Universal power law in crossover from integrability to quantum chaos

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We study models of interacting fermions in one dimension to investigate the crossover from integrability to non-integrability, i.e., quantum chaos, as a function of system size. Using exact diagonalization of finite-sized systems, we study this crossover by obtaining the energy level statistics and Drude weight associated with transport. Our results reinforce the idea that for system size \(L \to \infty\) non-integrability sets in for an arbitrarily small integrability-breaking perturbation. The crossover value of the perturbation scales as a power law \(\sim L^{-\delta}\) when the integrable system is gapless and the scaling appears to be robust to microscopic details and the precise form of the perturbation. We conjecture that the exponent in the power law is characteristic of the random matrix ensemble describing the non-integrable system. For systems with a gap, the crossover scaling appears to be faster than a power law.

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How isolated quantum systems thermalize, hitherto investigated theoretically in a few special cases \([1,2]\), is now the subject of active experimental study thanks to the advent of cold-atom systems \([3,4]\). Recall that in isolated classical systems that thermalize, a phase space trajectory samples all possible microstates at a given energy spending equal amounts of time in each, yielding the microcanonical prescription. On the other hand, for a system which does not thermalize, the trajectory typically follows regular, not chaotic, orbits constrained by conservation laws and samples only a low-dimensional subspace. This notion of thermalization underpins the Fermi-Pasta-Ulam problem of a classical system of masses connected by springs \([5]\). For harmonic springs the system does not thermalize and, even upon the introduction of anharmonicity, thermalization occurs only above an energy threshold which, however, scales to zero with increasing system size, as a power-law characterizing the nature of anharmonicity \([6]\). Signatures of lack of thermalization in classical systems can also be seen in transport \([3]\) (but note that singular size-dependence of thermal conductivity is distinct from a failure to thermalize \([6]\)).

In this paper we investigate analogous issues for quantum systems. Later in the paper we compare our study to the related work of Rabson et al. \([10]\). As quantum mechanics lacks a notion of phase space, we identify thermalization with non-integrability, i.e., quantum chaos, a now-standard prescription, and use the corresponding diagnostically tools. We would like to emphasize that while the integrable systems we study a) are exactly solvable, b) have an infinity of conservation laws in the thermodynamic limit and c) display Poissonian level-spacing statistics it is perhaps only the last one that is important to prevent thermalization: localized phases of disordered systems lacking properties a) and b) have been argued to not thermalize \([11]\).

Our main result is that the characteristic value of control parameter at which significant non-integrability is seen scales to zero with increasing system size as in the classical systems described above. For gapless systems, the approach to zero is a power law whose exponent appears robust to microscopic details such as variations in the type of integrable limit and integrability-breaking perturbation. We conjecture that this power law is determined only by the random matrix ensemble describing the non-integrable system. For systems with a gap our numerics suggest a faster-than-power-law dependence of the crossover on system size.

We consider two one-dimensional models of interacting fermions with periodic boundary conditions that have integrable limits. First is the \(t-t'-V-V'\) model of spinless fermions with Hamiltonian

\[
H = -t \sum_i c_i^\dagger c_{i+1} + h.c. - t' \sum_i c_i^\dagger c_{i+2} + h.c. + V \sum_i n_i n_{i+1} + V' \sum_i n_i n_{i+2}.
\]  

This model, which can be mapped on the spin 1/2 \(XXZ\) chain, is integrable and exactly solvable by the Bethe ansatz when \(t'=V'=0\) \([12]\). The other Hamiltonian we study is the Hubbard model with next nearest neighbor hopping and spin dependent hopping given by

\[
H = - \sum_{i \sigma} t_\sigma (c_i^\dagger c_{i+1\sigma} + h.c.) - \sum_{i \sigma} t'_{\sigma} (c_i^\dagger c_{i+2\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}.
\]  

This reduces to the regular one dimensional Hubbard model for \(t'_{\sigma} = 0\) and \(t_\uparrow = t_\downarrow\), which too is integrable and solvable by the Bethe ansatz \([13]\). For both of the above models, we set \(t = 1\) henceforth.

For the \(t-t'-V-V'\) model we have investigated the breaking of integrability by taking one or both of \(t'\) and
$V'$ to be non-zero \[14\]. The only conserved quantities in the non-integrable cases are particle number and crystal momentum \[15\].

Our Hubbard model is non-integrable in the presence of next-nearest neighbor hopping. In this case, in addition to particle number and crystal momentum, all components of the total spin are conserved if $t_r = t_l$ and $t'_r = t'_l$. To break this symmetry, we choose $t'_l = 0$ which breaks the $SU(2)$ symmetry of the model and only $S_z$ is conserved. Further, the $S_z = 0$ sector no longer has degeneracies arising from spin inversion.

We investigate the breaking of integrability through 1) The energy-level spacing distribution and 2) the Drude weight for charge transport.

**Energy level spacing:** An integrable system without disorder has an infinite number of conserved quantities in the thermodynamic limit whose values can be used to label the energy eigenstates of the system. The energy level spacing obtained from symmetry sectors labeled by any finite set of quantum numbers shows no level repulsion and in fact obeys a Poissonian distribution $P(s) = \exp(-s)$, for the energy spacing $s$ in units of the mean level spacing \[16\]. On the other hand, a non-integrable system of the type we study has a finite number of conserved quantities even in the thermodynamic limit. Once these have been accounted for the resultant symmetry sectors have no degeneracies left and the energy levels display level repulsion. $P(s)$ then corresponds to that of a random matrix ensemble even though there is no inherent microscopic randomness in the Hamiltonian. For most of our studies, the non-integrable system is described by $P(s) = \pi s/2 \exp(-\pi s^2/4)$, corresponding to the Gaussian Orthogonal Ensemble (GOE). We thus track $P(s)$ as a function of the strength of the appropriate integrability breaking parameter (say $p$) to locate the crossover from integrable to non-integrable behavior. Since our goal is to locate this crossover as a function of system size, we perform numerical exact diagonalization on finite-sized systems to obtain all the energy eigenvalues. We are thus restricted to a maximum system size of about $L = 22$ for the model of spinless fermions and about $L = 11$ for the Hubbard model \[17\]. We perform the diagonalization in momentum space and leave out the $k = 0$ and $k = \pi$ sectors to exclude the effect of parity symmetry. The system sizes we consider appear sufficient to quantify the crossover we are investigating. Having obtained $P(s)$ for a given system, we locate its peak $S$ by fitting to a Brody distribution \[18\]

\[P(s) = (\beta + 1)bs^\beta \exp(-bs^{\beta+1}),\]

where $b = \Gamma([\beta + 2]/(\beta + 1))^{\beta+1}$, which interpolates smoothly between Poissonian ($\beta = 0$) and GOE ($\beta = 1$). We assume that all our systems become non-integrable in the limit $p \to \infty$ \[19\]. Thus, knowing $S$ as a function of $p$, for a system size $L$, we locate the crossover value $p_L$ by fitting the values of $S$ to a function of $p$ that smoothly interpolates from 0 (Poisson) at $p = 0$ to 0.8 as $p \to \infty$ (GOE). We choose the function $S(p) = 0.8 \tanh(p/p_L)$ \[18\] for this purpose and have checked that other functions yield similar results.

The level spacing distribution for our largest system sizes for the $t-t'-V$ model (Fig. 1) and the Hubbard model (Fig. 2) for representative values of $V$ and $U$ respectively show that $P(s)$ evolves from being Poissonian to GOE as the integrability breaking parameter $t'$ is increased. For the $t-t'-V$ model, we show data for $V = 1.0$ at half filling while increasing the integrability breaking parameter $t'$ from 0. For the Hubbard model too we work at half filling, setting $S_z = 0(1)$ when the number of particles is even(odd). We show our data for $U = 1$ while increasing $t'$ from 0 in Fig. 2.

Fig. 3 shows peak positions of $P(s)$ for various $t'$ and $L$ obtained using the Brody distribution for representative values $V = 2.0$ and $U = 2.0$ for the $t-t'-V$ and Hubbard models along with fits to obtain the crossover scale for different $L$.

**Drude weight:** We assume that our system is in contact with an external heat bath which causes it to thermalize at a temperature $T$ even if it is integrable when isolated. One can then formally define a frequency dependent charge conductivity

\[\sigma_c(T, \omega) = D_c(T)\delta(\omega) + \sigma(\omega \neq 0, \omega),\]

where $\omega$ is the frequency and $D_c(T)$ is the Drude weight or charge stiffness \[20\]. For an integrable system with-
out a charge gap, \( D_c(T) \) can be argued to be non-zero for all finite values of \( T \) whereas for a non-integrable system it goes to zero in the thermodynamic limit at any finite temperature \( 20, 21, 23, 24 \). Thus, \( D_c(T) \) can be used as a diagnostic tool to determine the crossover from integrability to non-integrability. We consider the limit \( T \to \infty \) for better statistics for which \( 23 \).

\[
TD_c(T) = \frac{1}{LN} \sum_{\epsilon_m < \epsilon_n} | < n|J|m > |^2, \tag{5}
\]

where \( N \) is the size of the Hilbert space, \( n \) and \( m \) are energy eigenstates at the same energy and \( J \) is the charge current given by

\[
J = \lim_{k \to 0} \frac{1}{k} [n(k), H]. \tag{6}
\]

Here \( n(k) \) is the Fourier transform of the charge density. We emphasize that \( D_c(T) \) is a useful diagnostic tool only if the integrable system is gapless. For our specific systems, this is true for the \( t - t' - V \) model for all values of filling except half filling for \( V > 2|t| \), which we study later using only level spacing statistics. For the Hubbard model, we calculate \( D_c(T) \) away from half-filling, where it is gapless. At half filling, the integrable system has a charge gap but no spin gap for all values of \( U > 0 \). In this case, the spin Drude weight \( D_s(T) \) can be used instead of \( D_c(T) \). \( D_s(T) \) can be obtained from relations similar to \( 5 \) and \( 6 \) with the charge current and density replaced by the spin current and density respectively. We have verified that \( D_s(T) \) yields the same scaling of the integrability breaking parameter as \( D_c(T) \).

Fig. 4 shows \( D_c(T) \) for the \( t - t' - V \) model and the Hubbard model. In the integrable limit of the \( t - t' - V \) model \( (t' = 0) \), \( D_c(T) = 0 \) at half filling for an odd number of particles \( 20, 22 \). In order to obtain a sufficient number of data points for \( D_c(T) \) at different values of \( L \), we work away from half-filling. For the Hubbard model we set \( S_z = 0 \) always working with an even number of particles even when away from half-filling.

We extract the value of the crossover scale of \( t' \) for both models in the following way: It can be seen from Fig. 4 that \( TD_c(T) \) appears to decrease linearly for small values of \( t' \) before leveling off. Further, the value it appears to saturate to decreases with increasing system size. We expect that in the thermodynamic limit, this value will be equal to zero and will be attained for any non-zero value of \( t' \). The intercept on the \( x \) axis of the linear fit at small values of \( t' \) can thus be used to define the crossover...
The research was investigating the integrability-breaking parameter. Our systems sizes are slightly larger than theirs, which enables us to make better fits and we have verified to the extent possible that their numerical data is consistent with the power law that we obtain.

We have also conducted a similar study for gapped systems using energy level statistics. The specific system we have studied is the $t - t' - V$ model with $V > 2|t|$. The data for integrability breaking crossover scale as a function of system size is shown in Fig. 4. The value of $\tau_{cr}$ as obtained from energy level statistics is shown for $V = 1$ and 2 for which the integrable model is gapless and $V = 3$, 4 and 6 for which it is gapped. We have added a flux threading the loop since in its absence, one does not obtain the right gap when there are an odd number of particles [20]. For the system sizes we have studied, it appears that $\tau_{cr}$ does fall off faster than a power law when the system is gapped.

What is the origin of this power law? We do not have a very definite answer to that question yet. However, on the evidence of our numerical data and the robustness of the power law we conjecture that the exponent 3 is associated with the only universal feature of the different models we study, namely the GOE ensemble describing the non-integrable systems. If this is true, one will presumably obtain different exponents when the non-integrable systems are described by other ensembles. Our preliminary results on such microscopic models seems to bear out this fact and a detailed study will be published later.

The fall off of the crossover scale faster than a power law when the system is gapless is also intriguing. Naively,
one might have expected the energy level statistics, which is a property of the entire spectrum to not be affected by the presence or absence of a gap. Our studies might suggest that in the systems we study the entire spectrum is controlled by the properties of a few low lying energy states. A thorough validation of this claim would require larger scale numerics, perhaps of the sort using the Density Matrix Renormalization Group (DMRG) developed recently \cite{27} or tractable analytical calculations.

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