Time Evolution of a Quantum Many-Body System: Transition from Integrability to Ergodicity in the Thermodynamic Limit

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Numerical evidence is given for nonergodic (nonmixing) behavior, exhibiting ideal transport, of a simple nonintegrable many-body quantum system in the thermodynamic limit, namely, the kicked t-V model of spinless fermions on a ring. However, for sufficiently large kick parameters t and V we recover quantum ergodicity, and normal transport, which can be described by random matrix theory. [S0031-9007(98)05420-9]

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A simple question is addressed here: "Do intermediate quantum many-body systems, which are neither integrable nor ergodic, exist in the thermodynamic limit"? While it is clear that integrable systems are rather exceptional, it is an important open question whether a finite generic perturbation of an integrable system becomes ergodic or not in the thermodynamic limit (TL), $size \to \infty$ and *fixed density*. It is known that local statistical properties of quantum systems with few *degrees of freedom* whose classical limit is completely chaotic/*ergodic*, are universally described by *random matrix theory* (RMT); while in the other extreme case of *integrable systems*, Poissonian statistics may typically be applied [1,2] (with some notable nongeneric exceptions such as finite dimensional harmonic oscillator). This statement has also been recently verified numerically for integrable and *strongly* nonintegrable many-body systems of interacting fermions [3] which do not have a classical limit.

Having lost the reference to classical dynamics, we resort to the definition of *quantum ergodicity* (also termed *quantum mixing*) [4] as the decay of time correlations $\langle A(\tau)B(0)\rangle - \langle A\rangle\langle B\rangle$ of any pair of quantum observables A and B in TL, taking the time limit $\tau \to \infty$ in the end. In [4] a many-body system of interacting bosons has been studied, and it has been shown that quantum ergodicity corresponds to strongly chaotic (ergodic) dynamics of associated nonlinear mean-field equations. As a consequence of linear response theory, quantum ergodicity also implies normal transport and *finite* transport coefficients (such as dc electrical conductivity). On the other hand, integrable systems, which are solvable by Bethe ansatz or quantum inverse scattering, are characterized by (infinitely many) conservation laws and are thus *nonergodic*. It has been pointed out recently [5] that integrability implies nonvanishing stiffness, i.e., ideal conductance with infinite transport coefficients (or ideal insulating state). As we argue below, any deviation from quantum ergodicity generically implies nonvanishing long-time current autocorrelation and therefore an infinite transport coefficient. Since generic nonintegrable systems of finite size (number of degrees of freedom) are nonergodic (obeying *mixed* statistics smoothly interpolating from Poisson to RMT), it is thus important to question if and when such nonergodicity can survive TL.

In this Letter we introduce a family of simple many-body systems smoothly interpolating between integrable and ergodic regimes, namely, *kicked t-V model* (KtV) of spinless fermions with periodically switched nearest-neighbor interaction on a 1D lattice of size L and periodic boundary conditions $L \equiv 0$, with a time-dependent Hamiltonian,

$$H(\tau) = \sum_{j=0}^{L-1} [-\tfrac{1}{2} t(c_j^\dagger c_{j+1} + \text{H.c.}) + \delta_p(\tau) V n_j n_{j+1}], \tag{1}$$

and give numerical evidence for the existence of an *intermediate nonergodic regime* in TL by direct simulation of the time evolution. $c_j^\dagger, c_j, n_j$ are fermionic creation, annihilation, and number operators, respectively, and $\delta_p(\tau) = \sum_{m=-\infty}^{\infty} \delta(\tau - m)$. Deviations from quantum ergodicity (or mixing) are characterized by several different quantities as described below.

The KtV model (1) is a many-body analog of popular 1D nonintegrable kicked systems [2] such as, e.g., kicked rotor: Its evolution (Floquet) operator over one period, $U = \hat{T}\exp[-i\int_{0^+}^{1^+} d\tau H(\tau)]$ ($\hbar = 1$), factorizes into the product of a kinetic and potential part,

$$U = \exp\left(-iV\sum_{j=0}^{L-1} n_j n_{j+1}\right) \times \exp\left(it\sum_{k=0}^{L-1}\cos(sk+\phi)\tilde{n}_k\right), \tag{2}$$

where $s = 2\pi/L$. The flux parameter ϕ is used in order to introduce a *current operator* $J = (i/t)U^\dagger \partial_\phi U|_{\phi=0} = \sum_{k=0}^{L-1}\sin(sk)\tilde{n}_k$, elsewhere we put $\phi := 0$. The tilde denotes the operators which refer to *momentum* variable k, $\tilde{c}_k = L^{-1/2}\sum_{j=0}^{L-1}\exp(isjk)c_j$, $\tilde{n}_k = \tilde{c}_k^\dagger\tilde{c}_k$. The KtV model is integrable if either $t = 0$, or $V = 0$ (mod 2π), or $tV \to 0$ and t/V finite (continuous time t-V model

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[6]), while for $t \sim V \sim 1$ it is expected to be nonintegrable, either *quantum ergodic* or *intermediate*. We expect that unitary many-body quantum maps, such as (2), also mimic the dynamics of generic *autonomous* quantum many-body systems on the energy shell similar to the way 1D quantum maps describe quantum Poincaré sections of autonomous 2D quantum chaotic systems (e.g., [7]).

The total number of particles $N = \sum_j n_j$ is conserved, so the map U acts over Hilbert (Fock) space $\mathcal{H}$ of dimension $\mathcal{N} = \binom{L}{N}$. The dynamics of a given initial many-body state $|\psi(0)\rangle$, which is an iteration of the map $|\psi(m)\rangle = U|\psi(m-1)\rangle = U^m|\psi(0)\rangle$, can be performed most efficiently by observing that the kinetic part U_T is diagonal in the momentum basis $|k\rangle = \tilde{c}^\dagger_{k_1}, \ldots, \tilde{c}^\dagger_{k_N}|0\rangle, k_1 < \cdots < k_N$ while the potential part U_V is diagonal in the position basis $|j\rangle = c^\dagger_{j_1}, \ldots, c^\dagger_{j_N}|0\rangle, j_1 < \cdots < j_N$. The transformation between the two, $F_{\vec{j}\vec{k}} = \langle \vec{j} \,|\, \vec{k}\rangle$, is an antisymmetrized N-dimensional discrete Fourier transformation (DFT) on L sites which has been efficiently coded in $\sim \mathcal{N} \log_2 \mathcal{N}$ floating point operations (FPO) by factorizing L site DFT to the product of $\mathcal{O}(L \log_2 L)$ two-site transformations parametrized with 2×2 submatrices $(\alpha, \beta; \gamma, \delta)_{jj'}$, which are successively applied to creation operators, $(c^\dagger_j, c^\dagger_{j'}) \rightarrow (\alpha c^\dagger_j + \beta c^\dagger_{j'}, \gamma c^\dagger_j + \delta c^\dagger_{j'})$, in all Slater determinants $\Pi_n c^\dagger_{j_n}|0\rangle$ which contain a particle at sites j or j'. Our algorithm (fermionic fast Fourier transform) requires almost no extra storage apart from a vector of $\mathcal{N}$ c numbers and works for lattices of sizes $L = 2^p, 10, 12, 15, 20, 24, 30$, and 40. Therefore, the map (2) is iterated on a vector $\psi_{\vec{k}}(m) = \langle k \,|\, \psi(m)\rangle$, using the matrix composition $U = F^* U_V F U_T$ in roughly $2\mathcal{N} \log_2 \mathcal{N}$ FPO per time step which is by far superior to complete diagonalization techniques [$\mathcal{O}(\mathcal{N}^3)$ FPO], even for *long* time scales $m = \mathcal{O}(\mathcal{N})$ when quantum dynamics becomes quasiperiodic due to discreteness of the spectrum of U.

We now consider the current time-autocorrelation function $C_J(m) = (1/L)\langle J(m)J(0)\rangle$, where $J(m) = U^{\dagger m} J U^m$ and $\langle\cdot\rangle = (1/\mathcal{N})\mathrm{Tr}(\cdot)$ is a "microcanonical average." J is diagonal in the momentum basis $J|\vec{k}\rangle = J_{\vec{k}}|\vec{k}\rangle$, and $\langle J\rangle = 0$. So $C_J(m)$ can be evaluated by means of time evolution of momentum initial states $|\psi(0)\rangle = |\vec{k}'\rangle$,

$$C_J(m) = \frac{1}{L\mathcal{N}'} {\sum_{\vec{k}'}}' J_{\vec{k}'} \sum_{\vec{k}} J_{\vec{k}} p_{\vec{k}\vec{k}'}(m)\,, \tag{3}$$

where $p_{\vec{k}\vec{k}'}(m) = |\langle \vec{k} \,|\, \psi(m)\rangle|^2 = |\langle \vec{k} \,|\, U^m|\vec{k}'\rangle|^2$. For large sizes L, a smaller but uniformly random sample of $\mathcal{N}'$ initial states $|\vec{k}'\rangle$, $1 \ll \mathcal{N}' \ll \mathcal{N}$, is used in order to save computer time. Direct computation of $C_J(m)$ for $m \le M$ can be performed in $\sim(2M\mathcal{N}\mathcal{N}'/L)\log_2 \mathcal{N}$ FPO since, due to translational symmetry, one can simultaneously simulate the dynamics of L different states with different values of the conserved total momentum $K = \sum_n k'_n \pmod L$. Using the eigenphases η_n and eigenstates $|n\rangle$ of evolution operator U, $U|n\rangle = e^{-i\eta_n}|n\rangle, n = 1, \ldots, \mathcal{N}$, one can write the *dissipative* dc conductivity of such a kicked system $\sigma := \sum_{n=1}^{\mathcal{N}} (\partial_\phi \eta_n)^2 \approx C_J(0) + 2\sum_{m=1}^{\mathcal{N}/2} C_J(m)$. Note that $\partial_\phi \eta_n = \langle n|J|n\rangle$.

In Fig. 1 we present numerical computation of correlation function $C_J(m)$ for parameters $t = V = 1$ and $t = V = 4$, for various sizes L, but at fixed density $\rho = N/L = \frac{1}{4}$. Quite generally, $C_J(m)$ exhibits fast relaxation on a time scale M^* which is typically small, $M^* \sim 10$, and roughly independent of L, and afterwards it fluctuates around the averaged limiting value, the *stiffness*

$$D_J = \lim_{M\to\infty} \frac{1}{M} \sum_{m=1}^{M} C_J(m)\,, \tag{4}$$

where the strength of fluctuations decreases with increasing size L. Note again that TL $L \to \infty$ should be taken prior to the time-limit, $\lim_{M\to\infty}(1/M)\sum_{m=1}^{M}(\cdot)$ which, for systems of finite size L here and below, is estimated numerically as $(1/M')\sum_{m=M'+1}^{2M'}(\cdot)$ with sufficiently large but fixed averaging time $M' > M^*$; we take $M' = 30$. For sufficiently large control parameters the system is quantum ergodic (case $t = V = 4$ of Fig. 1), D_J goes to zero, and σ remains finite as $L \to \infty$ ($\mathcal{N} \to \infty$) and $\rho = N/L$ fixed, whereas in the other case ($t = V = 1$ of Fig. 1), D_J remains well above zero as we approach TL, whereas conductivity σ diverges [8]. In Fig. 2 we have analyzed $1/L$ scaling of D_J. Again, for large values of parameters, say $t = V = 4$, D_J is already practically zero for $L \approx 20$, while for smaller (but not small) control parameters $D_J \approx D_J^\infty + \beta/L$, where $D_J^\infty > 0$. In the *close-to-critical* case $t = V = 2$, we find a larger correlation time $M^* \sim 10^2$, and hence use a longer averaging time $M' = 200$. In Fig. 3 we illustrate an *ideal transport* for $t \sim V \sim 1$ by plotting a *persistent current* $J^p_{\vec{k}'} = \lim_{M\to\infty}(1/M)\sum_{m=1}^{M}\langle \vec{k}'|J(m)|\vec{k}'\rangle$ vs the initial

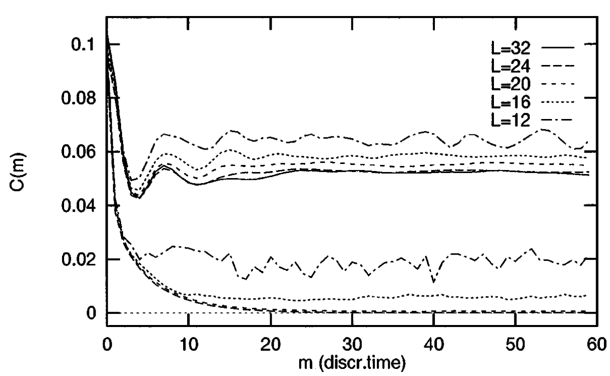

FIG. 1. Current autocorrelation function $C_J(m)$ against discrete time m for the quantum ergodic ($t = V = 4$, lower set of curves for various sizes L) and intermediate regimes ($t = V = 1$, upper set of curves) with density $\rho = \frac{1}{4}$. Averaging over the entire Fock space is performed, $\mathcal{N}' = \mathcal{N}$, for $L \le 20$, whereas random samples of $\mathcal{N}' = 12\,000$ and $\mathcal{N}' = 160$ initial states have been used for $L = 24$ and $L = 32$, respectively.

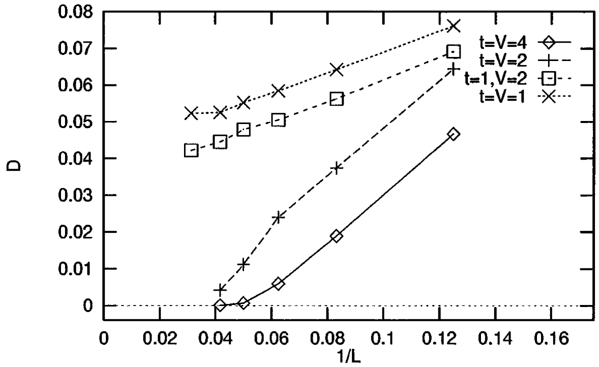

FIG. 2. Stiffness D_J vs $1/L$ at constant density $\rho = \frac{1}{4}$ and for different values of control parameters in the ergodic, $t = V = 4$ and $t = V = 2$, and intermediate, $t = 1, V = 2$ and $t = V = 1$, regimes. Other parameters are the same as in Fig. 1.

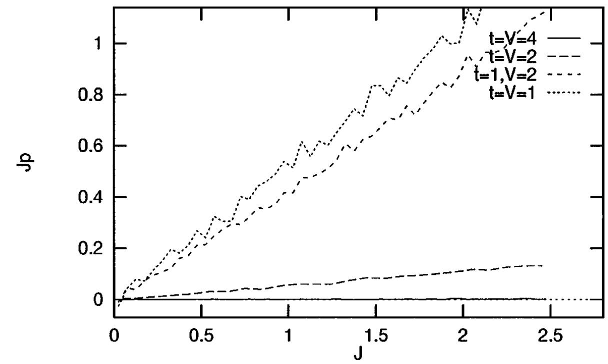

FIG. 3. Persistent current $J^p_{\vec{k}}$ against initial current $J_{\vec{k}}$ (averaged over bins of size $\Delta J = 0.05$) in the ergodic, $t = V = 4$, (nearly) ergodic, $t = V = 2$, and intermediate, $t = V = 1$ and $t = 1, V = 2$, regimes ($L = 24$ and $\rho = \frac{1}{4}$.)

current $J_{\vec{k}'}$. The normal transport in the ergodic regime $t = V = 4$ is characterized by $J^p_{\vec{k}'} = 0$, while for $t \sim V \sim 1$ we find the ideal transport with the persistent current being proportional to the initial current, $J^p_{\vec{k}'} = \alpha J_{\vec{k}'}$. Proportionality constant α can be computed from [Eq. (4)] $D_J = (1/L)\langle J_{\vec{k}'} J^p_{\vec{k}'}\rangle = (\alpha/L)\langle J^2\rangle$, so $\alpha = 2D_J/[\rho(1-\rho)]$, where $\langle J^2\rangle$ is given below [Eq. (5)].

Because of translational symmetry, the total momentum $K = \sum_k k\tilde{n}_k$ (mod$L$) is the only conserved quantity (apart from N and parity), so the evolution of the initial momentum state $|\vec{k}'\rangle$ takes place in $\mathcal{N}_K \approx \mathcal{N}/L$ dimensional subspace $\mathcal{H}_K$, spanned by $|\vec{k}\rangle$ with $K = |\vec{k}| := \sum_n k_n$. Starting with a momentum state $|\vec{k}'\rangle$, the number of "excited" states $|\vec{k}\rangle$ after time m is characterized by information entropy [9] (see also [7]) as $\exp[-\sum_{\vec{k}} p_{\vec{k}\vec{k}'}(m)\ln p_{\vec{k}\vec{k}'}(m)]$. Averaging the entropy over a uniformly random sample of $\mathcal{N}'$ initial states $|\vec{k}'\rangle$, we define *relative localization dimension* in Fock space as a measure of quantum ergodicity,

$$R(m) = \frac{L}{\mathcal{N}} \exp\left(-\frac{1}{\mathcal{N}'}\sum_{\vec{k}'}{}' \sum_{\vec{k}} p_{\vec{k}\vec{k}'}(m)\ln p_{\vec{k}\vec{k}'}(m)\right).$$

Again, similar behavior is found numerically for $R(m)$ as for $C_J(m)$, namely, it typically saturates within the same (short) correlation time M^* to a roughly constant value $\bar{R} = \lim_{M\to\infty}(1/M)\sum_{m=1}^{M} R(m)$. If there are no conservation laws then the unitary blocks $U^m|_{\mathcal{H}_K}$ should have no preferred basis other than eigenbasis, and hence they may be modeled by circular orthogonal ensemble (COE) of random matrices for sufficiently large m giving the maximal asymptotic (as $\mathcal{N} \to \infty$) value of relative localization dimension, $\bar{R}_{\rm COE} \approx 0.655$. This case corresponds to quantum ergodicity since $p_{\vec{k}\vec{k}'}(m)$, for $m > M^*$, become pseudorandom and independent of $\vec{k}$ and $\vec{k}'$, hence the correlation function (3) factorizes and yields $C(m) = \langle J\rangle^2 = 0$. Indeed, as we show in Fig. 4, such behavior is obtained only for sufficiently large parameters, say, $t = V = 4$, while for smaller values of parameters t, V, $R(m)$ saturates to a smaller value indicating that there may exist approximate conservation laws causing nontrivial localization inside the Fock space. Scaling with $1/L$ suggests that, even in TL, $\bar{R}$ is smaller than $\bar{R}_{\rm COE}$ for the intermediate regime $t \sim V \sim 1$ (Fig. 5).

Finally, we discuss current fluctuations, or more generally, current distribution $P_\psi(I) = \langle\psi|\delta(I - J)|\psi\rangle$ giving a probability density of having a current I in a state $|\psi\rangle$. We let the state ψ with a "good" known initial current I_0 evolve for a long time from which we compute a steady-state current distribution (SSCD),

$$P(I; I_0) = \lim_{M\to\infty}\frac{1}{M}\sum_{m=1}^{M}\langle\delta(I_0 - J(0))\delta(I - J(m))\rangle .$$

Of course, delta functions should have a finite small width providing averaging over several states $|\vec{k}\rangle$ with $J_{\vec{k}} \approx I_0$. In the quantum ergodic regime all states eventually become populated, so SSCD $P(I; I_0)$ should be independent of the initial current I_0 and equal to the *microcanonical current distribution* $P_{\rm mc}(I) = \langle\delta(I - J)\rangle$. It has been shown by elementary calculation that in TL the latter becomes a Gaussian, $P_{\rm mc}(I) \to P_{\rm Gauss}(I) = (1/\sqrt{2\pi\langle J^2\rangle})\exp(-\frac{1}{2}I^2/\langle J^2\rangle)$, while at any finite size L

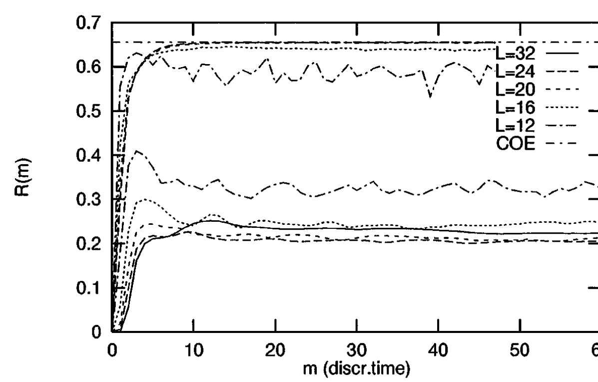

FIG. 4. Relative localization dimension in Fock space $R(m)$ for data of Fig. 1.

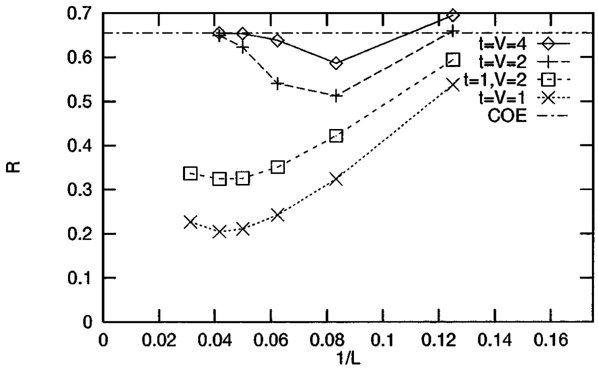

FIG. 5. Limiting relative localization dimension $\bar{R}$ vs $1/L$ for data of Fig. 2.

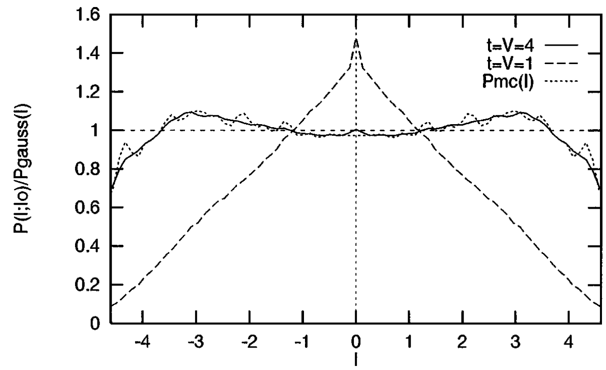

FIG. 6. Steady-state current distribution divided by a Gaussian $P(I, I_0)/P_{\rm Gauss}(I)$ averaged over 279 initial states with $|I_0| < 0.08$ in the ergodic, $t = V = 4$, and intermediate, $t = V = 1$, regimes, and the finite-size microcanonical current distribution $P_{\rm mc}(I)$. ($L = 24$ and $\rho = \frac{1}{4}$.)

the first few moments are

$$\langle J^2 \rangle = \frac{N(L-N)}{2(L-1)} \approx \frac{1}{2}\rho(1-\rho)L,$$
$$\frac{\langle J^4 \rangle}{\langle J^2 \rangle^2} = \frac{3(L-1)[2N(L-N)-L]}{2N(L-2)(L-N)} = 3 + \mathcal{O}\left(\frac{1}{L}\right). \tag{5}$$

Numerical results for $L = 24$ (see Fig. 6) indicate that in the ergodic regime, $t = V = 4$, SSCD is already in good agreement with microcanonical distribution $P_{\rm mc}(I)$, while in the nonergodic (intermediate) regime, $t = V = 1$, SSCD is *localized* on a smaller range indicating that the current fluctuation is smaller than $\langle J^2 \rangle$. Note that the mean $\bar{I} = \int dI I P(I; I_0)$ is just a persistent current, so $\bar{I} = \alpha I_0$ (see Fig. 3).

In this Letter we have presented numerical evidence, based on efficiently coded time evolution of a kicked fermionic system, in support of hypothesis, that intermediate (neither integrable nor ergodic) behavior of a quantum many-body system may survive TL provided that control parameters are not too far away from integrable points. In this regime ideal transport is possible due to nonvanishing current time correlations as a consequence of quantum nonergodicity (nonmixing). However, when the control parameters are sufficiently large we have a strong interaction between particles, hence we expect (according to ergodic hypothesis) and confirm quantum ergodicity compatible with RMT and normal transport properties. It is interesting to note that, at the transition point between the two regimes, where *order parameter—stiffness* $D_J|_{L=\infty}$ (inferred from $1/L$ scaling)—becomes zero, the correlation time scale M^* drastically increases what is reminiscent of a type of *dynamical* phase transition. This seems to be a discontinuous "order-to-chaos" transition in contrast to a smooth (KAM-like) transition in systems with a finite number of degrees of freedom. Although only data for quarter-filled lattice ($\rho = \frac{1}{4}$) are presented here, we should stress that the same conclusion follows from our data for other densities, $\rho = \frac{1}{3}, \frac{3}{8}, \frac{2}{5}$, and $\frac{1}{2}$, with a general rule that the border of a quantum ergodic regime moves to slightly smaller values of control parameters t, V as the density ρ approaches $\frac{1}{2}$. It should be noted that statistics of eigenphases of evolution operator U have been computed as well, and it has been found that, in the ergodic regime, level statistics are indeed that of COE while, in the intermediate regime, it interpolates smoothly between Poisson and COE.

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[8] Note that the case $t = V = 1$ is far beyond perturbative treatment of some integrable cases. For example, statistics of eigenphases η_n exhibit substantial level repulsion.

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