Collective tunnelling of strongly interacting cold atoms in a double well potential

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It is known that under resonance conditions, a group of strongly interacting bosonic atoms, trapped in a double-well potential, mimics a single particle, performing Rabi oscillations between the wells. By implication, all atoms need to tunnel at roughly the same time, even though the Bose-Hubbard Hamiltonian accounts only for one-atom-at-a-time transfers. We analyse the mechanism of this collective behaviour, evaluate the Rabi frequencies in the process, and discuss the limitation of this simple picture. In particular, it is shown that the small rapid oscillations superimposed on the slow Rabi cycle, result from splitting the transferred cluster at the sudden onset of tunnelling, and disappear if tunnelling is turned on gradually.

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I. INTRODUCTION

For a quantum particle, which can occupy several quantum states with roughly the same energy, even a small perturbation is capable of causing transitions between the states. If only a pair of states satisfies this resonance condition, these transitions would, in general, be in the form Rabi oscillations \cite{1}, moving the particle periodically from one state to the other. A more interesting case is the one where the resonance occurs between many-body states of interacting particles, which correspond to different spatial configurations of the system. A direct matrix element may or may not connect a pair of such states, say, $|\Psi_1\rangle$ and $|\Psi_2\rangle$. In the latter case the system would need to reach the final state via a pathway, passing through the states of the system, whose energies can lie far from the resonance. The passage must be, in some sense, rapid, since a measurement will almost always find the system either in $|\Psi_1\rangle$, or in $|\Psi_2\rangle$, and only rarely detect it elsewhere.

Examples of collective behaviour can be found, for example, in cold atom physics. In \cite{2} the authors observed coherent many-body Rabi oscillations in electronics transitions of interacting rubidium atoms. More relevant to our analysis is the direct observation of correlated tunnelling of pairs of strongly interacting cold atoms, reported in \cite{3}.

Recently developed laser techniques are capable of trapping such atoms in quasi one-dimensional traps \cite{4}, and the dynamics of interacting atomic systems has been extensively studied both by solving the Schrödinger equation numerically (see, e.g. \cite{5}, \cite{6}, \cite{7}), and by using a simplified Bose-Hubbard model, as was done, for example, in \cite{3}, \cite{8}, \cite{9}. In \cite{10}, \cite{11} and \cite{12} experimental and theoretical analysis of larger systems are presented, and the contributions from higher bands are included. In these systems, effects such as breathing are cradle modes can be observed as a consequence of this high-bands contributions, and tunnelling between wells as an effect of the lower modes. Similar dynamics may also be observed, for example, using mixtures of atoms, where different inter-species interaction regimes were studied \cite{13}, or spin chains \cite{14}. Other theoretical studies, with a large number of particles, address the dynamics of a BEC in a double-well using the Gross-Pitaevskii equations including many-body interactions studying the self-trapping effect induced \cite{15} or different regimes, from coherent oscillations to their suppression when the number of bosons is high \cite{16}. Important experimental results have also been obtained for BEC in double-well potentials, such as the first realization of a single Josephson junction \cite{17} or the more recent \cite{18}, where the dynamical control of correlated tunnelling processes of strongly interacting particles is presented.

The tunnelling frequencies for a symmetric trap were first evaluated in \cite{19}, where the authors relied on the time independent perturbation theory of \cite{20}, in order to obtain energy splitting between the resonant states. In their follow up paper \cite{21}, the authors of \cite{19} studied time evolution of the average difference of the wells’ populations, $\delta n(t)$, for various initial conditions, and analysed the frequency spectrum of quantum fluctuations, superimposed on the Rabi cycle.

However, this is not the whole story, and certain aspects of the collective tunnelling phenomenon require a further discussion. In particular, in the Rabi oscillations one would find all the transferred atoms in the same well, at all times. This suggests that the atoms must tunnel together, almost instantaneously, or at least during a time much shorter than the Rabi period \cite{22}. Neither the analysis of \cite{19}, \cite{21}, nor the form of the Bose-Hubbard Hamiltonian, which contains only single atom transfer terms, give an immediate clue as to how this may be possible. A study of the mechanism of this rapid collective transfer, and identification of the relevant time scales is the first of our aims.

Furthermore, the picture in which a cluster of transferred atoms behaves as a single particle, performing Rabi oscillations, is only approximate, and deserves further attention. The mean populations difference \cite{19},...
\[ \delta n(t) = \sum_{n=0}^{N} [p(n, t) - (N - n)(1 - p(n, t))], \]
where \( p(n, t) \) are the probabilities for finding \( n \) out of \( N \) bosons in the right well at a time \( t \), is a rather crude averaged quantity, and may not be best suited for such an analysis. Quantum fluctuations, evident in the \( \langle \delta n(t) \rangle \), come from the directly measurable individual probabilities \( p_n(t) \). These, in turn, are absolute squares of the sums of the probability amplitudes, corresponding to elementary processes, such as transfer of a single atom from one well to the other. Identification of interfering scenarios, responsible for the additional oscillatory patterns, specific to many body Rabi oscillations, is the second main subject of this paper.

Fortunately, with the tunnelling matrix element small, and the Rabi period large, the required analysis can be carried out already in the first non-vanishing order of the time dependent perturbation theory. With its help, we carried out in the first non-vanishing order of the main subject of this paper.

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It is convenient to describe the system by the number of bosons populating the right well, \( 0 \leq n \leq N \). If no tunnelling is possible, \( \Omega = 0 \), the eigenstates of \( H \)

\[ |n\rangle = (c^+_L)^{N-n}(c^+_R)^n|0\rangle/[n!(N-n)!]^{1/2} \]
correspond to the energies

\[ \mathcal{E}(n) = U(n - \nu)^2 + \mathcal{E}_0(N, \beta), \quad n = 0, 1, ..., N \]
where

\[ \nu \equiv (N - \beta/U)/2, \quad \mathcal{E}_0 \equiv U[N(N - 1)/2 - \nu^2] \]
The dependence of \( \mathcal{E}(n) \) on \( n \) is quadratic and, since \( \mathcal{E}(n) = \mathcal{E}(2\nu - n) \), whenever the minimum of the parabola, at \( n = \nu \) is an integer, or half integer,

\[ (N - \beta/U) = K, \quad K = 1, 2, ... \]
there are several pairs of doubly degenerate states. Fig. 2 shows the energy levels for an asymmetric potential with \( N = 8 \) and \( \beta/U = 1 \), so the minimum energy corresponds to \( \nu = 3.5 \). We have degeneracy between several pairs of states, for instance, between \(|1\rangle \) and \(|6\rangle \), that share the same energy, \( \mathcal{E}(1) = \mathcal{E}(6) \). In general, for \( \nu \leq N/2 \) the number of degenerate pairs is given by that of the integers in the interval \([0, \nu]\), and for \( \nu > N/2 \), by the number of integers inside \((\nu/2, N]\). We note that if \( \nu \) happens to be an integer, there is an unpaired non-degenerate ground state \(|n = \nu\rangle \), and \( \mathcal{E}(\nu) = \mathcal{E}_0 \).

Next we switch the tunnelling on, in such a manner that the tunnelling matrix element in Eq. (1) will remain small, compared to the interatomic interaction \( \Omega/U \ll 1 \). The perturbation will lift the degeneracy between the levels \(|n\rangle \) and \(|2\nu - n\rangle \), and introduce pairs of new eigenstates

\[ |n_{\pm}\rangle = (|n\rangle \pm |2\nu - n\rangle)/\sqrt{2} \]
with the energies

\[ \mathcal{E}(n_{\pm}) \equiv \mathcal{E}(n) \pm \omega_n = \mathcal{E}(2\nu - n) \pm \omega_n, \]
with the splitting \( 2\omega_n \) small, compared to other energy differences shown in Fig. 2.
If as a result, the atoms, initially prepared in the state \(|\Psi(0)\rangle = |n\rangle\rangle \) with \( n \) atoms in the right well, will perform collective Rabi oscillations between the states \(|n\rangle \) and \(|2\nu - n\rangle \), we expect their state at a time \( t \) to be given by

\[ \langle \Psi(t) \rangle \approx [\cos(\omega_n t)|n\rangle + \alpha \sin(\omega_n t)|2\nu - n\rangle] \exp(-i\mathcal{E}(n)t), \quad |\alpha| = 1. \]
For a symmetric setup, the frequencies $\omega_n$ were obtained in [19] within time-independent perturbation theory, using a rather complicated procedure [20] for diagonalising a tridiagonal matrix with degenerate eigenvalues. The authors of [19] correctly note that the shortest way to reach the state $|N-n\rangle$ from $|n\rangle$ is by “moving one boson per step”. There is, however, room for a further clarification. In the approximation [8], the atoms will never be observed in any other state $|m\rangle$, $m \neq n, 2n - 1$ (or rather the probability of such an observation will be negligibly small). For example, in the case shown in Fig. 2, for $|\Psi(0)\rangle = |1\rangle$, counting atoms in the right well will almost always give a result either 1, or 6. This suggests, and we will show below that this suggestion is correct, that the 5 atoms making the difference, will need to tunnel, in some sense, all at the same time. Next we demonstrate this by using time-dependent perturbation theory, and obtain, while we are at it, collective tunnelling frequencies for an asymmetric trap ($\beta \neq 0$).

\[ \langle \Psi(t) \rangle = \sum_{n=0}^{N} b_n(t) |n\rangle, \]  

where the equations for the coefficients $b_n(\tau)$

\[ i\partial_\tau b_n = \sum_{m=0}^{N} (E_n \delta_{nm} + \gamma_{n-1} \delta_{n,m+1} + \gamma_n \delta_{n,m-1}) b_m \]  

and introducing dimensionless time and energy,

\[ \tau \equiv U t, \quad E_n \equiv E(n)/U, \]

we obtain the equations for the coefficients $b_n(\tau)$

\[ \gamma_n \equiv U^{-1} \Omega[(n+1)(N-n)]^{1/2}. \]

FIG. 1. An asymmetric double-well potential supports two single-particle levels, with an energy difference $\beta$. Tunnelling across the barrier is described by the amplitude $\Omega$ in Eq. 1.

III. PERTURBATION THEORY AND THE COLLECTIVE FREQUENCIES

Writing the wave function of the system as

\[ \langle \Psi(t) \rangle = \sum_{n=0}^{N} b_n(t) |n\rangle, \]  

and introducing dimensionless time and energy,

\[ \tau \equiv U t, \quad E_n \equiv E(n)/U, \]

we obtain the equations for the coefficients $b_n(\tau)$

\[ i\partial_\tau b_n = \sum_{m=0}^{N} (E_n \delta_{nm} + \gamma_{n-1} \delta_{n,m+1} + \gamma_n \delta_{n,m-1}) b_m \]  

where

\[ \gamma_n \equiv U^{-1} \Omega[(n+1)(N-n)]^{1/2}. \]

FIG. 2. Energy levels for strongly interacting bosonic atoms, with $N = 8$ and $\beta/U = 1$, trapped in an asymmetric potential well. Degeneracy between the states with $n = 1$ and $n = 6$ atoms in the right well is lifted by tunnelling, which causes periodic transfer of $M = 5$ atoms between the wells. No matrix element connects the levels directly, and the transition has to follow the pathway shown by the arrows. In the strong coupling limit, all five atoms tend to tunnel together.

A probability to find $n$ atoms in the right well is, therefore, given by

\[ p(n) = |b_n(t)|^2. \]  

Equations (10) can be solved analytically only for $N \leq 3$ in general, and for $N \leq 7$ if the potential is symmetric, as discussed in Appendix B. In order to evaluate the Rabi frequencies for an arbitrary $N$, we note that since no matrix element connects the states $|n\rangle$ and $|2n - 1\rangle$ directly, and the latter can only be reached from the former via $2(\nu - n)$ intermediate steps, shown in Fig. 2.

For simplicity, we first consider the symmetric potential, $\beta = 0$, assume, for the moment, that the $\gamma_s$ depend on time, let the system start with $n$ bosons in the right well, and employ the time-dependent perturbation theory. To the leading approximation, the transition amplitude between the states $|n\rangle$ and $|N-n\rangle$ is given by ($M \equiv N-2n$, $n \leq N/2$)

\[ A_{n,N-n}(\tau) \equiv \langle N-n | \exp[-i \int_0^\tau H(\tau')d\tau'] | n \rangle = \]  

\[ (-i)^M \int_0^\tau d\tau_M \cdots \int_0^{\tau_3} d\tau_2 \int_0^{\tau_2} d\tau_1 \times \]  

\[ \exp[-iE_{N-n}(\tau - \tau_M)] \gamma_{N-n-1}(\tau_M) \times \exp[-iE_{N-n-1}(\tau_M - \tau_{M-1})] \cdots \times \gamma_{n+1}(\tau_2) \exp[-iE_{n+1}(\tau_2 - \tau_1)] \times \gamma_n(\tau_1) \exp(-iE_n \tau_1) + O(\Omega^{M+1}/U^{M+1}). \]
This expression has the standard interpretation: the first term corresponds to the first particle jump occurring at $t_1$, the second at $t_2$, and so on. The transition amplitude is then found by summing over all $t_j$, leaving the precise moments of jumps indeterminate. Perturbative treatment will limit us to times much shorter that the Rabi period, yet as we will see below, it captures the essential features of the collective transfer mechanism.

Next we demonstrate that for $\Omega/U < 1$, and $\Omega(t)$ slowly varying compared to the inverse of the separations between the system’s levels in Fig.2, the sum is dominated by the process in which all $N-2n$ atoms jump roughly at the same time. Returning to the original unscaled time variable, $t$, we have

$$A_{n,N-n}(T) = (-i)^{M} \exp[-i\mathcal{E}(N-n)T]$$

$$\times \int_0^T dt_{M}W_{N-n-1}(t_M)\exp[i\Delta_{M}t_M]...$$

$$\times \int_0^{t_2} dt_{2}W_{n+1}(t_2)\exp[i\Delta_{2}t_2]$$

$$\times \int_0^{t_2} dt_{1}W_{n}(t_1)\exp(i\Delta_{1}t_1) + O(\Omega^{M+1}/U^{M+1})$$

where $\Delta_m$ is the energy, separating two adjacent states,

$$\Delta_m \equiv \mathcal{E}(n+m) - \mathcal{E}(n+m-1) = U[1 - 2(n+m) - N],$$

and $W_{n}(t) \equiv \gamma_{n}U = \Omega(t)[(n+1)(N-n)]^{1/2}$ is the scaled tunnelling amplitude. Thus, we have to evaluate $M$ oscillatory integrals. Oscillations of $\exp(i\Delta_{n}t)$ become more rapid as $U$ increases, so that, for a large $U/\Omega$, the main contributions to the integrals will come from the endpoints (for details see Appendix A). For example, we may write

$$\int_0^{t_2} dt_{1}W_{n}(t_1)\exp(i\Delta_{1}t_1) =$$

$$[W_{n}(t_2)\exp(i\Delta_{1}t_2) - W_{n}(0)]/i\Delta_1 + O(\Omega/U).$$

Here the first term corresponds to the first particle jump occurring at the same time as the second, $t_1 = t_2$. The second term clearly corresponds to the first jump occurring at $t_1 = 0$, i.e., immediately after the tunnelling is switched on. Jumps at $0 < t_1 < t_2$ are suppressed, for large $U/\Omega$, due to destructive interference. Continuing in the same vein, we obtain a total of $2^{M}$ terms ranging from all particles jumping at $t = 0$ to all particles jumping at the same time. In the case of an exact resonance, $\sum_{m=1}^{M} \Delta_m = 0$, the contribution from all fully coordinated jumps between $0 < t < T$ is readily seen to be

$$i(-1)^{M} \int_0^{T} dt \prod_{j=0}^{M-1} W_{n+j}(t) \times$$

$$[\Delta_1(\Delta_1 + \Delta_2)...(\Delta_1 + \Delta_2 + ... + \Delta_{M-1})]^{-1}.$$

Note that since the amplitude results from the interference between all $t$’s, the exact moment in which the collective transfer takes place remains indeterminate, much like the number of the slit chosen by an electron in Young’s double-slit experiment. Returning to the case of constant $\Omega$, we, therefore, obtain

$$A_{n,N-n}(T) = i(-1)^{M} T^{\Omega M/UM-1} \exp[-i\mathcal{E}(N-n)T] \times$$

$$(n+1)...(N-n)/(E_{n+1} - E_{n})...(E_{N-n-1} - E_{n}) + R,$$

where the remainder $R$ contains the terms corresponding to, at least, one atom jumping immediately after tunnelling is turned on. In the next Section we will demonstrate that $R$ will vanish if tunnelling is switched on sufficiently slowly.

For a sufficiently small $T$, Eq. (8) predicts

$$A_{n,N-n}(T) = \alpha \omega_{n}T.$$

Comparing Eq. (19) with Eq. (18), and evaluating the products, yields

$$\omega_{n} = \frac{\Omega^{N-2n}}{U^{N-2n-1}/n![(N-2n-1)!]^2} \times \alpha = (-1)^n i,$$

which agrees with the result obtained by a different method in [17]. A calculation for an asymmetric well can be done in exactly the same way, and here we will only quote the final result. As discussed in Sec. II, the resonances between many-body states occur provided $\nu = 1/2, 1, ..., N/2$. The Rabi frequency for a process in which the atoms start in a state $|n\rangle$, and $2(\nu - n)$, $[0 < n < \nu - 1$ if $\nu$ is an integer, and $0 < n < \nu - 1/2$, if $\nu$ is odd] where the atoms are transferred simultaneously, is given by $[\nu = (N - \beta/U)/2]

$$\omega_{n} = \frac{\Omega^{2(\nu-n)}}{U^{2(\nu-n-1/2)}[2(\nu - n) - 1]!^2 \sqrt{(N-n)!(2\nu - n)!}} / n!(N + n - 2\nu)!].$$

For an asymmetric well, the leading probabilities $p(n)$, to find $n$ atoms in the right well, after switching the tunnelling on at $t = 0$, are shown in Fig.3, together with the Rabi oscillations at the frequency [21]. Superimposed upon the Rabi oscillations, there are much faster oscillations (see inset), which will be discussed in the next Section.

IV. SUDDEN VS. ADIABATIC SWITCHING ON OF THE TUNNELLING

These small rapid oscillations are much more pronounced in a system containing just $N = 2$ atoms, as shown in Fig. 4a. We have already used perturbation theory to obtain slow Rabi frequencies $\omega_{n}$, and next we will try to use it in order to explore the origin of these additional oscillatory patterns.
To the leading order in $\Omega$, the amplitude to find one atom in each well is given by Eq. (22), and we have (from [3], $\mathcal{E}(0) = U$, and $\mathcal{E}(1) = 0$)

$$A_{0,1}(T) \approx \frac{2\sqrt{2}\Omega}{U} \exp(-i\Omega T/2) \sin(i\Omega T/2),$$

so that the corresponding probability rapidly oscillates,

$$p(1) \approx 8\Omega^2/U^2 \sin^2(i\Omega T/2).$$

As discussed in Appendix A, by turning the tunnelling on gradually, we can avoid splitting the 2-atom cluster at $t = 0$, and quench the oscillations. This can be checked directly, e.g., by choosing

$$\Omega(t) = \Omega[1 - \exp(-\Gamma t)],$$

where $1/\Gamma$ is the characteristic switching time, over which the tunnelling matrix element is brought to its stationary value. Evaluation of the integral in Eq. (22) gives

$$A_{0,1}(T) \approx \sqrt{2}\Omega/\kappa U \{\exp(-i\Omega T/U) - \exp(-i(U-i\Gamma)T)/(U-i\Gamma) - 1/U + 1/(U-i\Gamma)\}. $$

For $\Gamma/U \ll 1$, and $\Gamma T >> 1$, this reduces to

$$A_{0,1}(T) \approx \sqrt{2}\Omega/\kappa U \{\exp(-i\Omega T/U), \quad \text{and} \quad p(1) \approx 2\Omega^2/U^2. $$

Oscillations of $p(1)$ disappear, and its largest value is reduced by a factor of four. The rapid oscillations also disappear from the amplitude to find 2 atoms in each well. This, as described in Appendix A, can be written as a sum of three terms,

$$A_{0,2}(T) \approx A_{0,2}^{(I)}(T) + A_{0,2}^{(II)}(T) + A_{0,2}^{(III)}(T) = \frac{2\Omega^2}{U} \exp(-i\Omega T) - \frac{2\Omega^2}{U^2} + \frac{2\Omega^2}{U^2} \exp(-i\Omega T),$$

related to the three scenarios shown in Fig. 5. The first term corresponds to both atoms being transferred together at some unspecified time between $t = 0$ and $t = T$. The second term comes from the process in which one of the atoms jumps immediately, at $t = 0$, while the second one is transferred later. The third term is the amplitude for both atoms jumping together at $t = 0$ (see Appendix A). With tunnelling switched on gradually from zero we, therefore, have

$$A_{0,1}(T) \approx A_{0,2}^{(I)}(T), \quad \text{and} \quad p(1) \approx 4\Omega^4 T^2/U^2. $$

What has been said so far should apply to times much shorter than the large Rabi period, $T_{Rabi} = \frac{2\pi}{\omega_0}$, $1/U << T << T_{Rabi}$, and we still need to check that this analysis remains correct for much longer times, shown in Fig. 4. We note first that the exact amplitude [cf. Eq. (17)] has a form, similar to $A_{0,2}$ in Eq. (22)

$$A_{0,1}(T) = -\frac{2\sqrt{2}\Omega}{\kappa U} \exp(-i\Omega T/2) \sin(i\kappa UT/2),$$

related to the three scenarios shown in Fig. 5.
Before giving our conclusions, we briefly discuss detuned extended, with similar results, to more than two atoms. This approach can be delayed until \( \Omega \) reaches its final magnitude, lack the rapid oscillations between the corresponding states \( \nu \) and \( \omega \), and the oscillations will be eliminated also from Fig.4b. The Rabi oscillations, \( \nu \) and \( \omega \) oscillations (dashed), \( \nu = \sqrt{1 + 16\Omega^2/U^2} \). The amplitude remains small, \( \sim \Omega \), at all times, since the system never stays in the one-atom-in-each-well configuration for long. We can, therefore, expect that, in the slow switching-on regime, the probability \( p(1) \) would reduce to

\[
p(1) = \frac{2\Omega^2}{\sqrt{U^2 + 16\Omega^2}^2},
\]

and the oscillations will be eliminated also from \( p(0) \) and \( p(2) \), which depend on \( p(1) \), through the condition \( p(0) + p(1) + p(2) = 1 \). The ultimate proof consists in solving numerically Eqs.(24) with an \( \Omega(t) \) given in Eq.(24). The results are shown in Fig.4b. The Rabi oscillations, delayed until \( \Omega \) reaches its final magnitude, lack the rapid oscillations seen in Fig. 4a, while \( p(1) \) does indeed have a constant value given by (20). This approach can be extended, with similar results, to more than two atoms. Before giving our conclusions, we briefly discuss detuned Rabi oscillations.

V. DETUNED RABI OSCILLATIONS

At the exact resonance, \( \mathcal{E}(n) = \mathcal{E}(2\nu - n) \) Rabi oscillations between the corresponding states \( |n\rangle \) and \( |2\nu - n\rangle \), \( \nu = (N - \beta/U)/2 \), can be described by an effective Hamiltonian, acting in a reduced two-dimensional Hilbert space, \( \hat{H}^{eff} = \omega_n \sigma_z \), with \( \sigma_z \) denoting the Pauli matrix.

In a slightly asymmetric well, with \( \beta \) replaced by \( \beta + \delta \beta \), the two levels are detuned by \( \Delta \mathcal{E}, |\Delta \mathcal{E}| = |2\delta \beta(n-\nu)| \) and the effective Hamiltonian acquires an additional term, proportional to \( \sigma_z \), \( \hat{H}^{eff} = \omega_n \sigma_z + \Delta \mathcal{E} \sigma_z/2 \). Here, as in the general case, the probabilities are given by the formulæ, known for detuned Rabi oscillations. In particular, starting with \( n \) atoms in the right well we should have

\[
P(2\nu - n) = 1 - P(n) \approx \\
\frac{\omega_n^2}{\omega_n^2 + \delta \mathcal{E}^2 (\nu - n)^2} \sin^2 \left[ \sqrt{\omega_n^2 + \delta \mathcal{E}^2 (\nu - n)^2} \delta t \right],
\]

where \( \nu \) and \( \omega_n \) are given by Eqs.(3) and (21), respectively. Detuned oscillations for \( N = 5, n = 0 \), in a slightly perturbed symmetric potential are shown in Fig. 6.

VI. CONCLUSIONS AND DISCUSSION

In summary, we show that a system of strongly interacting bosonic atoms in a not necessarily symmetric double-well potential is capable of performing collective Rabi oscillations of a frequency \( \omega_n \) given by Eq.(21). This will happen provided the resonance condition (5) is satisfied for the many body states containing \( n \) and \( n + M \) atoms in one of the wells. The frequencies of the Rabi oscillations are easily predicted with the help of time-dependent perturbation theory, which recovers the result obtained in [9] for the symmetric case. The physical picture is the one in which all \( M \) atoms are transferred together, as a single cluster, from one well to another, during a short period of time \( \delta t \sim U^{-1} \), while the precise moment of the transfer remains indeterminate, in accordance with the uncertainty principle.

This is achieved through destructive interference between other scenarios. Compared to the observation time, typically of the order of the large Rabi period, the rapid
transfer appears to be almost instantaneous. Accordingly, an observation made in either well will almost certainly find there either \( n \), or \( n + M \) atoms, with all other counts occurring only rarely. While it is difficult to probe directly the duration of the collective transfer, a less direct proof of this transfer mechanism is available. While the behaviour of the group of \( M \) atoms is broadly similar to that of a single particle, the composite nature of the group can be probed if tunnelling is switched on suddenly. If so, the immediate transfer of individual atoms, or smaller groups of atoms, will result in a rapid oscillatory pattern, superimposed on the much slower Rabi cycle. An analysis of the transition amplitude in Appendix A, as well as numerical results shown in Fig.4, show that these oscillations disappear, if tunnelling is turned on slowly, compared to \( \delta t \approx 1/|E_2 - E_1| \), the main contributions to the integral comes from the incomplete oscillations at the endpoints, i.e., from the regions around 0 and \( T \), of a width \( \sim \delta t \).

\[
A \approx -\Delta^{-1}[W(T)\exp(-E_1 T)W(0)\exp(-iE_2 T)] .
\]

Now the amplitude \( A \) has lost all the information about the overall behaviour of \( W(t) \), and depends only on its initial value at \( t = 0 \), and its current value at \( t = T \). The short time it takes for the system to ”jump” is, clearly \( \sim \delta t \). Moreover, if \( W(t) \) is gradually switched on from zero, the likelihood of finding the system in \( |2\rangle \), will depend only on the perturbation’s current value \( W(T) \).

A. Even number of atoms

Next in complexity is the case in which two atoms are transferred via a third state. For simplicity, we consider a symmetric well, \( \beta = 0 \), and start transferring an even number of atoms \( M = N = 2K \), so that the minimum of the parabola in Fig. 2 is at an integer value of \( n \). The transfer takes two steps, and the corresponding second-order amplitude is given by

\[
A \approx (-i)^2 \exp(-iE_3 T) \int_0^T dt_2 \int_0^{t_2} dt_1 \times \exp[i\Delta t_2]W_2(t_2)\exp(i\Delta_1 t_1)W_1(t_1),
\]

where, as before, \( \Delta_1 = E_{i+1} - E_i \), the resonance condition reads \( E_1 = E_3 \), and the ”jump time” is \( \delta t \approx 1/(E_2 - E_1) \). The diagram in Fig.7 helps to visualise the structure of the double integral in Eq. (34). Every integral, containing an exponential \( \exp(i\Phi t) \), splits into contributions from its endpoints. An exception is the second integral in the left branch, where the phase \( \Phi = \Delta_1 + \Delta_2 = 0 \) vanishes, and the integration has to be carried out over the whole interval \( 0 \leq t_2 \leq T \). This process, in which both atoms are transferred together at an unspecified moment \( t_2 \), contributes to the amplitude in Eq. (34) an amount

\[
A^{(I)} \approx i\Delta_1^{-1}\exp(-iE_3 T) \int_0^T dt_2 W_2(t_2)W_1(t_1). \quad (35)
\]

There is also a process, in which the first atom jumps at \( t = 0 \), and is followed by the second one at \( t = T \) Its contribution is

\[
A^{(II)} \approx -\Delta_1^{-2}\exp(-iE_2 T)W_2(T)W_1(0). \quad (36)
\]

(Note that the phase is \( E_2 t \), since the system continues in the state \( E_2 \), until the second jump at \( t = T \). Finally,
it is possible for both atoms to jump at \( t = 0 \), and we have

\[
A^{(III)} \approx \Delta_1^{-2} \exp(-iE_3 T) W_2(0) W_1(0),
\]

so that \( A = A^{(I)} + A^{(II)} + A^{(III)} \). We note that if \( W_1(t) \) is switched on from zero, slowly compared to the jump time \( \delta t \), the last two terms vanish, and the amplitude is fully determined by collective transfer of two atoms, \( A = A^{(I)} \) at an unspecified time \( t_2 \). The scheme in Fig. 7 is easily extended to collective transfer of more than two atoms, \( M > 2 \) provided \( N \) remains even. In general, such an amplitude is seen to be dominated by nearly instantaneous transfer of \( M \)-atom cluster, if \( W_1(t) \) varies slowly, compared to \( \delta t = 1/\min\{\Delta_m\} \). With the observation times typically of order of the large Rabi period \( T_{\text{Rabi}} \sim W^{-M} \), the pictures should hold in most practical cases.

\[
\int_0^t dt_2 e^{i\phi} W_1(t_1)\ldots W_0(t) W_0(t) e^{i\phi} W_1(t)\ldots W_1(t_1)
\]

\[
\int_{t_1}^t dt_2 e^{i\phi} W_2(t_1) W_2(t_2) e^{i\phi} W_2(t)
\]

\[
\int_{t_1}^t dt_2 W_1(t_2) W_2(t_2) e^{i\phi} W_1(t_2)
\]

FIG. 7. A diagram illustrating evaluation of the double integral in Eq. 33. Every integral, containing a rapidly oscillating exponential \( \exp(i\Phi) \), is split into the contributions from its lower and upper limits. This does not, however, happen in the last step of the left branch, where \( \Phi = \Delta_1 + \Delta_2 = 0 \), and the integration is over \( 0 \leq t_3 \leq T \).

B. Odd number of atoms

Although Eq. (13) is valid for any \( N \), the situation for \( M = 2K + 1 \), \( K = 1, 2, \ldots \) is slightly different, since now the two lowest states in Fig. 2, through which the system has to pass, are also in resonance. Thus, we have an integral

\[
A = (-i)^3 \exp(-iE_4 T) \int_0^T dt_3 \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 \times \exp(i\Delta_3 t_3) W_3(t_3) \exp(i\Delta_2 t_2) W_2(t_2) \exp(i\Delta_1 t_1) W_1(t_1),
\]

where \( \Delta_2 = 0 \), and \( \Delta_1 + \Delta_3 = 0 \). Four possible processes, which contribute to the amplitude (38) are shown in Fig. 9. The left branch on the diagram in Fig. 7 corresponds, as before, to all atoms jumping at the same, yet unspecified, time, for which we have,

\[
A^{(I)} = -i \exp(-iE_3 T) \Delta_1^{-2} \times \int_0^T W_1(t_3) W_2(t_3) W_3(t_3) dt_3.
\]

The process in which the first two atoms jump at \( t = 0 \), and the third at \( t = T \), contributes

\[
A^{(II)} = i \exp(-iE_3 T) \Delta_1^{-2} \Delta_3^{-1} \times W_1(0) W_2(0) W_3(0).
\]

Finally, it is possible for the first atom to jump at \( t = 0 \), for the second one to jump at some \( 0 \leq t_2 \leq T \), and for the third one to complete the transition at \( t = T \). The amplitude for this is

\[
A^{(IV)} = -i \exp(-iE_4 T) \Delta_1^{-1} \Delta_3^{-1} \times W_1(0) W_3(T) \exp(i\Delta_4 T) \int_0^T W_2(t_2) dt_2.
\]

The amplitude for the fifth process in Fig. 9 vanishes, since it involves \( \int_0^T W(t_2) dt_2 = 0 \), and the full amplitude is the sum of four terms \( A = A^{(I)} + A^{(II)} + A^{(III)} + A^{(IV)} \).

Typically, all \( W_i \) are of the same order of magnitude, \( W_1 \sim W_2 \sim W_3 \sim W_4 \), and in the strong interaction limit, \( W \delta t \ll 1 \), the second and the third terms, which contain an extra factor of \( \Delta_3^{-1} \), can be omitted. For all \( W_i \) chosen to be constant, both \( A^{(I)} \) and \( A^{(IV)} \) grow linearly with time,

\[
A^{(I)} \sim T, \quad A^{(IV)} \sim T \exp(i\Delta_3 T),
\]

FIG. 8. Transmission of \( M = 2 \) out of \( N = 2 \) atoms. The exact (solid), and the second order (dots) amplitudes, given by Eqs. (48) and (34), respectively, coincide to graphical accuracy. Also shown by dashed lines is \( A^{(I)} \) in Eq. (35). As in Eqs. (49), we use \( E_1 = E_3 = 0, E_2 = -U, \) constant values \( W_1 = W_2 = \sqrt{2} \Omega, \) and \( \Omega/T = 0.01 \).
as shown in the inset of Fig.10. However, $A^{IV}$ rapidly oscillates, compared to the large Rabi period, and can be omitted, when the Rabi frequency is calculated from the rate of change of $A$. Although not immediately seen from Eq. (42), this becomes clear from the graphs in the main panel of Fig. 10. The oscillations do not increase proportional to time, and the linear growth of the amplitude is determined, as one would expect, only by collective transfer of all three atoms. As before, switching tunnelling on slowly from zero, helps avoiding the splitting of the tunnelling cluster, and eliminates $A^{II}$, $A^{III}$, and $A^{IV}$, all proportional to $W_1(0)$. The diagram in Fig.9 can be extended to the transfer of more than three atoms, by adding integrations and branches, as appropriate. In general, the amplitude would contain the leading term, describing nearly simultaneous transfer of all $M$ atoms, as well as the additional sub-amplitudes, if the cluster is split at $t = 0$ by sudden onset of tunnelling.

\[ \int_0^T dt_1 e^{i\Delta_1} W_1(t_1) \cdots \frac{W_1(t_1)}{i\Delta_1} \frac{W_1(0)}{i\Delta_1} \frac{W_1(0)W_1(0)}{(i\Delta)^2} \int_0^T dt_3 e^{i\Delta_3} W_3(t_3) \cdots \]

\[ \left( \begin{array}{c} W \end{array} \right) = \left( \begin{array}{c} A^{(I)} \ A^{(II)} \ A^{(III)} \ A^{(IV)} \end{array} \right) \]

FIG. 9. Same as Fig. 7, except for the triple integral in Eq. (45). The phase of the integrand vanishes in the last step of the left branch, due to the resonance condition $\Delta_1 + \Delta_3 = 0$, and in the second step of the right branch, since $\Delta_2 = 0$. In the right branch, the contribution from $t_3 = 0$ vanishes, as marked by a cross.

VIII. APPENDIX B. EXACTLY SOLVABLE CASES

To write down a formal analytic solution to Eqs. (10), we need to diagonalise the Hamiltonian matrix $H_{mn} = \langle m|H|n \rangle$, $m, n = 0, 1, \ldots, N$. Since algebraic equations have analytical solutions up to the fourth order, this can be done for no more than $N = 3$ atoms, in the case of a general asymmetric well.

For a symmetric well, $\beta = 0$, a solution can be found for up to $N = 6$ atoms. Additional symmetry of $H_{mn}$, $H_{mn} = H_{N-m,N-n}$ requires that its eigenvectors $a^n = (a^n_0, a^n_1, \ldots, a^n_N)$ have a definite parity,

\[ a^n_m = \alpha a^n_{N-m}, \quad \alpha = \pm 1. \]

This, in turn, allows us to reduce the size of the matrix we need to diagonalise in order to obtain the eigenvalues of $H_{mn}$, and an analytical solution can, in principle, be obtained for $N \leq 7$. Below we analyse the $N = 2$ and $N = 3$ cases, assuming $\beta = 0$.

A. The two-particle case ($N = 2$)

For $N = 2$, we write $A_{n,N-n}(t) = \exp(-iUt)b_n(t)$, where $b_n(t)$ satisfy

\[ i\partial_0 b_0 = \sqrt{2}\Omega b_1 \]
\[ i\partial_1 b_1 = \sqrt{2}\Omega b_0 - Ub_1 + \sqrt{2}\Omega b_2 \]
\[ i\partial_2 b_2 = \sqrt{2}\Omega b_1 \]

with the initial condition $b_i(t = 0) = \delta_{i0}$, $i = 0, 1, 2$. This is equivalent to a second order equation for $b_1$

\[ \partial_0 b_1 - iU\partial_1 b_1 + 4\Omega^2 b_1 = 0 \]

with the initial condition $b_1(0) = 0$, $\partial_1 b_1(0) = -\sqrt{2}\Omega b_1$. The corresponding solution is

\[ b_1(t) = \frac{1}{\epsilon_1 - \epsilon_2} \left[ \exp(i\epsilon_1 t) - \exp(i\epsilon_2 t) \right] \]
where \( \epsilon_{1,2} = \frac{U}{2} \pm \sqrt{\frac{U^2}{4} + 4\Omega^2} \). For two other coefficients we then have

\[
b_2(t) = -\sqrt{2i\Omega} \int_0^t b_1(s) ds = \frac{2\Omega^2}{(\epsilon_1 - \epsilon_2)} \times (48)
\]

\[
[\exp(i\epsilon_1 t)/\epsilon_1 - \exp(i\epsilon_2 t)/\epsilon_2] + \frac{2\Omega^2}{\epsilon_1 \epsilon_2}
\]

and

\[
b_0(t) = 1 + b_2(t).
\]

Returning to the strong interaction case, \( \Omega/U \ll 1 \), we note then that

\[
\epsilon_1 - \epsilon_2 \approx \epsilon_1 \approx U, \quad \epsilon_2 \approx -4\Omega^2/U, \quad \epsilon_1 \epsilon_2 \approx -4\Omega^2. (49)
\]

With this we have

\[
b_0 = \exp(-i\omega_0 t) \cos(\omega_0 t), \quad b_2 = -i \exp(-i\omega_0 t) \sin(\omega_0 t), \quad \omega_0 = 2\Omega/U,
\]

which agrees with Eq. (50).

For the condensate prepared initially with one boson in each well we must change the initial condition for \( b_1(0) \) to \( b_1(0) = 1, \quad \partial_t b_1(0) = iU \). Hence we have

\[
b_1(t) = \frac{U - \epsilon_2}{\epsilon_1 - \epsilon_2} \exp(i\epsilon_1 t) + \frac{\epsilon_1 - U}{\epsilon_1 - \epsilon_2} \exp(i\epsilon_2 t)
\]

and \( b_0(t) = b_2(t) = -i\sqrt{2\Omega} \int_0^t b_1(s) ds \). It is readily seen that in the strong interaction limit \( \Omega/U \ll 1 \), when the energy separation from the two states corresponding to two bosons in the same well grows as \( U \), the system stays in its ground state \( |1 \rangle \). Indeed, rapid oscillations of \( b_1(t) \approx \exp(-iUt) \), guarantee that both \( b_0(t) \) and \( b_2(t) \) remain of order of \( \Omega/U \).

### B. The three-particle case \( (N = 3) \)

For three bosons, \( N = 3 \), in a symmetric well, \( \beta = 0 \), to evaluate \( b_n = \exp(2iUt)A_{n,N-n} \), we need to solve

\[
i\partial_t b_0 = \sqrt{3}\Omega b_1
\]

\[
i\partial_t b_1 = \sqrt{3}\Omega b_0 - 2U b_1 + 2\Omega b_2
\]

\[
i\partial_t b_2 = 2\Omega b_1 - 2U b_2 + \sqrt{3}\Omega b_3
\]

\[
i\partial_t b_3 = \sqrt{3}\Omega b_2.
\]

This is equivalent to

\[
i\partial_t b_0 = \sqrt{3}\Omega b_1
\]

\[
\partial_t b^\pm + 2iU^\pm \partial_t b^\pm + 3\Omega^2 b^\pm = 0
\]

\[
i\partial_t b_3 = \sqrt{3}\Omega b_2.
\]

where

\[
b^\pm = b_1 \pm b_2 \quad \text{and} \quad U^\pm \equiv \pm \Omega - U
\]

which are solved with appropriate initial conditions discussed below.

Initially, no particles in the right well \( (n = 0) \): \( b_n(0) = \delta_{n0}, \quad n = 0, 1, ..3 \). Introducing (subscripts 1 and 2 correspond to the + and − signs of the square root)

\[
\epsilon_{1,2}^\pm = [U^\pm] \pm \sqrt{(U^\pm)^2 + 3\Omega^2}
\]

we have

\[
b_0 = -\frac{3\Omega}{2} \left\{ \frac{\exp(i\epsilon_1^+ t)}{\epsilon_1^+(\epsilon_1^+ - \epsilon_2^+)} - \frac{\exp(i\epsilon_2^+ t)}{\epsilon_2^+(\epsilon_1^+ - \epsilon_2^+)} \right\}
\]

\[
\begin{align*}
b_1 &= -\frac{\sqrt{3}}{2} \Omega \left\{ \frac{\exp(i\epsilon_1^+ t)}{\epsilon_1^+(\epsilon_1^+ - \epsilon_2^+)} - \frac{\exp(i\epsilon_2^+ t)}{\epsilon_2^+(\epsilon_1^+ - \epsilon_2^+)} \right\} \\
b_2 &= -\frac{\sqrt{3}}{2} \Omega \left\{ \frac{\exp(i\epsilon_1^- t)}{\epsilon_1^-(\epsilon_1^- - \epsilon_2^-)} - \frac{\exp(i\epsilon_2^- t)}{\epsilon_2^-(\epsilon_1^- - \epsilon_2^-)} \right\} \\
b_3 &= -\frac{3\Omega}{2} \left\{ \frac{\exp(i\epsilon_1^- t)}{\epsilon_1^-(\epsilon_1^- - \epsilon_2^-)} - \frac{\exp(i\epsilon_2^- t)}{\epsilon_2^-(\epsilon_1^- - \epsilon_2^-)} \right\}
\end{align*}
\]

In the strong interaction limit \( \Omega/U \ll 1 \) we have

\[
\epsilon_{1,2}^\pm \approx \epsilon_{1,2}^\pm \approx 2U, \quad \epsilon_{1,2}^\pm \approx -3\Omega^2/2U \mp 3\Omega^3/2U^2
\]

so that

\[
b_0(t) \approx -\exp(-3\Omega^2 t/2U) \cos(3\Omega^2 t/2U^2),
\]

\[
b_1(t) \approx i \exp(-3\Omega^2 t/2U) \sin(3\Omega^2 t/2U^2),
\]

\[
b_2(t) \approx b_2(t) = o(\Omega/U)
\]

in accordance with \( \omega_0 \approx 3\Omega^3/2U^2 \), predicted by Eq. (50).

Initially, one particle in the right well \( (n = 1) \):

\[
b_n(0) = \delta_{n1}, \quad n = 0, 1, ..3.
\]

Solving Eqs. (51) with this initial condition we have

\[
b_0 = -\frac{\sqrt{3}\Omega}{2} \times (57)
\]

\[
\left\{ \begin{array}{l}
-\frac{\epsilon_2^+ + 2U^+}{\epsilon_1^+ (\epsilon_1^+ - \epsilon_2^+)} \exp(i\epsilon_1^+ t) + \frac{\epsilon_1^+ + 2U^+}{\epsilon_2^+ (\epsilon_1^+ - \epsilon_2^+)} \exp(i\epsilon_2^+ t) \\
-\frac{\epsilon_2^- + 2U^-}{\epsilon_1^- (\epsilon_1^- - \epsilon_2^-)} \exp(i\epsilon_1^- t) + \frac{\epsilon_1^- + 2U^-}{\epsilon_2^- (\epsilon_1^- - \epsilon_2^-)} \exp(i\epsilon_2^- t)
\end{array} \right\}
\]

\[
b_1 = \frac{1}{2} \left\{ \begin{array}{l}
-\frac{\epsilon_2^+ + 2U^+}{\epsilon_1^+ (\epsilon_1^+ - \epsilon_2^+)} \exp(i\epsilon_1^+ t) + \frac{\epsilon_1^+ + 2U^+}{\epsilon_2^+ (\epsilon_1^+ - \epsilon_2^+)} \exp(i\epsilon_2^+ t) \\
-\frac{\epsilon_2^- + 2U^-}{\epsilon_1^- (\epsilon_1^- - \epsilon_2^-)} \exp(i\epsilon_1^- t) + \frac{\epsilon_1^- + 2U^-}{\epsilon_2^- (\epsilon_1^- - \epsilon_2^-)} \exp(i\epsilon_2^- t)
\end{array} \right\}
\]
\[ b_2 = \frac{1}{2} \left\{ -\frac{e_2^+ + 2U^+}{e_1^+ - e_2^+} \exp(\imath e_1^+ t) + \frac{e_2^- + 2U^-}{e_1^- - e_2^-} \exp(\imath e_1^- t) + \frac{e_2^+ + 2U^+}{e_1^- - e_2^-} \exp(\imath e_1^- t) \right\} \]

\[ b_3 = -\frac{\sqrt{3} \Omega}{2} \times \left\{ -\frac{e_2^+ + 2U^+}{e_1^+ (e_1^+ - e_2^+)} \exp(\imath e_1^+ t) + \frac{e_2^- + 2U^-}{e_2^- (e_1^- - e_2^-)} \exp(\imath e_1^- t) + \frac{e_2^- + 2U^-}{e_1^- (e_1^- - e_2^-)} \exp(\imath e_1^- t) \right\}. \]

(\text{Note that the expressions for } b_0 \text{ and } b_3 \text{ do not contain the time-independent terms obtained in integrating } b_1 \text{ and } b_2. \text{ Since the hamiltonian matrix has four non-zero eigenvalues, } b_0 \text{ and } b_3 \text{ cannot contain an additional zero frequency.} \text{ In the strong interaction limit } \Omega/U << 1 \text{ we have}

\begin{align*}
\frac{b_1(t)}{\approx} & \approx - \exp(2\imath U t) \cos(2\Omega t), \\
\frac{b_2(t)}{\approx} & \approx - \imath \exp(2\imath U t) \sin(2\Omega t), \\
\frac{b_0(t)}{\approx} & \approx b_3(t) = O(\Omega/U),
\end{align*}

in accordance with } \omega_1 \approx 2\Omega, \text{ obtained from Eq. (20).}

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