On the relaxation toward equilibrium in an isolated strongly correlated one-dimensional Bose gas

Peter Schmitteckert

DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany
Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany
E-mail: Peter.Schmitteckert@kit.edu

Received 1 May 2012
Accepted for publication 27 July 2012
Published 30 November 2012
Online at stacks.iop.org/PhysScr/T151/014059

Abstract

In this work we study the time evolution of soft-core bosons on a one-dimensional lattice, where the particles are initially quenched into an atomic density wave. At time \( t = 0 \), the particles are released from the quench and can evolve under the dynamics of a soft-core Bose–Hubbard Hamiltonian on a lattice including a confining trap.

PACS numbers: 67.10.Jn, 37.10.Jk, 03.67.-a, 05.30.-d

Ultra-cold atoms in optical lattices have become a test bed for comparing simulations for strongly correlated quantum systems with experimental realizations [1–3]. In a recent work, Trotzky \textit{et al} [4] reported on the experimental realization and the numerical simulation of the dynamics of a quench of a strongly interacting Bose gas in one dimension. From their work they drew the remarkable conclusion that ‘for intermediate times the system fulfills the promise of being a dynamical quantum simulator, in that the controlled dynamics runs for longer times than present classical algorithms based on matrix product states can efficiently keep track of’. In this work, I present numerical simulations based on time-dependent density matrix renormalization (DMRG) as described in [5] for sample 2c of [4] to demonstrate that simulations on classical computers based on matrix product states can be performed reliably on a time scale which exceeds the time scale of the reported experimental data.

In the experiment under consideration, a one-dimensional Bose gas in a harmonic trap was subject to two optical lattices. The first lattice was used to provide a lattice, which can be modeled by the Hamiltonian

\[ H = \sum_x (\hat{a}_x^\dagger \hat{a}_x + \text{h.c.}) + \frac{U}{2} \sum_x (\hat{n}_x - 1) + \sum_x \frac{K x^2}{2} \hat{n}_x, \]

where \( \hat{a}_x^\dagger \) (\( \hat{a}_x \)) annihilates (creates) a particle at site \( x \), \( \hat{n}_x = \hat{a}_x^\dagger \hat{a}_x \) gives the number of particles at site \( x \), \( U \) is the on-site interaction and \( K \) is the potential of a harmonic trap. In the following, we use the parameter of sample (c) of [4]: \( U/J = 5.16 \), \( K/J = 9 \times 10^{-3} \), the number of lattice sites \( M = 121 \) with \( N = \sum_x \hat{n}_x = 43 \) particles, and the system is centered symmetrically around \( x = 0 \). We have set \( J = 1 \) for convenience. The second optical lattice is used to quench the particles on odd sites only for time \( t < 0 \) and is switched off at \( t = 0 \) so that the particles can now propagate between the odd and even sites and therefore through the complete system. In order to model the physical situation we start with an eigenstate of an Hamiltonian consisting of a staggered local potential, a strong on-site repulsion and a small coupling \( J \), see below, which is calculated via a standard DMRG [6]. In order to perform the time-dependent simulations, we applied the full time-dependent DMRG (td-DMRG) [5]. Specifically, our simulations consist of the following steps.

- First, we perform a ground state infinite lattice sweep as a warm-up.
We perform nine finite lattice sweeps where we target for the ground state $|\Psi_0\rangle$ of a Hamiltonian $\mathcal{H}_0$, $\mathcal{H}_0|\Psi_0\rangle = E_0|\Psi_0\rangle$.

At each DMRG step, we perform a time evolution of $N_t$ time steps of size $\Delta t$: $|\Psi_{t+1}\rangle = e^{-(i\mathcal{H}-E)\Delta t}|\Psi_t\rangle$, $E = \langle \Psi_0|\mathcal{H}|\Psi_0\rangle$. The density matrix used to select the basis states kept is given by the mixed density matrix $\rho = \text{Tr}\sum_n |\Psi_n\rangle \langle \Psi_n|$; that is, in each DMRG step we include the complete time evolution to select the target space.

The action of the matrix exponential $e^{-(i\mathcal{H}-E)\Delta t}$ is evaluated via a Krylov subspace expansion. There one expands the matrix exponential in the Krylov space $\mathcal{K}_{2n}(\mathcal{H}) = \text{span}\{|\Psi\rangle, \mathcal{H}|\Psi\rangle, \ldots, \mathcal{H}^n|\Psi\rangle\}$. The accuracy of this expansion is comparable with exact diagonalization using sparse matrix methods. Here we use a minimal residual of $10^{-10}$ for the accuracy of the matrix exponential [7, 8].

Once an initial short-time dynamics is finished, we continue the above-described finite lattice DMRG sweeping, where we then increase the number of time steps and the number of states kept per block. By restarting the DMRG at a given number of time steps and increasing the number of states $m$ kept per block, we can actually check for convergence. In our DMRG algorithm, we always used an $A \bullet B$ blocking scheme, where $m$ counts only the number of states kept per blocks $A$, $B$. The inserted sites are not included in $m$.

In order to perform simulations for soft-core bosons, we have to restrict the maximal occupation $n_{\text{max}}$ of a given site, where we use up to $n_{\text{max}} = 5$.

In figure 1 we show the evolution of the initially quenched atomic density wave on $M = 121$ lattice sites consisting of $N = 43$ particles in the center of the trap, where only the odd sites are occupied with a single particle at time $t = 0$. Within the time scale of the simulation, the system stays roughly homogeneous in the center of the trap—except the odd/even oscillation—and displays an expansion at the border of the particle cloud, which does not yet reach the boundary of the system.

In figure 2 we show results of the occupation of the odd sites, $N_{\text{odd}} = \langle N_{\text{odd}} \rangle$, $N_{\text{odd}} = \sum_{x=2y} N_x$, corresponding to the data of to sample (c) in figure 2 of [4]. We prepared our initial state by using a $J = 0.4$ and a staggered potential $V = V \sum_x (-1)^x \hat{n}_x$, $V = 1$ in addition to an on-site $U$ of 20. Once we found the ground state we restarted the DMRG lowering $J$ to 0.1 and then $J = 0$, performing five DMRG sweeps in each restart and performing $N_t = 10$ time steps of $\Delta t$. We then continued with $J = 0$ for the initial state and increased the number of states kept to 500, 750, 1500, 3000, 4000, performing five finite lattice sweeps for each restart, while at the same time we are increasing $N_t$ up to 25, 35 and 45. We report also the result for $N_t = 55$ time steps. However, this run was interrupted during the second sweep due to a hardware failure, which also destroyed the restart files. Therefore these data are not converged.

All these different runs display basically the same data; only the $n_{\text{max}} = 2$ run displays a slightly weaker damping of the oscillation of $N_{\text{odd}}$. In comparison with figure 2(c) of [4], we find a slightly smaller decay of the oscillations of $N_{\text{odd}}$ compared with the numerical simulations reported there, which can be attributed to the fact that there an ensemble average for different particle numbers were reported, while here we only calculated the system with the largest number of particles used in [4]. More interestingly, in extending the simulation time beyond the one reported in [4], we see a much smaller decay than the one reported in the experimental realization.

---

2 We actually use the full Arnoldi procedure [7, 8]. This is formally equivalent to a Lanczos version, where one only uses the tridiagonal elements of $\mathcal{H}$ projected on the Krylov space. We found that on finite precision arithmetic the full Arnoldi provides a higher accuracy.

3 Actually, in our simulation we find a different time scale as compared to [4]. However, we did not get a response from the authors whether we understood the parameter correctly.
we show the fluctuations plotted on a logarithmic level occupation averaged at x=-1,1

Figure 3. Level occupancy of the odd sites in the centre of the system. The solid line corresponds to the average occupation of the odd sites, as shown in figure 2. The ‘plus’ data show the average occupation of the two sites neighboring the center. In addition, we have resolved the particle occupation of these two sites into the individual level occupation of the single ($o_1$), double ($o_2$), triple ($o_3$) and quadruple ($o_4$) occupied levels; $n = \sum_{\ell=1}^{5} \ell \cdot o_\ell$.

In figure 3, we provide the individual level occupation for the single ($o_1$), double ($o_2$), triple ($o_3$) and quadruple ($o_4$) occupied levels averaged over site $\pm 1$, where the complete expectation value of the local particle number is given by $n = \sum_{\ell=1}^{5} \ell \cdot o_\ell$. The result demonstrates that the particle number is already dominated by the single and double occupied levels, the triple occupied level has still some non-vanishing contribution, while the higher occupied levels do not contribute significantly to the particle number. We also compare with the total average occupation $N_{\text{odd}}/N$, which shows only a small deviation from the occupation of the two innermost odd sites. Therefore, the boundary has only a small influence on the result. We show the same data in figure 4, where we use a logarithmic scale on the y-axis in order to make the values of the triple and quadruple occupied levels visible.

In contrast with the experiment, the numerical simulations give us direct access to the measured quantities. Specifically, in figure 5 we show the fluctuations $\langle \Psi_1 | (\hat{N}_{\text{odd}} - N_{\text{odd}})^2 | \Psi_1 \rangle$ of the occupation. Actually, with the techniques described in [9–11] the td-DMRG gives access to frequency resolved noise correlations. Within the time scale of our simulations they show basically the same decay as the oscillations for the average occupation, supporting the idea of a relaxation process for the particles. However, from the numerics it is not clear whether we see some kind of (local) thermalization or just a dephasing of the dynamics.

In order to gain a deeper insight we look at the nearest-neighbor correlation in the center of the trap. In figure 6 we display the nearest-neighbor density–density correlation $\langle \hat{N}_{\ell} \cdot \hat{N}_{\ell+1} | \Psi_1 \rangle$ and the nearest-neighbor hopping element $\langle \Psi_1 | (\hat{a}_{\ell}^+ \hat{a}_{\ell+1}^\dagger) | \Psi_1 \rangle$ for the two central bonds. While the density–density correlation and the nearest-neighbor correlation in the center of the trap do not contribute significantly to the particle number, we provide the individual level occupation of the single ($o_1$), double ($o_2$), triple ($o_3$) and quadruple ($o_4$) occupied levels; $n = \sum_{\ell=1}^{5} \ell \cdot o_\ell$.

Figure 4. The same data as in figure 3 plotted on a logarithmic y-axis.

Figure 5. The symbols show the average equal time fluctuations $\langle \Psi_1 | (\hat{N}_{\text{odd}} - N_{\text{odd}})^2 | \Psi_1 \rangle/N$, while the lines give the average occupation $N_{\text{odd}}$ of the odd sites for comparison.

Figure 6. Nearest-neighbor correlations for the two inner bonds connected to the center site. The blue symbols denote the density–density correlation $\langle \hat{N}_{\ell} \cdot \hat{N}_{\ell+1} | \Psi_1 \rangle$ and the green symbols are the nearest-neighbor correlation $\langle \hat{N}_{\ell} \cdot \hat{N}_{\ell+1} | \Psi_1 \rangle/N$. Finally, the circles correspond to bond currents $\text{Im}(\hat{a}_{\ell+1} \hat{a}_{\ell}^\dagger)$ of the $(0 \rightarrow 1)$ bond, and to the squares the bond currents $\text{Im}(\hat{a}_{\ell} \hat{a}_{\ell+1}^\dagger)$ of the negative of the $(1 \rightarrow 0)$ bond. The red line shows the average occupation of the odd sites $N_{\text{odd}}/N$ for comparison.
In summary we have shown that td-DMRG simulation can provide a deeper insight into the dynamics of strongly correlated Bose systems on a lattice. In comparison with the experimental realization, the numerics provides us with a large flexibility on the observables we want to look at. Of course, by the mere definition of science the experiment describes nature correctly. However, if we want to simulate the dynamics of the Hamiltonian equation (1), we claim that the numerics is currently not obsoleted by the experimental simulations. Furthermore, the numerics allows us to look at details, which are currently not accessible by the experimental realization. In addition, we have pointed out that the nature of the relaxation process in these systems is still an open issue. An interesting question that remains for future research is whether the (local) relaxation is due to a thermalization or a dephasing process. This question bears similarity to the difference between the $\tau_1$ and $\tau_2$ relaxation in nuclear magnetic resonance measurements.

Acknowledgments

We thank Avi Schiller and Frithjof Anders for encouraging discussions at the FQMT’11. Specifically, a discussion of the connection between Martin John Rees’s evening talk and Jens Eisert’s presentation led to the research reported in this paper. We also thank Václav Špička for his tremendous work in organizing the FQMT’11 conference.

References

[1] Jakšch D and Zoller P 2005 Ann. Phys. 315 52
[2] Lewenstein M, Sanpera A, Ahufinger V, Damski B, Sen A and Sen U 2007 Adv. Phys. 56 243
[3] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[4] Trotzky S, Chen Y A, Flesch A, McCulloch I P, Schollwöck U, Eisert J and Bloch I 2012 Nature Phys. 8 325
[5] Schmitteckert P 2004 Phys. Rev. B 70 R121302
[6] White S R 1992 Phys. Rev. Lett. 69 2863
White S R 1993 Phys. Rev. B 48 10345
[7] Saad Y 1998 SIAM J. Numer. Anal. 29 209
[8] Moler C and Van Loan C 2003 SIAM Rev. 45 3
[9] Boulat E, Saleur H and Schmitteckert P 2008 Phys. Rev. Lett. 101 140601
[10] Branschädel A, Boulat E, Saleur H and Schmitteckert P 2010 Phys. Rev. Lett. 105 146805
[11] Carr S T, Bagrets D A and Schmitteckert P 2011 Phys. Rev. Lett. 107 206801
[12] White S R and Feiguin A E 2004 Phys. Rev. Lett. 93 076401
Daley A J, Kollath C, Schollwöck U and Vidal G 2004 J. Stat. Mech. P04005