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# Block-diagonalization of pairing Hamiltonians using spin transpositions

**Jacob Szeftel**[1] **and Michel Caffarel**[2]

[1] Laboratoire de Physique Théorique de la Matière Condensée, Université Paris VII, Case Courrier 7020, 2 place Jussieu, 75251 Paris Cedex 05, France
[2] CNRS–Laboratoire de Chimie Théorique, Université Paris VI, Tour 22–23 Case Courrier 137, 4 place Jussieu, 75252 Paris Cedex 05, France

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**Abstract**
Using two-electron spin transpositions within BCS pairs, it is shown that an efficient block-diagonal decomposition of the Hamiltonian matrices associated with general pairing models is possible. The ratio of the dimension of the full Hilbert space to the size of the largest submatrix obtained grows exponentially with the number of electron pairs. This remarkable result holds for any electron filling. The approach is exemplified on the usual BCS model.

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## 1. Introduction

The long-standing interest in the Hubbard model stems from the conviction that understanding its basic properties would be helpful in unravelling the paramount role of electron correlation in magnetism and superconductivity. Unfortunately, only the one-dimensional version of the model has been solved [1]. For higher dimensions a large variety of approximate analytical approaches as well as numerous numerical studies on very small clusters are at our disposal (see, e.g., [2]). However, in all cases the approximations made are not controlled in a satisfactory way and therefore the search for exact information about the role of electron correlation in simplified—but still physically nontrivial—Hubbard-like models is highly desirable.

Among such models are the pairing models. Pairing models play an important role both in condensed matter and nuclear physics. In condensed matter physics, the fundamental model is the BCS model describing the dynamics of pairs of electrons as introduced by BCS in their celebrated work on superconductivity [3, 4]. This model can be viewed as a simplified version of the usual Hubbard model in which only one certain Cooper pairing channel is considered. In contrast with Hubbard-like models in which electrons can move independently, in pairing models the pairs of electrons cannot be broken; these pairs behave like true particles and have the characteristic features of hard-core bosons. In nuclear physics, the presence of pairing

  

effects in finite nuclei has been at the origin of the widespread use of BCS-type wavefunctions and pairing Hamiltonians (see, e.g., [5]). As remarked by Dukelsky *et al* [6], pairing is in fact a pervasive feature in nuclear physics.

Quite remarkably, the fundamental pairing problem was solved a long time ago by Richardson in a series of papers [7–10]. However, these works have escaped the attention of the physics community and it is only recently that the powerfulness of the approach of Richardson has been used to tackle a variety of problems: study of the crossover between the bulk and the few-electron limit in ultrasmall metallic grains [11, 12], description of various transitions in finite confined boson systems [13, 14], and very recently understanding of some new aspects of nuclear superconductivity [6]. More generally, new classes of exactly solvable models based on the pairing interaction and on the generalization of the ansatz used by Richardson have been presented [15]. Note also that very recently Krishnamurthy and Shastry (KS) have presented an exact solution of the BCS model for a purely repulsive interaction [16] without being aware of Richardson's solution. Their solution—independent and quite different from Richardson's one—has been developed within a functional-integral framework and rests on the fact that the Hubbard–Stratanovic field used to linearize the interaction admits only Gaussian fluctuations in the thermodynamic limit. Several interesting results regarding correlation functions have been obtained. In particular, a quasi-long-range order at half-filling, as well as large enhancements in the equal time pairing correlations in the neighbourhood of half-filling, have been found.

Very recently, one of us has shown that there exist some interesting consequences related to the use of spin transpositions in the BCS pairing problem [17]. Because of the existence of the Pauli principle for electrons, exchanging spins within a BCS pair is not a symmetry of the BCS Hamiltonian (the spin-transposition operators do not commute with the Hamiltonian). Because of that the use of standard group-theory machinery is not possible. However, Szeftel has shown that eigenfunctions still have some specific properties with respect to spin transpositions. More precisely, decomposing each eigenstate into a regular and a special part with respect to each transposition, it has been shown that the regular part still obeys the usual symmetry constraints resulting from group-theory.

In this paper, we show that this idea is quite general and can be used for block-diagonalizing very efficiently Hamiltonian matrices built from the pairing interaction operator. To exemplify the formalism, we shall consider the BCS model. However, it is important to emphasize that our approach can be applied without difficulty to various non-integrable pairing models. The main idea of this work rests on the construction of a new basis set adapted to spin transpositions. Using this new representation, it is shown that the full Hilbert space can be decomposed into independent (that is, not connected by the pairing Hamiltonian) subspaces. As a consequence, the Hamiltonian is decomposed into a set of block-diagonal submatrices whose size and structure can be completely elucidated. The remarkable result is that the ratio of the dimension of the full Hilbert space to the largest submatrix obtained grows exponentially as a function of the number of electron pairs. Accordingly, the gain in computational effort for getting the full spectrum as well as the complete set of eigenstates is also exponential. Finally, we show that there exists a well-defined relation between spin transpositions and more usual spin-symmetry operators. As a consequence, the exponential gain obtained using spin transpositions can also be understood as resulting from the existence of a hierarchical structure between eigenstates corresponding to various numbers of singlet and triplet elementary BCS pairs.

The organization of the paper is as follows. In section 2 the BCS model on which the formalism will be illustrated is presented. Section 3 is devoted to the construction of the so-called spin-transposition-adapted basis set. The block-diagonal structure of the full BCS

matrix is unravelled in section 4. Finally, a summary and some concluding remarks are given in the last section.

## 2. The BCS model

The BCS model is defined by the Hamiltonian $H = H_D + H_K$ where the diagonal and off-diagonal parts are written as

$$H_D = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{U}{N} N_\uparrow N_\downarrow \qquad H_K = \frac{U}{N} \sum_{k,k' \neq k} b^\dagger_{k'} b_k. \tag{1}$$

Here $c^{(\dagger)}_{k\sigma}$ are the standard one-electron annihilation (creation) operators associated with each Bloch state $k$ and spin state $\sigma$ ($=\uparrow, \downarrow$), $\epsilon_k$ is the band dispersion energy, $N$ the total number of Bloch states, $N_\sigma$ the number of electrons of spin $\sigma$, and $U$ the interelectronic coupling constant. In equation (1) $b^{(\dagger)}_k$ denote the pair annihilation (creation) operators defined as follows

$$b^\dagger_k = c^\dagger_{k\uparrow} c^\dagger_{K-k\downarrow} \qquad b_k = c_{K-k\downarrow} c_{k\uparrow} \tag{2}$$

where $K$ is the total momentum of the pairs, a quantity conserved by $H$.

In the BCS model the dimension of space is irrelevant; for simplicity, we shall therefore derive all results for a one-dimensional model. Regarding the dispersion energy we shall consider the expression given by a standard nearest-neighbour hopping model

$$\epsilon_{k_l} = -2 \cos\left(\frac{2\pi}{N} l\right) \tag{3}$$

where the integer $l$ takes the $N$ values $l = 0, \pm 1, \pm 2, \ldots$.

Denoting by $n$ the number of pairs and by $K$ the total momentum of the pairs, the total Hilbert space, $S_K$, is spanned by $2n$-electron Slater determinants of vanishing total projected spin and total momentum equal to $nK$. An arbitrary determinant is given by

$$\prod_{j=1}^{n} b^\dagger_{k_j} |0\rangle \tag{4}$$

where $|0\rangle$ denotes the no-electron state. Throughout this work the complete set of all possible determinants will be referred to as the *k-diagonal basis set*. The number of basis vectors is given by the binomial coefficient $\binom{N}{n}$.

Finally, it should be emphasized that the BCS Hamiltonian considered here can be viewed as a simplified version of the standard one-band Hubbard Hamiltonian in which only a certain Cooper pairing channel is considered. Indeed, using the notation introduced above, the Hubbard Hamiltonian can be written as $H_D + \sum_K H_K$ where the sum is carried out over all possible values of $K$ in the Brillouin zone, instead of one single value as in the BCS case. In sharp contrast with the Hubbard model, the Cooper pairs in the BCS model cannot be broken; these pairs behave like true particles and have the characteristic features of hard-core bosons. Note also that, in a way similar to what has been found for the Hubbard model [1], there exists some one-to-one correspondence between the eigenvalues of $H$ corresponding to positive and negative values of the coupling constant $U$ (relations are obtained by replacing electrons and holes). Denoting by $\varepsilon(\pm U, y)$ the eigenvalues of $H$ associated with $\pm U$, and by $y = \frac{2n}{N}$ the electron concentration, we have

$$\frac{\varepsilon(U, y) + \varepsilon(-U, 2 - y)}{N} = U(1 - 2y). \tag{5}$$

## 3. Spin-transposition-adapted (STA) basis

In order to build up our new basis set for the Hilbert space, we introduce a set of $N$ operators $T_k$ defined as follows:

$$T_k \equiv b^{\dagger}_{K-k} b_k. \tag{6}$$

These operators have a simple physical meaning: by applying $T_k$ the electron pair ($k\uparrow$, $K-k\downarrow$) is destroyed and a new pair ($K-k\uparrow, k\downarrow$) labelled by $K-k$ is created. Since all pairs have a total momentum $K$ the action of $T_k$ can also be interpreted as exchanging the spin $\uparrow$ and $\downarrow$ within a pair labelled by $k$. Because of that, the $T_k$ will be called 'spin-transposition' operators.

Now, our purpose is to construct a new basis set—called the spin-transposition-adapted (STA) basis—consisting of vectors which are all eigenstates of each spin-transposition operator $T_k$.

To avoid unnecessary difficulties related to lengthy notation, we shall only treat in detail the case of a zero pair momentum, $K = 0$, and an odd number $N$ of Bloch states. Extension to the general case is straightforward and will be briefly presented in section 3.2.

### *3.1. Construction of the STA basis*

*3.1.1. Case: $K = 0$ and $N$ odd.* For an odd number $N$ of Bloch states the allowed values of $k$ can be chosen as

$$0, \pm k_1, \pm k_2, \ldots, \pm k_p \tag{7}$$

where $k_i = \frac{2\pi}{N} i$ and $p = (N-1)/2$.

In the $k$-diagonal representation, equation (4), only some of the basis vectors are eigenstates of the spin-transposition operators. Precisely, denoting a $k$-diagonal basis vector as

$$\left|n_0, n_{k_1}, n_{-k_1}, \ldots, n_{k_p}, n_{-k_p}\right\rangle \tag{8}$$

where $n_k$ is the pair occupation number of Bloch state $k$ ($n_k = 0$, 1 and $\sum_k n_k = n$), we have the following eigenrelations:

$$T_0\left|n_0, n_{k_1}, n_{-k_1}, \ldots, n_{k_p}, n_{-k_p}\right\rangle = n_0\left|n_0, n_{k_1}, n_{-k_1}, \ldots, n_{k_p}, n_{-k_p}\right\rangle \tag{9}$$

$$T_{\pm k_i}\left|n_0, n_{k_1}, n_{-k_1}, \ldots, n_{k_p}, n_{-k_p}\right\rangle = 0 \qquad \text{when} \quad n_{k_i} = 1 \quad \text{and} \quad n_{-k_i} = 1 \tag{10}$$

$$T_{k_i}\left|n_0, n_{k_1}, n_{-k_1}, \ldots, n_{k_p}, n_{-k_p}\right\rangle = 0 \qquad \text{when} \quad n_{k_i} = 0. \tag{11}$$

Equation (9) means that all $k$-diagonal basis vectors are eigenvectors of the operator $T_0$. Here, this is true because the Bloch state $k = 0$ verifies the relation

$$K - k = k \mod(N) \tag{12}$$

when $K = 0$, and therefore $T_0$ reduces to the pair occupation number $n_0$. Remark that, more generally (arbitrary $K$ and $N$), Bloch states verifying equation (12) play in this problem a special role and must therefore be treated separately; we shall return to this point later. Equation (10) is a direct consequence of the Pauli principle which forbids the occupation of the same state by two electrons having the same spin and, finally, equation (11) is a trivial result.

In all other cases corresponding to $[n_{\pm k_i} = 1 \text{ and } n_{\mp k_i} = 0]$, the basis vectors are not eigenstates of the $T_{\pm k_i}$. However, it is easy to construct even and odd normalized eigenstates with respect to each transposition. This is done by defining

$$\left|s_{k_i}\right\rangle \equiv \frac{\left(1 + s_{k_i} T_{k_i}\right)}{\sqrt{2}} \left|n_0, n_{k_1}, n_{-k_1}, \ldots, n_{k_p}, n_{-k_p}\right\rangle \tag{13}$$

where $s_{k_i}$ is a signature (or parity) which can take the two values $\pm 1$. The symmetric $\left(s_{k_i} = +1\right)$ and antisymmetric $\left(s_{k_i} = -1\right)$ vectors verify

$$T_{k_i} \left|s_{k_i}\right\rangle = s_{k_i} \left|s_{k_i}\right\rangle. \tag{14}$$

Having these remarks in mind, it is convenient to relabel the $k$-diagonal basis vectors to make more explicit the various cases just described. An arbitrary basis vector is thus rewritten as

$$\left|n_0; \pm k_{i_1}, \ldots, \pm k_{i_q}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle \tag{15}$$

where $n_0 (= 0, 1)$ is the pair occupation number of the special Bloch state $k = 0$, $\left\{\pm k_{i_1}, \ldots, \pm k_{i_q}\right\}$ is the list of the $q$ values of $\pm k_{i_l}$ corresponding either to $[(n_{k_{i_l}} = 1 \text{ and } n_{-k_{i_l}} = 0) \rightarrow k_{i_l}$ is written in the list] or to $[(n_{k_{i_l}} = 0 \text{ and } n_{-k_{i_l}} = 1) \rightarrow -k_{i_l}$ is written in the list], and $\left\{\left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\}$ is the list of the $m$ doublets $\left(k_{j_l}, -k_{j_l}\right)$ corresponding to one pair in $k_{j_l}$ and one pair in $-k_{j_l}$. Of course, both ways of labelling a $k$-diagonal basis vector, equation (8) or (15), are strictly equivalent.

Using this notation we are now in a position to define the STA basis set. An arbitrary STA vector is given by

$$\begin{aligned}
&\left\|n_0; k_{i_1}{}^{(s_{i_1})}, \ldots, k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\right\rangle \\
&\qquad \equiv \prod_{l=1}^{q} \frac{\left(1 + s_{i_l} T_{i_l}\right)}{\sqrt{2}} \left|n_0; k_{i_1}, \ldots, k_{i_q}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\right\rangle
\end{aligned} \tag{16}$$

where $s_{i_l} = \pm 1$ are $q$ signatures associated with the $q$ spin-transposition operators $T_{i_l}$. Remark that only positive values of $k_{i_l}$ have been used in the right-hand side of equation (16) because both Bloch states $k_{i_l}$ and $-k_{i_l}$ lead to the same STA vector.

At this point, several remarks are in order. First, it is important to emphasize that each STA basis vector is now an eigenstate of all spin-transposition operators with three possible eigenvalues: 0, 1 or $-1$. To summarize, the complete set of eigenrelations is the following:

$$\begin{aligned}
&T_0 \left\|n_0; k_{i_1}{}^{(s_{i_1})}, \ldots, k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\right\rangle \\
&\qquad = n_0 \left\|n_0; k_{i_1}{}^{(s_{i_1})}, \ldots, k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\right\rangle \qquad \text{with} \quad n_0 = 0, 1 \\
&T_{\pm k_{i_l}} \left\|n_0; k_{i_1}{}^{(s_{i_1})}, \ldots, k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\right\rangle \\
&\qquad = s_{i_l} \left\|n_0; k_{i_1}{}^{(s_{i_1})}, \ldots, k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\right\rangle \\
&\qquad\quad s_{i_l} = \pm 1 \quad l = 1, q \\
&T_{\pm k_{j_l}} \left\|n_0; k_{i_1}{}^{(s_{i_1})}, \ldots, k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\right\rangle = 0 \qquad l = 1, m \\
&T_k \left\|n_0; k_{i_1}{}^{(s_{i_1})}, \ldots, k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\right\rangle = 0 \\
&\qquad\quad \text{otherwise} \quad k \neq 0, k \neq \pm k_{i_l}, k \neq \pm k_{j_l}.
\end{aligned}$$

Second, each basis vector of the STA basis is expressed as a linear combination of $2^q$ $k$-diagonal basis vectors. In addition, the $2^q$ STA vectors corresponding to all possible combinations of $s_{i_l}$ are orthonormal. This is true because each STA vector is the tensorial product of symmetric or antisymmetric normalized eigenstates for the $q$ transpositions involved. Thus, as a direct consequence of this remark, the entire STA basis set is an

orthonormal basis set. As we shall see later, the subset of STA vectors having positive signatures only will play a central role. We shall refer to this subset as the set of *positive* STA vectors.

Finally, an important aspect to discuss concerns the spin symmetry properties of the STA basis. As we shall show now, each STA basis vector defined in equation (16) is in fact an eigenstate of the total spin. To see this it is convenient to distinguish between the three possible cases for the pairs appearing in (16). The first case corresponds to pairs occupying one of the special Bloch states ($k$ verifying equation (12)). Such pairs are necessarily in a singlet state since they are described by a unique doubly occupied one-particle $k$-state. Using the same argument, this is also true for the four-electron sub-systems consisting of one pair in the state $k$ and one pair in the state $-k$ (denoted above as $(k, -k)$). For the remaining pairs (corresponding to pairs occupying a given $k$ with no pair occupying $-k$) the situation is different since they are not spin eigenstates. However, applying the operator $\frac{1+sT_k}{\sqrt{2}}$ ($s = 0, 1$) on one of such pairs corresponds to symmetrizing or antisymmetrizing its wavefunction to give either a singlet two-electron state (signature $s$ equal to zero) or a triplet two-electron state ($s = 1$). As a consequence, the full $2n$-particle STA basis vector describing the $n$ pairs is a spin eigenstate and its total spin is given by $S = \sum_{l=1}^{q} s_{i_l}$.

In order to help the reader to visualize the structure of the STA basis, let us give an illustrative example. We shall consider the case $N = 5$ and $n = 2$ for which there exist $5!/(3!2!) = 10$ basis vectors. The STA basis decomposes as follows:

- Four orthonormal vectors corresponding to the pattern $\left\|0; {k_1}^{(s_1)}, {k_2}^{(s_2)}\right\rangle\!\right\rangle$ (no pair in the special value $k = 0$, no double pairs in $k_i$ and $-k_i$),

$$\left\|0; {k_1}^{(+)}, {k_2}^{(+)}\right\rangle\!\right\rangle = \tfrac{1}{\sqrt{4}}(|0; k_1k_2\rangle + |0; -k_1k_2\rangle + |0; k_1 - k_2\rangle + |0; -k_1 - k_2\rangle)$$
$$\left\|0; {k_1}^{(+)}, {k_2}^{(-)}\right\rangle\!\right\rangle = \tfrac{1}{\sqrt{4}}(|0; k_1k_2\rangle + |0; -k_1k_2\rangle - |0; k_1 - k_2\rangle - |0; -k_1 - k_2\rangle)$$
$$\left\|0; {k_1}^{(-)}, {k_2}^{(+)}\right\rangle\!\right\rangle = \tfrac{1}{\sqrt{4}}(|0; k_1k_2\rangle - |0; -k_1k_2\rangle + |0; k_1 - k_2\rangle - |0; -k_1 - k_2\rangle)$$
$$\|0; {k_1}^{(-)}, {k_2}^{(-)}\rangle\rangle = \tfrac{1}{\sqrt{4}}(|0; k_1k_2\rangle - |0; -k_1k_2\rangle - |0; k_1 - k_2\rangle + |0; -k_1 - k_2\rangle).$$

- Four orthonormal vectors corresponding to the pattern $\|1; {k_i}^{(s_i)}\rangle\rangle$ (one pair in $k = 0$, no double pairs in $k_i$ and $-k_i$),

$$\left\|1; {k_1}^{(+)}\right\rangle\!\right\rangle = \tfrac{1}{\sqrt{2}}(|1; k_1\rangle + |1; -k_1\rangle)$$
$$\|1; {k_1}^{(-)}\rangle\rangle = \tfrac{1}{\sqrt{2}}(|1; k_1\rangle - |1; -k_1\rangle)$$
$$\left\|1; {k_2}^{(+)}\right\rangle\!\right\rangle = \tfrac{1}{\sqrt{2}}(|1; k_2\rangle + |1; -k_2\rangle)$$
$$\|1; {k_2}^{(-)}\rangle\rangle = \tfrac{1}{\sqrt{2}}(|1; k_2\rangle - |1; -k_2\rangle).$$

- Two orthonormal vectors corresponding to the pattern $\|0; (k_i, -k_i)\rangle\rangle$ (no pair in $k = 0$, one double pair in $k_i$ and $-k_i$),

$$\|0; (k_1, -k_1)\rangle\rangle = |(k_1, -k_1)\rangle$$
$$\|0; (k_2, -k_2)\rangle\rangle = |(k_2, -k_2)\rangle.$$

In this case there are five positive STA vectors. They are given by $\left\{\left\|0; {k_1}^{(+)}, {k_2}^{(+)}\right\rangle\!\right\rangle$, $\left\|1; {k_1}^{(+)}\right\rangle\!\right\rangle$, $\left\|1; {k_2}^{(+)}\right\rangle\!\right\rangle$, $\|0; (k_1, -k_1)\rangle\rangle$, $\|0; (k_2, -k_2)\rangle\rangle\right\}$.

*3.1.2. General case: K and N arbitrary.* The general case does not involve any particular difficulty. The main difference lies in the number of special values of $k$ verifying the equality $K - k = k \bmod(N)$ (equation (12)) and leading to $T_k = n_k$. Here, depending on the values of

$K$ and $N$, the number of special values may vary from zero to two. When $N$ is odd there is only one single special value. When $N$ is even there are zero or two special values depending on the parity of $K$ (strictly speaking, the parity of the integer associated with $K$). The even $K$ leads to two special values while there is no special value when $K$ is odd. The construction of the STA basis set is identical to what has been presented above. In the general case an arbitrary STA vector is defined as (same notation as in the previous section)

$$\begin{aligned}\left\|n^{(1)}\cdots n^{(r)}; k_{i_1}{}^{(s_{i_1})},\ldots,k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1}, K-k_{j_1}\right),\ldots,\left(k_{j_m}, K-k_{j_m}\right)\right\rangle\!\rangle \\ \equiv \prod_{l=1}^{q}\frac{\left(1+s_{i_l}T_{i_l}\right)}{\sqrt{2}}\left|n^{(1)}\cdots n^{(r)}; k_{i_1},\ldots,k_{i_q}; \left(k_{j_1}, K-k_{j_1}\right),\ldots,\left(k_{j_m}, K-k_{j_m}\right)\right\rangle\end{aligned} \tag{17}$$

where $n^{(i)}$ denotes the $r$ pair occupation numbers associated with the $r$ special values of $k$ and the list $\left\{k_{i_1},\ldots,k_{i_q}\right\}$ appearing on both sides of the equation must be understood as $\{(k_{i_1}\text{or } K-k_{i_1}),\ldots,(k_{i_q}\text{or } K-k_{i_q})\}$. The number of pairs $n$ is related to integers $r$, $q$ and $m$ as follows:

$$n=\sum_{i=1}^{r}n^{(i)}+q+2m. \tag{18}$$

## 4. Block-diagonalization

In order to shed some light on the structure of the BCS Hamiltonian matrix expressed within the STA basis let us calculate the action of $H$ on an arbitrary STA basis vector. As in the previous section we shall focus our attention on the case $K=0$ and $N$ odd, extension to the general case being, here also, straightforward. Our first step consists in rewriting the BCS Hamiltonian in a form adapted to spin transpositions. Note that the diagonal part of $H$ within the $k$-diagonal basis, equation (1), remains diagonal within the new STA basis and, therefore, does not need to be developed further here. Regarding the off-diagonal part, it can be rewritten as follows,

$$H_K=\frac{U}{N}\sum_{k\neq 0}\left(b_k^{\dagger}+b_{-k}^{\dagger}\right)b_0+\text{h.c.}+\frac{U}{N}\sum_{k\neq 0,k'\neq 0,k\neq k'}\left(b_{k'}^{\dagger}+b_{-k'}^{\dagger}\right)\left(b_k+b_{-k}\right)+\frac{U}{N}\sum_{k\neq 0}\left(T_k+T_{-k}\right) \tag{19}$$

where the third contribution on the right-hand side of the equation is now diagonal within the new basis. When applying $H_K$ on an arbitrary STA vector of the form

$$\left\|n_0; k_{i_1}{}^{(s_{i_1})},\ldots,k_{i_q}{}^{(s_{i_q})}; \left(k_{j_1},-k_{j_1}\right),\ldots,\left(k_{j_m},-k_{j_m}\right)\right\rangle\!\rangle \tag{20}$$

we just need to consider the off-diagonal contributions (within the new basis) resulting from

$$\begin{aligned}H_K=&\frac{U}{N}\sum_{l=1}^{q}\left(b_{k_{i_l}}^{\dagger}+b_{-k_{i_l}}^{\dagger}\right)b_0+\text{h.c.}+\frac{U}{N}\sum_{k\in\{k_{\text{ext}}\}}\left(b_k^{\dagger}+b_{-k}^{\dagger}\right)b_0+\text{h.c.}\\&+\frac{U}{N}\sum_{l\neq l'}\left(b_{k_{i_{l'}}}^{\dagger}+b_{-k_{i_{l'}}}^{\dagger}\right)\left(b_{k_{i_l}}+b_{-k_{i_l}}\right)+\frac{U}{N}\sum_{l,k\in\{k_{\text{ext}}\}}\left(b_k^{\dagger}+b_{-k}^{\dagger}\right)\left(b_{k_{i_l}}+b_{-k_{i_l}}\right)+\text{h.c.}\\&+\frac{U}{N}\sum_{l,k\in\{k_{\text{ext}}\}}\left(b_k^{\dagger}+b_{-k}^{\dagger}\right)\left(b_{k_{j_l}}+b_{-k_{j_l}}\right)+\text{h.c.}\end{aligned} \tag{21}$$

where $\{k_{\text{ext}}\}$ denotes the set of Bloch states different from 0, $\pm k_{i_l}$ and $\pm k_{j_l}$.

To proceed further two different cases must be distinguished, depending on whether or not the STA vector is positive.

### *4.1. Action of H on a positive STA vector*

Let us recall that a positive STA vector is defined by $s_{i_l} = 1$ for $l = 1, \ldots, q$ ($q$ may vary from 0 to $n$). To compute how the operator $H_K$, equation (21), acts on a positive STA vector, is just a matter of formal manipulations using the operators $b_k^{(\dagger)}$ and $T_k$. To do that, four basic relations turn out to be very useful:

$$\left(b_k^\dagger + b_{-k}^\dagger\right)\frac{(1+T_k)}{\sqrt{2}}b_k^\dagger|0\rangle = \sqrt{2}b_{-k}^\dagger b_k^\dagger|0\rangle \tag{22}$$

$$\left(b_k^\dagger + b_{-k}^\dagger\right)|0\rangle = \sqrt{2}\frac{(1+T_k)}{\sqrt{2}}b_k^\dagger|0\rangle \tag{23}$$

$$(b_k + b_{-k})\frac{(1+T_k)}{\sqrt{2}}b_k^\dagger|0\rangle = \sqrt{2}|0\rangle \tag{24}$$

$$(b_k + b_{-k})b_{-k}^\dagger b_k^\dagger|0\rangle = \sqrt{2}\frac{(1+T_k)}{\sqrt{2}}b_k^\dagger|0\rangle. \tag{25}$$

The derivation of these formulae is straightforward. Now, using the definition of the STA basis vector, equation (16), and the four previous relations, we get after some algebra the following five equalities associated with the five subparts in equation (21):

*Pattern 1.* $(n_0 = 1, q, m) \to (n_0 = 0, q-1, m+1)$ corresponding to the destruction of one $k_{i_l}$ and the creation of one double pair:

$$\begin{aligned}&\sum_{l=1}^{q}\left(b_{k_{i_l}}^\dagger + b_{-k_{i_l}}^\dagger\right)b_0\left\|1; {k_{i_1}}^{(+)}, \ldots, {k_{i_q}}^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle \\ &= \sqrt{2}\sum_{l=1}^{q}\left\|0; {k_{i_1}}^{(+)}, \ldots {k_{i_{l-1}}}^{(+)}, {k_{i_{l+1}}}^{(+)}, \ldots, {k_{i_q}}^{(+)}; \left(k_{i_l}, -k_{i_l}\right), \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle.\end{aligned} \tag{26}$$

*Pattern 2.* $(n_0 = 1, q, m) \to (n_0 = 0, q+1, m)$ corresponding to the destruction of one $k_{i_l}$ and the creation of another one:

$$\begin{aligned}&\sum_{k\in k_{\text{ext}}}\left(b_k^\dagger + b_{-k}^\dagger\right)b_0\left\|1; {k_{i_1}}^{(+)}, \ldots, {k_{i_q}}^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle \\ &\qquad = \sqrt{2}\sum_{k\in k_{\text{ext}}}\left\|0; {k_{i_1}}^{(+)}, \ldots, {k_{i_q}}^{(+)}k^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle.\end{aligned} \tag{27}$$

*Pattern 3.* $(n_0, q, m) \to (n_0, q-2, m+1)$ corresponding to the destruction of two $k_{i_l}$ and the creation of one double pair:

$$\begin{aligned}&\sum_{l\neq l'}\left(b_{k_{i_{l'}}}^\dagger + b_{-k_{i_{l'}}}^\dagger\right)\left(b_{k_{i_l}} + b_{-k_{i_l}}\right)\left\|n_0; {k_{i_1}}^{(+)}, \ldots, {k_{i_q}}^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle \\ &\qquad = 2\sum_{l\neq l'}\left\|n_0; \ldots, {k_{i_{l-1}}}^{(+)}, {k_{i_{l+1}}}^{(+)}, \ldots, {k_{i_{l'-1}}}^{(+)}, {k_{i_{l'+1}}}^{(+)}, \ldots; \right. \\ &\qquad\quad \left.\left(k_{i_l'}, -k_{i_l'}\right), \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle.\end{aligned} \tag{28}$$

*Pattern 4.* $(n_0, q, m) \to (n_0, q, m)$ corresponding to the destruction of one $k_{i_l}$ and the creation of a new one:

$$\sum_{lk_{\text{ext}}} \left(b_k^\dagger + b_{-k}^\dagger\right)\left(b_{k_{i_l}} + b_{-k_{i_l}}\right)\left\|n_0; {k_{i_1}}^{(+)}, \ldots, {k_{i_q}}^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle$$
$$= 2\sum_{lk\in k_{\text{ext}}} \left\|n_0; {k_{i_1}}^{(+)}, \ldots, {k_{i_{l-1}}}^{(+)}, k^{(+)}, {k_{i_{l+1}}}^{(+)}, \ldots, {k_{i_q}}^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle. \quad (29)$$

*Pattern 5.* $(n_0, q, m) \to (n_0, q+2, m-1)$ corresponding to the destruction of one double pair and the creation of two $k_{i_l}$.

$$\sum_{lk_{\text{ext}}} \left(b_k^\dagger + b_{-k}^\dagger\right)\left(b_{k_{j_l}} + b_{-k_{j_l}}\right)\left\|n_0; {k_{i_1}}^{(+)}, \ldots, {k_{i_q}}^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle$$
$$= 2\left\|n_0; {k_{i_1}}^{(+)}, \ldots, {k_{i_q}}^{(+)}, {k_{j_l}}^{(+)}, k^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_{l-1}}, -k_{j_{l-1}}\right),\right.$$
$$\left.\left(k_{j_{l+1}}, -k_{j_{l+1}}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle. \quad (30)$$

These different relations allow us to compute the matrix elements of $H$ between two arbitrary positive STA vectors. The key result is that the BCS Hamiltonian applied to an arbitrary positive STA basis vector leads to a linear combination of STA basis vectors which are still positive. In other words, $H$ can be exactly diagonalized within the subset of positive STA vectors. As we shall see later, the corresponding submatrix turns out to be the largest submatrix of the full block-diagonal decomposition of the Hamiltonian. The number of positive STA vectors is therefore the most important quantity which determines the linear size of the largest matrix to be diagonalized to get the full spectrum of the problem. Calculating this number is just a combinatorial problem. Considering the labelling of an arbitrary positive STA vector, $\left\|n_0; {k_{i_1}}^{(+)}, \ldots, {k_{i_q}}^{(+)}; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\!\rangle$, we need to count how many different vectors can be constructed. When $n_0 = 0$, $n$ pairs are to be distributed either in the $p = (N-1)/2$ different positive values of $k$ or in the doublets $(k, -k)$. Supposing an even number of pairs, the counting leads to

$$\sum_{m=0}^{n/2} \binom{p-m}{n-2m}\binom{p}{m}.$$

For $n_0 = 1$, $(n-1)$ pairs are to be distributed and a similar formula is obtained. Finally, the general formula for the number $D_{n,N}$ of positive STA vectors is given by

$$D_{n,N} = \sum_{m=0}^{n/2} \binom{p-m}{n-2m}\binom{p}{m} + \sum_{m=0}^{(n-1)/2} \binom{p-m}{n-2m-1}\binom{p}{m} \quad (31)$$

where the division must be understood as the division for integers. In table 1 the linear sizes $D_{n,N}$ of the largest matrices obtained for different number $n$ of pairs and number $N$ of Bloch states are shown. $D_0$ denotes the size of the full Hilbert space

$$D_0 = \binom{N}{n} \quad (32)$$

and the ratios $D_0/D_{n,N}$ are given. From formulae (31) and (32) it is quite clear that this ratio grows exponentially as a function of the number of pairs $n$. This illustrates the very important gain obtained by using spin-transposition operators in this problem.

**Table 1.** Sizes of the largest submatrices obtained. Gain in computational effort obtained by using the block-diagonalization as defined by equation (37).

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Number of Bloch states $N$ | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 |
| Number of pairs $n$ | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| Size of the full Hilbert space $D_0$ | 10 | 35 | 126 | 462 | 1716 | 6435 | 24 310 | 92 378 |
| Size of the largest submatrix $D_{n,N}$ | 5 | 13 | 35 | 96 | 267 | 750 | 2123 | 6046 |
| Ratio $D_0/D_{n,N}$ | 2 | 2.69 | 3.6 | 4.81 | 6.43 | 8.58 | 11.45 | 15.28 |
| Gain in computational effort | ∼7 | ∼16 | ∼38 | ∼88 | ∼202 | ∼463 | ∼1062 | ∼2433 |

### *4.2. Action of H on a non-positive STA vector*

A non-positive STA basis vector has at least one negative signature. In this case we have the central result

$$\left(b_{k_{i_l}} + b_{-k_{i_l}}\right)\left\|n_0; \ldots, k_{i_l}{}^{(s_{i_l})}, \ldots; \left(k_{j_1}, -k_{j_1}\right), \ldots, \left(k_{j_m}, -k_{j_m}\right)\right\rangle\rangle = 0 \tag{33}$$

for each $i_l$ such that $s_{i_l} = -1$. This equality is a simple consequence of the definition (16) of the STA basis vectors and of the relation

$$(b_k + b_{-k})\frac{(1 - T_k)}{\sqrt{2}} b_k^\dagger |0\rangle = 0.$$

From equation (33) follow some important consequences. The first one is that the operator $H$ acting on a STA basis vector does not modify the list of $k_{i_l}$ having a negative signature. Accordingly, two STA vectors with two different lists of Bloch states with negative signatures are not connected by $H$ (zero matrix elements between such STA vectors). This is the central result responsible for the block-diagonalization of the BCS matrix. The number of independent blocks is given by the number of ways of distributing $0, 1, \ldots, n$ negative signatures over the $p$ possible values for the positive $k_i$. The independent (not connected by $H$) subspaces of STA vectors are then characterized as follows:

- 1 subspace spanned by STA vectors with 0 negative signature (positive STA vectors);
- $p$ subspaces spanned by STA vectors with 1 negative signature. The $p$ possible locations for the negative sign (Bloch state $k_1, \ldots, k_p$) differentiate the $p$ subspaces;
- $p(p-1)/2$ subspaces corresponding to 2 negative signatures. Subspaces are labelled by all possible doublets $(k_i, k_j)$ $i \neq j$ giving all possible locations for the two negative signs; and so on
- up to $\binom{p}{n}$ subspaces associated with $n$ negative signs.

Remark that in the case $p = n$ ('half-filling') the number of independent subspaces is found to be $2^n$.

The second important remark concerns the structure of the BCS matrix within a given subspace of STA vectors with $r$ negative signatures. Because of equation (33) it is clear that the structure of the BCS matrix is identical to that obtained for $(n - r)$ pairs distributed over $(p - r)$ Bloch states having positive signatures. The sole difference between the BCS submatrix associated with $r$ negative signatures and the BCS matrix as expressed within the positive STA basis for $(n-r)$ pairs over $(p-r)$ Bloch states, is a diagonal contribution related to the $r$ Bloch states not affected by $H$. This diagonal contribution is just a global constant given by

$$\sum_{k \in \{k_{\text{neg}}\}} (\epsilon_k + \epsilon_{-k}) - \frac{2rU}{N} \tag{34}$$

where $\{k_{\rm neg}\}$ denotes the set of $r$ Bloch states having negative signatures. The first contribution in equation (34) results from the diagonal part in (1) and the second one from the third contribution in equation (19). Finally, the entire spectrum of the BCS matrix can be obtained by diagonalizing the set of matrices built from the set of all positive STA vectors associated with a number of pairs ranging from 0 to $n$ over a number of states varying from $p-n$ to $p$, respectively.

In summary, we can collect all these results as follows. Within the STA basis the matrix of $H$ for a number $n$ of pairs and a number $2p+1$ of Bloch states decomposes as a set of $\sum_{k=0}^{n}\binom{p}{k}$ block-diagonal matrices. Each matrix is defined over the set of $D_{k,p-k}$ positive STA vectors for $k$ pairs over $p-k$ Bloch states. The off-diagonal matrix elements are given by the set of relations (equations (26)–(30)). The diagonal part is given by

$$\left[n_0 2\epsilon_0+\sum_{l=1}^{q}\left(\epsilon_{k_{i_l}}+\epsilon_{-k_{i_l}}\right)+\sum_{l=1}^{m}2\left(\epsilon_{k_{j_l}}+\epsilon_{-k_{j_l}}\right)+\frac{Un^2}{N}+\sum_{k\in\{k_{\rm neg}\}}(\epsilon_k+\epsilon_{-k})+\frac{2(q-r)U}{N}\right]. \tag{35}$$

In terms of the sizes of the different subspaces the full Hilbert space is decomposed as follows:

$$\binom{N}{n}=\sum_{k=0}^{n}\binom{p}{k}D_{k,p-k}. \tag{36}$$

Finally, knowing that the calculation of the full spectrum of a matrix of size $N$ is a process of order $N^3$ the gain $\gamma$ in computational effort can be defined as

$$\gamma=\frac{\binom{N}{n}^3}{\sum_{k=0}^{n}\binom{p}{k}D_{k,p-k}{}^3}. \tag{37}$$

We have reported in table 1 the values of $\gamma$. Note that the gain in computational effort to compute the full spectrum grows exponentially as a function of the number of pairs $n$.

Let us return to our illustrative example corresponding to $N=5$ and $n=2$. In that case there exist $\sum_{k=0}^{2}\binom{2}{k}=4$ block-diagonal matrices. The matrix corresponding to zero negative signature is built from the five positive STA vectors $\|0;k_1{}^{(+)},k_2{}^{(+)}\rangle\rangle$, $\|1;k_1{}^{(+)}\rangle\rangle$, $\|1;k_2{}^{(+)}\rangle\rangle$, $\|0;(k_1,-k_1)\rangle\rangle$, $\|0;(k_2,-k_2)\rangle\rangle$ and we have

$$\begin{aligned}
H\|0;k_1{}^{(+)},k_2{}^{(+)}\rangle\rangle&=\left[\left(\epsilon_{k_1}+\epsilon_{-k_1}\right)+\left(\epsilon_{k_2}+\epsilon_{-k_2}\right)+\frac{Un^2}{N}+\frac{4U}{N}\right]\|0;k_1{}^{(+)},k_2{}^{(+)}\rangle\rangle\\
&\quad+\frac{2U}{N}[\|0;(k_1,-k_1)\rangle\rangle+\|0;(k_2,-k_2)\rangle\rangle]+\frac{\sqrt{2}U}{N}\left[\|1;k_1{}^{(+)}\rangle\rangle+\|1;k_2{}^{(+)}\rangle\rangle\right]\\
H\|1;k_1{}^{(+)}\rangle\rangle&=\left[2\epsilon_0+\left(\epsilon_{k_1}+\epsilon_{-k_1}\right)+\frac{Un^2}{N}+\frac{2U}{N}\right]\|1;k_1{}^{(+)}\rangle\rangle\\
&\quad+\frac{2U}{N}\|1;k_2{}^{(+)}\rangle\rangle+\frac{\sqrt{2}U}{N}[\|0;(k_1,-k_1)\rangle\rangle+\|0;(k_2,-k_2)\rangle\rangle]\\
H\|1;k_2{}^{(+)}\rangle\rangle&=\left[2\epsilon_0+\left(\epsilon_{k_2}+\epsilon_{-k_2}\right)+\frac{Un^2}{N}+\frac{2U}{N}\right]\|1;k_2{}^{(+)}\rangle\rangle\\
&\quad+\frac{2U}{N}\|1;k_1{}^{(+)}\rangle\rangle+\frac{\sqrt{2}U}{N}[\|0;(k_1,-k_1)\rangle\rangle+\|0;(k_2,-k_2)\rangle\rangle]
\end{aligned}$$

$$H\|0;(k_1,-k_1)\rangle\rangle = \left[2\left(\epsilon_{k_1}+\epsilon_{-k_1}\right)+\frac{Un^2}{N}\right]\|0;(k_1,-k_1)\rangle\rangle + \frac{\sqrt{2}U}{N}\left\|1;{k_1}^{(+)}\right\rangle\!\right\rangle + \frac{2U}{N}\left\|0;{k_1}^{(+)},{k_2}^{(+)}\right\rangle\!\right\rangle$$

$$H\|0;(k_2,-k_2)\rangle\rangle = \left[2\left(\epsilon_{k_2}+\epsilon_{-k_2}\right)+\frac{Un^2}{N}\right]\|0;(k_2,-k_2)\rangle\rangle + \frac{\sqrt{2}U}{N}\|1;{k_2}^{(+)}\rangle\rangle + \frac{2U}{N}\|0;{k_1}^{(+)},{k_2}^{(+)}\rangle\rangle.$$

Two matrices correspond to one negative signature. They are built from the two positive STA vectors corresponding to only one pair in $p = 1$ ($N = 3$ sites), $\left\|0;{k_1}^{(+)},{k_2}^{(-)}\right\rangle\!\right\rangle$, $\|1;{k_2}^{(-)}\rangle\rangle$ and $\left\|0;{k_1}^{(-)},{k_2}^{(+)}\right\rangle\!\right\rangle$, $\left\|1;{k_2}^{(+)}\right\rangle\!\right\rangle$ with the relations

$$H\left\|0;{k_1}^{(+)},{k_2}^{(-)}\right\rangle\!\right\rangle = \left[\left(\epsilon_{k_1}+\epsilon_{-k_1}\right)+\left(\epsilon_{k_2}+\epsilon_{-k_2}\right)+\frac{Un^2}{N}+\frac{U}{N}(1+1-1-1)\right] \times \left\|0;{k_1}^{(+)},{k_2}^{(-)}\right\rangle\!\right\rangle + \frac{\sqrt{2}U}{N}\|1;{k_2}^{(-)}\rangle\rangle$$

and

$$H\|1;{k_2}^{(-)}\rangle\rangle = \left[2\epsilon_0+\left(\epsilon_{k_2}+\epsilon_{-k_2}\right)+\frac{Un^2}{N}+\frac{U}{N}(-1-1)\right]+\frac{\sqrt{2}U}{N}\left\|0;{k_1}^{(+)},{k_2}^{(-)}\right\rangle\!\right\rangle$$

with some similar formulae for the second matrix. Finally, there is one matrix of size 1 corresponding to two negative signatures,

$$H\|0;{k_1}^{(-)},{k_2}^{(-)}\rangle\rangle = \left[\left(\epsilon_{k_2}+\epsilon_{-k_2}\right)+\left(\epsilon_{k_1}+\epsilon_{-k_1}\right)+\frac{Un^2}{N}+\frac{U}{N}(-1-1-1-1)\right] \times \|0;{k_1}^{(-)},{k_2}^{(-)}\rangle\rangle$$

associated with an exact eigenstate for the problem.

Before ending this section it is important to mention that the various results just presented can be rephrased using a spin-based language. As shown above, the total spin associated with a particular STA basis vector is given by the sum of its $q$ signatures. As a consequence, the various blocks obtained in the block-diagonalization of the Hamiltonian can be associated with some well-defined value of the total spin ($n + 1$ values of the total spin ranging from $S = 0$ to $S = n$). As just seen, the set of positive STA vectors (defined as having 0 negative signature) plays a central role here. Positive STA vectors correspond to singlet states and are used as a complete basis set for the singlet many-particle wavefunctions. Using this spin language the central result of this work can be summarized as follows. By using an iterative process (diagonalization within the set of singlet states for $n$ pairs; diagonalization within the set of singlet states for $n - 1$ pairs, one pair being fixed in a triplet state, and so on) the entire eigenspectrum of the Hamiltonian for $n$ pairs can be built by collecting the various eigenspectra of the very same Hamiltonian (up to a trivial diagonal shift) computed for a smaller number of pairs ranging from 1 to $n$ and defined within *singlet subspaces only*. The way the various sub-spectra are put together to obtain the complete spectrum is just a combinatorial problem and has been presented in detail above.

## 5. Summary and discussion

In this paper we have shown that by using operators associated with spin transposition within electron pairs, it is possible to construct a new basis set—the so-called spin-transposition-adapted (STA) basis set—consisting of vectors which are all eigenstates of each transposition

operator. Within this STA basis set it has been shown that the full BCS matrix can be decomposed into a series of block-diagonal submatrices. The ratio of the dimension of the complete Hilbert space over the size of the largest submatrix obtained grows exponentially as a function of the number of electron pairs considered. As a consequence, the gain in numerical effort to get the full set of energies and eigenstates is also exponential. This remarkable result is valid for any dimension of space and pair electron filling. We have also shown that spin transpositions and more usual spin-symmetry operators are not independent. Within a spin language, the main result presented here can be summarized by stating that the entire eigenspectrum associated with eigenstates of total spin $S = 0, 1, \ldots, n$ can be obtained by collecting *singlet* eigenspectra of identical problems with smaller number of pairs. The resulting gain resulting from this hierarchical structure is exponential.

In this paper, the results have been presented for the BCS model whose exact spectrum can be obtained using Richardson's method. However, it is clear that the STA basis set can be used without particular difficulty when considering more general non-integrable pairing models expressed in terms of transposition operators. A simple example of such models is a model where the interaction $U$ is not diagonal in $k$-space, $U_{kk'}$. Thanks to the results presented here, the linear sizes accessible to exact diagonalization studies of pairing models are now larger than the sizes usually considered. To give an example, using the Lanczòs algorithm—the standard tool for computing ground-state energies and Green functions—it is possible to treat linear subspaces of the maximum size of about $10^7$–$10^8$. Using the results of the present work we can hope to study systems including up to about 20 pairs. In the standard $k$-diagonal basis this would mean a Hilbert space of size $\sim 3 \times 10^{11}$, which is of course unattainable by present computers.

Finally, let us mention that it is natural to try to generalize the results presented here to the most important case of the Hubbard model. Of course, in this case the pairs are no longer conserved by the interaction. However, as shown by our preliminary investigations the presence of some residual pair structure seems to have also some interesting consequences.

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