

Computing Transfer Amplitude between BCS-Pair Condensates

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Abstract

I propose a new algorithm that uses recursive relations to compute spectroscopic factor, pair transfer amplitude and cluster transfer amplitude. I demonstrate the algorithm that it can be calculated very quickly and stored within small computer memory consumption. In BCS case, the particle number is always conserved and the time-consuming projection is avoided. I derive analytical expressions for the pair transfer amplitude and the cluster transfer amplitude expressed by asymmetry many-pair density matrix. This algorithm practically could be used in all of the nuclear double beta decay fields, the heavy cluster emission fields and the single-nucleon transfer of the odd-mass isotopes.

Keywords

BCS, Spectroscopic Factor, Pair-Transfer Amplitude, Cluster-Transfer Amplitude

1. Introduction

The Bardeen-Cooper-Schrieffer (BCS) theory was first proposed as a superconducting microscopic theory [1] [2]. Later, it was used to treat pairing correlations in nuclear physics [3] [4]. It is still one of the “standard” treatments after fifty years [5], owing to its simplicity and the ease with which higher-order correlations could be added [for example, via quasiparticle random-phase approximation (QRPA)]. However, as compared to macroscopic quantum systems, the theory applied to finite nuclei has two major drawbacks. First, it breaks particle-number conservation by introducing quasiparticles. Second, the BCS theory needs a minimum pairing strength for nuclear systems with finite level spacing. It only yields trivial (vanishing) solutions below that strength, whereas pairing always has an impact in reality.

The “pair condensate” [Equation (3), with determinate particle number] is a frequent improvement over the BCS “quasiparticle vacuum” as the variational ground state [6]. A method was recently proposed under the pair condensate to calculate pair-hopping amplitudes by computing the many-pair density matrices [7]. In the example of the spherical nuclear shell model, it is demonstrated that the many-pair density matrices can be calculated fast using recursive relations and stored easily in computer memory. The method is demonstrated in semi-magic nuclei $^{46,48,50}\text{Ca}$, ^{116}Sn , and ^{182}Pb .

However, this method can only compute the pair-hopping amplitude of one same nucleus with fixed particle number. Nuclear reactions such as the nuclear double beta decay, single-nucleon transfer and cluster decay of which the amplitudes are of two different nuclei play a crucial role in nuclear physics and particle physics.

One of the pair transfer nuclear reactions is the nuclear double beta decay. Mayer was the first to explore the nuclear double beta decay mode with obvious lepton number conservation in 1935 [8]. On the particle physics side, the inverse half-life of double beta decay is expressed as a product of a phase-space factor and the relevant double beta decay nuclear matrix element, which is free of unknown parameters. Thus, the value of the double beta decay nuclear matrix elements is directly determined by the measured experimental half lives of double beta decays. As a result, double beta decay provides a rigorous test of nuclear structure calculations. The double beta decay is already well established experimentally for a couple of isotopes. Because of the enormous energy release, the transition from the ground state 0^+ of the initial to the ground state 0^+ of the final nuclei is the most favored for experimental study of this unusual phenomenon. Transitions to the 2^+ and 0^+ excited states of the final nucleus have lately received more study [9]-[20].

Because many observable quantities are acquired from one-body operators, coefficients of fractional parentage (CFP) are quite useful. In addition, there is a resurgence of interest in experiments involving single nucleon transfer studies in the $1p$ shell region [21]. As an example, the odd-mass isotopes $^{5,7}\text{He}$ are particle-unbound [22]. In the framework of an R-matrix analysis, the data provide the neutron spectroscopic factor, which describes to what extent the total angular momentum quantum number $J^\pi = 3/2^-$ ground state of ^7He can be regarded as a $^6\text{He} \otimes 1p_{3/2}$ configuration, where the symbol \otimes means tensor product of the single-particle Hilbert space. The spectral factor is a fundamental quantity that characterizes the single-particle nature of nuclear excitation and is hence consequently an important test of wave functions derived using newly established methods [23].

Heavy cluster emission and super-asymmetric fission have been studied theoretically since the late 1970s [24]. Cluster radioactivity is the phenomena of radioactive nuclei emitting particles heavier than the alpha particle spontaneously [25]. This process can be thought of as a case of strong asymmetric fission [26]

or as a decay process involving cluster formation and tunneling through the barrier, analogous to alpha decay [27]. The penetrability of the pre-scission component of the barrier was proven to be similar to the super asymmetric fission model by interpreting the cluster preformation probability within a super asymmetric fission model as the penetrability of the pre-scission part of the barrier [28] [29] [30] [31]. Rose and Jones [32] validated this occurrence in the radioactive decay of ^{14}C from ^{223}Ra in 1984, and Alexandrov *et al.* [33] confirmed it a few months later. Since then, the ^{14}C decay of many isotopes of Ra nuclei and many other heavy cluster decays have been observed [34].

With the advent of heavy ion beams for inducing multi-particle transfer reactions, a wealth of data from nuclei with a large variety of nucleon numbers has become available. The no-recoil, zero-range distorted wave Born approximation (DWBA) algorithms that are typically used to analyze light ion single-particle transfer data have been demonstrated to be insufficient in assessing the new studies. There have been some questions about how to properly extract structure information from less restrictive exact finite range DWBA computations [35]. Studying transfer amplitude between BCS-pair condensates and a proper technique for computing it is needed.

In this work, I define the asymmetry many-pair density matrix and derive the recursive relations of the asymmetry many-pair density matrix. I demonstrate that it can be calculated very quickly and stored within small computer memory consumption. I also derive the pair transfer amplitude for double beta decay and the cluster transfer amplitude for cluster decay expressed by asymmetry many-pair density matrix. The manuscript is organized as following. In Section 2, I briefly introduce the pair condensate with zero generalized seniority of the $2N$ -particle system and the many-pair density matrix. Then in Section 3, I derive the relation between the cluster transfer amplitude and the asymmetry many-pair density matrix. Finally, Section 4 summarizes the work.

2. Basic Expressions

In this section I briefly review the many-pair density matrix and the simple relation between the Pauli-blocked normalizations and many-pair density matrix. The pair-creation operator

$$P_{\alpha}^{\dagger} = a_{\alpha}^{\dagger} a_{\tilde{\alpha}}^{\dagger} = P_{\tilde{\alpha}}^{\dagger} \quad (1)$$

creates a pair of particles on the single-particle level $|\alpha\rangle$ and its time-reversed partner $|\tilde{\alpha}\rangle$ ($|\tilde{\tilde{\alpha}}\rangle = -|\alpha\rangle$). The coherent pair-creation operator

$$P^{\dagger} = \frac{1}{2} \sum_{\alpha} v_{\alpha} a_{\alpha}^{\dagger} a_{\tilde{\alpha}}^{\dagger} = \sum_{\alpha} v_{\alpha} P_{\alpha}^{\dagger} \quad (2)$$

creates a pair of particles with the real structure coefficients v_{α} that are distributed coherently over the whole single-particle space. The summation index in Equation (2) is a pair index that only accounts for half of the single-particle space (for instance, only account for those single-particle levels with a positive magnetic quantum number m). The state with zero generalized seniority of the

2N-particle system in the presence of pairing correlations is

$$|\phi_N\rangle = \frac{1}{\sqrt{\chi_N}} (P^\dagger)^N |0\rangle, \tag{3}$$

where

$$\chi_N = \langle 0 | P^N (P^\dagger)^N | 0 \rangle \tag{4}$$

is the normalization factor. The pair creation and annihilation operators, P_α^\dagger , and P_α along with $\hat{N}_\alpha = \frac{1}{2}(a_\alpha^\dagger a_\alpha + a_{\bar{\alpha}}^\dagger a_{\bar{\alpha}})$ are the generators of a quasi-spin $su(2)$ algebra,

$$[P_\alpha, P_\beta^\dagger] = \delta_{\alpha\beta} (1 - 2\hat{N}_\alpha), \tag{5}$$

$$[\hat{N}_\alpha, P_\beta^\dagger] = \delta_{\alpha\beta} P_\beta^\dagger. \tag{6}$$

The many-pair density matrix is introduced as

$$t_{\alpha_1\alpha_2\cdots\alpha_p;\beta_1\beta_2\cdots\beta_q}^N \equiv \langle 0 | P^{N-p} P_{\alpha_1} P_{\alpha_2} \cdots P_{\alpha_p} \times P_{\beta_1}^\dagger P_{\beta_2}^\dagger \cdots P_{\beta_q}^\dagger (P^\dagger)^{N-q} | 0 \rangle, \tag{7}$$

where all the indices $\alpha_1\alpha_2\cdots\alpha_p, \beta_1\beta_2\cdots\beta_q$ are distinct, owing to the Pauli principle. Note that the $t_{\alpha_1\alpha_2\cdots\alpha_p;\beta_1\beta_2\cdots\beta_q}^N$ is real because of the real v_α , so $t_{\alpha_1\alpha_2\cdots\alpha_p;\beta_1\beta_2\cdots\beta_q}^N = t_{\beta_1\beta_2\cdots\beta_q;\alpha_1\alpha_2\cdots\alpha_p}^N$. The normalization χ_N defined in Equation (4) is the special case of Equation (7) when there is no α and β index,

$$\chi_N \equiv t_{;}^N. \tag{8}$$

For convenience, I introduce $[\gamma_1\gamma_2\cdots\gamma_r]$ to represent a subspace of the original single-particle space, by removing Kramers pairs $\gamma_1\gamma_2\cdots\gamma_r$ of single-particle levels from the latter. The Pauli-blocked many-pair density matrix is defined as

$$t_{\alpha_1\alpha_2\cdots\alpha_p;\beta_1\beta_2\cdots\beta_q}^{[\gamma_1\gamma_2\cdots\gamma_r],N} \equiv \langle 0 | P^{N-p} P_{\gamma_1} P_{\gamma_2} \cdots P_{\gamma_r} \times P_{\alpha_1} P_{\alpha_2} \cdots P_{\alpha_p} P_{\beta_1}^\dagger P_{\beta_2}^\dagger \cdots P_{\beta_q}^\dagger \times P_{\gamma_1}^\dagger P_{\gamma_2}^\dagger \cdots P_{\gamma_r}^\dagger (P^\dagger)^{N-q} | 0 \rangle, \tag{9}$$

and Pauli-blocked normalization

$$\chi_N^{[\gamma_1\gamma_2\cdots\gamma_r]} \equiv t_{;}^{[\gamma_1\gamma_2\cdots\gamma_r],N} = \langle 0 | P^N P_{\gamma_1} P_{\gamma_2} \cdots P_{\gamma_r} P_{\gamma_1}^\dagger P_{\gamma_2}^\dagger \cdots P_{\gamma_r}^\dagger (P^\dagger)^N | 0 \rangle \tag{10}$$

could be easily derived. Also, there is no duplicated P operator, and duplicated P^\dagger operator in Equations (9) and (10), owing to the Pauli principle. The many-pair density matrix (7) and the Pauli-blocked many-pair density matrix (9) could be expressed by normalizations, and normalizations could be computed by recursive relations [36], which means for a certain nucleus, if we know all v_α (or $n_\alpha = \langle \phi_N | \hat{n}_\alpha | \phi_N \rangle = \langle \phi_N | a_\alpha^\dagger a_\alpha | \phi_N \rangle$) of single-particle orbit, we could rapidly and accurately compute many-pair density matrix and normalizations [37].

3. Transfer Amplitude

In the Section 2, I introduce the many-pair density matrix, of which the bra and the ket are of a same nucleus (v_α is the same). In this section I drive the cluster

transfer amplitude to solve the issue with the inner product between two different nuclei. Defining

$$|\phi'_N\rangle = \frac{1}{\sqrt{\chi'_N}}(P'^{\dagger})^N |0\rangle, \tag{11}$$

where

$$\chi'_N = \langle 0|(P')^N (P'^{\dagger})^N |0\rangle, \tag{12}$$

the inner product between $|\phi_N\rangle$ and $|\phi'_N\rangle$ is

$$\begin{aligned} \langle \phi'_N | \phi_N \rangle &= \langle \phi_N | \phi'_N \rangle \\ &= \frac{1}{\sqrt{\chi'_N \chi_N}} \langle 0|(P')^N (P^{\dagger})^N |0\rangle \\ &= \frac{1}{\sqrt{\chi'_N \chi_N}} \langle 0|(P)^N (P^{\dagger})^N |0\rangle \\ &= \frac{\Upsilon_N}{\sqrt{\chi'_N \chi_N}}, \end{aligned} \tag{13}$$

where

$$P' = \sum_{\alpha} v'_{\alpha} P_{\alpha}, \tag{14}$$

and

$$\Upsilon_N = \langle 0|(P')^N (P^{\dagger})^N |0\rangle = \langle 0|(P)^N (P^{\dagger})^N |0\rangle. \tag{15}$$

The asymmetry many-pair density matrix is defined as

$$u_{\alpha_1 \alpha_2 \dots \alpha_p; \beta_1 \beta_2 \dots \beta_q}^N \equiv \langle 0|(P')^{N-p} P_{\alpha_1} P_{\alpha_2} \dots P_{\alpha_p} \times P_{\beta_1}^{\dagger} P_{\beta_2}^{\dagger} \dots P_{\beta_q}^{\dagger} (P^{\dagger})^{N-q} |0\rangle. \tag{16}$$

Now I drive the relation between $u_{\alpha_1 \alpha_2 \dots \alpha_p; \beta_1 \beta_2 \dots \beta_q}^N$ and Υ_N . By substituting Equation (14) into $(P')^{N-p}$ and polynomially expanding, terms with $P_{\alpha_1}, P_{\alpha_2}, \dots$ or P_{α_p} vanish due to the Pauli principle, which is equivalent to Pauli block the $\alpha_1 \alpha_2 \dots \alpha_p$ indices from $(P')^{N-p}$. Thus, $(P')^{N-p}$ could be replaced by $\left(P'_{[\alpha_1 \alpha_2 \dots \alpha_p]}\right)^{N-p}$, where

$$P'_{[\alpha_1 \alpha_2 \dots \alpha_p]} \equiv P' - v'_{\alpha_1} P_{\alpha_1} - v'_{\alpha_2} P_{\alpha_2} - \dots - v'_{\alpha_p} P_{\alpha_p}. \tag{17}$$

Next, use

$$\begin{aligned} \left(P'_{[\alpha_1 \alpha_2 \dots \alpha_p]}\right)^{N-p} &= \left(P'_{[\alpha_1 \alpha_2 \dots \alpha_p \beta_1 \beta_2 \dots \beta_q]} - v'_{\beta_1} P_{\beta_1} - v'_{\beta_2} P_{\beta_2} - \dots - v'_{\beta_q} P_{\beta_q}\right)^{N-p} \\ &= P_{N-p}^q v'_{\beta_1} P_{\beta_1} \dots v'_{\beta_q} P_{\beta_q} \left(P'_{[\alpha_1 \dots \beta_q]}\right)^{N-p-q} + \text{Others}, \end{aligned} \tag{18}$$

where ‘‘Others’’ do not contribute and each contributing term must have the factor $P_{\beta_1} P_{\beta_2} \dots P_{\beta_q}$ to annihilate $P_{\beta_1}^{\dagger} P_{\beta_2}^{\dagger} \dots P_{\beta_q}^{\dagger}$ resulting in the permutations P_{N-p}^q in the last step.

Treating $(P^{\dagger})^{N-q}$ similarly, Equation (16) becomes

$$\begin{aligned}
 u_{\alpha_1\alpha_2\cdots\alpha_p;\beta_1\beta_2\cdots\beta_q}^N &= P_{N-p}^q P_{N-q}^p v_{\alpha_1} v_{\alpha_2} \cdots v_{\alpha_p} v'_{\beta_1} v'_{\beta_2} \cdots v'_{\beta_q} \\
 &\times \langle 0 | \left(P'_{[\alpha_1\cdots\beta_q]} \right)^{N-p-q} P_{\beta_1} \cdots P_{\beta_q} P_{\alpha_1} \cdots P_{\alpha_p} \\
 &\times P_{\alpha_1}^\dagger \cdots P_{\alpha_p}^\dagger P_{\beta_1}^\dagger \cdots P_{\beta_q}^\dagger \left(P'_{[\alpha_1\cdots\beta_q]} \right)^{N-p-q} | 0 \rangle \\
 &= \frac{(N-p)!(N-q)!}{[(N-p-q)!]^2} \times v_{\alpha_1} v_{\alpha_2} \cdots v_{\alpha_p} v'_{\beta_1} v'_{\beta_2} \cdots v'_{\beta_q} \\
 &\times \Upsilon_{N-p-q}^{[\alpha_1\alpha_2\cdots\alpha_p\beta_1\beta_2\cdots\beta_q]},
 \end{aligned} \tag{19}$$

where

$$\begin{aligned}
 \Upsilon_{N-p-q}^{[\alpha_1\alpha_2\cdots\alpha_p\beta_1\beta_2\cdots\beta_q]} &= \langle 0 | \left(P'_{[\alpha_1\cdots\beta_q]} \right)^{N-p-q} P_{\beta_1} \cdots P_{\beta_q} P_{\alpha_1} \cdots P_{\alpha_p} \\
 &\times P_{\alpha_1}^\dagger \cdots P_{\alpha_p}^\dagger P_{\beta_1}^\dagger \cdots P_{\beta_q}^\dagger \left(P'_{[\alpha_1\cdots\beta_q]} \right)^{N-p-q} | 0 \rangle \\
 &= \langle 0 | (P')^{N-p-q} P_{\beta_1} \cdots P_{\beta_q} P_{\alpha_1} \cdots P_{\alpha_p} \\
 &\times P_{\alpha_1}^\dagger \cdots P_{\alpha_p}^\dagger P_{\beta_1}^\dagger \cdots P_{\beta_q}^\dagger (P')^{N-p-q} | 0 \rangle.
 \end{aligned} \tag{20}$$

From Equation (2), (5) and (6) it is easy to derive the identity

$$P_\alpha (P^\dagger)^{N+1} | 0 \rangle = v_\alpha (N+1) (P^\dagger)^N | 0 \rangle - (v_\alpha)^2 N(N+1) P_\alpha^\dagger (P^\dagger)^{N-1} | 0 \rangle. \tag{21}$$

Now premultiplication with $\langle 0 | (P')^N$ gives the result

$$u_{\alpha;}^{N+1} = v_\alpha (N+1) \Upsilon_N - (v_\alpha)^2 N(N+1) u_{\alpha;}^N. \tag{22}$$

Based on Equations (14) and (15), Υ_N could be expressed as

$$\Upsilon_N = \sum_\alpha v'_\alpha \langle 0 | (P')^{N-1} P_\alpha (P^\dagger)^N | 0 \rangle = \sum_\alpha v'_\alpha u_{\alpha;}^N. \tag{23}$$

Substituting $u_{\alpha;}^{N+1} = v_\alpha (N+1) \Upsilon_N^{[\alpha]}$ and $u_{\alpha;}^N = v'_\alpha N \Upsilon_{N-1}^{[\alpha]}$ implied from Equation (19) into (22) and (23), I get the recursive relations

$$\Upsilon_N = N \sum_\alpha v_\alpha v'_\alpha \Upsilon_{N-1}^{[\alpha]}, \tag{24}$$

$$\Upsilon_N - \Upsilon_N^{[\alpha]} = N^2 v_\alpha v'_\alpha \Upsilon_{N-1}^{[\alpha]}, \tag{25}$$

with initial value $\Upsilon_0 = \langle 0 | 0 \rangle = 1$ and $\Upsilon_0^{[\alpha]} = \langle 0 | P_\alpha P_\alpha^\dagger | 0 \rangle = 1$. This is because by definition the norm of all the orthonormal basis for the Hilbert space is 1 in quantum mechanics, with no exceptions for vacuum. Knowing $\Upsilon_0^{[\alpha]}$, I could compute Υ_1 by Equation (24), and then $\Upsilon_1^{[\alpha]}$ by Equation (25). Equations (24) and (25) are also valid in the blocked subspace $[\gamma_1\gamma_2\cdots\gamma_r]$. For example, in $[\beta]$ they read

$$\Upsilon_N^{[\beta]} = N \sum_\alpha v_\alpha v'_\alpha \Upsilon_{N-1}^{[\alpha\beta]}, \tag{26}$$

$$\Upsilon_N^{[\beta]} - \Upsilon_N^{[\alpha\beta]} = N^2 v_\alpha v'_\alpha \Upsilon_{N-1}^{[\alpha\beta]}, \tag{27}$$

with initial value $\Upsilon_0^{[\alpha\beta]} = \langle 0 | P_\alpha P_\beta P_\beta^\dagger P_\alpha^\dagger | 0 \rangle = 1$.

So by definition, the spectroscopic factor between an odd nucleus $a_\alpha^\dagger | \phi'_{N-1} \rangle$

and an even nucleus $|\phi_N\rangle$ is

$$\begin{aligned}\kappa_{\alpha\alpha_1} &= \langle \phi'_{N-1} | a_\alpha a_{\alpha_1} | \phi_N \rangle \\ &= \frac{\delta_{\bar{\alpha}\alpha_1}}{\sqrt{\chi'_{N-1}\chi_N}} \langle 0 | (P')^{N-1} P_\alpha (P^\dagger)^N | 0 \rangle \\ &= \frac{\delta_{\bar{\alpha}\alpha_1}}{\sqrt{\chi'_{N-1}\chi_N}} u_{\alpha_1}^N \\ &= \delta_{\bar{\alpha}\alpha_1} \frac{N v_\alpha \Upsilon_{N-1}^{[\alpha]}}{\sqrt{\chi'_{N-1}\chi_N}},\end{aligned}\quad (28)$$

the pair transfer amplitude is

$$\kappa_{\bar{\alpha}\alpha} = \langle \phi'_{N-1} | P_\alpha | \phi_N \rangle = \frac{N v_\alpha \Upsilon_{N-1}^{[\alpha]}}{\sqrt{\chi'_{N-1}\chi_N}}, \quad (29)$$

and the cluster transfer amplitude is

$$\begin{aligned}\kappa_{\alpha\alpha_1\bar{\alpha}_2\alpha_2\cdots\bar{\alpha}_p\alpha_p} &= \delta_{\bar{\alpha}\alpha_1} \langle \phi'_{N-1} | P_{\alpha_1} P_{\alpha_2} \cdots P_{\alpha_p} | \phi_N \rangle \\ &= \frac{\delta_{\bar{\alpha}\alpha_1}}{\sqrt{\chi'_{N-p}\chi_N}} \langle 0 | (P')^{N-p} P_{\alpha_1} \cdots P_{\alpha_p} (P^\dagger)^N | 0 \rangle \\ &= \frac{\delta_{\bar{\alpha}\alpha_1}}{\sqrt{\chi'_{N-p}\chi_N}} u_{\alpha_1\alpha_2\cdots\alpha_p}^N \\ &= \delta_{\bar{\alpha}\alpha_1} \frac{N! v_{\alpha_1} v_{\alpha_2} \cdots v_{\alpha_p} \Upsilon_{N-p}^{[\alpha_1\alpha_2\cdots\alpha_p]}}{(N-p)! \sqrt{\chi'_{N-p}\chi_N}}.\end{aligned}\quad (30)$$

The Equation (28), (29) and (30) can be used in computer program to compute any kinds of nuclear transfer amplitude between two given nuclei, since all parameters [the paired particle number N , the number of paired particle to transfer p , the structure coefficients v_α and v'_α , the normalization factors χ_N and χ'_N , and the transfer factors Υ_N which can be compute by recursive relations (24) and (25)] are known.

4. Summary

In summary, I propose a new algorithm that uses recursive relations to compute spectroscopic factor, pair transfer amplitude and cluster transfer amplitude. This work starts from the inner product between two different nuclei. In order to compute the product, I define the asymmetry many-pair density matrix and drive its recursive relations. The recursive relations can be calculated very quickly and stored within small computer memory consumption, which is the foundation of performing the next step. Due to the properties of the recursive relations, it could be easy to compute the transfer amplitude such as the spectroscopic factor, the pair transfer amplitude and the cluster transfer amplitude using the asymmetry many-pair density matrix.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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