Functional field integral approach to the quantum work

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We introduce the functional field integral approach to study the statistics of quantum work for arbitrary nonequilibrium process. For a general bilinear Hamiltonian with a sudden quench of the control parameters, we derive the analytical formalism for the characteristic function, the mean work density and mean irreversible work density. We show that the mean irreversible work may be used to detect quantum phase transitions and exhibit characteristic scaling at the quantum critical point for a single quench process. For a double quench process, a dynamical quantum phase transition may occur as a singularity in the so-called rate function. We examine our method in three models: the transverse Ising chain, the Su-Schrieffer-Heeger (SSH) model and the Bardeen-Cooper-Schrieffer (BCS) Hamiltonian for superconductivity. Our results for the Ising chain is in agreement with the Hamiltonian approach and yield the correct scaling exponents, while for the SSH model, we find nonuniversal quantum critical scaling due to the topological nature of its quantum phase transition. Quantum critical scaling and dynamical quantum phase transition were also obtained in the BCS model with single or double quench protocols in combination with the mean-field approximation. This suggests that our approach may be potentially extended to other many-body systems for future investigation of their dynamical properties under nonequilibrium condition.

I. INTRODUCTION

Nonequilibrium conditions provide an additional dimension in time domain for probing the many-body dynamics beyond the well-established equilibrium statistics and have recently led to the proposal of many novel phenomena such as the dynamical quantum phase transition\textsuperscript{1–4}, the time crystal\textsuperscript{5,6}, the fluctuation relations\textsuperscript{7–14}, and so on. While ultracold atoms in optical lattices can be easily tuned to be out of equilibrium\textsuperscript{15,16}, recent development of ultrafast pump-probe spectroscopy has enabled one to study the excitation and relaxation dynamics in real correlated materials\textsuperscript{17}. The study of nonequilibrium quantum physics is becoming one of the most active and exciting branches of modern condensed matter physics and attracted intensive attentions in recent years\textsuperscript{18}. Despite of many theoretical progresses including the nonequilibrium extension of the density matrix renormalization group, quantum master equations, Keldysh Green’s function technique and dynamical mean-field theory\textsuperscript{19–21}, we still lack a schematic framework to interpret the vast kinds of nonequilibrium phenomena.

Probability distribution of quantum work is arguably one of the most important quantities to characterize the nonequilibrium dynamics such as the dynamical fluctuations, quantum phase transitions (QPTs) and quantum criticality\textsuperscript{22–24}. Technically, it may be defined as

\[ p(w) = \sum_{n,m} \delta(W - E_m^f + E_n^i) P(m^f | n^i) P(n^i), \]

where \( w = W/N^d \) is the work density, \( N \) is the lattice size, \( d \) is the dimensionality, \( E_n^i \) is the \( n \)-th eigenvalue of the initial state \( (|n^i\rangle) \), and \( E_m^f \) is the \( m \)-th eigenvalue of the final state \( (|m^f\rangle) \). \( P(n^f) = \exp(-\beta E_n^f)/Z(0) \) denotes the probability distribution of the initial canonical state, and \( P(m^f | n^i) \equiv |\langle m^f | U(T_0,0) | n^i \rangle|^2 \) accounts for the transition probability between the initial and final states governed by the time-dependent evolution, \( U(T_0,0) = T \exp \left[ -i \int_0^{T_0} dt H(t) \right] \), where \( T \) is the time ordering operator and \( T_0 \) is the period for the time evolution. The reduced Planck constant \( \hbar \) is set to unity. The nonequilibrium dynamics is fully incorporated in the time-dependent Hamiltonian \( H(t) \) and the transition probability contains the key information characterizing the dynamical process.

The above method has been applied to a variety of many-body systems including the transverse Ising chain\textsuperscript{25–30}, the anisotropic XY model\textsuperscript{31}, the XXZ model\textsuperscript{32}, the Luttinger liquid\textsuperscript{33}, and the low-dimensional quantum gas\textsuperscript{34–38}. In most of these works, a Hamiltonian approach has been used by calculating explicitly the time evolution of the quantum state for quench protocol. However, such calculations can be very involved which makes it impossible to be extended to more general correlated many-body systems\textsuperscript{39,43}. To overcome this issue, here we propose to carry out the calculations straightforwardly using the functional field integral formalism. The latter has the advantage of numerical simplicity and may be extended to more complicated nonequilibrium processes beyond the quench protocol. Moreover, in combination with the auxiliary field method and mean-field approximation, it has the potential to be applied to more general correlated systems, in the cost of explicit state evolution.

The manuscript is organized as follows. In Section II, we first introduce the general formalism based on
the functional field integral approach and show that it can be used to identify both the equilibrium and dynamical QPTs. In Section III we apply it to three different models, including the well-studied transverse Ising model, the Su-Schrieffer-Heeger (SSH) model with topological phase transition and the Bardeen-Cooper-Schrieffer (BCS) model with superconductivity under mean-field approximation. We will discuss the QPTs in these models and derive the corresponding quantum critical exponents from the calculated mean irreversible work density. Section IV is the discussion and conclusions.

II. GENERAL FORMALISM

To proceed, we consider the bilinear model,

\[ H(t) = \sum_k \Psi^\dagger_k A_k(t) \Psi_k, \]

where \( A_k(t) = d_k(t) \cdot \sigma \) is a matrix and \( \sigma \) is the vector of the Pauli matrices. Although simple, it represents a large number of models in condensed matter physics. We first reformulate the functional field integral approach to calculate the Fourier transformation of the work distribution, namely the characteristic function:

\[ G(u) = \int_{-\infty}^{\infty} dw \exp \left( i u w N^d \right) p(w) \]

\[ = Z_0^{-1} \text{Tr} \left[ U^\dagger(T_0, 0) e^{i u H(T_0)} U(T_0, 0) e^{-(i u + \beta) H(0)} \right], \]

where \( Z_0 = \text{Tr} e^{-\beta H(0)} \) is the partition function at \( t = 0 \). The time contour of the functional field integral in \( G(u) \) is illustrated in Fig. 1. After some tedious calculations using the functional field integral techniques (see Appendix A), we obtain

\[ G(u) = \prod_k \frac{2 + \text{Tr} [B_k(T_0)]}{2 + \text{Tr} [e^{-\beta A_k(0)}]}, \]

where

\[ B_k(T_0) = C_k^\dagger(T_0) e^{i u A_k(T_0)} C_k(T_0) e^{-(i u + \beta) A_k(0)}, \]

where \( C_k(T_0) = C_k^\dagger(T_0) e^{i u A_k(T_0)} C_k(T_0) e^{-(i u + \beta) A_k(0)} \), with \( C_k(T_0) = T \exp \left[ -i \int_{T_0}^{T_0} dt A_k(t) \right] \). The mean work density is given by the first cumulant of the characteristic function,

\[ \langle w \rangle = -i \text{d} G(u) / \text{d} (N^d u) \big|_{u=0}, \]

yielding

\[ \langle w \rangle = \frac{1}{N^d} \sum_k \text{Tr} \left[ \left( D_k(T_0) - A_k(0) \right) e^{-\beta A_k(0)} \right], \]

with \( D_k(T_0) = C_k^\dagger(T_0) A_k(T_0) C_k(T_0) \), where \( C_k(T_0) \) can be computed numerically for arbitrary time dependence. Note that the mean work density \( \langle w \rangle \) always exceeds the free energy density difference \( \Delta f \) between the initial and final equilibrium states (both with the same inverse temperature \( \beta \)), as stated in the second law of thermodynamics. A mean irreversible work density can thus be defined as their difference, \( \langle w_{\text{irr}} \rangle = \langle w \rangle - \Delta f \geq 0 \), which characterizes the irreversibility of the nonequilibrium process and is directly related to the entropy increase between the final and initial equilibrium states, \( \Delta s = \beta \langle w_{\text{irr}} \rangle \), for a closed quantum system without heat transfer.

The mean work density \( \langle w \rangle \) and the mean irreversible work density \( \langle w_{\text{irr}} \rangle \) can be used to identify equilibrium phase transitions. Considering a quench process where the model Hamiltonian changes from \( A_k^0 = d_k^0 \cdot \sigma \) at time \( t = 0^- \) to \( A_k^1 = d_k^1 \cdot \sigma \) at \( t = T = 0^+ \), we have \( D_k(0^+) = A_k^1 \). As shown in Appendix B, one can derive an explicit formula for the free energy density difference,

\[ \Delta f = -\frac{1}{\beta N^d} \sum_k \ln \frac{\cosh^2 \left( \beta E_k^1 / 2 \right)}{\cosh^2 \left( \beta E_k^0 / 2 \right)}, \]

and the mean work density,

\[ \langle w \rangle = \frac{1}{N^d} \sum_k \left( E_k^1 - d_k^0 \cdot d_k^1 \right) \tan \left( \frac{\beta}{2} E_k^0 \right), \]

where \( E_k^{0,1} = \{ d_k^{0,1} \} \). Then the mean irreversible work density can be immediately obtained by definition. To see how these detect the phase transitions, we consider a small quench, \( d_k^{0,1} = \{ x_k^{0,1}, y_k^{0,1}, z_k^{0,1} \} \). It can be shown analytically (Appendix B) that \( \langle w \rangle = -\sum_k \frac{\delta^2}{\delta x_k} \left| x_k = x_k^0 \right. \) and \( \langle w_{\text{irr}} \rangle = \sum_k \frac{\delta^2}{2 N^d \delta x} \left| x_k = x_k^0 \right. \) at zero temperature, which connect directly to the first and second derivatives of the ground state energy with respect to the quench parameter. Thus the singularity in \( \langle w \rangle \) and \( \langle w_{\text{irr}} \rangle \) reflect the first or second-order phase transitions.

For a (second-order) QPT, scaling analysis of \( \langle w_{\text{irr}} \rangle \) can yield key information on the critical exponents. In the heat susceptibility limit, where \( \delta^{-\nu} \) is the largest length scale, the mean irreversible work density at zero temperature scales as

\[ \langle w_{\text{irr}} \rangle / \delta^2 \sim \lambda^{\nu(d+z)-2}, \quad \delta^{-\nu} > N > \lambda^{-\nu} \sim N^{2/\nu-(d+z)}, \quad \delta^{-\nu} > \lambda^{-\nu} > N, \]

where \( \nu \) is the correlation length exponent, \( z \) is the dynamical exponent, and \( \lambda \) reflects the distance from the

FIG. 1: (Color online) Time contour \( \mathcal{C} \) for the functional field integral. Dots on the forward and backward branches denote the discretized time points with \( \Delta t = T_0 / M \).
quantum critical point (QCP). In the thermodynamic limit, where $N$ is the largest length scale, one arrives at the scaling relation

$$\langle w_{\text{irr}} \rangle / \delta^2 \sim \delta^{(d+z)-2}, \quad N > \lambda - \nu > \delta - \nu$$

$$\sim \lambda^{(d+z)-2}, \quad N > \delta - \nu > \lambda - \nu. \quad (10)$$

On the other hand, if the system is prepared very close to the QCP such that $\lambda - \nu$ is larger than all other length scales, the scaling relation becomes

$$\langle w_{\text{irr}} \rangle / \delta^2 \sim \delta^{p(d+z)-2}, \quad \lambda - \nu > N > \delta - \nu$$

$$\sim N^2/(\nu - (d+z)), \quad \lambda - \nu > \delta - \nu > N. \quad (11)$$

Note that when the combination $\nu (d + z)$ exceeds 2, the scaling of $\langle w_{\text{irr}} \rangle$ is non-universal. In the marginal case, $\nu (d + z) = 2$, one may find additional logarithmic correction to above scaling.

Recently, it has also been shown that the work statistics in a double quench process, where the Hamiltonian changes from $A_0^0$ to $A_k^1$ at $t = 0$ and then back to $A_k^0$ for $t > T_0$, can be used to describe dynamical QPTs. In this case, the free energy density difference $\Delta f$ is zero and we have $\langle w_{\text{irr}} \rangle = \langle w \rangle$ and $D_k(T_0) = e^{i T_0 A_1^1 - i T_0 A_0^0}$. The mean irreversible work density is incapable of capturing the dynamical QPTs. On the other hand, the work distribution function, which in principle could be evaluated by inverse Fourier transformation of $G(u)$, is often ill-defined in numerical calculations. Lately, an alternative approach has been proposed based on the so-called Gärtner-Ellis theorem. Considering a global quench process, the quantum work grows exponentially with the system size, $p(w) \sim e^{-N^{\delta}r(w)}$, which defines the rate function $r(w) \geq 0$. The theorem states that $r(w)$ can be obtained via a Legendre-Fenchel transformation,

$$r(w) = -\inf_{R \in \mathbb{R}} \{w R - c(R)\}, \quad (12)$$

where $c(R) = -\lim_{N \to \infty} N^{-d} \ln G(u = i R)$ is a scaled cumulant generating function assumed to be differentiable with respect to the real variable $R \in \mathbb{R}$, and the infimum is evaluated within the domain of definition of $c(R)$ including $R = \pm \infty$. The dynamical QPT is then manifested as a singular point of $r(w)$, as discussed in Appendix B.

### III. NUMERICAL RESULTS

In this section, we use the above general formalism to study the work statistics and possible QPTs in three different models. The first model is the transverse Ising model, which has been extensively studied using the Hamiltonian approach and hence provides a good examination of our method. We then discuss the SSH model, where we will find corrections to the quantum work due to its topological properties. Last but not least, for possible extension to other correlated models in future studies, we discuss the well-known BCS model for superconductivity in combination with the mean-field approximation.

#### A. The transverse Ising model

The Hamiltonian of the transverse Ising model is:

$$H = -J \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x - h \sum_{j=1}^{N} \sigma_j^z, \quad (13)$$

where $\sigma_j^z (\alpha = x, z)$ are the Pauli matrices at site $j$, $J > 0$ is the ferromagnetic exchange coupling, $h$ is the transverse external field. Here we assume $N$ is even and consider the periodic boundary condition, $\sigma_{N+1}^z = \sigma_1^z$. This model has a quantum critical point at $h_0 = J$. Using the Jordan-Wigner transformation,

$$\sigma_j^+ = \frac{(\sigma_j^x + i \sigma_j^y)}{2} = c_j^\dagger \exp \left(i \pi \sum_{l < j} c_l^\dagger c_l \right), \quad (14)$$

it can be mapped to a spinless fermion model:

$$H = Nh - 2h \sum_{j=1}^{N} c_j^\dagger c_j - J \sum_{j=1}^{N} \left( c_j^\dagger - c_j \right) \left( c_{j+1}^\dagger - c_{j+1} \right), \quad (15)$$

where the fermionic operator $c_j$ satisfies either periodic or anti-periodic boundary conditions, $c_{j+1} = \pm c_j$, depending on odd or even number of the $c$-quasiparticles, $M = \sum_{j=1}^{N} c_j^\dagger c_j$. For simplicity, we confine ourselves to the subspace of even $M$ with anti-periodic boundary condition. Using $c_q = N^{-1/2} \sum_{j=1}^{N} c_j \exp(i q j)$, the fermionic Hamiltonian can be transformed into the bilinear form, $H = \sum_{k>0} \Psi_k^\dagger d_k \cdot \sigma \Psi_k$, where $\Psi_k^\dagger = (c_k^\dagger, c_{-k})$, $d_k = (0, -2J \sin k, -2h - 2J \cos k)$, and $k = \pm \pi (2m - 1)/N$ with $m = 1, \ldots, N/2$.

Below we set $J$ to unity and consider the quench protocol where the external field $h$ is tuned from its initial value $h_0$ to $h_1 = h_0 + \delta$. The dispersion relation is $\epsilon_k(h) = |d_k| = 2\sqrt{1 + h^2 + 2h \cos k}$. The characteristic function $G(u) = \prod_{k>0} G_k(u)$ for transverse Ising chain has an analytical form as shown in Eq. (13) of Appendix B. Figure 2 plots the characteristic function for a quench protocol across the QCP and the corresponding work distribution function obtained through the Gärtner-Ellis theorem at different temperatures. As discussed in Appendix B, the work distribution is restricted in the interval, $[w_{\text{min}}, w_{\text{max}}]$, where $w_{\text{min}}$ is the energy density difference of the highest excited state of the initial phase and the ground state of the final phase and $w_{\text{max}}$ is the energy density difference between the ground state of the initial phase and highest excited state of the final phase. At finite temperature, the small but finite $p(w)$ close to $w_{\text{min}}$ and $w_{\text{max}}$ reflects the finite weight of all possible configurations due to thermal effect. However, at zero temperature, since there is no weight for the excited state in the initial phase, $p(w)$ is strictly zero if $w$ is smaller than the energy density difference of the ground states of the initial and final Hamiltonians, as can be seen in Fig. 2(b). For all the temperatures, we have the normalization condition, $G(0) = \int_{-\infty}^{\infty} dw \, p(w) = 1$, as confirmed.
in Figs. 2(c) and (d). These results agree with those obtained using the Hamiltonian eigenstate approach.

The mean work density and mean irreversible work density at zero temperature can be obtained from Eqs. (7) and (8). Figure 3(a) plots the variation of \( \langle w_{\text{irr}} \rangle / \delta^2 \) as a function of \( h_0 \) and quenched back to \( h_0 = 0 \). We see clear cusp in the curve \( \delta \to 0 \) for different values of the lattice size \( N \), respectively. The lattice size is set to \( N = 20 \).

We now turn to the double quench protocol where the external field \( h \) is tuned from \( h_0 < 1 \) to \( h_1 > 1 \) at time \( t = 0 \) and quenched back to \( h_0 = 0 \) at \( t = T_0 \). Figure 4 plots the rate function as a function of \( h_0 \) and \( \lambda \) in the thermodynamic limit (\( N = 1000 \)) for \( \lambda = 0.01 \) in (d) and \( \delta = 0.01 \) in (e). (f) and (g) show the logarithmic scaling with \( N \) and \( \delta \) for \( \lambda = 0.0005 \), such that \( \lambda^+ \) is the largest length scale and the prequench Hamiltonian is very close to the quantum critical point. Other parameters are \( \delta = 0.001 \) in (f) and \( N = 1000 \) in (g).

a sequence of critical time, \( t_c = (n + 1/2)T^* \), with

\[
T^* = \frac{\pi}{2\sqrt{1 + (h_1)^2 - 2h_1 \frac{1 + h_1 h_0}{h_0 + h_1}}}.
\]

We should note that such singularity is not present in the the mean (irreversible) work density. As shown in the inset, the mean work density varies smoothly with \( T_0 \) and is insensitive to the dynamical QPT revealed in \( r(w, T_0) \).

The above results are in good agreement with previous studies using the Loschmidt echo, which is defined as \( L(t) = |\langle \psi | U(t) | \psi \rangle|^2 \) and represents the probability amplitude to recover the initial state after the time evolution \( U(t) \). For double quench process, the work probability function \( p(w = 0, T_0) \) also gives the return probability to the initial state and could therefore provide a signature when a dynamical QPT occurs. The excellent
agreement between our results and previous Hamiltonian eigenstate method confirms the validity of our functional field integral approach for both the single and double quench protocols. We may extend it to other models and examine there the effect of quantum criticality on nonequilibrium dynamics and the possible existence of dynamical QPTs under more general circumstances.

B. The SSH model

In this section, we study the SSH model which was originally proposed for electronic transport in polyacetylene with spontaneous dimerization\textsuperscript{53–57}. Despite its simplicity, the SSH model exhibits a variety of exotic phenomena, such as topological soliton excitation, fractional charge and nontrivial edge states, and has attracted extensive interest in past decades\textsuperscript{53–57}. The model Hamiltonian can be written as

\[ H = \sum_{j=1}^{N} \left( v c_{A,j}^\dagger c_{B,j} + v' c_{A,j+1}^\dagger c_{B,j} + h.c. \right), \]  

where \( A \) and \( B \) denote the two sublattices and \( N \) is the number of unit cells. For even \( N \) and open boundary condition, there exist two edge modes for \( v < v' \) but no edge mode for \( v > v' \). Thus the model undergoes a topological quantum phase transition at \( v = v' \). For periodic boundary condition, one may apply the Fourier transformation, \( c_{\alpha,j} = N^{-1/2} \sum_k c_{\alpha,k} \exp(ikj) \), where \( \alpha = A \) or \( B \), \( k = 2m\pi/N \) with \( m = 1 - N/2, \ldots, N/2 \). Then the bulk Hamiltonian gets the bilinear form, \( H = \sum_k \Psi_k^\dagger \mathbf{d}_k \cdot \sigma \Psi_k \), where \( \Psi_k = (c_{A,k}^\dagger, c_{B,k}^\dagger) \) and \( \mathbf{d}_k = (v + \cos k, \sin k, 0) \).

Details on the calculations of the mean work density and the mean irreversible work density can be found in the Appendix. Figure 5(a) plots the results as a function of \( v_0 \) for a single quench from \( v = v_0 \) to \( v_0 + \delta \) at \( v' = 1 \). In contrast to that of the transverse Ising model shown in Fig. 3, the mean work density exhibits a clear discontinuity at the critical point. Correspondingly, one observes a sharp resonance-like peak in the mean irreversible work density on a smooth background. As \( N \) increases, the background evolves into a broad peak, resembling that in the transverse Ising model, but the sharp resonance at the critical point becomes weakened. Except for a small region of the sharp peak around critical \( v_0 = 1 \), the mean irreversible work density in all other parameter ranges from the relatively smooth background exhibits

FIG. 4: (Color online) The rate function \( r(w, T_0) \) at zero temperature for a double quench process of the transverse Ising model from \( h_0 = 0.5 \) to \( h_1 = 2.0 \) and back to \( h_0 \) after time \( T_0 \). The lattice size is \( N = 100 \). The rate function for \( w = 0 \) corresponds to the Loschmidt echo and its nonanalyticity at \( T_0 = (n + 1/2)T^* \) manifests the dynamical QPTs. The inset shows the mean work density \( \langle w \rangle \), which exhibits no singularity and is a smooth function of \( T_0 \).

FIG. 5: (Color online) (a) The mean irreversible work density, \( \langle w_{irr} \rangle / \delta^2 \), as a function of \( v_0 \) for different lattice size \( N \). The inset plots the mean work density \( \langle w \rangle / \delta \) versus \( v_0 \), showing a clear jump at \( v_0 = 1 \) for small \( N \). (b) and (c) show the logarithmic dependence of \( \langle w_{irr} \rangle / \delta^2 \) on \( N \) and \( N = 100 \) in (c). (d) and (e) show its logarithmic scaling with respect to \( \delta \) and \( \lambda \) in the thermodynamic limit (\( N = 1000 \)) for \( \lambda = 0.01 \) in (d) and \( \delta = 0.01 \) in (e).
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We have \[ \text{rate function } r(w, T_0) \text{ at zero temperature for a double quench of the BCS Hamiltonian from } \Delta_0 = 0 \text{ to } \Delta_1 = 2 \text{ and back to } \Delta_0 \text{ after time } T_0 \text{ for } N = 50. \text{ In contrast to the singular behavior at } T_0 = (n + 1/2)T^* \text{ in the rate function, the mean work density } \langle w \rangle \text{ shown in the inset exhibits no singularity from dynamical QPTs.} \]

FIG. 9: (Color online) The rate function \( r(w, T_0) \) at zero temperature, as a function of the initial order parameter \( \Delta_0 \), for different lattice sizes \( N \). (b) shows the logarithmic scaling with respect to \( \delta \) and \( \lambda \) in the thermodynamic limit with \( N = 1000 \). Other parameters are \( \delta = 0.01 \) in (b) and \( \lambda = 0.01 \) in (c).

For single quench, we tune the mean-field parameter \( \Delta \) and the Nambu spinor \( \Psi \) from an initial value \( \Delta_0 \) to \( \Delta_1 = \Delta_0 + \delta \) such that \( \Psi_k = (-\Delta_0, 0, \xi_k) \) and \( \Psi_k = (-\Delta_1, 0, \xi_k) \). The irreversible work can then be calculated analytically (Appendix C). Figure 8(a) plots \( \langle w_{irr} \rangle / \delta^2 \) as a function of \( \Delta_0 \) for different lattice sizes \( N \). For large \( N \), a logarithmic divergence appears as \( \Delta_0 \) approaches zero. In this thermodynamical limit \( (N = \infty) \), as shown in Figs. 8(b) and 8(c), we also obtain logarithmic scaling with respect to \( \lambda \) and \( \delta \). This indicates that the critical exponents are \( \nu = 1/2 \) and \( z = 2 \) with \( d = 2 \).

For the double quench protocol, we change the order parameter from \( \Delta_0 \) to \( \Delta_1 \) at \( t = 0 \) and back to \( \Delta_0 \) at \( t = T_0 \). Using the Gärtner-Ellis theorem, we obtain the rate function \( r(w, T_0) \) in Fig. 9 with the initial order parameter \( \Delta_0 = 0 \). We see a clear nonanalytic behavior in \( r(w = 0, T_0) \) at the critical times \( t_c = (n + 1/2)T^* \), where \( T^* = \pi/\Delta_1 \). Once again, this indicates the existence of a dynamical QPT under double quench. Such a transition only occurs for \( \Delta_0 = 0 \) but is absent for any finite \( \Delta_0 \). It must be associated with the superconducting instability. We therefore speculate that the external driven field induces Cooper pair excitations around the initially free electron Fermi surface at \( \Delta_0 = 0 \). While the calculation of nonequilibrium dynamics might be otherwise involving for a general correlated Hamiltonian, extension of our approach to other strongly correlated phenomena is straightforward under the mean-field approximation.

IV. DISCUSSION AND CONCLUSIONS

Our proposal of the functional field integral approach provides an alternate way to calculate the quantum work in an arbitrary time evolution protocol with a general bilinear Hamiltonian. The characteristic function and its cumulants contain all the major information for evaluating the work distribution via the Gärtner-Ellis theorem and the mean (irreversible) work density, as well as the fidelity and Loschmidt echo in the double quench process. The applications of our approach to the transverse field Ising model, the SSH model, and the BCS model provide unambiguous evidences for signatures of quantum phase transitions and quantum criticality in the nonequilibrium process. In the sudden quench protocol, this is reflected in the quantum critical scaling of the mean irreversible work density, while in the double quench protocol, dynamical quantum phase transitions may be encoded as a

\[ H = \sum_k \Psi_k \left[ \begin{array}{cc} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{array} \right] \Psi_k, \]

where \( \xi_k = -2t[\cos(k_x) + \cos(k_y)] - 4t' \cos(k_x) \cos(k_y) - \mu \), with the chemical potential \( \mu \), the mean-field order parameter \( \Delta \) and the Nambu spinor \( \Psi_k = (c_k^\dagger, c_{-k}) \). The parameters \( t \) and \( t' \) denote the nearest-neighbor and next-nearest-neighbor hoppings on a two-dimensional lattice. We have \( k_x = 2\pi m/N \) and \( k_y = 2\pi l/N \) with \( m, l = 1 - N/2, \ldots, N/2 \), where \( N \) is the lattice size along both \( x \) and \( y \) directions. Hereafter we set \( t = 0.435 \), \( t' = 0.05 \) and \( \mu = 0.5 \).

For single quench, we tune the mean-field parameter \( \Delta \) from an initial value \( \Delta_0 \) to \( \Delta_1 = \Delta_0 + \delta \) such that \( \Psi_k = (-\Delta_0, 0, \xi_k) \) and \( \Psi_k = (-\Delta_1, 0, \xi_k) \). The irreversible work can then be calculated analytically (Appendix C). Figure 8(a) plots \( \langle w_{irr} \rangle / \delta^2 \) as a function of \( \Delta_0 \) for different lattice sizes \( N \). For large \( N \), a logarithmic divergence appears as \( \Delta_0 \) approaches zero. In this thermodynamical limit \( (N = \infty) \), as shown in Figs. 8(b) and 8(c), we also obtain logarithmic scaling with respect to \( \lambda \) and \( \delta \). This indicates that the critical exponents are \( \nu = 1/2 \) and \( z = 2 \) with \( d = 2 \).

For the double quench protocol, we change the order parameter from \( \Delta_0 \) to \( \Delta_1 \) at \( t = 0 \) and back to \( \Delta_0 \) at \( t = T_0 \). Using the Gärtner-Ellis theorem, we obtain the

\[ \langle w \rangle = \frac{1}{\delta} \left[ \xi_k - \Delta \right] \Psi_k, \]
singularity in the rate function. In the SSH model, we also see anomalous $1/N$ corrections due to the topological nature of the quantum phase transition. Compared to the Hamiltonian approach, the functional field integral formalism has the advantage to avoid tedious calculations of the second-order time differential equation and replace them by matrix products at different time intervals, which may be computed efficiently using optimized algorithms at the cost of explicit time evolution of the many-body wave function. Our approach may be extended to general interacting many-body systems in combination with the auxiliary field method to be solved under saddle-point or mean-field approximations. This was shown in our treatment of the BCS Hamiltonian, where a dynamical quantum phase transition is observed in a double quench process. It may be interesting to explore in the future how this dynamical transition is associated with the formation of Copper pairs near the Fermi surface. We also note that only global quench was considered throughout this work, so that translational invariance was kept and the momentum $k$ remains a good quantum number. In principle, our approach may also be applied to local quench or random systems by treating the matrix products in real space. An interesting future topic along this line would be the study of many-body localization within the framework of work statistics.

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Appendix A: Functional field integral approach to the characteristic function

The Hamiltonian we consider here is

$$H(t) = \sum_k \Psi_k^\dagger A_k(t) \Psi_k,$$

where $A_k(t) = d_k(t) \cdot \sigma$ and $\sigma$ is the vector of the Pauli matrices. Due to the Dirac delta in the work distribution function in Eq. (1), instead of calculating $p(u)$, it is often easier first to calculate its Fourier transformation, namely the characteristic function, $G(u) = \int_{-\infty}^{\infty} dw e^{iuw} N^d p(w)$. Because of translational invariance, we have $G(u) = \prod_k G_k(u)$ with

$$G_k(u) = \frac{\text{Tr} \left[ U_k(T_0, 0) e^{i u H_k(T_0)} U_k (T_0, 0) e^{-(i u + \beta) H_k(0)} \right]}{\text{Tr} \left[ e^{-\beta H_k(0)} \right]},$$

and

$$U_k (T_0, 0) = \lim_{M \to \infty} e^{-i H_k(t_{M,M+1}) \Delta t} \ldots e^{-i H_k(t_{1,2}) \Delta t},$$

where $T_0$ is divided into $M$ slices and $\Delta t = T_0/M$ is an infinitesimal time step as illustrated in Fig. (1). One may then write down the characteristic function by inserting a series of overcomplete bases of the fermionic coherent states on a closed time contour $(0 \to T_0 \to 0)^{\text{cts}}$,

$$\hat{\mathcal{S}} = \int d \left[ \bar{\psi}^\dagger, \psi^\dagger \right] e^{-\bar{\psi}^\dagger \bar{\psi} \psi^\dagger \psi} \langle \psi^\dagger | \psi^\dagger \rangle,$$

where $|\psi^\dagger \rangle$ is defined at $t_j$ with $j = 1, 2, \ldots, 2M + 2$ on the contour. This yields

$$G_k(u) = \frac{1}{\text{Tr} \left[ e^{-\beta H_k(0)} \right]} \left( \prod_{n=1}^{2M+2} d \left[ \bar{\psi}^n_k, \psi^n_k \right] \right) \exp \left( - \sum_{j=1}^{2M+2} \bar{\psi}^j_k \psi^j_k \right)$$

$$\times \left( - \bar{\psi}^{2M+2}_k \right) e^{i H_k(t_{2M+1,2M+2}) \Delta t} \left( \psi^{2M+1}_k \right) \ldots \left( \bar{\psi}^{M+3}_k \right) e^{i H_k(t_{M+2,M+3}) \Delta t} \left( \psi^M_k \right) \left( \psi^M_k \right) e^{i H_k(t_{1,2}) \Delta t} \left( \bar{\psi}^1_k \right) e^{-(i u + \beta) H_k(0)} \left( \psi^2_{M+2} \right).$$

(A5)
Using the definition $\langle \psi^n_k | \psi^n_k \rangle = \exp\left(\overline{\psi}^n_k \psi^n_k\right)$, we have for any $t$,
\[
\langle \psi^m_k | e^{\alpha H_k(t) \Delta t} | \psi^n_k \rangle \approx \exp\left(\overline{\psi}^m_k \ e^{\alpha \Delta t A_k(t)} \psi^n_k\right).
\]  
(A6)

Thus the partition function at a single model $k$ may be reformulated as
\[
Z_k(0) = \text{Tr} \left[ e^{-\beta H_k(0)} \right] = \int d \overline{\psi}, \psi \ e^{-\overline{\psi} \psi} \langle -\psi | e^{-\beta H_k(0)} | \psi \rangle
= \int d \overline{\psi}, \psi \ \exp \left[ -\overline{\psi} \left( I + e^{-\beta A_k(0)} \right) \psi \right] = \det \left( I + e^{-\beta A_k(0)} \right),
\]
(A7)

and similarly,
\[
G_k(u) = \frac{\det \left[ I + e^{\Delta t A_k(t_1,2)} \cdots e^{\Delta t A_k(t_{M,M+1})} e^{i u A_k(T_0)} e^{-i \Delta t A_k(t_{M,M+1})} \cdots e^{-i \Delta t A_k(t_{1,2})} e^{-(i u + \beta) A_k(0)} \right]}{\det \left[ I + e^{-\beta A_k(0)} \right]},
\]  
(A8)

where $I$ is the $2 \times 2$ identity matrix. In deriving above equations, we have used the relation $\text{det}(I + A) = 1 + \text{Tr} \ A + \text{det} \ A$ for any $2 \times 2$ matrix $A$ and the integral
\[
\int d \overline{\psi}, \psi \ \exp \left( -\overline{\psi} A \psi + \overline{\chi} \psi + \overline{\psi} \chi \right) = \text{det} \left( A \right) \exp \left( \overline{\chi} A^{-1} \chi \right).
\]  
(A9)

The above formula can be further simplified by defining $B_k(T_0) = C_k^1(T_0) e^{i u A_k(T_0)} C_k(T_0) e^{-(i u + \beta) A_k(0)}$, with $C_k(T_0) = \mathcal{T} \int_0^{T_0} dt A_k(t)$ for arbitrary time dependence of $A_k(t)$ between 0 and $T_0$. We have eventually
\[
G(u) = \prod_k \frac{\det \left[ I + B_k(T_0) \right]}{\det \left[ I + e^{-\beta A_k(0)} \right]} = \prod_k \frac{2 + \text{Tr} \left[ B_k(T_0) \right]}{2 + \text{Tr} \left[ e^{-\beta A_k(0)} \right]},
\]  
(A10)

The mean work density is given by the first cumulant of the characteristic function, $\langle w \rangle = -i \frac{dG(u)}{(Nd du)}|_{u=0}$, yielding
\[
\langle w \rangle = \frac{1}{N^d} \sum_k \frac{\text{Tr} \left[ \left(D_k(T_0) - A_k(0) \right) e^{-\beta A_k(0)} \right]}{2 + \text{Tr} \left[ e^{-\beta A_k(0)} \right]},
\]  
(A11)

where $D_k(T_0) = C_k^1(T_0) A_k(T_0) C_k(T_0)$. On the other hand, taking $u = i \beta$, one immediately derives the Jarzynski equality\cite{jarzynski1997},
\[
\langle e^{-\beta w N^d} \rangle = \langle e^{-\beta W} \rangle = \prod_k \frac{2 + \text{Tr} \left[ e^{-\beta A_k(T_0)} \right]}{2 + \text{Tr} \left[ e^{-\beta A_k(0)} \right]} = \frac{Z(T_0)}{Z(0)} = e^{-\beta \Delta F},
\]  
(A12)

where $\Delta F = F_1 - F_0$ is the free energy difference between the final and initial equilibrium states at the inverse temperature $\beta$, $Z(0)$ and $Z(T_0)$ are the partition functions at $t = 0$ and $t = T_0$, respectively. Recently, the quantum Jarzynski equality has been experimental verified in trapped ion system\cite{lever2021,martinez2021}.

**Appendix B: The work statistics and dynamical quantum phase transition**

For a single quench where the model Hamiltonian changes from $A_k^0 = d_k^0 \cdot \sigma$ at $t = 0^-$ to $A_k^1 = d_k^1 \cdot \sigma$ at $t = T_0 = 0^+$, the characteristic function is
\[
G(u) = \prod_k \frac{2 + \text{Tr} \left[ e^{i u A_k^1} e^{-(i u + \beta) A_k^0} \right]}{2 + \text{Tr} \left[ e^{-\beta A_k^0} \right]},
\]  
(B1)
An arbitrary matrix $A_k = d_k \cdot \sigma$ with $d_k = (x_k, y_k, z_k)$ may be diagonalized under the unitary transformation, $U_k^{-1} A_k U_k = D_k$, where

$$U_k = \begin{bmatrix} \mu_k & -\nu_k^* \\ \nu_k & \mu_k \end{bmatrix}, \quad D_k = \begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix}, \quad \text{(B2)}$$

with $E_k = |d_k|$, $\mu_k = \sqrt{(E_k + z_k)/2E_k}$, and $\nu_k = \frac{x_k + iy_k}{\sqrt{x_k^2 + y_k^2}} \sqrt{E_k - z_k}/2E_k$. The matrix exponential $e^{\alpha A_k}$ is then

$$e^{\alpha A_k} = U_k e^{\alpha D_k} U_k^{-1} = \begin{bmatrix} E_k \cosh(\alpha E_k) + z_k \sinh(\alpha E_k) & (E_k - i y_k) \sinh(\alpha E_k) \\ (x_k + i y_k) \sinh(\alpha E_k) & E_k \cosh(\alpha E_k) - z_k \sinh(\alpha E_k) \end{bmatrix}. \quad \text{(B3)}$$

We have

$$G_k(u) = \frac{1}{2} \operatorname{sech}^2 \left( \frac{\beta E_k^0}{2} \right) \left\{ 1 + \cos(u E_k^0) \cos \left[ E_k^0 (u - i \beta) \right] + \frac{d_k^0 \cdot d_k^1}{E_k^0 E_k^1} \sin \left[ E_k^0 (u - i \beta) \right] \right\}. \quad \text{(B4)}$$

where $E_k^{0,1} = |d_k^{0,1}|$.

From Eq. (A7), the free energy density difference between the final and initial states in a quench process can be written as,

$$\Delta f = \frac{\Delta F}{N^d} = -\frac{1}{\beta N^d} \sum_k \ln \frac{2 + \operatorname{Tr} \left[ e^{-\beta A_k(T_0)} \right]}{2 + \operatorname{Tr} \left[ e^{-\beta A_k(0)} \right]} = -\frac{1}{\beta N^d} \sum_k \frac{\ln \cosh^2 \left( \frac{\beta E_k^0}{2} \right)}{\cosh^2 \left( \frac{\beta E_k^0}{2} \right)}. \quad \text{(B5)}$$

From Eq. (A11) and considering $D_k(T_0) = A_k^1$ for the quench protocol, we have the mean work density,

$$\langle w \rangle = \frac{1}{N^d} \sum_k \frac{\operatorname{Tr} \left[ (A_k^1 - A_k^0) e^{-\beta A_k^0} \right]}{2 + \operatorname{Tr} \left[ e^{-\beta A_k^0} \right]} = \frac{1}{N^d} \sum_k \frac{\left( E_k^0 \right)^2 - d_k^0 \cdot d_k^1}{E_k^0} \tanh \left( \frac{1}{2} \beta E_k^0 \right). \quad \text{(B6)}$$

Combing above equations gives the mean irreversible work density, $\langle w_{irr} \rangle = \langle w \rangle - \Delta f$. For a small quench, $d_k^0 = (x_k^0, y_k^0, z_k^0) \rightarrow d_k^1 = (x_k^0 + \delta, y_k^0, z_k^0)$, we have the expansion,

$$E_k = E_k^0 + \frac{x_k^0 \delta}{E_k^0} + \frac{1}{2} \frac{(y_k^0)^2 + (z_k^0)^2}{(E_k^0)^3/2} + O(\delta^3). \quad \text{(B7)}$$

Thus at zero temperature

$$\langle w \rangle = \frac{1}{N^d} \sum_k \frac{-x_k^0 \delta}{E_k^0} = -\frac{1}{N^d} \sum_k \frac{\partial E_k}{\partial x_k} \bigg|_{x_k = x_k^0}, \quad \text{(B8)}$$

$$\langle w_{irr} \rangle = \frac{1}{N^d} \sum_k \left( \frac{-x_k^0 \delta}{E_k^0} + E_k^0 - E_k^0 \right) = \frac{1}{N^d} \sum_k \frac{\delta^2}{2} \left. \frac{E_k}{\partial x_k} \right|_{x_k = x_k^0}. \quad \text{(B9)}$$

We see that the singularity in $\langle w \rangle$ and $\langle w_{irr} \rangle$ reflects the first and second-order phase transitions, respectively.

The work distribution $p(w)$ may be calculated using the Fourier transformation of $G(u)$. In general, the energy density difference of the ground states, $\Delta w_{min} = \Delta f = -\frac{1}{N^d} \sum_k \left[ E_k^1 - E_k^0 \right]$ gives the minimal work that can be achieved at zero temperature, i.e., $p(w < \Delta w_{min}) = 0$ for $T = 0$. While at finite temperatures, even the highest excited state may have a small but finite weight due to thermal effect. Thus the minimal work $w_{min}$ that can be achieved is given by the energy density difference between the ground state of the postquench Hamiltonian with energy density $\epsilon^g = -\frac{1}{N^d} \sum_k E_k^1$ and the highest excited state of the initial Hamiltonian with the energy density $\epsilon^h = \frac{1}{N^d} \sum_k E_k^0$, yielding $w_{min} = -\frac{1}{N^d} \sum_k (E_k^1 + E_k^0)$. Oppositely, the maximal work $w_{max}$ is given by the energy density difference between the highest excited state of the postquench Hamiltonian with energy density $\epsilon^h = \frac{1}{N^d} \sum_k E_k^1$ and the ground excited state of the initial Hamiltonian with the energy density $\epsilon^g = -\frac{1}{N^d} \sum_k E_k^0$, yielding $w_{max} = \frac{1}{N^d} \sum_k (E_k^1 + E_k^0) = -w_{min}$. Beyond the interval $[w_{min}, w_{max}]$, the distribution function $p(w) = 0$ and the rate function $r(w) = \infty$ at all temperatures.
For a double quench, where the Hamiltonian changes from $A_0^t$ to $A_1^t$ at $t = 0$ and back to $A_0^t$ for $t \geq T_0$, we have $C_k(T_0) = e^{-i T_0 A_1^t_k}$. The characteristic function at zero temperature can be evaluated to be

\[
G(u) = \prod_k e^{i u E_k^0} \left\{ \cosh(-i u E_k^0) + \sinh(-i u E_k^0) \right\} \left\{ \cos^2(E_k^1 T_0) + \frac{2(d_k^1 \cdot d_k^0)^2 - (E_k^1 T_0)^2}{(E_k^1 T_0)^2} \right\}. \tag{B10}
\]

Because $c(R) = -\lim_{N \to \infty} \frac{1}{N} \ln G(u = i R)$ and $r(w = 0) = \inf_{R \in \mathbb{R}} c(R)$, the singularity in the rate function is associated with the roots of $G(R)$. Thus a dynamical quantum phase transition may occur at the critical time, $t_c = \left(\frac{(2n+1)\pi}{2 E_{k_c}}\right)$ $(n = 0, 1, 2, \ldots)$ if there exits a critical momentum $k_c$ satisfying $d_k^0 \cdot d_k^1 = 0$. Under this condition, we have at $T_0 = t_c$,

\[
G_{k_c}(R) = e^{-RE_{k_c}^0} \left\{ \cosh(RE_{k_c}^0) + \sinh(RE_{k_c}^0) \left[ \cos^2(n + \frac{\pi}{2}) - \sin^2(n + \frac{\pi}{2}) \right] \right\} = e^{-RE_{k_c}^0}. \tag{B11}
\]

Then the singularity occurs when $G(R) = \prod_k G_k(R) = 0$ as $R \to \infty$. While for all other $T_0 \neq t_c$ or $k \neq k_c$, there exists a term in the brace proportional to $e^{RE_{k_c}^0}$, which will cancel the prefactor $e^{-RE_{k_c}^0}$ and produce a nonzero $G(R)$ for all $R$.

Appendix C: Application to the models

For the transverse Ising chain, we have $d_k = (0, -2\sin k, -2h - 2\cos k)$. Using the dispersion relation $\epsilon_k(h) = |d_k| = 2\sqrt{1 + h^2 + 2h \cos k}$, we can calculate $\langle w_{irr} \rangle$ for the single quench from $h_0 < 1$ to $h_0 > 1$, 

\[
\langle w_{irr} \rangle = \frac{1}{N} \sum_k \left[ -\frac{\delta (h_0 + \cos k)}{\epsilon_k (h_0)} + \epsilon_k (h_1) - \epsilon_k (h_0) \right]. \tag{C1}
\]

Using $t_c = \left(\frac{(2n+1)\pi}{2 E_{k_c}}\right)$ and $d_k^0 \cdot d_k^1 = 0$ for the value of $k_c$, the critical times for the dynamical QPT during a double quench process are

\[
t_c = \frac{(n + 1/2) \pi}{2 \sqrt{1 + (h_1)^2 - 2h_1 \frac{1 + h_0}{\pi_0 + \pi_1}}}. \tag{C2}
\]

For the SSH model, we have $d_k = (v + \cos k, \sin k, 0)$ and $\epsilon_k(v) = |d_k| = \sqrt{1 + v^2 + 2v \cos k}$. Thus for a single quench from $v_0 < 1$ to $v_1 = v_0 + \delta > 1$,

\[
\langle w_{irr} \rangle = \frac{1}{N} \sum_k \left[ -\frac{\delta (v_0 + \cos k)}{\epsilon_k (v_0)} + \epsilon_k (v_1) - \epsilon_k (v_0) \right]. \tag{C3}
\]

Because of the topological nature of the QPT in the SSH model, there exists a band crossing at $k = \pi$ at the QCP. We can thus separate the mean irreversible work density into two terms, $\langle w_{irr} \rangle = \langle w_{irr} \rangle_{k \neq \pi} + \langle w_{irr} \rangle_{k = \pi}$. The results are shown in Fig. 4. While the first term gives the usual $\ln N$ scaling due to quantum criticality, the second term $\langle w_{irr} \rangle_{k = \pi} = \frac{1}{N} (\delta - \lambda)$ yields an additional $1/N$ contribution, which becomes dominant and leads to the anomalous $1/N$ scaling when $\lambda^{-\nu}$ is the largest length scale. For the double quench process, the critical times for the dynamical QPT are

\[
t_c = \frac{(n + 1/2) \pi}{\sqrt{1 + (v_1)^2 - 2v_1 \frac{1 + v_0 v_1}{v_0 + v_1}}} \tag{C4}
\]

For the BCS model with $d_k = (-\Delta, 0, \xi_k)$, the mean irreversible work density for the single quench process is

\[
\langle w_{irr} \rangle = \frac{1}{N^2} \sum_k \left[ -\frac{\delta \Delta_0}{\sqrt{\Delta_0^2 + \xi_k^2}} + \sqrt{\Delta_0^2 + \xi_k^2} - \sqrt{\Delta_0^2 + \xi_k^2} \right], \tag{C5}
\]

and the dynamical QPT during a double quench process with $\Delta_0 = 0$ occurs at

\[
t_c = \frac{(n + 1/2) \pi}{A_1}. \tag{C6}
\]

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\(^1\) M. Heyl, A. Polkovnikov, and S. Kehrein, Phys. Rev. Lett.
