

## Statistics of Schmidt coefficients and the simulability of complex quantum systems

Hannah Venzl,<sup>1</sup> Andrew J. Daley,<sup>2,3</sup> Florian Mintert,<sup>1</sup> and Andreas Buchleitner<sup>1</sup>

<sup>1</sup>Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

<sup>2</sup>Institut für Theoretische Physik, Universität Innsbruck, Technikerstr. 25, A-6020 Innsbruck, Austria

<sup>3</sup>Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria

(Received 27 August 2008; revised manuscript received 18 February 2009; published 26 May 2009)

We show that the transition from regular to chaotic spectral statistics in interacting many-body quantum systems has an unambiguous signature in the distribution of Schmidt coefficients dynamically generated from a generic initial state, and thus limits the efficiency of the time-dependent density-matrix renormalization-group algorithm. We investigate this mechanism on the tilted Bose-Hubbard model; however the emergence of universal spectral properties allows translation of our conclusions to generic many-body quantum systems.

DOI: 10.1103/PhysRevE.79.056223

PACS number(s): 05.45.Mt, 05.50.+q, 05.45.Pq, 67.85.Hj

Complexity is paradigmatic in many areas not only in physics but equally so in life and social sciences, and in economics [1]. The characteristic property of a “complex system” resides in the difficulty of its efficient simulation through reduction to manageable size. More formally, e.g., the minimum length of an algorithm designed to simulate the system under study can serve as a quantitative measure of complexity [2]. Complexity thus has its very tangible counterpart in the numerical overhead required for an accurate simulation, and implies a challenge for computational physics: any time we succeed in minimizing that overhead we actually prove that the underlying complexity is smaller than anticipated.

Complex systems abound in nature, from interacting many-particle systems to deterministic chaos in few degrees of freedom [3], and from macroscopic to microscopic scales. On the quantum level, complexity has its counterpart in complex spectral structures, described by random matrix theory, and by now is well established in nuclear [4] and atomic physics [5], mesoscopics [6], and photonics [7]. Recently, “designed complexity” moved into reach for state of the art experiments on ultracold atoms in periodic optical potentials, and considerable effort is devoted to implementing solid-state Hamiltonians with unprecedented control in such systems [8]. Since analytical treatments are often unavailable to describe such many-particle dynamics, efficient numerical tools are in need, and “efficient” here means that the required numerical resources as memory and/or execution time scale favorably as compared to the exponential growth of Hilbert-space dimension with system size.

For one-dimensional (1D) systems, density-matrix renormalization-group methods [9] have aided efficient simulation considerably. The underlying idea lies in the construction of a suitable local basis that makes it possible to represent a system state in terms of significantly fewer basis states than the total dimension of Hilbert space suggests. More specifically, this approach makes use of a truncated matrix product state (MPS) ansatz [10] to reduce the number of coefficients required to specify the state to a manageable number. In particular in perturbative regimes, where a system has a natural basis, such techniques work very successfully, and the ground states of 1D systems with local Hamiltonians are typically well represented in this form [11,12]. Also dynamics can be tackled by time-dependent density-

matrix renormalization-group (*t*-DMRG) techniques. These methods have been shown to work well for low-energy initial states [11,13] giving rise to near-equilibrium time evolution. For a generic initial state, however, they may work only for short times [14], and apparently depend strongly on the properties of the Hamiltonian [15].

Here we investigate the connection between complexity and *t*-DMRG methods: can *t*-DMRG efficiently simulate complex many-particle systems in general or does the efficiency of *t*-DMRG rather identify parameter regimes where the dynamics—governed by the underlying spectral structure—is actually rather “regular?” To assess this question, we need independent measures of complexity, which, on the spectral level, will be imported from the theory of quantum chaos [4]. As we show in the following, the appearance of universal “globally irregular” *ultra* “chaotic” spectral structure implies the breakdown of simulability by *t*-DMRG techniques. More specifically, we observe a characteristic qualitative change in the distribution of dynamically generated Schmidt coefficients that directly reflects the defining property of complexity, namely, the effective *irreducibility* of the Hilbert-space dimension: any basis truncation leads to the rapid accumulation of uncontrollable errors in the simulation.

In what follows, we investigate the tilted Bose-Hubbard model. However, our subsequent conclusions will build on the emergence of *universal* spectral properties, implying in turn *universal* properties of the associated eigenstates, which are *independent* of the specific form of the Hamiltonian [4]. Since all dynamical properties are encoded in the spectral decomposition of the Hamiltonian, we expect that, in particular, our conclusions for simulations of the dynamics are valid in general for *generic* many-body quantum systems.

The tilted Bose-Hubbard model corresponds to bosonic atoms trapped in the lowest band of an optical lattice subject to an additional static field. For *m* lattice sites, the system is described by the Hamiltonian

$$H = -\frac{J}{2} \sum_{l=1}^m (\hat{a}_{l+1}^\dagger \hat{a}_l + \text{H.c.}) + \frac{U}{2} \sum_{l=1}^m \hat{n}_l(\hat{n}_l - 1) + F \sum_{l=1}^m l \hat{n}_l, \quad (1)$$

where  $\hat{a}_l^\dagger$  ( $\hat{a}_l$ ) are creation (annihilation) operators for a particle at lattice site *l*, and  $\hat{n}_l = \hat{a}_l^\dagger \hat{a}_l$  is the corresponding number

operator. The system's dynamical properties are characterized by the tunneling constant  $J$ , the interaction strength  $U$ , and a linear potential with strength  $F$ , resulting, e.g., from gravity when the optical lattice is tilted with respect to gravitational equipotential lines. The rich dynamics of this system ranges from perfect oscillations [16] with the Bloch period  $T_B=2\pi/F$  for weak interactions to chaotic dynamics for situations in which interaction and tunneling are of comparable order of magnitude [17].

As mentioned above, simulability via  $t$ -DMRG relies on the possibility of effectively decimating the system's Hilbert space in the course of the propagation. It is based on the Schmidt decomposition for every possible bipartite splitting [18],

$$|\psi\rangle = \sum_{\alpha=1}^{\chi_{AB}} \lambda_{\alpha} |\Phi_{\alpha}^{[A]}\rangle |\Phi_{\alpha}^{[B]}\rangle, \quad (2)$$

where  $A$  and  $B$  label the two subsystems with Schmidt eigenstates  $\{|\Phi_{\alpha}^{[A]}\rangle\}$  and  $\{|\Phi_{\alpha}^{[B]}\rangle\}$ , and the real coefficients  $\lambda_{\alpha}$ , with normalization condition  $\sum_{\alpha} \lambda_{\alpha}^2 = 1$ , describe the quantum correlations between the two subsystems. In the truncated MPS, we make an approximation to the state by setting an upper bound  $\chi$  on  $\chi_{AB}$ , retaining only those eigenstates with the largest  $\lambda_{\alpha}$ . This approximation is good if the decreasingly ordered  $\lambda_{\alpha}$  decay rapidly as a function of the index  $\alpha$ . Thus, it relies on the assumption that the entanglement between two parts of the system, as, e.g., measured by the von Neumann entropy

$$S = - \sum_{\alpha} \lambda_{\alpha}^2 \log_2 \lambda_{\alpha}^2, \quad (3)$$

is never too large. The von Neumann entropy provides the estimate  $\chi \geq 2^S$  required for a reliable representation of the state, and is often used as an indicator of simulability of the system. If  $S$  grows rapidly as a function of time, simulation of the system will be difficult, whereas if  $S$  is bounded during the dynamics, then we can fix  $\chi$  and compute the dynamics over long-time periods.

We now consider this approximation for the time evolution of various initial states, in different parameter regimes of the Hamiltonian, Eq. (1), above. The subsequent averaging over these different initial states then ensures the generality of our results. In the following we always discuss the bipartition that yields the largest von Neumann entropy since this limits the efficiency of the  $t$ -DMRG algorithm (however, other bipartitions also yield qualitatively similar results). In order to permit our subsequent comparison with the system's spectral properties, we choose a relatively small system, beginning with eight bosons in eight neighboring sites at the center of a 64-site lattice, with Dirichlet boundary conditions, for different values of  $U/J$  and  $F/J$ . Note that, for  $F/J \geq 1$ , the particles hardly spread on the time scale of the simulation, which makes it possible to compare the dynamical behavior of the larger system to the spectrum of the Floquet-Bloch operator on nine sites. However, for very weak static fields the atoms rather diffuse through the system and travel into initially unoccupied regions so that the corre-

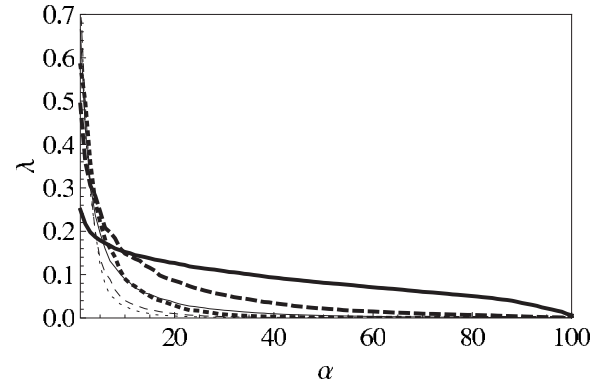


FIG. 1. Distribution of average Schmidt coefficients  $\lambda_{\alpha}$  obtained from averaging over ten initial states of eight particles initially distributed over eight lattice sites. The total lattice size was 64 to eliminate boundary effects. Shown are the  $\chi=100$  largest average Schmidt coefficients, sorted in descending order, for  $U/J=1$  (thick lines) and  $U/J=10$  (thin lines), and for different values of the static tilt  $F/J=1$  (solid), 1.5 (dashed), and 2 (dotted) at  $t=4.8 \times T_B$ .

spondence between spectral statistics and  $t$ -DMRG is lost. Therefore, our subsequent analysis does not extend to very small values of  $F/J$ , where diffusion sets in.

Figure 1 shows the averaged Schmidt coefficients after an evolution time  $t=4.8 \times T_B$ , (at this time, the state evolution has reached its asymptotic behavior for the given basis size—see also the inset of Fig. 3), with the average taken over ten separable initial states of the form  $|\psi_{\text{init}}\rangle \sim |n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes |n_8\rangle$  (each with a different random realization of occupation numbers  $n_{\ell}$  of eight initially occupied sites). The distributions can be divided into two qualitatively different categories: for strong interaction  $U/J=10$ , irrespective of the static field  $F/J$ , few comparably large coefficients dominate the distribution which exhibits a rapidly diminishing tail. The same holds for weak interaction  $U/J=1$  and medium static field  $F/J=2$ . However for  $U/J=1$  and medium to weak static field  $F/J=1.5$ , there is a transition to a distribution showing a slowly decaying tail with many non-negligible coefficients of comparable weight which is fully developed for weak static field  $F/J=1$ .

The eligibility of two such distributions for the basis truncation required to apply the  $t$ -DMRG algorithm is fundamentally different: while a distribution of the former type allows the truncation of the major portion of the Schmidt basis with virtually vanishing loss of accuracy, dropping a few basis states in the latter case already will lead to a sizable error. That is, we can identify situations that can be described efficiently with  $t$ -DMRG but there are parameter regimes of the *same* system where a faithful representation of the solution must be spanned essentially by the *complete* Hilbert space. *Any* numerical simulation then is plagued by highly unfavorable scaling. In particular, as immediately evident from Fig. 1, MPS basis truncation at  $\chi=100$  for  $U/J=1$  and  $F/J=1$  enforces a rapid decrease in the Schmidt coefficients for  $\alpha > 80$ , which, in turn, will induce artifacts in the simulated dynamics (as we confirmed by running computations for varying  $\chi$ ).

Such transition from an efficient to an inefficient representation in a MPS basis has its cause in a sudden and pro-

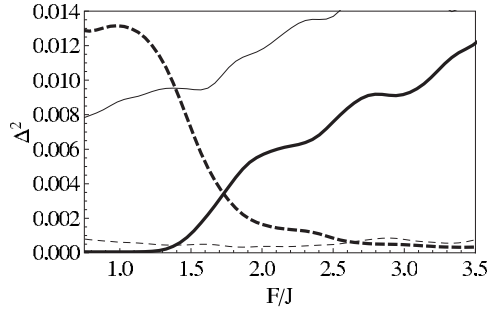


FIG. 2. Mean square deviation  $\Delta^2$ , Eq. (6), of the Floquet-Bloch operator's [Eq. (4)] nearest-neighbor distribution from Poissonian (dashed lines) and Wigner-Dyson statistics (solid lines), for eight particles on nine lattice sites, as a function of  $F/J$ .  $U/J=1$  (thick lines) and 10 (thin lines).

nounced transition in the underlying spectral structure, as we will now evidence by direct inspection of the spectrum of the time-evolution (or Floquet) operator,

$$U(T_B) = \hat{T} \exp \left[ -i \int_0^{T_B} \tilde{H}(t) dt \right], \quad (4)$$

generated by the time-dependent transformed Hamiltonian

$$H(t) = -\frac{J}{2} \sum_{l=1}^m (e^{iFt} \hat{a}_{l+1}^\dagger \hat{a}_l + \text{H.c.}) + \frac{U}{2} \sum_{l=1}^m \hat{n}_l (\hat{n}_l - 1) \quad (5)$$

( $\hat{T}$  denotes time ordering). Due to the translational invariance of  $H(t)$  with periodic boundary conditions,  $U(T_B)$  decomposes into the direct sum of operators labeled by distinct values of quasimomentum  $\kappa$  [17], and so does its spectrum. The statistical analysis therefore requires a diagonalization at fixed quasimomentum, and we chose  $\kappa=0$  here.

The integrated distribution  $I(s)$  of the spacings  $s$  between neighboring eigenfrequencies of  $U(T_B)$  allows distinguishing of regular spectral structure (tantamount to weakly coupled basis states), described by Poissonian statistics  $I_P(s) = \int_0^s P(s') ds' = 1 - \exp(-s)$  [19], from a chaotic spectrum that obeys Wigner-Dyson statistics  $I_W(s) = 1 - \exp(-\pi s^2/4)$  [4]. Figure 2 displays the mean-square deviation,

$$\Delta^2 = \int ds [f(s) - I(s)]^2, \quad (6)$$

of the numerically obtained distributions  $I(s)$  with respect to  $f(s)$  given by the universal [4] distributions  $I_W(s)$  and  $I_P(s)$ , respectively.

For  $U/J=10$ , the system obeys Poissonian statistics, irrespective of  $F/J$ . However, in the case of  $U/J=1$  there are two different regimes: for  $F/J \lesssim 1.3$ , the deviation from (irregular and chaotic) Wigner-Dyson statistics is negligible while for  $1.3 \lesssim F/J \lesssim 2$  the distribution changes its character, and turns (regular) Poissonian for  $F/J \gtrsim 2$ . Thus, in these two limiting parameter ranges of weak and strong tilts, the specific many-particle system under study exhibits the spectral properties of integrable (Poissonian) and random (Wigner-Dyson) Hamiltonians, respectively. These are *universal* in the sense that they are *independent* of the specific

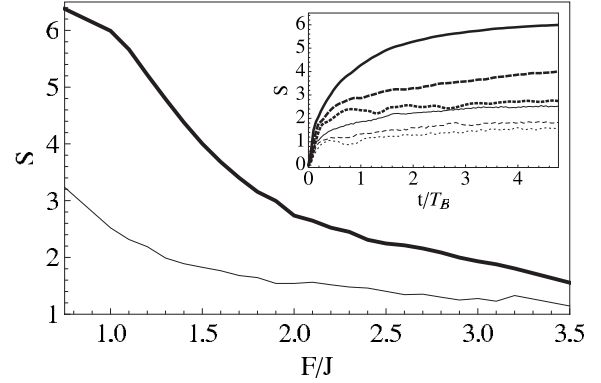


FIG. 3. Many-particle entanglement vs  $F/J$ , measured by the average von Neumann entropy  $S$ , extracted from  $t$ -DMRG simulations of eight particles for ten different initial states at  $t=4.8 \times T_B$ .  $U/J=1$  (thick) and 10 (thin line). Inset:  $S$  vs  $t/T_B$  for various tilt strengths  $F/J=1$  (solid), 1.5 (dashed), and 2 (dotted lines), and the same values of  $U/J$ .

form of the Hamiltonian and *exclusively* depend on its global symmetry properties. This renders the present system equivalent, e.g., to the three body Coulomb problem of the helium atom: the accurate simulation of the dynamics of the latter remains a challenge for modern computational physics [5] for the very same spectral reasons as identified here.

Focusing on the specific many-particle character of the Bose-Hubbard Hamiltonian, the above spectral transition is also reflected in the entropy of Schmidt coefficients  $S$ , Eq. (3), which is depicted as a function of  $F/J$  after a simulation time of  $t=4.8 \times T_B$  in Fig. 3. The inset shows the entropy as a function of time for different values of the static field strength  $F/J$ . In the regime of regular level statistics,  $S$  grows only initially, whereas it keeps increasing in the chaotic regime. As a matter of fact, the saturation of  $S$  for  $F/J \lesssim 1$  and  $U/J=1$  is once again a numerical artifact of the truncation at  $\chi=100$ : the simulation only approximates the real values of  $S$  from below, i.e., at given  $t$ ,  $S$  grows when increasing  $\chi$ . This behavior of  $S$  is perfectly consistent with our observations on Fig. 1. Note that the slight increase in  $S$  toward small values of  $F/J$ , for  $U/J=10$  in Fig. 3, corresponds to a narrow distribution of the Schmidt coefficients in Fig. 1, and therefore does not hinder efficient simulation—in perfect agreement with the regular spectral structure in this regime as spelled out by Fig. 2.

While the signature of the sharp “chaos transition” observed in Fig. 2 is somewhat smoother in the corresponding behavior of the von Neumann entropy in Fig. 3, the number of Schmidt coefficients larger than a certain threshold  $\epsilon$  turns out to provide an equally sensitive probe as the spectral statistics, as demonstrated in Fig. 4 (for  $\epsilon=0.01$ ): whereas in the regular regime ( $U/J=10$  or  $U/J=1$  with  $F/J \gtrsim 2$ ) less than 20% of the coefficients exceed the threshold  $\epsilon$ , essentially all of them contribute in the chaotic regime ( $U/J=1$ ,  $F/J \lesssim 1.3$ ). That is, whereas the  $t$ -DMRG algorithm allows an efficient simulation of the Bose-Hubbard dynamics in the regular regime, a basis truncation in the chaotic regime will rapidly lead to sizable errors in the simulation. An accurate description requires large numerical efforts that scale expo-

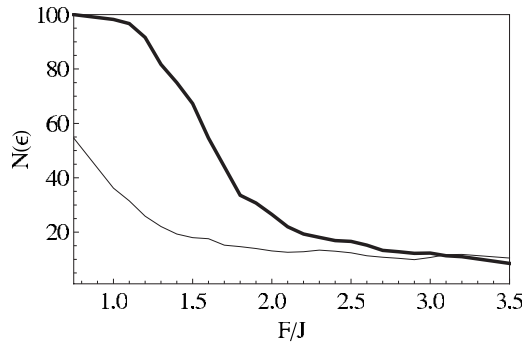


FIG. 4. Average number of Schmidt coefficients larger than  $\epsilon = 0.01$  vs  $F/J$ , after a simulation time  $t = 4.8 \times T_B$ .  $U/J=1$  (thick) and 10 (thin lines).

nentially, much as the system size itself. This observation also holds for larger systems, where  $t$ -DMRG is a powerful tool in the regime of regular spectral structure, and where an exact treatment of the dynamics becomes unfeasible: in  $t$ -DMRG calculations with 20 atoms in 20 sites, we observe precisely the same characteristic changes in the distribution of Schmidt coefficients as observed in Figs. 1 and 4. Therefore, the *inefficiency* of  $t$ -DMRG simulations, quantified by the statistical quantities evaluated in Figs. 2 and 4, is an

unambiguous indicator of the underlying complexity of the many-particle spectrum.

Moreover, also the eigenstates of generic quantum systems show universal behavior: in the chaotic regime they are delocalized in any generic basis. Likewise, any generic basis state is delocalized in the eigenbasis of the Hamiltonian. This in turn implies that generic initial states (even if initially localized in some particular basis) evolve to states broadly distributed in any basis when propagated by the unitary evolution generated by the Hamiltonian. This holds, in particular, for the Schmidt basis and thus our observations directly translate to generic many-body quantum systems, even in more than one dimension [4,5,20]. We conjecture that the distributions of Schmidt coefficients of typical states in spectrally regular and chaotic systems also exhibit universal features [21]—much like the energy-level distributions of regular and chaotic quantum systems.

We thank C. Kollath for helpful conversations. F.M. gratefully acknowledges financial support by the Alexander von Humboldt foundation. Work in Freiburg was supported by the German Research Foundation through Forschergruppe 760. Work in Innsbruck was supported by the Austrian Science foundation through SFB F15 and Project No. I118\_N16 (EuroQUAM\_DQS).

- 
- [1] *Extreme Events in Nature and Society*, edited by S. Albeverio, V. Jentsch, and H. Kantz (Springer, New York, 2005).
- [2] A. N. Kolmogorov, *IEEE Trans. Inf. Theory* **14**, 662 (1968).
- [3] A. Lichtenberg and M. Lieberman, *Regular and Stochastic Motion* (Springer, New York, 1983).
- [4] *Chaos and Quantum Physics*, edited by M.-J. Giannoni, A. Voros, and J. Zinn-Justin (North-Holland, Amsterdam, 1991).
- [5] J. Madroñero *et al.*, *Adv. At., Mol., Opt. Phys.* **53**, 33 (2006).
- [6] R. Ketzmerick, *Phys. Rev. B* **54**, 10841 (1996).
- [7] H.-J. Stöckmann and J. Stein, *Phys. Rev. Lett.* **64**, 2215 (1990); J. Zyss and I. Ledoux, *Chem. Rev.* **94**, 77 (1994).
- [8] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998); M. Greiner *et al.*, *Nature (London)* **415**, 39 (2002); D. Jaksch and P. Zoller, *Ann. Phys. (N.Y.)* **315**, 52 (2005); M. Lewenstein *et al.*, *Adv. Phys.* **56**, 243 (2007).
- [9] S. R. White, *Phys. Rev. Lett.* **69**, 2863 (1992); U. Schollwöck, *Rev. Mod. Phys.* **77**, 259 (2005).
- [10] M. Fannes, B. Nachtergaele, and R. F. Werner, *Commun. Math. Phys.* **144**, 443 (1992).
- [11] G. Vidal, *Phys. Rev. Lett.* **91**, 147902 (2003).
- [12] F. Verstraete and J. I. Cirac, *Phys. Rev. B* **73**, 094423 (2006).
- [13] A. J. Daley *et al.*, *J. Stat. Mech.: Theory Exp.* P04005 (2004); S. R. White and A. E. Feiguin, *Phys. Rev. Lett.* **93**, 076401 (2004); Á. Peralos and G. Vidal, *Phys. Rev. A* **78**, 042337 (2008).
- [14] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, *Phys. Rev. Lett.* **100**, 030504 (2008).
- [15] T. Prosen and M. Znidaric, *Phys. Rev. E* **75**, 015202(R) (2007).
- [16] M. Gustavsson, E. Haller, M. J. Mark, J. G. Danzl, G. Rojas-Kopeinig, and H. C. Nagerl, *Phys. Rev. Lett.* **100**, 080404 (2008); M. Fattori, C. D’Errico, G. Roati, M. Zaccanti, M. Jona-Lasinio, M. Modugno, and M. Inguscio, *ibid.* **100**, 080405 (2008).
- [17] A. R. Kolovsky and A. Buchleitner, *Phys. Rev. E* **68**, 056213 (2003).
- [18] E. Schmidt, *Math. Ann.* **63**, 433 (1907).
- [19] M. V. Berry and M. Tabor, *Proc. R. Soc. London, Ser. A* **356**, 375 (1977).
- [20] F. Verstraete and J. I. Cirac, e-print arXiv:cond-mat/0407066.
- [21] H. Kubotani, S. Adachi, and M. Toda, *Phys. Rev. Lett.* **100**, 240501 (2008).