

Eigenstate thermalization hypothesis versus Bohigas-Giannoni-Schmit conjecture: a comparison

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Thermalization of a closed chaotic quantum system is commonly addressed in terms of the “eigenstate thermalization hypothesis” (ETH). An alternative approach uses the Bohigas-Giannoni-Schmit (BGS) conjecture. The comparison shows that the two approaches differ significantly. In contrast to ETH, BGS fully uses the statistical properties of the chaotic Hamiltonian. In both approaches, the criterion for thermalization is similar. BGS goes beyond ETH in predicting quantitatively the time dependence of thermalization.

I. INTRODUCTION

Thermalization postulates that asymptotically (time $t \rightarrow \infty$) the expectation value $\text{Tr}(A\rho(t))$ of a classical observable (represented in Hilbert space by the Hermitean operator A) in a closed quantum system \mathcal{S} with density matrix $\rho(t)$ tends toward its equilibrium value,

$$\text{Tr}(A\rho(t)) \rightarrow \text{Tr}(A\rho_{\text{eq}}). \quad (1)$$

Thermalization is understood as the quantum analog of ergodicity in classical statistical mechanics. Therefore, the relation (1) is expected to hold in the semiclassical regime of high excitation energy E and for systems with small energy spread $\delta E \ll E$. Reviews are given in Refs. [1–3]. In recent years, thermalization has become a topic of considerable interest in several fields as for instance, quantum circuits [4], quantum lattice systems [5], open quantum systems [6], and low-entanglement states [7].

The asymptotic relation (1) cannot be expected to hold for every quantum system. For the system \mathcal{S} with Hamiltonian H , that is seen by writing $\text{Tr}(A\rho(t))$ in the eigenstate representation of H with eigenstates α, β, \dots and eigenvalues E_α, E_β, \dots where

$$\text{Tr}(A\rho(t)) = \sum_{\alpha\beta} A_{\alpha\beta} (\exp\{-iE_\beta t\} \Pi_{\beta\alpha} \exp\{+iE_\alpha t\}). \quad (2)$$

We put $\hbar = 1$ throughout. The terms in round brackets on the right-hand side represent the elements of the density matrix. The time-independent statistical operator Π has unit trace and defines the occupation amplitudes of the system \mathcal{S} in Hilbert space. The diagonal elements $\rho_{\alpha\alpha}$ of $\rho(t)$ are independent of time, and the non-diagonal elements $\rho_{\beta\alpha}$ oscillate periodically with frequency $(E_\alpha - E_\beta)$. Thus, $\text{Tr}(A\rho(t))$ is an oscillatory function of time, and thermalization does not occur in general. Indeed, integrable systems and systems showing many-body localization do not thermalize [2, 3]. The study of thermalization has been focused on quantum systems that are chaotic in the classical limit. The eigenfunctions and eigenvalues of such systems display statistical properties. Specifically, for a time-reversal-invariant chaotic quantum system (which we consider

in what follows), the Bohigas-Giannoni-Schmit (BGS) conjecture states [8] that the spectral fluctuations of eigenvalues and eigenfunctions are the same as for the GOE, the Gaussian Orthogonal Ensemble of Random Matrices [9]. Thermalization is a consequence of and follows from averaging over these statistical fluctuations.

In a seminal paper, M. Srednicki [10] used the “eigenstate thermalization hypothesis” to investigate thermalization in a closed chaotic quantum system. The statistical description of chaotic many-body quantum systems based on the Bohigas-Giannoni-Schmit conjecture [8] developed in Refs. [11, 12] offers an alternative access to thermalization. In the present paper, we compare the two approaches.

II. EIGENSTATE THERMALIZATION HYPOTHESIS

In Ref. [10], the statistical operator Π in Eq. (2) is defined in terms of a single normalized state $|\psi(t)\rangle$. In the eigenstate representation $|\psi(t)\rangle$ is written as

$$|\psi(t)\rangle = \sum_{\alpha} c_{\alpha} \exp\{-iE_{\alpha}t\} |\alpha\rangle \quad (3)$$

where

$$\sum_{\alpha} |c_{\alpha}|^2 = 1. \quad (4)$$

Density matrix and statistical operator are, respectively, given by

$$\rho(t) = |\psi(t)\rangle \langle \psi(t)|, \quad \Pi_{\alpha\beta} = c_{\alpha} c_{\beta}^* \quad (5)$$

so that

$$\text{Tr}(A\rho(t)) = \sum_{\alpha\beta} c_{\alpha} c_{\beta}^* \exp\{i(E_{\beta} - E_{\alpha})t\} A_{\alpha\beta}. \quad (6)$$

The elements $A_{\alpha\beta}$ of the operator A possess statistical properties and are written as [10]

$$A_{\alpha\beta} = \mathcal{A}(E) \delta_{\alpha\beta} + \exp\{-S/2\} f(E, \omega) R_{\alpha\beta}. \quad (7)$$

Here $\mathcal{A}(E)$ and $f(E, \omega)$ are smooth real functions of $E = (1/2)(E_{\alpha} + E_{\beta})$ and $\omega = E_{\alpha} - E_{\beta}$, $S(E)$ is the thermodynamic entropy of the system, and $R_{\alpha\beta} = R_{\beta\alpha}$ is a zero-centered real Gaussian random variable with variance

$$\langle R_{\alpha\beta} R_{\gamma\delta} \rangle = \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}. \quad (8)$$

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Here and in what follows, the angular brackets denote the ensemble average.

The function $\mathcal{A}(E)$ is the average of the diagonal elements of A . The average is taken over a large energy interval centered on energy E . It is argued [10] that for E in the semiclassical regime, $\mathcal{A}(E)$ is equal to the thermal average $\langle A \rangle_T$ of A . The function $f(E, \omega)$ describes the average dependence of the non-diagonal matrix elements of A on E and ω . The factor $\exp\{-S/2\}$ accounts for the smallness of these elements in the semiclassical regime. The factor $R_{\alpha\beta}$ accounts for their stochastic features.

In Ref. [10], the expansion coefficients c_α, c_β^* and the energies E_α, E_β in Eq. (6) are taken to be nonstatistical. Insertion of Eq. (7) into Eq. (6) and averaging over the distribution yields with Eq. (4) the result

$$\langle \text{Tr}(A\rho(t)) \rangle = \mathcal{A}(E). \quad (9)$$

The time dependence of $\text{Tr}(A\rho(t))$ disappears after averaging. The variance of $\text{Tr}(A\rho(t))$ is similarly found to be

$$\begin{aligned} \left\langle \left(\text{Tr}(A\rho(t)) - \mathcal{A}(E) \right)^2 \right\rangle &= \exp\{-S\} \\ &\times \sum_{\alpha\beta} \left[f^2(E, \omega) \left(\Pi_{\alpha\beta} \Pi_{\beta\alpha} \right. \right. \\ &\left. \left. + (\exp\{i(E_\alpha - E_\beta)t\} \Pi_{\alpha\beta})^2 \right) \right]. \end{aligned} \quad (10)$$

Since $\omega = E_\alpha - E_\beta$, the sum over (α, β) extends also over $f^2(E, \omega)$. Because of the factor $\exp\{-S\}$, the variance of $\text{Tr}(A\rho(t))$ and with it, the fluctuations of $\text{Tr}(A\rho(t))$ about its average are negligibly small in the semiclassical regime [10].

The time dependence of $\text{Tr}(A\rho(t))$ is determined as follows. For a general system with statistical operator Π , the average $\langle E \rangle$ and the quantum uncertainty Δ_S of the energy E of the system S are given by

$$\begin{aligned} \langle E \rangle &= \sum_{\alpha} E_{\alpha} \Pi_{\alpha\alpha}, \\ \Delta_S^2 &= \sum_{\alpha} (E_{\alpha} - \langle E \rangle)^2 \Pi_{\alpha\alpha}. \end{aligned} \quad (11)$$

In Ref. [10] it is shown that the difference of the thermal averages

$$\langle A^2 \rangle_T - (\langle A \rangle_T)^2 \quad (12)$$

is of order Δ_S^2 . With $\langle A \rangle_T = \mathcal{A}$, that fact accounts for finite-size fluctuations of $\text{Tr}(A\rho(t))$ about its mean value \mathcal{A} . The fluctuations are shown to decay in time. As a consequence, $\text{Tr}(A\rho(t))$ approaches $\text{Tr}(A\rho_{\text{eq}}) = \langle A \rangle_T$ for long times. The difference $\text{Tr}(A\rho(t)) - \text{Tr}(A\rho_{\text{eq}})$ is shown to be proportional to the Fourier transform $C(t)$ of $|f(E, \omega)|^2$ with respect to ω . The rate of change of $C(t)$ with time is determined by the band width in ω of $f(E, \omega)$. Since $|f(E, \omega)|^2 \geq 0$, the time-dependent function $C(t)$ oscillates about zero. Maxima and minima of the oscillations decrease monotonically with time. The analytical dependence of $|f(E, \omega)|^2$ on ω and that of $C(t)$ on time t are not given explicitly in Ref. [10] nor is it indicated how these might be determined from the Hamiltonian of the system.

III. BOHIGAS-GIANNONI-SCHMIT (BGS) CONJECTURE

In Ref. [11], the BGS conjecture has been applied to a chaotic many-body quantum system. We here repeat the arguments in a nutshell and focus attention on the results. For detailed justification, we refer to Ref. [11] and, for explicit calculations, to Ref. [12].

The Hamiltonian $H = H_{\text{HF}} + V$ is written as the sum of an (integrable) Hartree-Fock (HF) Hamiltonian H_{HF} and a residual interaction V . The HF eigenstates are labeled m, n, \dots , the HF energies are written as $\mathcal{E}_m, \mathcal{E}_n, \dots$. The residual interaction V mixes the HF eigenstates. Diagonalization of H by an orthogonal matrix with elements $O_{m\alpha}$ yields the eigenvalues E_α . In the HF basis, the diagonalized Hamiltonian is

$$H_{mn} = \sum_{\alpha} O_{m\alpha} E_{\alpha} O_{n\alpha}. \quad (13)$$

The system is assumed to be chaotic in the classical limit. In the quantum case, the BGS conjecture implies that V mixes the HF states locally sufficiently strongly to cause the eigenvalues E_α and the elements $O_{m\alpha}$ of the diagonalizing orthogonal matrix to obey GOE statistics. They do so at any energy E within an energy interval of size Δ centered on E . The system becomes analytically tractable by introducing an ensemble of random Hamiltonians that share with H these statistical properties. The ensemble is obtained by promoting the eigenvalues E_α and the elements $O_{m\alpha}$ of the orthogonalizing matrix to random variables. Within the interval Δ , the eigenvalues E_α obey Wigner-Dyson statistics. The elements $O_{m\alpha}$ are zero-centered Gaussian-distributed random variables with second moments

$$\langle O_{m\alpha} O_{n\beta} \rangle = \delta_{mn} \delta_{\alpha\beta} F(\bar{E}_\alpha - \mathcal{E}_m) \quad (14)$$

where

$$\begin{aligned} F(\bar{E}_\alpha - \mathcal{E}_m) &= \frac{1}{\sqrt{2\pi} \rho(\bar{E}_\alpha) \Delta} \\ &\times \exp\{-(\bar{E}_\alpha - \mathcal{E}_m)^2 / (2\Delta^2)\}. \end{aligned} \quad (15)$$

Here $\rho(E)$ is the average level density, and \bar{E}_α is the ensemble average of E_α . The statistical properties of the GOE are derived [9] in the limit of infinite matrix dimension. Full agreement with the statistical properties of the GOE is, therefore, only attained if the number

$$N = \rho(E) \Delta \quad (16)$$

of eigenvalues in the interval Δ obeys $N \gg 1$. That condition holds in the semiclassical regime.

The function $\text{Tr}(A\rho(t))$ is written as

$$\begin{aligned} \text{Tr}(A\rho(t)) &= \sum_{mnrs\alpha\beta} (O_{m\beta} A_{mn} O_{n\alpha}) \exp\{-iE_\alpha t\} \\ &\times (O_{r\alpha} \Pi_{rs} O_{s\beta}) \exp\{+iE_\beta t\}. \end{aligned} \quad (17)$$

Eq. (17) displays explicitly the dependence of $\text{Tr}(A\rho(t))$ on the random variables $O_{m\alpha}$ and E_α . The function $\text{Tr}(A\rho(t))$ is a stochastic process. The average and the variance of

$\text{Tr}(A\rho(t))$ are calculated in an asymptotic expansion in inverse powers of N where only terms of leading order are kept.

For the average of $\text{Tr}(A\rho(t))$ the result is [11]

$$\langle \text{Tr}(A\rho(t)) \rangle = \sum_k \frac{p_k}{\sqrt{2\pi\rho_k\Delta}} \text{Tr}_k(A) \quad (18)$$

$$+ \text{Tr}(A \exp\{-iH_{\text{HF}}t\} \Pi \exp\{+iH_{\text{HF}}t\}) \exp\{-\Delta^2 t^2\}.$$

For the first term on the right-hand side, the total spectrum has been divided into intervals labeled k of width Δ each, with ρ_k the average level density in the interval k , the trace Tr_k extending only over the states within the interval k , and p_k an approximation to the partial trace of Π extended over the HF eigenstates within the interval k .

In Ref. [12] it is shown that the correlation function

$$\langle \text{Tr}(A\rho(t_1)) \text{Tr}(A\rho(t_2)) \rangle - \langle \text{Tr}(A\rho(t_1)) \rangle \langle \text{Tr}(A\rho(t_2)) \rangle \quad (19)$$

vanishes for $N \rightarrow \infty$. It follows that the result (18) holds for almost all members of the random-matrix ensemble in Eq. (13), with the exception of a set of measure zero. The measure is the integration measure for the random variables $O_{m\alpha}$ and E_α . We use the result (19) to omit in Eq. (18) the angular brackets.

Eq. (18) shows that thermalization as defined in Eq. (1) does not hold in general. Thermalization occurs only if the statistical operator Π is confined to an energy interval bounded from above by Δ so that the quantum uncertainty Δ_S defined in Eq. (11) is less than Δ . Then only a single term (with index k_0 , say) contributes to the sum on the right-hand side of Eq. (18), we have $p_{k_0} = 1$, and $(1/\sqrt{2\pi\rho_{k_0}\Delta}) \text{Tr}_{k_0}(A)$ is equal to the equilibrium value $\text{Tr}(A\rho_{\text{eq}})$ because the Boltzmann factor is approximately constant within the energy interval Δ and cancels in numerator and denominator. Thus, for $\Delta_S < \Delta$, Eq. (18) takes the form

$$\text{Tr}(A\rho(t)) = \text{Tr}(A\rho_{\text{eq}}) \quad (20)$$

$$+ \text{Tr}(A \exp\{-iH_{\text{HF}}t\} \Pi \exp\{+iH_{\text{HF}}t\}) \exp\{-\Delta^2 t^2\}.$$

The condition $\Delta_S < \Delta$ quantifies the condition $\delta E \ll E$ mentioned in the Introduction.

IV. COMPARISON. DISCUSSION. CONCLUSIONS

In comparing results we refer to Ref. [10] with the letters ETH and to Ref. [11] with the letters BGS. Both ETH and BGS aim at a realistic description of the thermalization process in a chaotic system. Therefore, it is meaningful to compare the results of both approaches term by term. Comparing Eqs. (6) and (17), we identify

$$A_{\alpha\beta} \leftrightarrow \sum_{mn} (O_{m\beta} A_{mn} O_{n\alpha}),$$

$$c_\alpha c_\beta^* \leftrightarrow \sum_{rs} (O_{r\alpha} \Pi_{rs} O_{s\beta}). \quad (21)$$

The first identification is obvious. The second identification is valid because when Π has rank one we have $\Pi_{rs} = \pi_r \pi_s^*$ which yields $c_\alpha = O_{r\alpha} \pi_r$, $c_\beta^* = O_{s\beta} \pi_s^*$. We also identify

$$\exp\{-S\} \leftrightarrow 1/N. \quad (22)$$

That identification is consistent with the physical significance of $\exp\{-S\}$ and with the fact that in both approaches only terms of leading order in these small parameters are kept.

To compare the eigenstate thermalization hypothesis for $A_{\alpha\beta}$ in Eq. (7) with the statistical properties of $\sum_{mn} (O_{m\alpha} A_{mn} O_{n\beta})$ in Eq. (21) we calculate mean value and variance of $\sum_{mn} (O_{m\alpha} A_{mn} O_{n\beta})$. The average is given by

$$\langle \sum_{mn} (O_{m\alpha} A_{mn} O_{n\beta}) \rangle = \frac{\delta_{\alpha\beta}}{\sqrt{2\pi\rho(\bar{E}_\alpha)\Delta}} \quad (23)$$

$$\times \sum_m A_{mm} \exp\{-(\bar{E}_\alpha - \mathcal{E}_m)^2/(2\Delta^2)\}.$$

The variance is given in the Appendix. It is small of order $1/N$.

The expressions for $\langle A_{\alpha\beta} \rangle$ in ETH and BGS are similar. Both are diagonal in α, β , and are given in terms of energy averages. In ETH, the average \mathcal{A} of A is, in the semiclassical regime, given by the thermal average $\langle A \rangle_T$. In BGS, $\langle A_{\alpha\beta} \rangle$ is the normalized trace of A taken over an energy interval of width Δ centered on \bar{E}_α . In BGS, a thermal average cannot appear without explicit reference to the density matrix of the system. The last term in Eq. (7) and the terms on the right-hand side of Eq. (24) are small of first order in the parameters (22). BGS goes beyond ETH because Eq. (24) yields an explicit expression for the square of the function $f(E, \omega)$ in Eq. (7).

For $\langle \text{Tr}(A\rho(t)) \rangle$, both ETH and BGS yield a time-independent term, see Eqs. (9) and (20). These terms describe the asymptotic value of $\langle \text{Tr}(A\rho(t)) \rangle$ attained for large times. In ETH, the term is equal to $\mathcal{A}(E)$ in Eq. (7) and, in the semiclassical regime, to $\langle A \rangle_T$. In BGS, the term is equal to $\text{Tr}(A\rho_{\text{eq}})$ provided that $\Delta_S < \Delta$. The two results are basically equivalent but BGS states more explicitly the conditions for thermalization to occur.

Beyond the similarity shown by that comparison, the relations (21) actually point to a striking difference between ETH and BGS. In both approaches, the operator A , written in the eigenbasis of H , acquires statistical properties. However, in ETH the term $c_\alpha c_\beta^*$ is considered nonstochastic while in BGS the expression $\sum_{rs} (O_{r\alpha} \Pi_{rs} O_{s\beta})$ is taken as a stochastic variable in the same sense as $\sum_{mn} (O_{m\beta} A_{mn} O_{n\alpha})$. Consistency requires that both these expressions are treated on the same footing. The notation $c_\alpha c_\beta^*$ used for the matrix elements of the statistical operator blurs that need in ETH. The difference in statistical assumptions strongly affects the time dependence of $\text{Tr}(A\rho(t))$.

In BGS, the time-dependent term on the right-hand side of Eq. (20) is due to the correlation of the stochastic variables $\sum_{mn} (O_{m\beta} A_{mn} O_{n\alpha})$ and $\sum_{rs} (O_{r\alpha} \Pi_{rs} O_{s\beta})$ in Eq. (17). The term is the product of a factor the time dependence of which is determined by the HF Hamiltonian, and of the factor $\exp\{-\Delta^2 t^2/2\}$, the Fourier transform of the function F in Eq. (15). The scale of the time dependence is given by Δ , the correlation width of the BGS conjecture.

The analog of the time-dependent term in Eq. (18) is absent in Eq. (9). That is because the term $c_\alpha c_\beta^*$ is assumed to be non-statistical. As described below Eq. (12), deviations from

the mean value (9) are ascribed in ETH to the fluctuations of A around its mean value $\langle A \rangle_T$. The resulting non-monotonic time dependence of $C(t)$ differs qualitatively from the Gaussian form in Eq. (20).

In both ETH and BGS, $\text{Tr}(A\rho(t))$ is a stochastic process. In both approaches, the variance of $\text{Tr}(A\rho(t))$ vanishes in the limit where the small parameters (22) tend to zero. From a systematic point of view, $\text{Tr}(A\rho(t))$ should, therefore, be determined entirely by its mean value $\langle \text{Tr}(A\rho(t)) \rangle$. That desideratum is met in BGS. It is not met in ETH because the product $c_\alpha c_\beta^*$ is considered nonstatistical.

It must be borne in mind that BGS is obtained in the framework of the stochastic many-body Hamiltonian in Eqs. (13, 14) and (15) while ETH addresses chaotic quantum systems in full generality. Our comparison, therefore, applies strictly only to many-body systems. However, the problems of ETH displayed by the comparison are obviously generic. Moreover, the parametrization in Eqs. (13, 14) and (15) of the stochastic Hamiltonian is not as restrictive as it may seem, for the following reason. The parametrization uses the Hartree-Fock approach. The integrable HF Hamiltonian provides a scaffolding for the spectrum of the chaotic Hamiltonian H . The residual interaction V locally mixes the HF eigenstates and leads to GOE fluctuations within the correlation width Δ . For that to happen, it is not necessary to invoke statistical assumptions on V . That approach can be generalized. It is often the case that an integrable system with Hamiltonian H_{int} becomes chaotic upon adding a perturbation \tilde{V} to H_{int} . The integrable system then serves as a scaffolding for the spectrum. The perturbation \tilde{V} mixes the eigenstates of H_{int} locally in the same way as does V for the HF Hamiltonian H_{HF} . That fact, combined with the BGS conjecture, then leads to a parametrization of $H_{\text{int}} + \tilde{V}$ similar to that of Eqs. (13) to (15). If, in addition, the level density of the system increases strongly with excitation energy, one obtains a result of the form of Eq. (20). That is why we believe that Eq. (20) is valid for a class of chaotic quantum systems that encompasses but is wider than the class of chaotic many-body systems. In all these cases, BGS replaces

the semiquantitative ETH estimate for the time dependence of $\text{Tr}(A\rho(t))$ by an analytic result. The time scale is given by the inverse of the correlation width Δ of the BGS conjecture.

It seems plausible that our results apply in an even wider context because the BGS conjecture applies to chaotic quantum systems in general. The difficulty in extending our argument to a more general situation is technical. To formulate the BGS conjecture quantitatively, we need the scaffolding provided by the integrable Hamiltonian and the reference to its eigenvalues \mathcal{E}_m . That leads to Eq. (14). So far we have seen no way of bypassing that construction.

To sum up: ETH and BGS differ significantly. ETH uses a well-justified ad-hoc parametrization of the statistical matrix $A_{\alpha\beta}$ but disregards statistical properties of the term $c_\alpha c_\beta^*$. BGS fully uses the statistical properties of the Hamiltonian implied by the BGS conjecture. In contrast to ETH, BGS predicts quantitatively the time dependence of $\text{Tr}(A\rho(t))$.

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Appendix

The variance of $\langle O_{m\alpha} A_{mn} O_{n\beta} \rangle$ is obtained by calculating the correlated part of the square of that expression. For simplicity we assume that the matrix A_{mn} is real and symmetric. We obtain

$$\begin{aligned} \langle (O_{m\alpha} A_{mn} O_{n\beta})^2 \rangle_{\text{corr}} &= \frac{1}{2\pi\Delta^2 \rho(\bar{E}_\alpha) \rho(\bar{E}_\beta)} \quad (24) \\ &\times \text{Tr} \left(A \exp\{(\bar{E}_\alpha - H_{\text{HF}})^2 / (2\Delta^2)\} \right. \\ &\left. \times A \exp\{(\bar{E}_\beta - H_{\text{HF}})^2 / (2\Delta^2)\} \right). \end{aligned}$$

The right-hand side of that equation is the product of the normalized trace and of a factor $\propto 1/N$ and is, therefore, small of order $1/N$.

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