Thermalization of Interacting Fermions and Delocalization in Fock space

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By means of exact diagonalization, we investigate the onset of 'eigenstate thermalization' and the crossover to ergodicity in a system of 1D fermions with increasing interaction. We show that the fluctuations in the expectation values of the momentum distribution from eigenstate to eigenstate decrease with increasing coupling strength and system size. It turns out that these fluctuations are proportional to the inverse participation ratio of eigenstates represented in the Fock basis. We demonstrate that eigenstate thermalization should set in even for vanishingly small perturbations in the thermodynamic limit.

**Introduction.** – Statistical physics relies on the assumption that the system under investigation is in thermal equilibrium. However, what are the precise conditions for an isolated system to relax to thermal equilibrium? This question has a long history including the ground breaking numerical experiments initiated by Fermi, Pasta and Ulam [1] on an anharmonic chain of classical oscillators, where thermalization was not observed as expected [2]. Nowadays, the investigation of thermalization in quantum many-body systems attracts a lot of theoretical attention, inspired by the new experimental possibilities in systems of cold atoms [3–5].

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The trajectory of a classical ergodic system reaches all regions on the energy shell for sufficiently long times, establishing the microcanonical ensemble. As a consequence, suitable chosen subsystems obey the Boltzmann distribution. In the quantum case, switching on an interaction in a many-body system will combine the unperturbed eigenstates \(|i\rangle\) of similar energies into new energy eigenstates: \(|\alpha\rangle = \sum_i c_{\alpha i} |i\rangle\). If the expectation values \(A_{\alpha} = \langle \alpha | A | \alpha \rangle\) of observables in these new eigenstates approach their microcanonical values \(A_{\text{micro}}(E)\), as obtained by averaging over all unperturbed states in a small energy window around \(E\), then the properties of thermal equilibrium are established in each many-body eigenstate. This is the essential idea behind the 'eigenstate thermalization hypothesis' (ETH) [6, 7].

Recently, the ETH has been tested in numerical experiments [8–10], by means of exact diagonalization. For few-body observables like the momentum distribution, indeed it was demonstrated that \(A_{\alpha} \approx A_{\text{micro}}(E_{\alpha})\) and that the fluctuations around \(A_{\text{micro}}\) decrease with increasing interaction strength and system size.

In the present work, we address the important question of how fast thermal equilibrium is approached when increasing the system size. A direct, brute-force numerical approach would be prohibitive. Instead, we characterize the gradual delocalization of eigenstates in the many-body Fock space via the inverse participation ratio (IPR) \(\sum_{\alpha=1}^{D} (p_{\alpha}^2)^2\) (with \(p_{\alpha}^2 = |c_{\alpha i}|^2\)) which turns out to be connected with the fluctuations of \(A_{\alpha}\). While a connection between the IPR and the fluctuations was observed recently [11, 12], we are able to conjecture its functional form and its dependence on system size and interaction strength, based on earlier analytical results on Fock-space localization by P. Silvestrov. In particular, we have numerical evidence that the interaction strength needed for thermalization is below that needed for full quantum chaos. Moreover, we find that in the thermodynamic limit (TDL) thermalization (in the sense of the ETH) sets in for arbitrarily small interactions. This is in contrast to recent observations on relaxation in a classical 1D system [13].

Here, we address these questions by means of exact numerical diagonalization for a system of spinless 1D fermions on a lattice, where integrability is broken by an interaction of strength \(V\). As the observable of interest, we consider the fermionic momentum distribution \(\hat{f}_k\). Our main result is that for large enough \(V\) the fluctuations of \(\hat{f}_k^a = \langle \alpha | \hat{f}_k | \alpha \rangle\) are determined by the IPR which roughly can be considered as the inverse number of non-interacting Fock states \(|i\rangle\) contributing to \(|\alpha\rangle\) (see e.g. [14]). The IPR itself keeps track of the transition from integrability to quantum chaos [11, 15] and it was conjec-
tured only recently that it might directly determine the deviations of steady state expectation values from the corresponding microcanonical value \(10\).

We observe three different regimes, depending on the interaction strength. An important scale is set by the mean level spacing \(\Delta_f\) between Fock states that couple directly to a given initial Fock state. If the interaction is smaller than \(\Delta_f\), then the eigenstates are ‘localized’ in Fock space \(17, 18\) and experience only a perturbative correction due to the interaction (see Fig. 1a). For couplings beyond \(\Delta_f\), the eigenstates delocalize and remarkably the IPR decreases exponentially with \(V\) on a scale that depends on \(\Delta_f\). This scale essentially decreases polynomially in particle number and system size. Therefore, we expect the fluctuations of \(f^\alpha_k\) to be suppressed to zero in the TDL even for vanishingly small interaction strength, establishing eigenstate thermalization of the considered observable. Increasing the interaction even further, eigenstates become chaotic (see Fig. 1b) and the IPR as well as the fluctuations in \(f^\alpha_k\) decrease as the inverse many-body density of states as it was conjectured in \(9, 7\). These results should apply rather generically to few-body observables diagonal in the eigenbasis of the unperturbed Hamiltonian.

Model. – We consider \(n\) spinless 1D fermions with periodic boundary conditions on a lattice of \(N\) sites and with a next-nearest neighbor interaction breaking the integrability of the system. The Hamiltonian reads:

\[
\hat{H}_0 + \hat{V} = -t \sum_{i=1}^{N} c_i^\dagger c_{i+1} + H.c. + V \sum_{i=1}^{N} (\hat{n}_i - 1/2)(\hat{n}_{i+2} - 1/2). \tag{1}
\]

The eigenstates |\(i\rangle\) of \(\hat{H}_0\) with \(\xi_i = \langle i | \hat{H} | i \rangle\) are given by the Fock states of \(n\) fermions in momentum space. Due to the translational symmetry, the interaction does not mix Fock states with different total momentum \(K\). Therefore, each momentum sector \(K\) with dimension \(D_K\) will be considered separately. We exclude the \(K = 0\)-sector as it possesses a trivial extra symmetry under reflection. In our numerical examples \(n = 7\) and \(N = 21\).

Fluctuations and IPR. – In the following, we discuss the expectation values \(f^\alpha_k\) of the momentum occupation numbers \(f^\alpha_k = c_k^\dagger c_k\) (where \(c_k \equiv 1/\sqrt{N} \sum_{j=1}^{N} e^{-ikx_j} c_j\)). Being interested in the properties of typical eigenstates, we analyze the statistics of an ensemble of states \(|\alpha\rangle\) with similar eigenenergies \(E_\alpha \in E = [E - \delta E, E + \delta E]\), which will be called in the following ‘eigenstate ensemble’ (EE). The width of the energy window \(\delta E\) has to be chosen small enough to avoid artifacts resulting from systematic dependencies on \(E\). Averages with respect to the EE are denoted by \(\langle \ldots \rangle_E\). For not too large interactions, one can easily show that \(\langle f^\alpha_k \rangle_E \approx f_{k, \text{micro}}(E)\). However, the crucial statement of the ETH is that for each eigenstate itself \(f^{\alpha}_k \to f_{k, \text{micro}}\) when going to the TDL, i.e., that the fluctuations of \(f^{\alpha}_k\) from state to state vanish:

\[
\delta f^2_k \equiv \langle (f^\alpha_k - \bar{f}_k)^2 \rangle_{E} \xrightarrow{N \to \infty} 0. \tag{2}
\]

We introduced the EE-variance \(\delta f^2_k\) and \(\bar{f}_k = \langle f^\alpha_k \rangle_E\). Representing \(f^\alpha_k\) in the Fock basis \(f^\alpha_k = \sum_{i \in D_K} p_{\alpha i}^k f_{\alpha i}^k\) (with \(f_{\alpha i}^k = |i \rangle \langle \alpha | f_{\alpha i}^k\) this statement becomes plausible. For strong interaction, typical eigenstates are spread out widely in Fock space (Fig. 1b), i.e., they are composed of a large number of Fock states close in energy. Due to the law of large numbers, we thus expect the fluctuations to decay as the mean inverse number of Fock states contributing to \(|\alpha\rangle\), i.e., as the mean IPR

\[
\chi = \langle \sum_{i=1}^{D_K} (p_{\alpha i}^k)^2 \rangle_E. \tag{3}
\]

Before deriving the connection between \(\delta f^2_k\) and \(\chi\) formally, we focus on the numerical results for the present model. Fig. 2 shows \(\delta f^2_k\) as a function of \(V\) evaluated w.r.t. eigenstates at various energies. The eigenenergies can be re-expressed in terms of effective temperatures \(T\), with \(E_T \equiv \text{Tr}_K(\hat{H} e^{-\hat{H}/T})/\text{Tr}_K(e^{-\hat{H}/T})\). The results are compared to the IPR, or more precisely to
the sum over the variances \( \text{Var}_E(p_i^α) = \langle (p_i^α)^2 \rangle_E - \langle p_i^α \rangle_E^2 \) (see discussion below), clearly demonstrating that indeed \( δf_k^2 \propto \sum_i \text{Var}_E(p_i^α) \) even for small interactions. This is in stark contrast to the case of integrability conserving nearest-neighbor interaction (inset Fig.2), where the suppression of \( δf_k^2 \) with \( V \) is much smaller than in the prior case.

Formally, representing \( δf_k^2 \) in terms of \( p_i^α \), one finds

\[
δf_k^2 \simeq \bar{f}_k (1 - \bar{f}_k) \sum_i \text{Var}_E(p_i^α) + \sum_{i \neq j} (f_k^i f_k^j - \bar{f}_k^2) \text{Cov}_E(p_i^α p_j^α | k)
\]

with \( δf_k^i = (f_k^i - \bar{f}_k^i) \) and the covariance matrix \( \text{Cov}_E(p_i^α p_j^α | k) \equiv \langle p_i^α p_j^α | E \rangle - \langle p_i^α \rangle_E \langle p_j^α \rangle_E | k \). The first term in Eq.(4) contains the suppression of \( δf_k^2 \) with increasing number of Fock states contributing to a typical eigenstate. It is essentially determined by \( χ \) [we note \( χ \approx \sum_i \text{Var}_E(p_i^α) \) below the regime of full chaos (see below)]. We replaced \( \sum_i (f_k - \bar{f}_k) \text{Var}_E(p_i^α) \to (\bar{f}_k - \bar{f}_k^2) \sum_i \text{Var}_E(p_i^α) \), which is justified as \( \text{Var}_E(p_i^α) \) is a smooth function of \( i \). The prefactor \( \bar{f}_k (1 - \bar{f}_k) \) is nothing but the variance of the momentum occupation numbers for the non-interacting case.

The off-diagonal contributions in Eq.(4) are sensitive to residual correlations within eigenstates and are expected to become small for strong perturbations. Surprisingly, for strong enough interactions, it approximately reproduces the diagonal part of Eq.(4). Thus, even though \( δf_k^2 \) is still determined by the IPR, one observes a deviation of the prefactor of \( O(1) \). A very similar observation was made in [19] while investigating finite fermionic systems with random two-body interactions and was traced back to the strong correlations between matrix elements of two-body interaction matrices.

To sum up, we find that the fluctuations in the expectation value of \( f_k^i \) from eigenstate to eigenstate are determined by the IPR \( χ \). Thus, in the following, it will be discussed how \( χ \) decreases with increasing \( V \) and system size. Being a measure for the mean effective number of Fock states forming an eigenstate, \( χ \) indicates the ‘delocalization’ crossover in Fock space and serves as an indicator for the transition from integrability to quantum chaos.

Definitions – For the following discussion of the IPR, we need to set up a few technical definitions. We introduce the effective density \( ρ_f^j(ω) \) of Fock states \( |j⟩ \) coupling to a state \( |i⟩ \) of energy \( ξ_i ∈ I_E \) (i.e., \( ⟨i|V|j⟩ \neq 0 \)), where the energy difference between both states is \( ξ_i - ξ_j = ω \). Averaging over a couple of states \( |i⟩ \) (indicated by \( ⟨\cdots⟩_E = \{ ⟨i,ξ_i ∈ I_E⟩^{-1} [⟨i,ξ_i ∈ I_E⟩ \cdots] \} \)) one obtains the mean effective density of states \( ρ_f(ω, E) = \langle ρ_f^j(ω)⟩_E \). Furthermore, it will be convenient to introduce the interaction formfactor

\[
F(ω, E) = π \int f^+_{ω'} f^-_ω \sum_{j=1;i\neq j} \text{Var}_E(f^j_ω - f^j_{ω'}) | k | ω''}
\]

This can be rewritten as \( F = π ρ_f V^2 \), where \( V^2 \) denotes a mean matrix element squared. For \( ω \to 0 \) and small \( V \), the form factor \( F \) reduces to Fermi’s golden rule for a Fock state of energy \( E \). In the following, only the mean matrix element and the effective density of states with respect to states close in energy, i.e., \( V^2(ω \approx 0, E) \) and \( ρ_f(ω \approx 0, E) \) will appear. For brevity these will now be denoted by \( V^2 \) and \( ρ_f \), respectively.

Localized regime – As long as \( V^2 ≪ ρ_f^{-1} \), eigenstates can be obtained within standard perturbation theory (apart from a small set of eigenstates, which can be traced back to degenerate Fock states). A given Fock state gets perturbed by the set of directly coupling states and eigenstates consist of a small number of sharp peaks (Fig.1(k), i.e., they are localized in Fock space.

Delocalization – Increasing the coupling strength \( V^2 \sim ρ_f^{-1} \), one enters the regime of delocalized eigenstates [18]. Perturbation theory breaks down and the IPR starts to decrease rapidly (see Fig.3). In this regime, the fluctuations \( δf_k^2 \) become directly determined by \( χ \). Surprisingly, one observes an exponential decay of \( χ \) and we find good numerical evidence that

\[
χ \propto \exp(-C ρ_f V^2).
\]

The numerical constant \( C \) is independent of temperature and system size. In Figs.3a,c, the IPR is shown as a function of the scaling variable \( 2πρ_f V^2 \) for eigenstates.
ergodic eigenstates’, we understand states which in prin-
ciple are composed of all Fock states close in energy (cf.
Fig.1b). No Fock states are excluded a priori, e.g., due
to the two-body nature of \( \tilde{V} \) or further symmetries from
contributing to an ergodic eigenstate. The amplitudes \( c_i^\alpha \)
become Gaussian distributed random variables \([6, 7]\) as it is
shown in Fig.4 with a Lorentzian variance \([6, 21, 22]\)

\[
\langle p_i^\alpha \rangle_E \simeq \frac{1}{\pi \rho_K(E)} \frac{\Gamma(E - \xi_i, E)}{\xi_i - \bar{E}(E, \xi_i)^2 + \Gamma^2},
\]

where \( \rho_K \) denotes the full many-body density of states
for total momentum \( K \), scaling as \((N-1)!/(N-n)!n!\).
This indicates the crossover to full quantum chaos. We
checked that in this regime the nearest neighbor level spacing
agrees with the GOE-Wigner surmise, characteristic for GOE
random matrix ensembles. Due to the Gaussian distribution for \( c_i^\alpha \), one finds \( \chi = 3 \sum_n \langle p_i^\alpha \rangle_E^2 \) resulting in

\[
\chi \simeq \frac{3}{2\pi} \frac{1}{\langle 0|E\rangle \rho_K(E)},
\]

which is in fairly good agreement with the numerical
results in Fig.3a, demonstrating the suppression of
\( \delta f_n^2 \) by the inverse many-body density of states as it
was conjectured in \([3, 7]\). The mean spreading width \( \Gamma \)
(Fig.4h) can be extracted from the Fock state self-
energy \( \Sigma \) by averaging \(-\text{Im} \Sigma(\xi_i, \omega) \) over \( \xi_i, \omega \in I_E \).
\( \Sigma \) is obtained from \( G(\xi_i, \omega) \equiv \langle \omega + i0^+ - \hat{H} \rangle^{-1} |i \rangle \) via
\( G \equiv [\omega + i0^+ - \xi_i - \hat{\Sigma}]^{-1} \). Fig.4h shows a comparison of \( \langle p_i^\alpha \rangle_E \) and a Lorentzian of width \( \Gamma \) extracted
directly from \(-\text{Im} \Sigma \).

The important question remains, how the second
crossover scale (governing the crossover from delocalized
to ergodic eigenstates) depends on system size. We
found some indication that it might depend on the
intensive ‘energy range’ \( W \) of the coupling matrix \( \hat{V} \).
Consider the dependence of \( \Gamma \) on \( V \) in Fig.3a.
For small \( V \), Fermi’s golden rule applies and one finds \( \Gamma(0, E) \simeq
F(0, E) \propto V^2/t \). For large \( V \), one observes a crossover
\( \Gamma \propto V^2/t \to \Gamma \propto V \) indicating the entrance into
the strong coupling regime, where \( \Gamma \) and the finite width (in \( \omega \)) of the formfactor \( F \) become comparable \([21]\).
Comparing Figs.3a and 4a, there might exist a close relation
between this crossover and the onset of ergodicity of
eigenstates. This would imply that the interaction en-
ergy scale \( \rho_f^{-1} \) for the onset of thermalization is paramet-
rically smaller than the scale for the transition to chaos,
determined by \( W \).

Conclusions. – By means of exact diagonalization we
investigated the interaction induced onset of eigenstate
thermalization in a system of 1D fermions. We found
that the fluctuations of the expectation value of the
momentum occupation number from state to state are pro-
portional to the inverse participation ratio of eigenstates.
For small interactions the latter decays exponentially be-
fore one enters the chaotic regime. The interaction
scale for the onset of this decay is essentially set by the effective
mean level spacing between interacting Fock states,
and this vanishes in the TDL. Thus, we corroborate the physical expectation that in the TDL at arbitrarily small interactions, eigenstate thermalization sets in.

Acknowledgements. – We thank P.G. Silvestrov, Frank Göhmann and A. Polkovnikov for fruitful discussions related to this work. Financial support by DIP, NIM, the Emmy-Noether program and the SFB/TR 12 is gratefully acknowledged.