The Bloch-Messiah theorem and its application to overlaps

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Abstract

The Bogoliubov transformation is the starting point for the Hartree-Fock-Bogoliubov method and thus for many theoretical approaches that describe heavy nuclei. This transformation is based on two matrices, denoted by U and V, which are called Bogoliubov amplitudes. In this paper the properties of these matrices are investigated. Bogoliubov amplitudes are generated using BCS wavefunctions. The Bloch-Messiah theorem and the resulting Bloch-Messiah decomposition are discussed as well as a newfound restriction on the transformation matrix D from the BM decomposition. Different formulas are presented to compute the overlap between the generated wavefunctions.

Contents

Abbreviations

BM	Bloch-Messiah
BCS	Bardeen-Cooper-Schrieffer
HFB	Hartree-Fock-Bogoliubov
GCM	Generator Coordinate Method

1 Introduction

The theoretical description of nuclei and other many-fermion systems has advanced considerably during recent times. Computational technology and refined methods allow for an accurate picture of atomic nuclei. In comparison to real world experiments, computational models have the advantage that they are able to predict properties of nuclei in extreme conditions or during fission processes, that are difficult to observe in an experiment.

In many cases, in theoretical nuclear physics the aim is to solve a Hamiltonian to describe different nuclei. The Hartree–Fock method is the central starting point for most approaches that describe the many-nucleon system more accurately. Starting from a Slater determinant which is an antisymmetric linear combination of products of independent single particle wavefunctions, the variational principle is applied, which means that the energy is varied to find the Slater determinant that minimizes the energy. This solution is a good approximation for the actual wavefunction, for few particularly stable nuclei.

A more accurate method based on the Hartree-Fock approach is the Hartree-Fock-Boguliubov method. Its starting point is the Bogoliubov (or Bogoliubov-Valatin) transformation which transforms a single particle wavefunction into a quasi-particle wavefunction, where a quasi-particle represents a linear combination of particles and holes. This transformation, which was developed independently by Nikolay Bogolyubov and John George Valatin in 1958 ([1, 2]) finds a convenient basis to solve the nuclear many-body problem as we will show for the simple case of a BCS wavefunction. The BCS formalism was proposed by Bardeen, Cooper and Schrieffer in 1957 ([3]). The essential insight that time-reversed particles interact strongly made it possible to describe superconductivity through the formation of Cooper pairs. However, as the pairing interaction is a key attribute not only of electrons but of all fermions, this theory is applicable to nuclei as well. A generalization of the BCS approach is the Hartree-Fock-Bogoliubov (HFB) method [4] which is the core of many recent models describing heavy nuclei. In addition to that, the Bogoliubov transformation is useful for the description of many other processes in physics like for example Hawking radiation [5].

In a recent Model [6] developed in Lund nuclear spectra are computed using an effective Hamiltonian which is then solved using the Generator Coordinate method (GCM) [6, 7]. This framework of the GCM allows the implementation of collective and single particle dynamics, such as pair vibrations and shape transition starting from the HFB method. In this approach the actual wavefunction is calculated as the superposition of a weighted set of basis wave functions. Those trial wave functions, in most cases HFB states, can be freely chosen to define properties which are relevant for the actual state of the many-body system. This includes for example symmetries with respect to particle number, parity, rotational symmetry, etc [8]. Essentially, one uses the Generator Coordinate Method to define a certain set of basis wavefunctions that do not obey the symmetries that the final wavefunction needs to have. They can for example describe a many body system with different numbers of particles. This symmetry breaking is useful, since it allows to reduce the number of basis states considerably, without diminishing the accuracy. The weighing of the basis wavefunctions then restores the broken symmetries. A recurring problem for the implementation of this method is finding the exact weight that each basis wavefunction needs to be multiplied with, this requires the calculation of overlaps between two different basis wave functions. Most approaches calculate the overlaps using the Bogoliubov amplitudes, matrices U and V, that describe the relation between different sets of creation and annihilation operators. Important is the formula by Onishi and Yoshida [9] from 1966 as well as similar approaches by F. Dönau [10] and J. Dobaczewski [11, 12]. More recent formulations focus on the description of the phase of the overlap and include the formula by Bertsch and Robledo [13] as well as the formula derived by Carlsson and Rotureau [14].

An important tool when working with the Bogoliubov amplitudes is the Bloch-Messiah theorem [15] which describes the decomposition of the matrices U and V into more convenient matrices, a diagonal matrix $\bar{U}$ and a matrix $\bar{V}$ in a special canonical form. The theorem uses the results of a theorem by B. Zumino [16] which shows that skew-symmetric matrices can be brought into the canonical form. In the canonical basis it is possible to order the eigenvalues of $\bar{V}$ and cut off the eigenvalues with the smallest absolute values, thereby reducing the computational cost immensely. Apart from its applications in nuclear physics, the BM decomposition can also be used to determine eigenmodes for optical parametric amplifiers.

In this thesis, the Bogulibov amplitudes, their canonical basis and the calculation of overlaps will be studied. In the method section the concepts of second quantization, BCS pairing theory and HFB theory are introduced. The Bloch-Messiah theorem is stated and proven, in a complete and pedagogical way as an extension of the existing proofs in the literature ([15, 4]). Bogoliubov amplitudes in canonical form are created using BCS-theory combined with the potential of a 3D harmonic oscillator. Then a reverse process to the Bloch-Messiah decomposition is performed such that the matrices U and V are not in canonical form anymore. After artificially creating the U and V matrices, the BM decomposition is found again. Having established the BM-decomposition different approaches to calculate overlaps are described.

In the result section the restrictions on the matrix D, that have not yet been described in literature, are discussed as well as the observations of different overlaps using the different approaches.

2 Method

2.1 Theoretic background

2.1.1 Second quantization

If a quantum many-body system contains several indistinguishable particles it is not possible to label each particle. Hence, it is logical to introduce a formalism which only describes how many particles occupy each basis quantum state of the single particle basis. This is called the second quantization method. Another advantage is that it allows for the number and type of particles to change dynamically. It introduces creation and annihilation operators a_μ^+ and a_μ where the index μ specifies a single particle state. Depending on the context the states can be, for example, the levels of a harmonic oscillator or any other potential. This is the starting point for the nuclear shell model.

By acting on a vacuum state $|0\rangle$ the creation operator creates a particle,

$$a_\mu^+|0\rangle = |\psi_\mu\rangle \equiv |\mu\rangle. \tag{1}$$

In a similar way the annihilation operator takes away a particle from the state μ. We naturally have that

$$a_\mu|0\rangle = 0, \tag{2}$$

since no particle can be taken away from the vacuum.

We will consider the fermionic case, where we also have that the same quantum state cannot be occupied twice due to the Pauli exclusion principle and thus

$$a_\mu^+|\mu\rangle = 0. \tag{3}$$

This implies that the wavefunction has to be antisymmetric which requires that the creation operators of two different basis states anti-commute and similarly the annihilation operators,

$$\{a_\mu^+, a_\nu^+\} = 0, \quad \{a_\mu, a_\nu\} = 0. \tag{4}$$

Together with the additional condition,

$$\{a_\mu, a_\nu^+\} = \delta_{\mu\nu}, \tag{5}$$

the above equations (4,5) are called fermion anti-commutation Relations (see Appendix A).

The wavefunction of a single particle (1) is defined as a vector in a Hilbert space $\mathcal{H}$ (the so-called ket). The Hilbert space of an A-particle system then becomes

$$\mathcal{H}_A = \mathcal{H} \otimes \mathcal{H} \otimes \ldots \otimes \mathcal{H}, \tag{6}$$

where $\otimes$ denotes the usual tensor product. We then divide the new Hilbert space $\mathcal{H}_A$ into an asymmetric space $\mathcal{H}_A^{(-)}$ for fermions, a symmetric space $\mathcal{H}_A^{(+)}$ for bosons and the remaining orthogonal complement which until now does not have any connection to physical wavefunctions of elementary particles. We can see, however, that the creation and annihilation operators do not operate in a single space $\mathcal{H}_A$ but send wavefunctions from $\mathcal{H}_A$ to $\mathcal{H}_{A+1}$ or $\mathcal{H}_{A-1}$. To solve this problem we can introduce the Fock space

$$\mathcal{F}^{(\pm)} := \mathbb{C} \oplus \mathcal{H}_1^{(\pm)} \oplus \mathcal{H}_2^{(\pm)} \oplus \ldots \oplus \mathcal{H}_n^{(\pm)} \oplus \ldots, \tag{7}$$

where $\oplus$ denotes the direct sum. The Fermion creation and annihilation operators described above are now a simple transformation in the antisymmetric Fock space $\mathcal{F}^{(-)}$.

2.1.2 BCS pairing theory

The Bardeen–Cooper–Schrieffer theory (BCS) [3, 17] was introduced in solid state physics to explain phenomena like superconductivity and superfluidity. The essential insight is that any fermion interacts strongly with its time-reversed counterpart, i.e. a particle in a degenerate state but with the spin and the angular momentum pointing in the opposite direction. Since neutrons and protons are fermions, the same formalism has been applied immediately after to nuclei as well [18]. When it comes to superconductivity the strong attraction between such pairs is generally attributed to electron-lattice interactions, namely the interaction between lattice vibrations (the phonons) and electrons. A similar explanation can be made for the pairing in nuclei, the difference is that the interaction happens between nucleons and core vibrations.

For a single particle Hamiltonian any state $|\mu\rangle$ and the time-reversed counterpart, denoted by $|\bar{\mu}\rangle$ have the same energy. Thus $e_\mu = \langle\mu|H|\mu\rangle = \langle\bar{\mu}|H|\bar{\mu}\rangle$ which gives

$$H_{sp} = \sum_\nu e_\nu (a_\nu^+ a_\nu + a_{\bar{\nu}}^+ a_{\bar{\nu}}). \tag{8}$$

A general two particle operator in the second quantization formalism, given a potential V of the interaction strength, is given by

$$V = \sum_{k,l,m,n} a_k^+ a_l^+ a_m a_n \langle kl|V|nm\rangle. \tag{9}$$

The only interactions that are considered in BCS are the ones between time-reversed particles which specifies that the non-zero indices in equation (9) are $a_\mu^+ a_{\bar{\mu}}^+ a_{\bar{\nu}} a_\nu \langle\mu\bar{\mu}|V|\nu\bar{\nu}\rangle$. We will work with the seniority scheme which uses the first order term for this type of two body interaction. This term is constant and will be denoted by $-G$.

We thus have a two particle contribution to the Hamiltonian of the form

$$V_{2P} = -G \sum_{\mu,\nu} a_\mu^+ a_{\bar{\mu}}^+ a_{\bar{\nu}} a_\nu. \tag{10}$$

Hence, the total Hamiltonian is given by

$$H = \sum e_\nu (a_\nu^+ a_\nu + a_{\bar{\nu}}^+ a_{\bar{\nu}}) - G \sum\sum a_\mu^+ a_{\bar{\mu}}^+ a_{\bar{\nu}} a_\nu. \tag{11}$$

Bardeen, Cooper and Schrieffer proposed a trial wavefunction to solve this Hamiltonian,

$$|BCS\rangle = \prod_{\nu}(u_\nu + v_\nu a_\nu^+ a_{\bar{\nu}}^+ |0\rangle), \tag{12}$$

with the restriction $v_\nu^2 + u_\nu^2 = 1$. The solution of the given Hamiltonian finally gives the occupation probabilities v_ν^2 for the different single particle states as

$$v_\nu^2 = \frac{1}{2}\left(1 - \frac{E_\nu}{\sqrt{E_\nu^2 + \Delta^2}}\right), \tag{13}$$

where $E_\nu = \epsilon_\nu - \epsilon_f$ denotes the energy of the state ν relative to the Fermi energy ϵ_f and $\Delta = G\sum u_\nu v_\nu$ is the pairing gap, a parameter that describes the energy to break a pair of fermions. This implies that

$$u_\nu^2 = \frac{1}{2}\left(1 + \frac{E_\nu}{\sqrt{E_\nu^2 + \Delta^2}}\right). \tag{14}$$

The sum of the occupation probabilities v_ν has to equal a predetermined particle number, which gives

$$n = \sum_{\nu} v_\nu^2. \tag{15}$$

The coefficients u_ν and v_ν define a transformation of the single particle ν into a quasi-particle which is a linear combination of a particle and a hole. This defines new creation and annihilation operators

$$\alpha_\nu^+ = u_\nu a_\nu^+ - v_\nu a_{\bar{\nu}} \tag{16}$$

and

$$\alpha_\nu = u_\nu a_\nu - v_\nu a_{\bar{\nu}}^+. \tag{17}$$

This is in essence a change of basis and the BCS theory uses a special case of the Bogoliubov transformation.

2.1.3 Bogoliubov transformation

The general Bogoliubov transformation defines new operators as a linear combination of creation and annihilation operators which also fulfil the Fermion anti-commutation relations. As in BCS, the new operators do not represent the creation and annihilation of real particles anymore but are analogous to independent particles and are thus called quasi-particles,

$$\beta_k^+ = \sum_l U_{lk} a_l^+ + V_{lk} a_l \tag{18}$$

and

$$\beta_k = \sum_l U_{lk}^* a_l + V_{lk}^* a_l^+. \tag{19}$$

The transformation matrices U and V are called Bogoliubov amplitudes.

From the Fermion anti-commutation relations (Appendix B) we can show that in a model with M basis states the transformation

$$(a_1, \dots, a_\mu, a_1^+, \dots, a_\mu^+) \longrightarrow (\beta_1, \dots, \beta_\mu, \beta_1^+, \dots, \beta_\mu^+) \tag{20}$$

which acts in a 2M-dimensional space is unitary.

$$\begin{pmatrix} \beta \\ \beta^+ \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} a \\ a^+ \end{pmatrix} = W^\dagger \begin{pmatrix} a \\ a^+ \end{pmatrix} \tag{21}$$

Here a, a^+, β and β^+ are column vectors of the form $a = (a_1, \dots, a_\mu)^T$. Since equation (21) is a unitary transformation it is a simple rotation in the antisymmetric Fock space. This new basis is used in the Hartree-Fock-Bogoliubov method, a variational method which determines the single Slater determinant that minimizes the energy in the quasi particle basis and therefore finds the best approximation to the full wavefunction. The computational cost for the HFB method is relatively low, which is why it is the starting point for most theoretical approaches to describe heavy nuclei.

2.2 Bloch-Messiah theorem

The Theorem of Bloch and Messiah [15] now states that every unitary matrix of the form

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \tag{22}$$

can be decomposed into three matrices of the form

$$W = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix}, \tag{23}$$

where D and C are unitary and the matrices $\bar{U}$ and $\bar{V}$ are of the form

$$\bar{U} = \begin{pmatrix} 0 & & & & & & & & \\ & \ddots & & & & & & 0 & \\ & & 0 & & & & & & \\ & & & \boxed{\begin{matrix} u_1 & 0 \\ 0 & u_1 \end{matrix}} & & & & & \\ & & & & \ddots & & & & \\ & & & & & \boxed{\begin{matrix} u_n & 0 \\ 0 & u_n \end{matrix}} & & & \\ & & & & & & 1 & & \\ & 0 & & & & & & \ddots & \\ & & & & & & & & 1 \end{pmatrix} \tag{24}$$

and

$$
\bar{V} = \begin{pmatrix}
1 & & & & & & & \\
& \ddots & & & & & 0 & \\
& & 1 & & & & & \\
& & & \boxed{\begin{matrix} 0 & v_1 \\ -v_1 & 0 \end{matrix}} & & & & \\
& & & & \ddots & & & \\
& & & & & \boxed{\begin{matrix} 0 & v_n \\ -v_n & 0 \end{matrix}} & & \\
& & & & & & 0 & \\
& 0 & & & & & & \ddots \\
& & & & & & & & 0
\end{pmatrix}. \tag{25}
$$

In nuclear physics, where the matrices U and V in the BM theorem are the Bogoliubov amplitudes, it is a great advantage to be able to find their simplified forms (24,25). This makes it possible to reduce the matrix size by cutting away the beginning and tail of zeroth respectively ones on the diagonals of $\bar{U}$ and $\bar{V}$. The remaining 2×2 boxes represent a quasiparticle state and its time-reversed counterpart. This explains why the values u_i and v_i appear in pairs. The basis in which the Bogoliubov amplitudes are in the from of (24,25) is called the canonical basis.

2.2.1 Proof

The theorem is proved in [15, 4], however, here a more pedagogical proof is provided with many details. Furthermore, this proof, in contrast to existing proofs, is treating the general case without any assumptions. This means in particular that higher degeneracies and nonhermitian matrices U are considered. To prove the Bloch-Messiah theorem we need to show the spectral theorem for Hermitian matrices [19].

Lemma 1 (Göllmann [19])**.** *A Hermitian matrix $Q \in \mathbb{C}^{n \times n}$ can be diagonalized by a unitary matrix U such that*

$$\bar{Q} = U^{\dagger} Q U \tag{26}$$

is diagonal with real eigenvalues and an orthonormal set of eigenvectors.

Proof. First we show that the eigenvalues of a Hermitian matrix H are real. Let $Qv = \lambda v$, where v is an eigenvector and λ is an eigenvalue. We have

$$\lambda \langle v, v \rangle = \langle \lambda v, v \rangle = \langle Qv, v \rangle = \langle v, Qv \rangle = \langle v, \lambda v \rangle = \lambda^* \langle v, v \rangle. \tag{27}$$

Hence λ is real. We will show by induction that the eigenvectors of Hermitian matrices can be chosen to be orthogonal. Let Q be a $n \times n$ Hermitian matrix. The characteristic polynomial $\det(Q - \lambda I) = 0$ has at least one solution, which means that there exists at least one eigenvector, thus the base case is established.

In the induction step let $n < m$ be an integer. We want to show that if we know $n - m$ orthogonal eigenvectors which span the space W we can always find another eigenvector that is orthogonal to the previous ones. Let $u_1, \ldots, u_m$ be an orthonormal basis of the orthogonal complement $W^\perp$ of W in the vector space $\mathbb{C}^n$ and let U be the $n \times m$ matrix with columns u_1 to u_m. Now let w be an eigenvector of $U^\dagger QU$ with eigenvalue μ. Then

$$U^\dagger QUw = \mu w \Longrightarrow UU^\dagger QUw = \mu Uw. \tag{28}$$

We define $v = Uw$ which gives

$$UU^\dagger Qv = \mu v. \tag{29}$$

Thus v is clearly a linear combination of the basis vectors of $W^\perp$. Thus v is orthogonal to any other eigenvector x with eigenvalue λ and since Q is Hermitian

$$\langle \lambda x, v\rangle = 0 \Longrightarrow \langle Qx, v\rangle = \langle x, Qv\rangle = 0. \tag{30}$$

Hence Qv is a linear combination of basis vectors of $W^\perp$, $Qv = Uy$ for some vector y. Thus

$$UU^\dagger Qv = UU^\dagger Uy = UI_m y = Uy = Qv. \tag{31}$$

Combining this result with (29) we find a new orthogonal eigenvector,

$$Qv = \mu v. \tag{32}$$

Hence by induction for any Hermitian matrix there exist an orthogonal and hence orthonormal set of eigenvectors. Let us call this set of eigenvectors $t_1, \ldots, t_n$ and the corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$. Let $\bar{Q}$ be the diagonal matrix with $\lambda_1, \ldots, \lambda_n$ as entries and T the matrix with $t_1, \ldots, t_n$ as columns. The matrix T is unitary because the columns t_i are orthonormal. Then for any eigenvector t_i we have $Te_i = t_i \Longrightarrow e_i = T^\dagger t_i$ and thus

$$T\bar{Q}T^\dagger t_i = T\bar{Q}e_i = \lambda_i Te_i = \lambda_i t_i = Tt_i. \tag{33}$$

Since the vectors $t_1, \ldots, t_n$ span the whole space we have

$$T\bar{Q}T^\dagger = Q. \tag{34}$$

□

We also need to show the following lemma.

Lemma 2 (Becker [20, 16])**.** *Any skew-symmetric matrix P can be brought into the canonical form $\bar{P}$ as*

$$\bar{P} = S^\dagger PS^*, \tag{35}$$

where $\bar{P}$ is of the form

$$\bar{P} = \begin{pmatrix} \boxed{\begin{matrix} 0 & s_1 \\ -s_1 & 0 \end{matrix}} & & & & & 0 \\ & \boxed{\begin{matrix} 0 & s_2 \\ -s_2 & 0 \end{matrix}} & & & & \\ & & \ddots & & & \\ & & & \boxed{\begin{matrix} 0 & s_k \\ -s_k & 0 \end{matrix}} & & \\ & & & & 0 & \\ & 0 & & & & \ddots \\ & & & & & 0 \end{pmatrix} \tag{36}$$

and $s_1, s_2, \ldots$ are real numbers.

Proof. If a matrix P is skew symmetric ($P^T = -P$) then $P^\dagger P$ is Hermitian,

$$(P^\dagger P)^\dagger = ((P^\dagger P)^T)^* = (P^T P^*)^* = P^\dagger P. \tag{37}$$

Hence it has an orthonormal system of eigenvectors v_i. we define for each eigenvector v_j with eigenvalue $\lambda_j \neq 0$ a new vector given by

$$w_j = \frac{1}{\sqrt{|\lambda_j|}} P^\dagger v_j^* = -\frac{1}{\sqrt{|\lambda_j|}} P^* v_j^*. \tag{38}$$

We notice that this vector is normalized and orthogonal to v_j. The orthorgonality follows since

$$\langle w_j, v_j \rangle = -\frac{1}{\sqrt{|\lambda_j|}} \langle P^* v_j^*, v_j \rangle = \frac{1}{\sqrt{|\lambda_j|}} \langle v_j^*, P v_j \rangle, \tag{39}$$

where we used that $(P^*)^\dagger = -P$. The last two inner products have to be the same which is only possible if $\langle w_j, v_j \rangle = 0$. We proceed to show that w_j is an eigenvector of $P^\dagger P$,

$$P^\dagger P w_j = \frac{1}{\sqrt{|\lambda_j|}} P^\dagger P P^\dagger v_j^* = \frac{1}{\sqrt{|\lambda_j|}} P^\dagger (P^\dagger P v_j)^* = \frac{1}{\sqrt{|\lambda_j|}} P^\dagger \lambda_j v_j^* = \lambda_j w_j. \tag{40}$$

Thus every eigenvalue has an even degeneracy as both v_j and w_j are eigenvectors for the same eigenvalue. Higher degeneracies are possible, as long as they are a multiple of two. We create a matrix S where the eigenvectors are the columns such that all the v_j are odd columns and the corresponding w_j are the subsequent even columns. Also all eigenvectors with eigenvalue zero v_α are placed at the end of the ordering. Now for the eigenvectors with eigenvalue zero we have

$$\langle v_\alpha, P^\dagger P v_\alpha \rangle = \langle P v_\alpha, P v_\alpha \rangle = 0 \Longrightarrow P v_\alpha = 0. \tag{41}$$

And for the v_j and w_j we get (see equation (38))

$$P v_j = -\sqrt{|\lambda_j|} w_j^* \tag{42}$$

and

$$Pw_j = \sqrt{|\lambda_j|}PP^\dagger v_j^* = \sqrt{|\lambda_j|}v_j^* \tag{43}$$

This clearly gives

$$\bar{P} = S^\dagger P S^* \tag{44}$$

to be in the canonical form (36), with $s_i = \sqrt{|\lambda_i|}$. □

Bloch-Messiah theorem.

Proof. Let

$$Q = V^* V^T = I - UU^\dagger, \tag{45}$$

which follows from the unitary of W and

$$P = V^* U^T. \tag{46}$$

We can see that Q is hermitian since

$$Q^\dagger = V^* V^T = Q. \tag{47}$$

The skew-symmetry of P immediately follows from the unitarity of W (see Appendix B)

$$UV^\dagger + V^* U^T = 0 \Longrightarrow P^T = \left(V^* U^T\right)^T = UV^\dagger = -V^* U^T = -P \tag{48}$$

Furthermore we have that

$$QP = V^* V^T V^* U^T = -V^* V^T U V^\dagger = V^* U^T V V^\dagger = PQ^*, \tag{49}$$

since $U^T V = -V^T U$ (see Appendix B).

We want to show that P can be brought into canonical form and Q can be diagonalized simultaneously. Let B be the unitary matrix that diagonalizes Q and puts the eigenvalues in descending order for simplicity, i.e. $\bar{Q}$ is diagonal with $\bar{Q} = B^\dagger Q B = B^T Q^* B^*$ and real eigenvalues q_i. We now apply $B^\dagger$ from the left side and B^* from the right side to equation (49). This results in

$$\begin{aligned} B^\dagger Q P B^* = B^\dagger P Q^* B^* &\Longleftrightarrow B^\dagger Q B B^\dagger P B^* = B^\dagger P B^* B^T Q^* B^* \\ &\Longleftrightarrow \bar{Q} B^\dagger P B^* = B^\dagger P B^* \bar{Q}. \end{aligned}$$

Let now $\bar{P} = B^\dagger P B^*$. Thus $\bar{Q}\bar{P} = \bar{P}\bar{Q}$ and since $\bar{Q}$ is diagonal we have

$$\bar{P}_{ij} q_i = \bar{P}_{ij} q_j \Longleftrightarrow \bar{P}_{ij}(q_i - q_j) = 0. \tag{50}$$

This implies that the elements of $\bar{P}$ are nonzero for all i and k where the eigenvalues $q_i \neq q_j$. Thus we only need to consider the subspaces of degenerate eigenvalues which we denote by $\bar{Q}_i$ and $\bar{P}_i$. We know that $\bar{P}^T = B^\dagger P^T B^* = -B^\dagger P B^* = -\bar{P}$ is skew symmetric and thus all the subspaces are skew symmetric as well. Now from Lemma 2 we now that for each subspace $\bar{P}_i$ there exists a unitary matrix S_i such that $S_i^\dagger \bar{P}_i S_i^*$ is in canonical form. Furthermore the diagonal character of $\bar{Q}$ is unchanged since $S_i^\dagger \bar{Q}_i S_i = S_i^\dagger q_i I S_i = q_i S_i^\dagger S_i = q_i I$. Hence the matrix S which transform $\bar{P}$ for every subspace $\bar{Q}_i$ of $\bar{Q}$, i.e. the block-diagonal matrix with S_i on the diagonal, leaves $\bar{Q}$ untouched. Now let A be the real matrix that reorders the columns of $\bar{P}$ such that all zero columns are at the end. We then have that

$$D = BSA \tag{51}$$

simultaneously transforms P into canonical form and diagonalizes Q.

From equation (45) we know that $D^\dagger U U^\dagger D$ is diagonal as well. Let $D^\dagger U = \bar{U} C$ be the RQ decomposition, where $\bar{U}$ is upper triangular and C is unitary. Since

$$D^\dagger U U^\dagger D = \bar{U} C C^\dagger \bar{U}^\dagger = \bar{U}\bar{U}^\dagger \tag{52}$$

is diagonal $\bar{U}$ has to be diagonal as well. Furthermore C can be chosen such that the entries of $\bar{U}$ are real. This allows to define $\bar{U} = D^\dagger U C^\dagger$.

Furthermore $D^\dagger P D^* = D^\dagger V^* U^T D^*$ is in canonical form. Rewriting we get

$$D^\dagger V^* U^T D^* = D^\dagger V^* C^T C^* U^T D^* = D^\dagger V^* C^T \bar{U}. \tag{53}$$

Since $\bar{U}$ is diagonal and real, $D^\dagger V^* C^T$ has to be in canonical form with real entries. We define $\bar{V} = D^T V U^\dagger$. We consider now the eigenspace of U with eigenvalues 0, in this space $\bar{U}$ has zeros on the diagonal. Then equation (45) shows that V is unitary in this subspace and that in the Bloch Messiah decomposition this part of $\bar{V}$ can be represented by a unity matrix. On the other hand, in the subspaces of V that have eigenvalue zero, where $\bar{V}$ is zero, requires $\bar{U}$ to have ones on the diagonal such that equation (45) is satisfied. Thus the matrices $\bar{V} = D^T V U^\dagger$ and $\bar{U} = D^\dagger U C^\dagger$ are of the form seen in equations (24,25). The Bloch-Messiah decomposition of the matrices U and V is hence $U = D\bar{U}C$ and $V = D^*\bar{V}C$. □

2.3 Overlap formulae

The calculation of overlaps between different (basis) wavefunctions is a recurring task within the Generator Coordinate Method and thus an integral part of most theoretical models. Generally, the phase of the overlap needs to be considered as well, but for simplicity's sake we will focus on the absolute value of the overlap. There are different ways to calculate the overlap between two Bogoliubov vacua. One generally defines one vacuum to be a bra vector while the other one is a ket vector. This means that for two Bogoliubov vacua $|Z'\rangle$ and $\langle Z|$ the overlap is $\langle Z'|Z\rangle$. The Onishi Formula [4, 9] gives a simple way to calculate this overlap as the square root of the determinant of a certain matrix A. This matrix arises as a combination of the Bogoliubov transformation matrices U, V, U' and V', representing the vacua $|Z\rangle$ and $|Z'\rangle$ respectively. The formula reads

$$\langle Z'|Z\rangle = \sqrt{\det A} = \sqrt{\det(U^\dagger U' + V^\dagger V')}. \tag{54}$$

Because of the square root the Onishi Formula allows two possible solutions, thus being ambiguous about the sign. To remove this problem Bertsch and Robledo [13, 14] derived an expression using the pfaffian of the skew-symmetric matrix

$$\begin{pmatrix} V^T U & V^T V'^* \\ -V'^\dagger V & U'^\dagger V'^* \end{pmatrix}. \tag{55}$$

Furthermore the transformation matrices C and C' from the Bloch-Messiah decomposition are required, as well as the eigenvalues from the matrices V and V'. Those are the numbers v_i (respectively v'_j) that can be found in the canonical form. The formulation is then given by

$$\langle Z'|Z\rangle = (-1)^{\frac{N}{2}} \frac{(\det C)^* \det C'}{\prod_i v_i \prod_j v'_j} \mathrm{pf} \begin{pmatrix} V^T U & V^T V'^* \\ -V'^\dagger V & U'^\dagger V'^* \end{pmatrix}. \tag{56}$$

Since the matrices C and C' are unitary and we are foremost interested in the absolute value of the overlap we may ignore the nominator of the fraction in (56).

A third possibility to calculate the overlap makes use of the Thouless representation of Slater determinants or other product wave functions (see Appendix C). Thouless' Theorem [4, 21] states that we can express a general product wave function $|Z\rangle$ in terms of a quasi-particle vacuum $|-\rangle$ for quasi-particle operators β and β^+ as long as $|-\rangle$ and $|Z\rangle$ are not orthogonal.

The ket and bra vectors of the overlap $\langle Z|Z'\rangle$ in the usual representation and in the Thouless representation, which uses the exponential function, are

$$\langle Z| = \langle Z|-\rangle\langle -|\prod_{i<j}(1 + Z^*_{ij}\beta_i\beta_j) = \langle Z|-\rangle\langle -|e^{\frac{1}{2}\sum_{i,j} Z^*_{ij}\beta_i\beta_j} \tag{57}$$

and

$$|Z'\rangle = \langle -|Z'\rangle \prod_{i<j}(1 + Z'_{ij}\beta^+_i\beta^+_j) = \langle -|Z'\rangle e^{\frac{1}{2}\sum_{i,j} Z'_{ij}\beta^+_i\beta^+_j}|-\rangle. \tag{58}$$

For the calculation of the overlap to be numerically stable, it is necessary that the overlaps $\langle -|Z'\rangle$ and $\langle Z|-\rangle$ are sufficiently big (> 0.001).

The skew-symmetric matrix Z, and similarly Z', are obtained through the matrices A and B which depend on the U and V transformation matrices for $|Z\rangle$ (respectively $|Z'\rangle$) and $|-\rangle$, where the latter are indexed with a zero. The matrices are

$$A = U_0^\dagger U + V_0^\dagger V, \tag{59}$$

which we recognize from the Onishi formula if the unprimed state is considered to be the vacuum, and

$$B = V_0^T U + U_0^T V. \tag{60}$$

The matrix Z, and likewise Z', is now given as

$$Z = (BA^{-1})^*. \tag{61}$$

The matrix A is invertible since the state $|Z\rangle$ was required to be not orthogonal to the vacuum. The overlap can now be calculated as

$$\langle Z|Z'\rangle = \langle Z|-\rangle\langle -|Z'\rangle\sqrt{\det(I + Z^\dagger Z')}. \tag{62}$$

However, F. Dönau [10] and J. Dobaczewski [11, 12] recognized that if Z and Z' were brought simultaneously into canonical form the calculation of the overlap would be greatly simplified.

If both matrices are in canonical form we have

$$|Z'\rangle = \langle -|Z'\rangle e^{\sum_i z'_{i\bar{i}}\beta_i^+\beta_{\bar{i}}^+}|-\rangle = \langle -|Z'\rangle \prod_i (1 + z'_{i\bar{i}}\beta_i^+\beta_{\bar{i}}^+) \tag{63}$$

and

$$\langle Z| = \langle Z|-\rangle\langle -|Z\rangle e^{\sum_i z^*_{i\bar{i}}\beta_{\bar{i}}}\beta_i = \langle Z|-\rangle\langle -|\prod_i (1 + z^*_{i\bar{i}}\beta_{\bar{i}}\beta_i). \tag{64}$$

This simplifies the calculation of the overlap since

$$\langle Z|Z'\rangle = \langle Z|-\rangle\langle -|Z'\rangle \prod_{ij} [(1 + z^*_{i\bar{i}}\beta_{\bar{i}}\beta_i)(1 + z'_{j\bar{j}}\beta_j^+\beta_{\bar{j}}^+)] = \langle Z|-\rangle\langle -|Z'\rangle \prod_i (1 + z^*_{i\bar{i}}z'_{i\bar{i}}). \tag{65}$$

However to arrive at this simple solution one has to find Z and Z' in canonical form first. Let $E = Z^\dagger Z'$, then

$$EZ^\dagger = Z^\dagger Z' Z^\dagger = Z^\dagger E^T \tag{66}$$

and

$$Z'E = Z'Z^\dagger Z' = E^T Z'. \tag{67}$$

Now, if E can be diagonalized with e_i on the diagonal by a transformation S then

$$S^{-1}ESS^{-1}Z^\dagger(S^T)^{-1} = S^{-1}Z^\dagger(S^T)^{-1}S^T E^T (S^T)^{-1}. \tag{68}$$

Let a_{ik} be the elements of $S^{-1}Z^\dagger(S^T)^{-1}$ then

$$(e_i - e_k)a_{ik} = 0. \tag{69}$$

This means that if the eigenvalues of E are not the same, $e_i \neq e_k$, then $a_{ik} = 0$. A similar argument can be made for the matrix $S^T Z' S$. However, since Z and Z' are skew-symmetric $S^T Z' S$ and $S^{-1}Z^\dagger(S^T)^{-1}$ have to be skew-symmetric as well. This implies that the diagonal elements are zero. If each eigenvalue of E was only twofold degeneracy this would imply that $S^T Z' S$ and $S^{-1}Z^\dagger(S^T)^{-1}$ would be in canonical form. Since we know the structure of the U and V and hence Z and Z' matrices we know the degeneracies of the eigenvalues of E. They are the same degeneracies of the eigenvalues of U and V. The degeneracies are thus higher than two for some eigenvalues. This means that instead of the canonical form the matrices Z and Z' will be in block diagonal form.

3 Results

The following section discusses the results of a computational model that was created using the programming language Python.

3.1 BCS vacuum

As an example to study the Bloch-Messiah decomposition and the described overlap functions, we solve the BCS equations for the energy levels ϵ_n of the 3-dimensional harmonic oscillator which are given by,

$$\epsilon(n) = \hbar\omega \left(n + \frac{3}{2} \right) - V_0.$$

This simple case can approximate real medium-sized low energy nuclei (but is inadequate for some bound neutron states) [22]. The constant $\hbar\omega$ is defined in terms of the mass number A,

$$\hbar\omega = 41 A^{-\frac{1}{3}} \,\mathrm{MeV}, \tag{70}$$

and the depth V_0 of the harmonic oscillator is set as $V_0 = 57\,\mathrm{MeV}$. Since we want to use the BCS-theory approach we need to find the relative energy and thus a suitable Fermi energy. The n-th energy level has a degeneracy of $(n+1)(n+2)$ which means that v_n has to appear $(n+1)(n+2)$ times in the sum in equation (15). The particle number can now be calculated iteratively for different Fermi energies until a suitable Fermi energy with the desired particle number is found. Using the BCS approach we then get the coefficients u_k and v_k in the canonical basis. Thus, the matrices $\bar{U}$ and $\bar{V}$ can already be found since the elements on the diagonal of $\bar{U}$ are the coefficients u_k, similarly $\pm v_k$ are the real numbers in $\bar{V}$ (see section 2.2). The coefficients u_k and v_k are plotted in figure 1 for different values of Δ and one can clearly see how the occupation probabilities v_k follow a Fermi-Dirac-like distribution.

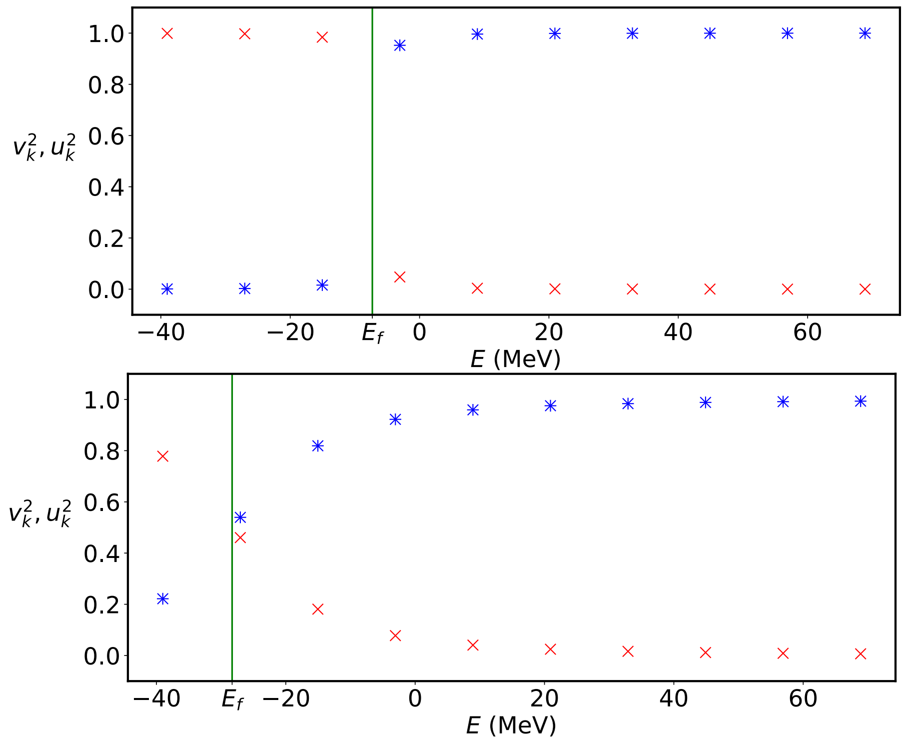

Figure 1: Coefficients u_k^2 (blue asterisk) and v_k^2 (red cross) for energy-gap parameters $\Delta = 2\,\text{Mev}$(upper plot) and $\Delta = 16\,\text{Mev}$ (lower plot) in terms of absolute energy. The Fermi energy is shown as a vertical green line.

3.2 Generating non-canonical Bogoliubov vacua

The Bloch-Messiah transformation takes matrices U and V, usually not in canonical form, as input. We will therefore artificially create such matrices by performing a random rotation in Fock space of the matrices $\bar{U}$ and $\bar{V}$, which means multiplying them with two random unitary matrices D and C such that $U = D\bar{U}C$ and $V = D^*\bar{V}C$. To create a random unitary matrix a random complex matrix was generated in the code, which then was made hermitian. The unitary matrix was then found by matrix exponentiation. Let the Hermitian matrix be called H, then

$$D = e^{iH} = \sum_{k=0}^{\infty} \frac{i^k H^k}{k!} \tag{71}$$

is unitary. This is true since $e^A e^B = e^{AB}$ for commuting matrices and thus

$$DD^\dagger = e^{iH}\left(e^{iH}\right)^\dagger = e^{iH}e^{-iH} = e^0 = I. \tag{72}$$

Through this process the random transformation matrices U and V were created. We are now able to look at the desired process of finding the Bloch-Messiah decomposition. The first step is to find the hermitian matrix $Q = V^*V^T$ in its diagonal form. To group degenerate eigenvalues we will sort them in descending order. The corresponding eigenvectors form the transformation matrix D. The diagonal matrix $\bar{Q}$ can be computed as $\bar{Q} = D^\dagger QD$. Since $\bar{U}$ is in diagonal form as well and $\bar{Q} = 1 - \bar{U}\bar{U}^\dagger = 1 - \bar{U}\bar{U}$, the diagonal elements u_k of $\bar{U}$ are determined by the diagonal elements q_k of $\bar{Q}$, where $u_k = \sqrt{|1 - q_k|}$. Applying the equation $V^* V^T + UU^\dagger = I$ will give the real numbers in the canonical form of V as $v_k = \pm\sqrt{|1 - u_k^2|}$. This process finds the decomposition of U and V into the diagonal and canonical form respectively. However, the matrix $P = V^* U^T$ is not necessarily in canonical form. In fact the matrix $D^\dagger P D^*$ is in block diagonal form such that each subspace of degenerate eigenvalues is a skew-symmetric square matrix P_j on the diagonal and any other values are zero. These square matrices are brought into tridiagonal form (using the skew_tridiagonalize command from the pfapack package by M. Wimmer [23]). Thus for each block P_j the package provides a matrix S_j such that

$$S_j^\dagger P_j S_j^* \tag{73}$$

is tridiagonal. Creating another block-diagonal matrix where the matrices S_j are on the diagonal gives a matrix S that brings $D^\dagger P D^*$ into tridiagonal form. Thus

$$S^\dagger D^\dagger P D^* S^* \tag{74}$$

is tridiagonal. To transform the skew-symmetric tridiagonal matrix into canonical form a simple transformation J is required, which is described in Appendix D. Then this gives

$$J^\dagger S^\dagger D^\dagger P D^* S^* J^* \tag{75}$$

in canonical form. Finally we can define a proper D matrix, where

$$D_{new} = DSJ \tag{76}$$

brings P into canonical form and Q into diagonal form.

The matrix C can then be found using the formula

$$C = (\bar{U} + \bar{V})^T (D^\dagger U + D^T V). \tag{77}$$

Since $D^\dagger U C^\dagger = \bar{U}$ as well as $D^T V C^\dagger = \bar{V}$ we have

$$(\bar{U} + \bar{V})^T (D^\dagger U + D^T V) C^\dagger = (\bar{U} + \bar{V})^T (\bar{U} + \bar{V}) = I. \tag{78}$$

Since inverses are unique the equation (77) is verified. A simpler method would be to avoid the degeneracies that are higher than 2 by introducing a small perturbation in the energy.

3.3 Observations for different calculation methods for the overlap of two BCS vacua

To test the different strategies of computing the overlap two different sets of wavefunctions were chosen. Firstly the overlap was computed between states with different pairing gap parameter Δ and secondly between states with different particle number. In this section the square of the overlap is plotted since the overlap itself has, depending on the formula, a complex phase.

3.3.1 Observations of the overlap between different BCS states

The different overlap formulas were tested and the difference of results was of the order of 10^{-29}. In figure 2 the square of the overlap $\langle\Psi(\Delta_1)|\Psi(\Delta_2)\rangle$ between the BCS state with $\Delta_1 = 7\,\mathrm{MeV}$ and a second state with varying Δ_2 is shown. The particle number is for both states 20 and, if considered in the context of nulcear physics, using this wavefunction for both neutrons and protons, would correspond to a nucleus of $^{40}\mathrm{Ca}$. Naturally, the overlap $\langle\Psi(\Delta_1)|\Psi(\Delta_1)\rangle$ between a state with itself is 1. On both sides of this maximum the overlap decreases. It decreases faster in the left side as the overlap $\langle\Psi(\Delta_1)|\Psi(2\,\mathrm{MeV})\rangle$ is considerably smaller than $\langle\Psi(\Delta_1)|\Psi(12\,\mathrm{MeV})\rangle$, for example.

Figure 2 also shows the results using the Onishi formula if the D and D' matrices that are used to generate both states are chosen separately at random. This shows that the restrictions on the matrices D and D' are necessary. If one wanted to use two states generated by two not related unitary matrices D and D' it would be necessary to bring the U and V matrices into canonical form before calculating the overlap.

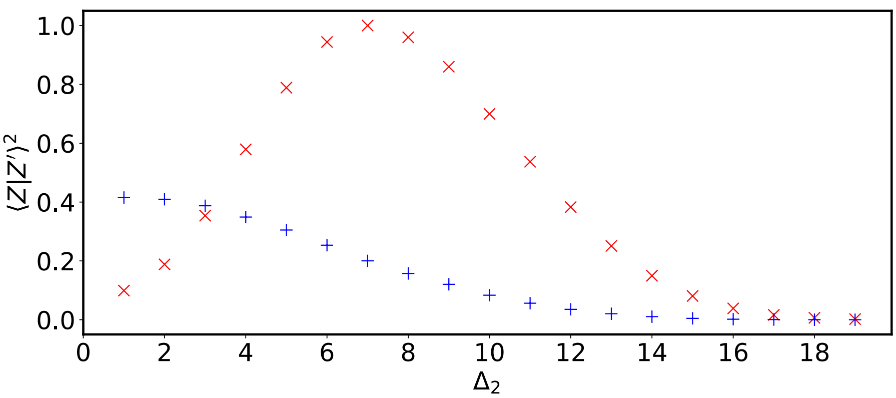

Figure 2: Overlap squared between state 1 with $\Delta_1 = 7\,\mathrm{MeV}$ and state 2 with varying Δ_2. All approaches for the overlap provide the same data points plotted in red as long as the matrix D and D' are related as shown in section 3.3.4. If the D matrices are randomly generated the result becomes very small the bigger the matrix size. The blue set of data points shows the result one would get when using the Onishi formula with randomly generated matrices D and D' for a very small matrix size (12×12).

In figure 3 the square of the overlaps $\langle\Psi(N_1)|\Psi(N_2)\rangle$ between the BCS state with particle number $N_1 = 20$ and states with different particle number N_2 are displayed both for $\Delta = 1\,\mathrm{MeV}$ and $\Delta = 5\,\mathrm{MeV}$. Figure 3 shows that states with different particle number are generally not orthogonal in the Bogoliubov basis. For this reason, in the GCM, wavefunctions can be written as a superposition of wavefunctions with different particle number. Similarly to figure 2 the overlap decreases as the parameters become more different, in this case the particle number. Additionally the plot shows that for a bigger pairing gap the distribution becomes more stretched out. As shown in figure 1 the occupation probabilities v_i tend from 1 to 0 slower, the bigger the pairing gap which exemplifies why the overlaps are bigger and hence the distribution wider. In other words, BCS wavefunctions are wave packets in particle number, and the pairing gap Δ identifies their width.

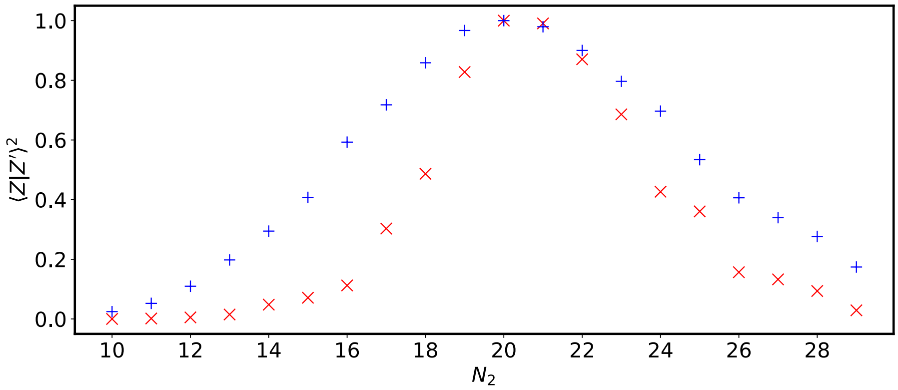

Figure 3: Overlap squared between state 1 and state 2 with particle number $N_1 = 20$ and varying particle number N_2 plotted for $\Delta = 1\,\mathrm{MeV}$ (red cross) and $\Delta = 5\,\mathrm{MeV}$ (blue plus).

3.3.2 Cutoffs

For a nonzero gap parameter Δ the coefficients v_i asymptotically approach zero. It is therefore sensible to introduce a cutoff to the $\bar{V}$ and $\bar{U}$ matrices. The cutoff was set such that any $v_i < 0.001$ would be cut off. This results in differently sized U and V matrices depending on the gap parameter. To calculate the overlap the smaller size of the matrices was chosen for both BCS states. The BM decomposition is extremely useful here in order to reduce the size of the U and V matrices to enhance the computational efficiency. Just cutting away two rows and columns from the original matrices completely changes the calculation of the overlap. However, in the canonical basis it is possible to reduce the size of the matrices from 70×70 matrices to 20×20 matrices with little effect. This is demonstrated in figure 4.

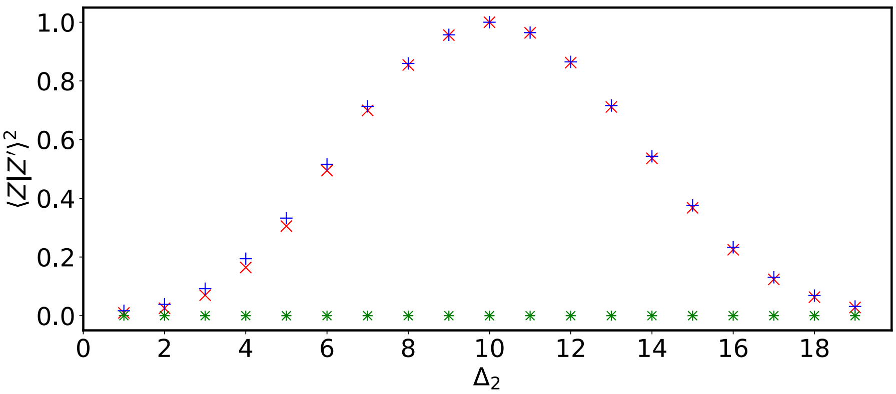

Figure 4: Square of the overlap between state 1 with $\Delta_1 = 10$ and state 2 with varying Δ_2. The Onishi formula has been used to calculate the overlap without any cutoffs, i.e 70×70 matrices (red crosses), with reduced 20×20 matrices in the canonical form (blue plus) and with reduced 40×40 matrices not in the canonical form (green asterisk).

This confirms that Bloch-Messiah decomposition is useful to derive a physically meaningful representation. The newfound canonical basis is computationally convenient, as most elements of the matrices are zero and because one can reduce the matrix size with only a minimal loss in precision, when calculating the overlap.

3.3.3 Overlap as described by F. Dönau in the canonical basis

A disadvantage of the overlap formula in [10] is that the diagonalization of $Z^\dagger Z'$ is computationally costly. Since the BM decomposition can be more efficient one could avoid the diagonalization of $Z^\dagger Z'$ by transforming all Bogoliubov amplitudes into canonical form. Then

$$A = \bar{U}_0^\dagger \bar{U} + \bar{V}_0^\dagger \bar{V} \tag{79}$$

is in diagonal form except if the number of ones on the diagonal varies for $\bar{V}_0$ and $\bar{V}$. In this case a number of anti-diagonal 2×2 boxes will remain. Thus the matrix A will be of the form

$$A = \begin{pmatrix} 1 & & & & & & & & & & & \\ & \ddots & & & & & & & & & & 0 \\ & & 1 & & & & & & & & & \\ & & & \boxed{\begin{matrix} 0 & a_1 \\ -a_1 & 0 \end{matrix}} & & & & & & & & \\ & & & & \ddots & & & & & & & \\ & & & & & \boxed{\begin{matrix} 0 & a_k \\ -a_k & 0 \end{matrix}} & & & & & & \\ & & & & & & \boxed{\begin{matrix} \alpha_l & 0 \\ 0 & \alpha_1 \end{matrix}} & & & & & \\ & & & & & & & \ddots & & & & \\ & & & & & & & & \boxed{\begin{matrix} \alpha_l & 0 \\ 0 & \alpha_1 \end{matrix}} & & & \\ & & & & & & & & & 1 & & \\ & & & 0 & & & & & & & \ddots & \\ & & & & & & & & & & & 1 \end{pmatrix} . \tag{80}$$

Similarly, the matrix

$$B = \bar{V}_0^T \bar{U} + \bar{U}_0^T \bar{V} \tag{81}$$

is in canonical form similar to $\bar{V}$ except for the same amount of boxes with coefficients b_i on the diagonal,

$$B = \begin{pmatrix} 0 & & & & & & & & & & \\ & \ddots & & & & & & & & 0 & \\ & & 0 & & & & & & & & \\ & & & \boxed{\begin{matrix} b_1 & 0 \\ 0 & b_1 \end{matrix}} & & & & & & & \\ & & & & \ddots & & & & & & \\ & & & & & \boxed{\begin{matrix} b_k & 0 \\ 0 & b_k \end{matrix}} & & & & & \\ & & & & & & \boxed{\begin{matrix} 0 & \beta_1 \\ \beta_1 & 0 \end{matrix}} & & & & \\ & & & & & & & \ddots & & & \\ & & & & & & & & \boxed{\begin{matrix} 0 & \beta_l \\ \beta_1 & 0 \end{matrix}} & & \\ & & & & & & & & & 0 & \\ & & & 0 & & & & & & & \ddots \\ & & & & & & & & & & & 0 \end{pmatrix}. \qquad (82)$$

Recognizing that the inverse of A has to be of exactly the same form as A it follows that $Z = (BA^{-1})^*$ is of the exact same form as $\bar{V}$ (25), i.e the canonical form. This implies that diagonalization of $Z^\dagger Z'$ is no longer required. The strategy of bringing all Bogoliubov amplitudes into canonical form first was tested and worked for the simple BCS wavefunction setup, where Ψ and Ψ' show the same basis for the canonical form, which is the original single particle basis. However, this is not generally true for HFB. In order to apply this formula it is necessary that the $Z^\dagger$ and Z' are canonical in the same basis. Any matrix in canonical form however is relatively well defined, as only the order of the antidiagonal 2×2 boxes can vary. Even though it has not been tested one could keep track of the reordering of eigenvalues of $V^* V^T$ and thus make sure that the the antidiagonal 2×2 boxes are in the right order. This could be the starting point for other investigation regarding an efficient implementation of the formula in [10] for HFB states.

3.3.4 Restrictions on the matrices D and D'

It was discovered that it is necessary to impose certain restriction on the matrices D and D' in order for the calculation of the overlap to work. When generating Bogoliubov amplitudes starting from a BCS wave function, this has to be taken into account. Considering the Onishi formula we want that the resulting overlap should be the same in the canonical as well as in the original bases. Thus

$$\sqrt{\det(\bar{U}\bar{U}' + \bar{V}^T\bar{V}')} = \sqrt{\det(\bar{U}\bar{U}' - \bar{V}\bar{V}')} = \sqrt{\det(U^\dagger U' + V^\dagger V')}. \qquad (83)$$

Rewriting the expression on the right side using the BM decomposition, i.e. $U = D\bar{U}C$ and $V = D^*\bar{V}C$, we get

$$\sqrt{\det(U^\dagger U' + V^\dagger V')} = \sqrt{\det(C^\dagger \bar{U} D^\dagger D' \bar{U}' C' + C^\dagger \bar{V} D^T D'^* \bar{V}' C')}$$
$$= \sqrt{\det(\bar{U} D^\dagger D' \bar{U}' + \bar{V} D^T D'^* \bar{V}')}.$$

Since C and C' are unitary they can be removed from the equation and for that reason the overlap does not depend on them. Thus they can be randomly chosen. The D matrices on the other hand do not cancel out. In fact, if one considers two unitary matrices D and $D' = e^{i\phi}D$ the equation becomes

$$\sqrt{\det(\bar{U} D^\dagger D' \bar{U}' + \bar{V} D^T D'^* \bar{V}')} = \sqrt{\det(\bar{U}\bar{U}' e^{i\phi} + \bar{V}\bar{V}' e^{-i\phi})}. \tag{84}$$

But this means that the U and V matrices are multiplied by different factors $e^{i\phi}$ and $-e^{-i\phi}$ and thus

$$\sqrt{\det(\bar{U}\bar{U}' + \bar{V}^T\bar{V}')} = \sqrt{\det(\bar{U}\bar{U}' e^{i\phi} + \bar{V}\bar{V}' e^{-i\phi})} \tag{85}$$

does not hold. The important result is that the unitary matrices D and D' cannot be chosen randomly when generating U and V. That does not imply though that the matrices D and D' have to be identical. We consider two D matrices D and $D' = DA$, where A is unitary. Let

$$DA\bar{U}C = U, \quad D^*A^*\bar{V}C = V. \tag{86}$$

Then if $A\bar{U} = \bar{U}A$ and $A^*\bar{V} = \bar{V}A$ we have

$$D\bar{U}AC = U, \quad D^*\bar{V}AC = V. \tag{87}$$

This shows that both D and D' are part of a valid Bloch-Messiah decomposition for the same state. To show that such a matrix A exist and does not have to be the identity matrix we observe the subspace of a single 2×2 block. Then $\bar{U}_i = u_i I$ and $A_i\bar{U}_i = \bar{U}_i A_i$ follows trivially. Now let

$$A_i = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \tag{88}$$

then

$$A_i^*\bar{V}_i = v_i \begin{pmatrix} a^* & b^* \\ -b & a \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = v_i \begin{pmatrix} -b^* & a^* \\ -a & -b \end{pmatrix} = v_i \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} = \bar{V}_i A_i. \tag{89}$$

Note that

$$A_i^\dagger A_i = \begin{pmatrix} a^* & -b \\ b^* & a \end{pmatrix} \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} = \begin{pmatrix} a^2 + b^2 & 0 \\ 0 & a^2 + b^2 \end{pmatrix}, \tag{90}$$

which gives the restriction $a^2 + b^2 = 1$. This shows that A in block diagonal form with 2×2 blocks A_i as described above fulfills all conditions.

4 Conclusion and Outlook

Using BCS wavefunctions to simulate Bogoliubov wavefunctions is a simple way to study the properties of Bogoliubov amplitudes. Using a reverse process to the BM decomposition allows the close inspection of the matrices involved. Thus the BM decomposition and the BM theorem could be studied. A pedagogical and complete proof of the BM theorem was provided. The usefulness of the BM decomposition was then demonstrated, when it comes to simplifying the form as well as the size of the involved matrices. A disadvantage of the approach of using the BCS wave function for a harmonic oscillator is that high degeneracies appear. Those degeneracies complicate the computation of the canonical form for example in the BM decomposition. The discussed overlap formulas are reliably implemented, even though more than twofold degenerate eigenvalues complicate the process of finding the canonical form for Z and Z' as the computation has to be slightly adapted. It was found that not any rotation in the Fock-space is allowed, as the unitary transformation matrix D can not be chosen randomly. As the Bogoliubov amplitudes are found as a solution to the HFB equations this restriction on the matrices D and D' has to be a result of those calculations. Since the calculation of overlaps is essential in the determination of nuclear wavefunctions it is a rewarding research topic.

In this project the computational cost of the different processes has not been tested, even though it would be important for example to determine, if a repeated BM decomposition is computationally more effective than the diagonalization of the matrix $Z^\dagger Z'$ in [10]. The computation time for each overlap formula for the calculation of the wavefunction of heavy nuclei could be studied and improved, possibly by implementing the BM decomposition and through that reducing the size of the matrices. Another approach would be to explore how symmetry breaking can be used to simplify computations. For that it would be necessary to apply the formulas and result of this project to the HFB method or a more advanced model which is based on the HFB theory. The phase of the overlap provided by the different formulas should also be discussed, as for example the Onishi formula does not provide a phase at all. Additional overlap formulas, as for example the formulation in [14] have to be taken into account as well. Considering the found restriction on the transformation matrix D it would be interesting to check how this transformation manifests itself in the HFB equations and the calculation of wavefunctions for real world nuclei.

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A Appendix

A.1 Appendix A: Fermion Anti-commutation

The Fermion Anti-commutation relations

$$\{a_\mu^+, a_\nu^+\} = 0, \quad \{a_\mu, a_\nu\} = 0, \quad \{a_\mu, a_\nu^+\} = \delta_{\mu\nu} \tag{91}$$

can be easily verified by checking the two possibilities of the state ν being occupied or not,

$$\langle\nu|a_\mu a_\nu^+|\nu\rangle = 0, \tag{92}$$

$$\langle\nu|a_\nu^+ a_\mu|\nu\rangle = \delta_{\mu\nu}.$$

This is clear since if the state ν is already occupied the creation operator acting on it gives zero. However, if the particle in the state ν is annihilated ($\nu = \mu$) the solution is nonzero. Similarly, we know

$$\langle 0|a_\mu a_\nu^+|0\rangle = \delta_{\mu\nu} \tag{93}$$

$$\langle 0|a_\nu^+ a_\mu|0\rangle = 0.$$

Since equation is valid for both possible cases we can conclude that it is true. Fermion Anti-commutation relations

$$\{a_\mu^+, a_\nu^+\} = 0, \quad \{a_\mu, a_\nu\} = 0, \quad \{a_\mu, a_\nu^+\} = \delta_{\mu\nu} \tag{94}$$

A.2 Appendix B: Unitarity of the transformation matrix

We want to show that

$$W^\dagger W = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = I, \tag{95}$$

where I is the identity matrix. This can be split into the equations

$$U^\dagger U + V^\dagger V = V^T V^* + U^T U^* = I \tag{96}$$

and

$$U^\dagger V^* + V^\dagger U^* = V^T U + U^T V = 0. \tag{97}$$

Recognizing that the second term of the equation (100) is just the transpose of the first term and similarly, the second term of the equation (101) is the complex conjugate of the first term we only need to show that

$$U^\dagger U + V^\dagger V = I \text{ and } V^T U + U^T V = 0. \tag{98}$$

We use the fermion anti-commutation relations for the quasi particle operators to find

$$\begin{aligned} \delta_{kn} &= \{\beta_k^+, \beta_n\} = \beta_k^+ \beta_n + \beta_n \beta_k^+ \\ &= \left(\sum_l U_{lk} a_l^+ + V_{lk} a_l\right) \left(\sum_m U_{mn}^* a_m + V_{mn}^* a_m^+\right) \\ &+ \left(\sum_m U_{mn}^* a_m + V_{mn}^* a_m^+\right) \left(\sum_l U_{lk} a_l^+ + V_{lk} a_l\right) \end{aligned}$$

Since $\{a_n, a_m\} = 0$ and $\{a_n^+, a_m^+\} = 0$ only the cross terms remain.

$$\begin{aligned} \delta_{kn} &= \sum_l U_{lk} a_l^+ \sum_m U_{mn}^* a_m + \sum_l V_{lk} a_l \sum_m V_{mn}^* a_m^+ \\ &+ \sum_m U_{mn}^* a_m \sum_l U_{lk} a_l^+ + \sum_m V_{mn}^* a_m^+ \sum_l V_{lk} a_l. \end{aligned}$$

Now we use that $\{a_n^+, a_m\} = \delta_{nm}$.

$$\delta_{kn} = \sum_l U_{lk} U_{ln}^* + \sum_l V_{lk} V_{ln}^* + \sum_l U_{ln}^* U_{lk} + \sum_l V_{ln}^* V_{lk}.$$

Since the inverse is unique we also have that

$$\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} = I, \tag{99}$$

which is equivalent to

$$UU^\dagger + V^*V^T = VV^\dagger + U^*U^T = I \tag{100}$$

and

$$VU^\dagger + U^*V^T = UV^\dagger + V^*U^T = 0. \tag{101}$$

A.3 Appendix C: Slater determinants

A good way to describe the wave function for a system of A is by introducing the concept of Slater determinants. We would like to write the wave function $\Phi_{\mu_1,\ldots,\mu_A}(x_1,\ldots,x_A)$ of the whole system as a linear combination of the orthogonal single particle wave functions $\phi_{\mu_i}(x_j)$. Here μ_i are the different basis quantum states and x_j the single particle coordinates. The simplest case would be to write the wave function of the system as the product of the single particle wave functions,

$$\Phi_{\mu_1,\ldots,\mu_A}(x_1,\ldots,x_A) = \prod_i^A \phi_{\mu_i}(x_i). \tag{102}$$

It is clear however that this approach results in a symmetric wave function. To achieve an anti-symmetric wave function the wave function can be written as a determinant with normalization constant $(A!)^{-1/2}$,

$$\Phi_{\mu_1,\ldots,\mu_A}(x_1,\ldots,x_A) = \frac{1}{\sqrt{A!}}\begin{vmatrix} \phi_{\mu_1}(x_1) & \phi_{\mu_2}(x_1) & \ldots & \phi_{\mu_A}(x_1) \\ \phi_{\mu_1}(x_2) & \phi_{\mu_2}(x_2) & \ldots & \phi_{\mu_A}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\mu_1}(x_A) & \phi_{\mu_2}(x_A) & \ldots & \phi_{\mu_A}(x_A) \end{vmatrix}. \tag{103}$$

A.4 Appendix D: Transformation of tridiagonal matrix into canonical form

A skew symmetric tridiagonal matrix is of the form

$$\begin{pmatrix} 0 & a_1 & & & 0 \\ -a_1 & 0 & a_2 & & \\ & -a_2 & 0 & a_3 & \\ & & -a_3 & 0 & \ddots \\ & 0 & & \ddots & \ddots \end{pmatrix}. \tag{104}$$

To bring it into canonical form one has to iteratively subtract a multiple of the first column from the third column and a multiple of the first row from the third row such that a_2 and $-a_2$ get annihilated [24]. Then the process has to be repeated to remove all even coefficient a_{2i}. This is done by using the unitary transformation matrix

$$J_1^\dagger = \begin{pmatrix} 1 & 0 & & 0 & \\ 0 & 1 & 0 & & \\ c\frac{a_2}{a_1} & 0 & c & 0 & \\ & & 0 & 1 & \ddots \\ & 0 & & \ddots & \ddots \end{pmatrix}, \tag{105}$$

where $c = \frac{1}{\sqrt{1+a_2^2/a_1^2}}$ is a normalization constant. Indeed

$$\begin{pmatrix} 1 & 0 & & 0 & \\ 0 & 1 & 0 & & \\ c\frac{a_2}{a_1} & 0 & c & 0 & \\ & & 0 & 1 & \ddots \\ & 0 & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} 0 & a_1 & & & 0 \\ -a_1 & 0 & a_2 & & \\ & -a_2 & 0 & a_3 & \\ & & -a_3 & 0 & \ddots \\ & 0 & & \ddots & \ddots \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & & 0 & \\ 0 & 1 & 0 & & \\ c\frac{a_2}{a_1} & 0 & c & 0 & \\ & & 0 & 1 & \ddots \\ & 0 & & \ddots & \ddots \end{pmatrix}$$

$$= \begin{pmatrix} 0 & a_1 & & & 0 \\ -a_1 & 0 & 0 & & \\ & 0 & 0 & ca_3 & \\ & & -ca_3 & 0 & \ddots \\ & 0 & & \ddots & \ddots \end{pmatrix}.$$

Through this process all the coefficient a_{2i} with even coefficients get removed by applying transformations similar to J_1. Thus one arrives at an almost canonical form, where the remaining coefficients (We will now call them s_i) that build the 2×2 boxes are not necessarily real which means that it is necessary to multiply by a phase (ϕ). This is done by creating a diagonal matrix K. Let $s_i = e^{i\phi} s_i'$, where s_i' is real and let $a_i = e^{-\frac{i\phi}{2}}$ be the diagonal elements of K such that even elements and the following odd element are the same, i.e the values are pairwise degenerate. Let J be the matrix product that consists of the matrices J_i which removes the even coefficients of the tridiagonal form and K which corrects the phase, then $J = J_1 J_2 \ldots J_{n/2-1} K$ brings a skew-symmetric matrix from tridiagonal form into canonical form.