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A Canonical Coordinate System Suitable for Adiabatic Treatment of Collective Motion

—— *An Illustrative Model* ——

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With the aid of the canonicity condition, we specify a canonical coordinate system suitable for the adiabatic treatment of "large" amplitude collective motion. We introduce a double transformation in order to specify a time-dependent Slater determinantal state. This specification follows that given by Baranger and Veneroni. The utility of the canonicity condition is shown with the use of an illustrative model.

The time-dependent Hartree-Fock (TDHF) method is one of the most promising candidates for the microscopic description of large amplitude collective motion. This method provides us physical information in a classical form. Hence, it is necessary to quantize the system obtained by TDHF method in order to extract all the information in a quantal form. However, the TDHF method does not involve the prescription of how to quantize in its framework. The canonicity condition introduced by Marumori, Maskawa, Sakata and one of the present authors (A. K.) enables us to specify exactly a certain canonical coordinate system of the collective submanifold and to adopt the prescription of canonical quantization.[1)]

In spite of this specification, there still remains the problem due to the ambiguity in the ordering of non-commutable operators. We have now two ways to deal with this problem: One is a way to exclude completely this ambiguity by introducing the remaining degrees of freedom, i.e., the independent-particle degrees of freedom, in addition to the collective ones. Following this way, we have expressed any physical quantity in terms of these two types of degrees of freedom and then quantized the quantity so as to reproduce its original quantal algebra.[2)] We have obtained, in this way, a boson or boson-fermion representation of physical operators in a useful version.[3)] The other way is to suppress the effect due to the ambiguity by taking advantage of the intrinsic property of the collective motion, the adiabaticity.[4)] It is expected that the ambiguity will give rise to the effect of $O(1/\Omega^2)$ on the potential term (where Ω is the so-called volume), when the collective coordinate system is properly chosen.

In this short note, we show how well the canonicity condition works in the specification of canonical coordinate system suitable for the adiabatic treatment of large amplitude collective motion, using an illustrative model ——coupled Lipkin model.[5)]

First, we give the coupled Lipkin model: The Hamiltonian is given as

$$\hat{H}=\sum_{\sigma}\hat{H}_{\sigma}-\sum_{\sigma}V_{\sigma\bar{\sigma}}\hat{S}_{\sigma+}\hat{S}_{\bar{\sigma}-}\,,$$

$$\hat{H}_{\sigma}=2\varepsilon_{\sigma}\hat{S}_{\sigma 0}-\frac{1}{2}V_{\sigma\sigma}(\hat{S}^2_{\sigma+}+\hat{S}^2_{\sigma-})\,;$$

$$\sigma=1,\,\bar{1}\,. \tag{1}$$

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

$$\hat{S}_{\sigma+}=\sum_{m}\hat{a}^{*}_{\sigma j_\sigma m}(-)^{j_\sigma-m}\hat{b}^{*}_{\sigma j_\sigma\bar{m}}\,,\quad \hat{S}_{\sigma-}=[\hat{S}_{\sigma+}]^{\dagger}\,,$$

$$\hat{S}_{\sigma 0}=\frac{1}{2}\sum_{m}(\hat{a}^*_{\sigma j_\sigma m}\hat{a}_{\sigma j_\sigma m}+\hat{b}^*_{\sigma j_\sigma m}\hat{b}_{\sigma j_\sigma m})-\Omega_\sigma ;$$

$$\Omega_\sigma=j_\sigma+\frac{1}{2}, \tag{2}$$

which obey the algebra of $SU(2)$. The Hamiltonian $\hat{H}_\sigma$ is just that of Lipkin model. In this note, we take up only the subspace with zero seniority number.

Following the specification of adiabatic coordinate system given by Baranger and Venenori,[4] we start with the following type of wave packet:

$$|c\rangle=VU|0\rangle, \tag{3}$$

$$\hat{a}_{\sigma j_\sigma m}|0\rangle=\hat{b}_{\sigma j_\sigma m}|0\rangle=0\,, \tag{4a}$$

$$U=\exp[S]\,;\quad S=\sum_\sigma(\hat{S}_{\sigma+}\Gamma_\sigma-\Gamma_\sigma^*\hat{S}_{\sigma-}), \tag{4b}$$

$$V=\exp[\mathring{S}]\,;\quad \mathring{S}=\sum_\sigma(\hat{\mathring{S}}_{\sigma+}\mathring{\Gamma}_\sigma-\mathring{\Gamma}_\sigma^*\hat{\mathring{S}}_{\sigma-}), \tag{4c}$$

where the quasi-spin operators $\hat{\mathring{S}}_{\sigma\pm}$ are defined in terms of the quasi-particle and quasi-hole operators

$$\hat{\mathring{\xi}}^*_{\sigma j_\sigma m}=U\hat{a}^*_{\sigma j_\sigma m}U^\dagger\,,\quad \hat{\mathring{\eta}}^*_{\sigma j_\sigma m}=U\hat{b}^*_{\sigma j_\sigma m}U^\dagger\,. \tag{5}$$

According to the specification of Branger-Veneroni, we require that the parameters Γ_σ, Γ_σ^*, $\mathring{\Gamma}_\sigma$ and $\mathring{\Gamma}_\sigma^*$ satisfy the following relations:

$$\Gamma_\sigma^*=\Gamma_\sigma=\gamma_\sigma^e\,,\quad \mathring{\Gamma}_\sigma^*=\mathring{\Gamma}_\sigma=i\gamma_\sigma^o\,;$$

$$\gamma_\sigma^e \text{ and } \gamma_\sigma^o \text{ are real numbers.} \tag{6}$$

Then, the quasi-particle and quasi-hole operators with respect to $|c\rangle$ are given as

$$\begin{pmatrix}\hat{\xi}^*_{\sigma j_\sigma m}\\ (-)^{j_\sigma-m}\hat{\eta}_{\sigma j_\sigma \bar{m}}\end{pmatrix}=VU\begin{pmatrix}\hat{a}^*_{\sigma j_\sigma m}\\ (-)^{j_\sigma-m}\hat{b}_{\sigma j_\sigma \bar{m}}\end{pmatrix}U^\dagger V^\dagger$$

$$=\begin{pmatrix}\mathring{U}_\sigma^* & -\mathring{V}_\sigma^*\\ \mathring{V}_\sigma & \mathring{U}_\sigma\end{pmatrix}\begin{pmatrix}U_\sigma^* & -V_\sigma^*\\ V_\sigma & U_\sigma\end{pmatrix}\times\begin{pmatrix}\hat{a}^*_{\sigma j_\sigma m}\\ (-)^{j_\sigma-m}\hat{b}_{\sigma j_\sigma \bar{m}}\end{pmatrix}, \tag{7}$$

$$U_\sigma=\cos\gamma_\sigma^e\,,\quad V_\sigma=\sin\gamma_\sigma^e\,, \tag{8a}$$

$$\mathring{U}_\sigma=\cos\gamma_\sigma^o\,,\quad \mathring{V}_\sigma=-i\sin\gamma_\sigma^o\,. \tag{8b}$$

Now we specify a canonical coordinate system with the aid of the canonicity conditions

$$\langle c|-i\partial_{p_\alpha}|c\rangle=0\,,$$

$$\langle c|i\partial_{q_\alpha}|c\rangle=p_\alpha\,;\quad \alpha=1,\bar{1}\,. \tag{9}$$

These conditions give rise to the following relations: The infinitesimal generators defined by

$$\hat{Q}_\alpha=i\partial_{p_\alpha}(VU)\cdot(VU)^\dagger,$$

$$\hat{P}_\alpha=i\partial_{q_\alpha}(VU)\cdot(VU)^\dagger, \tag{10}$$

satisfy the weak canonicity relations

$$\langle c|[\hat{Q}_\alpha,\hat{P}_{\alpha'}]|c\rangle=i\delta_{\alpha\alpha'}\,,$$

$$\langle c|[\hat{Q}_\alpha,\hat{Q}_{\alpha'}]|c\rangle=\langle c|[\hat{P}_\alpha,\hat{P}_{\alpha'}]|c\rangle=0\,. \tag{11}$$

After some calculations, we obtain the explicit forms of the canonicity conditions (9) as

$$\sum_\sigma 2\Omega_\sigma\sin 2\gamma_\sigma^o\cdot\partial_{p_\alpha}\gamma_\sigma^e=0\,,$$

$$\sum_\sigma 2\Omega_\sigma\sin 2\gamma_\sigma^o\cdot\partial_{q_\alpha}\gamma_\sigma^e=-p_\alpha\,. \tag{12}$$

Then, it is easily ascertained that the following is a possible solution of Eqs. (12):

$$\gamma_\sigma^e=\frac{1}{2}q_\alpha\,,\quad \sin 2\gamma_\sigma^o=-\frac{1}{\Omega_\sigma}p_\alpha\,. \tag{13}$$

The classical images of the quasi-spin operators, $\hat{S}_{\sigma\pm}$ and $\hat{S}_{\sigma 0}$, can be expressed in terms of these canonical variables as follows:

$$S_{\sigma x}=\langle c|\frac{1}{2}(\hat{S}_{\sigma-}+\hat{S}_{\sigma+})|c\rangle$$

$$=\Omega_\sigma\sqrt{1-(p_\sigma/\Omega_\sigma)^2}\,\sin q_\sigma\,,$$

$$S_{\sigma y}=\langle c|\frac{i}{2}(\hat{S}_{\sigma-}-\hat{S}_{\sigma+})|c\rangle$$

$$=-\Omega_\sigma(p_\sigma/\Omega_\sigma),$$

$$S_{\sigma z}=\langle c|\hat{S}_{\sigma 0}|c\rangle$$

$$=-\Omega_\sigma\sqrt{1-(p_\sigma/\Omega_\sigma)^2}\cos q_\sigma\,. \tag{14}$$

Here we check the canonicity of these

variables q_σ and p_σ with the use of the Poisson bracket

$$\{A, B\}_{(q,p)}=\sum_\sigma(\partial_{q_\sigma}A\cdot\partial_{p_\sigma}B-\partial_{p_\sigma}A\cdot\partial_{q_\sigma}B). \quad (15)$$

Then, we can easily ascertain the following commutation relations:

$$i\{S_{\sigma i}, S_{\sigma' j}\}_{(q,p)}=i\delta_{\sigma\sigma'}S_{\sigma i\times j};\quad i, j=x, y, z. \quad (16)$$

Further, we make clear the relation between these variables and those of usual boson representation. In the usual boson representation, the classical images of quasi-spin operators are given by

$$S_{\sigma+}=b_\sigma^*\sqrt{2\Omega_\sigma-b_\sigma^*b_\sigma},$$
$$S_{\sigma-}=\sqrt{2\Omega_\sigma-b_\sigma^*b_\sigma}\cdot b_\sigma,$$
$$S_{\sigma0}=b_\sigma^*b_\sigma-\Omega_\sigma. \quad (17)$$

Then, we define a set of canonical variables as

$$\mathring{q}_\sigma=(b_\sigma+b_\sigma^*)/\sqrt{2},\quad \mathring{p}_\sigma=(b_\sigma-b_\sigma^*)/\sqrt{2}i. \quad (18)$$

Comparing the expression (17) with (14), we obtain the following relations:

$$\mathring{q}_\sigma=\frac{\Omega_\sigma\sqrt{1-(p_\sigma/\Omega_\sigma)^2}\cdot\sin q_\sigma}{\sqrt{\Omega_\sigma\{1+\sqrt{1-(p_\sigma/\Omega_\sigma)^2}\cdot\cos q_\sigma\}/2}},$$
$$\mathring{p}=\frac{p_\sigma}{\sqrt{\Omega_\sigma\{1+\sqrt{1-(p_\sigma/\Omega_\sigma)^2}\cdot\cos q_\sigma\}/2}}. \quad (19)$$

The above relation is canonical, because of the relations

$$\{\mathring{q}_\sigma, \mathring{p}_{\sigma'}\}_{(q,p)}=\delta_{\sigma\sigma'},$$
$$\{\mathring{q}_\sigma, \mathring{q}_{\sigma'}\}_{(q,p)}=\{\mathring{p}_\sigma, \mathring{p}_{\sigma'}\}_{(q,p)}=0. \quad (20)$$

Further, the above two types of canonical variables have the following simple geometrical relation: We define another set of canonical variables from b_σ and b_σ^* as

$$\exp[-i\tilde{q}_\sigma]=-b_\sigma^*/\sqrt{b_\sigma b_\sigma^*},$$
$$\tilde{p}_\sigma=\Omega_\sigma-b_\sigma^*b_\sigma. \quad (21)$$

Then, the canonical coordinate system (q_σ, p_σ) is obtained from $(\tilde{q}_\sigma, \tilde{p}_\sigma)$ by a rotation of reference frame, where the quasi-spin is described as a vector $S_\sigma=(S_{\sigma x}, S_{\sigma y}, S_{\sigma z})$, through the angle $2\pi/3$ about the axis $(1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$.

Here, we give the classical image of the Hamiltonian (1) in terms of the present canonical variables:

$$H=\langle c|\hat{H}|c\rangle=\sum_\sigma H_\sigma-\sum_\sigma V_{\sigma\bar{\sigma}}S_{\sigma+}S_{\bar{\sigma}-},$$
$$H_\sigma=-\Omega_\sigma[2\varepsilon_\sigma\sqrt{1-(p_\sigma/\Omega_\sigma)^2}\cdot\cos q_\sigma$$
$$+V_{\sigma\sigma}(\Omega_\sigma-\frac{1}{2})\{(1-(p_\sigma/\Omega_\sigma)^2)\sin^2 q_\sigma$$
$$-(p_\sigma/\Omega_\sigma)^2\}]. \quad (22)$$

The Hamiltonian H_σ can be expressed in power series with respect to $(p_\sigma/\Omega_\sigma)^2$ as

$$H_\sigma=\frac{1}{2}M_\sigma(q_\sigma)^{-1}p_\sigma^2$$
$$+V_\sigma(q_\sigma)+O((p_\sigma/\Omega_\sigma)^4),$$
$$M_\sigma(q_\sigma)^{-1}=2\varepsilon_\sigma\{\cos q_\sigma+\chi_\sigma(1+\sin^2 q_\sigma)\}/\Omega_\sigma,$$
$$V_\sigma(q_\sigma)=-2\varepsilon_\sigma\Omega_\sigma(\cos q_\sigma+\frac{1}{2}\chi_\sigma\sin^2 q_\sigma),$$
$$\chi_\sigma=V_{\sigma\sigma}(\Omega_\sigma-\frac{1}{2})/\varepsilon_\sigma. \quad (23)$$

The above expression is nothing but that obtained with the use of ordinary adiabatic TDHF method by Holzwarth.[6]

The exact quantized form of the classical image of quasi-spin (14) is given as[7]

$$\hat{S}_{\sigma z}+i\hat{S}_{\sigma x}=-e^{-i\hat{q}_\sigma/2}\sqrt{\Omega_\sigma'^2-\hat{p}_\sigma^2}\,e^{-i\hat{q}_\sigma/2},$$
$$\hat{S}_{\sigma z}-i\hat{S}_{\sigma x}=-e^{i\hat{q}_\sigma/2}\sqrt{\Omega_\sigma'^2-\hat{p}_\sigma^2}\,e^{i\hat{q}_\sigma/2},$$
$$\hat{S}_{\sigma y}=-\hat{p}_\sigma;\quad [\hat{q}_\sigma, \hat{p}_{\sigma'}]=i\delta_{\sigma\sigma'}, \quad (24)$$

where Ω'_σ is equal to $\Omega_\sigma+\frac{1}{2}$. The replacement of Ω_σ by $\Omega_\sigma+\frac{1}{2}$ is due to the quantum fluctuation of the quasi-spin vector $\hat{S}_\sigma$ itself. Therefore, with the use of the present canonical coordinate system the ambiguity due to ordering brings about the effect of order $O(1/\Omega_\sigma^2)$ on the potential when we simply replace Ω_σ by $\Omega_\sigma+\frac{1}{2}$.

In this way, we can specify a canonical coordinate system suitable for the adiabatic treatment of large amplitude collective motion, with the aid of the canonicity condition. The above derivation is directly applicable to a system which can be described with the use of $SU(2)$ product space. Further, we can specify a canonical coordinate system for more general cases. On the other hand, we can study the structure of the adiabatic approximation in the specification of the collective submanifold, with the use of this exactly canonical coordinate system. These points will be discussed in succeeding papers.

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