Comment on: "Scaling and Universality at Noisy Quench Dynamical Quantum Phase Transitions"

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In Ref. [1], dynamical quantum phase transitions (DQPTs)—non-analyticities in the Loschmidt return rate at critical times—are investigated in the presence of noise for a two-band model. The authors report that DQPTs persist even after averaging over the noise and they use their results to derive dynamical phase diagrams. In this comment we rigorously prove that in any two-dimensional Hilbert space the Loschmidt echo of two density matrices can only become zero if and only if *both* density matrices are pure. As a consequence, the existence of DQPTs in the considered scenario is strictly ruled out for non-zero noise because the considered averaging leads to a mixed state. We also investigate alternative natural ways to average over noise realizations and show that in all of them DQPTs are smoothed out.

I. INTRODUCTION

A significant portion of research on non-equilibrium dynamics has concentrated on the behavior of systems subjected to quenches and ramps. Here, an initial quantum state $\rho(0)$ is prepared and then, in the case of a quench, time-evolved with a time-independent Hamiltonian or, in the case of a ramp, with a Hamiltonian which has a time-dependent parameter. One way to study the ensuing dynamics is to consider the Loschmidt echo $|L(t)|^2$ which provides a measure on how far the time-evolved state $\rho(t)$ is from the initial state $\rho(0)$. Of particular interest are critical times t_c where $L(t_c) = 0$. These times define what in the literature has been called a DQPT [2–4]. It is important to remark that this definition of a DQPT is not unique: another definition considers the dynamics of an order parameter and when it becomes zero [5]. The paper [1] deals with the former and this definition of a DQPT by the Loschmidt echo, also sometimes referred to as DQPT of type II, will be the sole focus of this comment.

In the most studied case, both the initial state $\rho(0)$ and the time-evolved state $\rho(t)$ are *pure states*. The Loschmidt amplitude is then simply defined by

$$L(t) = \langle\Psi(0)|\Psi(t)\rangle \tag{1}$$

with $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$. For the Loschmidt echo we can then write $|L(t)|^2 = \langle\Psi(0)|\rho(t)|\Psi(0)\rangle = \mathrm{tr}\,(\rho(0)\rho(t))$. This form suggests that it can also be applied for impure states $\rho(0)$ and $\rho(t)$. However, it is well known that this is not quite correct: If *both* $\rho(0)$ and $\rho(t)$ are impure then $\mathrm{tr}(\rho(0)\rho(t))$ does not induce a proper metric on the space of density matrices. Instead, one has to use the Uhlmann-Bures metric [6–8]

$$\mathcal{L}(t) = \mathrm{tr}\sqrt{\sqrt{\rho(0)}\rho(t)\sqrt{\rho(0)}} \tag{2}$$

which reduces to $|L(t)|$ with $L(t)$ defined in Eq. (1) if the density matrices are pure. We note that the arguments presented in the following are not fundamentally changed even if the not entirely correct version of the Loschmidt echo $|L(t)|^2 = \mathrm{tr}(\rho(0)\rho(t))$ is used for impure states. Because overlaps scale exponentially with system size, it is typically not the Loschmidt echo which is considered but rather the Loschmidt return rate. For a one-dimensional system of size N, this return rate is defined by

$$g(t) = -\lim_{N\to\infty}\frac{1}{N}\ln|L(t)|^2,\ \text{or}\quad \mathcal{G}(t) = -\lim_{N\to\infty}\frac{1}{N}\ln|\mathcal{L}(t)|^2, \tag{3}$$

respectively. In one dimension, zeroes of the Loschmidt echo manifest themselves as non-analyticities ('cusps') in the return rate.

II. CONSIDERED SETUP

The setup considered is shown in Fig. 1 of Ref. [1]. The system at the initial time t_i is prepared in the ground state, a pure state, of a given Hamiltonian $H^i = H_0 + h_i H_1$ with a magnetic field h_i. Then, in the time interval $[t_i, t_f)$ the system undergoes a linear ramp in the magnetic field $h_0(t) = h_i + \frac{h_f - h_i}{t_f - t_i}(t - t_i)$ so that at end of the ramp at time t_f—the authors choose $t_f = 0$—the magnetic field is given by h_f. Accordingly, the ramp velocity is $v = (h_f - h_i)/(t_f - t_i)$. During the entire ramp, classical Gaussian white noise is supposed to be present which is described by the field $R(t)$ with correlation function $\langle R(t)R(t')\rangle = \xi^2\delta(t-t')$. The total field acting during the ramp is thus $h(t) = h_0(t) + R(t)$. For times $t \geq t_f$ the field remains at h_f and there is no noise. Noise is present only during the ramp. The magnetic field $h(t)$ couples to the total staggered moment $H_1 = \sum_n (-1)^n S_n^z$ in Ref. [1]. The following general arguments, however, are valid for any coupling.

A step in Ref. [1] of crucial relevance for this comment is that at time $t = t_f = 0$ the *noise-averaged density matrix* $\rho(t)$ is calculated using the master equation

$$\dot{\rho}(t) = -i[H_0(t), \rho(t)] - \frac{\xi^2}{2}\Big[H_1, \Big[H_1, \rho(t)\Big]\Big]. \tag{4}$$

where $H_0(t) = H_0 + h_0(t)H_1$ with H_0 being the considered time-independent Hamiltonian. This is a Lindblad master equation of dephasing type for the density matrix $\rho(t)$. The authors then want to consider the Loschmidt echo between the noise-averaged $\rho(t_f = 0)$, obtained from Eq. (4), and the state $\rho(t)$ for $t > 0$ obtained by time-evolving $\rho(0)$ with the time-independent Hamiltonian $H^f = H_0 + h_f H_1$.

Surprisingly, the authors find that even after noise averaging over the initial state, the return rate shows non-analyticities (see Fig. 5 of Ref. [1]). I.e., DQPTs do still exist in the *noise-averaged* return rate. Based on these results, the authors also derive a dynamical phase diagram which consists of three phases (see Fig. 4 of Ref. [1]): a phase with no DQPTs and two phases with DQPTs. The phases with DQPTs are distinguished further by whether they show two critical momentum modes or multiple critical momentum modes (modes where the excitation probability is $1/2$). The latter phase, according to the phase diagram in Ref. [1], only exists in the presence of noise. I.e. it is a novel dynamical phase created by noise.

III. TWO RIGOROUS THEOREMS RULING OUT THE MAIN FINDINGS OF REF. [1]

In the following we prove two theorems which show that the main findings of Ref. [1] cannot hold.

Theorem 1: Except for trivial cases, the solution of the Lindblad Master equation (4) is a mixed state.
Proof: Consider the purity $P = \mathrm{tr}\rho^2(t)$. Then

$$\begin{aligned}\dot{P}(t) &= 2\mathrm{tr}(\rho\dot{\rho}) = 2\mathrm{tr}\left(\rho\left\{-i[H_0,\rho] - \frac{\xi^2}{2}[H_1,[H_1,\rho]]\right\}\right) \\ &= -\xi^2\mathrm{tr}\left(\rho[H_1,[H_1,\rho]]\right)\end{aligned} \tag{5}$$

where we have used $\mathrm{tr}(\rho[H_0,\rho]) = 0$ because of the cyclic invariance of the trace and, for brevity, have written $\rho = \rho(t)$ and $H_0 = H_0(t)$. We can now use that for Hermitian operators A, B the identity $\mathrm{tr}(B[A,[A,B]]) = \mathrm{tr}([A,B]^\dagger[A,B]) \geq 0$ holds which is straightforward to prove using again the cyclic invariance of the trace. We therefore find for the purity

$$\dot{P}(t) = -\xi^2\mathrm{tr}\left([H_1,\rho]^\dagger[H_1,\rho]\right) \leq 0 \tag{6}$$

which means that the purity is a non-increasing function. If we start from a pure state then the state remains pure if and only if $[H_1,\rho(t)] = 0$ for all times t. In this case we are in a decoherence-free subspace and the dissipator vanishes identically leaving only the unitary dynamics $\dot{\rho} = -[H_0,\rho]$. A typical example of such decoherence-free dynamics is the case $[H_0,H_1] = 0$ where we start in an eigenstate of H_0 which then in turn is also an eigenstate of H_1. If we want to study the effects of noise on DQPTs then we are obviously not interested in cases where the noise is inactive and the dynamics decoherence free. Indeed, in the example considered in Ref. [1], H_1 is the staggered magnetic field and $[H_0,H_1] \neq 0$. The purity is therefore a monotonically decreasing function and the fixed point of the Lindblad Master equation (4) is the maximally mixed state.

Theorem 2: In a two-dimensional Hilbert space, the Loschmidt echo $\mathcal{L}(t)$ can have zeroes if and only if *both* the initial state $\rho(0)$ and the final state $\rho(t)$ are pure. In this case $\mathcal{L}(t) = |L(t)| = |\langle\Psi(0)|\Psi(t)\rangle|$ and zeroes occur if critical times t_c exist where $|\Psi(0)\rangle$ and $|\Psi(t)\rangle$ are orthogonal.

Proof: Since $M(t) = \sqrt{\rho(0)}\rho(t)\sqrt{\rho(0)}$ is positive semidefinite, this implies

$$\mathcal{L}(t) = \mathrm{tr}\sqrt{M(t)} = 0 \Longleftrightarrow M(t) = 0\,. \tag{7}$$

Furthermore,

$$M(t) = 0 \Longleftrightarrow \mathrm{supp}[\rho(0)] \perp \mathrm{supp}[\rho(t)], \tag{8}$$

i.e., $M(t)$ vanishes if and only if the supports of the two density matrices are orthogonal to each other. This result is general and valid in any dimension.

In two-dimensional Hilbert spaces, the possible ranks of each of the two density matrices are 1 or 2. If either of the density matrices has rank 2 then their support is the entire two-dimensional Hilbert space and there is thus no orthogonal complement. It follows that $\mathcal{L}(t) = 0$ is possible if and only if both density matrices have rank 1 which means they are pure. In this case $\rho(0) = |\Psi(0)\rangle\langle\Psi(0)|$ and $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ implying that $\mathcal{L}(t) = |\langle\Psi(0)|\Psi(t)\rangle| = |L(t)|$, see Eq. (1) and Eq. (2), and $L(t) = 0$ if the two pure states $|\Psi(0)\rangle$ and $|\Psi(t)\rangle$ are orthogonal to each other. We note that in Hilbert spaces with dimensions larger than 2 it is possible for the Loschmidt echo to vanish also for impure states. For example, in $d = 4$ we can have $\rho(0) = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$ and $\rho(t) = \frac{1}{2}|2\rangle\langle 2| + \frac{1}{2}|3\rangle\langle 3|$ which have orthogonal support. Note, however, that even in higher dimensions this is not a generic scenario and will require some fine tuning.

In Ref. [1] a translationally invariant, one-dimensional, two-band model is considered. As a consequence, the Hilbert space factorizes into two-dimensional Hilbert spaces for each momentum mode, a result which is used throughout the paper. In particular,

$$\rho(t) = \bigotimes_k \rho_k(t) \tag{9}$$

where $\rho_k(t)$ are 2×2 matrices. It follows that

$$\mathcal{L}(t) = \prod_k \mathcal{L}_k(t) = \prod_k \mathrm{tr}\sqrt{\sqrt{\rho_k(0)}\rho_k(t)\sqrt{\rho_k(0)}} \tag{10}$$

and $\mathcal{L}(t) = 0$ if and only if at least one momentum k exists with $\mathcal{L}_k(t) = 0$. As we have shown in Theorem 2 this can happen if and only if both $\rho_k(0)$ and $\rho_k(t)$, which live in a two-dimensional Hilbert space, are pure. However, in Theorem 1 we have proven that the density matrix $\rho_k(0)$—obtained after the noisy ramp by taking the noise average—is an impure state. We have thus rigorously proven that there are no DQPTs under the noise-averaging procedure considered in Ref. [1] for any non-zero noise amplitude. For any noise amplitude $\xi \neq 0$ there is only a 'no-DQPT' phase, and not three phases including two with DQPTs as shown incorrectly in Fig. 4 of Ref. [1].

As a further check of Theorem 2 and as a tool useful to calculate the Loschmidt echo $\mathcal{L}_k(t)$ we note that in two dimensions we can write $\rho_k(t) = \frac{1}{2}(I + \boldsymbol{r}_k(t)\cdot\boldsymbol{\sigma})$ where $\boldsymbol{\sigma}$ is the vector of Pauli matrices and I is the 2×2 identity. From this representation it follows that

$$\mathcal{L}_k(t) = \sqrt{\frac{1}{2}\left(1 + \boldsymbol{r}_k(0)\cdot\boldsymbol{r}_k(t) + \sqrt{(1-\|\boldsymbol{r}_k(0)\|^2)(1-\|\boldsymbol{r}_k(t)\|^2)}\right)}\,. \tag{11}$$

This is just the standard expression for the Uhlmann fidelity of two qubit density matrices. From this formula it also immediately follows that $\mathcal{L}_k(t) = 0$ if and only if $\|\boldsymbol{r}_k(0)\| = \|\boldsymbol{r}_k(t)\| = 1$ (both states are pure) and $\boldsymbol{r}_k(0)\cdot\boldsymbol{r}_k(t) = -1$ (they are orthogonal).

To summarize, we have rigorously proven two theorems which are of general use when considering the Loschmidt echo in the presence of dissipation and which, more specifically, directly rule out the main findings of Ref. [1].

IV. MIXED STATES CANNOT FAITHFULLY BE REPRESENTED BY PURE STATES

Next, we will discuss the concrete issues leading to the incorrect dynamical phase diagram in Ref. [1]. The issues are general and we do not need to consider the concrete form of the Hamiltonian used in Ref. [1].

We can write an initial pure state for a translationally invariant model as $|\Psi(0)\rangle = \bigotimes_k |\Psi_k(0)\rangle$ and the Hamiltonian as $H = \bigoplus_k H_k$. Furthermore, for a two-band model as considered in Ref. [1] there are only two states for each k-mode so we can write $|\Psi_k(0)\rangle = v_k|\alpha_k\rangle + u_k|\beta_k\rangle$ with $|v_k|^2 + |u_k|^2 = 1$. We can also assume that $H_k|\alpha_k\rangle = -\varepsilon_k|\alpha_k\rangle$ and $H_k|\beta_k\rangle = \varepsilon_k|\beta_k\rangle$. The *pure-state Loschmidt echo* is then given by $L(t) = \prod_k L_k(t)$ and it is straightforward to show that

$$\begin{aligned} L_k(t) &= |\langle\Psi_k(0)|e^{-iH_kt}|\Psi_k(0)\rangle|^2 \\ &= 1 - 4p_k(1-p_k)\sin^2(\varepsilon_k t) \end{aligned} \tag{12}$$

where we have defined $p_k = |u_k|^2 = |\langle\Psi_k(0)|\beta_k\rangle|^2$. This is all well-known and the formula for the Loschmidt echo is correct for two-band models if (i) the initial state $|\Psi_k(0)\rangle$ is pure, and (ii) we time evolve the system with a time-independent Hamiltonian H_k.

The issue is that the authors of Ref. [1] use the Master equation (4) to obtain the noise-averaged initial state $\rho_k(0)$ but this state, as we have shown in Theorem 1, is impure and the formula (12) is therefore simply not applicable.

If we calculate, as the authors do, the probability

$$\tilde{p}_k = \langle\beta_k|\rho_k(0)|\beta_k\rangle \tag{13}$$

then this can indeed be interpreted as the probability of the mixed state $\rho_k(0)$ collapsing onto the pure state $|\beta_k\rangle$ in a measurement. However, this probability is not the pure-state amplitude p_k which enters into the Loschmidt echo formula (12), $\tilde{p}_k \neq p_k$. The authors assume that these two probabilities are the same, which is not so. We can ask though if by making this assumption the problem the authors set out to investigate—what happens to DQPTs under noise—is perhaps solved in some approximate way. To see whether or not this is the case, we start out from the general form of a 2×2 density matrix $\rho_k(0) = \frac{1}{2}(I + \boldsymbol{r}\cdot\boldsymbol{\sigma})$ where I is the 2×2 identity matrix. This form of $\rho_k(0)$ automatically fulfills $\mathrm{tr}\rho_k(0) = 1$ and also guarantees that $\rho_k(0)$ is hermitian. The condition that a density matrix has to be positive semidefinite further implies $\|\boldsymbol{r}\| \leq 1$. The pure states are lying on the surface of the Bloch sphere, i.e. for pure states we have $\|\boldsymbol{r}\| = 1$. W.l.o.g. we can assume, by an appropriate basis choice in the two-level space, that $\beta_k = (1\ 0)^T$. Then $\tilde{p}_k = \langle\beta_k|\rho_k(0)|\beta_k\rangle = (1+r_z)/2$. If we set $\tilde{p}_k = p_k$ then we assume that we can replace the mixed state $\rho_k(0)$ by the pure state $|\Psi_k(0)\rangle = \sqrt{(1-r_z)/2}|\alpha_k\rangle + \sqrt{(1+r_z)/2}|\beta_k\rangle$. In other words, the assumption is that the density matrix $\rho_k(0)$ is well approximated by the pure-state density matrix $\bar{\rho}_k = \frac{1}{2}(I + \boldsymbol{s}\cdot\boldsymbol{\sigma})$ with $\boldsymbol{s} = (\sqrt{1-r_z^2}, 0, r_z)$. This is the pure state obtained by keeping the z component the same and maximizing the coherence in the x component. However, this is *not* the pure state which best approximates the general mixed state $\rho_k(0)$. The best approximation is instead obtained by moving along the direction of the $\boldsymbol{r}$ vector to the surface of the Bloch sphere, i.e. the best approximation is the pure state $\tilde{\rho}_k(0) = \frac{1}{2}(I + \hat{\boldsymbol{r}}\cdot\boldsymbol{\sigma})$ with $\hat{\boldsymbol{r}} = \boldsymbol{r}/\|\boldsymbol{r}\|$. We can see this by considering the mixed-state fidelity

$$F(\rho_1,\rho_2) = \left(\mathrm{tr}\sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}}\right)^2 . \tag{14}$$

For the approximation chosen in Ref. [1] we find $\bar{F}_k(\rho_k,\bar{\rho}_k) = (1+\boldsymbol{r}\cdot\boldsymbol{s})/2 = (1 + r_z^2 + r_x\sqrt{1-r_z^2})/2$ whereas $\tilde{F}_k(\rho_k,\tilde{\rho}_k) = (1+\|\boldsymbol{r}\|)/2$ which is the maximal fidelity possible. We therefore see that the construction used in the paper only reproduces an optimal pure-state approximation of the mixed state $\rho_k(0) = (I + \boldsymbol{r}\cdot\boldsymbol{\sigma})$ if $\boldsymbol{r} = (r_x, 0, 0)$, i.e., if the $\boldsymbol{r}$-vector points in x direction.

More fundamentally, even if we choose the optimal pure-state approximation, we have $\tilde{F}_k < 1$ so that any such approximation is exponentially poor in system size

$$F = \prod_k F_k \sim \mathcal{O}(\mathrm{e}^{-N}) . \tag{15}$$

This can be most clearly seen if we consider the fixed point of the Lindblad Master equation (4) which is the completely mixed state $\rho_k^{\mathrm{fp}} = I/2$. In this case any pure state is an equally poor approximation with fidelity $F_k^{\mathrm{fp}} = 1/2$ leading to a total fidelity $F = 2^{-N}$.

To summarize, we have shown that the approach taken in Ref. [1] amounts to replacing the mixed state $\rho_k(0)$ obtained from the Master equation (4) by a non-optimal pure state. More importantly, even if an optimal pure-state approximation is chosen, the fidelity of the approximation diminishes exponentially with the length of the chain. This implies that such an approximation is meaningless—remember that DQPTs in the Loschmidt return rate are defined in the thermodynamic limit—and the results obtained in Ref. [1] using this approximation, which is also not justified by any small parameter, do not tell us anything about the original question which is what happens to DQPTs in the presence of noise.

V. NOISE AVERAGING ALWAYS DESTROYS DQPTS

Having shown that the approach used in Ref. [1] is incorrect, we now discuss three inequivalent and natural ways proper noise averages can be obtained. In this section we will denote quantities X which are noise averaged by $\bar{\bar{X}} = \mathbb{E}_R[X]$.

Case 1: As in the paper, the Master equation (4) is used to obtain the noise-averaged initial mixed state $\bar{\bar{\rho}}(0)$. Using the Loschmidt echo $\mathcal{L}[\bar{\bar{\rho}}](t)$ based on the noise-averaged density matrix we obtain the return rate

$$\bar{\bar{\mathcal{G}}}(t) = -\lim_{N\to\infty}\frac{1}{N}\ln|\mathcal{L}[\bar{\bar{\rho}}](t)|^2 . \tag{16}$$

Case 2: For each noise realization n, we obtain a new initial pure state $|\Psi_n(0)\rangle$. We then use the pure-state Loschmidt echo $|L_n(t)|^2 = |\langle\Psi_n(0)|\Psi_n(t)\rangle|^2$ and average over the noise realizations to obtain

$$\begin{aligned} |\bar{\bar{L}}(t)|^2 &= \lim_{M\to\infty}\frac{1}{M}\sum_{n=1}^{M}|L_n(t)|^2, \\ \bar{\bar{g}}(t) &= -\lim_{N\to\infty}\frac{1}{N}\ln|\bar{\bar{L}}(t)|^2 . \end{aligned} \tag{17}$$

Case 3: Similar to case 2, we start from the pure state $|\Psi_n(0)\rangle$ but calculate the return rate for each realization first and only take the noise average at the very end

$$\begin{aligned} g_n(t) &= -\lim_{N\to\infty}\frac{1}{N}\ln|L_n(t)|^2 \\ \bar{\bar{g}}'(t) &= \lim_{M\to\infty}\frac{1}{M}g_n(t) . \end{aligned} \tag{18}$$

Case 1 is the noise average the authors of Ref. [1] set out to consider. We have rigorously proven through Theorems 1 and 2 that for two-band models no DQPTs exist for any non-zero noise. We note that for generic noise, this is also expected to hold true for n-band models with $n > 2$. While orthogonal support is possible for $n > 2$, generic noise is not expected to produce such fine-tuned orthogonality. In case 2, each realization can have critical times $\tau_{n,k}$ $(k = 1, \cdots)$ such that $L_n(\tau_{n,k}) = 0$. However, the probability that a finite fraction of realizations has the exact same critical time is zero, because the critical times $\tau_{n,k}$ are continuous random variables that depend sensitively on the noise realization. Thus, $|\bar{\bar{L}}(t)|^2 \neq 0$ for all times t with probability 1 and $\bar{\bar{g}}(t)$ is smooth. A similar argument also holds for case 3: Each individual return rate $g_n(t)$ can have cusps at times $\tau_{n,k}$, however, these non-analyticities occur at different random times $\tau_{n,k}$ and thus do not add up coherently. As a result, $\bar{\bar{g}}'(t)$ is again a smooth function.

VI. CONCLUSIONS

Ref. [1] set out to study the effect of noise on DQPTs—non-analyticities of the Loschmidt return rate at critical times. We have shown here that the authors' approach amounts to replacing the mixed state, obtained after noise averaging, by a pure state. The obtained results for the return rates and the dynamical phase diagram based on these return rates therefore do not reflect the actual physics of the problem.

For the noise-averaging protocol considered in the paper—where the initial state after the ramp is obtained by averaging over the noise—we have rigorously proven two general theorems which demonstrate that a properly evaluated Loschmidt return rate will never show DQPTs for non-zero noise levels in two-band models. We note that the second theorem appears to be relevant beyond the purview of this comment by showing that in n-band models with $n > 2$ DQPTs are possible even for mixed states although this is expected to happen only in some fine-tuned models and not in generic noisy or finite-temperature systems.

In addition, we have also considered two other scenarios to obtain noise-averaged return rates. In these cases we are always working with pure states and individual noise realizations can show DQPTs because they correspond to unitary evolutions of pure states. However, the times at which DQPTs do occur are not coherent between different realizations. As a result, a noise averaging will always smooth out DQPTs also in these alternative approaches.

Overall, we have shown that there are no surprises and that previous results on the fate of DQPTs in the presence of finite temperatures or dissipation remain valid [8, 9]. As might have been expected on general physical grounds, averaging over noise always does smooth out dynamical quantum phase transitions.

The results in Ref. [1] do suggest that sharp dynamical quantum phase transitions can exist even in noisy environments which would not only be important from a fundamental point of view but would also be potentially relevant for quantum information applications. We therefore believe that it is important to correct the record given the potential implications of the original claim.

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