Symmetry Restoration in Hartree-Fock-Bogoliubov Based Theories

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We present a pfaffian formula for projection and symmetry restoration for wave functions of the general Bogoliubov form, including quasiparticle excited states and linear combinations of them. This solves a long-standing problem in calculating states of good symmetry, arising from the sign ambiguity of the commonly used determinant formula. A simple example is given of projecting good particle number and angular momentum from a Bogoliubov wave function in the Fock space of a single j-shell.

Introduction. The Bogoliubov transformation offers a powerful way to introduce correlations into multi-fermion wave functions. The variational theory based on it, the Hartree-Fock-Bogoliubov (HFB) theory, has been very useful in nuclear physics. However, the variational wave functions need not respect symmetries of the Hamiltonian, hindering its use for spectroscopic purposes. An obvious fix is to project the wave functions onto eigenstates of the conserved quantum numbers. However, present methods to carry out the projection are beset with technical difficulties. The purpose of this letter is to present a projection formula that is applicable to general Bogoliubov wave functions, including those for odd particle number. The results are generalized for the evaluation of overlaps, as those required in configuration mixing theories based on HFB wave functions, commonly referred to as Generator Coordinate Method (GCM).

We first remind the reader that an operator $\mathcal{P}_K$ for projecting onto a symmetry group representation K is given by the integral

$$\mathcal{P}_{Ki} = \frac{d_K}{\Omega_0} \int d\Omega \, R_{ii}^K(\Omega)\mathcal{R}(\Omega). \tag{1}$$

Here $\mathcal{R}$ is an operator of the symmetry group, R_{ij}^K is a diagonal element of a matrix representation of the group, d_K is the dimension of the representation matrix R^K and $\Omega_0 = \int d\Omega$ is the volume integral over the group. The main conserved quantum numbers that we wish to restore in nuclear physics are particle number N and angular momentum J. These are both very familiar but for concreteness we note that particle number is associated with the gauge group $U(1)$ and the group integral is $\int_0^{2\pi} d\phi$ where ϕ is the gauge angle. In the case of angular momentum, the integration is over the Euler angles $\sin(\beta)d\alpha d\beta d\gamma$ and the representation matrices are the Wigner D-functions. The probability of the component with quantum number K in the state $|w\rangle$ is given by the integral

$$\langle K|w\rangle^2 = \langle w|\mathcal{P}_K|w\rangle = \frac{d_K}{\Omega_0} \int d\Omega \, R_{ij}^K \langle w|\mathcal{R}|w\rangle. \tag{2}$$

In this letter we treat only the problem of calculating the overlaps; for applications one also needs to calculate matrix elements of physical operators. In the past, the computation of the overlap $\langle w|\mathcal{R}|w\rangle$ was carried out by the Onishi formula[1] (see also [2, Eq. E.49]). Unfortunately, the formula has square root sign ambiguity which makes it useless for projection, except in special cases. Several suggestions have been made in the past for overcoming this sign problem[3–6]. In ref. [6], Robledo proposed a promising new formula based on the pfaffian rather than the determinant. However, his formula requires the inverse of the Bogoliubov transformation matrix U, and is thus not applicable to wave functions for which the U matrix is singular. This is the case for all wave functions that have zero overlap with the vacuum. In particular, the formula cannot be used directly for states of odd particle number.

Here we propose a pfaffian expression which can be easily extended to odd-N wave functions, and indeed to states with more than one quasiparticle excitation. To establish the notation, we write the effect of the symmetry operation as

$$\mathcal{R}c_i^\dagger \mathcal{R}^{-1} = \sum_j R_{ij}c_j^\dagger; \quad \mathcal{R}c_i\mathcal{R}^{-1} = \sum_j R_{ij}^* c_j \tag{3}$$

where $c_i^\dagger$ and c_i are the usual Fock-space creation and annihilation operator in some convenient basis. Note that the matrix R depends on the specific details of the basis states and does not have to belong to an irreducible representation

of the group. The wave function is characterized by the U, V matrices of the Bogoliubov transformation. Use is made of the Bloch-Messiah decomposition (see [2] for details and notation) that expresses those matrices as the product of unitary matrices D and C and special block diagonal matrices $\overline{U}$ and $\overline{V}$, namely $U = D\overline{U}C$ and $V = D^*\overline{V}C$ [2, Eq. 7.8]. The unitary D transformation defines the "canonical" basis with creation and annihilation operators $a^\dagger$ and a.

We first consider the simpler case in which the wave function has a non-zero overlap with the vacuum. Then it can be expressed in the canonical basis as

$$|w\rangle = \prod_\alpha^n (u_\alpha + v_\alpha a_\alpha^\dagger a_{\bar\alpha}^\dagger)|\rangle. \tag{4}$$

Here n is the number of pairs in the wave function and the matrices U, V have dimension $(2n \times 2n)$. To specify the phase of the wave function, we may take all u_α positive definite. The overlap in this case is given by

$$\langle w|\mathcal{R}|w\rangle = \frac{(-1)^n}{\prod_\alpha^n (v_\alpha)^2}\mathrm{pf}\left[\begin{array}{cc} V^T U & V^T R^T V^* \\ -V^\dagger R V & U^\dagger V^* \end{array}\right] \tag{5}$$

where pf(M) is the pfaffian of the matrix M. We outline an alternative derivation below. Note that to use Eq. (5) the U, V matrices in the canonical basis must be truncated to omit columns for which $v_\alpha = 0$ (see also Ref. [8]). This simply means omitting the part of the Fock space that is not occupied.

The generalization of Eq. (5) to deal with arbitrary overlaps is straightforward but it requires to write the wave function $|w\rangle$ of Eq. (4) as

$$|w\rangle = \frac{\det C}{\prod_{\alpha=1}^n v_\alpha}\beta_1\beta_2\ldots\beta_{2n}|\rangle \tag{6}$$

where the β_μ are Bogoliubov quasiparticle annihilation operators with amplitudes U and V. Here an unnormalized wave function is obtained by the product of all the Bogoliubov-transformed annihilation operators acting on the vacuum, and $\prod_{\alpha=1}^n v_\alpha^{-1}$ is the normalization factor. The phase $\det C$ is required for consistency of all the definitions. The overlap is then given by

$$\langle w|\mathcal{R}|w'\rangle = (-1)^n\frac{\det C^* \det C'}{\prod_\alpha^n v_\alpha v'_\alpha}\mathrm{pf}\left[\begin{array}{cc} V^T U & V^T R^T V'^* \\ -V'^\dagger R V & U'^\dagger V'^* \end{array}\right] \tag{7}$$

This formula is useful in dealing with configuration mixing of symmetry restored HFB wave functions, as required in the implementation of the most general version of the Generator Coordinate Method (GCM). The connection between Eq. (7) and Eq. (7) of [6] is not straightforward and requires of some lengthy calculations, details are given in [7].

Eq. (7) may be extended to wave functions that are orthogonal to the vacuum by considering the more general canonical form

$$\prod_q c_q^\dagger \prod_\alpha^n (u_\alpha + v_\alpha a_\alpha^\dagger a_{\bar\alpha}^\dagger)|\rangle. \tag{8}$$

Again, if the canonical U, V (U', V') matrices are truncated to omit columns for which $v_\alpha = 0$ $(v'_\alpha = 0)$, Eq. (7) is still applicable. In the case of odd-N ground states, only a single additional operator is needed,

$$|qw\rangle = c_q^\dagger|w\rangle = \sum_j q_j c_j^\dagger|w\rangle. \tag{9}$$

We use the notation $\mathbf{q}$ for the row vector of the coefficients q_i ($q_{1,i}$ in matrix notation), and $\mathbf{0}$ for the row vector of zeros. Then the generalization of Eq. (7) is

$$\langle qw|\mathcal{R}|q'w'\rangle = (-1)^n\frac{\det C^* \det C'}{\prod_\alpha^n v_\alpha v'_\alpha}\mathrm{pf}\left[\begin{array}{cccc} V^T U & \mathbf{0}^T & V^T R^T \mathbf{q}'^T & V^T R^T V'^* \\ \mathbf{0} & 0 & \mathbf{q}^* R^T \mathbf{q}'^T & \mathbf{q}^* R^T V'^* \\ -\mathbf{q}' R V & -\mathbf{q}' R \mathbf{q}^\dagger & 0 & \mathbf{0} \\ -V'^\dagger R V & -V'^\dagger R \mathbf{q}^\dagger & \mathbf{0}^T & U'^\dagger V'^* \end{array}\right]. \tag{10}$$

The shape of this matrix is $(2n + 2 + 2n) \times (2n + 2 + 2n)$. To derive it and Eq. (7), first note that the expectation value of a product of single-fermion operators α_i is given by the pfaffian of all possible contractions[9, 10]

$$\langle \alpha_1 \alpha_2 \ldots \alpha_k\rangle = \mathrm{pf}\left(S_{i,j}\right) \tag{11}$$

where $S_{i,j}$ is a skew-symmetric matrix with upper triangular elements $S_{i,j} = \langle |\alpha_i \alpha_j| \rangle$ $(i < j)$ The overlaps can be written in this form using Eq. (6). The overlap in Eq. (10) is derived by evaluating the contractions in the operator product

$$\langle \beta^\dagger_{2n} \beta^\dagger_{2n-1} \ldots \beta^\dagger_1 c_q \tilde{c}^\dagger_{q'} \tilde{\beta}'_1 \tilde{\beta}'_2 \ldots \tilde{\beta}'_{2n} \rangle \tag{12}$$

where $\tilde{\beta}' = \mathcal{R}\beta'\mathcal{R}^{-1}$ etc. The matrices entering the pfaffian of Eq. (10) are easily identified:

$$(V^T U)_{\mu\nu} = \langle |\beta^\dagger_\mu \beta^\dagger_\nu| \rangle \tag{13}$$

$$(V^T R^T \mathbf{q}'^T)_\mu = \langle |\beta^\dagger_\mu \tilde{c}^\dagger_{q'}| \rangle = \sum_j q'_j \langle |\beta^\dagger_\mu \tilde{c}^\dagger_j| \rangle \tag{14}$$

$$(V^T R^T V'^*)_{\mu\nu} = \langle |\beta^\dagger_\mu \tilde{\beta}'_\nu| \rangle \tag{15}$$

$$\mathbf{q}^* R^T \mathbf{q}'^T = \sum_{jj'} q^*_j q'_{j'} \langle |c_j \tilde{c}^\dagger_{j'}| \rangle \tag{16}$$

$$(\mathbf{q}^* R^T V'^*)_\nu = \sum_j q^*_j \langle |c_j \tilde{\beta}'_\nu| \rangle \tag{17}$$

$$(U'^\dagger V'^*)_{\mu\nu} = \langle |\tilde{\beta}'_\mu \tilde{\beta}'_\nu| \rangle. \tag{18}$$

The generalization of Eq. (10) to multi-quasiparticle overlaps, with r annihilation operators $\bar{\beta}_{\mu_j}$ (Bogoliubov amplitudes $\bar{U}, \bar{V}$) to the left of $\mathcal{R}$ and s creation operators $\bar{\beta}'_{\nu_j}$ to the right, is tedious but straightforward

$$\langle w | \bar{\beta}_{\mu_r} \cdots \bar{\beta}_{\mu_1} \mathcal{R} \bar{\beta}'^\dagger_{\nu_1} \cdots \bar{\beta}'^\dagger_{\nu_s} | w' \rangle = (-1)^n (-1)^{r(r-1)/2} \frac{\det C^* \det C'}{\prod_\alpha^n v^*_\alpha v'_\alpha} \mathrm{pf} \begin{bmatrix} V^T U & V^T \mathbf{p}^\dagger & V^T R^T \mathbf{q}'^T & V^T R^T V'^* \\ -\mathbf{p}^* V & \mathbf{q}^* \mathbf{p}^\dagger & \mathbf{q}^* R^T \mathbf{q}'^T & \mathbf{q}^* R^T V'^* \\ -\mathbf{q}' R V & -\mathbf{q}' R \mathbf{q}^\dagger & \mathbf{p}' \mathbf{q}'^T & \mathbf{p}' V'^* \\ -V'^\dagger R V & -V'^\dagger R \mathbf{q}^\dagger & -V'^\dagger \mathbf{p}'^T & U'^\dagger V'^* \end{bmatrix}. \tag{19}$$

For this expression to make sense both r and s must have the same number parity. The objects $\mathbf{p}$ and $\mathbf{q}$ ($\mathbf{p}'$ and $\mathbf{q}'$) are matrices of dimension $r \times 2n$ ($s \times 2n$) with matrix elements $p_{\mu_j m} = \bar{V}_{m\mu_j}$ and $q_{\mu_j m} = \bar{U}_{m\mu_j}$. If some of the $\bar{\beta}$ annihilation operators are replaced by creation ones $\bar{\beta}^\dagger$ the appropriate rows of $\mathbf{q}$ and $\mathbf{q}$ have to be redefined accordingly. It is easy to check that Eq. (19) reduces to Eq. (10) in the limit $\mathbf{p} = 0$. Apart from the fact that Eq. (19) includes the phase of the matrix element, this expression has the advantage over more traditional approaches [12] that the combinatorial explosion in the evaluation of the left hand side of Eq. (19), namely the fact that $(r+s)!!$ contractions have to be considered if the multi-quasiparticle overlap is computed with the standard Generalized Wick's theorem, is completely avoided (see [11] for another approach based on the finite temperature formalism).

Example. As a proof of principle, we carry out the projection for an odd-N wave function having a nontrivial structure with respect to angular momentum and particle number. We take the Fock space as the 6-dimensional space of orbitals in a $j = 5/2$ shell. The creation operators $c^\dagger_m$ are labeled by azimuthal angular momentum $j_z = m$. The wave function for the test is

$$|qw\rangle = c^\dagger_{1/2} \left(u + v c^\dagger_{5/2} c^\dagger_{-5/2} \right) |\rangle \tag{20}$$

with $(u, v) = (0.8, 0.6)$. We project simultaneously on particle number and angular momentum with the operator $\mathcal{P}_N \mathcal{P}_{JJ_z}$. We use a 4-point uniform mesh for integrating the gauge angle and a 5-point Gauss-Legendre quadrature for integrating over the angular variable $\cos(\beta)$. There is no necessity to integrate over the other Euler angles because the wave function Eq. (20) is an eigenstate of J_z. The results are shown in Table I. The projected quantum numbers N and J are given in the first two columns. The third column gives the exact decomposition, and the fourth column the numerical projection. One sees that there is complete agreement to the level of numerical precision in the integrations.

Discussion. Besides the overlap function $\langle w | \mathcal{R} | w \rangle$ we need the matrix elements of various operators in the symmetry-restored states. For the most important operators they can be expressed as a single integral over matrix elements of the type $\langle w | \mathcal{O}\mathcal{R} | w \rangle$ where $\mathcal{O}$ is an operator such as the Hamiltonian. It is straightforward to calculate this operator matrix elements using the Balian-Brezin formula[12] or the multi-quasiparticle overlap of Eq. (19). Unlike the formulation in Ref. [6], our method here does not require one to construct quasiparticle states explicitly. Our procedure is easily extended to multi-quasiparticle matrix elements with a final result that avoids the combinatorial explosion that plagues other methods used to evaluate those overlaps. For an k-quasiparticle excitation, the pfaffian

TABLE I: Test of number and angular momentum projection for the wave function of Eq. (20), for which $J_z = 1/2$.

| N | J | $\langle NJJ_z|qw\rangle^2$ | |
		analytic	numerical
1	3/2	0	0.00000
1	5/2	$u^2 = 0.64$	0.64000
3	1/2	0	0.00000
3	3/2	$v^2/7 \approx 0.05143$	0.05143
3	5/2	$v^2/2 = 0.18$	0.18000
3	7/2	0	0.00000
3	9/2	$5v^2/14 \approx 0.12857$	0.12857

matrix is augmented by $2k$ rows and columns. A program that demonstrates the method for the example in Table I is provided in the supplementary material. After this work was posted on arXiv [13] we learned that a similar fully general formula for the overlap was obtained independently by Avez and Bender [14] and Oi and Mizusaki [15].

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