Breakdown of adiabaticity when loading ultra-cold atoms in optical lattices

Jakub Zakrzewski
Instytut Fizyki imienia Mariana Smoluchowskiego and Mark Kac Complex Systems Research Center, Uniwersytet Jagielloński, ulica Reymonta 4, PL-30-059 Kraków, Poland

Dominique Delande
Laboratoire Kastler-Brossel, UPMC, ENS, CNRS; 4 Place Jussieu, F-75005 Paris, France
(Dated: February 6, 2009)

Realistic simulations of current ultra-cold atoms experiments in optical lattices show that the ramping up of the optical lattice is significantly nonadiabatic, implying that experimentally prepared Mott insulators are not really in the ground state of the atomic system. The nonadiabaticity is even larger in the presence of a secondary quasi-periodic lattice simulating “disorder”. Alternative ramping schemes are suggested that improve the adiabaticity when the disorder is not too large.

PACS numbers: 03.75.Lm,67.85.Hj,03.75.Kk

Ultra-cold atoms in optical lattices form a wonderful toolbox for creating novel matter phases realizing a “condensed matter theorist dream”. This comes from the flexibility of parameters in cold atom physics where both the depth of the optical lattice (changing either the laser intensity or its detuning) as well as atom-atom interactions (via external magnetic field and Feshbach resonances) can be modified with unprecedented precision. By increasing the depth of the optical lattice where a Bose-Einstein condensate is loaded, one induces a transition between the superfluid (SF) phase and the Mott insulator (MI) phase, as suggested in [2] (basing a transition between the superfluid (SF) phase and the Mott insulator (MI) phase, as suggested in [2] (basing a transition between the superfluid (SF) phase and the Mott insulator (MI) phase, as suggested in [2] (basing a transition between the superfluid (SF) phase and the Mott insulator (MI) phase, as suggested in [2] (basing a transition between the superfluid (SF) phase and the Mott insulator (MI) phase, as suggested in [2] (basing a transition between the superfluid (SF) phase and the Mott insulator (MI) phase, as suggested in [2] (basing a transition between the superfluid (SF) phase and the Mott insulator (MI) phase, as suggested in [2] (basing a transition between the superfluid (SF) phase and the Mott insulator (MI) phase, as suggested in [2] (basing a transition 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the BH model [17, 18]; we use it here for parameters of a given experiment aiming at reproducing the processes taking place during ramping up of the lattices potential. Since the theory is based on the BH model, it cannot simulate the very initial stage of the experimental procedure that starts from a harmonically trapped Bose-Einstein condensate. In the first stage, the atomic gas is in a SF state; ramping up the lattice must be done sufficiently slowly to ensure that all atoms remain in the lowest band of the periodic potential. The optical potential must be increased from 0 to one recoil energy in a time longer than the recoil time (300 \(\mu s\)), which is largely fulfilled in the experiment. The atomic wave function then follows adiabatically the shrinking of the Wannier state in each site as long as tunneling between neighboring sites remains dominant. Following this reasoning, our simulations are performed starting from \(s_1 = 4\) or 5, where the system is already in the tight binding regime, in the SF phase. We have checked that our results are practically independent of this choice (proving that the initial stage is adiabatic). We choose 151 particles occupying roughly 80 lattice sites, in order to match the experimental parameters of [12]. Similar conclusions are obtained for different values of the parameters.

In the experiment [12], an absorption peak at frequency 1.9 kHz was observed, while the interaction energy for \(s_1 = 16\) is \(U = 2.3\) kHz. We thus believe that the \(s_1\) parameter was overestimated. To match the position of the peak, we modify all laser intensities by a 7/8 factor yielding \(s_1 = 14\) and \(s_2 = 35\). Attempts to simulate the absorption curve for the 30% modulation of the lattice lasting for 30 ms failed. Such a strong modulation apparently creates too much excitation and entanglement across the lattice for the TEBD algorithm to be reliable. The absorption spectra obtained for 10-30 times smaller modulation resemble those obtained in [17] with a prominent peak around \(U\) and a much smaller one around \(2U\) (in experiment this relation is reversed). In the presence of disorder, the absorption peaks broaden — both in the real experiments and in our numerical simulations — but it is hard to extract any information from this fact: firstly because of nonlinearities induced by the experimental strong modulation, and secondly because absorption spectra turn out to be almost insensitive to the details of the dynamics such as a breakdown of adiabaticity.

The numerical simulations make it possible to analyze the state of the system by different means. The first step in this direction is to test an assumption done in ultra-cold atoms “quantum phase transition” experiments [4, 5, 12], namely the adiabaticity of the optical lattice switching on. This assumption is especially critical in the laser intensity region corresponding to the transition from the SF to the MI phase. For the infinite system, due to the critical slowing down [19], such a transition cannot be fully adiabatic. For large 3D systems [4], an approximate mean-field simulation [20] showed that indeed adiabaticity is broken. For a collection of 1D tubes [3, 12], the small system size may assure the adiabaticity of the transition/crossover between phases. We can directly test the adiabaticity by comparing the state obtained dynamically by our procedure with the exact ground state of the system. The latter can be found by imaginary time propagation (using essentially the same algorithm). Next, the overlap between the dynamically created state and the ground state can be calculated.

This procedure yields for a single lattice (\(s_2 = 0\)) an overlap equal to 0.095; for weak disorder the corresponding overlap drops to 0.02-0.05, depending on the value of \(s_2\). For \(s_2\) greater than unity, the overlap drops dramatically to \(10^{-3}\) or smaller values (note that \(s_2 \approx 1\) corresponds to disappearance of the MI phase according to BH model predictions). The overlap values obtained indicate that the switching on of the lattices is not adiabatic. What is the character of the state prepared at the end of the ramping up? It is some kind of “wavepacket”, a coherent superposition of the ground state and some excited states. A crude way of measuring the wavepacket character is to compute the “excess energy”, i.e. \(\Delta E = E(\text{wavepacket}) - E(\text{ground state})\). Regardless of \(s_2\) it is about 0.15\(U\) meaning that the system is not highly excited.

More precise information can be obtained by considering the temporal autocorrelation function of the wavepacket. Indeed, the wavepacket can be expanded onto the eigenstates \(|\varphi_i\rangle\) (with energy \(E_i\)) of the Hamiltonian at the final values of \(s_1\) and \(s_2\): \(|\Psi\rangle = \sum_i a_i |\varphi_i\rangle\). If we now let \(|\Psi\rangle\) evolve freely with the final Hamiltonian, we obtain the autocorrelation function:

\[
C(t) = \langle \Psi(0)|\Psi(t)\rangle = \sum_i |a_i|^2 \exp(-i\frac{E_i t}{\hbar}).
\] (3)

Thus \(E_i\)’s and overlaps can be obtained by Fourier transforming \(C(t)\). For finite time evolution, a state of the art harmonic inversion technique [21] provides us with very accurate results. The exemplary results are shown in Fig. 1. In the absence of disorder, about 8 states contribute significantly to the wavepacket with surprisingly one excited state having 30% overlap. For strong disorder, the dynamically created wavepacket spreads over several tens of eigenstates. There are large fluctuations of the overlaps among neighboring states, meaning that the excitation brought by non adiabatic switching differs from a thermal excitation. Note also that real-time TEBD propagation brings here a spectral information not accessible to standard “quasi-exact” numerical methods such as DMRG or Quantum Monte-Carlo.

Let us underline that, while we have analyzed as closely as possible the ramping procedure in the recent “disorder” experiment [12], our findings should be applicable to other similar experiments in which both lattices and
The "best" pulse shape slowing down around confirmed by our numerical simulations shown in Fig. 2. Increase) is likely to improve adiabaticity. This is fully wards the final value (for example using an exponential ample ramp of the form

\[
s(t) = 1 + \exp(-\alpha(t - t_{\text{mid}})/T)
\]

Other shapes perform almost as well provided the region around than twice smaller than for the exponential pulse. Other ground state, a considerable improvement over the exponential transition function, eq. (3), showing peaks at the energy levels of the system, with an intensity equal to the squared overlap with the wavepacket (an exponential pulse is used). About eight (upper panel, no disorder) or several tens (lower panel, \( s_2 = 0.4375 \)) of states are significantly excited proving that the preparation is not adiabatic. Crosses indicate the values of overlap obtained via a harmonic inversion technique. Filled red circles are the corresponding overlaps for the improved ramp discussed in the text.

The solid line is the Fourier transform of the autocorrelation function, eq. (3), with a fast change in the vicinity of the SF-MI phase transition. While, for a homogeneous BH model, \( s_1 \approx 5 \) corresponds to the transition point higher in \( s_1 \), see [24]). Inspection of ground states for various \( s_1 \) shows that the crossover point is \( s_1 \approx 8 \), in agreement with experimental observations [12]. Therefore, a ramp which slows down around \( s_1 = 8 \), for example \( s_1(t) = 8\sin^2(2\pi t/T) \), and again speeds up towards the final value (for example using an exponential increase) is likely to improve adiabaticity. This is fully confirmed by our numerical simulations shown in Fig. 2. The "best" pulse shape slowing down around \( s_1 = 8 \) performs quite well, allowing to reach 53% overlap with the ground state, a considerable improvement over the exponential ramp. The excess energy for this pulse is more than twice smaller than for the exponential pulse. Other shapes perform almost as well provided the region around \( s_1 = 8 \) is passed slowly. In contrast, the "sigmoidal" ramp of the form

\[
s_1(t) = 14/[\exp(-\alpha(t - t_{\text{mid}})/T)]
\]

where \( T = 100 \text{ms} \) is the total ramp time, \( t_{\text{mid}} = T/2 \), \( \alpha = 20 \) as in [22], with a fast change in the vicinity of the phase transition, leads to a total loss of adiabaticity. For experiments exploring the insulator phase [23], this is certainly not a good choice.

While the current experiments exploring the MI regime appear not to be strictly adiabatic, this affects slightly properties such as occupation of different lattice sites or momenta distributions. The dynamically created wavepackets thus share with the corresponding ground states some global properties. In this approximate sense, the creation of MI state in 1D experiments without disorder [5] is confirmed by our simulations.

The situation is quite different in the presence of the secondary lattice creating quasi-disorder. Already for a relatively small disorder, \( s_2 = 0.4375 \), a few excited states are significantly populated, see Fig. 1. The situation becomes drastically worse for \( s_2 > 1 \) — the region where MI should disappear completely. There, the overlap between the dynamically created wavepacket and the ground state becomes vanishingly small, \( 10^{-6} \) or less for the exponential ramp at \( s_2 = 2.1875 \). However, the experimental results reported in [12] support the claim that a behavior characteristic of BG was observed.

The calculated momenta distributions averaged over different phase shifts between lattices, show a broad peak similar to the one for the ground state at \( s_1 = 14 \) and \( s_2 = 2.1875 \). The difference between the ground state
FIG. 3: (Color online) Average occupation (upper panel) and its variance (lower panel) of individual sites, for $s_1 = 14$ and $s_2 = 2.1875$, i.e. for parameters where a Bose glass phase is expected. Black circles (and solid line) correspond to the ground state of the system, with essentially only integer occupations and small variances, together with fluctuations of the occupations along consecutive sites, as expected for a Bose glass. Red crosses (and dashed line) correspond to the dynamically created wavepacket. Non-integer occupations and largely increased variances show significant excitation of the system and that its properties are different from a Bose glass.

and the wavepacket becomes evident looking at the occupations of sites and their variances $\Delta n_i = \sqrt{\langle n_i^2 \rangle - \langle n_i \rangle^2}$ as shown in Fig. 3. The ground state is characterized by integer occupations with relatively low number variance, while the dynamically excited wavepacket shows an average variance twice larger and non-integer occupation of some sites. The optimized pulse, working well for no disorder, leads to similarly disappointing results.

In summary, we have shown that the experimental preparation of a MI in recent experiment [12] is partially non adiabatic. Similar conclusion should apply to earlier experiments [4, 5]. Still the global properties of the created wavepackets resemble those for the ground states (in particular regions of integer occupations and low number fluctuations appear as in the MI phase). A careful reshaping of ramps used to switch on the lattices may lead to an adiabatic creation of MI.

The presence of disorder amplifies nonadiabaticity. Our simulations indicate that the properties of the ground state and of dynamically created wavepackets differ substantially indicating that a BG was not actually achieved in the experiment [12]. The observables measured in this experiment are not sufficiently sensitive to the state of the system to characterize unambiguously a BG. To that end, other tools suggested recently [25] might prove useful. A simple optimization of the pulse shape, successful in the absence of disorder, does not help. We are currently working on other schemes aiming at dynamical creation of a BG.

While competing this work we became aware of a recent work [26] which shows that adiabaticity is much harder to obtain in the presence of two lattices also for shallow lattices (Gross-Pitaevskii regime).

We are grateful to C. Fort, L. Fallani and M. Inguscio for discussions. DD was partially supported by IFRAF, J.Z. acknowledges support by Polish Ministry of Education and Sports (2008-2010). This work is realized within Marie Curie TOK scheme COCOS (MTKD-CT-2004-517186).

[1] D. Jaksch and P. Zoller, Ann. Phys. 315, 52 (2005).
[2] D. Jaksch et al., Phys. Rev. Lett. 81, 3108 (1998).
[3] M.P.A. Fisher, P.B. Weichman, G. Grinstein, & D.S. Fisher, Phys. Rev. B 40, 546 (1989).
[4] M. Greiner et al., Nature 415, 39 (2002).
[5] T. Stöferle et al., Phys. Rev. Lett. 92, 130403 (2004).
[6] I. B. Spielman, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. 98, 080404 (2007); arXiv:0803.3797
[7] M. Lewenstein et al., Adv. Phys. 56, 243 (2007).
[8] B. Damski et al., Phys. Rev. Lett. 91, 080403 (2003); R. Roth and K. Burnett, Phys. Rev. A 68, 023604 (2003).
[9] J. E. Lye et al., Phys. Rev. Lett. 95, 070401 (2005); D. Clément et al., Phys. Rev. Lett. 95, 170409 (2005); C. Fort et al., Phys. Rev. Lett. 95, 170410 (2005); T. Schulte et al., Phys. Rev. Lett. 95, 170411 (2005).
[10] J. Billy et al., Nature 453, 891 (2008); G. Roati et al. ibid. 453, 895 (2008).
[11] T. Giamarchi and H.J. Schulz, Phys. Rev. B 37, 325 (1988).
[12] L. Fallani et al., Phys. Rev. Lett. 98, 130404 (2007).
[13] T. Roscilde, Phys. Rev. A77, 063605 (2008); G. Roux et al., Phys. Rev. A78, 023628 (2008); X. Deng, R. Citro, A. Minguzzi and E. Orignac, Phys. Rev. A78, 013625 (2008).
[14] The heights of the optical lattice potentials $V_{latt}$ will be always expressed in units of the laser recoil energy $E_R = \hbar^2/(2m\lambda^2)$ through the dimensionless parameter $s = V_{latt}/E_R$.
[15] G. Vidal, Phys. Rev. Lett. 91, 147902 (2003).
[16] S. R. White and A. E. Feiguin, Phys. Rev. Lett. 93, 076401 (2004).
[17] C. Kollath et al., Phys. Rev. Lett. 97, 050402 (2006).
[18] S.R. Clark and D. Jaksch, New J. Phys. 8, 160 (2006).
[19] F.M. Cucchietti, B. Damski, J. Dziarmaga, and W. H. Zurek, Phys. Rev. A 75 023603 (2007).
[20] J. Zakrzewski, Phys. Rev. A 71, 043601 (2005); ibid. 72, 039904 (2005).
[21] B. Grémaud and D. Delande, Phys. Rev. A 61, 032504 (2000).
[22] T. Gericke et al., J. Mod. Opt. 54, 735 (2007).
[23] M. White et al., arXiv:0807.0446
[24] M. Rigol et al., arXiv:0811.2210
[25] T. Roscilde, arXiv:0804.2769; D. Delande and J. Zakrzewski, arXiv:0810.4111
[26] E.E. Edwards, M. Beeler, T. Hong, and S.L. Rolston, Phys. Rev. Lett. 101, 260402 (2008).