Full expectation-value statistics for randomly sampled pure states in high-dimensional quantum systems

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We explore how the expectation values $\langle\psi|A|\psi\rangle$ of a largely arbitrary observable A are distributed when normalized vectors $|\psi\rangle$ are randomly sampled from a high-dimensional Hilbert space. Our analytical results predict that the distribution exhibits a very narrow peak of approximately Gaussian shape, while the tails significantly deviate from a Gaussian behavior. In the important special case that the eigenvalues of A satisfy Wigner's semicircle law, the expectation-value distribution for asymptotically large dimensions is explicitly obtained in terms of a large deviation function, which exhibits two symmetric nonanalyticities akin to critical points in thermodynamics.

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I. INTRODUCTION

Consider any observable A of a quantum mechanical model system on a Hilbert space $\mathcal{H}$ with large but finite dimension N. Then the expectation value $\langle\psi|A|\psi\rangle$ will be almost identical for the vast majority of all normalized vectors $|\psi\rangle \in \mathcal{H}$. Equivalently, $\langle\psi|A|\psi\rangle$ will be very close to the microcanonical expectation value $\mathrm{Tr}\{\rho_{\mathrm{mc}}A\}$ for most $|\psi\rangle \in \mathcal{H}$, where $\rho_{\mathrm{mc}} := \mathbb{1}/N$ and $\mathbb{1}$ indicates the identity on $\mathcal{H}$. Similar properties are also found to apply simultaneously for several different observables $\{A_k\}_{k=1}^{K}$, as long as their number K remains much smaller than the Hilbert space dimension N. In particular, not only the mean value but also the statistical fluctuations (variance) of any given observable A in the microcanonical ensemble will thus be imitated practically perfectly by nearly any single pure state $|\psi\rangle \in \mathcal{H}$. Examples of foremost interest are isolated many body system at thermal equilibrium: If such a system is known to be in any of those typical pure states, then all fluctuation phenomena at thermal equilibrium can actually be ascribed to quantum fluctuations.

The quantitative derivation of those very general results, as well as the detailed discussion of their above mentioned, quite remarkable physical implications, can be traced back to the Ph.D. thesis by Seth Lloyd in 1988 [1] and are called pure state quantum statistical mechanics therein. Closely related variations have been independently rediscovered and then further developed under the name "canonical typicality" or "concentration of measure phenomena," e.g., in Refs. [2–9] and references therein, while some precursory ideas may also be attributed, e.g., to Ref. [10].

At the focus of our present paper is the so-called full expectation-value statistics, i.e., the entire probability distribution of expectation values $\langle\psi|A|\psi\rangle$, which arise when normalized vectors $|\psi\rangle$ are randomly sampled according to a uniform distribution on the unit sphere in $\mathcal{H}$. The mean value of this distribution is given by $\mathrm{Tr}\{\rho_{\mathrm{mc}}A\}$ and the variance is quantitatively well known [1]. Though never explicitly worked out so far to our knowledge, it is likely that the higher moments could in principle be determined along similar lines, but the resulting expressions are expected to become very involved and therefore would be of little practical or conceptual use. Accordingly, rather than going for the moments, we will derive here an alternative analytical approximation of the full expectation-value statistics for large Hilbert space dimensions N.

As said above, the majority of the pure states $|\psi\rangle$ imitate the microcanonical ensemble very well and, in particular, entail expectation values of A very close to the thermal equilibrium value $\mathrm{Tr}\{\rho_{\mathrm{mc}}A\}$. The remaining minority of states $|\psi\rangle$ thus corresponds to all the still possible nonequilibrium situations, and it is natural to classify them according to their expectation values $\langle\psi|A|\psi\rangle$. Especially, it seems quite interesting to quantify the relative measure of the far-from-equilibrium states along these lines. This is the main issue of our present work.

II. SETUP

We start by writing the observable (Hermitian operator) $A : \mathcal{H} \to \mathcal{H}$ in terms of its eigenvalues and eigenvectors as

$$A = \sum_{n=1}^{N} a_n\, |n\rangle\langle n|. \tag{1}$$

Without loss of generality, we assume that

$$\mathrm{Tr}\{A\} = 0 \tag{2}$$

and that the eigenvalues a_n are ordered by magnitude:

$$a_1 \leqslant a_2 \leqslant \cdots \leqslant a_N. \tag{3}$$

Excluding the trivial case $a_1 = a_N$, Eq. (2) implies that $a_1 < 0$ and $a_N > 0$.

Next, we introduce the function $y(a)$, which will play a key role in all that follows. To begin, we choose an arbitrary but

fixed $a \in (0, a_N)$ and define

$$g(x) := \frac{1}{N} \sum_{n=1}^{N} \frac{1}{1 + x(a - a_n)}. \tag{4}$$

One readily verifies that $g(0) = 1$, $g'(0) = -a < 0$, $g(x) \to \infty$ as x approaches $x_{\max}(a) := 1/(a_N - a)$ from below, $g(x) \to \infty$ as x approaches $x_{\min}(a) := -1/(a - a_1)$ from above, and $g''(x) > 0$ for all $x \in I_a := (x_{\min}(a), x_{\max}(a))$. These properties imply that there must be exactly one $x \in I_a$ with $g(x) = 1$. This x value is henceforth denoted as $y(a)$. One thus can conclude that $y(a) > 0$, that

$$p_n(a) := \frac{1}{N} \frac{1}{1 + y(a)\,(a - a_n)} > 0 \tag{5}$$

for all $n = 1, \ldots, N$, and that

$$\sum_{n=1}^{N} p_n(a) = 1. \tag{6}$$

Analogously, in the case $a \in (a_1, 0)$ there exists a unique $y(a) < 0$ which satisfies (5) and (6), while $y(a) = 0$ is the only solution of (5) and (6) in the case $a = 0$.

Altogether, $y(a)$ is thus well defined for any given $a \in (a_1, a_N)$ and can be obtained as the unique solution of the transcendental equation

$$\frac{1}{N} \sum_{n=1}^{N} \frac{1}{1 + y(a)\,(a - a_n)} = 1 \tag{7}$$

with the constraints $y(a) \in I_a$ and $y(a) \neq 0$ unless $a = 0$.

A second main ingredient of our approach consists in normalized random vectors of the form $|\psi\rangle = \sum_{n=1}^{N} c_n |n\rangle$, where the $(c_1, \ldots, c_N)$ are uniformly distributed on the unit sphere in $\mathbb{C}^N$ and thus all those $|\psi\rangle \in \mathcal{H}$ are equally likely. The probability that the expectation value of the observable A from (1) assumes some fixed value x can thus be written as

$$P(x) := \int d\mu(\psi)\, \delta(\langle\psi|A|\psi\rangle - x), \tag{8}$$

where the integration measure $\mu(\psi)$ in (8) is induced by the above uniform probability distribution on the unit sphere in $\mathbb{C}^N$. According to the previous findings in Refs. [1–8] the distribution $P(x)$ will be very sharply peaked for large N, hence it is natural to write $P(x)$ in the form

$$P(x) = \exp\{-N\, F(x)\}. \tag{9}$$

This equation amounts to an implicit definition of the function $F(x)$. To determine its detailed properties will be a main objective of our paper.

For the time being, (9) does not amount to any hypothesis of how $P(x)$ "scales" for large N in the spirit of large deviation theory [11]. Rather, we take N as large but fixed and then consider (9) as definition of $F(x)$. In order to draw conclusions about how $P(x)$ [and thus $F(x)$] behaves upon variations of N, one would first have to specify how the observable A changes with N, which is in general a quite subtle problem in itself. Particularly simple special cases will be considered in Sec. IV.

III. MAIN RESULTS

By means of the above ensemble of random vectors $|\psi\rangle$, yet another ensemble of random vectors $|\phi\rangle$ is defined via

$$|\phi\rangle := \frac{R|\psi\rangle}{\sqrt{\langle\psi|R^2|\psi\rangle}}, \tag{10}$$

$$R := \sum_{n=1}^{N} \sqrt{N p_n(a)}\, |n\rangle\langle n|, \tag{11}$$

where the dependence of R on a has been omitted. Similarly as in (8), we denote by

$$P_R(x) := \int d\mu_R(\phi)\, \delta(\langle\phi|A|\phi\rangle - x) \tag{12}$$

the probability that the expectation value x is realized, but now for the ensemble of normalized random vectors from (10). Accordingly, the integration measure $\mu_R(\phi)$ in (12) now generically corresponds to some nonuniform probability distribution on the unit sphere in $\mathbb{C}^N$. Quantitatively, this "nonuniformity" is captured by the following key result of our paper:

$$d\mu_R(\phi) = d\mu(\phi)\, \rho(\phi), \tag{13}$$

$$\rho(\phi) := c_R\, \langle\phi|R^{-2}|\phi\rangle^{-N}, \tag{14}$$

$$c_R := 1/\det[R^2], \tag{15}$$

where $\mu(\phi)$ is the uniform integration measure from above, and $\rho(\phi)$ quantifies the "density" or "probability distribution" of the $|\phi\rangle$'s on the unit sphere. Note that R from (11) is a positive operator due to (5), hence $R^{-2} := (R^{-1})^2$ in (14) is well defined and c_R in (15) is positive. The derivation of this result is the first main achievement of our paper, but since the details are quite technical, it has been postponed to the Appendix.

From (5) and (11) one can infer that

$$\begin{aligned}\langle\phi|R^{-2}|\phi\rangle &= 1 + y(a)a - y(a)\langle\phi| \sum_{n=1}^{N} a_n |n\rangle\langle n|\phi\rangle \\ &= 1 + y(a)(a - \langle\phi|A|\phi\rangle),\end{aligned} \tag{16}$$

where Eq. (1) was exploited in the last step. Likewise, (15) can be rewritten as

$$c_R = \det[1 + y(a)(a - A)]. \tag{17}$$

By introducing (16) into (12)–(14) one obtains

$$P_R(x) = \frac{c_R \int d\mu(\phi)\, \delta(\langle\phi|A|\phi\rangle - x)}{[1 + y(a)(a - x)]^N}. \tag{18}$$

The integral in (18) can be identified with $P(x)$ from (8), and with (9) it follows that

$$P_R(x) = c_R \exp\{-N\, G(x)\} \tag{19}$$

$$G(x) := F(x) + \ln[1 + y(a)(a - x)]. \tag{20}$$

The quantitative value of c_R in (17) may be difficult to determine, but the main point is that it is an x independent constant.

Finally, we exploit the following result, whose detailed derivation has been previously provided in Ref. [12]. (As expounded in Ref. [12], a largely equivalent result has also been obtained in Ref. [13], though its actual formulation is quite different. Another related, but less rigorous, investigation has been published even earlier in Ref. [14]). Namely, the overwhelming majority of all random vectors $|\phi\rangle$ in (10) entail expectation values $\langle\phi|A|\phi\rangle$ very close to the preset value a in (5), provided a has been chosen so that

$$p_1(a),\ p_N(a) \ll 1. \tag{21}$$

Conversely, if (21) is violated, then the random vectors in (10) yield a distribution of expectation values $\langle\phi|A|\phi\rangle$ without any pronounced concentration about some particular value. In general, condition (21) will be satisfied for all a values within a certain interval around zero [12], whose upper and lower limits depend on the detailed spectral properties of A in (1). More precisely, there exist two threshold values $a_+ \in (0, a_N)$ and $a_- \in (a_1, 0)$ so that (21) is satisfied if and only if $a \in (a_-, a_+)$. As will be seen in Sec. IV, the interval (a_-, a_+) about $a = 0$ is in many cases comparable or even almost equal to the maximally possible interval (a_1, a_N).

If $a \in (a_-, a_+)$ it follows that $P_R(x)$ in (12) exhibits a very narrow maximum around $x = a$. Since N is large this implies that $G(x)$ in (19) must exhibit a minimum very close to $x = a$ and thus $G'(a) = 0$ must be fulfilled in very good approximation. With (20) it follows that

$$F'(a) - y(a) = 0. \tag{22}$$

Next we turn to the case $a \notin (a_-, a_+)$. As mentioned below (21), the probability distribution in (19) thus exhibits no pronounced concentration about some particular value. Since N is large, the variations of $G(x)$ in (19) must therefore be small. As a consequence, $G'(a) = 0$, and thus (22) will again be satisfied in very good approximation.

So far, we tacitly considered a as arbitrary but fixed. In particular, the operator R in (11) and the function $G(x)$ in (20) in general still depend on the choice of a. However, by observing that the relation (22) applies to every given a value within the interval (a_1, a_N) we can conclude from (22) that

$$F(x) = F(0) + \int_0^x da\ y(a) \tag{23}$$

for all $x \in (a_1, a_N)$, where the value of $F(0)$ is fixed by the normalization of $P(x)$ in (8).

Equation (23) is the second main result of our paper: The very sharply peaked expectation-value statistics of A in (8) is governed via (9) and (23) by the function $y(a)$, which is implicitly defined as the solution of Eq. (7).

IV. DISCUSSION AND EXAMPLES

In the generic case, Eq. (7) cannot be solved for $y(a)$ in closed analytical form. However, by Taylor-expanding $y(a)$ in (5) about $a = 0$ and observing that (7) identically holds for all a, one can readily determine $y'(0)$, $y''(0)$, $y'''(0)$,...by comparing terms with equal powers of a. Introducing the result into (23), one obtains

$$F(x) = F(0) + \frac{1}{2m_2}x^2 - \frac{m_3}{3m_2^3}x^3 + \frac{2(m_3^2 + m_2^3) - m_2 m_4}{4m_2^5}x^4 + \cdots, \tag{24}$$

$$m_k := \frac{1}{N}\sum_{n=1}^{N}(a_n)^k = \frac{\mathrm{Tr}\{A^k\}}{N}. \tag{25}$$

It follows that the probability distribution in (9) closely resembles a sharply peaked Gaussian of variance m_2/N. However, the higher order terms in (24) give rise to corrections which become more and more important far away from the peak, i.e., in the very unlikely tails of the distribution.

We recall that the results (23) and (24) are based on the approximation (22), which is very good but not exact for large but finite N. For instance, (24) yields for the mean value (first moment) of $P(x)$ in (9) the approximation $m_3/\sqrt{N m_2^3}$, while the exact value is known to be zero [1]. In other words, our present approach may not necessarily be optimal if one is interested in the moments of $P(x)$. Rather, the main virtue of our results (23) and (24) is to provide insight about the properties of the distribution $P(x)$ outside its very narrow peak region, where very many moments play a notable role.

For example, by differentiating (7) with respect to a, one can show that $y(a)$ is a monotonically increasing function of a within the domain $[0, a_N)$ (the details are explicitly worked out in Ref. [12]). With (8), (9), and (10) it then follows that the vast majority of all normalized vectors $|\psi\rangle$ with the property $\langle\psi|A|\psi\rangle \geqslant x$ must exhibit expectation values $\langle\psi|A|\psi\rangle$ very close to x for an arbitrary but fixed $x \in [0, a_N)$, and analogously for $x \in (a_1, 0]$.

Another interesting feature arises in the very unlikely tails of $P(x)$: Focusing on $a > a_+$, one can infer from (5) and the discussion below (21) that $p_N(a)$ cannot not be small. Exploiting (5) once more, it follows that $y(a)(a - a_N) = -1$ and hence

$$y(a) = \frac{1}{a_N - a} \tag{26}$$

will be fulfilled in very good approximation for all $a \in (a_+, a_N)$. With (23) we can conclude that

$$F(x) = F(a_+) - \ln\left(\frac{a_N - x}{a_N - a_+}\right) \tag{27}$$

and with (9) that

$$P(x) = P(a_+)\left(\frac{a_N - x}{a_N - a_+}\right)^N \tag{28}$$

for all $x \in [a_+, a_N)$. On the one hand, this result continuously matches for $x \to a_N$ the obvious behavior $P(x) = 0$ for $x > a_N$, which readily follows from (1), (3), and (8). On the other hand, this result explicitly illustrates once more the pronounced non-Gaussian behavior of $P(x)$ far away from the narrow peak region. Analogous conclusions apply in the domain (a_1, a_-).

Recalling that $p_N(a) \ll 1$ for $a \notin (a_+, a_N)$ [see below (21)], it seems reasonable to expect in view of (5) that the

approximation (26) will *not* be fulfilled very well for $a \notin (a_+, a_N)$, apart from a small "transition region" very close to a_+. Furthermore, one may surmise that for sufficiently large N (and relevant choices of A as a function of N; see below), the approximation (26) becomes arbitrarily good and the above mentioned "transition region" becomes arbitrarily small. As a consequence, $y(a)$ may thus be supposed to develop a nonanalyticity at $a = a_+$, and likewise for $a = a_-$. In the following, these heuristic conjectures will be worked out in more quantitative detail.

To begin, we introduce the function

$$w_N(x) := \frac{1}{N}\sum_{n=1}^{N} \delta(a_n - x), \tag{29}$$

which is normalized to unity and thus may be viewed as an eigenvalue probability distribution. We thus can rewrite the implicit definition of $y(a)$ from (7) as

$$\int dx\; w_N(x)\, \frac{1}{1 + y(a)\,(a - x)} = 1. \tag{30}$$

In order to address the above expectations about $y(a)$, we next have to specify how $w_N(x)$ changes upon variation of N. To this end, we focus on cases where the eigenvalue probability distributions from (29) approach for asymptotically large N a well-defined limit $w_\infty(x)$ at least as far as the integral on the left hand side of (30) is concerned. It is thus necessary (but not sufficient; see below) that when slightly "smearing out" the delta functions in (29) then $w_N(x)$ approaches a reasonably well-behaving function $w_\infty(x)$ for $N \to \infty$. Moreover, a_1 and a_N in (3) are supposed to converge for $N \to \infty$. Without much loss of generality, we specifically assume that

$$a_N = 1 \tag{31}$$

for all N. An analogous relation for a_1 will not be needed in our examples below, since a_1 will already be fixed for any given N through (2) and (31). Note that also the thresholds $a_\pm$ introduced below Eq. (21) are in general N dependent, and we tacitly assume that they converge for $N \to \infty$.

From a different viewpoint, all these premises may be considered as assumptions about how the observable A changes upon variations of N; see also the remarks at the end of Sec. II.

A. Example 1

As a first example we assume that A is randomly sampled from a Gaussian orthogonal or unitary ensemble (GOE or GUE) [15], hence its spectrum satisfies for asymptotically large N a so-called semicircle law. Due to (2) and (31) this means that

$$w_\infty(x) = \frac{2}{\pi}\sqrt{1 - x^2} \tag{32}$$

for $|x| \leqslant 1$ and $w_\infty(x) = 0$ for $|x| > 1$. As a consequence, one can show that in the limit $N \to \infty$ the unique solution of (30) is

$$y(a) = 4\,a \text{ for } a \in [a_-, a_+]\,, \tag{33}$$

$$a_\pm := \pm 1/2, \tag{34}$$

while there exists no solution for $a \notin [a_-, a_+]$. These results can be verified either by quite tedious residue techniques or by quite elementary numerical methods. The details seem of little interest and are therefore omitted.

The interpretation is as follows: In view of (9), (23), and (33), the probability density $P(x)$ from (8) approaches for large N a Gaussian distribution with mean zero and variance $1/4N$ within the domain $x \in [a_-, a_+] = [-1/2, 1/2]$. This behavior is complemented by (26)–(28) for $x \in (a_+, a_N) = (1/2, 1)$ and analogous formulas for $x \in (a_1, a_-) = (-1, -1/2)$. In particular, the solutions $y(a)$ from (26) and (33) as well as their first derivatives coincide at the matching point $a = a_+$, while the second derivatives are different, and likewise for $a = a_-$; i.e., the function $y(a)$ indeed develops nonanalyticities at $a = a_\pm$ for $N \to \infty$, as heuristically anticipated above Eq. (29).

Moreover, the existence of well defined limits for $y(a)$ and thus for $F(x)$ in (23) when $N \to \infty$ means that $P(x)$ in (9) satisfies a so-called large deviation principle [11] [the limiting $F(x)$ being called rate function or large deviation function in this context]. From a different viewpoint, the role of $F(x)$ in (9) is reminiscent of a thermodynamic potential in the context of equilibrium statistical mechanic, and the nonanalyticities of $F(x)$ at $x = a_\pm$, inherited from $y(a)$ via (23), are then somewhat similar to critical points in the context of phase transitions (see also Sec. V).

In turn, from the asymptotic solution (26) in the domain (a_+, a_N) together with (3)–(6) one can infer that all the $p_n(a)$ are small quantities (approaching zero for $N \to \infty$) apart from $p_N(a)$, which converges to a positive (nonzero) value for $N \to \infty$. On the one hand, this explains why the continuum approximation (32) breaks down [does not admit solutions of (30)]. On the other hand, it suggests to interpret the nonanalyticity of $y(a)$ as a phase transition similar to Bose condensation: For x values beyond a_+, typical states $|\psi\rangle$ with the property $\langle\psi|A|\psi\rangle = x$ exhibit a "macroscopic" population of the eigenstate (or, in case of degeneracy, eigenspace) belonging to a_N in the "thermodynamic limit" $N \to \infty$.

A quantitative numerical illustration is provided by Fig. 1. For better visibility of the details, only a values within the domain $[0, a_N = 1]$ are shown [the function $y(a)$ is point symmetric about $a = 0$ apart from small fluctuations caused by the random matrices]. Since the variations of $y(a)$ are unbounded [see (26) and (33)] and since the nonanalyticity at $a_+ = 1/2$ is quite "weak" (jump in the second derivative; see above), rather than depicting $y(a)$ itself, we plotted in Fig. 1 the quantity

$$Y(a) := \frac{1}{4}\frac{d}{da}[y(a)\,(a_N - a)] = -\frac{1}{4}\frac{d}{da}\frac{1}{N p_N(a)}, \tag{35}$$

where the last identity follows from (5). Since $y(0) = 0$ [see below Eq. (6)], the function $Y(a)$ from (35) contains the

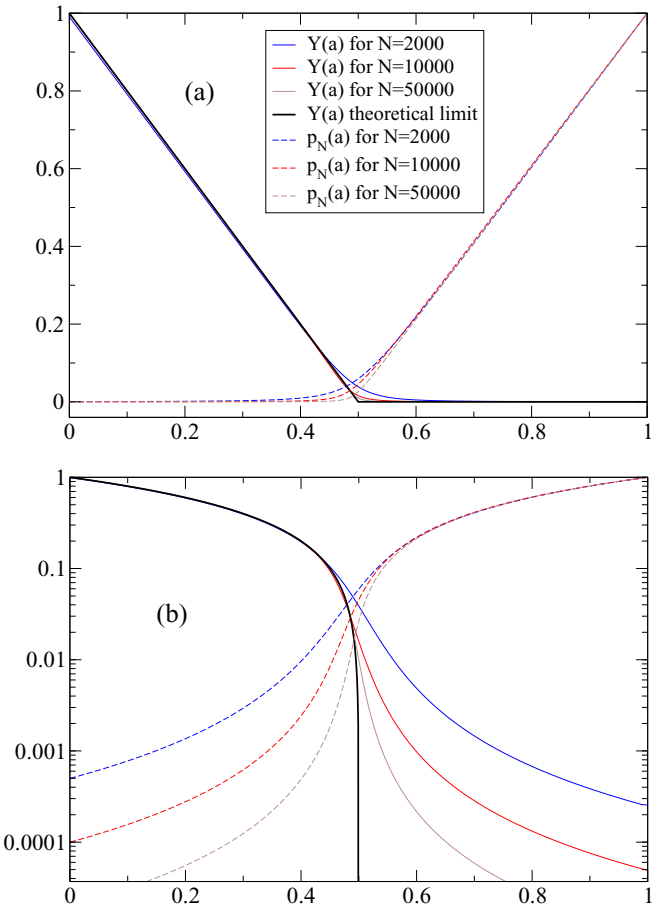

FIG. 1. Solid: The function $Y(a)$ from (35) by numerically evaluating $y(a)$ according to (7) for $N = 2000$ (blue), $N = 10\,000$ (red), and $N = 50\,000$ (brown). In each case, the a_n in (7) are the eigenvalues of an $N \times N$ matrix, randomly sampled from a GOE [15], and properly rescaled so that (2) and (31) are fulfilled. Bold black line: theoretical large N limit according to (26), (33), and (34). Dashed: The corresponding functions $p_N(a)$ from (5). The theoretical large N predictions are $p_N(a) = 0$ for $a \in [0, 1/2]$ and $p_N(1) = 1$ but are not shown in the plot. (a) and (b): Same data displayed on linear and logarithmic scales. The fluctuations for different samples of the random matrices turned out to be quite small (not shown). Some remnants are still visible close to $a = 1/2$ as apparent "irregularities" in the N dependence of the curves.

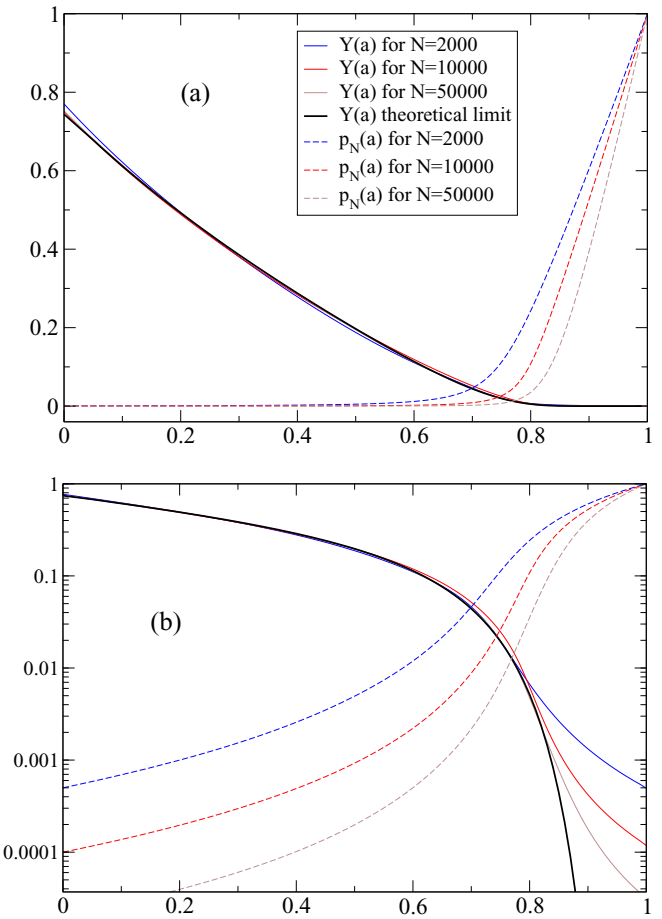

FIG. 2. Same as in Fig. 1 except that the eigenvalues a_n were randomly generated via Wigner distributed differences $a_{n+1} - a_n$ [15] and that the bold line was now obtained by numerically solving (37). Very similar results were also found for Poisson distributed differences $a_{n+1} - a_n$ (not shown).

same information as $y(a)$, but its variations are now bounded and it makes the nonanalyticity at $a = a_+$ better visible. The (approximate) symmetry between the solid and dashed curves in Fig. 1 seems to be a coincidence.

B. Example 2

As a second example, we assume that the eigenvalues of A give rise to a uniform eigenvalue probability distribution. Similarly as in (32), this means that

$$w_\infty(x) = 1/2 \tag{36}$$

for $|x| \leqslant 1$ and $w_\infty(x) = 0$ for $|x| > 1$. The corresponding relation (30) in the limit $N \to \infty$ gives rise to the following transcendental equation for $y(a)$:

$$\frac{1 + y(a)\,(1 + a)}{1 - y(a)\,(1 - a)} = e^{2y(a)}. \tag{37}$$

Similarly as below (4), the existence and uniqueness of a (nontrivial) solution $y(a)$ readily follows for any given $a \in (a_1, a_N) = (-1, 1)$. Moreover, one can show that $y(a)$ is analytic and monotonically increasing within the entire domain (a_1, a_N). To explicitly solve (37) for $y(a)$ is no longer possible in closed analytical form but is straightforward by numerical means; see Fig. 2.

Finally, it can be shown [12] that $p_N(a)$ tends to zero for $N \to \infty$ and any given $a \in (a_1, a_N)$. In particular, a_+ approaches $a_N = 1$ for $N \to \infty$, i.e., the situation is now reminiscent of a so-called quantum phase transition (occurring at zero temperature). A quantitative illustration is depicted in Fig. 2.

C. Outlook

It seems reasonable to expect that the behavior will be qualitatively similar to Fig. 1 whenever the spectrum of A can be approximated by an eigenvalue probability distribution

$w_\infty(x)$, which approaches zero for $x \to a_N$. Otherwise, a behavior similar to Fig. 2 is expected. Analogous conclusion are also suggested by Appendix D of Ref. [12].

More precisely, we recall that $w_\infty(x)$ approaches zero as $x \to a_N$ proportional to $(a_N - x)^\gamma$ with $\gamma = 1/2$ in the example depicted in Fig. 1 [see also Eq. (32)]. Upon decreasing the exponent γ, the position of the nonanalyticity (at $x = 1/2$ for the example in Fig. 1) is, roughly speaking, expected to increase until it hits the upper limit a_N when $\gamma = 0$.

V. SUMMARY AND CONCLUSIONS

Given a Hermitian operator (observable) A on a high-dimensional Hilbert space $\mathcal{H}$, what is the probability distribution $P(x)$ of the expectation values $\langle\psi|A|\psi\rangle$ when normalized vectors (pure states) $|\psi\rangle$ are randomly sampled according to a uniform distribution on the unit sphere in $\mathcal{H}$? The answer clearly depends on the spectrum of A (and on nothing else), but general quantitative statements are far from obvious. The main achievement of our paper is to show that $P(x)$ is connected to the eigenvalues $a_1, \ldots, a_N$ of A via the transcendental equation (7), whose solution $y(a)$ determines $P(x)$ according to (9) and (23).

It has been previously established in Refs. [1–9] that $P(x)$ exhibits a narrow peak about the microcanonical expectation $\mathrm{Tr}\{A\}/N$, which can be set to zero without loss of generality, so that the variance of the peak is (approximately) given by $\mathrm{Tr}\{A^2\}/N^2$. In other words (see also the Introduction), the majority of states $|\psi\rangle$ behave practically indistinguishable from the microcanonical ensemble and may thus be considered as equilibrium states. Accordingly, the remaining minority of $|\psi\rangle$'s are the nonequilibrium states, and $P(x)$ quantifies how many of them assume the nonequilibrium expectation value $\langle\psi|A|\psi\rangle = x$. In particular, the tails of $P(x)$ provide interesting information about the relative rareness of the far from equilibrium states.

We have shown that $P(x)$ exhibits an approximately Gaussian shape within the narrow peak region about $x = 0$, while the tails of $P(x)$ significantly deviate from a Gaussian behavior. Moreover, we found that $F(x)$ in (23) is a strictly monotonically increasing function of $|x|$, implying that the fraction of states $|\psi\rangle$ with a given nonequilibrium expectation value $\langle\psi|A|\psi\rangle$ decreases exponentially fast as this expectation value moves away from the equilibrium value.

In general, the transcendental equation (7) cannot be explicitly solved for $y(a)$ in closed analytical form. Yet further progress is possible under the assumption that the spectrum of A can be adequately approximated (as detailed in Sec. IV) by a well-defined eigenvalue distribution function $w_\infty(x)$ for asymptotically large Hilbert space dimensions N. Accordingly, the function $F(x)$ in (23) then plays the role of a so-called large deviation function. For example, if A is a typical random matrix from the Gaussian unitary or orthogonal ensemble, then the distribution $w_\infty(x)$ is determined by Wigner's semicircle law, and $F(x)$ exhibits two symmetric nonanalyticities, connecting the Gaussian peak region of $P(x)$ with the two distinctly non-Gaussian tails. A qualitatively similar behavior is expected whenever the observable A is so that $w_\infty(x)$ vanishes as x approaches the upper or the lower end of the spectrum. Conversely, if A is so that $w_\infty(x)$ remains nonzero as x approaches the upper or the lower end of the spectrum, then nonanalyticities of $F(x)$ are not to be expected, and likewise for the transition between the Gaussian peak region and the non-Gaussian tails of $P(x)$.

It is worth mentioning that we were not able to establish any physically meaningful connection between our present findings and the realm of equilibrium thermodynamics. In particular, there does not seem to exists a sensible relation between the function $P(x)$ and the key quantities in thermodynamics, namely, Boltzmann's entropy or any other thermodynamic potential. Despite this dissimilarity on the *physical* level, there are some remarkable similarities on a more *formal* level. Namely, the large N limit corresponds to the thermodynamic limit, and the large deviation function $F(x)$ in (9) plays a role analogous to that of the entropy in thermodynamics: it quantifies the logarithm of the state space volume (here the unit sphere in $\mathcal{H}$), which exhibits some common property (here a common expectation value). Accordingly, the nonanalyticities of $F(x)$ may be viewed as the analogues of critical points in thermodynamics.

It finally may be pointed out once more that our results are certainly of particular interest for, but not at all restricted to, closed many-body systems.

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APPENDIX

In this appendix we derive the relations (13)–(15). We do so by essentially starting from (10). In order to facilitate geometrical considerations, we change to the explicit representation of quantum states and operators exclusively by real numbers.

Let $\{|\psi_n\rangle\}$ be any orthonormal basis of the Hilbert space $\mathcal{H}$, for instance, the eigenvectors $|n\rangle$ of A from (1). Consider the $2N$ real numbers $\{\mathrm{Re}(\langle\psi|\psi_n\rangle), \mathrm{Im}(\langle\psi|\psi_n\rangle)\}$. Let those numbers be the components of the $2N$-dimensional, real vector $\vec{\psi}$. Let $\vec{\phi}$ be defined by a corresponding, completely analogous construction. Then (10) may be rewritten as

$$\vec{\phi} = \frac{\hat{R}\vec{\psi}}{\sqrt{\vec{\psi}\cdot\hat{R}^T\hat{R}\vec{\psi}}}. \tag{A1}$$

Here $\hat{R}$ is a $2N \times 2N$ real matrix, the components of which may be found from R in (11), and $\cdot$ denotes the standard, real Cartesian dot product. For the sake of generality, we do not require that $\hat{R}$ is a symmetric matrix and denote its transposed by $\hat{R}^T$.

The normalization of $|\psi\rangle$ caries over to a normalization of $\vec{\psi}$, i.e., $\vec{\psi}\cdot\vec{\psi} = 1$. Thus, in a Cartesian coordinate system, the vectors $\vec{\psi}$ lay on a $2N-1$-dimensional unit-hypersphere, and so do the vectors $\vec{\phi}$. However, whereas the $\vec{\psi}$ are

[by definition, see above (8)] uniformly distributed on the hypersphere, the $\vec{\phi}$ are not. It is the first aim of this appendix to find the density of the $\vec{\phi}$ on the hypersphere which essentially amount to calculating $\rho(\phi)$ from (13). Since (A1) maps a hypersphere onto a hypersphere it may be regarded as a coordinate transformation. To this coordinate transformation corresponds a Jacobian matrix. According to standard integral calculus of many variables, the density $\rho(\phi)$ may eventually be found from the (inverse of) the Gramian determinant of said Jacobian matrix; cf. below, (A4).

In order to arrive there, we start by a "locally Cartesian" parametrization of the surface of the above hypersphere formed by the $\vec{\psi}$. To be more explicit, consider a parametrization $\vec{\psi}(\theta_1, \ldots, \theta_i, \ldots, \theta_{2N-1})$ such that $\vec{\psi} \cdot \vec{\psi} = 1$ holds for any choice of the $\{\theta_i\}$. Furthermore, we require orthonormality, i.e., with the notation $\partial_i \vec{\psi} = \frac{\partial \vec{\psi}}{\partial \theta_i}$, the following is assumed to hold:

$$\partial_i \vec{\psi} \cdot \partial_j \vec{\psi} = \delta_{ij}, \quad \partial_i \vec{\psi} \cdot \vec{\psi} = 0. \tag{A2}$$

Thus the $\{\partial_i \vec{\psi}\}$ span a local tangent plain to the hypersphere. Using the analogous notation, the Jacobian matrix $\hat{j}$ which corresponds to the transformation (A1) may be defined by specifying its column vectors:

$$\hat{j} := (\partial_1 \vec{\phi}, \ldots, \partial_i \vec{\phi}, \ldots, \partial_{2N-1} \vec{\phi}). \tag{A3}$$

Obviously, $\hat{j}$ is a $2N \times (2N-1)$ real matrix. From this matrix the density $\rho(\phi)$ may be computed as

$$\rho(\phi) = (\det[\hat{j}^T \hat{j}])^{-\frac{1}{2}}. \tag{A4}$$

In order to calculate $\det[\hat{j}^T \hat{j}]$ (the Gramian determinant) we take a little detour. Consider the $2N \times 2N$ real matrix $\hat{J}$, defined by its column vectors as

$$\hat{J} := (\partial_1 \vec{\phi}, \ldots, \partial_i \vec{\phi}, \ldots, \partial_{2N-1} \vec{\phi}, \vec{\phi}), \tag{A5}$$

which is just $\hat{j}$ completed by the "radial vector" $\vec{\phi}$ itself. Since all the $\vec{\phi}$, just like the $\vec{\psi}$, lay on a hypersphere, the $\{\partial_i \vec{\phi}\}$ also span a local tangent plain to the sphere, not necessarily orthonormal though. Thus, nevertheless,

$$\partial_i \vec{\phi} \cdot \vec{\phi} = 0 \tag{A6}$$

holds. [This may be also seen more explicitly below, from (A11).] As a consequence, the matrix $\hat{J}^T \hat{J}$ may be denoted in the following schematic form:

$$\hat{J}^T \hat{J} = \begin{pmatrix} \hat{j}^T \hat{j} & 0 \\ & 0 \\ & \vdots \\ 00 \ldots & 1 \end{pmatrix}. \tag{A7}$$

Hence, one readily can infer that

$$\det[\hat{j}^T \hat{j}] = \det[\hat{J}^T \hat{J}]. \tag{A8}$$

In order to find the density $\rho(\phi)$ according to (A4), we now aim at finding a more explicit form of $\hat{J}$ that will allow for the computation of the determinant on the r.h.s. of (A8). Computing the column-vectors of $\hat{J}$ (from (A5), i.e., taking derivatives of (A1)) yields, for all but the last one,

$$\partial_i \vec{\phi} = \frac{\hat{R} \partial_i \vec{\psi}}{(\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi})^{1/2}} - \frac{Q}{2} \frac{\hat{R} \vec{\psi}}{(\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi})^{3/2}} \tag{A9}$$

$$Q := \partial_i \vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi} + \vec{\psi} \cdot \hat{R}^T \hat{R} \partial_i \vec{\psi}. \tag{A10}$$

Exploiting the properties of the dot product, this may be rewritten as

$$\partial_i \vec{\phi} = \frac{\hat{R} \partial_i \vec{\psi}}{\sqrt{\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi}}} - \left(\vec{\phi} \cdot \frac{\hat{R} \partial_i \vec{\psi}}{\sqrt{\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi}}} \right) \vec{\phi}. \tag{A11}$$

[Note that forming the dot-product of (A11) with $\vec{\phi}$ confirms (A6).] It may be seen from (A11) that the first $2N-1$ column vectors of $\hat{J}$ just consist of the vectors $\frac{\hat{R} \partial_i \vec{\psi}}{\sqrt{\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi}}}$, subtracted by multiples of $\vec{\phi}$ from each of them. However, $\vec{\phi}$ is the last column vector of $\hat{J}$. Since, according to basic linear algebra, adding multiples of column vectors to other column vectors of a matrix does not change determinant of the latter, we may conclude that

$$\det[\hat{J}] = \det[\hat{K}], \tag{A12}$$

where $\hat{K}$ is defined as

$$\hat{K} := \frac{(\hat{R} \partial_1 \vec{\psi}, \ldots, \hat{R} \partial_i \vec{\psi}, \ldots, \hat{R} \partial_{2N-1} \vec{\psi}, \hat{R} \vec{\psi})}{\sqrt{\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi}}}. \tag{A13}$$

Here the vectors in the numerator are again supposed to be the column vectors of the matrix $\hat{K}$ and the fraction bar notation is meant to indicate that each column vector has a prefactor given by the inverse of the expression in the denominator.

To repeat: (A12) and (A13) follow from (A5) and (A11). Due to the fact that the $\{\partial_i \vec{\psi}\}$ together with $\vec{\psi}$ form a complete, orthonormal basis [cf. (A2)], we may conclude that (A13) really just implements a specific representation (w.r.t. said basis) of

$$\hat{K} = \frac{\hat{R}}{\sqrt{\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi}}}. \tag{A14}$$

Hence the determinant of $\hat{K}$ and thus, according to (A12) the determinant if $\hat{J}$ is

$$\det[\hat{J}] = \det[\hat{R}] (\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi})^{-N}. \tag{A15}$$

Thus, using basic properties of determinants and (A4), (A8) we find for the probability density

$$\rho(\phi) = \frac{(\vec{\psi} \cdot \hat{R}^T \hat{R} \vec{\psi})^N}{\det[\hat{R}]}. \tag{A16}$$

While this is almost the final result, the r.h.s. of (A16) is still formulated in terms of $\vec{\psi}$ rather than in terms of $\vec{\phi}$. In order to convert we "invert" (A1),

$$\vec{\psi} = \frac{\hat{R}^{-1} \vec{\phi}}{\sqrt{\vec{\phi} \cdot (\hat{R} \hat{R}^T)^{-1} \vec{\phi}}}, \tag{A17}$$

where existence of $\hat{R}^{-1}$ is justified in the main text below (15). Plugging (A18) into (A16), we eventually obtain

$$\rho(\phi) = \frac{(\vec{\phi}\cdot(\hat{R}\hat{R}^T)^{-1}\vec{\phi})^{-N}}{\det[\hat{R}]}. \tag{A18}$$

Going back to standard quantum notation and realizing that any eigenvalue of R appears twice in the eigenvalues of $\hat{R}$, this reads

$$\rho(\phi) = \frac{\langle\phi|(RR^\dagger)^{-1}|\phi\rangle^{-N}}{\det[R^2]}. \tag{A19}$$

Observing that the specific operator R in (11) is Hermitian, we finally recover (14) and (15).

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