Letter

Entropy of the quantum work distribution

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The statistics of work done on a quantum system can be quantified by the two-point measurement scheme. We show how the Shannon entropy of the work distribution admits a general upper bound depending on the initial diagonal entropy, and a purely quantum term associated to the relative entropy of coherence. We demonstrate that this approach captures strong signatures of the underlying physics in a diverse range of settings. In particular, we carry out a detailed study of the Aubry-André-Harper model and show that the entropy of the work distribution conveys very clearly the physics of the localization transition, which is not apparent from the statistical moments.

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Introduction. Work in a quantum mechanical setting has proven to be a difficult concept to define [1], with several approaches developed [2–7]. Among them the two-point measurement (TPM) approach [8] has received significant attention: it recovers important results from stochastic thermodynamics [9,10], can be measured experimentally [11,12], and naturally connects with other areas, such as out-of-time-order correlators [13], information scrambling [14,15], Kibble-Zurek scaling [16,17], and many-body physics [18]. Often the focus is on cumulants of work (in particular, the mean and variance) rather than the full distribution. While in several contexts this is warranted, particularly when the underlying distribution tends to a Gaussian [19], several recent works have highlighted that studying the full distribution can reveal nontrivial features of the dynamics that, while perhaps present in the statistical cumulants, are nevertheless obfuscated [19,20].

Recently, it has been shown that coherence plays a subtle role in establishing a proper thermodynamic framework [21–24]. Indeed, quantum coherences present a viable source of useful work [25] and, as such, there is an intrinsic thermodynamic cost associated with their creation [26,27]. However, while potentially useful, the presence or creation of coherence when a system is driven out of equilibrium can lead to significant fluctuations [28]. A more careful analysis of such nonequilibrium dynamics reveals that one can identify uniquely quantum aspects in the thermodynamics of quantum systems, in particular, by splitting the irreversible work into distinct coherent and incoherent contributions [29,30]. While these, and related studies [18], have focused on the moments, it is intuitive that the full distribution should encapsulate and extend these insights.

We rigorously demonstrate the veracity of this intuition through the entropy H_W of the work distribution, which serves as a measure of its underlying complexity. This measure has been applied to the distribution of entropy production [31]. We derive a general and saturable bound on H_W that consists of two distinct contributions: one which stems from the diagonal ensemble and, in suitable limits, corresponds simply to the Gibbs equilibrium entropy, and a second term which is purely quantum in nature, related to the coherence established by the driving protocol and given by the relative entropy of coherence (REC). We first illustrate the utility of our results in the Landau-Zener model, which reveals that the entropy of the distribution succinctly captures the salient features of the model around the avoided crossing, features which are completely absent in the moments. We then carry out a detailed analysis of work fluctuations in the Aubry-André-Harper (AAH) model, a paradigmatic model for studying localization. We show that H_W is related to a modified inverse participation ratio (IPR) and provides a remarkably sensitive indicator of the localization transition.

Entropy of the work distribution. We consider a system, prepared in a generic state ρ and with initial Hamiltonian $\mathcal{H}_i = \sum_n E_n^i |n_i\rangle\langle n_i|$, that is driven according to a work protocol, which changes the state to $\rho' = U\rho U^\dagger$. The unitary U depends on the details of the protocol and its duration. The Hamiltonian at the end of the process is $\mathcal{H}_f = \sum_m E_m^f |m_f\rangle\langle m_f|$. The TPM consists of measuring in the bases of $\mathcal{H}_i$ and $\mathcal{H}_f$ before and after the unitary [8]. The probability that a certain amount of work, W, is injected or extracted is given by

$$P(W) = \sum_{n,m} p_n p_{m|n} \delta_{W, E_m^f - E_n^i}, \tag{1}$$

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where $p_n = \langle n_i|\rho|n_i\rangle$ is the initial state distribution and $p_{m|n} = |\langle m_f|U|n_i\rangle|^2$ are the transition probabilities. The support of $P(W)$ corresponds to all possible *Bohr (transition) frequencies* $E_m^f - E_n^i$ between the initial and final energy levels. We assume these form a discrete (possibly infinite) set. Note how in Eq. (1) they are collected in different pairs (n, m) which give rise to the same value of W.

The work distribution can be very complex, so one often focuses on summary statistics, such as the moments $\langle W^n\rangle = \sum_W W^n P(W)$ or cumulants. Here, we shift focus to another summary statistic, namely, the entropy of $P(W)$ [32],

$$H_W = -\sum_W P(W)\ln P(W), \tag{2}$$

which characterizes the complexity of $P(W)$. It is zero when the work is deterministic and can range up to $\ln N^2$ when $P(W)$ is uniform.

H_W is in general different from

$$H_{\rm u} = -\sum_{n,m} p_n p_{m|n} \ln p_n p_{m|n}, \tag{3}$$

which is the entropy of the *uncollected* distribution $p_n p_{m|n}$. We first quantify the relation between H_W and $H_{\rm u}$. Let $\gamma_{\max}$ denote the maximal degeneracy of the Bohr frequencies ($\gamma_{\max} \geqslant g_i g_f$, where $g_{i(f)}$ are the degeneracies of $\mathcal{H}_{i(f)}$). Then [33]

$$H_{\rm u} - \ln\gamma_{\max} \leqslant H_W \leqslant H_{\rm u}, \tag{4}$$

with equality if the values of work are all nondegenerate. We now show that $H_{\rm u}$ directly quantifies the degree of quantum coherence generated in the process. The REC [34] of a state σ in the basis $|m_f'\rangle = U^\dagger|m_f\rangle$ is

$$C(\sigma) = S(D_f(\sigma)) - S(\sigma) \geqslant 0, \tag{5}$$

where $S(\sigma) = -\mathrm{tr}\,\sigma\ln\sigma$ is the von-Neumann entropy and $D_f(\sigma) = \sum_m \langle m_f'|\sigma|m_f'\rangle|m_f'\rangle\langle m_f'|$ is the full dephasing operation in the basis $|m_f'\rangle$. It follows that $-\sum_m p_{m|n}\ln p_{m|n} = C(|n_i\rangle\langle n_i|)$, so Eq. (3) can be written as

$$H_{\rm u} = S(\bar\rho) + \sum_n p_n C(|n_i\rangle\langle n_i|), \tag{6}$$

where $\bar\rho = \sum_n \langle n_i|\rho|n_i\rangle|n_i\rangle\langle n_i|$ is the initial state dephased in the basis of $\mathcal{H}_i$.

Equation (6) summarizes the rich physics behind the entropy of the work distribution. The first term is the entropy of the initial outcomes p_n of the TPM, i.e., the entropy of the so-called diagonal ensemble [35–39]. If $[\rho, \mathcal{H}_i] = 0$, it reduces to the von Neumann entropy of ρ and if $\rho = e^{-\beta\mathcal{H}_i}/Z_i$ is a thermal state, it reduces to the Gibbs thermal entropy. If $\rho = |k_i\rangle\langle k_i|$ is any eigenstate of $\mathcal{H}_i$, $S(\bar\rho)$ vanishes and Eq. (6) reduces to $H_{\rm u} = C(|k_i\rangle\langle k_i|)$. The second term in Eq. (6) establishes that the relevant coherences are those of each $|n_i\rangle$ in the eigenbasis $|m_f'\rangle$. Therefore, this term contains information on both the dynamics (work protocol) and of how $\mathcal{H}_f$ differs from $\mathcal{H}_i$. The process is incoherent if $p_{m|n} = |\langle m_f|U|n_i\rangle|^2 = \delta_{m,n}$, which occurs when $[\mathcal{H}_i, U^\dagger\mathcal{H}_f U] = 0$. In this case, Eq. (6) reduces to $H_{\rm u} = S(\bar\rho)$.

We can take this a step further. Using the concavity of the von Neumann entropy, we can write $\sum_n p_n C(|n_i\rangle\langle n_i|) \leqslant S(D_f(\bar\rho)) = C(\bar\rho) + S(\bar\rho)$, which leads to

$$H_{\rm u} \leqslant 2S(\bar\rho) + C(\bar\rho). \tag{7}$$

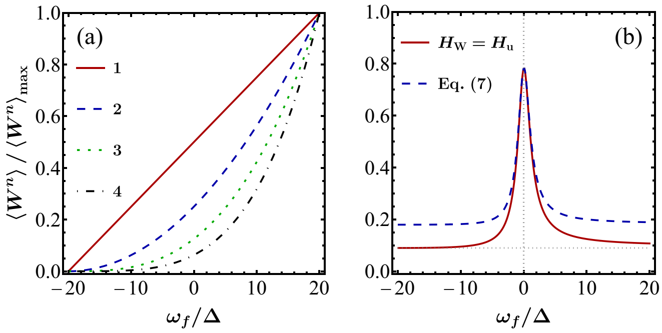

FIG. 1. Work fluctuations in the Landau-Zener model under a sudden quench. (a) First four moments $\langle W^n\rangle$ of $P(W)$ as a function of ω_f/Δ (normalized by their maximum value, at $\omega_f = \Delta$). (b) Entropy of the work distribution, Eq. (2) (red, solid), and the corresponding bound (7) (blue, dashed). Parameters: $\beta = 0.1(\hbar\Delta)^{-1}$ and $\omega_i = -20\Delta$.

The tightness of this bound is related to the purity of $\bar\rho$, being saturated when ρ is an eigenstate of $\mathcal{H}_i$ or for thermal states in the zero temperature limit.

Combining Eqs. (4), (6), and (7), we arrive at our main result: the entropy of the work distribution is bounded as

$$H_W \leqslant S(\bar\rho) + \sum_n p_n C(|n_i\rangle\langle n_i|) \leqslant 2S(\bar\rho) + C(\bar\rho). \tag{8}$$

The first inequality is often quite tight and relates H_W to the coherences of each individual transition $C(|n_i\rangle\langle n_i|)$. The second inequality bounds H_W to the full REC of $\bar\rho$ and its tightness is related to the purity of $\bar\rho$. Eq. (8) also allows us to estimate the dependence of H_W with temperature T, in the case of an initial thermal state. Both $S(\bar\rho)$ and the p_n depend on T. However, by convexity,

$$H_W \leqslant S(\bar\rho) + C_{\max}, \tag{9}$$

where $C_{\max} = \max_n C(|n_i\rangle\langle n_i|)$. The last term is now T independent, pushing the temperature dependence solely to the Gibbs thermal entropy. We next turn to the study of H_W in different models and show that it conveys crucial information about the work statistics.

Landau-Zener model. Consider a qubit with $\mathcal{H}_{\rm LZ}(\omega) = \hbar\Delta\sigma_x + \hbar\omega\sigma_z$, where σ_i are the Pauli matrices. This model has an avoided crossing at $\omega_c \equiv 0$, with minimal energy gap $\Delta > 0$. The eigenenergies are $E_0 = -\sqrt{\omega^2+\Delta^2}\hbar$ and $E_1 = \sqrt{\omega^2+\Delta^2}\hbar$. We assume the system starts in a thermal state at inverse temperature β and consider a sudden quench ($U = \mathbb{1}$) from $\mathcal{H}_i = \mathcal{H}_{\rm LZ}(\omega_i)$, with $\omega_i < 0$, to $\mathcal{H}_f = \mathcal{H}_{\rm LZ}(\omega_f)$. There are four allowed values of W, given by $E_{0(1)}(\omega_f) - E_{0(1)}(\omega_i)$. For $\omega_f \neq \pm\omega_i$ and fixed Δ, these will always be nondegenerate and thus $H_W \equiv H_{\rm u}$.

Figure 1(a) shows the first four moments $\langle W^n\rangle$ of $P(W)$, as a function of ω_f/Δ, while Fig. 1(b) shows H_W. Clearly the moments show no obvious evidence of the avoided crossing at $\omega_f = \omega_c$ (the same is true for the cumulants). The entropy H_W, on the other hand, portrays an entirely different picture.

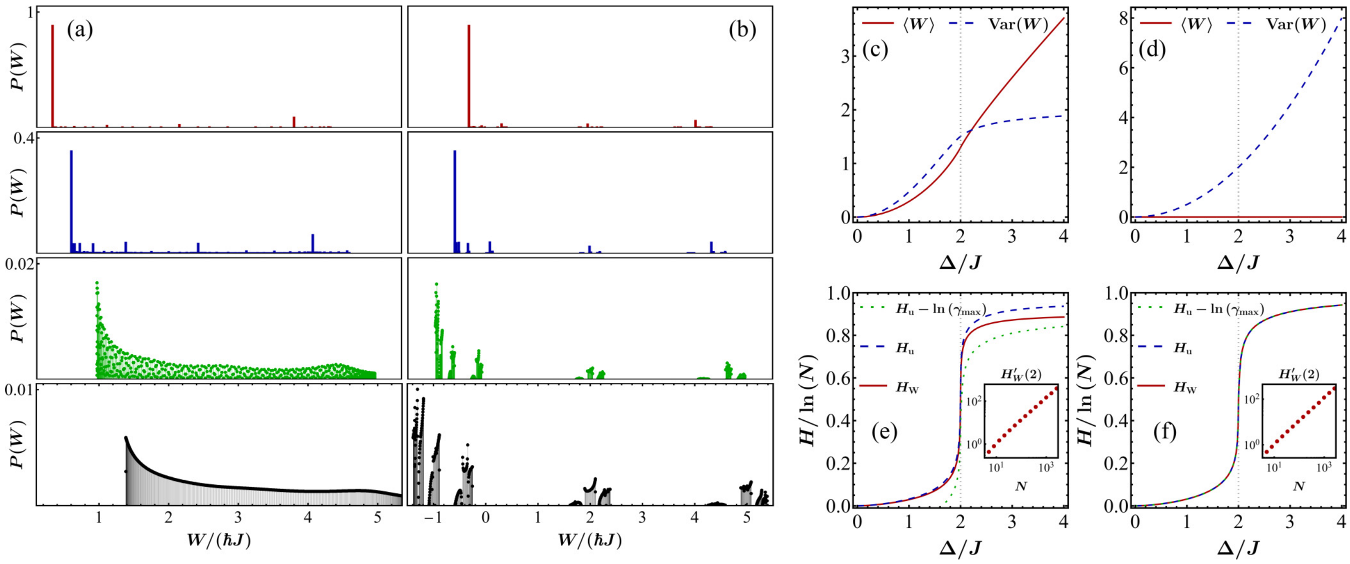

FIG. 2. Work statistics of the AAH model Eq. (10). (a) $P(W)$ for the $\Delta \to 0$ protocol, for $\Delta/J = 1.5, 2, 2.5$, and 3. (b) Similar, but for $0 \to \Delta$. (c), (d) Corresponding mean and variance versus Δ/J, for the two protocols. In (d), $\langle W\rangle \equiv 0$ [33]. (e), (f) H_W vs Δ/J [Eq. (2)] for the two protocols along with the upper and lower bounds derived in Eq. (6). Inset: $dH_W/d\Delta|_{\Delta=2J}$ as a function of a Fibonacci number N, showing that in the thermodynamic limit H_W will change discontinuously at $\Delta/J = 2$. In all simulations, the system starts in the ground state, $N = F_{16} = 987$ and $\eta = 1.2$, except in the insets of (e), (f), which were averaged over 50 values of η.

The first term in Eq. (6) yields a constant base value, as it depends only on the initial condition. The second term, on the other hand, presents a peak at $\omega_f = \omega_c$. By probing H_W we can therefore highlight the avoided crossing, which is the most important feature of the Landau-Zener model, and which is masked in the moments. In Fig. 1(b), we also plot the bound Eq. (7), which becomes tightest around $\omega_f = 0$. This reflects the coherence, which is largest at the avoided crossing.

AAH model. We next turn to a highly nontrivial application of our results. We consider a single particle in a lattice with N sites, labeled by states $|i\rangle$. The Hamiltonian is [40–42]

$$\mathcal{H}_{\rm AAH}(\Delta) = \hbar \sum_{i=1}^{N} [\Delta \cos(2\pi\gamma i + \eta)|i\rangle\langle i| - J(|i\rangle\langle i+1| + |i+1\rangle\langle i|)], \quad (10)$$

with periodic boundary conditions. The first term denotes the on-site potentials, with overall magnitude Δ, phase η, and modulation γ. Following Refs. [42–44], we choose the lattice size N to be a Fibonacci number, F_n, and $\gamma = F_{n-1}/F_n$ to be a rational approximation to the inverse golden ratio [45].

The AAH model undergoes a localization transition at $\Delta = 2J$. For $\Delta < 2J$ all eigenvectors are delocalized in space, while for $\Delta > 2J$, they become localized around specific sites in the lattice. We focus on the work distribution associated with turning the quasiperiodic potential off/on, i.e., in going from $\mathcal{H}_{\rm AAH}(\Delta) \to \mathcal{H}_{\rm AAH}(0)$, and vice versa. We refer to these as $\Delta \to 0$ and $0 \to \Delta$, respectively, and in what follows we focus on sudden quenches ($U = \mathbb{1}$).

Figures 2(a) and 2(b) shows the work distribution Eq. (1) for the two protocols, assuming the system starts in the ground state. The bandwidth of the distribution is discussed in Ref. [33]. For $\Delta \to 0$, $W > 0$, while for $0 \to \Delta$, $W \lessgtr 0$. Thus, work can be extracted by turning the potential on but not by turning it off. The overall behavior of $P(W)$ clearly reflects the localization transition at $\Delta = 2J$. For both protocols, quenches that keep the system in the delocalized phase, i.e., $\Delta < 2J$ [corresponding to the first two upper panels of Figs. 2(a) and 2(b)], result in a $P(W)$ with small support, and mostly concentrated around a minimum work value. In this regime, the work cost of turning the potentials on or off is overall small and fluctuates very little. This is also evidenced in Figs. 2(c) and 2(d), which plots the mean and variance of W, for the two protocols. Conversely, when $\Delta/J > 2$ the support of $P(W)$ increases significantly. For $\Delta \to 0$ [Fig. 2(a)], the distribution reflects the smooth energy spectrum, while for $0 \to \Delta$ [Fig. 2(b)] it is very irregular due to the fractal nature of the localized spectrum.

H_W is plotted in Figs. 2(e) and 2(f). It shows a jump at $\Delta/J = 2$, the sharpness of which depends on the lattice size N. To illustrate this, the insets of Figs. 2(e) and 2(f) show the slope $H'_W(2) := dH_W/d\Delta$, evaluated at $\Delta = 2J$, for different sizes N. A fit of the data reveals the relation, $H'_W(2) \propto \sqrt{N}$, which implies that, in the thermodynamic limit, H_W will change discontinuously at the localization transition. The entropy therefore succinctly captures the criticality of the AAH model. The two bounds in Eq. (4) are also shown in Figs. 2(e) and 2(f). For any $\Delta \neq 0$, the spectrum of the AAH model is nondegenerate. This explains why for $\Delta \to 0$ [Fig. 2(e)] the curves differ from H_W, but for $0 \to \Delta$ [Fig. 2(f)] they coincide: the former depends on the degeneracies of $\mathcal{H}_{\rm AAH}(0)$, leading to $\gamma_{\rm max} = 2$, while the latter does not since we start in the (nondegenerate) ground state.

$H_{\rm u}$ can be connected to a modified IPR, a widely used measure to characterize disordered systems. The conventional IPR of a state $|\psi\rangle$ is defined as $\sum_i |\langle i|\psi\rangle|^4$, where $|i\rangle$ are the position states. Instead, consider the quantity $\mathcal{I} := \sum_m p_{m|0}^2 = \sum_m |\langle m_f|0\rangle|^4$, where 0 indexes the ground state. This is

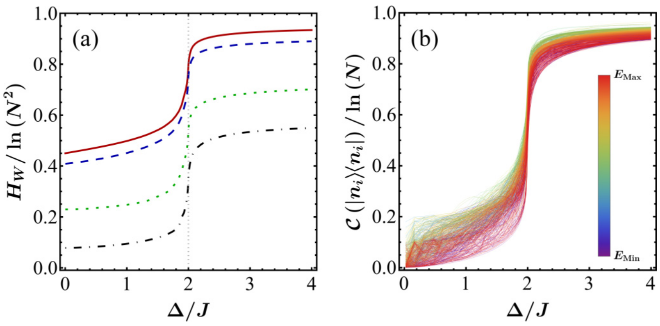

FIG. 3. The entropy of $P(W)$ for (a) initial thermal states with temperatures $J\beta = \{10^{-2}, 10^0, 10^2, 10^4\}$ (red [top], blue, green, black [bottom]) and (b) every eigenstate of the initial Hamiltonian, $\mathcal{H}_{\rm AAH}(0)$. These are all for the $0 \to \Delta$ case but the $\Delta \to 0$ case is very similar. The choice of phase and system size are as in Fig. 2.

known as the inverse of the "effective dimension" [46,47], and represents a type of IPR where $|m_f\rangle$ replaces the position states $|i\rangle$ (they coincide if $\Delta_f \to \infty$). Noticing that $-\ln \mathcal{I}$ is the Rényi-2 entropy of $p_{m|0}$, it then follows that $H_{\rm u} \geqslant -\ln \mathcal{I}$. Hence, the physics of H_W will reflect that of the modified IPR (the argument can also be extended to arbitrary initial states).

While Fig. 2 was concerned with the ground state, in the AAH model H_W shows a qualitatively similar behavior at finite temperatures [Fig. 3(a)]. As the temperature increases, H_W tends to grow but maintains the same overall shape as a function of Δ, and still exhibits strong signatures of the transition. This is due to the fact that in a localization transition *all* eigenvectors undergo a sudden change. As a consequence, all terms $C(|n_i\rangle\langle n_i|)$ in Eq. (6) will behave similarly, causing the bound Eq. (9) to be fairly tight. We confirm this numerically in Fig. 3(b), where we plot $C(|n_i\rangle\langle n_i|)$ for all eigenvectors. We thus reach the conclusion that the monotonic vertical shift in H_W, observed in Fig. 3(a), is essentially due to the Gibbs entropy $S(\bar{\rho})$. Our bounds therefore allow us to pinpoint different physical origins for different effects, namely, thermal fluctuations and the localization transition.

Conclusions. We have demonstrated that the entropy of the quantum work distribution provides a useful tool in characterizing the nonequilibrium response of a quantum system. The entropy captures the complexity of the full distribution and we have shown that it is acutely sensitive to sudden changes in the system, such as avoided crossings and localization transitions. Our main result, Eq. (8), shows that H_W can be understood as stemming from two distinct contributions, one given by the entropy of the initial state, dephased by the TPM, and a second term related to the coherences created by the work protocol. More specifically, what matters are the coherences of the initial eigenstates $|n_i\rangle$ in the basis $|m_f'\rangle = U|m_f\rangle$. It therefore accounts not only for the change in Hamiltonian, from $\mathcal{H}_i \to \mathcal{H}_f$, but also for the entire work protocol, summarized by U. The contribution of quantum coherence to work has been explored in the past [30,48,49] but only for initial thermal states, and with a focus on the average or the first few moments. Our results hold for any initial state and also focus on a different quantity, thus being complementary. By means of examples, we have shown that the entropy is capable of conveying a richness of information that is not immediately visible in the moments. We therefore believe that it could serve as a powerful tool for characterizing work statistics away from equilibrium.

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[33] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevResearch.5.L022010 for proofs of the bounds on the entropy and expression of the minimal, maximal and average work.

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