Impact of local integrals of motion onto metastable non-equilibrium states

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We analyse the stationary behaviour of correlations in a strongly correlated Bose gas in an optical lattice out of equilibrium. The dynamics are triggered by a quench of the interaction starting from the strongly interacting limit where the system is in a perfect Mott state. Despite the complete integrability of our theoretical description, we find seemingly thermal behaviour for the experimentally measurable correlations at large interactions. Quite opposed, away from the strongly interacting regime these correlation functions show highly non-thermal quasi-stationary values. Both situations are explained by overlaps of the integrals of motion with the observable and the initial state in an effective thermal ensemble. The results are obtained using approximate non-equilibrium Mazur equalities. The good agreement with the time-dependent calculations suggest that non-equilibrium Mazur equalities are an efficient way to calculate short range correlations for arbitrary integrable models.

Recent experimental developments in solid state and atomic physics enable the preparation of metastable non-thermal states of correlated quantum matter. Ultrafast optical pulses [11] uncover aspects of strongly correlated materials which are unreachable by conventional manipulation such as doping or application of pressure. In certain systems, for example in optically excited cuprate superconductors [4], long lived states with remarkable properties can be excited. The relaxation in materials not only stems from the interaction with the electronic degrees of freedom, but typically many phononic relaxation channels are present. In contrast, non-equilibrium states of ultracold atoms [5-11], can evolve coherently over long times with only little dissipation into external environments. Motivated by the experimental realizations, the theoretical description of such non-equilibrium phenomena and in particular of metastable non-thermal states has attracted a lot of interest recently. Several time-dependent numerical and approximative methods have been developed in the past decade. However, accessing long-time properties remains still an open challenge.

A special role in the understanding of non-equilibrium states take integrable models. For our purposes it is suitable to define an integrable system as quantum model exhibiting a macroscopic number of local operators which commute with the Hamiltonian. We classify operators as local if they act on a finite number of lattice sites. Different classes of such integrable models are quadratic systems, Gaudin-type models [12, 13] and Bethe ansatz solvable models [4]. Also the few body problems derived by perturbative treatments (e.g. [15]) can be seen as exactly solvable systems. It is important to note that a real physical system will never be integrable in a strict sense. Exactly solvable models should be seen as a tool to effectively describe metastable non-equilibrium states. In principle, the knowledge of the complete set of integrals of motions would enable the exact treatment of non-equilibrium states of exactly solvable models. The standard approach is the so-called ‘generalized Gibbs ensemble’ (GGE) [16], which implements constraints due to conservation laws by means of Lagrange multipliers. However, the usage of the GGE can be difficult and it has so far mainly been used for quadratic systems (e.g. [17, 20]). For non-trivially integrable models the GGE has so far only been evaluated in special cases [21, 24] or for weakly perturbed states [25, 26].

In this work we will make use of conserved quantities in order to gain further insights into the non-equilibrium states of integrable systems and to calculate their properties efficiently. The main idea is to approximate expectation values by a truncated series of projections onto independent integrals of motions. This can be realized by using an adaptation of Mazur bounds [28] to the non-equilibrium regime [29]. In Ref. [29] a condition for thermalization has been derived using these Mazur-type equalities. We specifically investigate a strongly interacting one-dimensional Bose gas in an optical lattice for which metastable states after an interaction quench have been predicted theoretically [30, 32] and observed in experiment [11]. Within an effective integrable model, we find that only few conserved quantities are sufficient to describe relevant physical properties. Besides its conceptual importance, an advantage of our strategy is, that it is not restricted to quadratic models. It can be straightforwardly extended to non-trivially exactly solvable systems, such as one-dimensional fermions and spin chains. The long-time expectation value is expressed in terms of thermal averages of observables and integrals of motions, which (unlike the time-evolution) can be calculated efficiently by standard equilibrium methods such as the density matrix renormalization group (DMRG) or exact diagonalizations.

Our starting point are bosonic atoms in a 1D tube subjected to a deep longitudinal optical lattice. This situation is accurately described by the Bose-Hubbard model.
FIG. 1. (Color online) Comparison of different averages for the parity-parity correlations for \(d = 1\) (upper curves) and \(d = 2\) (lower curves). (a) DMRG results obtained by a real-time evolution averaging over the time interval \(h/J \leq t \leq 3hJ\) (error bars reflect the mean square deviations from the average) and corresponding thermal expectation values. Experimental results are taken from Ref. 11. The inset shows the effective temperature. (b) Results for different ensembles averages (See text) derived from the approximate quadratic model (1).

\[
\hat{H} = \sum_j \left\{ -J \hat{a}_j^\dagger \hat{a}_{j+1} + \text{h.c.} + \frac{U}{2} \hat{n}_j (\hat{n}_j - 1) \right\}
\]

\(\hat{a}_j^{(t)}\) is a bosonic annihilation (creation) operator on site \(j\), \(\hat{n}_j = \hat{a}_j^{(t)\dagger} \hat{a}_j^t\) counts the number of bosons. Interaction \(U\) and tunneling \(J\) can be determined from first principles 33. The tunneling is exponentially suppressed upon increasing the intensity of the longitudinal lattice beam. Therefore, using a large lattice depth an atomic Mott state with a single localized atom per site \(|\psi_0\rangle = \prod_j \hat{a}_j^\dagger |0\rangle\) can be prepared with high fidelity 33 35. Here \(|0\rangle\) is the vacuum state. We work at filling one and assume a homogeneous system in the thermodynamic limit. For the times considered here effects of trapping potentials are weak 11.

Paired doublons and holes start propagating with well defined velocities in opposite directions when suddenly ramping down \(U/J\) from an effectively infinite value to a finite one. This gives rise to experimentally detectable parity correlations \(C_{j-j'} = \langle \hat{p}_j \hat{p}_{j'} \rangle - \langle \hat{p}_j \rangle \langle \hat{p}_{j'} \rangle\), \(\hat{p}_j = e^{i \pi (\hat{n}_j - 1)}\) \(34\). These correlations exhibit a pronounced propagation front at \(t \sim h(j - j')/6J\) 11 36. After the passage of this front, they show damped oscillations around a finite value. At large \(U/J\) it can be shown that the envelope of the oscillations decays algebraically as \(t^{-3/2}\) for the nearest neighbour and \(t^{-3}\) for the longer distance correlations 36. With time-dependent DMRG simulations (See also 36), we can study the evolution of the parity correlations up to \(t \sim 3h/J\). If interactions are sufficiently strong \((U/J > 4)\) a meaningful stationary value can be extracted from the time interval \(1h/J \leq t \leq 3h/J\). The result of this time average is displayed in Fig. 1. Only short range pair correlations show significant magnitudes and we focus on \(C_{d=1}\) and \(C_{d=2}\). The time average of \(C_{d=1}\) vanishes in the limit of \(U/J \to \infty\). It increases when lowering \(U/J\) before dropping relatively quickly to zero after \(U/J \sim 8\). \(C_{d=2}\) behave similarly, but at a much lower amplitude. From the experiment 11 the \(C_{d=1}\) stationary values can be extracted. These lie somewhat below the theoretical predictions. This discrepancy can be fully accounted for by defects in the initial state of the experimental realization.

Under ergodic assumptions 37, one expects that the large-time limit is described by the Boltzmann distribution \(\hat{\rho} = e^{-\beta (H - \mu \sum \hat{n}_j)}/Z\), where \(\beta\) and \(\mu\) are chosen such that \(\langle \psi_0 | \hat{H} | \psi_0 \rangle = \beta H \hat{\rho}\) and \(\sum_j \langle \psi_0 | \hat{a}_j^\dagger | \psi_0 \rangle = \sum_j \text{tr} \hat{n}_j \hat{\rho}\). This thermal ensemble is simulated using the finite-temperature DMRG method 38. The obtained effective temperature (Fig. 1(a) inset) is relatively large \(k_B T \gtrsim 0.4J\) and varies little in the shown region 5 \(U/J < 20\). As evident in Fig. 1(a), there are significant differences between thermal and time-averaged ensembles, but qualitatively they correspond unexpectedly well (see also 32). In particular the thermal average shows the same basic features: At large interactions coherent excitations only emerge perturbatively on the order \(J^2/U\) 38 39 and parity correlations become highly suppressed at these high effective temperatures. The vanishing correlations at weaker interactions are mainly due to the fact that correlations are no more purely doublon-hole-like, but mix with doublon-doublon and holon-holon correlations. In the strongly interacting regime \(U/J \geq 12\) the thermal values even quantitatively reproduce the time-averaged ones. In contrast, at intermediate interactions the non-equilibrium values are significantly larger than the thermal ones. In the following we analyze this crossover between apparently thermal and non-thermal regimes and relate it to the sensitivity of observables to conserved quantities.

The considered stationary state can be described approximately by a quadratic model of fermionized doublons and holes. Following Ref. 39, this model can be derived by first truncating the local Hilbert space to contain maximally two atoms per site, i.e. the site basis is spanned by the states \(|0\rangle, |1\rangle, |2\rangle\). Further, Jordan-Wigner fermion operators are introduced to describe the doublons \(\hat{c}_{j,+}^\dagger \propto |2\rangle |1\rangle\) and holes \(\hat{c}_{j,-}^\dagger \propto |0\rangle |1\rangle\) (the atomic Mott state at filling one \(|\psi_0\rangle\) is a vacuum of auxiliary fermions in this representation). By retaining only quadratic terms and neglecting a constant energy shift
the Bose-Hubbard model reduces to:

\[
\hat{H} = \sum_j \left\{ -2J \hat{c}^\dagger_{j,+} \hat{c}_{j+1,+} - J \hat{c}^\dagger_{j+1,-} \hat{c}_{j,-} - J \sqrt{2} \left( \hat{c}^\dagger_{j,+} \hat{c}^\dagger_{j+1,-} - \hat{c}_{j,-} \hat{c}_{j+1,+} \right) + \text{h.c.} \right\} + \frac{U}{2} \left( \hat{n}_{j,+} + \hat{n}_{j,-} \right).
\]

The Hamiltonian neglects the constraint that multiple occupancies of different auxiliary species on the same site are not allowed. This leads to a systematic overestimation of the number fluctuations, but otherwise reproduces well the physics of the intermediate time regime. The Hamiltonian is diagonalized in momentum space by using Bogolyubov transformations, \( \gamma_{k,\sigma} = u_k \hat{c}_{k,\sigma} - v_k \hat{c}^\dagger_{-k,-\sigma} \) with \( \sigma = \pm \), \( u_k = \cos \left( \frac{\sqrt{4 J \sqrt{2} \sin(k) - U}}{-J \cos(k) + U} \right) \) and \( v_k^2 = u_k^2 - 1 \). In this representation \( \hat{H} = \sum_{k,\sigma} \epsilon_\sigma(k) \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} \) where the quasiparticle energies are given by \( \epsilon_\sigma(k) = -\sigma J \cos(k) + \frac{1}{2} \sqrt{(-6 J \cos(k) + U)^2 + (4 J \sqrt{2} \sin(k))^2} \).

Unlike in DMRG simulations, it is possible to access the long-time limit within the quadratic fermionic model. We will evaluate the quadratic fermionic model in different ensembles. For all of them, two-point correlations are solely determined from momentum distributions for auxiliary fermions:

\[
\langle \hat{c}^\dagger_{k,\sigma} \hat{c}_{k,\sigma} \rangle = u_k^2 f_{k,\sigma} - v_k^2 (1 - f_{k,\sigma}), \\
\langle \hat{c}_{k,\sigma} \hat{c}_{-k,-\sigma} \rangle = u_k v_k (f_{k,+} + f_{k,-} - 1),
\]

where the quasiparticle distributions \( f_{k,\sigma} = \langle \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} \rangle \) are evaluated in a given ensemble (\( \bullet \) is a placeholder for the type of the ensemble). For example, in the long-time limit after the quench from the perfect Mott state expectation values are determined by the diagonal ensemble [17]:

\[
\langle \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} \rangle_{\text{diag}} := -v^2(k),
\]

which is equivalent to the 'generalized Gibbs ensemble' [10]. In the thermal ensemble we fix the energy and the total number of particles to the initial values by an effective temperature and a chemical potential. This leads to the Fermi-Dirac distributions,

\[
\langle \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} \rangle_{\text{therm.}} := n_{F,\sigma}^E (\epsilon_\sigma(k) - \sigma \mu),
\]

with \( n_{F,\sigma}^E (\epsilon) = 1/(e^{\beta \epsilon} + 1) \), which is fundamentally different from the quasiparticle distribution of the diagonal ensemble [3].

We also introduce a natural extended ensemble which fixes energies and number operators for both species individually:

\[
\langle \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} \rangle_{\text{ext.}} := n_{F,\sigma}^E (\epsilon_\sigma(k) - \sigma \mu). 
\]

The effective inverse temperatures \( \beta_\sigma \) and chemical potentials \( \mu_\sigma \) are chosen such that expectation values of \( \sum_k \epsilon_\sigma(k) \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} \) and \( \sum_k \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} \) are equal to those of the initial state.

The parity correlations in the diagonal, thermal, and extended ensembles for the quadratic approximation [1] are shown in Fig 1b. As demonstrated previously in time-dependent simulations [20], the correlations are somewhat overestimated as compared to exact DMRG simulations for the original Bose-Hubbard models (displayed in Fig. 1a). Apart from that it is justified to explain the properties of the metastable state in the Bose-Hubbard model within the quadratic model [1].

As in the full Bose-Hubbard model (see Fig. 1a), the diagonal ensemble of the effective integrable model exhibits a crossover between a seemingly thermalized behavior at large \( U \gtrsim 15 \) and non-thermal expectation values at smaller interactions. This behaviour is found for both the thermal ensemble and the extended ensemble. Whereas the thermal ensemble underestimates the correlations compared to the diagonal ensemble, the extended ensemble overestimates them. We find that this crossover is rather robust and occurs also for larger-distance correlations and other observables such as single particle and string [34] correlations. Other quantities, such as momentum distributions of quasiparticles, differ from their thermal values. A similar effect has been observed in a quantum Ising chain [18], where off-diagonal correlators approach thermal values while diagonal ones do not.

In order to understand such behaviour, we propose to use a hierarchy of conserved quantities out of which only few turn out to be relevant. In the context of the generalized Gibbs ensemble one typically resorts to the occupancies \( \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} \). In the considered quadratic model this ensemble is equivalent to the diagonal ensemble and therefore does not provide new physical insight. A promising idea has been put forward by Fagotti et al. [20] who used a truncated GGE formed by a limited number of local integrals of motions [5]. This is a valuable approach but the evaluation of this ensemble is technically difficult especially when non-quadratic models shall be considered. Similarly to Ref. [20] we use local integrals of motions but we avoid the evaluation of the truncated GGE by expanding the observables in a series of projections onto these local integrals of motions. Such expansion technique has been developed by Mazur [27] and is employed to estimate the influence of the conserved quantities to response functions [27, 28, 40–43].

For non-equilibrium setups, a Mazur-type equality has been used to estimate finite size effects [42] and a condition for thermalization [29].

We construct the local integrals of motion in the effective model using

\[
\hat{I}_{\sigma} = \sum_k \cos(\alpha k) \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma},
\]

where \( \alpha = \pi / (2L) \). The local integrals of motion are different from the momentum-dependent ones [5]. For this reason we consider a diagonal ensemble which is equivalent to the diagonal ensemble of the effective integrable model [1].
for \( \alpha \geq 0 \). These quantities are linear combinations of integrals of motion and thus remain integrals of motions. In addition, it is convenient to define \( \hat{I}_{\sigma,-1} = \sum_k \epsilon_k (k) \hat{\gamma}^+_k \hat{\gamma}_k,\sigma \).

The hierarchy of integrals of motions should be such that lower integrals are not contained in the higher ones. This can be achieve by orthogonalizing the integrals. One can use different ensemble averages as a measure for the overlap of conserved quantities and we formulate our procedure for a general ensemble \( \langle \cdot \rangle \). In order to achieve a set of orthogonal integrals we first shift expectation values of integrals of motions to zero, \( \hat{I}_{\sigma,\alpha} = \hat{I}_{\sigma,\alpha} - \langle \hat{I}_{\sigma,\alpha} \rangle \) and then apply the Gramm-Schmidt scheme

\[
\hat{J}_{\sigma,-1} = \hat{I}_{\sigma,-1}:
\]

\[
\hat{J}_{\sigma,0} = \hat{I}_{\sigma,0}² - \langle \hat{I}_{\sigma,0} \rangle \langle \hat{J}_{\sigma,-1}² \rangle
\]

such that

\[
\langle \hat{J}_{\sigma,\alpha} \hat{J}_{\sigma',\alpha'} \rangle = \delta_{\sigma,\sigma'} \delta_{\alpha,\alpha'} \langle \hat{J}_{\sigma,\alpha}² \rangle \quad \text{and} \quad \langle \hat{J}_{\sigma,\alpha} \rangle = 0.
\]

With this transformed set, we can closely follow Mazur’s arguments \(27,28\) and expand the observable in the diagonal ensemble in the conserved quantities \(29\):

\[
\langle \hat{O} \rangle_{\text{diag.}} = \sum_{\sigma,\alpha} \langle \hat{O} \hat{J}_{\sigma,\alpha} \rangle \text{tr} \left( \hat{\rho}_0 \hat{J}_{\sigma,\alpha} \right) / \langle \hat{J}_{\sigma,\alpha}² \rangle.
\]

This modified Mazur equation measures the distance between the diagonal and an approximate ensemble \(\langle \cdot \rangle\) for a given quantity \(\hat{O}\) (We recall that \(\langle \hat{O} \rangle_{\text{diag.}} = \langle \hat{O} \rangle_{\text{ext.}} - \langle \hat{O} \rangle_{\text{diag.}}\)). In the original linear response formula of Mazur \(27,28\) all terms are positive and the equation turns into an inequality when the series is truncated. In the present case such an inequality cannot be derived. However, in practice there is nevertheless no need to evaluate the entire series. Strictly speaking, Eq. \(9\) is only exact when all local \([\alpha]\) and non-local integrals of motion (i.e. projections onto eigenstates) are included. But on rather general grounds, one can argue that eigenstates become irrelevant for local observables in the thermodynamic limit \(29,42\). For short range correlations one can even go one step further and truncate the series to contain few terms. In the considered case the amplitudes of the contributions of higher order terms decay rapidly and already the first few are sufficient to obtain accurate results.

To demonstrate this we stick to the extended ensemble \(\langle \cdot \rangle\) in which all terms with \(\alpha \leq 0\) in Eq. \(0\) vanish by definition. For the experimentally relevant parity-parity correlations the first relevant term in the

\[
\hat{C}_d^{(1)} = \sum_{\sigma} \langle \hat{p}_d \hat{p}_{d+1} \rangle_{\text{ext.}} \text{tr} \left( \hat{\rho}_0 \hat{J}_{\sigma,1} \right) / \langle \hat{J}_{\sigma,1}² \rangle_{\text{ext.}}.
\]

As shown in Fig. 2 for small distances \(d\), this term almost fully describes the deviation from the extended thermal ensemble. Only at distances \(d \geq 4\) higher terms become significant. For large distances or higher precision one could include higher integrals of motion \(\alpha \geq 1\).

With this result we can interpret the crossover from thermal to non-thermal behaviour upon decreasing interaction (See Fig. 1) in terms of equilibrium expectation values of integrals of motions and the observable: Both, overlaps of the integral of motion with the observable \(\langle \hat{p}_d \hat{p}_{d+1} \rangle_{\text{ext.}}\) and the initial state \(\text{tr} \left( \hat{\rho}_0 \hat{J}_{\sigma,1} \right)\) are negligibly small at large \(U\) and small \(d\) and become significant only at weaker interactions. It is important to note that this effect goes beyond second order perturbation theory – even in the strongly interacting regime the \(\frac{d^2}{d^2} \) expansion \(36,39\) is not sufficient to describe the observed behaviour. The effective integrals of motion \(\hat{J}_{\sigma,1}\) are fermionic two-point correlators which mainly extend over distances \(d = 1\) and \(d = 2\).

For future investigations, it will be interesting to approach also non-quadratic integrable systems. In Ref. \(44\) for example, a weak interaction quench in the 1D Hubbard model for fermions has been studied. This model is integrable by the Bethe ansatz \(45\). The time-dependent DMRG simulations show a relatively quick relaxation \(44\) of the double occupancy to a value which is not completely far off the thermal one. The first
non-trivial integral of motion for the 1D fermionic Hubbard model is an energy current formed by operators on three neighboring sites \( \hat{I}_3 \), which is similar to \( \hat{I}_{n,1} \) used here. Therefore, we expect that mainly the first integral of motion will contribute to the local double occupancy. Overlaps with the conserved current in the modified Mazur equation \( \mathcal{H}_{\text{M}} \) can be accessed by finite temperature DMRG or other methods such as high-temperature series expansions, allowing to make predictions for the long time limit which is inaccessible to time-dependent DMRG simulations. Another interesting perspective is the calculation of the effect of non-integrable perturbations within the Mazur expansion. This may be a feasible way to extract thermalization time scales in near-integrable systems.

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