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Angular Momentum Projection with Pfaffian

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Abstract. Recent developments to rewrite the Onishi formula for an evaluation of the so-called norm overlap kernel necessary in angular momentum projection are to be discussed. The essential ingredients in the development, that is, the Fermion coherent states, the Grassmann numbers, and the Pfaffian, are explained.

1 Introduction

The Hartree-Fock-Bogoliubov (HFB) method is greatly successful in descriptions of nuclear many-body systems [1]. Particularly, correlations to cause nuclear deformation and pairing are effectively taken into account through the HFB ansatz

$$|\mathrm{HFB}\rangle = \mathfrak{N} \exp\left(\frac{1}{2}\sum_{ij} Z_{ij} a_i^\dagger a_j^\dagger\right)|0\rangle, \tag{1}$$

where the creation and annihilation operators for nucleons are denoted as $(a, a^\dagger)$ and the associated vacuum $|0\rangle$ is defined as

$$a_i|0\rangle = 0. \tag{2}$$

The variation parameter Z_{ij} is expressed as a skew-symmetric matrix and it is written in terms of the Bogoliubov transformation

$$Z = (VU^{-1})^*. \tag{3}$$

The Bogoliubov transformation is a canonical transformation from the particle basis $(a, a^\dagger)$ to a quasi-particle basis $(\beta, \beta^\dagger)$

$$a_i = \sum_j U_{ij}\beta_j + V_{ij}^*\beta_j^\dagger. \tag{4}$$

The condition for a canonical transformation restricts U and V to satisfy the following relations.

$$U^\dagger U + V^\dagger V = 1, \qquad UU^\dagger + V^* V^T = 1, \tag{5}$$

$$U^T V + V^T U = 0, \qquad UV^\dagger + V^* U^T = 0. \tag{6}$$

The normalization constant $\mathfrak{N}$ is written as

$$\mathfrak{N} = \sqrt{\det(U)} \tag{7}$$

thanks to the Onishi formula [2, 3].

The HFB ansatz breaks the rotational symmetry, so that it is a wave packet with respect to angular momentum projection. To compare with experimental data from a quantum mechanical viewpoint, it is necessary to project out a component with a good angular momentum.

$$|IM\rangle = \sum_K g_K \hat{P}^I_{MK} |\text{HFB}\rangle, \tag{8}$$

where an angular momentum projection operator is given as

$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2} \int\int\int d\alpha \sin\beta d\beta d\gamma D^{I*}_{MK}(\alpha\beta\gamma) \hat{R}(\alpha\beta\gamma). \tag{9}$$

The rotational operator $\hat{R}(\alpha\beta\gamma)$ is defined as

$$\hat{R}(\alpha\beta\gamma) = \exp(-i\alpha\hat{J}_3)\exp(-i\beta\hat{J}_2)\exp(-i\gamma\hat{J}_3). \tag{10}$$

Wigner's D function, a representation of the group SO(3), is denoted as $D^I_{MK}(\alpha\beta\gamma)$ [4]. Hereafter, the Euler angles α, β, γ are collectively expressed as Ω.

To carry out the angular momentum projection calculation, the Hill-Wheeler equation needs to be solved [5].

$$\sum_{K'} (H^I_{KK'} - E^I N^I_{KK'}) g_{K'} = 0. \tag{11}$$

The energy and norm matrices are written as

$$\begin{pmatrix} H^I_{KK'} \\ N^I_{KK'} \end{pmatrix} = \int d\Omega D^{I*}_{KK'}(\Omega) \begin{pmatrix} \mathcal{H}(\Omega) \\ \mathcal{N}(\Omega) \end{pmatrix}, \tag{12}$$

where $\mathcal{N}(\Omega)$ and $\mathcal{H}(\Omega)$ are called respectively as the norm and energy overlap kernels, and they are defined as

$$\begin{pmatrix} \mathcal{N}(\Omega) \\ \mathcal{H}(\Omega) \end{pmatrix} = \langle \text{HFB}| \begin{pmatrix} \hat{1} \\ \hat{H} \end{pmatrix} \hat{R}(\Omega)|\text{HFB}\rangle. \tag{13}$$

The evaluation of these overlap kernels has been difficult, particularly for cranked HFB states to simulate high-spin states. The problem lies in the assignment of the sign of the norm overlap kernel because it is evaluated with help of the Onishi formula

$$\mathcal{N}(\Omega) = \sqrt{\det(U^\dagger D^\dagger(\Omega) U + V^\dagger D^T(\Omega) V)}. \tag{14}$$

The determinant inside the square root is generally a complex function of the Euler angle. This means that it is necessary to find a proper branch for given Ω of the norm overlap kernel.

2 The Sign Problem and Nodal Lines

The sign assignment of the norm overlap kernel can be carried out by tracking the change of the phase $\theta(\Omega)$ of $\mathcal{N}(\Omega) = r(\Omega)\exp(i\theta(\Omega))$. This approach relying on the continuity and differentiability of the norm overlap kernel was first developed by Hara, Hayashi and Ring [6].

However, it was found later that such a method does not always work, in particular, in the cases that high-spin states are considered [7]. According to my previous work [7], angular momentum projection can be executed successfully for non-cranked HFB states as well as low-spin states. However, the highly cranked HFB shows a peculiar feature which prevents a successful angular momentum projection. The feature is originated from the zeros of the norm overlap kernel, that is, $\mathcal{N}(\Omega) = 0$. Due to the three dimensionality of the Euler space, the collection of such zeros forms a closed loop, which is named "nodal line". The sign assignment method developed by Hara, et al. does not work in the vicinity of the nodal lines in numerical calculations. As a result, wrong sign assignments are made to give rise to negative eigenvalues for the Norm matrix $N^I_{KK'}$, which need to be positive definite by definition.

The improvement was found recently by the author, and it solves the sign assignment problem in the framework of the Onishi formula. The work is in preparation for publication [8].

Another new approach was proposed recently by Robledo [9], and several new works followed quite recently [10–12]. In the following, I would like to concentrate on the latter approach.

3 Pfaffian and a Square Root of Determinant

Like a determinant of a matrix A, a Pfaffian is a polynomial consisting of matrix elements of a matrix A. But it is defined only for skew-symmetric matrix $A^T = -A$. When the dimensionality of A is odd, the corresponding Pfaffian identically vanishes. In the even dimensional cases, there is a relation between the determinant and the Pfaffian of a skew-symmetric matrix A, as

$$\det(A) = \{\mathrm{Pf}(A)\}^2. \tag{15}$$

In many cases, the relation is inverted to define the Pfaffian in terms of the determinant, as

$$\mathrm{Pf}(A) = \sqrt{\det(A)}. \tag{16}$$

Of course, it is possible to chose the negative sign in taking the square root, but it is not natural in many cases.

Robledo found that the Onishi formula can be expressed in terms of the Pfaffian [9]. Without a square-root operation, there would not be the sign assignment problem in the norm overlap kernel.

Nonetheless, Pfaffian is just a result in an attempt to rewrite the Onishi formula. What is more essential is an introduction of the Fermion coherent states, associated with eigenvalues expressed in terms of Grassmann numbers [13].

4 Fermion Coherent States and Grassmann Numbers

The Fermion coherent state $|\boldsymbol{\xi}\rangle$ is defined as an eigenstate of the annihilation operator a_i, that is,

$$a_i|\boldsymbol{\xi}\rangle = \xi_i|\boldsymbol{\xi}\rangle, \tag{17}$$

where $\boldsymbol{\xi}$ means $(\xi_1, \xi_2, \cdots, \xi_M)$. If a_i satisfies the anticommutation relations, $a_i a_j = -a_j a_i$ and $a_i a_j^\dagger = -a_j^\dagger a_i + \delta_{ij}$, then ξ_i needs to be a Grassmann number, which satisfies the anticommuation relation as well.

$$\xi_i \xi_j + \xi_j \xi_i = 0. \tag{18}$$

The special case happens when $i = j$, which results in $\xi_i^2 = 0$. This means that the algebra related to the Grassmann number contains only bilinear polynomials [13].

An extension of the Fock space with the Grassmann numbers is necessary so as to consider a space spanned by the Fermion coherent states. The Fermion coherent states form a complete set, and its completeness relation is given as

$$\int \prod_i d\xi_i^* d\xi_i \exp(-\sum_j^M \xi_j^* \xi_j)|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}| = \hat{1}. \tag{19}$$

However, the Fermion coherent states are not orthogonal, so that an overlap between two Fermion coherent states is calculated to be

$$\langle\boldsymbol{\xi}|\boldsymbol{\xi}'\rangle = \exp(\sum_i \xi_i^* \xi_i'). \tag{20}$$

Like the generator coordinate method, an expansion in terms of the Fermion coherent states cannot avoid an issue of the overcompleteness. At any rate, an arbitrary quantum state Φ in the Fock space is expanded through the Fermion coherent states as

$$|\Phi\rangle = \int \prod_i d\xi_i^* d\xi_i \exp(-\sum_j^M \xi_j^* \xi_j)\Phi(\xi^*)|\boldsymbol{\xi}\rangle, \tag{21}$$

where $\Phi(\xi^*) = \langle\xi|\Phi\rangle$.

The Fermion coherent state can be expressed as

$$|\boldsymbol{\xi}\rangle = \exp\left(-\sum_i^M \xi_i a_i^\dagger\right)|0\rangle, \tag{22}$$

which is similar to the Bosonic coherent state.

5 Calculation of Norm Overlap with Fermion Coherent States

In the following discussions, we consider HFB states without the normalization constant, or $\mathfrak{N} = 1$ for the sake of simplicity. (An amendment can be easily done for the normalization in later stages.)

Thus, a norm overlap is written as

$$\mathcal{N}(\Omega) = \langle \text{HFB}|\hat{R}(\Omega)|\text{HFB}\rangle = \langle 0|\mathrm{e}^{\frac{1}{2}\sum_{ij} Z^*_{ij} a_j a_i}\hat{R}(\Omega)\exp^{\frac{1}{2}\sum_{kl} Z_{kl} a^\dagger_k a^\dagger_l}|0\rangle. \quad (23)$$

Thanks to $\hat{R}(\Omega)|0\rangle = |0\rangle$, a rotated HFB state can be expressed as

$$\hat{R}(\Omega)|\text{HFB}\rangle = \exp\Big(\frac{1}{2}\sum_{ij} Z_{ij}\hat{R}(\Omega)a^\dagger_i a^\dagger_j \hat{R}^\dagger(\Omega)\Big)\hat{R}(\Omega)|0\rangle \quad (24)$$

$$= \exp\Big(\frac{1}{2}\sum_{ij} Z_{ij} a^\dagger_i(\Omega) a^\dagger_j(\Omega)\Big)|0\rangle. \quad (25)$$

Using the Baker-Hausdorff formula, the "rotated" creation operator is expressed in terms of the original creation operator as

$$a^\dagger_j(\Omega) = \hat{R}(\Omega)a^\dagger_i \hat{R}^\dagger(\Omega) = \sum_i D_{ji}(\Omega)a^\dagger_i. \quad (26)$$

Therefore, in the original basis, the rotated HFB state is expressed as

$$\hat{R}(\Omega)|\text{HFB}\rangle = \exp\Big(\frac{1}{2}\sum_{ij} Z_{ij}(\Omega)a^\dagger_i a^\dagger_j\Big)|0\rangle, \quad (27)$$

where

$$Z(\Omega) = D(\Omega) Z D^T(\Omega). \quad (28)$$

As a result of the above expression and Eq.(3), the Bogoliubov transformation matrix in the rotated framework is given as

$$U(\Omega) = D(\Omega)U, \quad V(\Omega) = D^*(\Omega)V. \quad (29)$$

The rotated norm overlap is hence simplified to

$$\mathcal{N}(\Omega) = \langle \text{HFB}|\hat{R}(\Omega)|\text{HFB}\rangle = \langle 0|\mathrm{e}^{\frac{1}{2}\sum_{ij} Z^*_{ij} a_j a_i}\exp^{\frac{1}{2}\sum_{kl} Z_{kl}(\Omega) a^\dagger_k a^\dagger_l}|0\rangle. \quad (30)$$

Inserting the completeness relation of the Fermion coherent state, the norm overlap kernel becomes

$$\mathcal{N}(\Omega) = \int\prod_\alpha d\xi^*_\alpha d\xi_\alpha \mathrm{e}^{-\sum_\alpha \xi^*_\alpha\xi_\alpha}\langle 0|\mathrm{e}^{\frac{1}{2}\sum_{ij} Z^*_{ij} a_j a_i}|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}|\exp^{\frac{1}{2}\sum_{kl} Z_{kl}(\Omega) a^\dagger_k a^\dagger_l}|0\rangle \quad (31)$$

$$= \int\prod_\alpha d\xi^*_\alpha d\xi_\alpha \mathrm{e}^{-\sum_\alpha \xi^*_\alpha\xi_\alpha}\mathrm{e}^{\frac{1}{2}\sum_{ij} Z^*_{ij}\xi_j\xi_i}\exp^{\frac{1}{2}\sum_{kl} Z_{kl}(\Omega)\xi^\dagger_k\xi^\dagger_l}\langle 0|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}|0\rangle.$$

Using a fact that $\langle \boldsymbol{\xi} | 0 \rangle = 1$, the above integral can be summarised to the Gaussian integral form:

$$\mathcal{N}(\Omega) = \int \prod_i d\xi_i^* d\xi_i G(\bar{\xi}), \tag{32}$$

where the Gaussian of the Grassmann numbers ξ_i is defined as

$$G(\bar{\xi}) \equiv \exp\left(\frac{1}{2}\bar{\xi}^T \mathbb{X} \bar{\xi}\right). \tag{33}$$

Here, the $2M$-dimensional Grassmann vector $\bar{\xi}$ is defined as

$$\bar{\xi} = \begin{pmatrix} \xi_1^* \\ \xi_2^* \\ \vdots \\ \xi_M^* \\ \xi_1 \\ \xi_2 \\ \vdots \\ \xi_M \end{pmatrix}. \tag{34}$$

In this basis, the $2M$-dimensional matrix $\mathbb{X}$ is given as

$$\mathbb{X} = \begin{pmatrix} Z(\Omega) & -I \\ I & -Z^* \end{pmatrix}. \tag{35}$$

Following the rules of the Grassmann integral carefully, the Gaussian integral gives rise to

$$\mathcal{N}(\Omega) = s_M \mathrm{Pf}(\mathbb{X}), \tag{36}$$

where the phase factor is given as $s_M = (-1)^{M(M+1)/2}$. This formula was first derived by Robledo [9].

6 Normalisation

The above formula does not take the normalization into account, which is given in Eq.(7). Together with Eq.(29), the normalization constant of the rotated HFB state is calculated to be

$$\mathfrak{N}(\Omega) = \sqrt{\mathrm{Det}(U(\Omega))} = \sqrt{\mathrm{Det}(D(\Omega)U)} = \sqrt{\mathrm{Det}(U)}, \tag{37}$$

which means that the normalisation is invariant against rotation. (The unitarity of the rotational group is used in the above result.)

Therefore, the complete expression for the Pfaffian formula becomes

$$\mathcal{N}(\Omega) = s_M \mathrm{Det}(U) \mathrm{Pf}(\mathbb{X}). \tag{38}$$

In my preliminary numerical calculations using the above formula, I found that the Pfaffian part tends to become an extremely big number, while the Determinant of U tends to be very small. A product of a very small and a very large numbers may cause a numerical error in obtaining the norm overlap kernel, which needs a careful numerical treatment. On the contrary, there is no sign problem with the new Pfaffian formula because there is no square root operation in the formula.

7 Conclusion

A new formula was derived by Robledo for the calculation of the norm overlap kernel, with help of the Fermion coherent state and the Grassmann numbers. The result is expressed in terms of the Pfaffian. I have added a modification coming from the normalization to complete the formula. The sign problem can be avoided with the new Pfaffian formula, but there can be a need for a careful numerical treatment to avoid errors in the evaluation of the norm overlap kernel with the Pfaffian formula.

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