Few-Boson Dynamics in Double Wells: From Single-Atom to Correlated Pair Tunneling

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We investigate few-boson tunneling in a one-dimensional double well, covering the full crossover from weak interactions to the fermionization limit of strong correlations. Based on exact quantum-dynamical calculations, it is found that the tunneling dynamics of two atoms evolves from Rabi oscillations to correlated pair tunneling as we increase the interaction strength. Near the fermionization limit, fragmented-pair tunneling is observed and analyzed in terms of the population imbalance and two-body correlations. For more atoms, the tunneling dynamics near fermionization is shown to be sensitive to both atom number and initial configuration.

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The double well is a paradigm model for some of the most fundamental quantum effects, like interference or tunneling. Using ultracold atoms, it has become possible to study this system at an unprecedented level of control. This has led, e.g., to the observation of Josephson oscillations [1–3] and nonlinear self-trapping [1,4,5] of Bose-Einstein condensates. In the first case, the weakly interacting atoms—prepared mostly in one well—simply tunnel back and forth between the two wells in analogy to a Josephson current. However, above a critical interaction strength, the atoms essentially remain trapped in that well for the experimental lifetime even though they repel each other. On the few-body level, this resembles the situation of repulsive atom pairs, whose stability [6] and dynamics [7] have recently been observed.

All of these effects are confined to the regime of relatively weak interactions, where the dynamics can be understood qualitatively (up to phases) by means of a single parameter: the number of atoms in one well. However, interactions in ultracold atoms can be adjusted experimentally over a wide range, e.g., via Feshbach resonances [8]. In particular, in one dimension (1D) one can tune the effective interaction strength at will by exploiting a confinement-induced resonance [9], which makes it possible to explore the limit of strong correlations. If the bosons repel each other infinitely strongly, they can be mapped to noninteracting fermions [10] in the sense that the exclusion principle mimics the *hard-core* interaction. While local properties like the densities are shared with their fermionic counterparts, nonlocal aspects such as their momentum distribution are very different. Sparked also by its experimental demonstration [11,12], this *fermionization* has attracted broad interest (see [13,14] and references therein).

In this Letter, we investigate the case where a few atoms are loaded into the same well and explore the tunneling dynamics as we vary the interaction strength from zero up to the fermionization limit. For two atoms, we show that the character of the tunneling changes from Rabi oscillations to correlated pair tunneling. Near fermionization, the strongly interacting atoms tunnel back and forth as a fragmented pair. For three or more atoms, the tunneling dynamics turns out to depend strongly on the atom number and the initial imbalance.

Model and computational method.—The double-well dynamics is described by the many-body Hamiltonian $H = \sum_{i=1}^{N}[\frac{1}{2}p_i^2 + U(x_i)] + g\sum_{i<j}\delta_\sigma(x_i - x_j)$. Here the double well $U(x) = \frac{1}{2}x^2 + h\delta_w(x)$ is modeled as a superposition of a harmonic oscillator and a central barrier shaped as a Gaussian $\delta_w(x) = e^{-x^2/2w^2}/\sqrt{2\pi}w$ (we choose $w = 0.5$ and $h = 8$, where harmonic-oscillator units are employed throughout). The effective interaction resembles a 1D contact potential [9], but is mollified with a Gaussian $\delta_{\sigma=0.05}$ so as to alleviate the well-known numerical difficulties of the δ function. We focus on repulsive forces $g \in [0, \infty)$.

Our goal is to investigate the few-atom quantum dynamics in the crossover to the highly correlated fermionization limit $g \to \infty$ in a numerically *exact* fashion. This is a challenging task, and most studies on the double-well dynamics so far have relied on two-mode models [2,15] valid for sufficiently weak coupling. Our approach rests on the multiconfiguration time-dependent Hartree method [16], a wave-packet dynamics tool which has been applied successfully to few-boson systems (see [14] for details).

From uncorrelated to pair tunneling.—To prepare the initial state $\Psi(0)$ with a population imbalance—in our case, such that almost all atoms reside in the right-hand well—we make that side energetically favorable by adding a linear external potential $-d \cdot x$ $(d > 0)$ and let the system relax to its ground state $\Psi_0^{(d>0)}$. For sufficiently large d, this amounts to preparing nearly all atoms in one well. To study their time evolution in the *symmetric* double well, in our simulations the asymmetry will be ramped down, $d \to 0$, within some time $\tau > 0$.

Let us now study how the tunneling changes as we pass from uncorrelated tunneling $(g = 0)$ to tunneling in the presence of correlations and finally to the fermionization limit $(g \to \infty)$. It is natural to first look at the conceptually clearest situation where $N = 2$ atoms initially reside in the

right-hand well. Absent any interactions, the atoms simply *Rabi* oscillate back and forth between both wells, which materializes in the percentage of atoms in the right well $p_R(t) = \langle \Theta(x) \rangle_{\Psi(t)} = \int_0^\infty \rho(x;t)dx$ (ρ being the one-body density) or, correspondingly, the population imbalance $\delta = p_R - p_L = 2p_R - 1$. By contrast, if the atoms repel each other, then the tunneling process will be modified, as can be seen in Fig. 1(a). For $g = 0.2$, one sees that the tunneling oscillations have become a two-mode process: There is a fast (small-amplitude) oscillation which modulates a much slower oscillation in which the atoms eventually tunnel completely ($p_R \approx 0$). In case g is increased further, we have found that the tunnel period becomes indeed so long that complete tunneling is hard to observe. For example, at $g = 1.3$ the period is as large as 2×10^3. What remains is a very fast oscillation with only a minute amplitude—the two-body analog of quantum self-trapping. As we go over to much stronger couplings (see $g = 4.7$), we find that the time evolution becomes more and more complex, even though this is barely captured in the reduced quantity p_R [Fig. 1(a)]. What is striking, though, is that near the fermionization limit (see $g = 25$) again a simple picture emerges: A fast, larger-amplitude motion is superimposed on a slightly slower tunneling oscillation whose period roughly equals that of the Rabi oscillations.

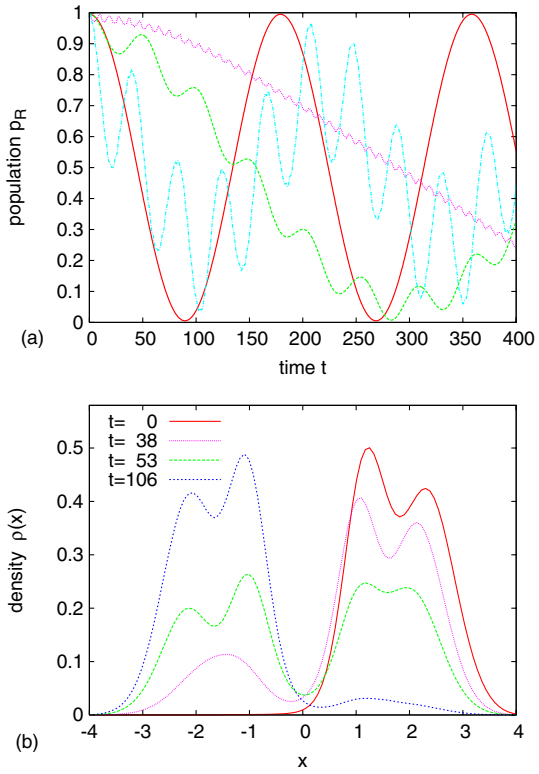

FIG. 1 (color online). Two-atom dynamics. (a) Relative population of the right-hand well over time, $p_R(t)$, for different interaction strengths $g = 0$ (solid line), $g = 0.2$ (dashed line), $g = 4.7$ (dotted line), and $g = 25$ (dash-dotted line). (b) Snapshots of the one-body density $\rho(x)$ for different times t in the fermionized case $g = 25$. (All quantities are in harmonic-oscillator units throughout; see the text.)

To get an understanding of the oscillations, Fig. 2 explores the evolution of the two-body spectrum $\{E_m(g)\}$ as g is varied. In the noninteracting case, the low-lying spectrum is given by distributing the N atoms over the lowest antisymmetric or symmetric orbital of the trap. This yields the $N + 1$ energies $\{E_m = E_0 + m\Delta^{(0)}\}_{m=0}^N$, where $\Delta^{(0)} = \epsilon_1 - \epsilon_0$ is the energy gap between these two orbitals, or the splitting of the lowest *band*. Assuming that for sufficiently small g still only $N + 1 = 3$ levels are populated, then the imbalance $\delta(t)$ (and likewise p_R) can be computed to be [17]

$$\delta(t) = \delta_{01} \cos(\omega_{01} t) + \delta_{12} \cos(\omega_{12} t), \qquad (1)$$

where $\omega_{mn} = E_m - E_n$ and $\delta_{mn} = 4\langle \Psi_m | \Theta(x) | \Psi_n \rangle c_m c_n$ are determined by the participating many-body eigenstates and their weight coefficients c_m. At $g = 0$, due to the levels' equidistance, only a single mode with Rabi frequency $\omega_{01} = \omega_{12} = \Delta^{(0)}$ contributes. However, as the interaction is "switched on," the two upper lines $E_{1,2}$ virtually glue to one another to form a doublet, whereas the gap to E_0 increases (Fig. 2 inset). For times $t \ll T_{12} \equiv 2\pi/\omega_{12}$, we see only an oscillation with period $T_{01} \ll T_{12}$, offset by δ_{12}, which on a longer time scale modulates the slower oscillation determined by ω_{12}. For small initial imbalances, $|c_0/c_2| = |\delta_{01}/\delta_{12}| \gg 1$, so for short times we observe the few-body analog of Josephson tunneling. In our case of an almost complete imbalance, in turn, $|\delta_{12}|$ dominates, which ultimately corresponds to *self-trapping*, viz., extremely long tunneling times. These considerations convey a simple yet essentially exact picture for the two-body counterpart of the crossover from Rabi oscillations to self-trapping beyond the bare two-mode approach common for condensates [2].

It is obvious that the two-frequency description above breaks down as the gap to higher-lying states melts, as for $g = 4.7$. Concordantly, the dynamics becomes more com-

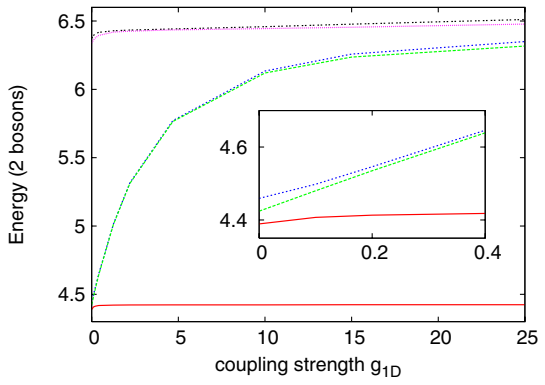

FIG. 2 (color online). Low-lying spectrum of two bosons in a double well as a function of the interaction strength g. Inset: Doublet formation with increasing g.

plicated. However, in the fermionization limit (exemplified for $g = 25$), the system becomes integrable again by mapping it to noninteracting fermions [10]. As an idealization, assume that at $t = 0$ we put two (auxiliary) fermions in the ground state of the *right* well, where they would occupy the lowest two orbitals. Expressing this through the fermionic eigenstates $|\boldsymbol{n}\rangle_-$ of the full system leads to [17] $\Psi(t = 0) = \frac{1}{2}\sum_{a,b\in\{0,1\}}|1_a^{(0)}, 1_b^{(1)}\rangle_-$, where $1_a^{(\beta)}$ denotes occupation of the symmetric ($a = 0$) or antisymmetric ($a = 1$) orbital in band β. Analyzing the corresponding energies, one finds that the frequencies contributing to the imbalance dynamics are exactly $\Delta^{(0)}$ (the lowest-band Rabi frequency, corresponding to the longer tunneling period) and $\Delta^{(1)}$ (the splitting of the upper band). This intriguing result states that only *two* modes determine the imbalance dynamics, so that the strongly repulsive atoms coherently tunnel back and forth almost like a single particle. As an illustration, snapshots of the density at different t are displayed in Fig. 1(b). This demonstrates the tunneling of a *fragmented* pair.

In order to unveil the physical content behind the tunneling dynamics, let us now investigate the two-body correlations. Noninteracting bosons simply tunnel independently, which is reflected in the two-body density (or correlation function) $\rho_2(x_1, x_2)$. As a consequence, if both atoms start out in one well, then in the equilibrium point of the oscillation it will be as likely to find both atoms in the same well as in opposite ones. This is illustrated in Fig. 3, which exposes ρ_2 at the equilibrium points and visualizes the temporal evolution of the *pair* (or *same-site*) *probability* $p_2 = \int_{\{x_1x_2\geq 0\}}\rho_2(x_1, x_2)dx_1dx_2$. As we introduce small correlations, the pair probability does not drop to 0.5 anymore—at $g = 0.2$ it notably oscillates about a value near 100%. This is apparent from the equilibrium-point snapshot of ρ_2: Both atoms remain essentially in the same well in the course of tunneling. In other words, they tunnel *as pairs*. On top of this, Fig. 3 in hindsight also lays bare the nature of the fast (small-amplitude) modulations of $p_R(t)$ encountered in Fig. 1(a) by linking them to temporary reductions of the pair number p_2. Thus it is fair to interpret them as attempted one-body tunneling. As before, the time evolution becomes more involved as the interaction energy is raised to the fermionization limit (cf. $g = 25$). The two-body correlation pattern is fully fragmented not only when the pair is captured in one well (corresponding, e.g., to the upper right corner $x_1, x_2 \geq 0$), but also when passing through the equilibrium point $t = 53$. Similarly, the evolution of $p_2(t)$ is governed by two modes, $\Delta^{(0)} \pm \Delta^{(1)}$, and over time p_2 passes through just about any value from 1 (fragmented pair) to almost zero (complete isolation).

Many-body effects.—Although we have focused so far on the case of $N = 2$ atoms, the question of higher atom numbers is interesting from two perspectives. For one thing, it is fascinating because for $g \gg 1$ many results become explicitly N dependent, including distinctions between even or odd atom numbers [14]. (The experimental preparation of definite $N = 3, 4, \ldots$ is feasible, if harder to achieve due to losses. In fact, the experimental setup in [12] requires only an additional central barrier created by a Gaussian light sheet.) On the other hand, in a setup consisting of a whole *array* of 1D traps as in [11,12], number fluctuations may automatically admix states with $N > 2$.

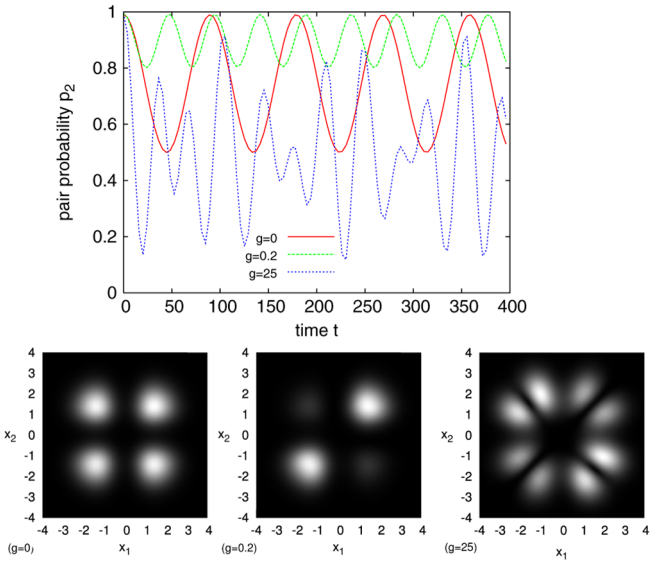

FIG. 3 (color online). Top: Probability $p_2(t)$ of finding two atoms in the same well for $g = 0, 0.2$, and 25. Bottom: Snapshots of the two-body correlation function $\rho_2(x_1, x_2)$ at equilibrium points, $\delta(t) = 0$, for $g = 0$ ($t = 44$), $g = 0.2$ ($t = 128$), and $g = 25$ ($t = 53$)—from left to right.

For $N \geq 3$, the weak-interaction behavior does not differ conceptually. In fact, Eq. (1) carries over but with the sum now running over $m < n \leq N$. While the dynamics is no longer determined by strictly two frequencies, the separation of time scales (related to the formation of doublets in the spectrum) persists—ultimately, this should connect to the condensate dynamics valid for $N \gg 1$. Things become more intricate if we leave the two-mode regime, though. In particular, the fermionization limit reveals a clear N dependence (Fig. 4). Generally, an idealized state with N fermions initially in one well has contributions from all excitations $|1_{a_0}^{(0)}, \ldots, 1_{a_{N-1}}^{(N-1)}\rangle_-$ ($a_\beta = 0, 1\ \forall\ \beta$) in the N lowest bands. Hence all tunnel splittings $\Delta^{(\beta)}$ for each band are expected to be present [17]. Figure 4(a) conveys an impression of the complexity of the dynamics by exhibiting $p_R(t)$ for $N = 3, 4$. This somewhat erratic pattern may wash out the clear signature of the two-atom case upon averaging over an array. In an experiment, it is therefore desirable to reduce number fluctuations, e.g., by having sufficiently high barriers in between different copies of the double well.

In the context of many-body effects, it is interesting to consider what happens if *not* all $N \geq 3$ atoms are prepared in one well, but rather, say, $N - 1$ in one well and one in

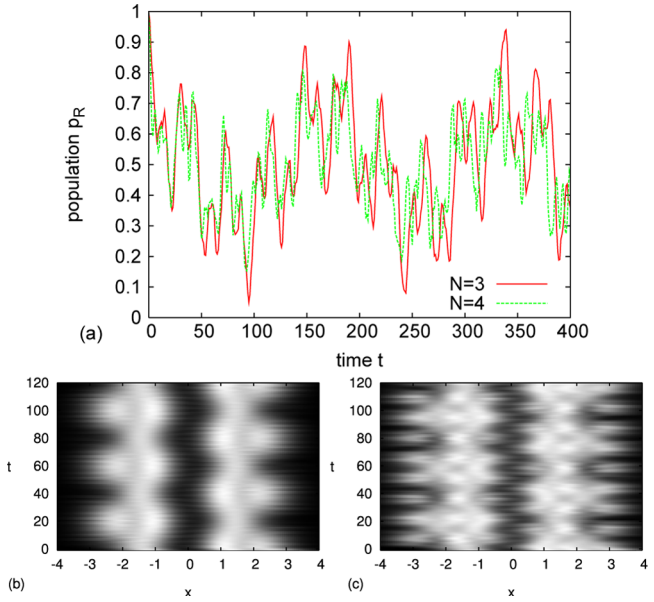

FIG. 4 (color online). Many-body effects in the fermionization limit ($g = 25$). (a) Population of the right-hand well, $p_R(t)$, for $N = 3, 4$ atoms initially in one well. Bottom: Density evolution $\rho(x;t)$ for $N-1=2$ atoms (b) and $N-1=3$ atoms (c) initially in the right-hand well if exactly one atom is present on the left.

the other. Paraphrased in the case $N = 3$, this is the question of the fate of an atom pair if the target site is already occupied by an atom. The striking answer, as evidenced in Fig. 4(b), is that the process can be viewed as single-atom tunneling on the background of the symmetric two-atom ground state. The tunneling frequency in the fermionization limit is simply the tunnel splitting $\Delta^{(1)} \approx 2\pi/40$. This has the intuitive interpretation of a fermion which—lifted to the band $\beta = 1$—tunnels independently of the two lowest-band fermions. From that point of view, it should come as no surprise that adding another particle destroys that simple picture. In fact, Fig. 4(c) reveals that if we start with $N-1=3$ atoms on the right, then the tunneling oscillations appear erratic at first glance, and a configuration with three atoms per site becomes an elusive event. (For example, at $t \approx 22$, three atoms are on the left site, whereas at $t \approx 44, 72$ three atoms are on the right.) In the spirit of the Fermi map above, this can be understood as superimposed tunneling of one atom in the first excited band ($\Delta^{(1)}$) and another in the second band ($\Delta^{(2)} \approx 2\pi/15$), while the remaining zeroth-band fermions stay inactive.

Finally, we mention that one may not only use the tilt d to load the atoms into one well, but also to study tunneling oscillations in *asymmetric* wells in order to actively tune the tunneling. A detailed investigation [17] reveals that, for medium g, single-particle tunneling can be resonantly *enhanced* if the right well is lowered enough to compensate the interaction-energy shift. In the fermionization limit, in turn, single-atom tunneling turns out resonant already for $d = 0$, while tuning d makes other resonances accessible.

In conclusion, we have performed an *ab initio* investigation of the full crossover from uncorrelated to fermionized tunneling of a boson pair in a double well. Remarkable features of this pathway are the strongly delayed pair tunneling encountered for medium interactions and, in the fermionization limit, fragmented-pair tunneling at the Rabi frequency. Having pushed the notion of tunneling toward strongly interacting systems, this opens up intriguing perspectives, ranging from resonantly tuning the tunneling to considering multiwell setups.

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[1] M. Albiez *et al.*, Phys. Rev. Lett. **95**, 010402 (2005).
[2] G. J. Milburn *et al.*, Phys. Rev. A **55**, 4318 (1997).
[3] A. Smerzi *et al.*, Phys. Rev. Lett. **79**, 4950 (1997).
[4] T. Anker *et al.*, Phys. Rev. Lett. **94**, 020403 (2005).
[5] J. Javanainen, Phys. Rev. Lett. **57**, 3164 (1986).
[6] K. Winkler *et al.*, Nature (London) **441**, 853 (2006).
[7] S. Fölling *et al.*, Nature (London) **448**, 1029 (2007).
[8] T. Köhler, K. Góral, and P. S. Julienne, Rev. Mod. Phys. **78**, 1311 (2006).
[9] M. Olshanii, Phys. Rev. Lett. **81**, 938 (1998).
[10] M. Girardeau, J. Math. Phys. (N.Y.) **1**, 516 (1960).
[11] B. Paredes *et al.*, Nature (London) **429**, 277 (2004).
[12] T. Kinoshita, T. Wenger, and D. S. Weiss, Science **305**, 1125 (2004); Nature (London) **440**, 900 (2006).
[13] M. D. Girardeau and E. M. Wright, Phys. Rev. Lett. **84**, 5691 (2000); K. K. Das, M. D. Girardeau, and E. M. Wright, Phys. Rev. Lett. **89**, 170404 (2002); T. Busch and G. Huyet, J. Phys. B **36**, 2553 (2003); A. Minguzzi and D. M. Gangardt, Phys. Rev. Lett. **94**, 240404 (2005); O. E. Alon and L. S. Cederbaum, Phys. Rev. Lett. **95**, 140402 (2005); F. Deuretzbacher *et al.*, Phys. Rev. A **75**, 013614 (2007).
[14] S. Zöllner, H.-D. Meyer, and P. Schmelcher, Phys. Rev. A **74**, 053612 (2006); **74**, 063611 (2006); **75**, 043608 (2007).
[15] A. P. Tonel, J. Links, and A. Foerster, J. Phys. A **38**, 1235 (2005); A. N. Salgueiro *et al.*, arXiv:quant-ph/0608222; C. E. Creffield, Phys. Rev. A **75**, 031607 (2007); D. R. Dounas-Frazer and L. D. Carr, arXiv:quant-ph/0610166.
[16] H.-D. Meyer, U. Manthe, and L. S. Cederbaum, Chem. Phys. Lett. **165**, 73 (1990); M. H. Beck *et al.*, Phys. Rep. **324**, 1 (2000).
[17] S. Zöllner, H.-D. Meyer, and P. Schmelcher, arXiv:0801.1090v1.