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Multiple-timescale quantum dynamics of many interacting bosons in a dimer

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Abstract
The full quantum dynamics of many bosons that are initially completely localized on one site of a symmetric dimer is investigated in the small tunnelling amplitude regime. The number difference of bosons between the two equivalent sites of the dimer exhibits rich behaviour on different timescales, ranging from small amplitude oscillations and collapses and revivals, to coherent tunnelling. We show that this complex quantum evolution is completely accounted for by analytical expressions. A general formula is obtained at a higher order of perturbation theory for the splitting of quasi-degenerate energy levels. The splittings of the two highest pairs provide the characteristic frequencies of the intermediate and long timescale dynamics.

The boson-Hubbard dimer Hamiltonian has been used for describing both

(i) two coupled intra-molecular symmetric stretching vibrational modes, taking into account the anharmonicity of the bond [1, 2], and
(ii) a Bose–Einstein condensate (BEC) confined in a double-well potential, in the framework of the so-called two-mode approximation [3].

For more details see [4] and references therein. In the BEC context, recent theoretical studies [3, 5] address the full quantum dynamics of the system beyond the mean-field Gross–Pitaevskii equation. Experimentally, this quantum regime has been investigated not in the double-well potential but in an optical lattice [6, 7].

Here, we investigate the many-body quantum evolution of the initial state in which all the bosons are localized on one site of the symmetric dimer, in the case where the tunnelling amplitude between the two traps is relatively small. Although at short timescales the dynamics is identical with mean-field predictions, richer behaviour is observed at larger timescales. On the one hand, the self-trapped dynamics exhibits collapses and revivals, which correspond to the vanishing and the subsequent restoring, respectively, of the oscillation amplitude. Collapses and revivals constitute characteristic signatures of quantum evolution, and they have also been observed in quantum optics [8, 9]. On the other hand, at even longer timescales, coherent tunnelling takes place at the initially unoccupied trap of the double well, due to the Schrödinger-cat relevant eigenstates that are implied by the symmetry of the system. A detailed understanding of this multiple-timescale dynamics is provided in terms of the energy spectrum, through precise analytical relations derived using results obtained from perturbation theory.

The boson-Hubbard Hamiltonian reads

$$\mathcal{H} = -\kappa(b_1^\dagger b_2 + b_2^\dagger b_1) + U(b_1^\dagger b_1^\dagger b_1 b_1 + b_2^\dagger b_2^\dagger b_2 b_2). \tag{1}$$

In this equation $b_i^\dagger$ and b_i are creation and annihilation operators, respectively, of bosons at the ith well ($i = 1, 2$), κ is the tunnelling amplitude between the two sites and U represents the interaction energy between pairs of bosons that are confined in a particular well [4].

From now on we use dimensionless quantities. The interaction energy U defines the unit of energy and the dimensionless tunnelling amplitude $k = \kappa/U$ remains the only parameter in the Hamiltonian. In the BEC case this parameter can be conveniently tuned by varying both κ, through alterations of the power of the laser that induces the barrier of the double-well [10], and U, by tuning the s-wave scattering length through Feshbach resonance [11]. In this study, we restrict ourselves to the small k regime. The dimensionless time is $\tau = \frac{U}{\hbar}t$, and ω represents a dimensionless frequency (the actual frequency is $\omega\frac{U}{\hbar}$).

In figure 1, we show the time evolution of the difference, $N_2 - N_1$, of the number of bosons occupying the two traps, divided by the total number of bosons, N. The initial condition is $N_2 = N$ and $N_1 = 0$. The numerical solution is obtained through direct diagonalization of the Hamiltonian (1) and decomposition of the initial state in the basis of the energy eigenstates. At short timescales we observe small amplitude oscillations around the initial condition (figure 1(a)). This oscillatory dynamics coincides with the corresponding behaviour of the solutions of the discrete nonlinear Schrödinger (DNLS) dimer [12–14], which constitutes the mean-field limit of the boson-Hubbard Hamiltonian (1) [15]. For small k, we are in the strongly self-trapped regime of DNLS. At longer times, while the bosons still remain localized in the initially occupied trap, the full quantum dynamics differentiates from that of DNLS, and exhibits collapses and complete revivals (figure 1(b)). As we see below, the two sufficiently close frequencies that are responsible for the resulting beat at this timescale are provided by the splitting of the second highest quasi-degenerate pair of energy levels. Finally, at very large times (figure 1(c)), all the bosons coherently tunnel back and forth between the two traps (notice the scale on the abscissa of figure 1(c)). This behaviour is due to the fact that there is no eigenstate of the system that is localized in one trap, and as a result the initial state has to be decomposed to the symmetric and antisymmetric combinations of localized states at each trap. The splitting of the quasi-degenerate pair of those higher lying energy levels provides the corresponding tunnelling frequency [2, 16].

Before interpreting these numerical results with the help of analytical solutions, we briefly recall the structure of the energy spectrum of Hamiltonian (1) for small values of k [4]. For a system with N bosons the energy spectrum comprises $N+1$ eigenvalues. At $k = 0$, degenerate pairs of energy levels are formed. The degenerate eigenvalues are given by

$$E_{m^\pm} = 2m^2, \qquad m = \frac{1}{2} \text{ or } 1, \ldots, \frac{N}{2} - 1, \frac{N}{2}, \tag{2}$$

where m is a positive integer or half-integer, depending on whether N is even or odd, respectively. For even N, the ground state is non-degenerate, and has energy $E_{m=0} = 0$. As k increases from zero, the degeneracy is gradually lifted, starting from the lower levels (smaller m), with the sense that for fixed k the amount of splitting $\Delta E_{m^\pm}$ decreases exponentially with m.

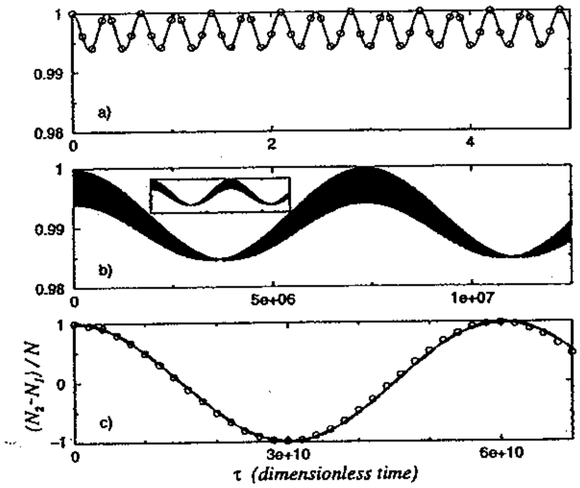

Figure 1. Time evolution of the relative boson number difference between the two sites of the dimer for different timescales. The dimensionless tunnelling amplitude is $k = 0.5$ for a system with $N = 10$. The continuous curves represent numerical results. The inset in (b) and the open circles in (a) and (c) correspond to analytical results provided by equation (3).

(This figure is in colour only in the electronic version)

For example, the splittings $\Delta E_{\frac{1}{2}\pm}$ and $\Delta E_{1\pm}$ are of the order of k and k^2, respectively [4], while for the highest energy levels, $E_{\frac{N}{2}\pm}$, their splitting is of the order of k^N [2]. As a result, the higher energy levels form quasi-degenerate pairs for relatively small k (up to a value of k depending on N and the specific level $E_{m\pm}$ [4]). Below, we derive an expression for the splitting of the arbitrary quasi-degenerate pair, $\Delta E_{m\pm}$, by generalizing the method used in [2] for the calculation of $\Delta E_{\frac{N}{2}\pm}$.

Using perturbative results for the eigenstates of the boson-Hubbard dimer [4], we are able to obtain an analytical formula governing the dynamics of the relative number difference. We have used the standard formula for the evolution of an observable in quantum mechanics, in terms of its matrix elements among the energy eigenstates and the corresponding projections of the initial state. Having available a perturbative expansion for the energy eigenstates allows a successive calculation of different order terms describing the dynamics of the observable. Leaving the details of the calculation for an extended article [17], where different initial conditions are also considered, we show the final result for our present case up to second order in k at the amplitudes of the corresponding Bohr frequencies provided by the energy spectrum of Hamiltonian (1):

$$\frac{N_2 - N_1}{N} = \cos(\omega_0\tau) + \frac{k^2}{2(N-1)^2}\left[\frac{N}{2}[\cos(\omega_1\tau) - \cos(\omega_0\tau)] + 2\cos(\omega_\mu\tau)\cos\left(\frac{\omega_1}{2}\tau\right) - \cos(\omega_1\tau) - \cos(\omega_0\tau)\right]. \tag{3}$$

In this expression, the frequencies ω_0 and ω_1 correspond to the splittings $\Delta E_{\frac{N}{2}\pm}$ and $\Delta E_{(\frac{N}{2}-1)\pm}$ of the two highest quasi-degenerate energy pairs, respectively (see equations (8) and (9) below). The other frequency ω_μ represents the difference $E_{\frac{N}{2}\pm} - E_{(\frac{N}{2}-1)\pm}$, which, up to second order in k, is given by [4]

$$\omega_\mu = 2(N-1) - k^2 \frac{N+1}{N^2-4N+3}. \tag{4}$$

Before we proceed to the derivation of the analytical expressions providing ω_0 and ω_1, we comment on some characteristic terms of equation (3). This formula provides an accurate description of the quantum dynamics, as can be seen from figure 1. The frequency ω_μ (of order k^0) is much larger than both ω_0 (of order k^N) and ω_1 (of order k^{N-2}), and is responsible for the short time dynamics appearing in figure 1(a). If we consider that ω_0 and ω_1 are small enough to be neglected, i.e. $\omega_0 = 0$ and $\omega_1 = 0$, then equation (3) reduces [17] to the corresponding result of DNLS [14]. On the other hand, the $\cos(\frac{\omega_1}{2}\tau)$ which multiplies the higher frequency term, $\cos(\omega_\mu\tau)$, provides the beat that is responsible for the exhibited collapses and revivals at timescales determined by ω_1 (figure 1(b)). All the harmonic functions containing the frequencies ω_μ and ω_1 in equation (3) are of small amplitude (of the order of k^2) and are unable to completely transfer the bosons from one trap to the other (which requires oscillations of $\frac{N_2-N_1}{N}$ from 1 to -1). Only the first term of the right-hand side of equation (3), $\cos(\omega_0\tau)$, can provide this coherent tunnelling, that, consequently, takes place at timescales determined by ω_0 (figure 1(c)).

The frequency $\omega_0 = \Delta E_{\frac{N}{2}\pm}$ appearing in equation (3) is already known from Bernstein *et al* [2]. We can calculate the $\omega_1 = \Delta E_{(\frac{N}{2}-1)\pm}$ by applying similar arguments as those used in that work. In particular, we derive a more general result for the splitting of any quasi-degenerate pair, $\Delta E_{m\pm}$, and, from this, we directly obtain ω_1 for $m = \frac{N}{2} - 1$. Since we are following the same lines as in [2], we merely give the main points of the calculation here.

For our purposes, we define the diagonal $(N+1) \times (N+1)$ matrix H_0 with elements $(H_0)_{n,n} = 2n^2$, $n = -\frac{N}{2}, \ldots, \frac{N}{2}$, and the tridiagonal coupling matrix V with non-zero elements $V_{n,n-1} = k\sqrt{\frac{N}{2}(\frac{N}{2}+1) - n(n-1)} = V_{n-1,n}$ (all the other matrix elements of V are zero). H_0 corresponds to the unperturbed Hamiltonian (1) for $k = 0$, and the symmetric V describes the tunnelling term (apart from a sign that has no effect in the following calculation). For any particular splitting of interest, $\Delta E_{m\pm}$, $m = 0$ or $\frac{1}{2}, \ldots, \frac{N}{2}$, we define the diagonal matrix $L_m = H_0 - E_m I$, where $E_m = 2m^2$ is the doubly degenerate eigenvalue and I is the $(N+1) \times (N+1)$ identity matrix. We then have $(L_m)_{n,n} = 0$ for $n = \pm m$, while $(L_m)_{n,n} = 2(n^2 - m^2)$ for $n \neq \pm m$. We also define the diagonal matrix

$$(L_m^{-1})_{n,n} = \begin{cases} 0, & n = \pm m \\ \dfrac{1}{2(n^2-m^2)}, & n \neq \pm m. \end{cases} \tag{5}$$

Taking into account the arguments of [2], we obtain that the splitting $\Delta E_{m\pm}$ is provided at the $2m$th order of perturbation theory, through the non-diagonal elements, $\Omega_{1,2} = \Omega_{2,1}$, of the projection on the 2×2 subspace of degeneracy, of the matrix that describes the coupling between the two degenerate (at $k = 0$) states $|\Psi_m^1\rangle$ and $|\Psi_m^2\rangle$. These are the states containing $\frac{N}{2} + m$ bosons in one well and $\frac{N}{2} - m$ in the other: $|\Psi_m^1\rangle \equiv |N_1 = \frac{N}{2} + m, N_2 = \frac{N}{2} - m\rangle$ and $|\Psi_m^2\rangle \equiv |N_1 = \frac{N}{2} - m, N_2 = \frac{N}{2} + m\rangle$. In particular,

$$\begin{aligned}\Delta E_{m\pm} = 2|\Omega_{1,2}| &= 2|V(L_m^{-1}V)^{2m-1}|_{m\to -m} = 2|V_{m,m-1}(L_m^{-1})_{m-1,m-1} \\ &\quad \times V_{m-1,m-2}(L_m^{-1})_{m-2,m-2} \times \cdots \times (L_m^{-1})_{-m+1,-m+1} V_{-m+1,-m}|.\end{aligned} \tag{6}$$

The physical interpretation of this expression is the following: since the coupling V represents transfer of just a single boson from one well to the other, the 'shortest' (most direct) way to directly couple the degenerate states $|\Psi_m^1\rangle$ and $|\Psi_m^2\rangle$ by moving one boson per step—as indicated by the perturbation—involves $2m$ steps, provided by the $2m$ matrix elements of V in

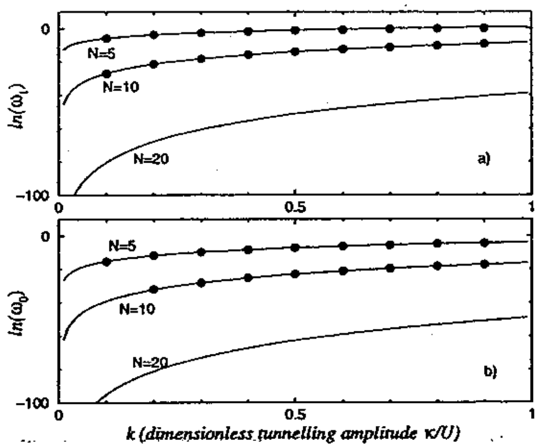

Figure 2. The logarithms of the characteristic frequencies (a) ω_1, determining the collapses and revivals at intermediate timescales, and (b) ω_0, determining the coherent tunnelling at very long timescales, as a function of k for different numbers, N, of bosons. The continuous curves show the analytical results obtained from equations (9) and (8), respectively, while the filled circles correspond to direct numerical calculations.

equation (6). This is the reason that the degeneracy is lifted at $2m$th order. The specific result of equation (6) is obtained by the particular form of the matrix that couples the $|\Psi_m^1\rangle$ and $|\Psi_m^2\rangle$, and represents the unique strongest connection between them [2].

Taking into account the matrix elements of V and L_m^{-1}, the calculation of the product appearing in equation (6) is straightforward. The final result is

$$\Delta E_{m^\pm} = \frac{k^{2m}}{2^{2m-2}[(2m-1)!]^2} \frac{(\frac{N}{2}+m)!}{(\frac{N}{2}-m)!}. \tag{7}$$

For the special cases $m = 1$ and $\frac{1}{2}$, we obtain that $\Delta E_{1^\pm} = 2|V_{1,0}(L_1^{-1})_{0,0}V_{0,-1}| = k^2\frac{N}{2}(\frac{N}{2}+1)$ and $\Delta E_{\frac{1}{2}^\pm} = 2V_{\frac{1}{2},-\frac{1}{2}} = 2k\sqrt{\frac{N}{2}(\frac{N}{2}+1)+\frac{1}{4}} = k(N+1)$, in accordance with the perturbative results presented in [4]. Regarding the frequencies ω_0 and ω_1 appearing in expression (3), equation (7) yields that for $m = \frac{N}{2}$

$$\omega_0 = \Delta E_{\frac{N}{2}^\pm} = k^N \frac{N}{2^{N-2}(N-1)!}, \tag{8}$$

while for $m = \frac{N}{2} - 1$

$$\omega_1 = \Delta E_{(\frac{N}{2}-1)^\pm} = k^{N-2} \frac{(N-1)(N-2)}{2^{N-4}(N-3)!}. \tag{9}$$

The result (8) coincides with that of [2].

In figure 2, we compare the analytical expressions (8) and (9) with the corresponding splittings obtained through direct diagonalization of Hamiltonian (1). We see that the above formulas are in excellent agreement with the numerical results. Although the long timescale phenomena (collapses/revivals and coherent tunnelling) occur for systems with any number of bosons, the time needed for their manifestation is abruptly increased with N. Since the Hamiltonian (1) conserves the number of atoms, in the BEC case it does not allow losses of the condensate due to decoherence, finite temperature effects etc. This fact, combined with the rapid decrease of the characteristic frequencies ω_1 and ω_0 with the number of bosons, prevents the observation of the intermediate and long time behaviour, as revealed in figures 1(b) and (c), in current BEC experiments. However, these phenomena may be relevant in the context of the intra-molecular symmetric stretching modes, where a few vibrational quanta can be excited.

In summary, we have discussed the full quantum dynamics of a system of many interacting bosons initially occupying one site of a symmetric dimer. Rich behaviour is exhibited on multiple timescales. These results make contact with previous multiple-timescale investigations of a related problem [18], as well as with a study of BEC tunnelling [5] in which the exponential dependence of the tunnelling time on atom number has been numerically demonstrated. Accurate analytical results have been obtained in the present paper that explain in detail the different characteristics of the evolution and provide a full physical interpretation of the observed behaviour. The long and intermediate timescale dynamics, which differentiates from the corresponding mean-field evolution, is determined by small splittings of the highest lying quasi-degenerate pairs of energy levels. An analytical formula has been derived for the splitting of any quasi-degenerate level that appears in the energy spectrum at relatively small values of tunnelling amplitude.

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Note added in proof. The result of equation (7) has been alternatively derived in equation (29) of [19].

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