Relaxation Theory for Perturbed Many-Body Quantum Systems versus Numerics and Experiment

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An analytical prediction is established of how an isolated many-body quantum system relaxes towards its thermal longtime limit under the action of a time-independent perturbation, but still remaining sufficiently close to a reference case whose temporal relaxation is known. This is achieved within the conceptual framework of a typicality approach by showing and exploiting that the time-dependent expectation values behave very similarly for most members of a suitably chosen ensemble of perturbations. The predictions are validated by comparison with various numerical and experimental results from the literature.

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The long-standing task to adequately explain the time-dependent relaxation and ultimate equilibration of isolated many-body quantum systems has recently witnessed a veritable renaissance, driven, among others, by very impressive new experimental and numerical capabilities [1–4]. On the other hand, quantitative analytical interpretations of the so-acquired data are still rather scarce. For instance, a paradigmatic setup for probing the temporal relaxation behavior of strongly correlated cold atoms was originally proposed in the numerical works [5,6] and then experimentally explored in Ref. [7], concluding that "the exact origin of this enhanced relaxation in the presence of strong correlations constitutes one of the major open problems posed by the results presented here" [8]. The main objective of our Letter is to better understand several such experimental and numerical findings by considering model Hamiltonians of the form

$$H = H_0 + \lambda V, \tag{1}$$

and asking how the temporal relaxation of the reference system H_0 is altered by a small perturbation λV.

Setting.—Given a (pure or mixed) initial state $\rho(0)$, the system (1) evolves in time as $\rho(t) = e^{-iHt}\rho(0)e^{iHt}$ ($\hbar = 1$), resulting in expectation values $\langle A\rangle_{\rho(t)} := \mathrm{Tr}\{\rho(t)A\}$ of an observable (self-adjoint operator) A. Of foremost interest to us are the deviations of those $\langle A\rangle_{\rho(t)}$ from the corresponding expectation values $\langle A\rangle_{\rho_0(t)}$ when the same initial state $\rho(0)$ evolves according to the unperturbed Hamiltonian H_0 in Eq. (1).

Denoting by E_n and $|n\rangle$ the eigenvalues and eigenvectors of H, we assume as usual [1–4] that only energies E_n within a macroscopically small but microscopically large interval $I := [E, E+\Delta]$ entail non-negligible level populations $\langle n|\rho(0)|n\rangle$. Put differently, the system must exhibit a macroscopically well-defined energy, while the number of $E_n \in I$ is still exponentially large in the degrees of freedom [9,10], and the mean level spacing ε is approximately constant throughout I [1–4]. Very low system energies (close to the ground state) are incompatible with these requirements and are thus tacitly excluded. Finally, ε is assumed to be (practically) independent of the perturbation strengths λ considered in Eq. (1). Since the level density $1/\varepsilon$ is—according to the textbook microcanonical formalism—directly connected to the system's thermodynamics, we thus concentrate on sufficiently weak perturbations in the sense that phase transitions or other significant changes of the thermal equilibrium properties are ruled out.

Next we adopt the common idea of statistical mechanics that the system's many-body character inevitably implies some uncertainties about the microscopic details. Hence, we temporarily consider an entire class of similar perturbations instead of one particular V in Eq. (1). More precisely, denoting by $V^0_{\mu\nu} := {}_0\langle\mu|V|\nu\rangle_0$ the matrix elements of V in the eigenbasis $|\nu\rangle_0$ of H_0, we choose an ensemble of matrices whose statistics still reflects the essential properties of the "true" perturbation V in Eq. (1) as closely as possible. For instance, if H_0 models noninteracting particles and V some few-body interactions, the true matrix $V^0_{\mu\nu}$ is known to be sparse (most entries are zero) [11–14]. Similarly, the true perturbation may give rise to a so-called banded matrix [14–18]. Accordingly, it is appropriate to work with a possibly (but not necessarily) sparse and/or banded random matrix ensemble.

Denoting ensemble averages by $[\cdots]_V$, the $V^0_{\mu\nu}$'s are considered as unbiased and—apart from $V^0_{\nu\mu} = (V^0_{\mu\nu})^*$—independent random variables, with second moments

$$[|V^0_{\mu\nu}|^2]_V = \sigma_v^2 F(|\mu-\nu|), \tag{2}$$

where the "band profile" $F(n)$ approaches unity for small n, and σ_v^2 sets the overall scale. Moreover, $F(n)$ is usually a slowly varying function of n and upper bounded by a constant of order unity. In particular, the matrices $V^0_{\mu\nu}$ may still be sparse, while $B := \sum_{n=1}^{\infty} F(n)$ characterizes the bandwidth if the matrix is banded, and $B = \infty$ otherwise. A more detailed discussion is provided in Ref. [19].

Results.—Our main result is the following analytical prediction of how the unperturbed behavior $\langle A\rangle_{\rho_0(t)}$ is modified by a typical perturbation, i.e., for the vast majority of V's from a given ensemble,

$$\langle A\rangle_{\rho(t)} = \langle A\rangle_{\mathrm{mc}} + |g(t)|^2\{\langle A\rangle_{\rho_0(t)} - \langle A\rangle_{\mathrm{mc}}\}. \tag{3}$$

Here $\langle A\rangle_{\mathrm{mc}}$ is the microcanonical expectation value corresponding to the energy window I, and $g(t)$ depends on the mean level spacing ε, the coupling λ, and the properties of the random matrix ensemble from Eq. (2). In particular, for sufficiently weak perturbations we find that

$$g(t) = \exp\{-\Gamma t/2\}, \qquad \Gamma := 2\pi\lambda^2\sigma_v^2/\varepsilon, \tag{4}$$

where "sufficiently weak" means—besides the requirements in the section "Setting"—that $\Gamma \ll \varepsilon B$. Likewise, we find that

$$g(t) = 2J_1(\gamma t)/\gamma t, \qquad \gamma := \sqrt{8B}\lambda\sigma_v, \tag{5}$$

for $\gamma \gg \varepsilon B$ ("sufficiently strong" perturbations), where $J_\nu(x)$ are Bessel functions of the first kind. In between, $g(t)$ exhibit as transition from Eq. (4) to Eq. (5) as detailed in Ref. [19].

Before turning to their derivation, we further discuss and exemplify those results (3)–(5): So far, these are predictions regarding the vast majority of a given V ensemble. As usual in random matrix theory [10,11,13–16], one thus expects that the true (nonrandom) perturbation V in Eq. (1) belongs to that vast majority, provided its main properties are well captured by the considered ensemble. Note that the microscopic dynamics of a many-body system is commonly expected to be extremely sensitive against perturbations (chaotic [37]), so that it is virtually impossible to theoretically predict its response exactly or in terms of well-controlled approximations [38]. Hence, some kind of "uncontrolled" approximation is practically unavoidable. One of them is random matrix theory, which in fact has been originally devised by Wigner for the very purpose of exploring chaotic quantum many-body systems, and is by now widely recognized as a remarkably effective tool in this context [37]. Another common justification is by comparison with particular examples, to which we now turn. These will be state-of-the-art numerical and experimental results from previous publications, which, however, do not contain the corresponding (numerical) data for the variances required in Eq. (2). We will thus concentrate on the weak perturbations regime, where Eq. (4) applies. Again, the quantitative values of σ_v^2/ε required in Eq. (4) can, in principle, be computed, but have not been provided in those publications, and will therefore be treated as fit parameters.

Examples.—Our first example is the numerical exploration by Flesch *et al.* [6] (see also Ref. [5]) of the bosonic Hubbard chain

$$H := -J\sum_{i=1}^{L}(\hat{b}_{i+1}^\dagger\hat{b}_i + \hat{b}_i^\dagger\hat{b}_{i+1}) + \frac{U}{2}\sum_{i=1}^{L}\hat{n}_i(\hat{n}_i - 1), \tag{6}$$

with periodic boundary conditions, creation (annihilation) operators $\hat{b}_i^\dagger$ ($\hat{b}_i$), and $\hat{n}_i := \hat{b}_i^\dagger\hat{b}_i$. For the initial state $\rho(0)$ considered in Ref. [6] and Fig. 1, the model (6) can be recast as an effective spin-1/2 chain by means of a mapping that becomes asymptotically exact for large interaction parameters U [39]. In the limit $U \to \infty$, the so-obtained "unperturbed" effective Hamiltonian H_0 amounts to an XX model. The leading finite-U correction takes the form $U^{-1}H_1$, where H_1 contains nearest neighbor, next-nearest neighbor, as well as three-spin terms [39]. In other words, H_1 plays the role of the perturbation V in Eq. (1), and $1/U$ that of λ. Since $\langle A\rangle_{\rho_0(t)}$ and $\langle A\rangle_{\mathrm{mc}}$ are known (see Ref. [6] and Fig. 1), the only missing quantity is σ_v^2/ε in Eq. (4), which is, as mentioned above, not provided by Ref. [6], and hence treated as a fit parameter, yielding $\Gamma = 4.98\lambda^2$. The resulting agreement with the numerics in Fig. 1 speaks for itself.

An experimental realization of Eq. (6) by a strongly correlated Bose gas has been explored by Trotzky *et al.* in Ref. [7] and is compared in Fig. 2 with our theory Eqs. (3), (4). Adopting $\Gamma = 4.98\lambda^2$ from before, this amounts to an entirely analytic prediction without any fit

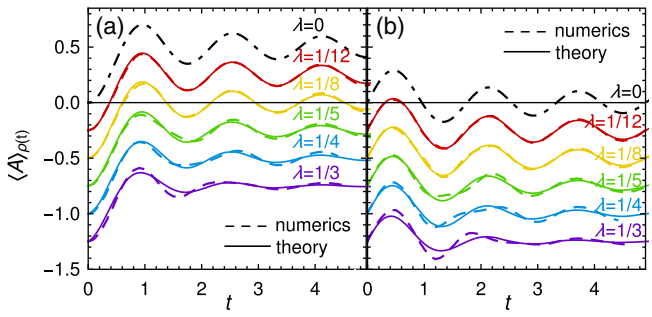

FIG. 1. Bosonic Hubbard chain. Dashed lines: Numerical results from Ref. [6] for the Hubbard model (6) with $L = 32$, $J = 1$, and various $\lambda := 1/U$, vertically shifted in steps of -0.25 for better visibility. The initial state consists of singly occupied even and empty odd sites. The observables are $A := \hat{n}_1$ in (a) and $A := (\hat{b}_1^\dagger\hat{b}_2 - \hat{b}_2^\dagger\hat{b}_1)/2i$ in (b), implying $\langle A\rangle_{\mathrm{mc}} = 1/2$ in (a) and $\langle A\rangle_{\mathrm{mc}} = 0$ in (b). Dash-dotted lines: Unperturbed analytical solutions $\langle A\rangle_{\rho_0(t)} = [1 - J_0(4t)]/2$ in (a) and $\langle A\rangle_{\rho_0(t)} = J_1(4t)/2$ in (b) [6]. Solid lines: Eqs. (3), (4) with $\Gamma = 4.98\lambda^2$.

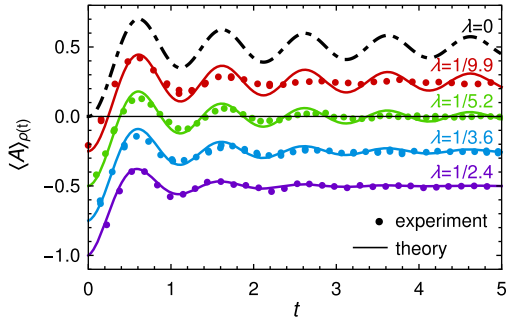

FIG. 2. Cold atom experiments. Dots: Experimental data for repulsively interacting Rb atoms in a 1D optical superlattice, adopted from Fig. 2 in Ref. [7]. Initial condition, observable, and dynamics experimentally emulate the theoretical ones from Fig. 1(a). All further details (dash-dotted and solid lines, vertical shifts) are as in Fig. 1.

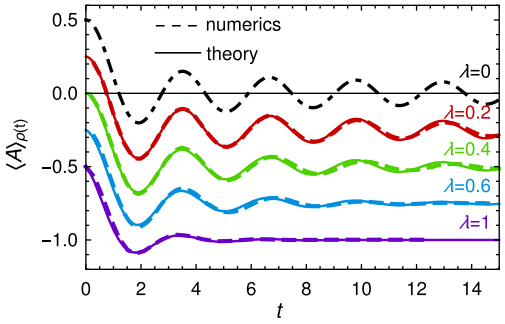

FIG. 3. Spin-1/2 XXZ model of the form (1) with $H_0 := \sum_{i=1}^{L-1}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$, $V := \sum_{i=1}^{L-1} S_i^z S_{i+1}^z$, observable $A := \sum_{i=1}^{L}(-1)^i S_i^z/L$, and Néel initial state (see Ref. [40] for more details). Dashed lines: Numerical results from Ref. [40] for different λ, vertically shifted in steps of -0.25. Dash-dotted line: Unperturbed analytical solution $\langle A\rangle_{\rho_0(t)} = J_0(2t)/2$ [40]. Solid lines: Eqs. (3), (4) with $\langle A\rangle_{\mathrm{mc}} = 0$, and $\Gamma = 0.46\lambda^2$.

parameter. Incidentally, the agreement in Fig. 2 improves as λ increases. The same tendency is recovered when comparing the numerical results from Fig. 1(a) with the experimental data, suggesting that the model (6) itself may not capture all experimentally relevant details for large U (small λ).

Next we turn to the spin-1/2 XXZ chain with anisotropy parameter λ as specified in Fig. 3, exhibiting a gapless "Luttinger liquid" and a gapped, Ising-ordered antiferromagnetic phase for $\lambda \leq 1$ and $\lambda > 1$, respectively [40]. Similarly as before, σ_v^2/ε in Eq. (4) is unknown and hence treated as a fit parameter. The analytics in Fig. 3 explains the numerics by Barmettler *et al.* from Ref. [40] remarkably well all the way up to the critical point at $\lambda = 1$.

Our last example in Fig. 4 is a model of hard-core bosons, numerically explored by Mallayya *et al.* in Ref. [41], and exhibiting so-called prethermalization [3,42,43] for small λ. Treating σ_v^2/ε again as a fit parameter, our theory also explains very well such a prethermalization scenario.

For lack of space, further examples have been moved to the Supplemental Material [19], namely, the fermionic systems from Refs. [44,45] and a case in which $g(t)$ exhibits a crossover from Eqs. (4) to (5) without any fit parameters. Moreover, a scaling behavior $\Gamma \propto \lambda^2$ as in Eq. (4) has also been reported, among others, in Refs. [3,46–49].

Derivation.—Adopting the notation as introduced below Eq. (1), one readily confirms that

$$\langle A\rangle_{\rho(t)} = \sum_{m,n} e^{i(E_n - E_m)t}\rho_{mn}(0)A_{nm}, \tag{7}$$

where $\rho_{mn}(t) := \langle m|\rho(t)|n\rangle$ and $A_{nm} := \langle n|A|m\rangle$. Given that in Eq. (7) only levels $E_n \in I$ actually matter (see Sec. Setting), and that their spacings $E_{n+1} - E_n$ generically exhibit a Poisson- or Wigner-Dyson-like statistics [37] of mean value ε, the random fluctuations of those $E_{n+1} - E_n$ will also be of order ε and (practically) uncorrelated. Hence, the $E_n - E_m$ exhibit typical deviations from their mean value $(n-m)\varepsilon$ of order $|n-m|^{1/2}\varepsilon$. Recalling that ε is exponentially small [9,10] and $|n-m|\varepsilon \simeq |E_n - E_m| \leq \Delta$, it is reasonable to expect—and justified in more detail in Ref. [19]—that the deviations between $(E_n - E_m)t$ and $(n-m)\varepsilon t$ are negligible in Eq. (7) for all t of later relevance. Employing this approximation and the unitary basis transformation

$$U_{m\nu} := \langle m|\nu\rangle_0 \tag{8}$$

we rewrite Eq. (7) in terms of the unperturbed basis $|\nu\rangle_0$ as

$$\langle A\rangle_{\rho(t)} = \sum_{\mu_1,\mu_2,\nu_1,\nu_2} \rho^0_{\mu_1\nu_2}(0)A^0_{\mu_2\nu_1}W^{\mu_1\mu_2}_{\nu_1\nu_2}(t), \tag{9}$$

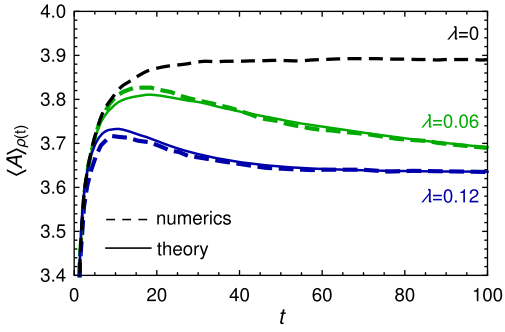

FIG. 4. Hard-core boson model of the form (1) with $H_0 := \sum_i[-\hat{b}_i^\dagger(\hat{b}_{i+1} + 0.7\hat{b}_{i+2}) + \mathrm{H.c.} + (\hat{n}_i - \frac{1}{2})(\hat{n}_{i+1} + 0.7\hat{n}_{i+2} - 0.85)]$ and $V := \sum_i[\hat{b}_i + \frac{1}{2}(\hat{b}_i - b_i^\dagger)\hat{b}_{i+1} + \mathrm{H.c.}]$ [see also Eq. (6) and Ref. [41]]. The initial state is thermal with respect to $H_I := H_0 + \frac{1}{2}\sum_i[\hat{b}_i^\dagger\hat{b}_{i+1} + \mathrm{H.c.} + (\hat{n}_i - \frac{1}{2})(\hat{n}_{i+1} - \frac{1}{2})]$, and the observable is $A := \frac{1}{L}\sum_i[\hat{b}_i^\dagger\hat{b}_{i+1} + \mathrm{H.c.}]$. Dashed lines: Numerical results from Ref. [41] for different λ. Solid lines: Eqs. (3), (4) using the dashed line for $\lambda = 0$ as $\langle A\rangle_{\rho_0(t)}$, the numerical values for $\langle A\rangle_{\mathrm{mc}}$ quoted in Ref. [41], and $\Gamma = 4.2\lambda^2$.

$$W^{\mu_1\mu_2}_{\nu_1\nu_2}(t) \coloneqq \sum_{m,n} e^{i(n-m)\varepsilon t} U_{m\mu_1} U_{n\mu_2} U^*_{m\nu_1} U^*_{n\nu_2}, \quad (10)$$

where $\rho^0_{\mu\nu}(0) \coloneqq {}_0\langle\mu|\rho(0)|\nu\rangle_0$, and $A^0_{\nu\mu} \coloneqq {}_0\langle\nu|A|\mu\rangle_0$.

The randomness of V [see above Eq. (2)] is inherited via Eq. (1) by the eigenvector overlaps $U_{m\nu}$ in Eq. (8). A particularly important role is played by their second moments, $[|U_{m\nu}|^2]_V$, which due to Eq. (2) only depend on $m-\nu$,

$$[|U_{m\nu}|^2]_V =: u(m-\nu). \quad (11)$$

Specifically, the function $g(t)$ from Eq. (3) is defined as their Fourier transform,

$$g(t) \coloneqq \sum_n e^{in\varepsilon t} u(n). \quad (12)$$

As a first basic result of our present work, we show in Ref. [19] that the function $u(n)$ itself follows as $(\varepsilon/\pi)\lim_{\eta\to 0+}\mathrm{Im}G(n\varepsilon - i\eta)$ from the ensemble-averaged (scalar) resolvent or Green's function $G(z)$ of H, which in turn can be obtained as the solution of

$$G(z)[z - \lambda^2\sigma_v^2\varepsilon^{-1}\int G(z-E)F(|E|/\varepsilon)dE] = 1. \quad (13)$$

Along these lines one readily recovers [19] for weak perturbations as specified below Eq. (4) the previously known Breit-Wigner distribution [14–16]

$$u(n) = \frac{1}{2\pi}\frac{\Gamma/\varepsilon}{(\Gamma/2\varepsilon)^2 + n^2}, \quad (14)$$

with Γ from Eq. (4), and provided that $\delta \coloneqq \varepsilon/\Gamma \ll 1$. Our next goal is to evaluate the ensemble-averaged time evolution (9), hence we need the average of four $U_{m\nu}$'s in Eq. (10). The solution of this technically quite challenging problem by means of supersymmetry methods [37,50,51] is provided in the Supplemental Material [19]. There, we also establish that δ is indeed exponentially small in the system's degrees of freedom f,

$$\delta \approx \exp\{-\mathcal{O}(f)\} \ll 1. \quad (15)$$

Introducing those averages of four $U_{m\nu}$'s into Eqs. (9) and (10) finally yields

$$[\langle A\rangle_{\rho(t)}]_V = \langle A\rangle_{\tilde\rho} + |g(t)|^2\{\langle A\rangle_{\rho_0(t)} - \langle A\rangle_{\tilde\rho}\} + R(t). \quad (16)$$

Here, $\tilde\rho$ is defined via ${}_0\langle\mu|\tilde\rho|\nu\rangle_0 \coloneqq \delta_{\mu\nu}\sum_\kappa \tilde u(\nu-\kappa)\rho^0_{\kappa\kappa}(0)$ with $\tilde u(n) \coloneqq \sum_m u(n-m)u(m)$, essentially amounting to a "washed-out" descendant of the so-called diagonal ensemble [longtime average of $\rho_0(t)$] [1–3]. Following Deutsch [16], $\langle A\rangle_{\tilde\rho}$ is thus commonly considered [1,52,53] to closely approximate the microcanonical expectation value $\langle A\rangle_{\mathrm{mc}}$ [see below Eq. (3)]. Furthermore, we can infer from Eqs. (12), (14), and (15) that $g(t) \simeq \int e^{in\varepsilon t}u(n)\mathrm{d}n = e^{-\Gamma|t|/2}$, i.e., we recover Eq. (4). Finally, the last term in Eq. (16) is given by

$$R(t) \coloneqq \sum_{\mu,\nu}\rho^0_{\mu\mu}(0)A^0_{\nu\nu}r(|t|,\mu-\nu), \quad (17)$$

$$r(t,n) \coloneqq e^{-\Gamma t}\tilde u(n)\left\{1 - \cos(tn\varepsilon) - \frac{\Gamma\sin(tn\varepsilon)}{n\varepsilon}\right\}. \quad (18)$$

Because of similar arguments as in the above approximation $\langle A\rangle_{\tilde\rho} \simeq \langle A\rangle_{\mathrm{mc}}$, this term is usually negligibly small. For example, if the unperturbed system satisfies the eigenstate thermalization hypothesis (ETH), the $A^0_{\nu\nu}$ are well approximated by $\langle A\rangle_{\mathrm{mc}}$ [2,16,54,55]. Observing that $\sum_n r(t,n) \simeq \int r(t,n)dn = 0$ then immediately implies $R(t) \simeq 0$. However, similar cancellations so that $R(t) \simeq 0$ can be shown to persist under much more general conditions [56] (some ETH violating examples are also provided above and in Ref. [19]). Altogether, we thus obtain

$$[\langle A\rangle_{\rho(t)}]_V = \langle A\rangle_{\mathrm{mc}} + |g(t)|^2\{\langle A\rangle_{\rho_0(t)} - \langle A\rangle_{\mathrm{mc}}\}; \quad (19)$$

see also Refs. [3,13,57–64] for somewhat similar findings.

The advantage of Eq. (19) over Eq. (16) is that $\langle A\rangle_{\tilde\rho}$ and $R(t)$ are often hard to determine in concrete examples. For the rest—especially if the above approximations leading to Eq. (19) might not apply—one also could continue to employ Eq. (16) (for an example, see Sec. I B in Ref. [19]).

So far, we focused on sufficiently weak perturbations as specified below Eq. (4). Beyond this regime, the solution $G(z)$ of Eq. (13) and hence $g(t)$ from Eq. (12) will be different, yet we still recovered [19] the same final conclusion as in Eq. (19). In particular, for "sufficiently strong" perturbations as specified below Eq. (5) one finds [14,15,19] that $u(n)$ approaches a semicircular distribution with radius γ/ε and hence one recovers Eq. (5), while in the intermediate regime, $g(t)$ can still be readily obtained by solving Eq. (13) numerically.

Our final objective is to quantify the fluctuations $\xi_V(t) \coloneqq \langle A\rangle_{\rho(t)} - [\langle A\rangle_{\rho(t)}]_V$ about the average behavior in terms of the variance $[\xi^2_V(t)]_V$. In view of Eqs. (9) and (10), averages over eight $U_{m\nu}$'s are thus required. Referring to Ref. [19] for their quite tedious evaluation, we finally obtain the estimate

$$[\xi^2_V(t)]_V \le c\delta\|A\|^2, \quad (20)$$

where $\|A\|$ indicates the operator norm and c is some positive real number, which does not depend on any further details of the considered system and is at most on the order of 10^3. Exploiting Chebyshev's inequality, the probability

that $|\xi_V(t)| \leq \delta^{1/3}\|A\|$ when randomly sampling V's from the ensemble can thus be lower bounded by $1-\delta^{1/3}c$. In view of Eq. (15), the deviations from the average behavior (19) are thus negligibly small for most V's and any preset t. Moreover, one can show similarly as in Ref. [65] that for most V's the deviations $\xi_V(t)$ must be negligibly small not only for any given t, but even for the vast majority of all t within any given time interval $[t_1, t_2]$. Overall, we thus recover our main result from Eq. (3).

Conclusions.—We derived an analytical prediction for the ensemble-averaged, time-dependent deviations of the perturbed from the unperturbed expectation values in isolated many-body quantum systems. Moreover, we showed that nearly all members of the ensemble behave very similarly to the average. Provided the ensemble has been chosen appropriately, the same behavior is thus typically expected to also apply when dealing with a specific physical model, resulting in our main analytical prediction (3). As a validation, we demonstrated good agreement with a variety of numerical and experimental findings from the literature. Technically speaking, substantial extensions of previously established, nonperturbative supersymmetry methods were indispensable to arrive at those results [19]. Related analytical [14,66] and numerical [63] studies suggest that such methods may in the future even be further extended to considerably more general ensembles than those we admitted here. On the conceptual side, a better understanding of when a given physical system is *not* a typical member of any permitted ensemble [62,67,68] remains as yet another important issue for further studies.

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[19] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.124.120602, which includes Refs. [20–36], for additional numerical examples and for further details regarding the V ensembles in Eq. (2) and the calculations outlined in "Derivation."
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