Effect of pairing on one- and two-nucleon transfer below the Coulomb barrier: a time-dependent microscopic description.

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The effect of pairing correlation on transfer reaction below the Coulomb barrier is investigated qualitatively and quantitatively using a simplified version of the Time-Dependent Hartree-Fock + BCS approach. The effect of particle number symmetry breaking on the description of reaction and dedicated methods to extract one and two-nucleon transfer probabilities (\(P_{1n}\) and \(P_{2n}\)) in a particle number symmetry breaking approach are discussed. Influence of pairing is systematically investigated in the \(^{40}\)Ca\(^+\) on \(^{40,42,44,46,48,50}\)Ca reactions. A strong enhancement of the two-particle transfer probabilities due to initial pairing correlations is observed. This enhancement induces an increase of the ratio of probabilities \(P_{2n}/(P_{1n})^2\) compared to the case with no pairing. It is shown that this ratio increases strongly as the center of mass energy decreases with a value that could be larger than ten in the deep sub-barrier regime. An analysis of the pair transfer sensitivity to the type of pairing interaction, namely surface, mixed or volume, used in the theory is made. It is found that the pair transfer is globally insensitive to the type of force and mainly depends on the pairing interaction strength.

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I. INTRODUCTION

The possibility to access cross section much below the Coulomb barrier has revealed new aspects like the hindrance of fusion cross section (see for instance [1]) whose origin is still debated [2, 3]. Among possible interpretation, other competing processes like single- or multi-nucleon transfer might eventually be enhanced and/or modify the capture process [4, 5]. New experimental observations [6, 7] in the moderate and deep sub-barrier regime might lead to important new insight especially on the process of pair transfer. The description of such pair transfer is particularly complex since it requires to treat the quantum tunneling of a composite, eventually correlated, system. In particular, pairing correlations among last bound nucleons is anticipated to play a crucial role.

Following the pioneering work of Refs [6, 12], an important effort is currently being made to improve the description of pair transfer in superfluid systems [13, 24]. These approaches have usually in common that transition probabilities from the initial to the final nucleus are estimated using state of the art Hartree-Fock Bogolyubov (HFB) and Quasi-Particle Random Phase Approximation (QRPA) nuclear models while the reaction dynamics part is treated in a completely separated steps using coupled channels technique.

The present work is an attempt to treat nuclear structure and nuclear reaction aspects in a common microscopic framework that includes pairing. Recently, active research has been devoted to include pairing correlations into the nuclear dynamics using the Time-Dependent HFB (TDHFB) approach [13, 24, 25]. While current applications can be performed in an unrestricted space, due to the required effort, applications of TDHFB have been essentially made on process involving one nucleus, like giant resonances. The use of TDHFB to nuclear reactions remains tedious. A simplified version of TDHFB based on the BCS approximation is considered. This theory has been proposed already some times ago [26] and recently applied with some success either to collective motion in nuclei [27], to reactions in 1D models [28]. First step toward collisions have been reported in ref. [29]. The TDHF+BCS approach has the advantage to be simpler than the original TDHFB theory while keeping part of the physics of pairing. Note that, time-dependent microscopic theories have several advantages compared to other techniques. Many effects, like possible dynamical deformation or core polarization during the reaction are automatically accounted for. In addition, other competing phenomena like emission to the continuum and/or fusion are simultaneously treated. Since, many aspects of the theory applied here have been extensively discussed in Refs. [27, 28], only main aspects features are recalled below.

II. NUCLEAR REACTIONS WITH PAIRING

Time-Dependent Hartree-Fock (TDHF) has become a standard tool to describe nuclear reactions like fusion or transfer reactions (see [31] and ref. therein). In the present work, the TDHF3D code of ref. [32] is extended to include pairing correlations. Below, specific aspects related to the introduction of pairing are discussed.
A. Initial conditions

The reaction is simulated on a 3-dimensional mesh. Following the standard procedure, the two nuclei are initiated separately and then positioned consistently with the desired impact parameter \( b \) and center of mass energy \( E_{\text{c.m.}} \). The initial wave function can be written as

\[
|\Psi(t_0)\rangle = |\Phi_1(t_0)\rangle \otimes |\Phi_2(t_0)\rangle
\]

where \(|\Phi_\alpha(t_0)\rangle\) denotes the many-body wave-function of nucleus \( \alpha = 1, 2 \). Usually, these wave-functions corresponds to Slater determinants. It is assumed here to take the more general form of a quasi-particle vacuum written as

\[
|\Phi_\alpha(t_0)\rangle = \prod_{k>0} \left( u_k^\dagger(t_0) + v_k(t_0) a_k^\dagger(t_0) a_k(t_0) \right)|-\rangle.
\]

where \( a_k^\dagger(t_0) \) stands for the creation operator associated to the canonical single-particle states, denoted hereafter by \( |\varphi_k(t_0)\rangle \) while \((u_k(t_0), v_k(t_0))\) are the standard upper and lower components of the quasi-particle states. Note that due to the spatial separation of the two nuclei, a common single-particle basis can be used. Accordingly, we can omit the \( \alpha \) index and directly write the total wave-function as:

\[
|\Psi(t_0)\rangle = \prod_{k>0} \left( u_k(t_0) + v_k(t_0) a_k^\dagger(t_0) a_k(t_0) \right)|-\rangle.
\]

In practice, initial states for each nucleus have been obtained using the EV8 code that solve the self-consistent BCS equations in the Energy Density Functional framework. Single-particle states are written in \( r \)-space and spin space, denoted by \( \sigma = \uparrow, \downarrow \) as:

\[
a_k^\dagger = \sum_\sigma \int d\mathbf{r} \varphi_k(\mathbf{r}, \sigma) \Psi_\sigma^\dagger(\mathbf{r}),
\]

where \( \Psi_\sigma^\dagger(\mathbf{r}) \) are standard spinors creation operators. In EV8, time-reversal symmetry is assumed and single-particle states can be grouped by pairs of time-reversed states \((k, \bar{k})\). Associated quasi-particle creation operators \((\beta_k^\dagger, \beta_{\bar{k}}^\dagger)\) are written using the following convention for the Bogolyubov transformation:

\[
\begin{aligned}
\beta_k^\dagger &= \sum_\tau u_k^\dagger(r, t_0) \Psi_\tau^\dagger(\mathbf{r}) + v_k(r, t_0) \Psi_{\bar{\tau}}^\dagger(\mathbf{r}), \\
\beta_{\bar{k}}^\dagger &= \sum_\tau u_k(r, t_0) \Psi_\tau^\dagger(\mathbf{r}) - v_k^*(r, t_0) \Psi_{\bar{\tau}}^\dagger(\mathbf{r}),
\end{aligned}
\]

where, using time-reversal properties, we have

\[

\begin{aligned}
&u_k(\mathbf{r}, t_0) = u_k \varphi_k(\mathbf{r}, \uparrow) = u_k \varphi_{\bar{k}}(\mathbf{r}, \downarrow), \\
v_k(\mathbf{r}, t_0) = v_k \varphi_k(\mathbf{r}, \downarrow) = v_k \varphi_{\bar{k}}(\mathbf{r}, \uparrow).
\end{aligned}
\]

The Skyrme Sly4d functional is used in the mean-field channel while for pairing, the following effective neutron-neutron interaction is used:

\[
V_\tau(\mathbf{r}, \sigma; \mathbf{r}', \sigma') = V_0^{\tau\tau} \left( 1 - \eta \frac{\rho_\tau(\mathbf{r} + \mathbf{r}')/2}{\rho_0} \right) \delta_{\tau, \tau'} [1 - P_{\sigma, \sigma'}]
\]

where \( P_{\sigma, \sigma'} \) is the spin exchange operator and where \( \rho_0 = 0.16 \text{ fm}^{-3} \). Here \( \tau = n, p \) stands for neutron or proton channel, only neutron-neutron and proton-proton interaction are considered. Three different forces, standardly called volume \((\eta = 0)\), mixed \((\eta = 0.5)\) and surface \((\eta = 1)\) will be used below. In each case, the neutron pairing interaction strength \( V_0^{nn} \) was adjusted to properly reproduce the experimental gap for the calcium isotopic chain deduced from masses using the 5 points formula. Theoretical odd systems binding energies have been computed using blocking techniques. Values of the interaction parameters are reported in table I. The proton interaction strength is taken from ref. 36 but do not play any role due to the proton closed shell. Illustration of the pairing gap obtained for the three results of the fit are shown in Fig. 1 for the three types of pairing interaction. A comparison of the neutron pairing gap \( \Delta_0^{(5)} \) obtained using the different interactions is done in Fig. 1. The three interactions lead to gaps that are compatible with each others and compatible with the experimental gaps along the calcium isotopic chains especially in the mid-shell. In the following, we consider systematically reactions between the doubly magic \( ^{40}\text{Ca} \) nucleus and other \( ^{42}\text{Ca} \) isotopes. The two reactions \( ^{40}\text{Ca} + ^{40}\text{Ca} \) and \( ^{40}\text{Ca} + ^{48}\text{Ca} \) will correspond to reactions between two normal systems, while in other cases, one of the nucleus will present pairing.

![Figure 1: Experimental (red star) and theoretical neutron gaps](image)

| interaction | \( V_0^{nn} \) [MeV.fm\(^3\)] | \( V_0^{pp} \) [MeV.fm\(^3\)] |
|-------------|-----------------|-----------------|
| volume 0    | 585             | 490             |
| mixed 0.5   | 798             | 755             |
| surface 1   | 1256            | 1462            |

TABLE I: Parameters of the neutron-neutron and proton-proton pairing strength used in the present work.
B. Time-dependent equation of motion

Once the two nuclei have been initiated, the reaction is simulated by performing the dynamical evolution of the many-body wave-packet given by Eq. (3). Here, the TDHF+BCS approximation that may be derived from a variational principle [22] or by an approximate reduction of the TDHF equations [23] is used. Since, properties as well as numerical aspects of the TDHF+BCS method are discussed in Refs. [27, 28], only main ingredients of the theory are summarized here. In this theory, the wave-function remains at all time in its canonical basis, Eq. (3), and the single-particle states evolution identifies with the mean-field dynamics with:

$$i\hbar \partial_t \phi_k = (\hat{h}[\rho] - \eta_k)\phi_k$$

(8)

where \( \eta_k(t) = \langle \phi_k(t) | \hat{h}[\rho]| \phi_k(t) \rangle \) is a time-dependent phase that is conveniently chosen to minimize the effect of the \( U(1) \) symmetry breaking. \( \hat{h}[\rho] \) corresponds here to the self-consistent mean-field derived from the Skyrme functional including time-odd components.

Along the dynamical path, the information is contained in the normal and anomalous densities, denoted by \( \rho \) and \( \kappa \) written in \( r \)-space as:

$$\rho_{\sigma\sigma'}(r, r') = \sum_{k, \tilde{k}} n_k \phi^*_k(r, \sigma) \phi_k(r', \sigma')$$

(9)

$$\kappa_{\sigma\sigma'}(r, r') = \sum_{k, \tilde{k}} \kappa_k (\phi^*_k(r, \sigma) \phi_k(r', \sigma') - \phi^*_k(r, \sigma) \phi_k(r', \sigma')).$$

(10)

\((k, \tilde{k})\) corresponds to pair of single-particle states that were originally degenerated in the static calculation due to time-reversal symmetry. \( n_k = v^*_k v_k \) denote the occupation numbers while \( \kappa_k = u^*_k u_k \) are the components of the anomalous density in the canonical basis. Conjointly to the single-particle evolution, the equation of motion of the components \((n_k, \kappa_k)\) or equivalently of \((n_k, \kappa)\) should be specified. Following Ref. [27], we have:

$$i\hbar \frac{d}{dt} n_k(t) = \kappa_k(t) \Delta_k(t) - \kappa^*_k(t) \Delta_k(t),$$

(11)

$$i\hbar \frac{d}{dt} \kappa_k(t) = \kappa_k(t) (\eta_k(t) + \eta_k(t)) + \Delta_k(t) (2n_k(t) - 1),$$

where \( \Delta_k(t) \) correspond to the pairing field components given by:

$$\Delta_k(t) = -\sum_{l>0} \pi_{kl} \kappa_l(t) g_k(t_0).$$

(12)

g_k(t_0) corresponds to the cut-off function that select the pairing window. This cut-off should be taken consistently with the static calculation [23]. Here, a slightly different prescription is used compared to the original EV8 with:

$$g_k(t_0) = f(\eta_k(t_0) - \lambda) f(\lambda - \eta_k(t_0)) \theta(-\eta_k(t_0)).$$

(13)

\( f \) here corresponds to a Fermi distribution with a cutoff at 5 MeV and a stiffness parameter equal to 0.5 MeV [32], while \( \eta(\eta) \) equals one for \( \eta > 0 \) and zero elsewhere. This additional cut-off insures that only states that are initially bound are considered during the evolution.

As discussed in ref. [28], the reduction of the TDHFB to TDHF+BCS leads to some inconsistencies, especially regarding the one-body continuity equation, making the interpretation of the dynamics difficult. To avoid this problem, we used here the Frozen Occupation Approximation (FOA). In the FOA, it is assumed that the main effect of pairing originates from the initial correlations that induce partial occupations of the orbitals and non-zero components of the two-body correlation matrix, denoted by \( C_{12} \). Possible reorganization in time of occupation numbers and components of \( C_{12} \) are neglected. Said differently, occupation numbers \( n_k \) and components \( \kappa_k \) are kept fixed in time and equal to their initial values. Note that similar ideas have been used recently to describe two-particle break-up reaction using the Time-Dependent Density-Matrix approach [33]. This simplification is motivated by the fact that (i) it solves the problem of continuity equation [28] (ii) in the simple one dimensional model considered in the same reference, it gives rather good description of the emission of particles and is sometimes more predictive than the full TDHFB theory (iii) the FOA approximation applied to collective motion in nuclei [37] gives results that are very close to the full TDHF+BCS dynamics reported in [27].

C. Illustration of reactions

In the present work, we are interested in reactions below the Fusion barrier like the one presented in Ref. [7] where the probabilities to transfer \( x \) neutrons, denoted by \( P_{xn} \) can be extracted as a function of the minimal distance of approach \( D \) during the collision. Assuming a Coulomb trajectory, \( D \) is related to the center of mass energy \( E_{c.m.} \) through:

$$D = \frac{Z_P Z_T e^2}{2E_{c.m.}} \left( 1 + \frac{1}{\sin(\theta_{cm}/2)} \right)$$

(14)

where \( Z_P \) and \( Z_T \) are the target and projectile proton number while \( \theta_{cm} \) is the center of mass scattering angle. Following Ref. [32], only central collisions will be considered here and different distances \( D \) are simulated by varying the center of mass energy. Initial conditions are obtained on a lattice of \( 2L_x \times 2L_y \times 2L_z = 22.4 \times 22.4 \times 22.4 \) \( \text{fm}^3 \) noting that the EV8 code uses symmetries to reduce the calculation in one octant of this space. The dynamical evolution are performed in the center of mass frame using a Runge-Kutta 4 algorithm on a spatial grid of \( L_x \times L_y \times 2L_z = 60.8 \times 22.4 \times 22.4 \) \( \text{fm}^3 \) with a lattice spacing \( \Delta x = 0.8 \) \( \text{fm} \). The time-step is \( \Delta t = 0.015 \times 10^{-22} \) s. Note that, non-equilibrium particle emission is negligible due to the small center of mass energy in the entrance channel.
reaction plan

FIG. 2: Evolution of the neutron density projected onto the reaction plan $z = 0$, for the reaction $^{46}\text{Ca}^{+40}\text{Ca}$ at impact parameter $b = 0$ fm and center of mass energy $E_{\text{c.m.}} = 49$ MeV. At initial time (top), $t = 20 \times 10^{-22}$ s (middle) and $t = 37 \times 10^{-22}$ s (bottom). The neck position is indicated by the dashed vertical line.

As an illustration, the neutron density profiles of the reaction $^{40}\text{Ca}^{+40}\text{Ca}$ are shown at different stages of the reaction in Fig. 2. During the reaction, the two nuclei approach from each other, stick together during a certain time and then re-separate. During the contact time that strongly depends on the initial center of mass energy, they eventually exchange particles.

D. Particle transfer probability in normal systems

In practice, the system can be cut into two pieces at the neck position to calculate the expectation value of the number of exchanged nucleons from one-side to the other. By convention, we will denote by $B$ the subspace where the lightest nucleus is initially (right side of the neck position in Fig. 2) and $\bar{B}$ the rest of the total space. In a mean-field approach, the simplest way to obtain the number of exchanged particles is to estimate the operator $\hat{N}_B$ defined through [32]:

$$\hat{N}_B = \sum_\sigma \int dr \Psi_\sigma^\dagger(r) \Psi_\sigma(r) \Theta(r)$$

(15)

with the time-dependent wave-function [32]. Here $\Theta(r)$ is zero on the left side of the neck and 1 elsewhere.

An illustration of the mean number of transferred particle, denoted by $N_{tr} = \langle \hat{N}_B \rangle - 20$, from $^{46}\text{Ca}$ to $^{40}\text{Ca}$ at center of mass energy $E_{\text{c.m.}} = 49$ MeV is shown in Fig. 3 (solid line). As discussed in ref. [38], a deeper understanding of the transfer process can be achieved by introducing projection onto good particle numbers in the sub-space $B$ (or equivalently $\bar{B}$). The projection operator on a given number of particles $N$ inside the subspace $B$ can be written as (see [38]):

$$\hat{P}_B(N) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i\varphi (\hat{N}_B - N)},$$

(16)

where $\varphi$ is the standard gauge angle. Then the probability to find $N$ particles in the subspace $B$ is:

$$P_B(N) = \langle \Psi(t) | \hat{P}_B(N) | \Psi(t) \rangle$$

$$= \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-i\varphi N} \langle \Psi(t) | \Psi_B(\varphi, t) \rangle$$

(17)

where $|\Psi_B(\varphi, t)\rangle = e^{i\varphi \hat{N}_B} |\Psi(t)\rangle$ is a new quasi-particle vacuum obtained from the original one by making a rotation $\varphi$ in the gauge space from the original state.

The probabilities extracted by projection are linked to the mean number of particles through the sum rule:

$$\langle \hat{N}_B \rangle = \sum_N NP_B(N).$$

(18)

FIG. 3: Evolution of the mean number of particles transferred from $^{46}\text{Ca}$ to $^{40}\text{Ca}$ as a function of time during the reaction illustrated in Fig. 2. The probability $P_{1n}$ (dashed line) and $P_{2n}$ (dotted line) to exchange 1 and 2 particles obtained by making projection on the side $B$ are also presented as well as the quantity $P_{1n} + 2P_{2n}$ (open circles). Top: mean-number of particles and probabilities obtained without projecting on good particle number in the total space. Bottom: same with an additional projection on neutron number $N = 46$ in the total space.
$P_{1p}, P_{2p}, \ldots, P_{xp}$). In the present reaction, these probabilities are defined through $P_{zn} = P_B(20+x)$ while the above sum rule reads $N_{tr} = \sum x \times P_{zn}$.

In the present work, probabilities have been evaluated using the Pfaffian technique of ref. [40] and explicit formulas for the wave-packet are given in appendix A. An illustration of $P_{1n}$ and $P_{2n}$ probabilities obtained using the projection method is shown in top panel of Fig. 4 for the $^{46}$Ca. As already noted in ref. [38], the $1n$ and $2n$ channels are often dominating over other multi-nucleon transfer channels leading to $N_{tr} \simeq P_{1n} + 2P_{2n}$, that is perfectly fulfilled in Fig. 4 after the two nuclei re-separate.

E. Particle transfer probability in superfluid systems

Strictly speaking, the above method to extract transfer probabilities is only valid for normal systems, i.e. when the wave-function \[1\] identifies with a Slater determinant that is an eigenstate of particle number. For nuclei that present pairing, the initial wave-function explicitly breaks the particle number symmetry and the BCS states is obtained by imposing the particle number only in average. This is for instance the case for the $^{46}$Ca discussed above. Said differently, the ground state that is used for $^{46}$Ca not only presents a component with $N = 26$ neutrons but also with surrounding number of neutrons. These components lead to spurious contributions in the probabilities extracted in previous section. A possible way to remove this contamination is to first select the relevant component with $N_0 = 20 + 26$ particles in the full space and then consider the projection onto different particle numbers in the sub-space $B$. In the following, we denote by $\hat{P}(N_0)$ the projector on $N_0$ particles in the full space:

$$\hat{P}(N_0) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i\varphi(N-N_0)},$$

(19)

where $\hat{N}$ is now the complete particle number operator. More generally, to estimate the possible effect of contribution from components $N \neq N_0$, one can compute the probability $P(N)$ that the initial state belongs to the Hilbert space of $N$ particles. This probability is defined through:

$$P(N) = \langle \Psi(t_0) | \hat{P}(N) | \Psi(t_0) \rangle$$

(20)

and is shown in Fig. 4 (top panel). Since $^{40}$Ca has a well defined number of particles, by convention, $N$ in the x axis of Fig. 4 is taken here as the number of particles of its collision partner. Only even components are non-zero due to the specific form of the state (Eq. 13). While the distribution is properly centered around the imposed mean number of particles, non negligible contributions coexist, especially for $N = N_0 \pm 2$ in the initial state.

To remove possible influence of these spurious components, it is possible to define at all time a state with good number of neutrons

$$|N_0(t)\rangle \equiv \frac{1}{\sqrt{\langle \Psi(t) | \hat{P}(N_0) | \Psi(t) \rangle}} \hat{P}(N_0) | \Psi(t) \rangle.$$  

(21)

Then, the mean number of transferred particle as well as probabilities $P_{zn}$ can be computed using the same technique as in section II D. Note that since $^{46}$Ca has a good particle number, $N$ is defined here as the number of particles in the wave-function describing the $^{46}$Ca and is centered around $N = 26$.

FIG. 4: Illustration of the distribution of probabilities to have $N$ particles initially for the $^{40}$Ca + $^{46}$Ca reaction in the TDHF+BCS case (top) and TDHF with initial filling approximation (bottom). Note that since $^{46}$Ca has a good particle number, $N$ is defined here as the number of particles in the wave-function describing the $^{46}$Ca and is centered around $N = 26$.

A second difficulty arises, that could already be seen in Fig. 8 when pairing is non-zero. While $N_{tr}$ after collisions converges to a well defined asymptotic value, small oscillations of $P_{1n}$ and $P_{2n}$ are only slightly affected by the removal of spurious components. This is a quite general feature we observed in applications presented in the article. However, the difference between $P_{2n}$ with and without projection can be as large as several orders of magnitude. This conclusion also holds for a larger number of particles transferred.
two-body continuity equation. This difficulty is not specific to the TDHF+BCS theory but is also present in TDHFB. Indeed, we have checked in the 1D model developed in ref. [28], adapted to treat transfer, that similar oscillations occur even if the full TDHFB is solved. In the following, results obtained for nuclei with non-vanishing pairing will be presented with error-bars with height equal to oscillation amplitudes. In most cases displayed below, error-bars will be too small to be seen.

F. Sensitivity to the pairing residual interaction

Three different pairing interactions, presented in section IIIA have been used to initialize the collision partners. These interactions lead to different spatial properties of the pairing field but have been adjusted to reproduce the experimental gaps (see Fig. 1). In figure 5 asymptotic values of one- and two-nucleon transfer probabilities are reported as a function of center of mass energy for the $^{40}\text{Ca} + ^{48}\text{Ca}$ for the three pairing interactions below the Fusion barrier. As seen in the figure, the extracted transfer probabilities are insensitive to the type of interaction used. It turns out, that whatever is the form of the pairing effective zero-range vertex, if the interaction is carefully adjusted to reproduce the same experimental gap (Fig. 1), the final transfer rate is also the same. Note that the present finding is not in contradiction with ref. [22] where different types of interactions (mixed and surface) were shown to give different two-particle transfer from ground state to ground state. The two forces used in ref. [22] have been adjusted to reproduce the same two neutrons separation energies but lead to different pairing gap. In the present work, we do not see any evidence of a dependence of the pair transfer process on the shape of the pairing force that is used.

Since all types of force lead to the same probabilities, below only results of one of the interaction (mixed) are shown.

G. The no-pairing limit

Here, we are interested in the enhancement of pair transfer probabilities as the pairing is introduced in the transport theory. To quantify this enhancement, it is necessary to also perform calculation without pairing interaction, i.e. TDHF. An additional difficulty arises in the comparison between systems with and without pairing. Quite often, especially when a given j-shell is partially occupied, nuclei initialized with EV8 in the Hartree-Fock limit are deformed. The introduction of pairing stabilizes the spherical shape. Therefore, a direct comparison of the case with and without pairing not only probes the effect of pairing but also the effect of deformation that is (i) not correct for calcium isotopes (ii) not the objective of the present work.

To avoid, possible effects of deformation, we used the filling approximation for the last occupied shell, i.e. we assume that the last shell has partial occupations $n_k$ such that all angular momentum projections $m$ are occupied in the same way. This insures the convergence of the mean-field theory towards non-deformed systems. This approach implies that the initial system is not anymore described by a wave-packet like in Eq. (9), that would identify with a Slater determinant in the usual TDHF, but by a many-body density matrix of the form:

$$\hat{D}(t) = \frac{1}{Z} \exp(-\sum_k \lambda_k a_k^\dagger(t) a_k(t))$$

(22)

where $Z = \text{Tr}(\exp(-\sum_k \lambda_k a_k^\dagger(t) a_k(t)))$. The trace here is taken on the complete Fock space while $a_k^\dagger(t)$ corresponds to creation operator of the canonical states $\varphi_k(t)$. In the filling approximation, the density operator corresponds to a statistical density and the information on the system reduces to the knowledge of the one-body density matrix $\rho = \sum_k |\varphi_k(t)| n_k (\varphi_k(t))$ where the occupation numbers are related to the coefficients through $n_k = 1/(1 + e^{\lambda_k})$. The evolution of $\hat{D}(t)$ is performed by generalizing the TDHF approach where the single-particle states evolve according to the standard self-consistent equation of motion (Eq. (8)) while the occupation numbers are kept fixed in time. As far as we know, this is the only way to avoid possible mixing of deformation and pairing effects and this procedure will be taken below as the no-pairing reference.

Similarly to the pairing case, for non doubly magic nuclei, the density $\hat{D}(t)$ mixes systems with different particle numbers and similar treatment based on double projections is necessary to extract transfer probabilities. In appendix A some helpful formulas to perform projection
on statistical densities of the form (Eq. 22) are given. An illustration of the decomposition of the initial state with a mean neutron number \( \langle N \rangle = 26 \) corresponding to the \( ^{46}\text{Ca} \) is given in bottom panel of Fig. 4. This figure illustrates that the width of the distribution is comparable to the BCS case (top panel) with the difference that odd components are also present in the filling approximation. Probabilities obtained with the filling approximation will be labelled by \( P_{xn}(\text{MF}) \) while those with pairing will be labelled by \( P_{xn}(\text{BCS}) \).

As a first illustration of the enhancement of pair transfer probabilities when pairing is introduced, we have extracted systematically the ratios between probabilities with and without pairing as the pairing interaction strength \( V_{nn}^{\text{pair}} \) is varied in the mixed interaction for the reaction \( ^{46}\text{Ca}+^{46}\text{Ca} \) at \( E_{c.m.} = 43.7 \text{ MeV} \). These ratios are shown in Fig. 4 as a function of \( V_{nn}^{\text{pair}} \). When pairing is accounted for, the two nucleons probabilities have been computed using either non-zero components of the anomalous density (open triangles) or neglecting them (open squares). While the former case corresponds to the appropriate treatment of pairing effects, the latter case can be regarded as a reference calculation where only the sequential transfer of the two neutrons is treated while taking properly the occupation number dispersion of single-particle states around the Fermi energy. The increase is interpreted as the contribution from direct simultaneous processes.

### III. RESULTS AND DISCUSSION

In the present work, we have systematically investigated the effect of initial pairing correlations on the single- and multi-nucleon transfer by comparing the TDHF+BCS with frozen correlations to the mean-field dynamics with the filling approximation for collision between \( ^{40}\text{Ca} \) and different calcium isotopes below the Fusion barrier. In Table II the fusion threshold energy \( B_0 \) deduced from the mean-field transport theories using the technique described in ref. 11 are systematically reported for the different reactions considered here. When available, experimental fusion barrier are also shown. It is clear from the table, that the introduction of pairing has a very weak influence on the barrier height.

| system       | \( B_0 \) (Exp.) | \( B_0 \) (Filling) | \( B_0 \) (BCS) |
|--------------|------------------|--------------------|-----------------|
| \( ^{40}\text{Ca}+^{40}\text{Ca} \) | 53.6             | 53.090             | 53.090          |
| \( ^{40}\text{Ca}+^{42}\text{Ca} \) | 52.735           | 52.735             | 52.735          |
| \( ^{40}\text{Ca}+^{44}\text{Ca} \) | 51.8             | 52.343             | 52.332          |
| \( ^{40}\text{Ca}+^{46}\text{Ca} \) | 52.069           | 52.049             | 52.049          |
| \( ^{40}\text{Ca}+^{48}\text{Ca} \) | 51.8             | 51.935             | 51.935          |
| \( ^{40}\text{Ca}+^{50}\text{Ca} \) | 51.200           | 51.247             | 51.247          |

**TABLE II:** Fusion barrier \( B_0 \) (in MeV) for the reaction \( ^{40}\text{Ca}+^{42}\text{Ca} \). Experimental barrier are taken from the systematic [12], theoretical barrier are computed with a precision of 0.005 MeV.

### A. Systematic study of two-particle transfer versus one-particle transfer

In Figure 4 one- and two-particle transfer probabilities obtained for the collision between calcium isotopes are displayed as a function of center of mass energy for the TDHF+BCS case and no-pairing case. In all cases, when one of the collision partner presents pairing, the two-particle transfer probabilities are significantly enhanced. Conjointly, the one-particle transfer is also increased but to a less extend. This implies that the mean number of particles exchanged is also influenced by the pairing correlations due to the sum-rule (Eq. 18). Comparing the TDHF results where the effect of \( \kappa \) is included (direct+sequential process) to the case where it is neglected (sequential only), several conclusions can be drawn. First, the one-particle probability is almost unchanged. Therefore, the enhancement in \( P_{1n} \) observed in BCS theory compared to the pure mean-field case is a direct consequence of the specific fragmentation of occupation numbers due to pairing that reduces Pauli blocking effect during the transfer process and is unaffected by
the simultaneous component. A second important conclusion is that the main source of enhancement observed in \( \langle P \rangle \) is coming from the initial two-body correlations themselves that lead to direct process during the collision. This confirms the observation made in Fig. 7.

### B. Correlations between two-particle transfer and pairing gap

To further quantify the influence of pairing correlations on the enhancement of two-particle transfer and possible dependence with center of mass energy, the ratio \( \frac{\langle P \rangle_{BCS}}{\langle P \rangle_{MF}} \) is displayed as a function of the mass of the heaviest nucleus participating to the collision and for two different fixed center of mass energies below the Coulomb barrier reported in table II. Open triangles and open squares correspond to 4 MeV and 6 MeV below the Coulomb barrier respectively.

**C. Relationship between \( P_{2n} \) and \( P_{1n}^2 \)**

Experimentally, the no-pairing limit that would be a reference for a given reaction, cannot be measured. It is therefore important to compare quantities that could be measured simultaneously. Usually, the two-particle transfer \( P_{2n} \) is compared to \( \langle P_{1n} \rangle^2 \), where the latter quantity is considered as the probability for a completely sequential transfer \[ 7, 8, 44 \]. Such a comparison has the advantage that both quantities contain all possible effects that might influence the transfer of particles as well as possible pollution from coming from experimental set-ups. In figure 11 this ratio is presented for different theories considered here. This figure gives interesting insight in the two-particle transfer. First, both mean-field and TDHF+BCS where only the fragmentation of single-particle state is accounted for while \( C_{12} = 0 \), lead to almost identical ratios. This aspect was not clear from Fig. 7 where different fragmentations obtained with the filling approximation and from BCS with \( C_{12} = 0 \) lead to differences for both \( P_{1n} \) and \( P_{2n} \). The mean-field theory or equivalently the BCS where initial correlations are neglected could be considered as a way to mimic independent transfer of the two-particles.

It turns out that simple combinatorial arguments can be used to understand analytically the sequential limit. Let us denote by \( p \) the average probability to transfer one particle from the \( ^{40}\text{Ca} \) to \( ^{40}\text{Ca} \). Here ”average” means that we disregard the fact the the probability depends on the initial and final single-particle states. It turns out that the total probability to transfer \( 1, 2, ..., k \) nucleons
where the last approximation holds if \( p \ll 1 \).

This simple approximation turns out to work very well in the mean-field case (or equivalently in the pairing case when \( \kappa \) is neglected). In figure 10 the quantity \( P_{2n}/(P_{1n})^2 \) is compared to the left side of Eq. (24) for the different reactions considered here. We see that for a wide range of center of mass energy, mean-field results perfectly matches the relation (25). The fact that such a simple description is adequate in mean-field theory is not trivial. Indeed, in this theory, nucleons are quantal objects interacting first with two cores (the emitter and the receiver nucleus) that are not fully inert and second with each other through the self-consistent mean-field. Last, the two transferred nuclei are fermions and are subject to the Pauli exclusion principle. This induces automatically correlations during the transfer. If a particle is already transferred to a certain single-particle level, this automatically forbid the other particles to be transferred to the same level. The latter effect is automatically included in the present theory and partially described through the factor \( \Omega_{kn} \) in Eq. (24).

![FIG. 9: Ratio \( P_{2n}/(P_{1n})^2 \) as a function of beam energies. The different panel correspond to different reactions: (a) \( ^{40}\text{Ca}+^{42}\text{Ca} \), (b) \( ^{40}\text{Ca}+^{44}\text{Ca} \), (c) \( ^{40}\text{Ca}+^{46}\text{Ca} \) and (d) \( ^{40}\text{Ca}+^{48}\text{Ca} \). The TDHF+BCS results obtained by neglecting (crosses) or not (open circles) the anomalous density contribution are systematically compared with the mean-field case (open triangles).](image)

![FIG. 10: Ratio \( P_{2n}/(P_{1n})^2 \) as a function of center of mass energy for the reaction \( ^{42}\text{Ca}+^{40}\text{Ca} \) (open circles), \( ^{44}\text{Ca}+^{40}\text{Ca} \) (open triangles), \( ^{48}\text{Ca}+^{40}\text{Ca} \) (cross) and \( ^{48}\text{Ca}+^{44}\text{Ca} \) (open squares). The horizontal lines correspond in each case to the value of left side of Eq. (24) where \( N_f = 8 \) while \( N_v = x \) for \( ^{42}\text{Ca}+^{40}\text{Ca} \) reactions.](image)
ations of two-body observables. However, pairing alone does not contain all physical effects to treat this problem. This is clearly illustrated close to magicity where pairing vanishes. In that case, TDHF dynamics is known to fail to reproduce transfer cross section. Recently, a stochastic mean-field approach was shown to properly describe quantal collective fluctuations especially in magic nuclei [15, 48] and leads to realistic description of the nucleon exchange process. It would be interesting, in the near future to explore the possibility to combine stochastic methods with the present BCS approach.

IV. CONCLUSION

The TDHF+BCS theory with frozen correlations is used here to investigate the effect of pairing on one- and two-nucleon transfer below the Coulomb barrier. A method based on projection onto particle number is developed to properly extract transfer probabilities from theories that break the U(1) symmetry. In addition, a particular attention is paid to compare with a no-pairing technique, the enhancement of two-particle transfer due to pairing correlations is studied qualitatively and quantitatively for reactions involving different calcium isotopes. A developed to properly extract transfer probabilities from theories that break the U(1) symmetry. In addition, a particular attention is paid to compare with a no-pairing technique, the enhancement of two-particle transfer due to pairing correlations is studied qualitatively and quantitatively for reactions involving different calcium isotopes. A

Appendix A: Formulas for projection

In the present appendix, formulas useful for the numerical estimate of particle number projection are given for many-body quasi-particle states and density operators respectively given by Eqs. [3] and [22].

1. Particle number projection of density operators

Starting from the density [22], the probability to have N particles in the subspace B can be written as:

\[ P_B(N) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-i\varphi N} \text{Tr} \left( e^{i\varphi N_B} \hat{D} \right). \]  

(A1)

The estimate of the trace can be made by writing the operator \( \hat{N}_B \) in the canonical basis \( \{ \varphi_i \} \) associated to the density. Using the expression of \( \hat{N}_B \) and the fact that the canonical basis forms a complete basis of the total single-particle space, it could be easily shown that:

\[ P_B(N) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-i\varphi N} \text{Tr} \left( e^{i\varphi \sum_j O^B_{ij} a^j_k a^j_k} \right), \]  

(A2)

where

\[ O^B_{ij} = \sum_{\sigma} \int d\varphi \varphi^*(r, \sigma) \varphi^*_j(r, \sigma) \Theta(r) = \langle i | j \rangle_B. \]  

(A3)

Then, using formula (A.16) of ref. [49] leads to

\[ \text{Tr} \left( e^{i\varphi N_B} \hat{D} \right) = \frac{1}{z} \exp[\text{Tr} \ln(1 + e^{-i\varphi O^B} e^{-M})] \]  

\[ = \frac{1}{z} \text{det}(1 + e^{-i\varphi O^B} e^{-M}) \]  

(A4)

where

\[ (e^{-i\varphi O^B})_{ij} = F_{ij}(\varphi) = \delta_{ij} + \langle i | j \rangle_B (e^{i\varphi} - 1), \]  

(A5)

while from formula (8.11) of ref. [49], we have:

\[ (e^{-M})_{ij} = \delta_{ij} + \frac{n_i}{1 - n_i} \]  

(A6)

and \( z = \prod_i (1 + \frac{n_i}{1 - n_i}) \). Altogether, we obtain:

\[ P_B(N) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-i\varphi N} \text{det}((1 - n_j)\delta_{ij} + F_{ij}(\varphi)n_j). \]

Note that in the case where the statistical density identifies with a Slater determinant (\( n_i = 0, 1 \)), the formula given in ref. [38] is properly recovered. Formulas for the double-projection technique can be derived using a similar technique.

2. Projection with quasi-particle states

To perform projection of quasi-particle vacuum onto good particle number, we used the recently proposed Pfaffian method [40, 50, 51]. Since the Pfaffian technique has been largely discussed recently, here, only specific formulas useful in the present article are given. Again, we first consider the projection on the B subspace as an illustration. We need to perform the overlap between the quasi-particle state [4] and its gauge angle rotated counterpart:

\[ |\Psi\rangle = \prod_{k>0} \left( u_k + v_k a^i_k a^i_k \right) |\rangle. \]  

\[ |\Psi_B(\varphi)\rangle = \prod_{k>0} (u_k + v_k b^i_k(\varphi) b^i_k(\varphi)) |\rangle, \]  

where

\[ b^i_k(\varphi) = \sum_{\sigma} \int d\varphi \varphi^*_i(r, \sigma) \varphi^*_j(r, \sigma) \Psi^i_j(r), \]  

(A7)

\[ = \sum_j F_{ij}(\varphi) a^i_j. \]  

(A8)

The matrix F plays the role of the matrix R in ref. [40] and the overlap between the non-rotated and rotated
state are given by Eq. (5) of this reference. In the present case, we obtain:

$$\langle \Psi_0 | \Psi_B(\varphi) \rangle = \frac{(-1)^n}{\prod_{i=1}^{2n} v_i} \mathrm{pf} \left[ \begin{array}{cc} \mathcal{K} & \mathcal{M}(\varphi) \\ -\mathcal{M}^\dagger(\varphi) & -\mathcal{K}^\dagger \end{array} \right],$$

where $\mathcal{K}$ and $\mathcal{M}$ are matrix of size $2n \times 2n$ where $n$ is the number of single-particle states with $\iota > 0$. These matrices can be decomposed in $2 \times 2$ matrix blocks as:

$$\mathcal{K} = \begin{bmatrix} 0 & [\kappa_{ij} \delta_{ij}] \\ -[\kappa_{ij} \delta_{ij}] & 0 \end{bmatrix},$$

and

$$\mathcal{M}(\varphi) = \begin{bmatrix} [v_i v_j F_{ij}(\varphi)] & [v_i v_j F_{ij}(\varphi)] \\ [v_i v_j F_{ij}(\varphi)] & [v_i v_j F_{ij}(\varphi)] \end{bmatrix},$$

where matrix elements are directly indicated in each $n \times n$ block.

For the double projection, the probability to find $N'$ particles in the space $B$ for a system of $N$ particles in the total space is given by

$$P_B(N, N') = \frac{\langle N | \hat{P}_B(N') | N \rangle}{\langle N | N \rangle} = \frac{\langle \Psi | \hat{P}_B(N') \hat{P}(N) | \Psi \rangle}{\langle \Psi | \hat{P}(N) | \Psi \rangle}.$$ (A9)

Therefore, we need to integrate with respect to two gauge angles.

$$\langle \Psi | \hat{P}_B(N') \hat{P}(N) | \Psi \rangle = \frac{1}{4\pi^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' e^{-i\varphi N - \varphi' N'} \langle \Psi | \Psi_B(\varphi, \varphi') \rangle,$$

where $\langle \Psi | \Psi_B(\varphi, \varphi') \rangle$ can be calculated using formula (A9) except that $F_{ij}(\varphi)$ is now replaced by $F_{ij}(\varphi, \varphi') = e^{i\varphi} f_{ij}(\varphi').$

Numerically, the gauge integral are discretized using the Fomenko method with 20 points. Note that during the time evolution, due to accumulated numerical errors, small violation of orthonormalization between single-particle states can occur, this might lead to large errors in the extracted transfer probabilities. To avoid this problem, a Gram-Schmidt orthonormalization algorithm is used prior to applying the Pfaffian formula.

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