


Quantum work: Reconciling quantum mechanics and thermodynamics

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It has been claimed that no protocol for measuring quantum work can satisfy standard physical principles, casting doubts on the compatibility between quantum mechanics, thermodynamics, and the classical limit. In this Letter, we present a solution for this incompatibility. We demonstrate that the standard formulation of these principles fails to address the classical limit properly. By proposing changes in this direction, we prove that all the essential principles can be satisfied when work is defined as a quantum observable, reconciling quantum work statistics and thermodynamics.

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The concept of work lies at the heart of thermodynamics, being crucial to determine the processes permissible under the first and second laws [1–4]. Moreover, work’s statistical properties have paved the way for ground-breaking results, among which the Jarzynski equality [5] and Crook’s fluctuation relation [6] certainly stand out. These so-called fluctuation theorems have unveiled the tight connection of work with equilibrium free energy, the reversibility of thermodynamic processes, and information theory [7–21].

In the quantum realm, the pursuit of a universal definition of work resulted in multiple definitions [21–44], allowing the thermodynamic analysis of various quantum systems [22,45–47]. Nevertheless, the statistical characterization of work continues to be the subject of intense debate [48–72]. For instance, in scenarios without heat flux, work average is expected to equal the variation of mean energy, a feature not generally fulfilled by broadly used work measurement schemes, such as the two-point-measurement (TPM) [28,62,65,68], the Gaussian [28,72], and postselection [53] schemes. Other significant discussions in the literature include the definition of work in scenarios encompassing the energetic effects of measurements and quantum resources [14,15,53,73–80]. Successfully overcoming these challenges can propel advancements in quantum thermodynamics and the design of efficient quantum devices [45–47,81–84].

To elucidate quantum work, it has been generally considered that its statistics should comply with the following *criteria*, provided by the basic structure of quantum mechanics and thermodynamics [68,69]: work statistics should (i) be described by a positive operator-valued measure (POVM) [85,86] independent of the system’s initial state, (ii) yield an average work equal to the variation of energy over time

for externally controlled systems not interacting with a heat bath, and (iii) reproduce the classical limit. Surprisingly, it was demonstrated that no protocol for raising work statistics would comply simultaneously with criteria (i) and (ii) and a *condition* inspired by (iii) [68]. These findings have prompted the quest for new measurement protocols and a better understanding of the statistics of work [48–53,63,64,69–71]. Remarkably, there is still no statistical framework for describing work that aligns with criteria (i)–(iii), suggesting an incompatibility between quantum mechanics, its convergence to the classical limit, and thermodynamics.

In this Letter, we propose a solution to this challenge. We demonstrate that there is at least one protocol for raising work statistics in consonance with the basic criteria (i)–(iii). To demonstrate our results, we adopt criteria (i) and (ii) in a manner analogous to Ref. [68] while imposing necessary conditions for the classical limit as stipulated by criterion (iii). Specifically, we require that in the classical limit, the average of general quantum observables approximates their corresponding classical counterpart and that the commutation of quantum observables is sufficiently small. Guided by these conditions, we demonstrate that treating work as a two-time quantum observable [87–89], criteria (i)–(iii) are satisfied. Furthermore, we shed light on previous forms of imposing criterion (iii), highlighting their reliance on the two-point-measurement (TPM) methodology [21,67,72], which we show neither guarantees the recovery of the classical limit nor represents the unique approach capable of achieving it. We expect that our study showcases the feasibility of achieving a satisfactory reconciliation between quantum and classical work statistics and contributes to the ongoing quest for a unified framework for quantum work statistics.

Requirements for consistent work statistics. We first present criteria (i)–(iii) in detail. Our analysis consists of a closed system whose initial state is described by ρ governed by an externally controlled time-dependent Hamiltonian $H(t)$ with eigenbasis $\{|e_j(t)\rangle\}$. The system’s dynamics are dictated by the evolution operator U_t , which satisfies the Schrödinger equation $i\hbar\partial_t U_t = H(t)U_t$. Since the system is isolated, no heat is exchanged, and work equals the system energy

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variation. We thus posit that there exists a general protocol for measuring work, such that for any process defined by operators $H(t)$ and U_t , this protocol can describe the probability $P(w)$ of obtaining a value of work w . Following the quantum mechanics paradigm [85,86], we require that $P(w) = \text{Tr}[M(w)\rho]$, where $M(w)$ are the elements of a POVM $\{M(w)\}$, i.e., a set of non-negative Hermitian operators $M(w)$ satisfying the relation $\sum_w M(w) = 1$. Considering this formalism, a work measurement scheme implemented by $\{M(w)\}$ should satisfy the following criteria:

(i) *The operators $M(w)$ may depend on $H(t)$ and U_t , but are independent of ρ .* With this criterion, we anticipate that the measurement protocol must depend on the process described by U_t and $H(t)$ but is independent of the initial state, as one should not expect to adjust the measurement apparatus to the system's initial state [68]. Importantly, an equivalent formulation of criterion (i) allows for state-dependent POVM, as long as $P(w)$ exhibits linear dependence on the state [68,69].

(ii) *For any state ρ , the work average equals the variation in the average energy over time, i.e., $\langle W \rangle = \sum_w w P(w) = \text{Tr}[H(t)U_t\rho U_t^\dagger] - \text{Tr}[H(0)\rho] = \langle H(t) \rangle - \langle H(0) \rangle$.* Considering the convention in which work is deemed positive when the energy $H(t)$ increases, this statement aligns with the first law of thermodynamics, as there is no heat flux for this nonautonomous and closed quantum scenario.

(iii) *In the classical limit, the statistics raised via the POVM $M(w)$ must approach the classical results.* More precisely, it is anticipated that as the system approaches the classical limit, the quantum distribution $P(w)$ obtained through $M(w)$ should exhibit the same statistics as the classical distribution associated with the classical limit. This criterion put forward the expectation that the classical world can be reproduced within quantum mechanics in semiclassical regimes [78,90–94].

Criteria (i)–(iii) collectively provide a comprehensive framework that aligns with the foundations of quantum mechanics and thermodynamics and the convergence to classical behavior. In fact, these have served as the basis for many recent works (see [53,64,68–71] and references therein).

We can straightforwardly examine how criteria (i) and (ii) can constrain work POVMs considering two notable examples that shall be treated frequently in this Letter. On the one hand, we consider the two-point-measurement (TPM) POVM, which is succinctly described as follows [21,67,72]. At an initial time, the system is submitted to a projective measurement of energy, collapsing to an $H(0)$ eigenstate $|e_n(0)\rangle$ with probability $p_n = \langle e_n(0)|\rho|e_n(0)\rangle$. The system then evolves unitarily until the instant τ , when a second measurement is performed and a random eigenvalue $e_m(\tau)$ of $H(\tau)$ is obtained with probability $p_{m|n} = |\langle e_m(\tau)|U_t|e_n(0)\rangle|^2$. The TPM work probability is thus computed as [68,72] $P_{\text{TPM}}(w) = \sum_{mn} p_{m|n} p_n \delta[w - (e_m(\tau) - e_n(0))] = \text{Tr}[M_{\text{TPM}}(w)\rho]$, where $M_{\text{TPM}}(w) = \sum_{mn} \delta[w - (e_m(\tau) - e_n(0))] p_{m|n} |e_n(0)\rangle \langle e_n(0)|$ are the elements of the TPM POVM and δ is the Dirac's delta. Although TPM complies with criterion (i), it generally does not satisfy criterion (ii), as the first measurement destroys any coherence the initial state may possess [64,68,69].

On the other hand, the observable (OBS) POVM is connected with the two-time work observable [49,50,87–89]

$$W(\tau, 0) = H_h(\tau) - H(0), \quad (1)$$

where $H_h(t) = U_t^\dagger H(t) U_t$ represents the Hamiltonian in the Heisenberg picture at time t . Notably, $W(\tau, 0)$ is a Hermitian operator possessing a set of eigenvalues $w_j(\tau, 0)$ and corresponding eigenvectors $\{|w_j(\tau, 0)\rangle\}$, such that $W(\tau, 0) = \sum_j w_j(\tau, 0) |w_j(\tau, 0)\rangle \langle w_j(\tau, 0)|$. Accordingly, the probability of finding a value w of work is defined as $P_{\text{OBS}}(w) = \text{Tr}[M_{\text{OBS}}(w)\rho]$, where $M_{\text{OBS}}(w) = \sum_j \delta(w - w_j(\tau, 0)) |w_j(\tau, 0)\rangle \langle w_j(\tau, 0)|$. As can be checked from the discussion in [49], there always exists a corresponding Schrödinger operator S diagonalized by the same basis as $\{|w_j(\tau, 0)\rangle\}$ for each arbitrary interval $[0, \tau]$. Therefore, by measuring S at time 0 and collapsing the state to an eigenstate $|w_j(\tau, 0)\rangle$, one is thus “preparing” a state whose amount of work done on the system is known to be $w_j(\tau, 0)$ during $[0, \tau]$. By making several measurements of S at time 0, one thus raises $P_{\text{OBS}}(w)$.

We remark that criteria (i) and (ii) are fulfilled if and only if $M(w)$ are state-independent operators that satisfy the relation $\sum_w w M(w) = H_h(\tau) - H(0)$ [68,69]. Comparing this equation with Eq. (1) and considering the explicit form of $M_{\text{OBS}}(w)$, we readily confirm that the OBS POVM satisfies criteria (i) and (ii).

TPM and the classicality criterion. Unlike criteria (i) and (ii), verifying criterion (iii) for a specific POVM is challenging due to the elusive nature of the classical limit in the quantum realm—a topic that has been intensely debated since the inception of quantum mechanics [95–100]. Still, there is no unique form of characterizing the classical limit in the quantum context [101–105]. Notwithstanding these difficulties, Perarnau-Llobet *et al.* [68] boldly proposed what we refer to as the classical stochastic (CS) hypothesis, aiming to implement criterion (iii): *for initial states with no quantum coherences in the energy basis, the results of classical stochastic thermodynamics should be recovered.* More specifically, they suggested that for incoherent initial states where $[\rho, H(0)] = 0$, the work probability should be equal to the TPM probability, i.e., $[\rho, H(0)] = 0 \Rightarrow P(w) = P_{\text{TPM}}(w)$. The CS hypothesis was justified on the basis that the TPM scheme used for incoherent states enabled classical stochastic thermodynamics relations to be reproduced similarly in the quantum regime [10–13,21,26,30,106] and because of its good convergence in the classical limit [78,90–94]. Remarkably, the authors demonstrated that no POVM could simultaneously satisfy criteria (i) and (ii) along with the CS hypothesis. However, even though the CS hypothesis has been considered in many works aiming to recover the classical limit [53,64,69], we present throughout this section three arguments showing that demanding CS as a way of implementing criterion (iii) may not be the most general or accurate approach.

(1) *There is no fundamental principle dictating that quantum processes beginning with initial incoherent states should recover classical stochastic thermodynamic results* [49,63,65,78]. Because the Hamiltonian is time-dependent, an initial incoherent state will not always time-evolve to an incoherent state with respect to the instantaneous Hamiltonian energy bases. The emergence of coherences throughout the

process may result in a different amount of work exchange relative to what is classically expected. Moreover, for incoherent states quantum corrections can still display significant thermodynamics effects [107,108], as has been recognized ever since Wigner’s seminal paper [109].

(2) *TPM is not the unique approach successful in reproducing classical outcomes when coherences are absent.* Indeed, the agreement of TPM with the classical results in the semi-classical regime [78,90–94] has served as a justification for its selection in the CS hypothesis [68,69]. However, TPM is not necessarily unique in this sense. To prove this statement, consider a process described by $H(t)$ and U_t and a initial state ρ taking place within the time interval $[0, \tau]$. Consider also that the average of energy is bounded, i.e., $\langle H(t) \rangle < \infty$, for any $t \in [0, \tau]$. Let $C(\rho(t))$ be the 1-norm measure of coherences [110] for the evolved state $\rho(t) = U_t \rho U_t^\dagger$:

$$C(\rho(t)) = \|\rho(t) - \Phi_{H(t)}(\rho(t))\|_1 = \sum_{j \neq k} |\langle e_j(t) | \rho(t) | e_k(t) \rangle|, \tag{2}$$

where $\Phi_{H(t)}(\rho(t)) = \sum_j |e_j(t)\rangle \langle e_j(t) | \rho(t) | e_j(t)\rangle \langle e_j(t) |$ is the dephasing map at time t , accounting for the incoherent part of $\rho(t)$. Within this scenario, we prove the first result of this Letter:

Result 1. *If there is a real non-negative scalar ϵ_1 in which for any initial incoherent state ρ , $C(\rho(t)) \leq \epsilon_1$ during the entire interval $[0, \tau]$, then $\int_{-\infty}^{\infty} dw |P_{\text{TPM}}(w) - P_{\text{OBS}}(w)| \leq C_1 \epsilon_1$, where C_1 is a bounded real positive scalar independent of ϵ_1 . Therefore, $\lim_{\epsilon_1 \rightarrow 0} \int_{-\infty}^{\infty} dw |P_{\text{TPM}}(w) - P_{\text{OBS}}(w)| = 0$.*

Result 1 arises from the fact that processes with a small amount of coherence require the Hamiltonians at different times to *almost* commute. Otherwise, a large amount of coherences will emerge. The difference between TPM and OBS, as well as the creation of coherences, stem from the lack of Hamiltonian commutation and will be reduced as the Hamiltonians approach to a perfect commutation. Therefore, the TPM protocol will approach the OBS scheme for processes close to the classical limit where coherences are *all the time* small. Consequently, justifying the preference for TPM over OBS based on its convergence to classical results can be misleading. We confirm this physical intuition by rigorously showing that C_1 is bounded and independent of ϵ_1 (see the Supplemental Material (SM) [111]). The case of zero coherence, $\epsilon_1 = 0$, can be directly proved considering the results presented in Ref. [67].

(3) *The CS hypothesis lacks the necessary generality to encompass a broader range of processes in the classical limit.* Consider, for instance, an oscillator with a time-dependent frequency described by the Hamiltonian operator [90,91]

$$H(t) = \frac{P^2}{2m} + \frac{m\omega^2(t)}{2} X^2, \tag{3}$$

where $\omega^2(t) = \omega_0^2 + (\omega_1^2 - \omega_0^2) \frac{t}{\tau}$, and $\omega_{0,1}$ and τ are fixed parameters. When initialized in a coherent state $\rho = |\alpha\rangle \langle \alpha|$, defined as

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |e_n(0)\rangle, \tag{4}$$

then, for a sufficiently large $|\alpha|$, the center of the wave packet exhibits classical particle-like behavior [112], following dy-

namics governed by a classical Hamiltonian analogous to Eq. (3). On the one hand, following criterion (iii), if we consider this scenario a classical limit, the quantum work statistics should converge to its classical counterpart. Under this perspective, this example extends beyond the scope of the CS hypothesis, exposing its limited coverage of the classical limit by associating it solely with incoherence in the energy basis. On the other hand, despite the oscillator’s classical behavior, one might expect that a large amount of coherence could lead to work statistics diverging from the classical counterpart. This example thus highlights the need to clarify the classical limit beyond the CS hypothesis and when we expect the quantum statistics to converge to it. We address this issue in the next section and in [111], where we explicitly calculate the work statistic for a coherent state, revealing that the OBS protocol appropriately converges in the classical limit while the TPM does not.

OBS protocol and the classical limit. As exemplified above, formally characterizing criterion (iii) is daunting and the CS hypothesis is not able to implement it. In order to circumvent these difficulties and still obtain valuable results from criterion (iii), we propose an alternative strategy. Here, we first identify some necessary conditions for a quantum process to approach the classical limit. Then, we show that these are enough to obtain general results for quantum work statistics.

We consider again a process described by U_t and $H(t)$, but now the Hamiltonian $H(t)$ depends on a Schrödinger coordinate observable X and its conjugate momentum P ($[X, P] = i\hbar \mathbb{1}$), and time t within the interval $[0, \tau]$. Consequently, U_t and the Heisenberg version of the Hamiltonian $H_h(t)$ are continuous functions of X, P , and t . We can identify $H_h(t) = G(X, P, t)$, where G is a *smooth* function that can be written as powers of X, P , and t .

In order to establish the necessary conditions for the convergence to the classical limit of an initial preparation ρ and the quantum process described by $U_t, H_h(t)$, it is essential to introduce the following quantities: the classical probability distribution $q(\Gamma_0)$, representing the likelihood of finding a classical system at the phase points $\Gamma_0 = (x_0, p_0)$ at time 0; and a classical Hamiltonian function $H_{\text{CL}}^t(\Gamma_t, t)$, characterizing the energy of the system at time t with respect to the phase point $\Gamma_t = (x_t, p_t)$. Importantly, within the Hamiltonian formalism, the evolution of $\Gamma_t(\Gamma_0, t) = (x_t(\Gamma_0, t), p_t(\Gamma_0, t))$ can be expressed in terms of Γ_0 and t , allowing the Hamiltonian function to also be written as a function of Γ_0 and t , so that $H_{\text{CL}}^t(\Gamma_t, t) = H_{\text{CL}}(\Gamma_0, t)$. Here, H_{CL} corresponds to the energy at time t related to the system that was at Γ_0 at time 0. With these definitions in place, the following conditions are required for the convergence to the classical limit of the process characterized by $\{X, P, \rho, H_h(t)\}$:

(A) *There exists at least one classical distribution $q(\Gamma_0)$ along with a Hamiltonian function $H_{\text{CL}}(\Gamma_0, t)$, such that*

$$\left| \text{Tr}[P^m X^n \rho] - \int d\Gamma_0 p_0^m x_0^n q(\Gamma_0) \right| \leq \epsilon_A |\text{Tr}[P^m X^n \rho]| \tag{5}$$

for any integers m and n , and

$$H_{\text{CL}}(\Gamma_0, t') \equiv H_{\text{CL}}(x_0, p_0, t) = G(x_0, p_0, t'), \tag{6}$$

where $G(x_0, p_0, t)$ has the same functional form as $G(X, P, t)$, previously defined, t' can be either 0 or τ , and $\epsilon_A \ll 1$. Equation (5) asserts that there must be at least one classical scenario whose averages approach the quantum ones at $t = 0$. Furthermore, Eq. (6) states that the quantum energy in the classical limit should be described in terms of the same quantities that define its classical version at $t' = 0, \tau$.

(B) For any functions $g_l \equiv g_l(X, P)$ and $g_r \equiv g_r(X, P)$ describing the product of powers of X and P , it follows that

$$|\text{Tr}[g_l [X, P] g_r \rho]| \leq \epsilon_B |\text{Tr}[g_l X P g_r \rho]| \quad (7)$$

and

$$|\text{Tr}[g_l [X, P] g_r \rho]| \leq \epsilon_B |\text{Tr}[g_l P X g_r \rho]|, \quad (8)$$

where $\epsilon_B \ll 1$. This requirement resembles the usual classical limit assumption $\hbar \rightarrow 0$. In our formulation, however, we allow the noncommutation to have a non-null yet significantly small value compared to the system's inherent scales.

It is important to emphasize that conditions (A) and (B) alone are not sufficient to certify the classical limit. Specifically, they do not rule out the effects of quantum correlations, measurement's disturbance, or any other quantum phenomena. In our framework, processes influenced by these quantum effects may still adhere to conditions (A) and (B) without truly approximating the classical limit. Conversely, these conditions are *necessary* for the classical limit. Therefore, we expect that any quantum scenario genuinely approaching the classical limit rigorously satisfies conditions (A) and (B). In these circumstances, the set $\{x_0, p_0, \varrho, H_{\text{CL}}\}$ describe the classical scenario to which the process characterized by $\{X, P, \rho, H_h(t)\}$ converges. Interestingly, we demonstrated in [111] that the system described in Eqs. (3) and (4) satisfies conditions (A) and (B) for $|\alpha| \rightarrow \infty$.

Now, consider a scenario fulfilling conditions (A) and (B) converging to the classical limit. Within this context, the classical work is described as $W_{\text{CL}}(\Gamma_0, \tau, 0) = H_{\text{CL}}(\Gamma_0, \tau) - H_{\text{CL}}(\Gamma_0, 0)$, with the associated classical distribution defined as

$$P_{\text{CL}}(w) = \int_{\Gamma_0} d\Gamma_0 \varrho(\Gamma_0) \delta[w - W_{\text{CL}}(\Gamma_0, \tau, 0)]. \quad (9)$$

According to criterion (iii), a consistent approach to describing quantum work statistics should converge to the results provided by $P_{\text{CL}}(w)$ in the classical limit. Following this reasoning, we derived the central result of this Letter.

Result 2. *If conditions (A) and (B) are satisfied, then*

$$\lim_{\epsilon_{\text{max}} \rightarrow 0} \int_{-\infty}^{\infty} dw |P_{\text{OBS}}(w) - P_{\text{CL}}(w)| = 0 \quad (10)$$

and

$$\int_{-\infty}^{\infty} |P_{\text{OBS}}(w) - P_{\text{CL}}(w)| dw \leq K \epsilon_{\text{max}}, \quad (11)$$

where $P_{\text{OBS}}(w)$ is the probability related to the OBS protocol, $P_{\text{CL}}(w)$ is defined in Eq. (9), ϵ_{max} is the maximal value of ϵ_A and ϵ_B as defined in conditions (A) and (B), and K is a bounded real positive scalar independent of ϵ_A and ϵ_B .

The OBS protocol, derived from classical work using standard quantization rules, reveals differences between classical and quantum observables in scenarios with significant lack of commutation. This suggests that the difference in quantum and classical probabilities is tied to the lack of commutation, approaching zero when commutation is negligible [condition (B)], and the quantum scenario exhibits similar averages as a classical counterpart [condition (A)]. This intuition supports result 2, which we rigorously proved in [111], employing the Cauchy-Hadamard formula [113,114] to demonstrate the boundedness of K .

According to result 2, the OBS protocol will converge to the description via Eq. (9) for any given quantum state ρ and process $\{U_t, H(t)\}$ that satisfies conditions (A) and (B). Since these conditions are necessary for the classical limit, then we can deduce that the statistics of work obtained through the OBS protocol invariably replicate the classical work statistics in the classical limit, thereby satisfying criterion (iii). Furthermore, from the review conducted in Ref. [69], the OBS protocol is the only well-known protocol that generally adheres to (i) and (ii). As a consequence of the result 2 and given our current understanding, we can also assert that OBS is the only well-known protocol capable of meeting criteria (i)–(iii) simultaneously.

Conclusions. Quantum work is a fundamental concept for extending thermodynamics to general quantum scenarios. Its statistical description, however, still presents intriguing challenges. Therefore, testing its consistency with criteria (i)–(iii), expressing general features that any quantum work protocol should possess, is a paramount goal. By adopting a novel strategy to consider the classical limit, we demonstrated that OBS is the only well-known scheme for quantum work measurement that complies with all these criteria simultaneously.

Our results are entirely general concerning the internal structure of the closed system. The latter may comprise multiple subsystems, including scenarios where heat is transferred among them. However, we did not address open quantum scenarios with *external* sources transferring heat to the system of interest. Although we showed that the OBS POVM is the only well-known scheme capable of satisfying simultaneously all the criteria (i)–(iii) in the closed-case scenario, it is not necessarily expected that an observable precisely as it is defined in Eq. (1) should be the correct observable describing thermodynamics work in the open quantum case. This leads to an intriguing question: Is there a broader, more encompassing quantum work observable that not only adheres to criteria (i)–(iii) in open quantum scenarios but also aligns with the observable in Eq. (1) in the specific closed case? We believe our current work lays the groundwork for addressing this question, hopefully inspiring future research to expand and refine our understanding of the concept of work.

Interestingly, our results pave the way for many research opportunities exploring superposition, entanglement, and other correlations regarding OBS statistics of work and other two-time quantities [49]. Conditions (A) and (B) introduced here could be used to study the classical limit in diverse fields like quantum chaos [115], quantum optics [103–105,116], and the semiclassical formalism. A promising avenue in these lines involves conducting a comparative study between the results obtained in [78,90–94] and result 2.

Moreover, our findings support the viewpoint that conventional fluctuation theorems aimed at recovering classical expressions necessitate a departure from their conventional forms [117], revealing new connections between equilibrium properties and information resources with quantum work statistics. Furthermore, we hope our approach stimulates the analysis of the relation between work and other quantum thermodynamic facets, such as the lack of detailed balance at equilibrium (nonreciprocity) and persistent quantum currents [118,119]. These lines of research, we expect, will propel the field of quantum thermodynamics to new frontiers.

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