

Dynamical creation of entangled bosonic states in a double well

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Abstract

We study the creation of a bosonic N00N state from the evolution of a Fock state in a double well. While noninteracting bosons disappear quickly in the Hilbert space, the evolution under the influence of a Bose–Hubbard Hamiltonian is much more restricted. This restriction is caused by the fragmentation of the spectrum into a high-energy part with doubly degenerate levels and a nondegenerate low-energy part. This degeneracy suppresses transitions to states of the high-energy part of the spectrum. At a moderate interaction strength, this effect supports strongly the dynamical formation of a N00N state. The N00N state is suppressed in a double well, where one well has attractive and the other has repulsive interaction, because the double degeneracy is absent.

1. Introduction

Recent experiments on ultracold gases in optical potentials [1–3] and experiments on photons in microwave cavities [4, 5] have demonstrated that it is possible to prepare a Fock state as a pure state in a finite-dimensional system. After the preparation of the Fock state, the parameters of the system can suddenly be changed (performing a ‘quench’) such that the Fock state is not an eigenstate of the new system Hamiltonian H . Then, the evolution of the many-body state due to the evolution operator $\exp(-iHt)$ will lead to a random walk inside the available Hilbert space. The visited states include other Fock states as well as superpositions of Fock states. Typical questions in this context are: what is the probability for visiting different states and how is this affected by the interaction of the particles? A natural quantity for measuring this probability is the spectral density function of the Hamiltonian H with respect to the initial Fock state [6–8].

A classical candidate for modelling the evolution of a Fock state is the Hubbard model [9, 10]. The corresponding discrete Hamiltonian describes the tunnelling of a particle between neighbouring potential wells and a local particle–particle interaction. The Hubbard model for bosons (the Bose–Hubbard model) was realized as an atomic system in an optical lattice [11]. A possible realization of the Bose–Hubbard model by photons in coupled microwave cavities was proposed recently by Hartmann *et al* [12]. An anharmonicity

of the microwave cavities plays the role of the photon–photon interaction [8].

The simplest system for discussing the evolution of a Fock state within the Hubbard model is a double well, where particles can tunnel between the two wells. For N bosons the underlying Hilbert space is spanned by the $(N+1)$ -dimensional Fock base $\{|0, N\rangle, |1, N-1\rangle, \dots, |N, 0\rangle\}$, where l bosons are in one well and $N-l$ in the other well [13–16]. The initial state is prepared as a Fock state, where all the bosons are in one of the two wells (i.e. $|0, N\rangle$ or $|N, 0\rangle$), while the tunnelling between the wells is turned off. To start the evolution, a ‘quench’ is provided by switching on the tunnelling between the two wells. This is realized by a sudden reduction in the potential barrier between the wells in an atomic system [1] or by connecting the two microwave cavities with an optical fibre [8, 12, 17]. A similar experiment was performed with two atomic clouds subject to weak interaction and separated by an adjustable potential barrier [18, 19].

On the theoretical side, mean-field descriptions of the Bose–Hubbard model, such as a Hartree approximation or the Gross–Pitaevskii equation, may work well for clouds with many bosons and weak boson–boson interaction [14]. However, they provide a rather poor approximation for the dynamics of small many-body systems (cf [13]). This was also observed in a recent study by Streltsov *et al* who compared the results of a simple Hartree (Gross–Pitaevskii) approximation with a sophisticated (multiconfigurational time-dependent)

Hartree approximation for bosons [20]. The latter reveals that the bosonic clouds are related to superpositions of Fock states in the form of NOON states

$$|\text{NOON}\rangle = \frac{1}{\sqrt{2}}[|0, N\rangle + e^{i\phi N}|N, 0\rangle]. \quad (1)$$

In the following, we will study the Hubbard dynamics of bosons in a double well in more detail. In particular, we are interested in the connection of spectral properties and the formation of NOON states, based on a Fock state with all particles in one well as the initial state. To avoid problems with uncontrolled approximations, we will rely on a full quantum calculation. An exact solution is available in a Fock-state base, as described previously in [6, 8].

The paper is organized as follows. In section 2, the model based on the Bose–Hubbard Hamiltonian is defined, and in section 2.1, the dynamics of an isolated quantum system is explained. Then, we discuss the dynamics of a noninteracting Bose gas in section 3, and the dynamics of an interacting Bose gas in section 4. The latter is divided into a study of a symmetric double well (section 4.1) and a double well with mixed interaction, where one well has attractive and the other repulsive interaction (section 4.2). Finally, we summarize the results of our calculation in section 5 and discuss them in section 6.

2. The model

The many-body Hamiltonian \hat{H} of N bosons with mass m reads

$$\hat{H} = \sum_{j=1}^N \left[\frac{\mathbf{p}_j^2}{2m} + V(\mathbf{r}_j) \right] + \sum_{j,k=1}^N U(\mathbf{r}_j, \mathbf{r}_k), \quad (2)$$

where \mathbf{p}_j is the momentum of a boson, $V(\mathbf{r}_j)$ is the one-body potential of the double well and $U(\mathbf{r}_j, \mathbf{r}_k)$ is the two-body interaction potential. For the latter, we assume that it decays very quickly with the distance $|\mathbf{r}_j - \mathbf{r}_k|$ of the particles. This implies that particles located in different wells do not interact with each other. In a general situation, the two-body interaction can be attractive in one and repulsive in the other well. Then, the many-body Hamiltonian is expressed in Fock-state representation as

$$\begin{aligned} & \int \cdots \int \langle N-k, k | \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N \rangle \langle \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N | \hat{H} \\ & \quad \times | \mathbf{r}'_1, \mathbf{r}'_2, \dots, \mathbf{r}'_N \rangle \langle \mathbf{r}'_1, \mathbf{r}'_2, \dots, \mathbf{r}'_N | \\ & \quad \times | N-k', k' \rangle d^3 \mathbf{r}_1 \cdots d^3 \mathbf{r}'_N \\ & = \langle N-k, k | H | N-k', k' \rangle. \end{aligned} \quad (3)$$

For the new Hamiltonian H , which acts in the Hilbert space spanned by the Fock base, we can use a generalized Bose–Hubbard Hamiltonian with different local interaction parameters U_1, U_2 in the corresponding wells as a reasonable approximation:

$$H = J(a_1^\dagger a_2 + a_2^\dagger a_1) + U_1(a_1^\dagger a_1)^2 + U_2(a_2^\dagger a_2)^2, \quad (4)$$

where $a_j^\dagger(a_j)$ are creation (annihilation) operators for bosons in the Fock states. H , which describes tunnelling between the two wells and the local interaction inside the well with interaction strength U_j , gives us a complete quantum description of the different Fock states and their superpositions. In particular, we

can employ it to study the evolution of a Fock state to a NOON state of equation (1). This will be used subsequently for two special cases. The first case is a symmetric double well, where $U_1 = U_2$. The second case has opposite signs of interactions $U_1 = -U_2$, which describes an attractive interaction in one well and a repulsive interaction in the other well.

2.1. Evolution of isolated systems

We consider a system which is isolated from the environment. Furthermore, we assume that the system lives in an $(N+1)$ -dimensional Hilbert space. With the initial state $|\Psi_0\rangle$, we can obtain for the time evolution of the state

$$|\Psi_t\rangle = e^{-iHt} |\Psi_0\rangle \quad (5)$$

or the evolution of the return probability $|\langle \Psi_0 | \Psi_t \rangle|^2$ with the amplitude

$$\langle \Psi_0 | \Psi_t \rangle = \langle \Psi_0 | e^{-iHt} | \Psi_0 \rangle. \quad (6)$$

In general, the amplitude $\langle \Psi_1 | \Psi_t \rangle$ can be expressed via an integral transformation of the resolvent as

$$\langle \Psi_1 | \Psi_t \rangle = \langle \Psi_1 | e^{-iHt} | \Psi_0 \rangle = \int_{\Gamma} \langle \Psi_1 | (z - H)^{-1} | \Psi_0 \rangle e^{-izt} dz, \quad (7)$$

where the contour Γ encloses all the eigenvalues E_j ($j = 0, 1, \dots, N$) of H . With the corresponding eigenstates $|E_j\rangle$, the spectral representation of the resolvent is a rational function:

$$\langle \Psi_1 | (z - H)^{-1} | \Psi_0 \rangle = \sum_{j=0}^N \frac{\langle \Psi_1 | E_j \rangle \langle E_j | \Psi_0 \rangle}{z - E_j} = \frac{P_N(z)}{Q_{N+1}(z)}, \quad (8)$$

where $P_N(z), Q_{N+1}(z)$ are polynomials in z of orders $N, N+1$, respectively, with the common denominator

$$Q_{N+1}(z) = \prod_{j=0}^N (z - E_j).$$

These polynomials are readily evaluated by the recursive projection method (RPM) [6].

The expression in equation (8) for $|\Psi_1\rangle = |\Psi_0\rangle$ can be interpreted as the bosonic spectral density $\rho_\epsilon(E)$ with respect to the state $|\Psi_0\rangle$:

$$\begin{aligned} \rho_\epsilon(E) &= \frac{1}{\pi} \text{Im} \langle \Psi_0 | (E - i\epsilon - H)^{-1} | \Psi_0 \rangle \\ &= \frac{\epsilon}{\pi} \sum_{j=0}^N \frac{|\langle \Psi_0 | E_j \rangle|^2}{\epsilon^2 + (E - E_j)^2}. \end{aligned} \quad (9)$$

The amplitude of the return probability then reads as the Fourier transform of the spectral density

$$\langle \Psi_0 | \Psi_t \rangle = \lim_{\epsilon \rightarrow 0} \int \rho_\epsilon(E) e^{-iEt} dE. \quad (10)$$

Analogously, the overlap $\langle \Psi_1 | \Psi_t \rangle$ reads in terms of the resolvent

$$\langle \Psi_1 | \Psi_t \rangle = \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \int \text{Im} \langle \Psi_1 | (E - i\epsilon - H)^{-1} | \Psi_0 \rangle e^{-iEt} dE, \quad (11)$$

with

$$\begin{aligned} & \lim_{\epsilon \rightarrow 0} \text{Im} \langle \Psi_1 | (E - i\epsilon - H)^{-1} | \Psi_0 \rangle \\ &= \pi \sum_j \langle \Psi_1 | E_j \rangle \langle E_j | \Psi_0 \rangle \delta(E - E_j), \end{aligned} \quad (12)$$

provided that the matrix elements are symmetric. The latter is the case for the Hubbard Hamiltonian.

The purpose of the subsequent calculation is to determine the evolution of the Fock state under the influence of the Bose–Hubbard Hamiltonian of equation (4). In general, this is expressed in the Fock base as

$$|\Psi_t\rangle = \sum_{j=0}^N c_j(t) |N-j, j\rangle, \quad (13)$$

with coefficients $c_j(t) = \langle N-j, j | \Psi_t \rangle$. For the NOON state we only need to focus on the coefficients $c_0(t)$ and $c_N(t)$. Although we do not anticipate that the other coefficients vanish, for the existence of a NOON state it is sufficient to have simultaneously $c_0(t), c_N(t) \neq 0$. Moreover, the resulting entangled state may in general not have $c_0(t) = c_N(t)$ but is still called a NOON state.

Comparing the result in equation (13) with the expressions in equations (10), (11) and (12), it turns out that the Fourier transforms of $c_0(t)$ and $c_N(t)$ are just the imaginary parts of the matrix elements of the resolvent:

$$\begin{aligned} \tilde{c}_0(E) &= \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \text{Im} \langle N, 0 | (E - i\epsilon - H)^{-1} | N, 0 \rangle \\ &= \sum_j \langle N, 0 | E_j \rangle \langle E_j | N, 0 \rangle \delta(E - E_j) \end{aligned} \quad (14)$$

and

$$\begin{aligned} \tilde{c}_N(E) &= \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \text{Im} \langle 0, N | (E - i\epsilon - H)^{-1} | N, 0 \rangle \\ &= \sum_j \langle 0, N | E_j \rangle \langle E_j | N, 0 \rangle \delta(E - E_j). \end{aligned} \quad (15)$$

These two expressions will be called spectral coefficients, where $\tilde{c}_0(E)$ measures the relative weight $|\langle N, 0 | E_j \rangle|^2$. Integration over the energy E gives 1 for this coefficient. The coefficient $\tilde{c}_N(E)$ measures the correlation between $|N, 0\rangle$ and $|0, N\rangle$ due to the product $\langle 0, N | E_j \rangle \langle E_j | N, 0 \rangle$. The latter is real for a symmetric Hamiltonian. Integration over the energy E gives 0 for this coefficient.

3. Double well: noninteracting Bose gas

The Bose–Hubbard Hamiltonian has two simple limits: the local limit $J = 0$ and the noninteracting limit $U_1 = U_2 = 0$. In the local limit for a symmetric double well with $U_1 = U_2$ pairs, Fock states $|N-k, k\rangle, |k, N-k\rangle$ are doubly degenerate eigenstates with energy $E_k = U[(N-k)^2 + k^2]$. A perturbation by a small tunnelling term will break the degeneracy. This effect is stronger at lower energies because the parabolic spectrum is denser there. This agrees with a numerical study [13]. The fact that the states $|N, 0\rangle$ and $|0, N\rangle$ are very close in energy may support the formation of a NOON state.

In the absence of the particle–particle interaction the Bose–Hubbard Hamiltonian H_t (i.e. the Hamiltonian in

equation (4) with $U_1 = U_2 = 0$) only describes tunnelling. A straightforward calculation shows that the eigenstate $|N-k; k\rangle$ of H_t with $H_t |N-k; k\rangle = J(N-2k) |N-k; k\rangle$ has an overlap with the Fock states $|N, 0\rangle$ and $|0, N\rangle$ as

$$\begin{aligned} \langle N, 0 | N-k; k \rangle &= 2^{-N/2} \sqrt{\binom{N}{k}}, \\ \langle 0, N | N-k; k \rangle &= (-1)^k 2^{-N/2} \sqrt{\binom{N}{k}}. \end{aligned} \quad (16)$$

This implies that the spectral coefficients of equations (14) and (15) have a binomial form:

$$\tilde{c}_0(E) = 2^{-N} \sum_{k=0}^N \binom{N}{k} \delta(E + J(2k - N)), \quad (17)$$

$$\tilde{c}_N(E) = 2^{-N} \sum_{k=0}^N \binom{N}{k} (-1)^k \delta(E + J(2k - N)). \quad (18)$$

A Fourier transformation reveals a periodic behaviour of the evolutionary coefficients as

$$\begin{aligned} c_0(t) &= \langle N, 0 | e^{-iHt} | N, 0 \rangle = \cos^N(Jt), \\ c_N(t) &= \langle 0, N | e^{-iHt} | N, 0 \rangle = (-i)^N \sin^N(Jt). \end{aligned} \quad (19)$$

Thus, the evolution of the Fock state leads to a NOON state with a probability that decays exponentially with N . This is a consequence of the fact that for an increasing N , the particles disappear in the $(N+1)$ -dimensional Hilbert space because there is no constraint due to interaction.

4. Double well: interacting Bose gas

The double well with the two Fock states $|N, 0\rangle, |0, N\rangle$ as possible initial states can be treated within the RPM. This method is based on a systematic expansion of the resolvent $\langle \Psi_1 | (z - H)^{-1} | \Psi_0 \rangle$, starting from the initial base $\{|N, 0\rangle, |0, N\rangle\}$. The method can also be understood as a directed random walk in Hilbert space. This means that in comparison with the conventional random walk the directed random walk of the RPM visits a subspace \mathcal{H}_{2j} only once and never returns to it. In terms of N bosons, distributed over the double well, the subspace \mathcal{H}_{2j} is spanned by the base $\{|N-j, j\rangle, |j, N-j\rangle\}$. A step from \mathcal{H}_{2j} to \mathcal{H}_{2j+2} is given by the Hamiltonian H in such a way that \mathcal{H}_{2j+2} is created by acting H on \mathcal{H}_{2j} (see the [appendix](#)). This step is provided by the tunnelling of a single boson. Thus, the directed random walk follows a path with increasing numbers j . The directed random walk is the main advantage of the RPM which allows us to calculate the matrix elements $\langle \Psi_0 | (z - H)^{-1} | \Psi_0 \rangle, \langle \Psi_1 | (z - H)^{-1} | \Psi_0 \rangle$ of the resolvent on an $(N+1)$ -dimensional Hilbert space exactly.

4.1. Symmetric double well

Now we choose $U_1 = U_2 \equiv U$ for the Bose–Hubbard Hamiltonian. Assuming that N is even, all projected spaces \mathcal{H}_{2j} are two-dimensional and spanned by $\{|N-j, j\rangle, |j, N-j\rangle\}$ ($j = 0, \dots, N/2$). This leads to a recurrence relation in

the base of the two Fock states ($|N, 0\rangle, |0, N\rangle$) as initial states. The recurrence relation reads (see the [appendix](#))

$$g_{k+1} = \begin{pmatrix} a_{k+1} & b_{k+1} \\ b_{k+1} & a_{k+1} \end{pmatrix}, \quad g_0 = \frac{1}{z - UN^2/2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (k = 0, 1, \dots, N/2 - 1), \quad (20)$$

with coefficients

$$a_{k+1} = \frac{z - \tilde{f}_{k+1} - J^2 a_k (N/2 + k + 1)(N/2 - k)}{[z - \tilde{f}_{k+1} - J^2 a_k (N/2 + k + 1)(N/2 - k)]^2 - J^4 b_k^2 (N/2 + k + 1)^2 (N/2 - k)^2} \quad (21)$$

$$b_{k+1} = \frac{J^2 b_k (N/2 + k + 1)(N/2 - k)}{[z - \tilde{f}_{k+1} - J^2 a_k (N/2 + k + 1)(N/2 - k)]^2 - J^4 b_k^2 (N/2 + k + 1)^2 (N/2 - k)^2} \quad (22)$$

and

$$\tilde{f}_{k+1} = U(N/2 + k + 1)^2 + U(N/2 - k - 1)^2.$$

The iteration terminates after $N/2$ steps with

$$g_{N/2} = \begin{pmatrix} a_{N/2} & b_{N/2} \\ b_{N/2} & a_{N/2} \end{pmatrix}, \quad (23)$$

where

$$a_{N/2} = \langle N, 0 | (z - H)^{-1} | N, 0 \rangle = \langle 0, N | (z - H)^{-1} | 0, N \rangle \quad (24)$$

and

$$b_{N/2} = \langle 0, N | (z - H)^{-1} | N, 0 \rangle = \langle N, 0 | (z - H)^{-1} | 0, N \rangle. \quad (25)$$

An invariance of the recurrence relation under the following simultaneous sign changes in equations (21) and (22) exists:

$$z \rightarrow -z, \quad U \rightarrow -U, \quad a_j \rightarrow -a_j, \quad b_j \rightarrow -b_j. \quad (26)$$

This implies that a change from a repulsive to an attractive Hubbard interaction results in a mirror image with respect to energy of the spectral coefficients

$$\tilde{c}_0(E, U) = \tilde{c}_0(-E, -U), \quad \tilde{c}_N(E, U) = \tilde{c}_N(-E, -U). \quad (27)$$

4.2. Double well with mixed interaction

In the case $U_1 = -U_2 \equiv U$, we have one more variable, namely a_k, b_k and c_k with the following recurrence relations (see the [appendix](#)):

$$g_{k+1} = \begin{pmatrix} a_{k+1} & c_{k+1} \\ c_{k+1} & b_{k+1} \end{pmatrix}, \quad g_0 = \frac{1}{z} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (k = 0, 1, \dots, N/2 - 1), \quad (28)$$

with matrix elements ($n = N/2$):

$$a_{k+1} = \frac{z + 4Un(k+1) - J^2(n+k+1)(n-k)b_k}{D_{k+1}} \quad (29)$$

$$b_{k+1} = \frac{z - 4Un(k+1) - J^2(n+k+1)(n-k)a_k}{D_{k+1}} \quad (30)$$

$$c_{k+1} = -\frac{J^2(n+k+1)(n-k)c_k}{D_{k+1}} \quad (31)$$

and with

$$D_{k+1} = [z - 4Un(k+1) - J^2 a_k (n+k+1)(n-k)] \times [z + 4Un(k+1) - J^2 b_k (n+k+1)(n-k)] - J^4 c_k^2 (n+k+1)^2 (n-k)^2.$$

The final result of the iteration is

$$g_{N/2} = \begin{pmatrix} a_{N/2} & b_{N/2} \\ b_{N/2} & c_{N/2} \end{pmatrix}, \quad (32)$$

with

$$a_{N/2} = \langle N, 0 | (z - H)^{-1} | N, 0 \rangle, \quad (33)$$

$$b_{N/2} = \langle 0, N | (z - H)^{-1} | 0, N \rangle,$$

$$c_{N/2} = \langle N, 0 | (z - H)^{-1} | 0, N \rangle = \langle 0, N | (z - H)^{-1} | N, 0 \rangle. \quad (34)$$

5. Results

The iteration of equations (21) and (22) for a symmetric double well and the iteration of equations (29)–(31) for a double well with mixed interaction give us, according to equations (24), (25) and (33), (34), the following four matrix elements of the resolvent:

$$\langle N, 0 | (z - H)^{-1} | N, 0 \rangle, \quad \langle 0, N | (z - H)^{-1} | 0, N \rangle, \\ \langle 0, N | (z - H)^{-1} | N, 0 \rangle = \langle N, 0 | (z - H)^{-1} | 0, N \rangle.$$

These are rational functions of z as shown in equation (7). For N bosons these are lengthy expressions with $N + 1$ poles. Therefore, it is convenient to present the results as plots with respect to energy. The examples of the spectral coefficients $\tilde{c}_0(E)$ and $\tilde{c}_N(E)$ are shown for a symmetric double well with 100 bosons in figure 1 and with 20 bosons in figure 2, and for a double well with mixed interaction for 100 bosons in figure 3. A larger number of bosons show a richer spectral structure. The diagonal coefficient $\tilde{c}_0(E)$ in the case of 100 bosons is remarkably different from the off-diagonal coefficient $\tilde{c}_N(E)$ because the latter does not have spectral weight from eigenstates whose energy E_j is larger than the energy of the initial Fock state $\bar{E} = UN^2$. The reason for this feature is the double degeneracy of the eigenvalues mentioned in section 3: the signs of the product $\langle 0, N | E_j \rangle \langle E_j | N, 0 \rangle$ for adjacent eigenvalues are opposite to each other. Since the eigenvalues get closer pairwise as we increase their energy, the contribution of the two levels cancels each other for each pair inside the sum of equation (15). This interaction effect is also visible for 20 bosons (figure 2), although the cancellation is incomplete then due to a larger level distance. This can be considered as an effect of spectral fragmentation, where the spectrum has a nondegenerate low-energy part and a degenerate high-energy part, caused by the competition of tunnelling and interaction.

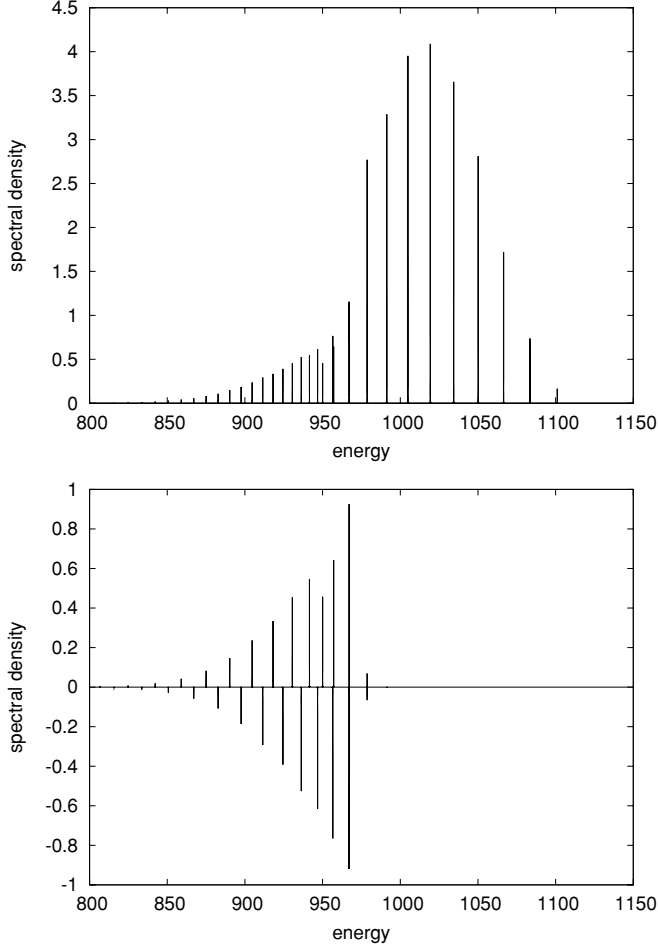


Figure 1. Spectral coefficients of equations (14) and (15) for 100 bosons with $U/J \approx 0.023$ and $\epsilon = 0.01$. The energy of the initial Fock state is $\bar{E} = 1000$. The spectral fragmentation appears around $E \approx 970$, where the levels are nondegenerate at lower energies but almost degenerate for higher energies. This is a consequence of the competition between tunnelling and interaction, in which the latter wins at higher energies.

The contribution of the two Fock states $|0, N\rangle$, $|N, 0\rangle$ to the evolution in equation (13) is given by the coefficients $c_0(t) = \langle N, 0 | \Psi_t \rangle$, $c_N(t) = \langle 0, N | \Psi_t \rangle$. In figure 4, the real parts of these coefficients are plotted for 100 bosons. Their evolution indicates a collapse and revival behaviour. The latter is mainly due to a rapidly changing phase factor, since $|c_0(t)|$, $|c_N(t)|$ has a much smoother behaviour. This allows us to plot the evolution of the two-dimensional vector $(|c_0(t)|, |c_N(t)|)$ to characterize the dynamics of the NOON state. Examples of the complex dynamical behaviour are shown for 100 bosons and for 20 bosons in figure 5. These results suggest a statistical description with a probability $P(|c_0(t)|, |c_N(t)|)$ that measures how often certain values of $|c_0(t)|$, $|c_N(t)|$ are visited during the evolution in a period of time. The result for 20 bosons is plotted in figure 6 for $U = 0.1$, $J = \sqrt{15}$. It indicates that there is a strong correlation between the coefficients, where the most favoured values are $|c_0(t)| \approx |c_N(t)| \approx 0.35$.

For a double well with interaction strength $\pm U$ the spectrum is different because of the absence of double degeneracy of the eigenvalues (cf figure 3). There are

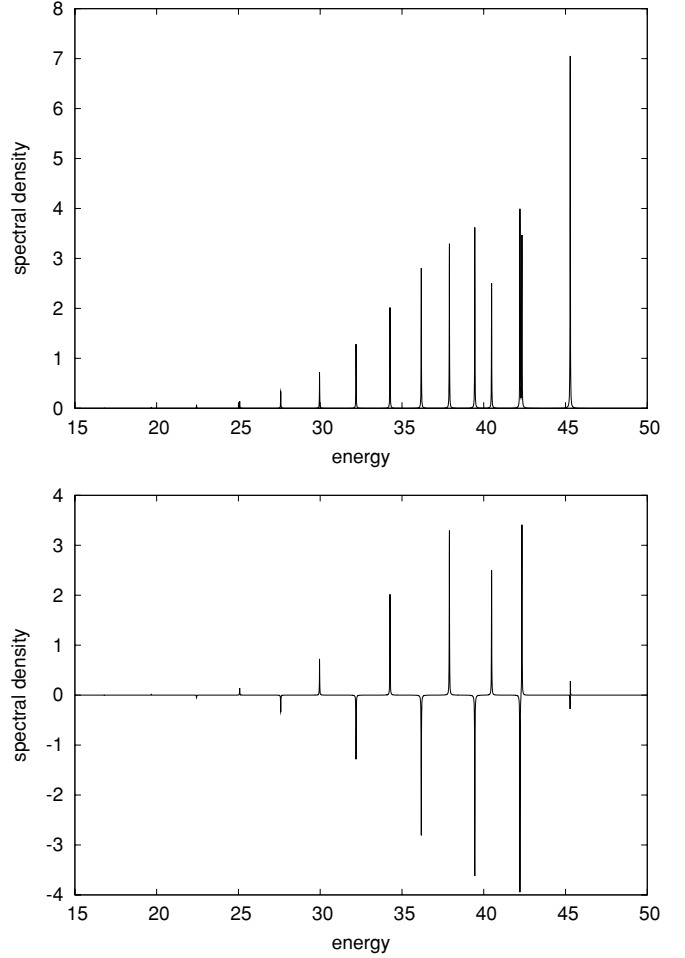


Figure 2. Spectral coefficients for 20 bosons with $U/J \approx 0.1$ and $\epsilon = 0.01$. The energy of the initial Fock state is $\bar{E} = 40$. The almost degenerate states appear above 42.

two ‘bands’, one around $E = UN^2$ and the other around $E = -UN^2$, where the widths of the bands are characterized by the tunnelling rate J . Moreover, the off-diagonal part $\tilde{c}_N(E)$ appears closer to zero energy and its values are very small. This indicates that the off-diagonal part overlaps with energy levels which are different from those of the diagonal part $\tilde{c}_0(E)$. For the evolution only the latter contribute substantially, preventing the system from creating a NOON state.

6. Discussion and conclusions

In order to understand the evolution of an isolated many-body bosonic system, we start with noninteracting bosons (i.e. $U_1 = U_2 = 0$) of section 3. The spectral properties are characterized by (i) equidistant energy levels with distance J and (ii) a binomial weight distribution of the energy levels. The evolution of a Fock state is characterized by a periodic behaviour with a single frequency $\omega = J/2\pi$ as a direct consequence of the equidistant energy levels. The amplitudes for visiting the initial Fock state $|N, 0\rangle$ or the complementary Fock state $|0, N\rangle$ vary with $\cos^N(Jt)$ or $(-i)^N \sin^N(Jt)$, respectively. This implies for a large number N of bosons that (i) these states are visited only for a very short period

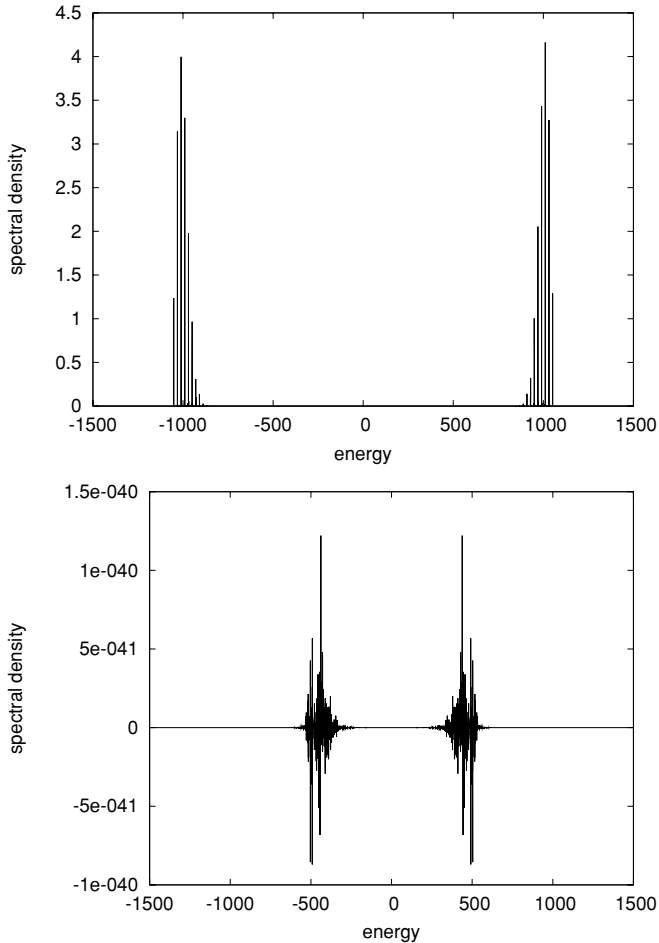


Figure 3. Spectral coefficients for 100 bosons in a double well with $U/J \approx \pm 0.023$ and $\epsilon = 0.01$. The energy of the Fock states $|0, N\rangle$ and $|N, 0\rangle$ is $\bar{E} = \pm 1000$, respectively.

of time and (ii) the two Fock states are visited at different times. Thus, the formation of a NOON state is very unlikely for noninteracting bosons.

A simple qualitative picture for the general evolution of the Fock state is the random walk in Hilbert space. In the case of noninteracting bosons the particles can walk independently of each other, which enables them to explore the entire Hilbert space spanned by the Fock states without restriction. Then, a simultaneous overlap of $|\Psi_t\rangle$ with both Fock states $|N, 0\rangle$ and $|0, N\rangle$ is very unlikely, as discussed above. Once we have turned on the boson–boson interaction the particles experience a mutual influence which restricts their individual random walks. This is related to the fact that the system stays much longer in the energetically (almost) degenerate Fock states $|N, 0\rangle$ and $|0, N\rangle$ than it would for noninteracting bosons (cf figure 5) and, what is even more important here, they can have a simultaneous overlap with both Fock states, such that they create a NOON state. In terms of the spectral properties the interaction modifies (i) the energy levels, which are not equally spaced, and (ii) the weight distribution of the levels, which are not binomial any longer (cf figures 1–3). This, of course, also affects the evolution of the Fock state which is more complex now, since many different frequencies are involved. A particular feature is the spectral fragmentation

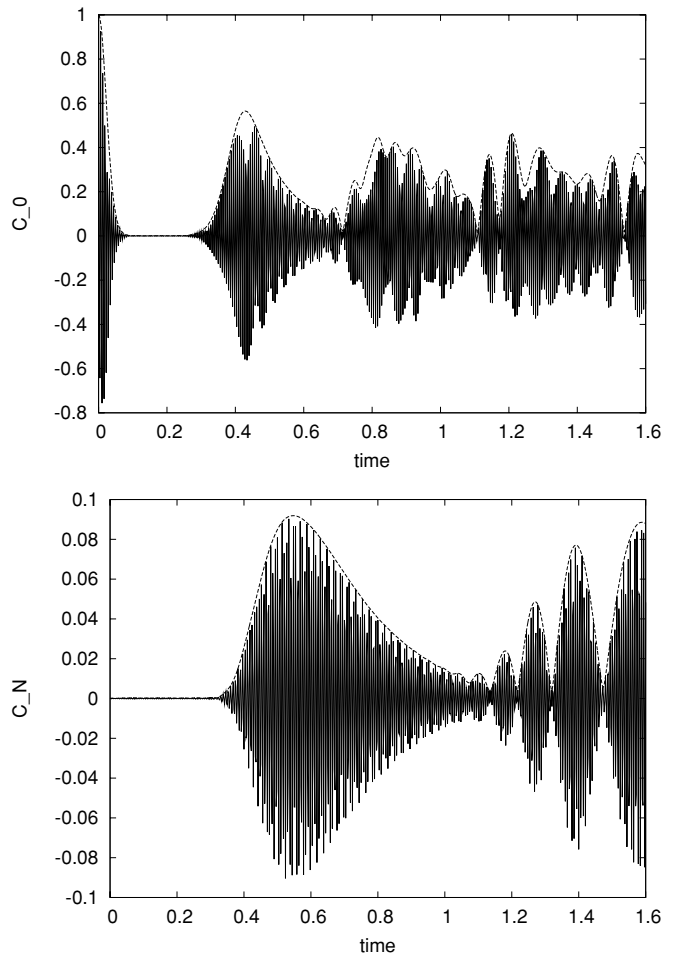


Figure 4. Evolution of the real part of the evolutionary coefficients $c_0(t) = \langle N, 0 | \Psi_t \rangle$ (upper panel), $c_N(t) = \langle 0, N | \Psi_t \rangle$ (lower panel) for 100 bosons with $U/J \approx 0.023$. The time scale is given in inverse units of the interaction strength $0.1\hbar/U$ and the energy of the initial state is $\bar{E} = 1000$. The dashed curves are $|c_0(t)|$ and $|c_N(t)|$ in the two plots, respectively.

(cf figure 1), where only a part of the spectrum contributes to the off-diagonal coefficient $\tilde{c}_N(E)$. This is a kind of Hilbert-space localization, where transitions to the high-energy part of the Hilbert space are completely suppressed, similar to the self-trapping found in the Hartree approximation of the Bose–Hubbard model [13]. It should be noted, however, that spectral fragmentation appears at a much weaker interaction strength than the self-trapping effect. For $U \approx J$, which is the threshold for self-trapping [13], there is only one eigenvalue with significant weight $|\langle N, 0 | E_j \rangle|^2$ [6]. Thus, it is unlikely that the two effects are directly connected.

For the double well with mixed interaction the situation is different due to the existence of two ‘bands’ and the absence of the double degeneracy. The main consequence is the absence of a support for the formation of NOON states because the off-diagonal coefficient $c_N(t)$ is strongly suppressed. From this observation, we can conclude that the evolutionary entanglement is much more favourable in the symmetric double well. This is in qualitative agreement with the results of a multiconfigurational Hartree calculation

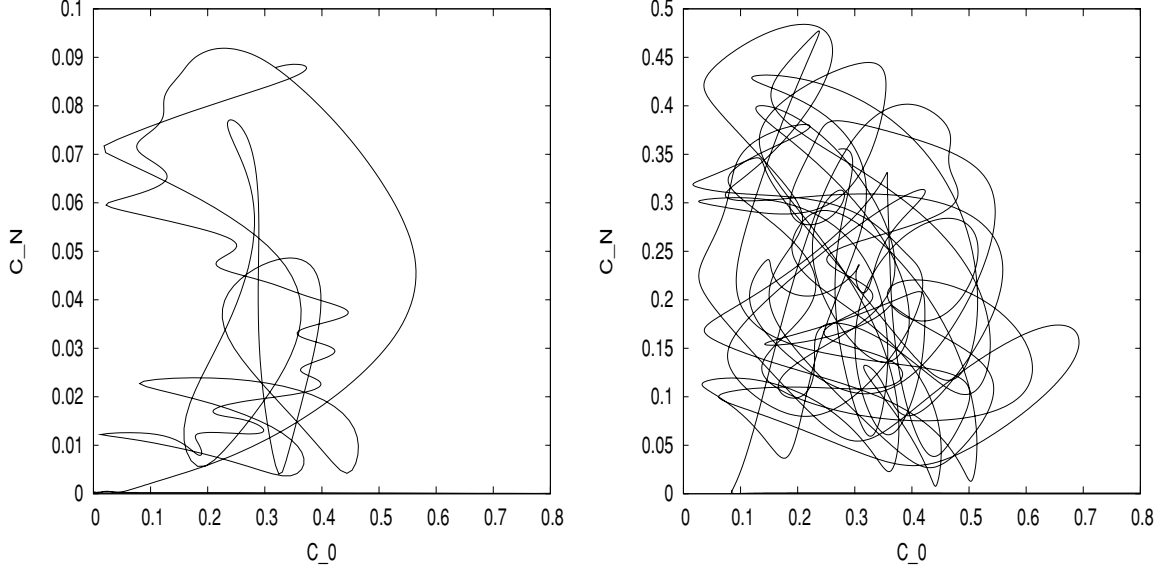


Figure 5. Evolution of $C_0 = |c_0(t)|$, $C_N = |c_N(t)|$ for the system shown in figure 4 (left panel) and for 20 bosons with $U/J \approx 0.1$ over a time period of $0.4\hbar/U$ (right panel). The trajectories $(|c_0(t)|, |c_N(t)|)$ start at 1 on the abscissa (outside the shown plots).

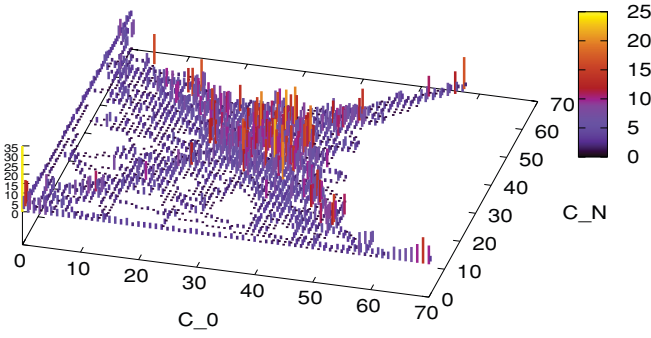


Figure 6. Distribution $P(|c_0(t)|, |c_N(t)|)$ of $|c_0(t)|$, $|c_N(t)|$ over a time period of $0.4\hbar/U$ for 20 bosons with $U/J \approx 0.026$. The axes are scaled by a factor 100 and the vertical axis is in arbitrary units. This plot indicates a strong correlation between the two spectral coefficients, supporting the formation of a NOON state.

for a one-dimensional Bose gas with a Gaussian barrier in [20].

In conclusion, we have studied the evolution of a bosonic Fock state $|N, 0\rangle$ in a double well and found that a local particle–particle interaction supports the formation of a NOON state, provided that the interaction is not too strong. This is accompanied by a fragmentation of the spectrum. The latter is characterized by the fact that only eigenstates with energies less than the energy of the initial Fock state can be reached in the evolution. This interaction effect causes a Hilbert-space localization and prevents the evolution of the Fock state to disappear in the depth of the Hilbert space. This is the main reason for a favourable creation of a NOON state. The appearance of a NOON state is suppressed though for strong interaction because then the restriction of the Hilbert space is too severe and does not allow us to reach the complementary Fock state $|0, N\rangle$.

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Appendix. Recursive projection method

A sequence of projectors P_j ($n \geq j \geq 0$) is given, defined by the recurrence relation

$$P_{2k+1} = P_{2k-1} - P_{2k} \quad (n \geq k \geq 0),$$

with initial conditions $P_{-1} = \mathbf{1}$, P_0 and by the Hamiltonian H through the properties

$$P_{2k} H P_{2k+1} = P_{2k} H P_{2k+2}, \quad P_{2k+1} H P_{2k} = P_{2k+2} H P_{2k}. \quad (\text{A.1})$$

The projection of the resolvent $(z - H)^{-1}$ defines

$$g_k = P_{2(n-k)} (z - H)_{2(n-k)-1}^{-1} P_{2(n-k)} \quad (0 \leq k < n), \quad (\text{A.2})$$

where $(\dots)_{2(n-k)}^{-1}$ is the inverse on the $P_{2(n-k)}$ -projected Hilbert space. Then, g_k satisfies the recurrence relation

$$g_k = (z - h_k)_{2(n-k)}^{-1} \quad (\text{A.3})$$

with

$$h_k = \begin{cases} P_{2n} H P_{2n} & k = 0 \\ P_{2(n-k)} H P_{2(n-k)} + P_{2(n-k)} H g_{k-1} H P_{2(n-k)} & 1 \leq k \leq n. \end{cases} \quad (\text{A.4})$$

Of interest here is only the case $k = n$, where we have from equation (A.2)

$$g_n = P_0 (z - H)^{-1} P_0.$$

For the specific case of the double well we choose $n = N/2$ and the projectors

$$P_0 = |N, 0\rangle\langle N, 0| + |0, N\rangle\langle 0, N|,$$

$$P_2 = |N-1, 1\rangle\langle N-1, 1| + |1, N-1\rangle\langle 1, N-1|, \dots,$$

$$P_N = |N/2, N/2\rangle\langle N/2, N/2|.$$

With the Hubbard Hamiltonian of equation (4), the diagonal terms of the effective Hamiltonian in equation (A.4) read

$$\begin{aligned} P_{2(n-k)} H P_{2(n-k)} &= P_{N-2k} H P_{N-2k} \\ &= [U_1(N/2+k)^2 + U_2(N/2-k)^2] \\ &\quad \times |N/2+k, N/2-k\rangle\langle N/2+k, N/2-k| \\ &\quad + [U_1(N/2-k)^2 + U_2(N/2+k)^2] \\ &\quad \times |N/2-k, N/2+k\rangle\langle N/2-k, N/2+k|. \end{aligned}$$

The off-diagonal terms of the effective Hamiltonian in equation (A.4) read

$$\begin{aligned} P_{2(n-k)} H P_{2(n-k+1)} &= P_{2N-2k} H P_{N-2k+2} \\ &= -J\sqrt{N/2+k}\sqrt{N/2-k+1} \\ &\quad \times (|N/2+k, N/2-k\rangle\langle N/2+k-1, N/2-k+1| \\ &\quad + |N/2-k, N/2+k\rangle\langle N/2-k+1, N/2+k-1|). \end{aligned}$$

For $U_1 = U_2$ this leads to equations (21) and (22) and for $U_1 = -U_2$ to equations (29), (30) and (31).

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