ABOUT THE SIGN AMBIGUITY IN THE EVALUATION OF GRAND CANONICAL TRACES FOR QUASI-PARTICLE STATISTICAL DENSITY OPERATORS

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A simple and general prescription for evaluating unambiguously the sign of the grand canonical trace of quasi-particle statistical density operators (the so-called sign ambiguity in taking the square root of determinants) is given. Sign ambiguities of this kind appear in the evaluation of the grand canonical partition function projected to good quantum numbers (angular momentum, parity and particle number) in the Hartree–Fock–Bogoliubov approximation at finite temperature, since traces are usually expressed as the square root of determinants. A comparison is made with the numerical continuity method.

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1. Introduction

Nuclei at finite temperature are usually studied microscopically using the finite temperature Hartree–Fock (HF) or Hartree–Fock–Bogoliubov (HFB) approximations (Refs. [1,2]), at least at first level of approximation. The basic quantity is the grand canonical partition function or equivalently the grand potential. Such a quantity contains an average of all possible contributions from different conserved quantum numbers such as angular momentum, parity and particle number. It is, of course, of great physical interest to study the partition function and related thermal averages using the partition function projected to the exact quantum numbers. This is especially true if the projection to good angular momentum is carried out without any assumption about axial symmetry, that is, if the full three dimensional angular momentum projector is used. As the temperature increases, we expect triaxial shapes to play a role and it is interesting to see how shape transitions are obtained at different excitation energies.

Sometimes the full projector is replaced by a partial projector to good z-component of the angular momentum J_z. The partition function for a specified value of the angular momentum J is then obtained by subtraction between the partition function at a J_z and the partition function at $J_z + 1$. This recipe, however, has a basic limitation that requires the exact evaluation of the partition function. This limitation is of course a problem when using even accurate approximations such as the HFB. Moreover, in the limit of 0 temperature, the HFB ground state for a specified value of J_z is not as accurate as the ground state obtained with a specified value of J. Also, the above recipe would pose severe problems for odd and odd–odd nuclei. Therefore, the use of the exact angular momentum projector is highly desirable.

In the case of the temperature dependent HFB approximation, a standard result for the trace of the statistical density operator (the exponential of a quadratic form in the quasi-particle operators) states that it can be recast as a square root of a determinant (Ref. [3]). This is a problem if the projected partition function is required, since an improper sign can lead to erroneous results. In the past the cure for this problem has been given with the so-called continuity argument. This argument states that the proper sign can be determined by constructing the statistical density operator from unity and then by determining the appropriate sign by imposing the continuity of the phase of the trace as we progressively rebuild the statistical density operator. This has been the recipe followed in Ref. [3].

Recently this problem has been considered anew using the Grassmann algebra (Ref. [4]) for the determination of the sign for both overlaps of HFB wave functions and the trace of the statistical density operator (Ref. [5]). Although the results obtained were not previously reported in the literature, in the case of the trace of the statistical density operator, the sign ambiguity was not fully resolved since the vacuum contribution was still left as the square root of a determinant.

The purpose of this work is to show how all possible ambiguities can be resolved without referring to a numerical continuity argument, which may not be easy to implement. In the next section we shall derive the construction of the proper sign for the trace of the statistical density operator in rather general terms starting from the properties of the Lie algebra of the generators of the statistical density operators as described in Ref. [6]. Therefore, the HFB approximation is only a special case of the recipe described below.

2. Determination of the sign of the trace of the statistical density operator

2.1. Symbols, definitions and basic properties

As mentioned in the introduction we shall keep the discussion as general as possible. Let $N_{\rm s}$ be the total number of the single particle states (that is neutrons plus protons). Let us consider an arbitrary antisymmetric complex $2N_{\rm s} \times 2N_{\rm s}$ matrix A and let us define the row vector $\gamma_{\rm r} = (a, a^\dagger)$, the collection of all annihilation and of all creation operators. In order to use consistently the matrix notations let us denote the column vector $\gamma_{\rm c} = {\rm col}(a, a^\dagger)$. A general statistical density operator (SDO for short) is written as

$$\hat{W} = \exp\left(\tfrac{1}{2}\,\gamma_{\rm r} A \gamma_{\rm c}\right) . \tag{1}$$

No other limitations are imposed on this operator, except for the antisymmetry of the matrix A. Also let us define the $2N_{\rm s} \times 2N_{\rm s}$ matrix

$$\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2}$$

and the vectors

$$\overline{\gamma}_{\rm r} = \gamma_{\rm r}\sigma\,, \qquad \overline{\gamma}_{\rm c} = \sigma\gamma_{\rm c}\,. \tag{3}$$

Eq. (1) can be recast as

$$\hat{W} = \exp\left(\tfrac{1}{2}\overline{\gamma}_{\rm r} S \gamma_{\rm c}\right)\,, \qquad S = \sigma A\,. \tag{4}$$

This is the form of the SDO we shall use in the following. In the case of the HFB approximation S is Hermitian. To any operator of the form of Eq. (4) one can associate the matrix (without the caret)

$$W = \exp(S)\,. \tag{5}$$

Following Ref. [6], the exponents of operators as in Eq. (4) form a Lie algebra, and therefore the product of any two exponential operators of this form is an operator of the same form, moreover the product preserves the association of Eq. (5) that is, if

$$\hat{W}_1\hat{W}_2 = \hat{W} \tag{6}$$

also

$$W_1 W_2 = W\,. \tag{7}$$

For example, $\hat{W}_1$ is the rotation operator in terms of the Euler angles. In general, an arbitrary SDO is constructed as a product of several operators of the class of Eq. (4), and for each one of them we know unambiguously the matrix S of Eq. (4). Eq. (6) tells us that the matrix S corresponding to the product $\hat{W}$ exists, but we cannot reconstruct this matrix from Eq. (7) because of the $2\pi i$ ambiguity of the logarithm of the eigenvalues of W. This is the source of the sign ambiguity is the evaluation of the traces. From Ref. [6], the operators of the class (4) transform the vectors γ in the following way

$$\hat{W}^{-1}\gamma_{\rm c}\hat{W} = W\gamma_{\rm c}\,, \qquad \hat{W}^{-1}\gamma_{\rm r}\hat{W} = \gamma_{\rm r}\tilde{W}\,, \qquad \hat{W}^{-1}\overline{\gamma}_{\rm r}\hat{W} = \overline{\gamma}_{\rm r}W^{-1}\,, \tag{8}$$

where $\tilde{W}$ denote the transpose of the matrix W. Moreover, the following relation holds (*cf.* Ref. [6])

$$\sigma\tilde{W}\sigma = W^{-1}\,. \tag{9}$$

It ensures that the transformed operators in Eq. (8) obey the anticommutation relations.

2.2. The trace in the case the matrix S is known

If the matrix S in Eq.(5) is known, the grand canonical trace of $\hat{W}$ can easily be evaluated without ambiguities. Let us prove it in the most general case, assuming S is known. Consider a SDO $\hat{T}$, then

$$\begin{aligned}\mathrm{Tr}\left(\hat{W}\right) &= \mathrm{Tr}\left(\hat{T}^{-1}\hat{W}\hat{T}\right) = \mathrm{Tr}\left(\exp\left(\tfrac{1}{2}\hat{T}^{-1}\overline{\gamma}_{\rm r}S\gamma_{\rm c}\hat{T}\right)\right)\\ &= \mathrm{Tr}\left(\exp\left(\tfrac{1}{2}\overline{\gamma}_{\rm r}T^{-1}ST\gamma_{\rm c}\right)\right)\,,\end{aligned} \tag{10}$$

where Eq. (8) has been used. We shall prove that the matrix T that diagonalizes S satisfies Eq. (9).

It is easy to see that the eigenvalues of S come in opposite pairs. In fact, the eigenvalue problem for $S = \sigma A$ written in the form (T is the matrix of the eigenvectors and the λ's are the eigenvalues written in block form for convenience)

$$ST = T\begin{pmatrix}\lambda & 0\\ 0 & \lambda'\end{pmatrix} \tag{11}$$

can be rewritten as

$$A\sigma(\sigma T\sigma) = (\sigma T\sigma)(\sigma\begin{pmatrix}\lambda & 0\\ 0 & \lambda'\end{pmatrix}\sigma) = (\sigma T\sigma)\begin{pmatrix}\lambda' & 0\\ 0 & \lambda\end{pmatrix}$$

but $A\sigma = -\tilde{S}$ hence $\lambda = -\lambda'$. The trace can now be trivially evaluated and the result is

$$\mathrm{Tr}(\hat{W}) = \exp\left(-\tfrac{1}{2}\sum_i^{N_{\rm s}}\lambda_i\right)\prod_i^{N_{\rm s}}\left(1+\exp\left(\lambda_i\right)\right) \tag{12}$$

provided one can show that $\hat{T}$ is an element of the class of Eq. (4), that is, provided its associated matrix T satisfies Eq. (9) (which guarantees the legitimacy of the chain of steps in Eq. (10)). In order to see this, consider the eigenvalue problem for W written as

$$WT = T\begin{pmatrix} e^{\lambda} & 0 \\ 0 & e^{-\lambda} \end{pmatrix} \tag{13}$$

by applying at the left and at the right the matrix σ ($\sigma^2 = 1$) and taking into account Eq. (9) one has

$$(\tilde{W})^{-1}\sigma T\sigma = \sigma T\sigma \begin{pmatrix} e^{-\lambda} & 0 \\ 0 & e^{\lambda} \end{pmatrix}. \tag{14}$$

Taking the inverse and the transpose of the above we obtain

$$W(\sigma\tilde{T}\sigma)^{-1} = (\sigma\tilde{T}\sigma)^{-1}\begin{pmatrix} e^{\lambda} & 0 \\ 0 & e^{-\lambda} \end{pmatrix}. \tag{15}$$

Therefore T_{ik} and $(\sigma\tilde{T}\sigma)^{-1}_{ik}$ coincide apart a normalization constant $f_k \neq 0$. If f is the diagonal matrix of elements f_k then

$$f = (\sigma\tilde{T}\sigma)T\,. \tag{16}$$

Evaluating the above product one can show that f has the doublet structure $f = \mathrm{diag}(f_1, f_2, \ldots\, f_1, f_2, \ldots)$. Therefore, $\sigma f^{-1/2}\sigma = f^{-1/2}$ and from this it follows that if T does not satisfy Eq. (9) and the matrix $T/\sqrt{f}$ does.

Eq. (12) for the trace does not have any sign ambiguity since we had access to the eigenvalues of S. If we do not have access to the matrix S, from Eq. (12) taking the square, we have

$$\mathrm{Tr}(\hat{W})^2 = \det(1+W) \tag{17}$$

since we always have access to eigenvalues of W. This is where the sign ambiguity comes from. If we work with W obtained from Eq. (7), we never have access to the matrix S although we know it exists.

2.3. The contribution of the vacuum

Consider now the fugacity dependent trace

$$Z_{gc}(z) = \mathrm{Tr}\left(\exp(\alpha\hat{N})\hat{W}\right), \tag{18}$$

where $z = \exp(\alpha)$ and $\hat{N}$ is the particle number operator. For $z = 0$ we isolate the contribution of the vacuum. Let us define the operator of the class (4)

$$\hat{\mathcal{N}} = \exp \frac{1}{2} \overline{\gamma}_{\mathrm{r}} \begin{pmatrix} \alpha & 0 \\ 0 & -\alpha \end{pmatrix} \gamma_{\mathrm{c}} \tag{19}$$

and its associated matrix

$$\mathcal{N} = \begin{pmatrix} z & 0 \\ 0 & 1/z \end{pmatrix} . \tag{20}$$

Let us set $\hat{W}(z) = \hat{\mathcal{N}}\hat{W}$. This operator has an associated matrix $W(z) = \mathcal{N}W$. Explicitly

$$W = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix} . \tag{21}$$

Then

$$Z_{gc}(z)^2 = z^{N_{\mathrm{s}}} \det(1 + W(z)) = \det \begin{pmatrix} 1 & 0 \\ 0 & z \end{pmatrix} \det(1 + \mathcal{N}W) . \tag{22}$$

This expression can be recast as

$$Z_{gc}(z)^2 = \det(S_v + zS_p) = \det(S_v) \det \left(1 + zS_v^{-1}S_p\right) , \tag{23}$$

where

$$S_v = \begin{pmatrix} 1 & 0 \\ W_{21} & W_{22} \end{pmatrix} , \qquad S_p = \begin{pmatrix} W_{11} & W_{12} \\ 0 & 1 \end{pmatrix} . \tag{24}$$

Since $Z_{gc}(z)$ is a polynomial in z the eigenvalues of $S_v^{-1}S_p$ must come in degenerate pairs (μ_k, μ_k) , $k = 1, , , N_{\mathrm{s}}$. This argument is the similar to the one used in Ref. [7].Therefore

$$Z_{gc}(z) = \det(W_{22})^{1/2} \prod_{k=1}^{N_{\mathrm{s}}} (1 + z\mu_k) . \tag{25}$$

It follows that, if we know the matrix S (the log of W) then, using Eq. (12),

$$\det(W_{22})^{1/2} = \frac{\exp\left(-\frac{1}{2}\sum_i^{N_{\mathrm{s}}} \lambda_i\right) \prod_i^{N_{\mathrm{s}}} (1 + \exp(\lambda_i))}{\prod_k^{N_{\mathrm{s}}} (1 + \mu_k)} , \tag{26}$$

where we have set $z = 1$. There are no sign ambiguities in $\prod_{k=1}^{N_{\mathrm{s}}}(1 + z\mu_k)$ since its sign must be a continuous function of z. The only ambiguity is the $\det^{1/2}(W_{22})$ and it is removed by Eq. (12). Eq. (26) is the basic equation that allows us to remove the sign ambiguity also in the general case when we do not know the matrix S and its eigenvalues unambiguously, as shown in the next subsection. Before leaving this section let us note that for $z = 0$ we obtain the vacuum contribution to the grand canonical trace of $\hat{W}$

$$\langle 0|\hat{W}|0\rangle = \det(W_{22})^{1/2}\,, \tag{27}$$

where $|0\rangle$ is the particle vacuum.

2.4. The trace in the general case

Consider the SDO of the type

$$\hat{W} = \hat{W}^{(b)}\hat{W}^{(a)}\,, \tag{28}$$

where $\hat{W}^{(b,a)}$ are of the type of Eq. (4), and let us assume we know explicitly the matrices $S^{(b)}$ and $S^{(a)}$. As previously mentioned, we do not know unambiguously the matrix S associated with $\hat{W}$, although we know the matrix W associated with $\hat{W}$, since $W = W^{(b)}W^{(a)}$. In what follows we shall need the following matrices

$$D^{(b)} = W_{22}^{(b)-1}W_{21}^{(b)}\,, \qquad C^{(a)} = W_{12}^{(a)}W_{22}^{(a)-1}\,. \tag{29}$$

Using Eq. (25) (with $z = 1$) we have

$$Z_{gc} = \left(\det\left[W^{(b)}W^{(a)}\right]_{22}\right)^{1/2}\prod_{k=1}^{N_\mathrm{s}}(1+\mu_k)\,. \tag{30}$$

The square root of the determinant can be evaluated in the following way. Consider the vacuum expectation value $\langle 0|\hat{W}^{(b)}\exp(\alpha\hat{N})\hat{W}^{(a)}|0\rangle$. Then (*cf.* Eq. (27))

$$\langle 0|\hat{W}^{(b)}\exp(\alpha\hat{N})\hat{W}^{(a)}|0\rangle = z^{N_\mathrm{s}/2}\left(\det\left[W^{(b)}\mathcal{N}W^{(a)}\right]_{22}\right)^{1/2}. \tag{31}$$

Direct evaluation of the matrix product gives

$$\langle 0|\hat{W}^{(b)}\exp(\alpha\hat{N})\hat{W}^{(a)}|0\rangle = \left(\det\left[W_{22}^{(b)}W_{22}^{(a)} + z^2W_{21}^{(b)}W_{12}^{(a)}\right]\right)^{1/2} \tag{32}$$

or

$$\langle 0|\hat{W}^{(b)}\exp(\alpha\hat{N})\hat{W}^{(a)}|0\rangle = \left(\det W_{22}^{(b)}\right)^{1/2}\left(\det W_{22}^{(a)}\right)^{1/2} \times \det\left(1+z^2D^{(b)}C^{(a)}\right)^{1/2}. \tag{33}$$

Since this vacuum contribution must be a polynomial in z, the eigenvalues of $D^{(b)}C^{(a)}$ must come in degenerate pairs (ν_k, ν_k). Therefore, considering only one eigenvalue for each degenerate pair

$$\langle 0|\hat{W}^{(b)}\exp(\alpha\hat{N})\hat{W}^{(a)}|0\rangle = \left(\det W_{22}^{(b)}\right)^{1/2}\left(\det W_{22}^{(a)}\right)^{1/2}\prod_{k=1}^{N_{\rm s}}\left(1+z^2\nu_k\right). \tag{34}$$

Finally setting $z=1$, we obtain for the grand canonical trace

$$Z_{gc} = \det\left(W_{22}^{(b)}\right)^{1/2}\det\left(W_{22}^{(a)}\right)^{1/2}\prod_k(1+\nu_k)\prod_k(1+\mu_k)\,. \tag{35}$$

The only sign ambiguity in Eq. (35) comes from the contributions of the two square roots. From Eq. (34) (for $z=0$), one can see that each square root is again the vacuum contribution from $\hat{W}^{(b)}$ and $\hat{W}^{(a)}$, but we know already as to remove this ambiguity using Eq. (26) for each $W^{(b)}, W^{(a)}$, since we know the matrices $S^{(b)}$ and $S^{(a)}$. These considerations can easily be extended to a product of several SDOs.

As a final remark, it is possible (using Eq. (9)) to prove that the matrices $D^{(b)}$ and $C^{(a)}$ are antisymmetric and therefore these arguments amount to a quantum mechanical proof of the statement that the product of two antisymmetric matrices has eigenvalues in degenerate pairs (even $N_{\rm s}$) or the odd one is zero (odd $N_{\rm s}$).

2.5. A numerical test

Essentially, our method to fix the sign of the square root in the general case is based on an analytical continuity argument, supplemented by the fact that we know the contribution of the vacua of the factors $W^{(a)}, W^{(b)}, \ldots$, because of Eqs. (12) and (26). We performed extensive numerical tests of Eq. (35), by considering an ensemble of 12×12 antisymmetric random matrices with matrix elements uniformly distributed in the interval $-a$ and a ($a \simeq 3$). This random set generates the matrices $A^{(b)}$ and $A^{(a)}$ and from Eq. (4) the matrices $S^{(b)}$ and $S^{(a)}$. To test the above method we consider the matrices $bS^{(b)}$ and $bS^{(a)}$ with b varying from 0 to 1 in sufficiently small steps, so that a numerical continuity argument can be tested. We also have used the conventional way of evaluating the grand canonical trace, by taking the square of Eq. (35) and then numerically evaluating the square root and then following the phase of this square root as b is varied from 0 to 1. More precisely, we evaluate the phase of the grand canonical trace and, if the phase changes between consecutive values of b by an amount larger than some value $\delta\phi_{\rm max}$ we change the phase by π. In many cases the numerical continuity argument agrees with Eq. (35) but in some case we found a sign disagreement. It is instructive to analyze these latter cases. In Fig. 1 we

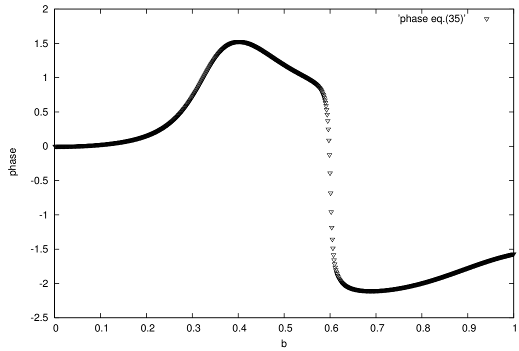

Fig. 1. The phase of Eq. (35) as a function of b.

show the phase of Eq. (35) as a function of b for one of these instances, and in Fig. 2 we show the phase for the same trace evaluated with the numerical continuity argument with two different step sizes. For a relatively small number of steps ($N_{\text{steps}} = 200$), the phase shows a discontinuity, while for a much larger number of steps ($N_{\text{steps}} = 800$), the continuity of the phase as a function of b is restored. The maximum phase change from one step to the next has been kept fixed for both cases to $\delta\phi_{\max} = 0.5$. From Fig. 2 we see that the source of the discontinuity is the rather large change in the phase for small variations of b, which is associated with a vertical slope of the phase. In this instance even 400 steps fail to reproduce the continuity of the phase. This rather surprising result, was obtained because of the

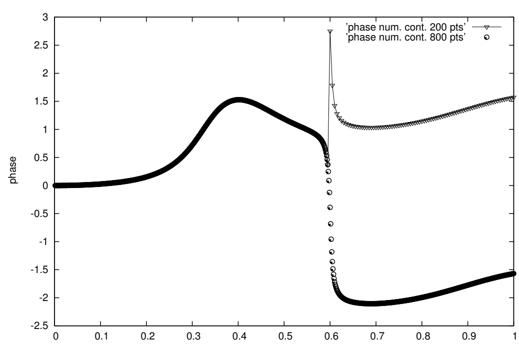

Fig. 2. The phase of the square root of the square of Eq. (35) as a function of b, obtained with the numerical continuity method.

disagreement with Eq. (35), otherwise it would have gone undetected. If we have to check the continuity of the phase for hundreds of cases (as it is in the case of the angular momentum projection), we can hardly check every single instance to insure the proper phase. If we consider smaller values of $\delta\phi_{\rm max}$ we may need several thousands steps to restore continuity. This pathological behavior of the numerical continuity argument was found in presence of a vertical slope.

This example does show the limitations of the numerical continuity method.

3. Conclusions

In this work we have shown that the sign ambiguity in the evaluation of the trace of statistical density operator written as a product of elementary statistical density operators (this is usually the case in physical applications) can be effectively removed by considering all factors separately, evaluating the vacuum contributions using Eq. (12), then reconstructing the vacuum contribution of the full statistical density operator without taking any square root of determinant using Eq. (35). Quite surprisingly, a numerical continuity argument, computationally more involved, can fail to reproduce the proper sign in some numerical test cases, unless we use a large number of steps. The recipe presented in this work opens the possibility to perform calculations of grand canonical partition functions within the HFB formalism with projectors to good quantum numbers.

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