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 as-
sumption that the system under investigation is in ther-
mal equilibrium. However, what are the precise con-
tions for an isolated system to relax to thermal equi-
librium? 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 exper-
imental possibilities in systems of cold atoms [3–5].

The trajectory of a classical ergodic system reaches
all regions on the energy shell for sufficiently long times,
establishing the microcanonical ensemble. As a conse-
quence, suitable chosen subsystems obey the Boltzmann
distribution. In the quantum case, switching on an in-
teraction in a many-body system will combine the un-
perturbed eigenstates |i⟩ of similar energies into new energy
eigenstates: |α⟩ = ∑_i c_α^i |i⟩. If the expectation values
A_α = ⟨α| A |α⟩ of observables in these new eigenstates
approach their microcanonical values A_{micro}(E), as ob-
tained by averaging over all unperturbed states in a small
energy window around E, then the properties of ther-
mal equilibrium are established in each many-body eigen-
state. This is the essential idea behind the ‘eigenstate
thermalization hypothesis’ (ETH) [3, 7].

Recently, the ETH has been tested in numerical experi-
ments [8–10], by means of exact diagonalization. For few-
bodies observables like the momentum distribution, indeed
it was demonstrated that A_α ≈ A_{micro}(E_α) and that the fluctua-
tions around A_{micro} decrease with increasing in-
teraction strength and system size.

In the present work, we address the important ques-
tion of how fast thermal equilibrium is approached when
increasing the system size. A direct, brute-force numerical
approach would be prohibitive. Instead, we char-
acterize the gradual delocalization of eigenstates in the
many-body Fock space via the inverse participation ra-
tio (IPR) \( \sum_{i=1}^{D} (p_\alpha^i)^2 \) (with \( p_\alpha^i = |c_\alpha^i|^2 \)) 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 in-
teraction 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 thermo-
dynamic 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 in-
terest, we consider the fermionic momentum distribution
\( \hat{f}_k \). Our main result is that for large enough \( V \) the fluctuations
of \( f_k^\alpha \equiv ⟨\alpha | \hat{f}_k | \alpha⟩ \) are determined by the IPR which
roughly can be considered as the inverse number of non-
interacting Fock states |i⟩ contributing to |α⟩ (see e.g.
\[13\]). The IPR itself keeps track of the transition from
integrability to quantum chaos [11, 15] and it was conjec-

![Figure 1. Probability distribution \( p_\alpha^i = |\langle i | \alpha⟩|^2 \) of a many-
body eigenstate |\alpha⟩ in the non-interacting Fock basis (energies \( \xi_i \)). a) For weak interaction \( V/t = 0.1 \), the eigenstate
is localized in Fock space, consisting of a few isolated peaks.
b) At large \( V/t = 1.3 \), all Fock states with energies \( \xi_i \) close
to \( E_\alpha \) contribute. c) \( p_\alpha^i \) averaged over a couple of nearby
eigenstates in a range \( \delta E/t = 0.05 \), for \( V/t = 0.45, 1.45 \) (top,
bottom). It can be approximated by a Lorentzian of width \( Γ \) (red line).
The energy was chosen to correspond to infinite
effective temperature (see main text).]
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 in-
teraction 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 perturba-
tive correction due to the interaction (see Fig. 1b). For
couplings beyond $\Delta_f$, the eigenstates delocalize and re-
markably 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. There-
fore, we expect the fluctuations of $f_k^0$ 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. 1d) and the
IPR as well as the fluctuations in $f_k^0$ decrease as the in-
verse many-body density of states as it was conjectured
in [6, 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 pe-
riodic boundary conditions on a lattice of $N$ sites and
with a next-nearest neighbor interaction breaking the in-
tegrability of the system. The Hamiltonian reads:

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

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 $f_k^0$ of the momentum occupation numbers $f_k = c_k^\dagger c_k$ (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 $E_\alpha \in E_E = [E - \delta E, E + \delta E]$, 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 systemati-
cal 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 $\langle f_k^0 \rangle_E \approx f_{k, \text{micro}}(E)$. However,
the crucial statement of the ETH is that for each eigenstate
itself $f_k^0 \rightarrow f_{k, \text{micro}}$ when going to the TDL, i.e., that the
fluctuations of $f_k^0$ from state to state vanish:

$$
\delta f_k^2 \equiv \langle (f_k^0 - \bar{f}_k)^2 \rangle_E \underset{N \rightarrow \infty}{\rightarrow} 0. \quad (2)
$$

We introduced the EE-variance $\delta f_k^2$ and $\bar{f}_k = \langle f_k^0 \rangle_E$. Representing $f_k^0$ in the Fock basis $f_k^0 = \sum_{i=1}^{D_K} p_i^0 f_k^0$ (with $f_k^0 = \langle i | f_k^0 | i \rangle$) 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 fluctua-
tions to decay as the mean inverse number of Fock states
contributing to $|\alpha\rangle$, i.e., as the mean IPR

$$
\chi = \langle (\sum_{i=1}^{D_K} (p_i^0)^2 \rangle_E. \quad (3)
$$

Before deriving the connection between $\delta f_k^2$ and $\chi$ for-
malement, we focus on the numerical results for the present
model. Fig. 2 shows $\delta f_k^2$ as a function of $V$ evaluated w.r.t.
eigenstates at various energies. The eigenener-
gies can be re-expressed in terms of effective tempera-
tures $T$, with $E_T \equiv \text{tr}_K(\hat{H} e^{-H/T}/tr_K(e^{-H/T})$. The
results are compared to the IPR, or more precisely to

![Figure 2. Fluctuations of expected occupation number $\langle f_k^0 | \alpha \rangle$ between eigenstates decrease with increasing interaction strength $V$, indicating eigenstate thermalization. Plot shows the variance $\delta f_k^2$ for states with an effective temperature $T/t = 1.2, 1.7, \infty$ (from top to bottom), with energy shells of width $\delta E/t = 0.25$. Solid lines show $\text{const} \times f_{k=0} (1 - f_{k=0}) \sum_i \text{Var}_E(p_i^0)$, with a slightly $T$-dependent constant. Finally, we averaged the results over all total momentum sectors $K$. Inset: As in main figure, but with $\delta f_k^2$ averaged over all $k$. The red dots show $\delta f_k^2$ averaged over all $k$ for an integrable model with nearest-neighbor interactions (at $T = \infty$ and $K/(2\pi/N) = 1$). $K$-averages are only performed to improve statistics. The same results are obtained for individual $K$-sectors.](image-url)
the sum over the variances $\text{Var}_E(p_i^0) = \langle (p_i^0)^2 \rangle_E - \langle p_i^0 \rangle_E^2$ (see discussion below), clearly demonstrating that indeed $\delta f_k^2 \propto \sum_i \text{Var}_E(p_i^0)$ 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 $\delta f_k^2$ with $V$ is much smaller than in the prior case.

Formally, representing $\delta f_k^2$ in terms of $p_i^0$, one finds

$$\delta f_k^2 \approx \frac{1}{2K} \sum_i \text{Var}_E(p_i^0) + \sum_{i \neq j} \delta f_k^{ij} \text{Cov}_E(p_i^0, p_j^0),$$

with $\delta f_k^{ij} = (f_k^i f_k^j - \bar{f}_k^2)$ and the covariance matrix $\text{Cov}_E(p_i^0, p_j^0) = \langle p_i^0 p_j^0 \rangle_E - \langle p_i^0 \rangle_E \langle p_j^0 \rangle_E$. The first term in Eq. (4) contains the suppression of $\delta f_k^2$ with increasing number of Fock states contributing to a typical eigenstate. It is essentially determined by $\chi$ [we note $\chi \approx \sum_i \text{Var}_E(p_i^0)$ below the regime of full chaos (see below)]. We replaced $\sum_i (f_k^i - \bar{f}_k^i) \text{Var}_E(p_i^0) \to (\bar{f}_k^i - \bar{f}_k^i) \sum_i \text{Var}_E(p_i^0)$, which is justified as $\text{Var}_E(p_i^0)$ is a smooth function of $i$. The prefactor $\frac{1}{2K}(1 - \bar{f}_k)$ 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 $\delta f_k^2$ 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 $\chi$. Thus, in the following, it will be discussed how $\chi$ decreases with increasing $V$ and system size. Being a measure for the mean effective number of Fock states forming an eigenstate, $\chi$ 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 $\rho_f(\omega)$ of Fock states $|j\rangle$ coupling to a state $|i\rangle$ of energy $\xi_i \in I_E$ (i.e., $\langle i| \hat{V} |j\rangle \neq 0$), where the energy difference between both states is $\xi_i - \xi_j = \omega$. Averaging over a couple of states $|i\rangle$ (indicated by $(\ldots)_{\infty} = \sum_{i, \xi_i \in I_E}^{-1} [\sum_{i, \xi_i \in I_E} \ldots ]$) one obtains the mean effective density of states $\rho_f(\omega, E) = \langle \rho_f(\omega) \rangle_E$. Furthermore, it will be convenient to introduce the interaction formfactor

$$F(\omega, E) = \pi \int \omega' d\omega' \frac{d\omega'}{\delta \omega} \sum_{j=1}^K \sum_{i \neq j} V_{ij}^2 \delta(\xi_j - \xi_i - \omega').$$

This can be rewritten as $F = \pi \rho_f \sqrt{V}$, where $\sqrt{V}$ denotes a mean matrix element squared. For $\omega \to 0$ and small $V$, the form factor $F$ reduces to Fermi’s golden rule rate 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., $\sqrt{V} (\omega \approx 0, E)$ and $\rho_f(\omega \approx 0, E)$ will appear. For brevity these will now be denoted by $\sqrt{V}$ and $\rho_f = \Delta_f^{-1}$, respectively.

Localized regime – As long as $\sqrt{V} \ll \rho_f^{-1}$, 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. 1b), i.e., they are localized in Fock space.

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

$$\chi \propto \exp\{-\mathcal{C} \rho_f \sqrt{V}\}.$$

The numerical constant $\mathcal{C}$ is independent of temperature and system size. In Figs. 3b,c, the IPR is shown as a function of the scaling variable $2\pi \rho_f \sqrt{V}$ for eigenstates.
ergodic eigenstates, we understand states which in principle decrease drastically in the thermodynamic limit even in the plane: energy dependent standard deviation of width $\langle (\alpha_i^\lambda)^2 \rangle_E$ increases linearly in $t/\omega$.

Figure 4. a) Fock state decay rate $\tilde{\Gamma}$ vs. $V$ (at $T = \infty$), extracted from the imaginary part of the self-energy (red dots). For small $V$, Fermi’s golden rule $\Gamma = \rho_f V^2$ holds, while $\Gamma$ increases linearly in $V$ for large $V$. For this plot, $\text{Im}\Sigma(\omega)$ was averaged in both $\omega$ and energy $\xi_i$ over the energy interval of width $\delta E = 0.25t$ centered around $E_f$. Black dots show the results of a direct fit of $\langle p_i^\lambda \rangle_E$. Here $K = 2\pi/N$. b) Amplitude distribution $P(\alpha_i^\lambda)$ for eigenstates at $T/t = \infty$ with $\delta E/t = 0.25$ and $V/t = 1$ demonstrating that for very large $V$ one enters the chaotic regime. In this regime, the amplitudes $\alpha_i^\lambda$ are gaussian distributed as originally conjectured in [6]. In plane: energy dependent standard deviation $\pm (\langle (\alpha_i^\lambda)^2 \rangle_E)^{1/2}$ of $P$ (blue lines). Out of plane: Cuts of $P$ (black lines), which can be described by gaussians of variance $\langle (\alpha_i^\lambda)^2 \rangle_E$ (red lines).

at different energies $E$ and for various $N$ and $n$. Indeed, in good accordance to Eq. (6) all curves collapse to the same scaling curve. An explanation of this exponential decay of $\chi$ might be found in the two-particle nature of the interaction, following P. Silvestrov. In [20] it was argued (in a random matrix setting) that for moderate interaction strength, typical eigenstates are composed of independent pairs of interacting fermions. Thus, eigenstates decompose into direct products of pairs of Fock states, resulting in an exponential decay of $\chi$, of the form given by Eq. (6). While this exponential decay (and additional corrections) have been confirmed numerically in a random quantum dot Hamiltonian [14], here we find it in a translationally invariant many-body system without disorder.

We now discuss the dependence on system size. The effective density of states $\rho_f(\omega)$ scales as $N^3$. For example, at large $T$, we have $\rho_f(\omega) t \simeq N^3 \rho^2(1 - \rho)^2 t(\omega)$, with the density $\rho$. For our particular model, $\rho(\omega) \propto \ln(t/\omega)$ for $\omega \to 0$ due to transitions of particle pairs around the inflection point of the $-2t\cos(k)$ dispersion, resulting in $\rho_f^\lambda \propto t/N^3 \ln N$ (assuming a cutoff scale $\omega/t \sim 1/N$). Together with the scaling of the matrix elements $\sqrt{\tilde{\Gamma}}(\omega, E) = v(\omega, E) V/N$, this would yield $\chi \propto \exp\left\{-\tilde{C}N^2 \ln N \rho^3(1 - \rho)^2 V/t\right\}$, with $\tilde{C}$ being independent of $N$. Thus, we expect the fluctuations to decrease drastically in the thermodynamic limit even in this intermediate regime, where eigenstates are not yet ergodic.

Chaos – Only by increasing the interaction even further, one enters the regime of ergodic eigenstates. By ‘ergodic eigenstates’, we understand states which in principle are composed of all Fock states close in energy (cf. Fig. 4b). No Fock states are excluded a priori, e.g., due to the two-body nature of $V$ or further symmetries from contributing to an ergodic eigenstate. The amplitudes $\alpha_i^\lambda$ become Gaussian distributed random variables [6, 7] as it is shown in Fig. 4 with a Lorentzian variance $\langle \delta f_i^\lambda \rangle_E = \frac{1}{\pi \rho_K(E) (\xi_i - E - \delta(E, \xi_i))^2 + \Gamma^2}$, 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 statistics agrees with the GOE-Wigner surmise, characteristic for GOE random matrix ensembles. Due to the Gaussian distribution for $\alpha_i^\lambda$, one finds $\chi = \sum_\lambda \langle \alpha_i^\lambda \rangle^2_E$ resulting in

\[
\chi \simeq \frac{3}{2\pi} \frac{1}{\Gamma(0, E)/\rho_K(E)},
\]

which is in fairly good agreement with the numerical results in Fig. (4), demonstrating the suppression of $\delta f_i^\lambda$ by the inverse many-body density of states as it was conjectured in [6, 7]. The mean spreading width $\tilde{\Gamma}$ (Fig. 4b) can be extracted from the Fock state self-energy $\Sigma$ by averaging $-\text{Im}\Sigma(\xi_i, \omega)$ over $\xi_i, \omega \in \mathbb{I}_E$. $\Sigma$ is obtained from $G(\xi_i, \omega) \equiv \langle \alpha_i | \omega + i\delta^+ - \hat{H}^{-1} | \alpha_i \rangle$ via $G \equiv \left[ \omega + i\delta^+ - \xi_i - \Sigma \right]^{-1}$. Fig. 4b shows a comparison of $\langle \alpha_i^\lambda \rangle_E$ and a Lorentzian of width $\tilde{\Gamma}$ 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 $V$. Consider the dependence of $\tilde{\Gamma}$ on $V$ in Fig. 4a. For small $V$, Fermi’s golden rule applies and one finds $\tilde{\Gamma}(0, E) \simeq F(0, E) \propto V^2/t$, for large $V$, one observes a crossover $\tilde{\Gamma} \propto V^2/t \to \tilde{\Gamma} \propto V$ indicating the entrance into the strong coupling regime, where $\tilde{\Gamma}$ and the finite width (in $\omega$) of the formfactor $F$ become comparable [21]. Comparing Figs. 3a and 4b, there might exist a close relation between this crossover and the onset of ergodicity of eigenstates. This would imply that the interaction energy scale $\rho_f^{-1}$ for the onset of thermalization is parametrically 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 proportional to the inverse participation ratio of eigenstates. For small interactions the latter decays exponentially before 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.

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