Momentum correlations between two ultra-cold bosons escaping from an open well

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The dynamical properties of a one-dimensional system of two bosons escaping from an open potential well are studied in terms of the momentum distributions of particles. It is shown that the single- and two-particle momentum distributions undergo a specific transition as the interaction strength is tuned through the point where tunneling switches from the pair tunneling to the sequential one. Characteristic features in the momentum spectra can be used to quantitatively determine the participation of specific decay processes. For completeness, the time-dependent Tan’s contact of the system is also examined and its dynamics is found to undergo a similar transition. The results provide a new insight into the dynamics of decaying few-body systems and offer potential interest for experimental research.

I. INTRODUCTION

The quantum tunneling of a particle through a classically impenetrable barrier is one of the oldest problems in quantum mechanics. This problem arises in the analysis of such phenomena as the α-decay of an atomic nucleus [1], proton emission [2, 3], fusion, fission, photodissociation, and photodissociation [4, 5]. While the tunneling of a single particle is well understood [6], and the tunneling of a Bose-Einstein condensate of a large number of particles is well described by a mean-field approximation [7, 8], the escape behavior of interacting few-body systems is a more complicated problem which has not yet been completely understood [9, 10].

Current experimental advancements in the field of ultra-cold physics allow realizing a variety of formerly purely theoretical scenarios in the lab [11]. In particular, it is possible to precisely control the shape of the external confinement [12, 13], the inter-particle interactions [14–16], as well as engineer the initial state of the system [17–19] and mimic low-dimensional physics [20–22]. The recent experiments on the tunneling of a few interacting atoms escaping from an effectively one-dimensional potential well [23–25] provide fresh motivation for the study of such tunneling problems. One suspects that the presence of inter-particle interactions affects the tunneling of few-body systems in interesting and complex ways. Therefore a deeper understanding of this issue could become important also from a theoretical point of view [26, 27].

Although the system of two tunneling particles is the simplest possible case of the few-body tunneling problem, many open questions still remain unanswered, and it continues to be explored in recent research [28, 29]. In [13, 14] the properties of the system were partially studied from the momentum distribution point of view for repulsive interactions. Here we extend this description by also taking the attractive branch of interactions into account. This allows us to examine how the momenta of the system are changed when the interaction strength is tuned across the point of transition between sequential and pair tunneling [30, 31, 32]. Precise relationships can be established that connect the form of the momentum spectra to quantities such as the system energy and the relative participation of the different tunneling processes. In addition, we touch upon the time evolution of the Tan’s contact, a quantity related to the interaction energy between the particles.

The work is organized as follows. In Section II we describe the model system under study. In Section III we describe the decay dynamics of a two-boson system, showing the basic nature of the tunneling dynamics, and the transition between distinct regimes that occurs at a specific value of the interaction strength. In Section IV we discuss the momentum distribution of the decaying system. In Section V we focus on the ways in which the transition between different regimes is reflected in the center-of-mass momentum distribution and the Tan’s contact. Section VII is the conclusion.

II. THE MODEL

We consider a system of two indistinguishable ultra-cold bosons of mass $m$, interacting via a point-like δ potential and confined in an effectively one-dimensional external trap. The many-body Hamiltonian of this system has the form:

$$H = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + V(x_1) + V(x_2) + g\delta(x_1 - x_2),$$

(1)

where $x_i$ represents the position of the $i$-th boson and $V(x)$ is the external potential. The effective inter-particle interaction strength $g$ is related to the three-dimensional s-wave scattering length [33, 34] and its magnitude can be tuned experimentally via the Feshbach resonances [35, 36] or by changing the confinement in perpendicular directions [37].

We assume that at $t < 0$ bosons are confined within a closed asymmetric well potential $V_0(x)$ (dashed line in
where the modified frequency $\Omega \approx \Omega_0/2.26$. Accordingly, the initial many-body state at $t = 0$ is chosen as the ground state of an interacting two-boson system confined inside $V_0(x)$. For given interaction $g$, we find the ground state numerically by propagating a trial many-body wave function in imaginary time. At $t = 0$ the trap is suddenly opened and the external potential is changed to $V(x)$, given by the following expression ($x_0 = \sqrt{\hbar/m\Omega_0}$ is the harmonic oscillator length unit):

$$V(x) = \begin{cases} 
    m\Omega_0 x^2/2, & x < 0 \\
    m\Omega x^2/2, & x > 0,
\end{cases}$$  \hspace{1cm} (2)

The resulting shape of $V(x)$ is that of a potential well separated from open space by a finite barrier (solid line in Fig. 1). The numerical coefficients are chosen to ensure that the function $V(x)$ and its first derivative are continuous everywhere.

The time evolution of the many-body state for $t > 0$ is performed straightforwardly by solving numerically the time-dependent Schrödinger equation in position representation. The boundaries of the simulated region are chosen large enough to ensure that reflections from the boundaries do not affect the main results.

For convenience, in all further discussion we employ harmonic oscillator units, i.e. energy, length, and the interaction are given in $\hbar\Omega_0$, $\sqrt{\hbar/m\Omega_0}$, and $\sqrt{\hbar^2\Omega_0/m}$, respectively.

III. DYNAMICS OF THE ESCAPING BosONS

After the well is suddenly opened at $t = 0$, the bosons start escaping through the barrier into open space. Before we analyze the system from the momentum distribution point of view, let us recall recent results from [40] and shortly discuss the dynamical properties of the system from the point of view of density distributions. It is known that the dynamical properties of the system depend significantly on the strength of inter-particle interactions. As the interaction strength is changed from strong repulsions to strong attractions, the dynamics of the two-boson system undergoes a transition between two distinct scenarios, characterized by the dominance of different decay processes. Below a critical value of interactions (approximately $g = -0.9$ in the case studied), essentially the entire decay is dominated by sequential tunneling, i.e., both bosons leave the well simultaneously as a bound pair. Conversely, for $g$ above the critical value, the decay is dominated by a sequential tunneling, in which the bosons leave the well one by one. In such a regime, pair tunneling plays only a subordinate role.

To illustrate this transition, in Fig. 2 (exactly as in [40]) we show snapshots of the two-particle density profile $\rho(x_1, x_2; t) = |\Psi(x_1, x_2; t)|^2$ for different moments after the opening of the well, and different interaction strengths $g$. For better visibility we indicate the well boundary $x_B \approx 3x_0$ with dashed lines.

In the most trivial scenario of vanishing interactions ($g = 0$) both bosons tunnel entirely independently of each other. After a short time ($t = 40$) a significant amount of the density is present in the region $(x_1-x_B)(x_2-x_B) < 0$ indicating a high probability of exactly one boson being outside the well. For longer times both bosons are likely
to end up outside the well. Due to the absence of interactions, the two-body wave function is simply a product of two identical one-body wave functions during the entire process.

For a repulsive system ($g = 1.0$) the dynamics is also dominated by the sequential tunneling, indicated by the initial accumulation of the probability density in $(x_1 - x_B)(x_2 - x_B) < 0$ region. However, the inter-particle repulsion causes a significant anticorrelation in the boson positions, so that the probability density vanishes close to the $x_1 = x_2$ diagonal. It is clear that simultaneous tunneling of bosons is strongly suppressed in this case.

For strong attractions the scenario is completely different (see example results for $g = -1.0$ in Fig. 2). The sequential tunneling is suppressed and the bosons leave the well only as a composite pair. This can be seen from the density distribution, which during the whole evolution is nonzero only in the regions with $(x_1 - x_B)(x_2 - x_B) > 0$ and remains concentrated around the line $x_1 = x_2$.

IV. MOMENTUM DISTRIBUTIONS

Now let us discuss how the different tunneling regimes are reflected in the particle momenta. For this purpose we study the time evolution of the two- and one-particle momentum distributions defined as

$$
\pi_2(k_1, k_2; t) = \frac{1}{4\pi^2} \left| \int dx_1 dx_2 e^{-i(k_1 x_1 + k_2 x_2)} \Psi(x_1, x_2; t) \right|^2
$$

(4a)

$$
\pi_1(k; t) = \int dk' \pi_2(k, k'; t).
$$

(4b)

From the experimental point of view, measuring momentum distributions is quite feasible, since appropriate techniques have been developed for measuring positions andvelocities of individual untrapped atoms. For the specific problem of bosons escaping from a potential well, a relevant experimental scheme to measure the momenta of the emitted particles has been proposed in [13].

Initially ($t = 0$) both momentum distributions have nearly-Gaussian shapes centered at $k_1 = 0, k_2 = 0$. For larger times, depending on the tunneling mechanism dominating the dynamics, characteristic features in $\pi_2$ and $\pi_1$ emerge in these distributions. On Fig. 3 we show the one-body and two-body momentum distributions for a few different interaction strengths, after the bosons have been allowed to tunnel for some time $t$. To increase understanding of the results, we show these distributions for the same interactions and time moments as in Fig. 2.

In the simplest, non-interacting case ($g = 0$), as the particles tunnel from the well, a narrow peak appears in the distribution $\pi_1$, centered around the value $k_0 \approx 0.89$. It is clear that the two bosons are emitted with a very well-defined momentum. The two-body momentum distribution is a simple product of two identical one-body fixed.
distributions $\pi_2(k_1, k_2; t) = \pi_1(k_1; t)\pi_1(k_2; t)$ and clear horizontal/vertical lines at $k_1 = k_0$ and $k_2 = k_0$ are visible. They indicate that the emitted boson has a narrowly defined momentum, while the trapped boson still has a nearly-Gaussian distribution of momenta.

The momentum dynamics become more complicated for interacting systems. In the case of repulsive interactions ($g = +1.0$, second row in Fig. [3]) the dynamics is dominated by the sequential tunneling of bosons. This behavior is reflected in the one-body momentum distribution $\pi_1(k; t)$ by two distinct peaks. One of them is centered around the non-interacting value $k_0$ while the second one is shifted to larger momenta $k' \approx 1.15$. These two different momenta can be directly associated with momenta of the sequentially emitted bosons. Due to the repulsive interaction energy, the first boson which leaves the well carries this additional energy and in consequence has a higher momentum $k'$. The second boson no longer feels any interaction and therefore it tunnels with the momentum $k_0$. All this means that the momenta of the emitted particles are also causally correlated, i.e., the boson can be emitted with the momentum $k_0$ only if the other has been already emitted with momentum $k'$. This specific time-correlation is directly reflected in the two-particle momentum distribution $\pi_2(k_1, k_2; t)$. It is clearly seen that probability of finding the boson with momentum $k_0$ almost vanishes whenever the remaining boson has momentum different than $k'$. Contrary, probability of finding the boson with momentum $k'$ is associated with almost gaussian distribution of the second boson centered around $k = 0$, i.e., distribution which is characteristic for the trapped boson in the well.

Particular values for the momenta of emitted bosons $k_0$ and $k'$ can be easily found from the relevant system energies. In the case studied ($g = +1.0$) one finds that the initial energy of two confined bosons $E_{INI}(g) \approx 1.07$, while the ground-state energy of a single boson in the well $E_1 \approx 0.4$. These energies correspond to $k' = \sqrt{2(E_{INI}(g) - E_1)} \approx 1.16$ and $k' = \sqrt{2E_1} \approx 0.89$, respectively (vertical dashed lines in the left middle and left upper plot on Fig. [3]). Our numerical results are in full agreement with this phenomenological analysis. Note that this argument also predicts that, for sufficiently strong attractions, when $E_{INI}(g) < E_1$, sequential tunneling is strongly suppressed by the energy conservation.

Finally, let us discuss the momentum distributions in a case of strong attractions ($g = -1.0$, bottom row in Fig. [3]) for which the pair tunneling is the dominating mechanism of the decay. Although the single-particle momentum distribution $\pi_1(k; t)$ is quite broad, a clear correlation between momenta of emitted bosons along the line $k_1 + k_2 = K = \text{const}$ is visible in the two-particle distribution $\pi_2(k_1, k_2; t)$. This indicates that bosons are emitted simultaneously as a bounded pair with a clearly defined center-of-mass momentum $K$ (in this case $K \approx 1.50$), with the particles oscillating around the center-of-mass with opposite relative momenta. Note that in the distribution $\pi_2(k_1, k_2; t)$ also some additional gaussian background centered around $k_1 = k_2 = 0$ is visible. This part of the momentum distribution reflects the momenta of bosons which still remain in the well (see Fig. [3] for the corresponding density distribution of the remaining particles).

It is worth noticing that in the case of strong attractions, where the pair tunneling dominates the dynamics of the system, the wave function can be well approximated as a superposition of two non-overlapping wave functions, $\Psi(x_1, x_2; t) \approx \Psi_{INI}(x_1, x_2; t) + \Psi_{OUT}(x_1, x_2; t)$, where $\Psi_{INI/OUT}$ encodes the state of both bosons being inside/outside the well. Therefore in this case, it is possible to study the momentum distribution of the escaping bosons independently of the state of bosons remaining in the well. This approach corresponds to a simple modification of definitions [1] by limiting the wave function to the $\Psi_{OUT}$ part. This approach is also justified experimentally since it is possible to measure the momenta of the escaping particles solely. With this redefinition, the single-particle distribution is significantly modified since the threshold from confined particles is removed (thin black solid line in the left-bottom plot on Fig. [3]). After this modification a significant enhancement at momentum $K/2$ (half of the center-of-mass momentum) is clearly visible (vertical dashed line in the left bottom plot on Fig. [3]).

The particular value of the center-of-mass momentum $K$ can be predicted with simple phenomenological argumentation. In this case the initial energy of the system $E_{INI}(g)$ is fully converted to the energy of the emitted interacting pair $E_{pair}(g)$. Since the wave function of the emitted pair (for $g < 0$) can be well approximated as [52]

$$\Psi_{pair}(x_1, x_2) \approx \sqrt{\frac{|g|}{2}} e^{-\frac{|g|}{2} |x_1 - x_2|} e^{i\frac{K}{2}(x_1 + x_2)},$$

the corresponding pair energy is $E_{pair}(g) = (K^2 - g^2)/4$. Consequently, $K = (4E_{INI}(g) + g^2)^{1/2}$. In the case studied ($g = -1.0$) one finds $E_{pair}(g) \approx 0.31$ and $K \approx 1.50$, which agrees very well with the momentum distribution obtained with our numerical approach.

To make this analysis more comprehensive one can discuss inter-particle correlations not only in terms of the two-particle momentum distribution but also via the so-called noise correlation [53–57]. This quantity is defined straightforwardly as the difference between the full two-particle distribution and the product of corresponding single-particle distributions:

$$G(k_1, k_2; t) = \pi_2(k_1, k_2; t) - \pi_1(k_1; t)\pi_1(k_2; t).$$

Phenomenologically, the noise correlation can be interpreted as a distribution of the amount of correlations which are forced by inter-particle interactions that cannot be captured by any single-particle description. In Fig. [3], we plot the noise correlation for two different interactions corresponding to the dominance of two different decay channels ($g = \pm 1.0$). It is evident that a single-particle description strongly underestimates probabilities
FIG. 4: The center-of-mass momentum distributions $\pi_{CM}(K; t)$ of the two-boson system for various values of $g$, at a specific moment $t = 120$. For the repulsive ($g = 1.0$) and strongly attractive ($g = -1.0$) systems, only one decay process is available (sequential and pair tunneling, respectively) and it is reflected in the distribution as a single peak. For a system with weaker attractions ($g = -0.5$) both sequential and pair tunnelings are possible, and two peaks appear in the spectrum, each corresponding to a different process. Momenta are in units of $\sqrt{\hbar m} \Omega_0$, interaction strength in units of $\sqrt{\hbar^2} \Omega_0/\hbar$, and time in units of $1/\Omega_0$.

FIG. 5: The relative participation of pair and sequential tunneling in the overall dynamics of the two-boson system, for various interaction strengths $g$. Green and red symbols show the participation of pair tunneling and sequential tunneling, respectively, calculated from the areas of the corresponding peaks in the center-of-mass momentum distribution $\pi_{CM}$ at $t = 180$. For comparison, the corresponding results from Ref. [40] are shown as green dashed and red solid lines, respectively. It can be seen that sequential tunneling dominates in a wide range of interaction strengths, but its participation falls abruptly to zero as $g$ approaches the critical value $g = -0.9$. Interaction strength is given in units of $\sqrt{\hbar^2} \Omega_0/\hbar$.

of finding particles in cases when two-particle momentum distributions display strong correlations (green areas). More importantly, the noise correlation nicely exposes the aforementioned causal correlations between sequentially emitted particles (vertical/horizontal lines localized around $k' \approx 0.89$ for $g = +1.0$).

V. THE TRANSITION

The specific transition between different tunneling channels can be analyzed and well described when the momentum of the center of mass $K = k_1 + k_2$ is considered. Its distribution can be extracted from the two-particle momentum distribution as follows:

$$\pi_{CM}(K; t) = \int dk_1 \pi_1(K - k_1, k_2; t).$$

(7)

On Fig. 4 we display this distribution for three different interactions $g$, after the system has been allowed to evolve for some time $t$. In the case of strong repulsions ($g = +1.0$) as well as strong attractions ($g = -1.0$) a single peak in the center-of-mass momentum emerges. It is centered around the sum of the individual emitted boson momenta $k_0 + k' \approx 2.05$ or the bound pair momentum $K \approx 1.50$, respectively. However, for intermediate interactions $g = -0.5$ both tunneling mechanisms are present, and the distribution $\pi_{CM}(K; t)$ displays two distinct peaks which can be directly associated with one of the tunneling processes. By comparing integrated intensities of both peaks it is possible to determine a relative participation of different tunneling mechanisms in the overall dynamics. In Fig. 5 we show the relative participation of pair tunneling (green crosses) and of sequential tunneling (red triangles) obtained this way for a few example interaction strengths $g$. For comparison, we include similar quantities (red and green lines) obtained recently by a theoretical analysis of different probability fluxes through the potential barrier [40]. A qualitative agreement between both results opens an additional, much less demanding from the experimental point of view, method for detecting the transition between different tunneling mechanisms.

Dynamical properties of the system in the vicinity of the transition are also encoded in the interaction energy between particles $\mathcal{I}(t) = g \int dx |\Psi(x; x; t)|^2$. It is worth noticing that interaction energy is closely related to the Tan’s contact $\mathcal{C}$ [58]

$$\mathcal{C}(t) = \frac{m^2 g^2}{\pi \hbar^4} \frac{\partial \mathcal{E}}{\partial g} = \frac{m^2 g}{\pi \hbar^4} \mathcal{I}(t)$$

(8)

which is known to be a very universal quantity connected with many different features of atomic systems such as the dependency of energy on interaction strength, the pair correlation function, and the relation between pressure and energy density [59, 62]. Furthermore, it is accessible to experimental measurements [63, 64]. Note that,
although the total energy of the system $E$ is conserved, its derivative with respect to $g$ changes during the evolution due to the dynamical changes of the system's wave function.

In Fig. 6 we plot the time evolution of the Tan’s contact (relative to its initial value at $t = 0$) for different interaction strengths. As it is seen, the contact displays exponential decay. Moreover, the decay rate (inset in Fig. 6) strongly depends on the interaction strength and near the transition between sequential and pair tunneling channel at $g \approx -0.9$ it approaches 0.

These results can be explained intuitively when the different decay processes are considered. One suspects that the interaction energy, due to the short-range form of interactions, rapidly decreases when particles are sequentially emitted from the trap. Accordingly, when sequential tunneling dominates the dynamics, the magnitude of the contact is closely tied to the probability that the system remains in the initial trapped state. For systems such as the one under study, this probability obeys an exponential decay law to a very good approximation [65], hence $C(t)/C(0)$ decays exponentially.

The rate of this exponential decay decreases as the interaction energy in the trapped system is lowered [28]. Additionally, as the interactions become more attractive, the system dynamics are increasingly dominated by the process of pair tunneling. During pair tunneling the interaction energy remains almost unchanged throughout the evolution since particles in all stages of the dynamics form a bound pair. Due to the combination of these effects, the decay rate of the contact decreases and eventually almost plateaus at zero as $g$ approaches $-0.9$.

**VI. CONCLUSION**

We have analyzed the decay of a system of two ultracold bosons, initially trapped in an open one-dimensional potential well. In particular, we have examined the influence of the interaction strength $g$ on the dynamics of the momentum distributions of the system, as well as the Tan’s contact. We find that there is an essential difference in the behavior of these quantities when the interaction strength $g$ is tuned across a critical value that corresponds to strong suppression of sequential tunneling. These findings are in full agreement with previous results, based on careful analysis of many-body probability fluxes [40]. We show that it is possible to establish a relationship between the dominant tunneling process and the form of the momentum distributions. In particular, from the center-of-mass momentum distribution of the system one can quantitatively determine the relative participation of the different tunneling processes in the dynamics. Additionally, we examine the evolution of the Tan’s contact and show that its behavior also reflects the dominant tunneling process.

Since the single- and two-particle momentum distributions as well as the Tan’s contact are accessible to experimental measurements, the presented results have potential significance for upcoming experiments with ultracold bosons in quasi-one-dimensional potentials. The theoretical and experimental analysis of these quantities can give increased insight into the system dynamics.

**VII. ACKNOWLEDGMENTS**

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