Physics Letters A 377 (2013) 1854–1861

Contents lists available at SciVerse ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Probability density of quantum expectation values

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ARTICLE INFO

Article history:
Received 9 March 2013
Received in revised form 17 May 2013
Accepted 20 May 2013
Available online 22 May 2013
Communicated by P.R. Holland

Keywords:
Haar measure
Typicality
Probability density
Measure concentration

ABSTRACT

We consider the quantum expectation value $\mathcal{A} = \langle\psi|A|\psi\rangle$ of an observable A over the state $|\psi\rangle$. We derive the exact probability distribution of $\mathcal{A}$ seen as a random variable when $|\psi\rangle$ varies over the set of all pure states equipped with the Haar-induced measure. To illustrate our results we compare the exact predictions for few concrete examples with the concentration bounds obtained using Levy's lemma. We also comment on the relevance of the central limit theorem and finally draw some results on an alternative statistical mechanics based on the uniform measure on the energy shell.

1. Introduction

The role of probability distributions in quantum theory cannot be overestimated. Arguably the most important of those distributions is the one describing the statistics of possible outcomes of the measurement of the observable associated with the self-adjoint operator A while the system is in the pure state $|\psi\rangle$: $P_A(a) := \langle\psi|\delta(A-a)|\psi\rangle$. This function is supported on the numerical range of A and, for bounded A can be equivalently characterized by the set of its moments (see e.g. [1]): $m_k := \langle\psi|A^k|\psi\rangle$ $(k \in \mathbf{N})$, i.e., the expectation values of the family of observables $\{A^k\}_{k\in\mathbf{N}}$ in the state $|\psi\rangle$. This latter, quite often, can be itself regarded as a random variable distributed according to some prior density that depends on the problem under consideration. For example, in the context of equilibration dynamics of closed quantum systems [2,3] one is interested in the quantity $a(t) := \langle\psi(t)|A|\psi(t)\rangle$, where $|\psi(t)\rangle := e^{-itH}|\psi\rangle$ and H is the Hamiltonian operator of the system. If one monitors A by sampling time instants uniformly over a the interval $[0,T]$ the underlying probability space for the $|\psi(t)\rangle$'s is the segment $[0,T]$ equipped with the uniform measure dt/T. In this case averaging over the quantum states amounts to perform the time average $1/T\int_0^T a(t)\,dt$.

Another possibility that recently gained relevance for the foundation of statistical mechanics [4] is to consider $\langle\psi|A|\psi\rangle$ and let $|\psi\rangle$ vary over the full unit sphere of the, say d-dimensional, Hilbert space. This manifold is transitively acted upon by the group of all $d\times d$ unitary matrices $\mathbb{U}(d)$ and therefore inherits a natural invariant measure from the unique group-theoretic invariant measure over $\mathbb{U}(d)$ i.e., the Haar measure.

In this Letter we will address precisely this latter setting and compute the probability distribution for the quantum expectations $\langle\psi|A^k|\psi\rangle$ seen as random variables over the unit sphere of the Hilbert space equipped with the measure induced by the Haar measure. In this way the function P_A itself becomes a probability-density valued random variable that can be partially characterized by the probability densities of its moments m_k over the unit sphere. We will show that these probability densities can be determined with elementary tools and explicit analytical expressions for their characteristic functions can be obtained. To be specific we will concentrate on the probability density defined as $P_{\mathcal{A}}(a) := \overline{\delta(\langle\psi|A|\psi\rangle - a)}$ where the overline $\overline{f(\psi)} = \int D\psi\, f(\psi)$ indicates Haar-induced averages over pure states. The probability distribution for $\langle\psi|A^k|\psi\rangle$ is trivially obtained with the substitution $A \to A^k$.

The probability density $P_{\mathcal{A}}(a)$ has been first considered in a series of works [5–9] which introduced the so-called "quantum microcanonical equilibrium" (QME), an alternative statistical mechanics based on a generalization of the postulate of equal a-priori probability. This postulate states that, at equilibrium, all the energy eigenstates in a given energy shell are equally probable and it leads to the familiar microcanonical equilibrium state $\rho_{MC} = \Pi_E/d$ where Π_E is the projection onto the space of energies between E and $E+\Delta$, [d is the dimension of its range and Δ is a small parameter (see e.g. [10])]. In the QME setting instead one also allows for quantum superposition of energy eigenstates. This leads one to consider all normalized states in the Hilbert space of the

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0375-9601/$ – see front matter
http://dx.doi.org/10.1016/j.physleta.2013.05.041

energy shell taken with uniform probability, that is, the Haar induced measure over the pure states. We will come back to QME in Section 6. In particular we will answer the question whether QME gives rise to extensive free energy and the typical size of fluctuations.

Studies investigating the form and the properties of $P_{\mathcal{A}}(a)$ have recently appeared [11–13] (see also [14] for an entry into the mathematical literature) where $P_{\mathcal{A}}(a)$ is sometimes referred to as "numerical shadow". In the present Letter we give extra care to the physical situation where the total Hilbert space is that of a many-body systems and observables are extensive operators. Moreover, for the first time, we give explicit formulae for the moment generating function and the probability density for the general case where A is not necessarily a non-degenerate operator.

2. Preliminaries

Our key object is $\mathcal{A}(\psi) = \langle\psi|A|\psi\rangle$. Computing the first few moments of $\mathcal{A}(\psi)$ is a relatively easy task. The first moment reads

$$m_1 = \overline{\mathcal{A}} = \int D\psi\, \mathrm{tr}\big(A|\psi\rangle\langle\psi|\big) = \frac{\mathrm{tr}(A)}{d}, \tag{1}$$

a result which follows from $\overline{|\psi\rangle\langle\psi|} = \mathbb{1}/d$ [15]. A closed formula for the general moment can be obtained by noting that

$$\overline{|\psi\rangle\langle\psi|^{\otimes n}} = \frac{1}{\binom{d+n-1}{n}} \frac{1}{n!} \sum_{\pi\in S_n} P_\pi. \tag{2}$$

Here P_π is the operator that enacts the permutation π in $\mathcal{H}^{\otimes n}$ and S_n is the symmetric group of n elements. For a proof of (2) see e.g. [16]. The proportionality constant is obtained noting that $\binom{d+n-1}{n}$ is the dimension of the totally symmetric space, and the remaining operator is an orthogonal projector. Using Eq. (2) one obtains the following closed expression for the n-th moment

$$m_n = \frac{(d-1)!}{(d+n-1)!} \sum_{\pi\in S_n} \mathrm{tr}\big(P_\pi A^{\otimes n}\big) \tag{3}$$

$$= \frac{(d-1)!}{(d+n-1)!} \times \sum_{\pi\in S_n} \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_n=1}^{d} [A_{\sigma_1,\sigma_{\pi(1)}} \cdots A_{\sigma_n,\sigma_{\pi(n)}}]. \tag{4}$$

This expression can be thought of as a sum of contractions and represents a sum of products of traces of A. For instance for $n = 2, 3$ one has

$$m_2 = \frac{\mathrm{tr}(A)^2 + \mathrm{tr}(A^2)}{d(d+1)}, \tag{5}$$

$$m_3 = \frac{\mathrm{tr}(A)^3 + 3\,\mathrm{tr}(A^2)\,\mathrm{tr}(A) + 2\,\mathrm{tr}(A^3)}{d(d+1)(d+2)}. \tag{6}$$

With a little extra work one gets for $n = 4$

$$m_4 = \big[d(d+1)(d+2)(d+3)\big]^{-1} \times \big[\mathrm{tr}(A)^4 + 6\big[\mathrm{tr}\big(A^2\big)\big]\big[\mathrm{tr}(A)\big]^2 + 3\big[\mathrm{tr}\big(A^2\big)\big]^2 + 8\,\mathrm{tr}(A)\,\mathrm{tr}\big(A^3\big) + 6\,\mathrm{tr}\big(A^4\big)\big]. \tag{7}$$

Although the moments can be obtained in closed form it seems difficult to obtain the probability density following this approach. Instead our procedure will be that of computing directly the characteristic function $\chi(\lambda) := \overline{e^{i\lambda\mathcal{A}(\psi)}}$ and obtain the probability density via Fourier transform.

Choosing a basis $|j\rangle$ $(j = 1,\dots,d)$ and calling $z_j = \langle j|\psi\rangle$ we observe that we can write the average over $|\psi\rangle$ as

$$\overline{f(\psi)} = C\int \delta\left(\sum_{j=1}^{d} |z_j|^2 - 1\right) f(\psi)\, d^2\boldsymbol{z} \tag{8}$$

where we defined

$$\int d^2\boldsymbol{z} = \prod_{i=1}^{d} \int_{\mathbb{R}\times\mathbb{R}} \frac{dx_i\, dy_i}{\pi}. \tag{9}$$

The normalization constant C can be computed with the same technique that we are going to show and it turns out to be equal to $(d-1)!$. Using the Fourier representation for the delta function in Eq. (8) we obtain a Gaussian integral that can be computed. For simplicity we use the basis that diagonalizes A: $A = \sum_j a_j |j\rangle\langle j|$. Calling $D_A = \mathrm{diag}\{a_1, a_2, \dots, a_d\}$ we can write the characteristic function as

$$\chi(\lambda) = (d-1)! \int d^2\boldsymbol{z} \int_{\mathbb{R}} \frac{dr}{2\pi} e^{ir(z^\dagger z - 1)} e^{i\lambda z^\dagger D_A z - \epsilon z^\dagger z}. \tag{10}$$

As customary we introduced a small positive ϵ in order to make the Gaussian integral absolutely convergent. The Gaussian integration gives

$$\chi(\lambda) = \frac{(d-1)!}{(-i)^d} \int_{\mathbb{R}} \frac{dr}{2\pi} \frac{e^{-ir}}{\prod_j (r - r_j)}, \tag{11}$$

with $r_j = -\lambda a_j - i\epsilon$. At this point we make the important assumption that all eigenvalues of A are non-degenerate. We will treat the general case in Section 3. Under these conditions the integrand in Eq. (11) has only simple poles and the integral is easily evaluated with residues closing the circle in the in the lower half-plane. The result is, after sending $\epsilon \to 0$,

$$\chi(\lambda) = \frac{(d-1)!}{(i\lambda)^{d-1}} \sum_{k=1}^{d} \frac{e^{i\lambda a_k}}{\prod_{j\neq k}(a_k - a_j)}. \tag{12}$$

Although it might not be readily apparent from Eq. (12), $\chi(\lambda)$ is actually regular in $\lambda = 0$. This fact follows from a set of identities proven in Appendix A stating that

$$\sum_{k=1}^{d} \frac{(a_k)^n}{\prod_{j\neq k}(a_k - a_j)} = \begin{cases} 0, & 0 \leqslant n \leqslant d-2, \\ 1, & n = d-1. \end{cases} \tag{13}$$

Applying Eq. (13) to Eq. (12) we thus see that $\chi(\lambda)$ is regular at $\lambda = 0$ and being a linear combination of analytic functions it is in fact analytic in the whole complex plane (entire). A simple way to remember that $\chi(\lambda)$ must be regular at $\lambda = 0$ is to note that $\chi(\lambda) = 1 + m_1(i\lambda) + O(\lambda^2)$. In fact this very same approach can be used to prove Eq. (13). Using Eq. (13) and Eq. (12) we readily obtain the Taylor series of $\chi(\lambda)$

$$\chi(\lambda) = \sum_{n=0}^{\infty} m_n \frac{(i\lambda)^n}{n!}, \tag{14}$$

$$m_n = \frac{1}{\binom{n+d-1}{n}} \sum_{k=1}^{d} \frac{(a_k)^{n+d-1}}{\prod_{j\neq k}(a_k - a_j)}. \tag{15}$$

Eq. (15) is a quite compact expression in place of the complicated Eq. (4). Equating Eq. (15) with Eq. (4) we obtain the following non-trivial set of matrix identities valid when the spectrum of A is non-degenerate