Comment on "Equilibration Time Scales of Physically Relevant Observables"

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Putting a generally valid upper bound on equilibration times of physically relevant observables is a much pursued endeavor. Recently, such a bound has been suggested by Garcia-Pintos *et al.* While the mathematical correctness of the bound as such is undisputed, its concrete calculation requires the knowledge of certain quantities, which Garcia-Pintos *et al.* assess by means of assumptions. We show that, e.g., in standard cases of slow, exponential equilibration, (at least) one of these assumptions is not valid. This demonstration highlights the difficulty to judge the validity of the above assumptions without further information. Such information is, in general, very hard to obtain.

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I. INTRODUCTION

For self-containedness, we (re)state the main result of Ref. [1] [hereafter called the García-Pintos bound (GPB)] in a comprehensive form. (It should be a quick read-through for those familiar with this result.) Furthermore, we define the function $w(G)$, cf. Eq. (2), which is directly calculated from the probability distribution denoted by p_{jk} in Ref. [1].

The GPB addresses an equilibration time T_{eq}. To further specify T_{eq}, we introduce some notation. Let ρ be the initial state of the system. Moreover, let $A(t)$ denote an observable A in the Heisenberg picture and $\langle A(t)\rangle := \mathrm{Tr}\{A(t)\rho\}$ its time-dependent expectation value. Because the closed system dynamics is unitary (and the system is finite), $\langle A(t)\rangle$ has a well-defined "infinite-time average" $\overline{\langle A\rangle} =: \langle A\rangle_{\mathrm{eq}}$, which is routinely considered as the equilibrium value of A, if the observable A equilibrates at all [2]. Now, consider a deviation $D(t)$ of the actual expectation value from its equilibrium, i.e., $D(t) := (\langle A(t)\rangle - \langle A\rangle_{\mathrm{eq}})^2/4\|A\|^2$, where $\|A\|$ is the largest absolute eigenvalue of A. Furthermore, consider an average of $D(t)$ over the time interval $[0,T]$ denoted by $\bar{D}_T$. The condition that defines T_{eq} is that $\bar{D}_T \ll 1$ must hold for $T \gg T_{\mathrm{eq}}$ (for nonequilibrating systems, such a T_{eq} may not exist [2]). The GPB is an explicit expression for such a T_{eq} [see Eq. (4)] based on ρ, $A(0)$ and the Hamiltonian of the system H. As the GPB involves somewhat refined functions of the above three operators, we need to specify these before stating the GPB explicitly. A central role is taken by the probability distribution p_{jk}, which is defined as

$$p_{jk} \propto |\rho_{jk}A_{kj}| \quad \text{for } E_j - E_k \neq 0,$$
$$p_{jk} = 0 \quad \text{for } E_j - E_k = 0, \qquad \sum_{j,k} p_{jk} = 1, \tag{1}$$

where E_j, E_k are energy eigenvalues corresponding to energy eigenstates $|j\rangle$, $|k\rangle$. Additionally, matrix elements are abbreviated as $\rho_{jk} := \langle j|\rho|k\rangle$, $A_{jk} := \langle j|A(0)|k\rangle$. While the GPB is not limited to this case, here, we focus on the p_{jk} that may be described in terms of a probability density function $w(G)$. The examples we present below conform with such a description, and it is plausible that this applies to generic many-body scenarios. Prior to defining $w(G)$, we define $w(G,\epsilon)$ as

$$w(G,\epsilon) := \frac{1}{\epsilon}\sum_{j,k}\Theta\left(\frac{\epsilon}{2} - |E_j - E_k - G|\right)p_{jk}, \tag{2}$$

where Θ is the Heaviside function. This definition is the standard construction of a histogram in which the p_{jk} are sorted according to their respective energy gaps $E_j - E_k$. It is now assumed that there exists a range of (small but not too small) ϵ such that $w(G,\epsilon)$ is essentially independent of variations of ϵ within this range. The $w(G,\epsilon)$ from this "independence regime" are simply abbreviated as $w(G)$. Let the standard deviation of $w(G)$ be denoted by σ_G. [In Ref. [1], σ_G denotes the standard deviation of $w(G,0)$; however, here we focus on situations where this difference is negligible.]

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Furthermore, let $w_{\max}$ denote the maximum of $w(G)$. The quantities a and Q that eventually enter the GPB are now defined as

$$a := w_{\max}\sigma_G, \qquad Q := \sum_{i,j:E_i\neq E_j} \frac{|\rho_{ij}A_{ji}|}{\|A\|}. \tag{3}$$

We can now state the GPB:

$$T_{\mathrm{eq}} = \frac{\pi a \|A\|^{1/2} Q^{5/2}}{\sqrt{|\mathrm{Tr}\{[[\rho,H],H]A\}|}} = \frac{\pi a \|A\|^{1/2} Q^{5/2}}{\sqrt{\left|\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle A(t)\rangle|_{t=0}\right|}}. \tag{4}$$

II. GENERAL PROBLEM OF UPPER BOUNDING a, Q IN THE CASE OF SLOW EXPONENTIAL DECAY DYNAMICS

Obviously, the GPB links T_{eq} to the initial "curvature" of the observable dynamics $\partial_t^2\langle A(t)\rangle|_{t=0}$ [which is often practically computable, simply from its form in the denominator in the middle of the double equation in Eq. (4)]. An actual, concrete value or upper bound for T_{eq}, however, may only be computed from Eq. (4) if the numerator can also be computed or upper bounded. Let us stress that this (rather obvious) statement is pivotal for the argument in this Comment. The three main results, which are formulated further below, attain their significance only in connection with this statement. The crucial quantities in the numerator are a and Q. As it is practically impossible to calculate a from its definition for many-body quantum systems, García-Pintos *et al.* instead resort to an assumption concerning a. They argue that $a \sim 1$ may be expected for $w(G)$ that are "unimodal." Unimodal means that $w(G)$ essentially consists of one central elevation like a Gaussian or a box distribution, etc. Indeed, a is invariant with respect to a rescaling $w(G) \to sw(sG)$, as it would result from rescaling the Hamiltonian as $H \to sH$ (here, s is some real, positive number). García-Pintos *et al.* also offer various upper bounds on Q for different situations.

In contrast to the argument in Ref. [1], we show in the following that the assumption of any two fixed upper bounds on a and Q is necessarily violated for generic, sufficiently slow, exponential decays of $\langle A(t)\rangle$. To this end, two standard scenarios of slow dynamics are analyzed below. In Sec. III, we also provide a concrete spin-based example (along the lines of Scenario 1) in which a is found to diverge while the bound on Q from Ref. [1] applies. This result occurs even though $w(G)$ is unimodal.

Scenario 1: Dynamics of quantities that are conserved except for a weak perturbation to the Hamiltonian.—Consider first a Hamiltonian consisting of an unperturbed part H_0 and a perturbation λH_{int}.

$$H = H_0 + \lambda H_{\mathrm{int}}. \tag{5}$$

Furthermore, consider an observable A, which is conserved under H_0, i.e., $[A, H_0] = 0$. If H_0 has a sufficiently wide and dense spectrum and λ is small, exponential decay, in the simplest case, monoexponential decay, i.e.,

$$\langle A(t)\rangle = (\langle A(0)\rangle - \langle A\rangle_{\mathrm{eq}})\mathrm{e}^{-t/\tau_{\mathrm{rel}}} + \langle A\rangle_{\mathrm{eq}}, \tag{6}$$

occurs, where $\tau_{\mathrm{rel}} = r\lambda^{-2}$ and r is a real, finite, positive number that depends on the details of the setup. Many well-understood approaches, such as the Weisskopf-Wigner theory and projection operator techniques (Nakajima-Zwanzig, Mori, etc.), arrive at such exponential decay dynamics [3–7] for standard, physical, nonequilibrium situations. A bold numerical demonstration for the emergence of dynamics in accordance with Eq. (6) in closed quantum systems is given in Ref. [8]. For even more evidence, see Refs. [9,10]. If $\partial_t\langle A(t)\rangle|_{t=0} = 0$, obviously Eq. (6) cannot apply at $t = 0$. In this case, Eq. (6) is meant to apply after a short "Zeno time" τ_{zeno}, which is usually exceedingly short compared to the relaxation time τ_{rel} [4,7]. Note, however, that the denominator of Eq. (4) necessarily addresses a time below the Zeno time, namely, $t = 0$. We now aim to find the principal dependence of quantities in Eq. (4) on the interaction strength λ. From the definition of T_{eq} given at the beginning of Sec. I, it follows that

$$T_{\mathrm{eq}} \geq \tau_{\mathrm{rel}}. \tag{7}$$

For the denominator of Eq. (4), we find, with Eq. (5),

$$\sqrt{\left|\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle A(t)\rangle|_{t=0}\right|} = \sqrt{|c_1\lambda + c_2\lambda^2|}, \tag{8}$$

where $c_1 = \mathrm{Tr}\{[H_{\mathrm{int}},A][\rho,H_0]\}$, $c_2 = \mathrm{Tr}\{[H_{\mathrm{int}},A][\rho,H_{\mathrm{int}}]\}$. While initial states ρ such that $c_2 = 0$ are possible, they are not generic; rather, they are very rare (untypical) for a given, nonvanishing $\langle A(0)\rangle$ [11]. Plugging Eqs. (6)–(8) into Eq. (4) yields

$$\pi a \|A\|^{1/2} Q^{5/2} \geq r\frac{\sqrt{|c_1\lambda + c_2\lambda^2|}}{\lambda^2} \tag{9}$$

for the numerator of Eq. (4). Obviously, the numerator of Eq. (4) diverges in the limit of weak interactions, i.e., $\lambda \to 0$. The latter holds even if $c_1 = 0$. The divergence of the numerator of Eq. (4) necessarily implies the divergence of a or Q or both. Thus, no concrete, finite T_{eq} may be computed from Eq. (4) in this case. This is the first main result of the present Comment.

Scenario 2: Dynamics of long-wavelength Fourier components of spatial densities of conserved quantities.—In Scenario 1, the exponential decay is due to some "conservation breaking" part of the Hamiltonian being small. However, exponential decay also often occurs without some part of the Hamiltonian being particularly small.

Consider, e.g., a spatially more or less homogeneous system in which some quantity Z (like energy, particles, magnetization, etc.) is totally conserved. Nevertheless, the spatial density of this quantity $p(x,t)$ may undergo some time evolution. If this evolution complies with a diffusion equation, a Fourier component of this density, e.g., $\langle A_k(t)\rangle = \langle \int \cos(kx)p(x,t)\mathrm{d}x\rangle$, will decay exponentially, i.e.,

$$\langle A_k(t)\rangle = \langle A_k(0)\rangle \mathrm{e}^{-\kappa k^2 t}, \tag{10}$$

where κ is the non-negative, finite diffusion coefficient. However, just like in Scenario 1, we additionally need to find $\partial_t^2\langle A_k(t)\rangle|_{t=0}$ in order to find the scaling of a and Q with k. While the following consideration, in principle, applies to all spatial dynamics of conserved quantities, here we resort to a specific example, for clarity. We consider the XXZ chain of length N with periodic boundary conditions ($N+1\equiv 1$) and anisotropy Δ described by the Hamiltonian

$$H_{\mathrm{XXZ}} = \sum_{j=1}^{N}(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z). \tag{11}$$

The total magnetization of the system, i.e., $Z=\sum_i S_i^z$, is conserved. The Fourier components of the spatial distribution of the magnetization are

$$A_k = \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\cos(ki)S_i^z, \tag{12}$$

where $k = 2\pi m/N$ are the discrete wave numbers and $m = 0,1,\ldots,N-1$. The scaling in N guarantees the convergence of the variances of the spectra of the A_k to finite values of order unity at large N. (This case may be inferred from considering the corresponding Hilbert-Schmidt norms.) Calculating the second temporal derivatives of the A_k yields

$$\begin{aligned} &-[H_{\mathrm{XXZ}},[H_{\mathrm{XXZ}},A_k]] \\ &\quad = 2(\cos(k)-1)(A_k+B_k) - \sin(k)C_k, \end{aligned} \tag{13}$$

where

$$\begin{aligned} B_k &= \frac{2}{\sqrt{N}}\sum_{j=1}^{N}\cos(kj)(S_{j-1}^x S_j^z S_{j+1}^x + S_{j-1}^y S_j^z S_{j+1}^y) \\ &\quad -\frac{\Delta}{\sqrt{N}}\sum_{j=1}^{N}\cos(kj)(S_{j-1}^z S_j^x S_{j+1}^x - S_{j-1}^x S_j^x S_{j+1}^z \\ &\quad + S_{j-1}^z S_j^y S_{j+1}^y - S_{j-1}^y S_j^y S_{j+1}^z), \\ C_k &= -\frac{2\Delta}{\sqrt{N}}\sum_{j=1}^{N}\sin(kj)(S_{j-1}^z S_j^x S_{j+1}^x - S_{j-1}^x S_j^x S_{j+1}^z \\ &\quad + S_{j-1}^z S_j^y S_{j+1}^y - S_{j-1}^y S_j^y S_{j+1}^z). \end{aligned} \tag{14}$$

For small k, this result may be approximated as

$$[H_{\mathrm{XXZ}},[H_{\mathrm{XXZ}},A_k]] \approx k^2(A_k+B_k) + kC_k. \tag{15}$$

Note that the variances of the spectra of B_k and C_k are all of order unity for any k, just like the spectra of the A_k. Relying on the small-k approximation yields

$$\sqrt{\left|\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle A_k(t)\rangle|_{t=0}\right|} = \sqrt{\left|c_3 k + c_4 k^2\right|}, \tag{16}$$

where $c_3 = \mathrm{Tr}\{C_k\rho\}$ and $c_4 = \langle A_k(0)\rangle + \mathrm{Tr}\{B_k\rho\}$. While initial states ρ resulting in $\mathrm{Tr}\{B_k\rho\} = -\langle A_k(0)\rangle$ are mathematically possible, they are not generic or typical at all. Instead, typical values are $\mathrm{Tr}\{B_k\rho\}\approx 0$—even, and especially, for a given $\langle A_k(0)\rangle$ [11]. Thus, exploiting Eq. (16) yields, in general, by the same line of argumentation employed before in Scenario 1 [cf. Eqs. (7)–(9)],

$$\pi a \|A_k\|^{1/2} Q^{5/2} \geq \kappa \frac{\sqrt{|c_3 k + c_4 k^2|}}{k^2}, \tag{17}$$

where the rhs diverges in the limit $k\to 0$, analogous to Eq. (9). Again, this divergence occurs even for $c_3 = 0$. Thus, no concrete, finite T_{eq} may be computed from Eq. (4) in this limiting case either. This is the second main result of the present Comment. We want to emphasize the following. The XXZ chain exhibits, depending on (nonsmall) Δ and ρ, various sorts of transport behavior, such as diffusive, ballistic, and possibly superdiffusive, with the inclusion of some disorder, possibly subdiffusive, etc., [12,13]. The constants a and Q cannot be simultaneously finite in the long-wavelength limit ($k\to 0$, $N\to\infty$) if the transport is diffusive. They may be finite if the transport is, e.g., ballistic. Thus, determining whether or not a and Q are both finite is as difficult as determining whether transport is ballistic or diffusive. The latter is, however, a long-standing and only recently to a good extent answered research question for the XXZ chain [12,14–17].

III. CONCRETE, PHYSICAL EXAMPLE ENTAILING $a \nsim 1$

Here, we present a concrete, physical example, which is nevertheless simple enough to allow for analytical analysis. This analysis unveils that, in this particular instance, indeed a diverges while the bound on Q, as provided in Ref. [1], applies. The exemplary setup consists of a single spin (hereafter, called the "system") subject to a magnetic field of strength B along the z direction, weakly coupled to a large (but finite) environmental system (hereafter, called the "bath"). Thus, the unperturbed Hamiltonian is given by $H_0 = BS_{\mathrm{sys}}^z + H_{\mathrm{bath}}$ and the coupling interactions by λH_{int}. The observable of choice is the magnetization in the z direction of the system spin, i.e., $A = S_{\mathrm{sys}}^z$. For a numerical analysis of such an example, see Ref. [8]. We consider the

simple case of a product initial state, where the system is maximally aligned with the magnetic field and the bath is in an infinite-temperature state, i.e., $\rho = (S^z_{\mathrm{sys}} + 1_{\mathrm{sys}}/2) \otimes 1_{\mathrm{bath}}/d_{\mathrm{bath}}$. According to Ref. [1] [Sec. V, Eq. (29)], this case entails $Q \leq 2$. Furthermore, we obtain

$$\langle S^z_{\mathrm{sys}}(t)\rangle = \mathrm{Tr}\{S^z_{\mathrm{sys}}(t)\rho\} = \mathrm{Tr}\{S^z_{\mathrm{sys}}(t)S^z_{\mathrm{sys}}\} \quad (18)$$

for the dynamics of the observable $\langle S^z_{\mathrm{sys}}(t)\rangle$, which may be rewritten as

$$\langle S^z_{\mathrm{sys}}(t)\rangle = \sum_{j,k} |\langle j|S^z_{\mathrm{sys}}|k\rangle|^2 e^{\mathrm{i}(E_j - E_k)t}. \quad (19)$$

Now, consider the distribution p_{jk} as defined in Eq. (1) for the given setting:

$$p_{jk} \propto |\langle j|S^z_{\mathrm{sys}}|k\rangle^2| = |\langle j|S^z_{\mathrm{sys}}|k\rangle|^2 \quad \text{for } j \neq k. \quad (20)$$

For nonintegrable systems, the eigenstate thermalization hypothesis is expected to hold, yielding $|\langle j|S^z_{\mathrm{sys}}|j\rangle|^2 \approx 0$. Exploiting this case, the insertion of Eq. (20) into Eq. (19) yields

$$\langle S^z_{\mathrm{sys}}(t)\rangle \propto \sum_{j,k} p_{jk} e^{\mathrm{i}(E_j - E_k)t}. \quad (21)$$

To the extent that p_{jk} may indeed be replaced by a smooth probability density as discussed around Eq. (2), Eq. (21) may be rewritten as

$$\langle S^z_{\mathrm{sys}}(t)\rangle \propto \int w(G) e^{\mathrm{i}Gt} \mathrm{d}G. \quad (22)$$

Thus, for the present example, $w(G)$ is essentially the Fourier transform of the observable dynamics $\langle S^z_{\mathrm{sys}}(t)\rangle$. If the expectation value $\langle S^z_{\mathrm{sys}}(t)\rangle$ decays strictly exponentially, i.e., if Eq. (6) strictly applies, $w(G)$ would be strictly Lorentzian. While a Lorentzian distribution is clearly unimodal with one well-behaved maximum, its variance diverges. Consequently, a, as defined in Eq. (3), would diverge as well. This is the third main result of the Comment at hand. A strict mathematical divergence of a is only hindered by the small deviations of the true dynamics in a finite system from Eq. (6). These deviations are captured by the aforementioned Zeno time. As is well known, Zeno times may become arbitrarily small in systems with arbitrarily broad energy spectra [4]. Thus, a may indeed become arbitrarily large, i.e., $a \nsim 1$. In many standard scenarios, rather large a may be expected if the coupling is sufficiently weak and the baths are large. For a numerical illustration of this statement, see Ref. [8].

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