Physics Letters B 779 (2018) 237–243

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Why does the sign problem occur in evaluating the overlap of HFB wave functions?

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ARTICLE INFO

Article history:
Received 7 September 2017
Received in revised form 29 January 2018
Accepted 5 February 2018
Available online 12 February 2018
Editor: W. Haxton

ABSTRACT

For the overlap matrix element between Hartree–Fock–Bogoliubov states, there are two analytically different formulae: one with the square root of the determinant (the Onishi formula) and the other with the Pfaffian (Robledo's Pfaffian formula). The former formula is two-valued as a complex function, hence it leaves the sign of the norm overlap undetermined (i.e., the so-called sign problem of the Onishi formula). On the other hand, the latter formula does not suffer from the sign problem. The derivations for these two formulae are so different that the reasons are obscured why the resultant formulae possess different analytical properties. In this paper, we discuss the reason why the difference occurs by means of the consistent framework, which is based on the linked cluster theorem and the product-sum identity for the Pfaffian. Through this discussion, we elucidate the source of the sign problem in the Onishi formula. We also point out that different summation methods of series expansions may result in analytically different formulae.

1. Introduction

The Hartree–Fock–Bogoliubov (HFB) theory gives a simple but profound basis for the nuclear many-body problem where the competition between the nuclear pairing and deformation plays a primary role in the determination of the ground state as well as the excited states. Especially, a combination of the HFB method with the technique of angular momentum projection allows the direct comparison between the theoretical calculations and the experimental data. The projected HFB states can produce more elaborate and accurate calculations although the simplicity of the HFB wave functions is kept from a mean-field point of view. In this way, not only the simple HFB state but also a superposition of different HFB states (i.e., the projected HFB state) have been extensively used for nuclear-structure studies. Behind this success of the HFB theory, there was a hidden problem for the overlap matrix element between the HFB states.

Half a century ago, a formula for the overlap matrix element was derived by Onishi and Yoshida [1] and is called the Onishi formula [2]. To derive the Onishi formula, we begin with the Thouless representation [2], [3] of the HFB wave functions, $|\phi^{(k)}\rangle$ $(k=0,1)$ defined as

$$|\phi^{(k)}\rangle = e^{\frac{1}{2}\sum_{p,q=1}^{N} Z^{k}_{p,q} c^{\dagger}_{p} c^{\dagger}_{q}}|-\rangle, \tag{1}$$

where $c^{\dagger}$'s are the creation operators and $|-\rangle$ is the bare Fermion vacuum with $c_i|-\rangle = 0$ $(i = 1, \cdots, N)$. The dimension of the Fermion single-particle space is N. Z is an $N \times N$ complex skew-symmetric matrix. The Thouless representation is a specific one of the Bogoliubov quasiparticle states. In this representation, the overall phase is fixed for two HFB wave functions $|\phi^{(0)}\rangle$ and $|\phi^{(1)}\rangle$, respectively, as in Refs. [4], [5].

The overlap matrix element between these two HFB wave functions is defined as

$$\langle\phi^{(0)}|\phi^{(1)}\rangle = \langle -|e^{\frac{1}{2}\sum_{p',q'=1}^{N} Z^{0*}_{p',q'} c_{q'} c_{p'}} e^{\frac{1}{2}\sum_{p,q=1}^{N} Z^{1}_{p,q} c^{\dagger}_{p} c^{\dagger}_{q}}|-\rangle, \tag{2}$$

which can be expressed as

$$\langle\phi^{(0)}|\phi^{(1)}\rangle = \sqrt{\mathrm{Det}(I - Z^{0*}Z^{1})}. \tag{3}$$

This formula is known as the Onishi formula [1]. Due to the square root function, the Onishi formula is two-valued and does not give a definite sign if Z's are complex matrices. This indefiniteness of the sign assignment is referred to as the sign problem of the Onishi formula, which becomes quite serious in the application of the full

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https://doi.org/10.1016/j.physletb.2018.02.012

angular momentum projection. So far, there are several approaches known to remedy the problem [4], [5], [6], [7], [8].

Among them, Robledo [5] has recently derived an alternative and ambiguity-free formula for the overlap matrix element by the Pfaffian as

$$\langle\phi^{(0)}|\phi^{(1)}\rangle = s_N Pf\begin{bmatrix} Z^1 & -I \\ I & -Z^{0*}\end{bmatrix}, \tag{4}$$

where $s_N = (-)^{N(N+1)/2}$ and I is the $N\times N$ identity matrix. This formula is proved with rather advanced techniques, that is, the Fermion coherent state and Grassmann integral. His proof is mathematically very elegant and interesting [5]. Moreover, these techniques led us to a relation to the generalized Wick's theorem and its related topics [9], [10], [11], [12], [13]. The proof by Robledo is, however, rather abstract and it somewhat keeps us from an intuitive understanding of the reason for the disappearance of the sign ambiguity.

In the present paper, we derive both formulae in Eqs. (3) and (4) directly from Eq. (2) and elucidate an origin of the sign problem. First, we expand the exponential operators in Eqs. (1), (2). After handling the vacuum expectation values of the product of the creation-annihilation operators, the overlap matrix element can be, in principle, expressed as a polynomial of the matrix elements of Z. The overlap is, therefore, single-valued.

Next, we will consider two summation methods. We show that an expansion of the HFB wave function in Eq. (1) can be expressed by the Pfaffians and that the overlap matrix element can be, thereby, revealed by a finite series of the product-sum of the Pfaffians. This finite series can be summed up into Robledo's Pfaffian formula in Eq. (4). By this derivation, Robledo's Pfaffian formula is turned out to be obviously single-valued and to be free of the sign problem. We also show that the other summation method with the linked cluster theorem [14] brings us to the Onishi formula. We present that this summation concerning the connected diagrams involves an infinite series, which is in sharp contrast to the original finite series and that it gives rise to the square root function in the Onishi formula. We also clarify that the skew-symmetric property of the Thouless matrix Z can remove the sign problem from the Onishi formula completely.

The present paper is organized as follows. In Sec. 2, we show a basic structure of the overlap matrix element through the series expansion of the HFB wave functions and present an alternative derivation of Robledo's Pfaffian formula. In Sec. 3, we show a relation between the Onishi formula and the linked cluster theorem, and we discuss the origin of the sign problem. In Sec. 4, we give a conclusion. In the appendices, we summarize useful identities concerning the Pfaffian and show the derivation of the connected term.

2. Overlap formula with the Pfaffian

2.1. Basic structure of the overlap matrix element

First, we show a basic mathematical structure of the overlap matrix element by expanding the exponential operators in Eq. (2). Defining pair-annihilation and pair-creation operators, $\hat{A}$ and $\hat{B}$ as

$$\hat{A} = \frac{1}{2}\sum_{p,q} Z^{0*}_{p,q} c_q c_p = \sum_{q>p} Z^{0*}_{p,q} c_q c_p, \tag{5}$$

$$\hat{B} = \frac{1}{2}\sum_{p,q} Z^{1}_{p,q} c^\dagger_p c^\dagger_q = \sum_{q>p} Z^{1}_{p,q} c^\dagger_p c^\dagger_q, \tag{6}$$

the HFB wave functions are shown by

$$\langle\phi^{(0)}| = \langle -|e^{\hat{A}},$$
$$|\phi^{(1)}\rangle = e^{\hat{B}}|-\rangle. \tag{7}$$

The overlap matrix element is simply denoted by

$$\langle\phi^{(0)}|\phi^{(1)}\rangle = \langle -|e^{\hat{A}}e^{\hat{B}}|-\rangle. \tag{8}$$

By expanding exponential operator, the HFB wave function can be shown as

$$|\phi^{(1)}\rangle = (1+\hat{B}+\frac{1}{2!}\hat{B}^2+\frac{1}{3!}\hat{B}^3+\cdots+\frac{1}{(\frac{N}{2})!}\hat{B}^{\frac{N}{2}})|-\rangle, \tag{9}$$

where this series expansion terminates in order $N/2$ because the number of single particle states, namely, the dimension of the matrices Z^0 and Z^1 is N. The overlap matrix element is rewritten by

$$\langle\phi^{(0)}|\phi^{(1)}\rangle = \sum_{k=0}^{N/2}\langle -|\frac{\hat{A}^k}{k!}\frac{\hat{B}^k}{k!}|-\rangle. \tag{10}$$

Note that $\langle -|\frac{\hat{A}^l}{l!}\frac{\hat{B}^k}{k!}|-\rangle$ vanishes if $l\neq k$ because $\hat{A}$ and $\hat{B}$ are pair-annihilation and pair-creation operators, respectively.

Next, we investigate an expanded form of the $\frac{1}{k!}\hat{B}^k$ operator. The $\frac{1}{k!}\hat{B}^k$ operator is generally expressed by the $2k$ creation operators with the coefficients in terms of matrix elements of Z^1 as,

$$\frac{1}{k!}\hat{B}^k = \frac{1}{k!}\frac{1}{2^k}\sum Z^1_{p_1,q_1}\cdots Z^1{}_{p_k,q_k} c^\dagger_{p_1}c^\dagger_{q_1}\cdots c^\dagger_{p_k}c^\dagger_{q_k}. \tag{11}$$

As the $\hat{A}^k$ operator is also similarly shown, the overlap matrix element can be straightforwardly expressed as a function of matrix elements of Z^{0*} and Z^1 as,

$$\begin{aligned}&\langle\phi^{(0)}|\phi^{(1)}\rangle \\ &= \sum_{k=0}^{N/2}\frac{1}{(k!)^2}\frac{1}{2^{2k}}\sum_{p,q,p',q'} Z^{0*}_{p'_1,q'_1}\cdots Z^{0*}{}_{p'_k,q'_k} Z^1_{p_1,q_1}\cdots Z^1{}_{p_k,q_k} \\ &\langle -|c_{q'_k}c_{p'_k}\cdots c_{q'_1}c_{p'_1}c^\dagger_{p_1}c^\dagger_{q_1}\cdots c^\dagger_{p_k}c^\dagger_{q_k}|-\rangle.\end{aligned} \tag{12}$$

The matrix element in the third line of the above equation gives intricate restriction concerning p's, q's, p''s, q''s by taking the contractions. The above formula shows a very complicated structure regarding the matrix elements of Z^{0*} and Z^1. It is, however, quite evident that the overlap matrix element is a polynomial of the matrix elements of Z^{0*} and Z^1 and has, thereby, no sign ambiguity.

In the subsequent subsections, we will show that Eq. (12) can be rewritten by the Pfaffians and will directly derive Robledo's Pfaffian formula from Eq. (12). Furthermore, in the next section, by handling Eq. (12) with the linked cluster theorem, we will derive the Onishi formula.

2.2. Overlap formula with product-sum of the Pfaffians

In this subsection, we consider to rewrite Eq. (12) by investigating the detailed structure of Eq. (11).

For example, the 2nd order term is expressed as

$$\begin{aligned}\frac{1}{2!}\hat{B}^2 &= \frac{1}{2!}\sum_{p_1<q_1,p_2<q_2} Z^1_{p_1,q_1}Z^1_{p_2,q_2}c^\dagger_{p_1}c^\dagger_{q_1}c^\dagger_{p_2}c^\dagger_{q_2}, \\ &= \sum_{p_1<q_1,p_2<q_2,p_1<p_2} Z^1_{p_1,q_1}Z^1_{p_2,q_2}c^\dagger_{p_1}c^\dagger_{q_1}c^\dagger_{p_2}c^\dagger_{q_2},\end{aligned} \tag{13}$$

where 2! is removed due to the additional condition $p_1 < p_2$. Now let us change the integer indices p_1, q_1, p_2, q_2 to new indices n_1,