Quantum Chaos in the Bose-Hubbard model

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We present a numerical study of the spectral properties of the 1D Bose-Hubbard model. Unlike the 1D Hubbard model for fermions, this system is found to be non-integrable, and exhibits Wigner-Dyson spectral statistics under suitable conditions.

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During the last two decades much attention has been paid to the spectral properties of quantum systems which exhibit chaotic dynamics in the classical limit. The intrinsic complexity of these systems (due to underlying chaos) leads to an irregular energy spectrum with universal statistical properties – a phenomenon often referred to as ‘quantum chaos’ \cite{1}. One of the recent developments in the field is related to ‘many-body quantum chaos’ \cite{2}. Here the systems of interest consist of many interacting (identical) particles and usually have no classical counterpart. Notwithstanding, numerical studies of some simple models (like, for example, a 1D chain of interacting spins \cite{3}) have shown that the spectrum of a deterministic many-body system \cite{4} can also exhibit universal statistics. In the present paper we numerically study the spectrum of the 1D Bose-Hubbard model \cite{5}. Our particular interest in this system is due to its possible laboratory realization with cold atoms loaded into optical lattices \cite{6}. It is shown below that, unlike the 1D Hubbard model for fermions, the 1D Bose-Hubbard model is generally non-integrable. Moreover, in a certain parameter regime its spectrum obeys the Wigner-Dyson statistics for Gaussian Orthogonal Ensembles and, hence, this system can be considered as a quantum chaotic system.

The Hamiltonian of the 1D Bose-Hubbard (BH) model reads

\[
\hat{H} = -J \sum_{l} \cos \left( \frac{2\pi k}{L} \right) \hat{b}_{l}^{\dagger} \hat{b}_{l+1} + W \sum_{l} \hat{n}_{l} (\hat{n}_{l} - 1). \tag{1}
\]

Having in mind spinless atoms in a quasi 1D optical lattice, the creation, \( \hat{a}_{l}^{\dagger} \), or annihilation operator \( \hat{a}_{l} \) in \( \hat{H} \) ‘creates’ or ‘annihilates’ an atom in the \( l \)th well of the optical potential, in a Wannier state \( \psi_{l}(x) \). The parameter \( J \) is the hopping matrix element, the parameter \( W \) the on-site interaction energy for atoms sharing one and the same well. The Hilbert space of the system is spanned by Fock states given (in the coordinate representation) by symmetrised products of single-particle Wannier states. Assuming a finite size of the lattice, \( l = 1, \ldots, L \), and a finite number \( N \) of the atoms (which is a conserved quantity), the dimension of the Hilbert space is \( \mathcal{N} = (N + L - 1)!/N!(L - 1)! \).

It is worth noting that instead of the Wannier basis one can use a basis given by symmetrised products of Bloch waves \( \phi_{n}(x) = (1/\sqrt{L}) \sum_{l} \exp(\im \kappa l) \psi_{l}(x) \), where \( \kappa = 2\pi k/L \) is the single-particle quasimomentum (\( \kappa = 2\pi \) corresponds to the centre of the Brillouin zone). In second quantisation, this change of the basis amounts to the substitution \( \hat{b}_{l} = (1/\sqrt{L}) \sum_{l} \exp(\im 2\pi k l/L) \hat{a}_{l} \). Then the Hamiltonian \( \hat{H} \) takes the form (up to an additive term \( WN/2 \))

\[
\hat{H} = -J \sum_{k} \cos \left( \frac{2\pi k}{L} \right) \hat{b}_{k}^{\dagger} \hat{b}_{k} + \frac{W}{2L} \sum_{k_{1},k_{2},k_{3},k_{4}} \hat{b}_{k_{1}}^{\dagger} \hat{b}_{k_{2}} \hat{b}_{k_{3}}^{\dagger} \hat{b}_{k_{4}} \delta(k_{1} - k_{2} + k_{3} - k_{4}),
\]

where \( \delta(k) = 1 \) if \( k \) is a multiple of \( L \), and \( \delta(k) = 0 \) otherwise (conservation of total quasimomentum).

We proceed with our analysis of the spectrum of the BH model. In the limits \( J = 0 \) (no hopping) and \( W = 0 \) (non-interacting bosons), the BH model is completely integrable, with eigenstates given by symmetrised products of the single-particle Wannier states \( |n_{1}, \ldots, n_{L} \rangle \), or by symmetrised products of Bloch states \( |n_{1}, \ldots, n_{k}, \ldots, n_{L} \rangle \), respectively. The corresponding eigenvalues are

\[
E_{\mu} = W \mu, \quad \mu = \frac{1}{2} \sum_{i=1}^{L} n_{i} (n_{i} - 1), \quad \sum_{i=1}^{L} n_{i} = N, \tag{3}
\]

for \( J = 0 \), and

\[
E_{\nu} = -J \nu, \quad \nu = \sum_{k=1}^{L} \cos \left( \frac{2\pi k}{L} \right) n_{k}, \quad \sum_{k=1}^{L} n_{k} = N, \tag{4}
\]

for \( W = 0 \). Note that in both cases the majority of the energy levels are multiply degenerate, i.e. different combinations of integers \( n_{l} (n_{k}) \) may result in the same values of \( \mu (\nu) \).

Now we demonstrate the non-integrability of the BH model for \( J, W \neq 0 \). The left panel in Fig. \ref{fig:fig1} shows its spectrum for finite size \( L = N = 5 \), as a function of the parameter \( u = W \), with \( J = 1 - u \). The first step of the analysis is to account for the trivial symmetry of the spectrum, due to the translational invariance of the Hamiltonian. This implies that the Hamiltonian \( \hat{H} \)
Thus, the spectrum in Fig. 1(a) is a superposition of the Shannon entropy basis. To quantify such delocalisation, we consider the spectrum of the system in any generic basis. The lev-
terum of the 1D Hubbard model can be decomposed further until only one (possibly degenerate) level is left. Moreover, there is a vicinity of $J = 0$ where the eigenfunctions of the system do not depend on $J$. These states form the $\mu$-basis. More formally, the $\mu$-basis is given by the eigenstates of the Hamiltonian \( H_{\mu} \) where the matrix elements between Fock states with different $\mu$ are set (by hand) to zero. Analogously, the $\nu$-basis is given by the eigenstates of the Hamiltonian \( H_{\nu} \) where the matrix elements between states with different $\nu$ are set to zero.

The entropy \( S(u) \) calculated in the $\nu$-basis (solid line) and in the $\mu$-basis (dashed line), respectively, is depicted in the left panel of Fig. 2 for a filling factor $\bar{n} = N/L = 1$. There is a relatively wide interval of $u$ where the functions $S^{(\nu)}(u)$ and $S^{(\mu)}(u)$ simultaneously take large values. Thus, the eigenfunctions of the system are essentially delocalised in either of the two basis sets, and one may expect universal spectral statistics. Indeed, a statistical analysis of the spectrum confirms this expectation. The histogram in the upper panel of Fig. 3 shows the distribution of eigenenergies $E$ for $L = N = 8$ and $u = 0.3$. The numerically obtained density of states is well approximated by a Gaussian distribution, $\rho(E) \sim \exp[-(E - \bar{E})^2/\sigma^2]$, where $\bar{E}$ and $\sigma$ are fit-

![FIG. 1: Energy level dynamics of the BH model, as a function of the parameter $u \equiv W$, $J = 1 - u$, for $L = N = 5$ and periodic boundary conditions. The left panel shows the complete spectrum, the right panel singles out the ‘odd $\kappa = 2\pi’\) symmetry component.](image1)

$$H = \bigoplus_{k=1}^{L} H^{(\kappa)}, \quad \text{(5)}$$

where $\kappa = 2\pi k/L$ is now the total quasimomentum. Thus, the spectrum in Fig. 1(a) is a superposition of $L$ independent spectra. Next we account for the ‘odd-even’ symmetry of the $\kappa = \pi$ and $\kappa = 2\pi$ subspaces. The levels of the odd $\kappa = 2\pi$ symmetry are shown in the right panel of Fig. 1. No crossings between levels are left (on the scale of the figure, some tiny avoided crossings are not resolved), and, thus, no further decomposition of the spectrum is possible. This proves the non-integrability of the system. It is interesting to note in this context that the 1D Hubbard model for fermions is integrable for arbitrary $u$. In the latter case, in addition to the trivial ($u$-independent) symmetries (i.e., quasimomentum and odd-even symmetry), the system has a number of non-trivial ($u$-dependent) integrals. Therefore, the spectrum of the 1D Hubbard model can be decomposed further until only one (possibly degenerate) level is left.

The above non-integrability of our system (manifest in the avoided crossings in the right panel of Fig. 1) does not yet guarantee that the spectrum of the BH model has the universal statistical properties associated with quantum chaos. Loosely speaking, the latter requires a delocalisation of the eigenfunctions of the system in any generic basis. To quantify such delocalisation, we consider the Shannon entropy

$$S(u) = \left\langle -\frac{1}{\log N} \sum_{j=1}^{N} |c_j|^2 \log(|c_j|^2) \right\rangle, \quad \text{(6)}$$

where the $c_j$ are the expansion coefficients of an arbitrary eigenstate of the system in a given basis, and the angular brackets denote an average over all eigenstates. It is reasonable to choose as a basis the ‘$\nu$-basis’, when our starting point is $u = 0$ (no interaction), or the ‘$\mu$-basis’, when starting at $u = 1$ (no hopping). First let us clarify the notion of $\nu$- and $\mu$-basis. As mentioned above, and as apparent from Fig. 1, the spectrum of the system at $u = 1$ ($J = 0$) consists of a number of degenerate levels with energies given in Eq. 6. An arbitrarily small $J$ removes this degeneracy, and the levels split into a $\mu$-band with a width proportional to $J$. Moreover, there is a vicinity of $J = 0$ where the eigenfunctions of the system do not depend on $J$. These states form the $\mu$-basis. More formally, the $\mu$-basis is given by the eigenstates of the Hamiltonian $H_{\mu}$ where the matrix elements between Fock states with different $\mu$ are set (by hand) to zero. Analogously, the $\nu$-basis is given by the eigenstates of the Hamiltonian $H_{\nu}$ where the matrix elements between states with different $\nu$ are set to zero.

The entropy \( S(u) \) calculated in the $\nu$-basis (solid line) and in the $\mu$-basis (dashed line), respectively, is depicted in the left panel of Fig. 2 for a filling factor $\bar{n} = N/L = 1$. There is a relatively wide interval of $u$ where the functions $S^{(\nu)}(u)$ and $S^{(\mu)}(u)$ simultaneously take large values. Thus, the eigenfunctions of the system are essentially delocalised in either of the two basis sets, and one may expect universal spectral statistics. Indeed, a statistical analysis of the spectrum confirms this expectation. The histogram in the upper panel of Fig. 3 shows the distribution of eigenenergies $E$ for $L = N = 8$ and $u = 0.3$. The numerically obtained density of states is well approximated by a Gaussian distribution, $\rho(E) \sim \exp[-(E - \bar{E})^2/\sigma^2]$, where $\bar{E}$ and $\sigma$ are fit-

![FIG. 2: Left panel: Mean entropy $S(u)$ in the $\nu$-basis (solid line) and in the $\mu$-basis (dashed line), as a function of the interaction parameter $u$ ($N = L = 8$). Right panel: Entropy $S(u)$ of the individual eigenstates (dots), for $u = 0.3$.](image2)
We now address the conditions for quantum chaos to prevail in the BH model. Obviously, the above criterion based on the mean entropy \( S(\nu) \) provides only a rough estimate on the parameter region where one may expect an irregular spectrum. Moreover, besides the interaction parameter \( u \) and the filling factor \( \bar{n} \), also the energy \( E \) should be considered as a relevant parameter. As a an illustration of this statement, the right panel in Fig. 2 shows the entropy of the individual eigenstates,

\[
S(E) = \min[S^{(\nu)}(E), S^{(\bar{n})}(E)],
\]

which are labeled here by the individual level’s energy \( E \). Obviously, there is a nonvanishing fraction of localised eigenstates associated with the lower and upper parts of the spectrum. Hence, one has to distinguish regular and chaotic spectral components [11]. In the presently considered case \((u = 0.3, \bar{n} = 1)\) the regular component is negligible (less than 1/10 of the total number of levels) and, hence, the level spacing distribution follows the universal Wigner-Dyson law. However, when the ratio \( J/W \) approaches either one of the integrable limits, the regular component gradually increases at the expense of the irregular one, what causes a deviation from the universal distribution. The same holds true if we decrease the value of the filling factor. In this latter case the chaotic component (typically located in the central part of the spectrum) is small even for \( J/W \sim 1 \). Further studies are needed for a precise mapping of the chaotic region of the BH model in the parameter space spanned by \( u, \bar{n}, \) and \( E \).

Let us now discuss the physical manifestations of the irregular spectrum of the BH model, i.e. its relevance for ongoing experiments with cold atoms in optical lattices [6, 12, 13]. Obviously, to probe the irregular part of the spectrum one has to excite the system. This can be done, for example, by applying a static force, i.e., adding a term \( F \sum_i \hat{n}_i \) to the Hamiltonian [11]. Note that the translational symmetry of the system, broken by...
this term, can be recovered by a suitable gauge transformation of
the form
\[
\hat{H}(t) = -\frac{J}{2} \left( e^{-iFt} \sum l a_{l+1} a_l + h.c. \right) + \frac{W}{2} \sum l \dot{\alpha}_l (\dot{n}_l - 1),
\]
and a parametric dependence of the eigenvalues of the Hamiltonian on \(\theta = Ft\), as illustrated in Fig. 4 (for \(L = N = 5, \kappa = 2\pi, \) as in Fig. 1 and \(u = 0.1\)). Let us assume for a moment that there are no atom-atom interactions and, thus, all avoided crossings in Fig. 4 are true crossings. Then, in the course of time, the static force will drive the system along the continuation of the ground state (the grey shaded energy level in Fig. 4), representing nothing else than bona fide Bloch oscillations, where the system comes back to its initial state after one Bloch period \(T_B = 2\pi/F\). It is clear, however, that for \(u \neq 0\) the system generally does not come back to the initial state, because of Landau-Zener transitions at the avoided crossings encountered during one Bloch cycle [14]. In other words, after the Bloch cycle is completed, some excited states will be populated as a consequence of (a)diabatic transitions along the diabatic continuation of the ground state. (The branching ratio between diabatic and adiabatic transitions is obviously determined by the time derivative of \(\theta\), i.e., by the field amplitude \(F\).)

In the case of strong static forcing, \(F \gg J\), this excitation process is reversible, leading to quasiperiodic Bloch oscillations [15]. In contrast, for moderate forcing (and chaotic instantaneous spectrum) the excitation is irreversible, leading to decoherence of the one-particle density matrix and, as a consequence, to decay of the Bloch oscillations [16]. Since Bloch oscillations of the atoms are easily measured in laboratory experiments [12, 13], their irreversible decay provides a direct indication of chaos in the BH system [13].

In conclusion, we have shown that the 1D Bose-Hubbard model is a generic quantum chaotic system with characteristic spectral irregularity. This is in stark contrast to the 1D Hubbard model for fermions, which is known to be an integrable system with regular spectrum. It is also worth noting that the many-site character of the BH model is crucial for the appearance of quantum chaos – the two site BH model, which is often used to study Bose Einstein condensates of cold atoms in double-well potentials [17], has a regular spectrum.

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