Hidden symmetries in the HFB norm overlap functions

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Abstract. A brief consideration about hidden symmetries in the HFB norm overlap functions is presented, in particular, in association with the presence of pair-wise degeneracy of the eigenvalue spectrum of a product of two antisymmetric matrices.

1 Introduction

The mean field approximation, such as the Hartree-Fock-Bogoliubov (HFB) method, has been successful to describe various nuclear properties such as the moment of inertia of the ground-state rotational band. There are types of physics, however, demanding higher order correlations beyond the mean field approximation. Collective phenomena, such as surface vibration and pairing vibration, are such. The generator coordinate method (GCM) is one of the methods that can take such dynamical collective degrees of freedom into account. However, there had been a problem in implementing the GCM to numerical calculations, which is the sign problem in obtaining the norm overlap function for the GCM equation.

In 1983, Neergård and Wüst proposed a method [1] how to calculate the HFB norm overlap functions without the sign ambiguity, which damages the Onishi formula [2], the first exact and compact formula to enable the calculation of the HFB overlap. This method exploits the pairwise degeneracy of the norm overlap function. For some technical reasons, however, the Neergård-Wüst method was not widely employed by many authors [3]. The primary reason is that their method requires the diagonalisation of a matrix without any symmetries and special properties, such as hermiticity and antisymmetry. Many feared that this lack of speciality may result in serious numerical errors in the evaluation of the HFB overlap.

But we recently found that this "general matrix" possess a hidden symmetry, which can allow numerical calculation with high precision for the pairwise degeneracy obtained from a general matrix.

2 The Onishi formula and the Neergård-Wüst method

The Onishi formula reads

$$\langle \Psi_0 | \Psi_1 \rangle = \sqrt{\det(I - Z_0^* Z_1)}, \qquad (1)$$

where the n-by-n identity matrix is denoted as I and the HFB state Ψ_m is expressed as

$$|\Psi_\alpha\rangle = \exp\left(\frac{1}{2}\sum_{i,j}^{n}(Z_\alpha)_{ij}c_i^\dagger c_j^\dagger\right)|0\rangle. \qquad (2)$$

This form of the HFB state is also referred to as the Thouless ansatz. Here, the single-particle creation and annihilation operators for fermion are $(c, c^\dagger)$ and its model-space dimension is n, which is an even integer for even-even nuclear systems. The variational parameter Z_α is an n-by-n antisymmetric matrix, $Z_\alpha^T = -Z_\alpha$.

In general, the Onishi formula has a form of the square root of a complex function, so that it has the sign ambiguity. Neergård and Wüst believed that the HFB norm overlap function should not possess such a complicated mathematical structure because the Thouless ansatz is essentially an exponential. Based on this consideration, they believed that the matrix $Z_0^* Z_1$, which does not hold any special properties and symmetries, must give rise to pairwise eigenvalues. In other words, the pair-wise degeneracy can be a solution to avoid the mathematical complexity, but they did not demonstrate that the other ways are excluded theoretically. Only a numerical demonstration was given to support their claim. In accordance with their approach, once the diagonalisation is done, the norm overlap function should be expressed as

$$\langle \Psi_0 | \Psi_1 \rangle = \prod_{i=1}^{n/2}(1 - \lambda_i), \qquad (3)$$

where λ_i is one of the paired eigenvalues. Due to absences of any symmetries and special properties, λ_i is a complex number.

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There were many who doubted that such a general matrix can produce the well-structured pairs of eigenvalues, but our recent numerical investigation showed that such a structure is well maintained for a practical HFB calculations with the pair-plus-quadrupole model. We then decided to analyse why this pair-wise eigenvalues are guaranteed for such a general matrix $Z_0^* Z_1$.

3 Demonstration of the pair-wise degeneracy

Although the matrix $Z_0^* Z_1$ does not hold any symmetries and special properties, it is obvious that it is a product of two antisymmetric matrices Z_0^* and Z_1. It is natural to suspect that the pair-wise degeneracy is a consequence of this "hidden" symmetric properties of $Z_0^* Z_1$. In other words, the necessity of the pair-wise degeneracy is naturally derived from the "hidden symmetries" that I noticed in the present work, which will be demonstrated in the following.

For the sake of simplicity, we will employ simpler expressions in the consideration of the eigenvalues of a product of two antisymmetric matrices. Such antisymmetric matrices are denoted as A and B hereafter, so that the eigenvalue equation of our interest becomes

$$AB\boldsymbol{v}^i = \lambda^i \boldsymbol{v}^i, \tag{4}$$

and we want to demonstrate that the eigenvalue spectrum has pair-wise degeneracies. It can be justified that the rank of the matrix AB is n, because $\det(AB) = \det A \cdot \det B \neq 0$.

First of all, a vector $\boldsymbol{w}^i = B\boldsymbol{v}^i$ is introduced. The transpose of this new vector corresponds to the left eigenvector of AB,

$$(\boldsymbol{w}^i)^T AB = \lambda^i (\boldsymbol{w}^i)^T, \tag{5}$$

which can be easily verified by multiplying eq.(4) with B from left. Operating A to $\boldsymbol{w}^i$ from left gives rise to the equivalent expression to the original eigenvalue equation, eq.(4),

$$A\boldsymbol{w}^i = \lambda^i \boldsymbol{v}^i. \tag{6}$$

Here, we introduce collective expressions for eigenvalues λ^i and the eigenvectors $\boldsymbol{v}^i$ and $\boldsymbol{w}^i$ in the form of n-by-n matrices,

$$\Lambda = \mathrm{diag}(\lambda^1, \cdots, \lambda^n), \tag{7}$$
$$V = (\boldsymbol{v}^1 \quad \boldsymbol{v}^2 \quad \cdots \quad \boldsymbol{v}^n), \tag{8}$$
$$W = (\boldsymbol{w}^1 \quad \boldsymbol{w}^2 \quad \cdots \quad \boldsymbol{w}^n). \tag{9}$$
$$\tag{10}$$

Then, the above expressions are rewritten

$$W = BV, \tag{11}$$
$$AW = V\Lambda. \tag{12}$$

From the first equation in the above, that is, eq.(11), we can derive a antisymmetric relation

$$V^T W = -(V^T W)^T, \tag{13}$$

by demanding B to be antisymmetric.

From the second equation in the above, that is, eq.(12), we can also derive a commutation relation

$$\left[\Lambda, W^T V\right] = 0, \tag{14}$$

by demanding A to be antisymmetric. This commutation relation can be equivalently expressed as

$$(\lambda_i - \lambda_j)(W^T V)_{ij} = 0, \tag{15}$$

Let us assume that there is no degeneracy in the eigenvalue spectrum. Then, we have $W^T V = 0$, which implies that $B = 0$. which is contradictory from the original condition that B is antisymmetric. Therefore, the eigenvalue spectrum of AB must be degenerate.

Let us now suppose that the eigenvalues of $i = 1$ and of $i = 2$ are pair-wise degenerate, $\lambda^1 = \lambda^2$. Then, $(W^T V)_{12} = -(W^T V)_{21} \neq 0$, and the antisymmetric matrices B is expressed as

$$B_{pq} = -(W^T V)_{12} \begin{vmatrix} (V^{-1})_{1p} & (V^{-1})_{1q} \\ (V^{-1})_{2p} & (V^{-1})_{2q} \end{vmatrix}. \tag{16}$$

The eigenvalue equation now reads

$$(ABV)_{ij} = (W^T V)_{12} \left\{ -(V^{-1}A)_{2i}\delta_{1j} + (V^{-1}A)_{1i}\delta_{2j} \right\}. \tag{17}$$

This means that if $j \neq 1, 2$, we have $AB\boldsymbol{v}^j = 0$, which contradicts the fact that AB is a full-rank matrix.

References

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