ and $A^{02}_{\beta\alpha}$ are given by the relations

$$A^0 = \int_0^1 d\,\beta\, \mathrm{Tr}[A(-\beta)\Gamma^\dagger_{,X} B(-\beta) - B(-\beta)^\dagger \Gamma_{,X} A(-\beta)], \qquad \text{(A1·7a)}$$

$$A^{11}_{\beta\alpha} = \int_0^1 d\,\beta [B(-\beta)^\dagger \Gamma_{,X} A(-\beta)^\dagger - A(-\beta)\Gamma^\dagger_{,X} B(-\beta)^\dagger]_{\beta\alpha} , \qquad \text{(A1·7b)}$$

$$A^{20}_{\alpha\beta} = \int_0^1 d\,\beta [A(-\beta)\Gamma_{,X} A(-\beta) + B(-\beta)\Gamma^\dagger_{,X} B(-\beta)]_{\alpha\beta} , \qquad \text{(A1·7c)}$$

$$A^{02}_{\beta\alpha} = \int_0^1 d\,\beta [A(-\beta)\Gamma^\dagger_{,X} A(-\beta)^T + B(-\beta)^\dagger \Gamma_{,X} B(-\beta)^\dagger]_{\beta\alpha} . \qquad \text{(A1·7d)}$$

In the above equations, we have used the notations

$$A(\beta)=\cos\beta\sqrt{\Gamma^\dagger\Gamma}\,,\qquad B(\beta)=\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}\,. \tag{A1·8}$$

Now we perform the integration of RHS of Eq. (A1·7) with the aid of the method of integration by parts.

$$\begin{aligned}
A^0=&\int_0^1 d\beta\,\mathrm{Tr}[\sin\beta\sqrt{\Gamma^\dagger\Gamma}\cdot(\Gamma^\dagger\Gamma)^{-1/2}\Gamma^\dagger\Gamma_{,x}\cos\beta\sqrt{\Gamma^\dagger\Gamma}\\
&\qquad-\cos\beta\sqrt{\Gamma^\dagger\Gamma}\cdot\Gamma_{,x}^\dagger\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}]\\
=&\int_0^1 d\beta\,\mathrm{Tr}[\sin\beta\sqrt{\Gamma^\dagger\Gamma}\cdot(\Gamma^\dagger\Gamma)^{-1/2}\Gamma^\dagger(\Gamma\cos\beta\sqrt{\Gamma^\dagger\Gamma})_{,x}\\
&\qquad-(\cos\beta\sqrt{\Gamma^\dagger\Gamma}\cdot\Gamma^\dagger)_{,x}\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}]\\
=&\mathrm{Tr}[B^\dagger B_{,x}-B_{,x}^\dagger B]\\
&-\int_0^1 d\beta\,\mathrm{Tr}[\cos\beta\sqrt{\Gamma^\dagger\Gamma}\cdot\Gamma^\dagger(\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma})_{,x}\\
&-(\sin\beta\sqrt{\Gamma^\dagger\Gamma}\cdot(\Gamma^\dagger\Gamma)^{-1/2}\Gamma^\dagger)_{,x}\Gamma\cos\beta\sqrt{\Gamma^\dagger\Gamma}]\\
=&\mathrm{Tr}[B^\dagger B_{,x}-B_{,x}^\dagger B]\\
&-\int_0^1 d\beta\,\mathrm{Tr}[\sin\beta\sqrt{\Gamma^\dagger\Gamma}\cdot(\Gamma^\dagger\Gamma)^{-1/2}\Gamma^\dagger\Gamma_{,x}\cos\beta\sqrt{\Gamma^\dagger\Gamma}\\
&\qquad-\cos\beta\sqrt{\Gamma^\dagger\Gamma}\cdot\Gamma_{,x}^\dagger\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}].
\end{aligned} \tag{A1·9}$$

Then

$$A^0=\frac{1}{2}\mathrm{Tr}[B^\dagger B_{,x}-B_{,x}^\dagger B]. \tag{A1·10}$$

In the above derivation, we have used the relation

$$B=\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\sqrt{\Gamma^\dagger\Gamma}=\sin\sqrt{\Gamma\Gamma^\dagger}\cdot(\Gamma\Gamma^\dagger)^{-1/2}\Gamma. \tag{A1·11}$$

$$\begin{aligned}
A_{\beta\alpha}^{11}=&\int_0^1 d\beta[\cos\beta\sqrt{\Gamma^\dagger\Gamma}\cdot\Gamma_{,x}^\dagger\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}\\
&\qquad-\sin\beta\sqrt{\Gamma^\dagger\Gamma}\cdot(\Gamma^\dagger\Gamma)^{-1/2}\Gamma^\dagger\Gamma_{,x}\cos\beta\sqrt{\Gamma^\dagger\Gamma}]_{\beta\alpha}\\
=&\int_0^1 d\beta[(\cos\beta\sqrt{\Gamma^\dagger\Gamma}\cdot\Gamma^\dagger)_{,x}\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}\\
&\qquad-(\cos\beta\sqrt{\Gamma^\dagger\Gamma})_{,x}(\Gamma^\dagger\Gamma)^{1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}\\
&\qquad-\sin\beta\sqrt{\Gamma^\dagger\Gamma}\cdot(\Gamma^\dagger\Gamma)^{-1/2}\Gamma^\dagger(\Gamma\cos\beta\sqrt{\Gamma^\dagger\Gamma})_{,x}\\
&\qquad+\sin\beta\sqrt{\Gamma^\dagger\Gamma}\cdot(\Gamma^\dagger\Gamma)^{1/2}(\cos\beta\sqrt{\Gamma^\dagger\Gamma})_{,x}]_{\beta\alpha}\\
=&[B_{,x}^\dagger B-B^\dagger B_{,x}+A_{,x}A-AA_{,x}]_{\beta\alpha}\\
&-\int_0^1 d\beta[\cos\beta\sqrt{\Gamma^\dagger\Gamma}\cdot\Gamma_{,x}^\dagger\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}
\end{aligned}$$

$$-\sin\beta\sqrt{\Gamma^\dagger\Gamma}\cdot(\Gamma^\dagger\Gamma)^{-1/2}\Gamma^\dagger\Gamma_{,x}\cos\beta\sqrt{\Gamma^\dagger\Gamma}\,]_{\beta\alpha}\,. \tag{A1·12}$$

Then

$$A^{11}_{\beta\alpha}=\frac{1}{2}[B^\dagger_{,x}B-B^\dagger B_{,x}+A_{,x}A-AA_{,x}]_{\beta\alpha}\,. \tag{A1·13}$$

In the above derivation, we have used the relation

$$((\Gamma^\dagger\Gamma)^{1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma})_{,x}=\Gamma^\dagger_{,x}\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma}+\Gamma^\dagger(\Gamma(\Gamma^\dagger\Gamma)^{-1/2}\sin\beta\sqrt{\Gamma^\dagger\Gamma})_{,x}\,. \tag{A1·14}$$

In the same way, we can easily derive the explicit forms of $A^{20}_{\alpha\beta}$ and $A^{02}_{\beta\alpha}$:

$$A^{20}_{\alpha\beta}=\frac{1}{2}[A^TB_{,x}-A^T_{,x}B+B^TA_{,x}-B^T_{,x}A]_{\alpha\beta}\,, \tag{A1·15}$$

$$A^{02}_{\beta\alpha}=\frac{1}{2}[A_{,x}B^*-AB^*_{,x}+B^\dagger_{,x}A^T-B^\dagger A^T_{,x}]_{\beta\alpha}\,. \tag{A1·16}$$

Now we have derived the explicit form of Eq. (A1·6). Then the first term of Eq. (A1·2) can be easily obtained as follows:

$$\begin{aligned}\partial_xU\cdot U^\dagger&=U\cdot U^\dagger\partial_xU\cdot U^\dagger\\&=\frac{1}{2}A^0+\sum_{\alpha\beta}A^{11}_{\beta\alpha}\hat{a}_\alpha{}^*\hat{a}_\beta+\frac{1}{2}\sum_{\alpha\beta}(A^{20}_{\alpha\beta}\hat{a}_\alpha{}^*\hat{a}_\beta{}^*-A^{02}_{\beta\alpha}\hat{a}_\beta\hat{a}_\alpha).\end{aligned} \tag{A1·17}$$

The second term of Eq. (A1·6) can also be easily derived by noticing the relation (A1·3) and the relation

$$U\partial_x(U^\dagger\mathring{U}U)\cdot(U^\dagger\mathring{U}U)^\dagger U^\dagger=W\cdot(U^\dagger\mathring{U}U)^\dagger\partial_x(U^\dagger\mathring{U}U)\cdot W^\dagger\,. \tag{A1·18}$$

We can derive its explicit form by simply replacing A and B by $\mathring{A}$ and $\mathring{B}$ in the derivation of the first term.

After all, we have the explicit form of (A1·1) as follows:

$$\begin{aligned}\hat{O}_X=&\,i\left\{\frac{1}{2}A^0+\sum_{\alpha\beta}A^{11}_{\beta\alpha}\hat{a}_\alpha{}^*\hat{a}_\beta+\frac{1}{2}\sum_{\alpha\beta}(A^{20}_{\alpha\beta}\hat{a}_\alpha{}^*\hat{a}_\beta{}^*-A^{02}_{\beta\alpha}\hat{a}_\beta\hat{a}_\alpha)\right\}\\&+i\left\{\frac{1}{2}\mathring{A}^0+\sum_{\alpha\beta}\mathring{A}^{11}_{\beta\alpha}\hat{a}_\alpha{}^*\hat{a}_\beta+\frac{1}{2}\sum_{\alpha\beta}(\mathring{A}^{20}_{\alpha\beta}\hat{a}_\alpha{}^*\hat{a}_\beta{}^*-\mathring{A}^{02}_{\beta\alpha}\hat{a}_\beta\hat{a}_\alpha)\right\},\end{aligned} \tag{A1·19}$$

where $\mathring{A}^0$, $\mathring{A}^{11}_{\beta\alpha}$, $\mathring{A}^{20}_{\alpha\beta}$ and $\mathring{A}^{02}_{\beta\alpha}$ are given respectively by Eq. (A1·10), Eq. (A1·13), Eq. (A1·15) and Eq. (A1·16) with the use of $\mathring{A}$ and $\mathring{B}$ in place of A and B, respectively.

Appendix B

—— *Canonical Form for Particle-Hole Correlation* ——

For the case of general particle-hole correlation, we can also introduce a similar CCS of TDHF symplectic manifold to that discussed in the text for the case of general particle-pair correlation. We give here only the result.

We denote the particle creation operator in the particle state λ by $\hat{a}_\lambda{}^*$ and the hole creation operator in the state i by $\hat{b}_i{}^*$. Then the starting Slater determinantal state is given by

$$|c\rangle = W|0\rangle;$$
$$\hat{a}_\lambda|0\rangle = \hat{b}_i|0\rangle = 0\,. \tag{A2·1}$$

The unitary operator W is defined as follows:

$$W = \mathring{U}U\,; \tag{A2·2a}$$
$$U = \exp[S]; \qquad S = \sum_{\lambda i}(\hat{a}_\lambda{}^*\hat{b}_i{}^*\Gamma_{i\lambda} - \Gamma^*_{i\lambda}\hat{b}_i\hat{a}_\lambda), \tag{A2·2b}$$
$$\mathring{U} = \exp[\mathring{S}]; \qquad \mathring{S} = \sum_{\lambda i}(\mathring{\hat{a}}_\lambda{}^*\mathring{\hat{b}}_i{}^*\mathring{\Gamma}_{i\lambda} - \mathring{\Gamma}^*_{i\lambda}\mathring{\hat{b}}_i\mathring{\hat{a}}_\lambda), \tag{A2·2c}$$

where we have used the notations

$$\mathring{\hat{a}}_\lambda{}^* = U\hat{a}_\lambda{}^*U^\dagger, \qquad \mathring{\hat{b}}_i{}^* = U\hat{b}_i{}^*U^\dagger\,. \tag{A2·3}$$

The parameters $\Gamma_{i\lambda}$ and $\mathring{\Gamma}_{i\lambda}$ satisfy the time-reversal relation

$$\Gamma_{\bar{i}\bar{\lambda}} = \Gamma^*_{i\lambda}, \qquad \mathring{\Gamma}_{\bar{i}\bar{\lambda}} = -\mathring{\Gamma}^*_{i\lambda}\,. \tag{A2·4}$$

Then we obtain a possible canonical form of classical image of one-body operators:

$$\langle c|\hat{a}_\lambda{}^*\hat{b}_i{}^* - \hat{b}_{\bar{i}}\hat{a}_{\bar{\lambda}}|c\rangle = -i[p^\dagger + q^*pq^*]_{\lambda i}\,, \tag{A2·5a}$$

$$\begin{aligned}\langle c|\hat{a}_\lambda{}^*\hat{b}_i{}^* + \hat{b}_{\bar{i}}\hat{a}_{\bar{\lambda}}|c\rangle = [&(1+q^*q^T)^{-1/2}q^*\{1-(1+q^Tq^*)^{1/2}p(1+q^*q^T)p^\dagger\\ &\times(1+q^Tq^*)^{1/2}\}^{1/2}(1+q^Tq^*)^{-1/2}\\ &+(1+q^*q^T)^{-1/2}\{1-(1+q^*q^T)^{1/2}p^\dagger(1+q^Tq^*)p(1+q^*q^T)^{1/2}\}^{1/2}\\ &\times(1+q^*q^T)^{-1/2}q^*]_{\lambda i}\,,\end{aligned} \tag{A2·5b}$$

$$\langle c|\hat{a}_\lambda{}^*\hat{a}_{\bar{\mu}} + \hat{a}_\mu{}^*\hat{a}_{\bar{\lambda}}|c\rangle = -i[p^\dagger q^T - q^*p]_{\lambda\bar{\mu}}\,, \tag{A2·5c}$$

$$\begin{aligned}\langle c|\hat{a}_\lambda{}^*\hat{a}_{\bar{\mu}} - \hat{a}_\mu{}^*\hat{a}_{\bar{\lambda}}|c\rangle = [&1+(1+q^*q^T)^{-1/2}q^*\{1-(1+q^Tq^*)^{1/2}p(1+q^*q^T)p^\dagger\\ &\times(1+q^Tq^*)^{1/2}\}^{1/2}q^T(1+q^*q^T)^{-1/2}\\ &-(1+q^*q^T)^{-1/2}\{1-(1+q^*q^T)^{1/2}p^\dagger(1+q^Tq^*)p(1+q^*q^T)^{1/2}\}^{1/2}\\ &\times(1+q^*q^T)^{-1/2}]_{\lambda\bar{\mu}}\,,\end{aligned} \tag{A2·5d}$$

$$\langle c|\hat{b}_i{}^*\hat{b}_{\bar{j}} + \hat{b}_j{}^*\hat{b}_{\bar{i}}|c\rangle = i[q^\dagger p^T - p^*q]_{i\bar{j}}\,, \tag{A2·5e}$$

$$\begin{aligned}\langle c|\hat{b}_i{}^*\hat{b}_{\bar{j}} - \hat{b}_j{}^*\hat{b}_{\bar{i}}|c\rangle = [&1+(1+q^\dagger q)^{-1/2}q^\dagger\{1-(1+qq^\dagger)^{1/2}p^T(1+q^\dagger q)p^*\\ &\times(1+qq^\dagger)^{1/2}\}^{1/2}q(1+q^\dagger q)^{-1/2}\\ &-(1+q^\dagger q)^{-1/2}\{1-(1+q^\dagger q)^{1/2}p^*(1+qq^\dagger)p^T(1+q^\dagger q)^{1/2}\}^{1/2}\\ &\times(1+q^\dagger q)^{-1/2}]_{i\bar{j}}\,.\end{aligned} \tag{A2·5f}$$

The matrices q^* and p have only the following elements:

$$q^*_{\lambda i}, \qquad p_{i\lambda}\,. \tag{A2·6}$$

They satisfy the following time-reversal relation:

$$q_{\lambda\bar{i}}=q^*_{\lambda i}\,,\qquad p_{\bar{i}\lambda}=p^*_{i\lambda}\,. \tag{A2·7}$$

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