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Comparison of Various HFB Overlap Formulae

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Abstract. The nuclear many-body approach beyond the mean-field approximation demands overlap calculations of different many-body states. Norm overlaps between two different Hartree-Fock-Bogoliubov states can be calculated by means of the Onishi formula. However, the formula leaves the sign of the norm overlap undetermined. Several approaches have been proposed by Hara-Hayashi-Ring, Neergård-Wüst, and Robledo. In the present paper, the Neergård-Wüst formula is examined whether it is applicable to practical numerical calculations, although the formula was dismissed by many nuclear theoreticians so far for unknown reasons.

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1 Introduction

The Hartree-Fock-Bogoliubov (HFB) theory has been successful in descriptions of interacting nuclear many-body systems. It can deal with two types of many-body correlations: nuclear deformation and nuclear pairing. However, it is based on the variational theory, which results in the framework of the mean field approximation.

In order to take more complicated correlations into account beyond the mean field approximation, the generator coordinate method (GCM) was proposed by Wheeler and his collaborators [1]. For example, the surface oscillation of a nucleus can be handled within GCM as a superposition of different HFB states having different deformation q

$$|\Psi\rangle = \int f(q)|\mathrm{HFB}(q)\rangle dq. \tag{1}$$

The weight function $f(q)$ is determined through the variational principle, which results in the so-called Hill-Wheeler equation [2]. The Hill-Wheeler equation consists of the overlap kernels

$$\begin{pmatrix} N(q,q') \\ H(q,q') \end{pmatrix} = \langle \mathrm{HFB}(q)| \begin{pmatrix} \hat{I} \\ \hat{H} \end{pmatrix} |\mathrm{HFB}(q')\rangle, \tag{2}$$

where $\hat{I}$ and $\hat{H}$ denote the identity and Hamiltonian operators, respectively. The deformation parameter q here can be generalised to the generator coordinate, which characterises the HFB states.

The progress in the application of GCM based on HFB has been unfortunately quite slow due to the difficulty in the calculation of the norm overlap kernel $N(q, q')$.

In principle, $N(q, q')$ can be calculated with the Onishi formula [3,4]. However, the formula undetermines the sigh of $N(q, q')$. To solve this "sign problem", various approaches were proposed to date. Hara, Hayashi and Ring proposed a method based on the continuity of the norm overlap kernel as a function of the generator coordinate q [5]. This approach is widely employed at present. However, it was demonstrated recently in the context of the angular momentum projection (an application of GCM) that it is difficult to calculate the norm overlap kernels between the cranked HFB states because of the presence of "nodal lines" [6]. Quite recently, Robledo demonstrated that an introduction of the Pfaffian can eliminate the problem in the Onishi formula [7].

Already in the 1980s', however, Neergård and Wüst proposed an different approach [8], which is based on the diagonalisation of the Bogoliubov transformation matrix. For unknown reasons, their approach was not widely approved as an effective method. In this paper, I would like to consider the reasons why the Neergård-Wüst method has been ignored so far, and investigate its validity through comparisons with other effective methods.

2 Neergård-Wüst Formula for HFB Norm Overlap

The HFB state can be expressed as

$$|\mathrm{HFB}(Z)\rangle = \exp\left(\frac{1}{2}\sum_{ij} Z_{ij} c_i^\dagger c_j^\dagger\right)|0\rangle, \tag{3}$$

where Z is a skew-symmetric matrix of dimension M (M is the dimension of the single-particle model space). $(c, c^\dagger)$ represent the annihilation-creation operators for the single-particle state. The vacuum $|0\rangle$ is defined as $c_i|0\rangle = 0$.

The norm overlap between different HFB states is

$$\langle \mathrm{HFB}(Z)|\mathrm{HFB}(Z')\rangle = \langle 0|\exp\left(\frac{1}{2}\sum_{ij} Z^*_{ij} c_j c_i\right)\exp\left(\frac{1}{2}\sum_{i'j'} Z'_{i'j'} c^\dagger_{i'} c^\dagger_{j'}\right)|0\rangle. \tag{4}$$

One can evaluate the above quantity through the Onishi formula as

$$\langle \mathrm{HFB}(Z)|\mathrm{HFB}(Z')\rangle = \sqrt{\det\left(I + Z^* Z'^T\right)}. \tag{5}$$

Quantity inside the square root, that is, $\det(I + Z^* Z'^*)$ takes a complex value. If $|\mathrm{HFB}(Z)\rangle$ can be constructed smoothly and continuously from the original HFB state $|\mathrm{HFB}(Z')\rangle$ through canonical transformations, the norm overlap can be regarded as a continuous and differentiable function of $Z = Z' + \delta Z$. An example is the case when $|\mathrm{HFB}(Z)\rangle$ is constructed by three-dimensional rotational operator $\hat{R}(\Omega)$, where Ω stands for the Euler angles. In that case, we can demonstrate that $\hat{R}(\Omega)|\mathrm{HFB}(Z')\rangle = |\mathrm{HFB}(Z)\rangle$, and that

$$Z = Z(\Omega) = D(\Omega) Z' D(\Omega)^T. \tag{6}$$

$D(\Omega)$ is a representation of the group O(3), or the Wigner function. This is the case for angular momentum projection, and the norm overlap is regarded as a function of the Euler angles Ω. A complex function with a square root is a multi-valued function unless a proper Riemann surface is introduced beyond the branch cut.

Without setting up a proper Riemann surface, a simple computation of a square root for a complex function $\sqrt{z(\Omega + \Delta\Omega)}$ leaves its sign ambiguous relative to $\sqrt{z(\Omega)}$. The sign depends on whether the path $\Delta\Omega$ passes through the branch cut or not. Hara, Hayashi and Ring carefully determined the sign at $\Omega + \Delta\Omega$ by checking the continuity of the norm overlap numerically. The accuracy of the sign determination depends on the size $\Delta\Omega$, which the smaller the better. But the fine mesh size for $\Delta\Omega$ costs computational time and memory.

Neergård and Wüst proposed an alternative method to remove the square root operation from the Onishi formula, which leads to a removal of the sign ambiguity. First of all, a replacement of Z' with xZ' is made, where x is an arbitrary number. The expression in Eq.(4) is then regarded as a polynomial in x with degree $M/2$ [1]. On the contrary, the expression in Eq.(5) implies an algebraic function in x, not a polynomial in x. To overcome this inconsistency, the eigenvalues of matrix $Z^* Z'^T$ should be pairwise degenerate. Then, using the eigenvalues λ_i, the norm overlap can be written as

$$\langle \mathrm{HFB}(Z)|\mathrm{HFB}(xZ')\rangle = \prod_{i=1}^{M/2} (1 + x\lambda_i)\,, \tag{7}$$

where the product above is considered only for a half of the degenerate pair. Finally, putting $x = 1$, the Neergård-Wüst formula is obtained

$$\langle \mathrm{HFB}(Z)|\mathrm{HFB}(Z')\rangle = \prod_{i=1}^{M/2} (1 + \lambda_i)\,, \tag{8}$$

where λ_i is an eigenvalues of complex matrix $Z^* Z'^T$, which is not Hermitian, nor symmetric. The matrix is not even skew-symmetric. It is just a general complex square matrix of order M.

[1] Although the expression looks a transcendental function in x, a Taylor expansion of the exponential in Eq.(3) does not reach the infinite order due to the Fermi statistics, $(c_i^\dagger)^2 = 0$.

3 Reputation of the Neergård-Wüst Formula

Although the Neergård-Wüst formula is employed in few cases, such as the VAMPIR project [9], it is not so popular for unknown reasons. Avez and Bender recently remarked that "the practical application of the Neergård-Wüst technique becomes cumbersome in realistic cases, and has been rarely used in practice" [10]. Robledo mentioned about the Neergård-Wüst formula that "handling the eigenvalues of non-Hermitian matrices is a difficult task, that increases its complexity if the pairwise degenerate eigenvalues have to be obtained numerically without any symmetry enforcing degeneracy" [7].

From the remarks by Robledo, it seems numerically difficult to choose proper eigenvalues to form a pair due to a lack of numerical accuracy in the diagonalisation of a complex matrix without any symmetries.

I tried to apply the Neergård-Wüst formula by myself, and confirmed such a difficulty which eigenvalues to discard in the calculation of Eq.(8). However, after several attempts, I can find an optimised value for ϵ for the degeneracy condition $|\lambda_i - \lambda_j| < \epsilon$. In addition, there was no particular problem in evaluating the eigenvalues of a general complex matrix $Z^* Z'^T$ by using the widely distributed mathematical subroutines (LAPACK). The calculated result was compared with the one obtained through the Pfaffian formula [7]. The agreement between the two approaches was fairly satisfactory.

It seems that the main reason for the unpopularity of the Neergård-Wüst formula is neither the numerical difficulty to find a proper pair nor to perform a diagonalisation of a complex matrix without any symmetries.

4 Effect of Typographical Error

Through careful readings of the original paper, that is, Ref. [8], I found a typographical error in the main texts. As shown in Eq.(5), the matrix to diagonalise is $Z^* Z'^T$, but in the paper Neergård and Wüst repeatedly mentioned that it is $Z^T Z'$ that should be diagonalised. This typographical error can be the main reason because those who blindly implemented the formula to their numerical calculation might have failed to obtain the physically correct consequences.

Recalling the skew-symmetry of Z, the above two matrices were rewritten to be $-Z^* Z'$ and $-Z Z'$, respectively. I calculated the eigenvalues for the both cases for comparison. The obtained eigenvalues for the different complex matrices were found to be related as a complex conjugate. As a result, the norm overlaps calculated with the different matrices are mutually complex conjugate.

The norm overlap can be regarded as a Hermitian matrix if we write $N_{qq'} = \langle \Psi(q) | \Psi(q') \rangle$, which means that the eigenvalues of this matrix are real numbers. As a result, $N_{qq'}$ and $N^*_{qq'}$ have the identical eigenvalue spectrum, meaning that

the final result of the GCM calculation can be correctly obtained even with the typographical error. In fact, I solved the Hill-Wheeler equation numerically and confirmed that the both matrices give rise to the identical result.

After an analytical consideration, I understand that this consistency was achieved by chance. In my calculation, the HFB states are calculated for ^{170}Dy by means of the self-consistent one-dimensional cranking model. The effective two-body interaction is the pairing-plus-quadrupole force. Then, I performed the angular momentum projection, which is regarded as a special case of GCM (the generator coordinates are chosen to be the Euler angle).

In the one-dimensional and two-dimensional cranking calculations, the Bogoliubov transformation matrix is obtained as a real matrix, as seen in the Pauli matrix for spin (σ_x and σ_z are the real unitary matrix, while only σ_y is a complex matrix). In other words, unless the three-dimensional cranking calculation is carried out, the matrix Z' is a real matrix. On the contrary, Z is a complex matrix as shown in Eq.(6).

As far as the angular momentum projection for the one(two)-dimensionally cranked HFB states is concerned, the correct and wrong expressions for the matrix to be diagonalised in the formula happens to be related as a complex conjugate, $(Z^*Z')^* = ZZ'$. Therefore, the typographical error turns out not to damage the final result.

However, if the original HFB state $|\mathrm{HFB}(Z')\rangle$ gives rise to the complex Z', such as in the case of the three-dimensionally cranked HFB states, the matrix obtained through the typographical error has nothing to do with the correct expression. This means that the error leads to the wrong conclusion in the final result.

Nonetheless, there has been no work to date to set a complex Z' in the GCM calculation (including the quantum number projection), as far as I know. Therefore, the typographical error in the paper by Neergård and Wüst cannot be the primary reason for the unpopularity of their formula.

5 Conclusion

As far as my calculation (the cranked HFB calculation with the pairing-plus-quadrupole force) is concerned, the Neergård-Wüst method works perfectly, so that there is no reason to criticise their formula. In the modern computational environment, I confirmed that the Neergård-Wüst formula allows the numerical calculation of the norm overlap kernels slightly faster than the one through the Pfaffian formula, at least, in the present calculation that I have executed for this paper.

I have considered several reasons in the present paper why the formula was dismissed by many nuclear theoreticians, but none of them is found to be relevant. There may be other reasons why the formula has not been widely used in the

past. If more realistic interactions are chosen for the HFB calculation, such reasons might be clarified. However, in my opinion, the Neergård-Wüst formula is a reasonably practical formula to evaluate the HFB norm overlap in the GCM calculation.

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