Chapter 17
Quantum Thermodynamics at Impurity Quantum Phase Transitions

Abolfazl Bayat, Gabriele De Chiara, Tony J. G. Apollaro, Simone Paganelli, Henrik Johannesson, Pasquale Sodano and Sougato Bose

Abstract The study of quantum thermodynamics, i.e. equilibrium and non-equilibrium thermodynamics of quantum systems, has been applied to various many-body problems, including quantum phase transitions. An important question is whether out-of-equilibrium quantities from this emerging field, such as fluctuations of work, exhibit scaling after a sudden quench. In particular, it is very interesting to explore this problem in impurity models where the lack of an obvious symmetry breaking at criticality makes it very challenging to characterize. Here, by considering a spin emulation of the two impurity Kondo model and performing density matrix

A. Bayat (✉)
Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, Chengdu 610051, China
e-mail: abolfazl.bayat@uestc.edu.cn

A. Bayat · S. Bose
Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

G. De Chiara
School of Mathematics and Physics, Centre for Theoretical Atomic, Molecular, and Optical Physics, Queen's University Belfast, BT7 1NN London, UK

T. J. G. Apollaro
Department of Physics, University of Malta, MSD 2080, Msida, Malta

S. Paganelli
Dipartimento di Scienze Fisiche e Chimiche, Università dell'Aquila, via Vetoio, 67010 Coppito-LAquila, Italy

H. Johannesson
Department of Physics, University of Gothenburg, 412 96 Gothenburg, Sweden

Beijing Computational Science Research Center, Beijing 100094, China

P. Sodano
International Institute of Physics, Universidade Federal do Rio Grande do Norte, 59078-400 Natal, RN, Brazil
e-mail: pasquale.sodano01@gmail.com

INFN, Sezione di Perugia, Via A. Pascoli, 06123 Perugia, Italy

A. Ferraz et al. (eds.), *Strongly Coupled Field Theories for Condensed Matter and Quantum Information Theory*, Springer Proceedings in Physics 239,
https://doi.org/10.1007/978-3-030-35473-2_17

renormalization group computations, we establish that the irreversible work produced in a quench exhibits finite-size scaling at quantum criticality. Our approach predicts the equilibrium critical exponents for the crossover length and the order parameter of the model, and, moreover, implies a new exponent for the rescaled irreversible work.

17.1 Introduction

Impurities in the bulk of a material are the heart of solid state technologies which is exemplified by the computing revolution driven by the invention of transistors. In fact, even the addition of a single impurity can change the properties of matter. The theory of quantum impurities underpins much of the current understanding of correlated electrons. A case in point is the two-impurity Kondo model (TIKM) [1], with bearing on heavy fermion physics [2], correlation effects in nanostructures [3], spin-based quantum computing [4, 5], and more. The model describes two localized spin-1/2 impurities in an electron gas, coupled by the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction via their spin exchange with the electrons. In addition to the RKKY coupling, the model exhibits a second energy scale, the Kondo temperature T_K, below which the electrons may screen the impurity spins. For the sake of simplicity, in numerical computations, a spin chain emulation of the TIKM has been introduced which faithfully reproduces its physics [6]. Universal quantum quenches [7] and entanglement properties [8] of the TIKM model have been investigated.

Out-of-equilibrium thermodynamics of closed many-body systems subject to a variation of a Hamiltonian parameter has received considerable attention in the past few years, both experimentally and theoretically [9]. The increasing level of control over few-particle quantum systems has allowed to demonstrate experimentally the information-to-energy conversion and the Jarzynski equality [10–14]. On the one hand, the increasing level of control of simple systems consisting of a few quantum particles has led to the experimental possibility both of building the first quantum engines [15–17] and of investigating nonequilibrium theoretical predictions [11]. On the other hand, studies of the interplay between quantum thermodynamics, many-body physics, and quantum information, have shed light on fundamental aspects of thermalisation of closed quantum systems [19], fluctuation theorems [20], and prospects for quantum coherent thermal machines [21, 22].

A central issue is how the presence of a quantum phase transition (QPT) manifests itself in the out-of-equilibrium thermodynamics after a sudden quench of a Hamiltonian parameter [9, 19, 23–32]. In the sudden quench approach, the thermodynamic properties of a quantum system, initially at thermal equilibrium and experiencing a sudden variation of some global hamiltonian parameter, are investigated. It is now well established [24] that a second-order QPT is signaled by a discontinuity in the derivative of the *irreversible entropy production* (with the derivative taken with respect to the QPT driving parameter which is being quenched), as well as of the *variance of the work* [20]. This is to be contrasted with a first-order QPT, where the derivative of the *average work* (i.e. the first moment of the probability distribution function of the work) exhibits a discontinuity at the transition [28] (with a peak in the irreversible entropy production when the QPT is induced by a local quench [32]). The obvious parallels to the diverging behavior of response functions at a second-order equilibrium QPT prompts the question whether out-of-equilibrium quantities, like the *irreversible work* [20] (which is a measure of the nonadiabaticity of a quantum quench), may also exhibit scaling at criticality. Here, via a novel inroad—studying the quantum thermodynamics for a sudden quench across an impurity quantum critical point—we are able to provide an affirmative answer. Recent studies have also demonstrated a similar conclusion for first order transitions [33].

While for an ordinary bulk QPT the behavior of thermodynamic quantities after a sudden quench reflects the discontinuity of a corresponding equilibrium average value of a global observable [25], the same is not so obvious in an impurity quantum phase transition (iQPT) [34]. Local quenches in many-body quantum systems displaying iQPTs have not been investigated adequately. The lack of such works can be related both to the fact that iQPTs are a relatively new concept compared to the more well-established theory of QPTs classified according to the Ehrenfest-Landau scheme, and, most importantly but related, the identification of an order parameter exhibiting scaling properties according to some critical exponents for the iQPT has been only recently tackled [35, 36]. In ordinary QPTs the fact that the out-of-equilibrium thermodynamics of a global sudden quantum quench highlights the QPT point in the moments of the work probability distribution function (PDF) is due, in the final analysis, to the discontinuity of a corresponding equilibrium average value of a global observable, the latter being the order parameter. This holds, for instance, in spin models where the magnetization and the susceptibility show, respectively, discontinuities for 1st- and 2nd-order QPTs, thus reflecting in nonequilibrium quantum thermodynamics variables, which, as a consequence, inherit also the corresponding universality class scaling behaviour [37]. Moreover, as the irreversible entropy production can be related to the relative entropy of pre- and post-quenched thermal states, the abrupt change induced by the QPT of the latter (at low temperatures) is responsible for the its divergence at the critical point [25]. Based on these, one may ask whether, after a local quench of the impurity coupling, the behaviour of nonequilibrium quantum thermodynamic variables can reveal the iQPT?

In this paper, we elaborate on our results in [38] for the two-impurity Kondo model (TIKM) [39], one of the best studied models supporting an iQPT [2, 40–48]. Here, two spin-1/2 quantum impurities are coupled to each other by a Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction, and, in the simplest variant of the theory [45], to separate bulk reservoirs of conduction electrons by Kondo interactions. When the RKKY interaction dominates, the two impurities form a local spin-singlet state (RKKY phase), while in the opposite limit each of the impurities form a spatially extended singlet state with the electrons in the reservoir to which it is coupled (Kondo-screened phase). We shall show that the iQPT between these two phases is signaled both by the irreversible work production and the variance of work following a sudden quench. Remarkably, the irreversible work shows clear scaling with well-defined critical exponents, related to known equilibrium critical exponents by scaling laws. Moreover, by means of a small quench approximation for the irreversible work production, we are able to link the latter to the two-impurity spin correlation function, which is amenable to experimental determination. While our findings have broad ramifications, they are particularly timely considering recent breakthroughs in designing and performing measurements on tunable nanoscale realizations of the TIKM [3, 49, 50].

17.2 Two Impurity Kondo Model

For the purpose of exploring quantum critical properties of the TIKM, it is sufficient to focus on the spin sector of the model by considering its spin chain emulation which is sufficient to reproduce the underlying physics [6]. This can be emulated by the Kondo spin-chain Hamiltonian $H(K) = \sum_{m=L,R} H_m + H_I$ [6], where

$$\begin{aligned} H_m &= J' \left(J_1 \boldsymbol{\sigma}_1^m \cdot \boldsymbol{\sigma}_2^m + J_2 \boldsymbol{\sigma}_1^m \cdot \boldsymbol{\sigma}_3^m \right) + \\ &\quad + J_1 \sum_{i=2}^{N_m - 1} \boldsymbol{\sigma}_i^m \cdot \boldsymbol{\sigma}_{i+1}^m + J_2 \sum_{i=2}^{N_m-2} \boldsymbol{\sigma}_i^m \cdot \boldsymbol{\sigma}_{i+2}^m, \\ H_I &= J_1 K \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R. \end{aligned} \tag{17.1}$$

Here $m = L, R$ labels the left and right chains with $\boldsymbol{\sigma}_i^m$ the vector of Pauli matrices at site i in chain m, and with J_1 (J_2) nearest- (next-nearest-) neighbor couplings (see Fig. 17.1). In the following we set $J_1 = 1$ as our energy unit. The parameter $J' > 0$ plays the role of antiferromagnetic Kondo coupling and K represents the dimensionless RKKY coupling between the impurity spins $\boldsymbol{\sigma}_1^L$ and $\boldsymbol{\sigma}_1^R$. The total size of the system is thus $N = N_L + N_R$. By fine tuning J_2/J_1 to the critical point $(J_2/J_1)_c = 0.2412$ of the spin chain dimerization transition [51, 52] all logarithmic scaling corrections vanish, allowing for an unambiguous fit of numerical data using the Density Matrix Renormalization Group (DMRG) [53–55]. Indeed, a DMRG study reveals that the Hamiltonian (17.1) faithfully reproduces the features of the iQPT in the TIKM [6].

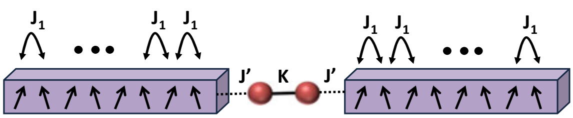

Fig. 17.1 Schematic of the two impurity Kondo mode. The two-impurity Kondo spin chain model consists of two spin-1/2 impurities, each interacting with an array of spin-1/2 particles via a Kondo coupling J'. The two impurity interacts with each other via an inter-impurity RKKY coupling K which serves as the control parameter. By varying K system exhibits a second order quantum phase transition at a critical value $K = K_c$ which depends on the impurity coupling J'

17.3 Thermodynamic Properties: Work Distribution

We assume that the impurity coupling is initially K. The system is at zero temperature in its ground state $|E_0(K)\rangle$ with energy $E_0(K)$. The impurity coupling is then quenched infinitesimally from K to $K + \Delta K$, with the Hamiltonian $H(K)$ suddenly changed to $H(K + \Delta K)$. The work performed on the system becomes a stochastic variable W described by the probability distribution function (PDF) [20]

$$p(W) = \sum_m \left|\left\langle E'_m \right| E_0(K)\rangle\right|^2 \delta\left[W - (E'_m - E_0(K))\right], \tag{17.2}$$

where $\{E'_m\}$ and $\{\left|E'_m\right\rangle\}$ are the eigenenergies and eigenvectors of $H(K + \Delta K)$, respectively. Notice that the work PDF is an experimentally accessible quantity [56, 57] and that from its knowledge all the statistical moments can be derived as

$$\left\langle W^n \right\rangle = \int W^n p(W) dW. \tag{17.3}$$

Due to the nature of the sudden quench in the Hamiltonian, the system is driven out of equilibrium and, by means of the Jarzynski fluctuation relation [10], it is possible to define the so-called *irreversible work*:

$$W_{irr} = \langle W \rangle - \Delta F \geq 0\,, \tag{17.4}$$

where ΔF is the difference between the free energies after and before the quench. Since we assume zero temperature, ΔF is simply the difference of the post- and pre-quench ground state energies. The irreversible work has a simple physical explanation as the amount of energy which has to be taken out from the quenched system in order to bring it to its new equilibrium state which, for our case, is the ground state of $H(K + \Delta K)$ [27]. For the instantaneous quantum quench we have

$$W_{irr} = \langle E_0(K)|\, H(K + \Delta K)\, |E_0(K)\rangle - E'_0(K + \Delta K)\,, \tag{17.5}$$

i.e., the irreversible work is given by the difference between the expectation value of the post-quenched Hamiltonian evaluated on the pre-quenched ground state and the post-quench ground state energy. It is worth emphasizing that the (17.2) and (17.5) are truly out-of-equilibrium quantum thermodynamic quantities, although evaluated at equilibrium due to the sudden quench approximation. In fact, for quasi-static processes, the work PDF would be a delta function peaked at the energy difference between the pre- and post-quenched ground states, whereas the irreversible work would result identically null. Instead, in the sudden quench case, which approximates the case where the quench is performed at a rate much faster than the typical time evolution scale of the pre-quenched ground state, both quantities give a measure of the irreversibility by performing the quench [10, 27].

17.4 Scaling of the Irreversible Work

In order to capture the iQPT between the Kondo regime and the RKKY phase, we introduce the rescaled quantity

$$\widetilde{W}_{irr} = \frac{W_{irr}}{\Delta K^2}\,, \tag{17.6}$$

and study the variation of $\widetilde{W}_{irr}$ when the coupling K is varied. In this paper we only consider infinitesimal quantum quenches, $\Delta K \ll 1$. In Fig. 17.2a, b we plot the irreversible work $\widetilde{W}_{irr}$ for two impurity couplings $J' = 0.4$ and $J' = 0.5$ respectively. It is clear from the plots that $\widetilde{W}_{irr}$ shows a sharp peak which becomes even more pronounced by increasing the system size N (apart from slightly shifting towards lower values of K's). This signifies that $\widetilde{W}_{irr}$ exhibits non-analytic behaviour at the critical point in the thermodynamic limit. In finite-size systems, such as the ones considered here, the position of the peak determines the critical point K_c which slowly moves towards the left by increasing N.

By considering the specific value of the RKKY coupling K at which $\widetilde{W}_{irr}$ diverges, one can determine numerically the critical point K_c, which then shows a particular

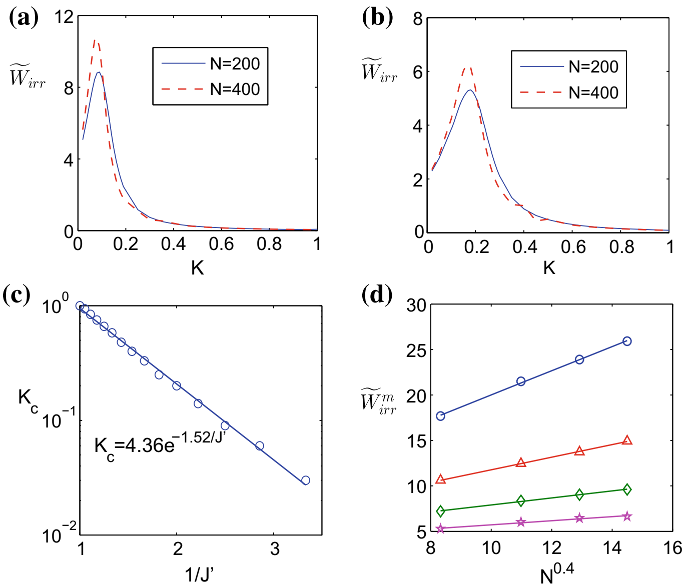

Fig. 17.2 The rescaled irreversible work near criticality. The irreversible work $\widetilde{W}_{irr}$ in terms of K in a chain with **a** $J' = 0.4$; **b** $J' = 0.5$. **c** The critical coupling K_c (blue circles) versus $1/J'$ in a semi-logarithmic scale and its exponential fit (blue line). **d** The maximum of the irreversible work W^m_{irr} versus $N^{0.4}$ and the linear fits. From top to bottom: $J' = 0.4$; $J' = 0.5$; $J' = 0.6$ and $J' = 0.7$. From [38]

dependence on $1/J'$, just as the Kondo temperature T_K (which sets the energy scale for the weak-to-strong of the renormalized Kondo coupling [39]). This can be seen in Fig. 17.2c in which the critical coupling K_c is plotted as a function of $1/J'$. The manifest linear trend in a semi-logarithmic scale confirms that

$$K_c \sim e^{-a/J'} \sim T_K \tag{17.7}$$

for some constant a, in agreement with other studies of the two-impurity Kondo spin chain [6, 35].

In the finite-size systems studied here, the divergence of $\widetilde{W}_{irr}$ at $K = K_c$ appears as a finite peak becoming more prominent for increasing system size, as shown in Fig. 17.2a, b. We define the maximum of the irreversible work as $\widetilde{W}^m_{irr} = \widetilde{W}_{irr}(K = K_c)$. Since $\widetilde{W}^m_{irr}$ increases by increasing the system size N one can try to fit it by an algebraic map of the form

$$\widetilde{W}^m_{irr} \sim N^{\lambda}, \tag{17.8}$$

where λ is a positive exponent. In fact, a perfect match is found for various impurity couplings J' by choosing $\lambda = 0.4$ as depicted in Fig. 17.2d. Note that the exponent λ governs the scaling of a purely non-equilibrium quantity with system size. Note that, whereas for a *global* quench the irreversible work is expected to have a functional dependence on the system size because in (17.4) both the work and the free energy become extensive quantities, it is far from trivial that the same holds for a *local* quench. Nevertheless, in the TIKM here considered, this behavior of $\widetilde{W}^m_{irr}$ is determined by the distinctive nature of the iQPT, where a local change in the RKKY coupling induces a global rearrangement of the ground state of the total system at criticality.

The above analysis for $\widetilde{W}_{irr}$ suggests the Ansatz:

$$\widetilde{W}_{irr} = \frac{A}{|K - K_c|^{\kappa} + BN^{-\lambda}}, \tag{17.9}$$

where A and B are two constants that may vary with J'. This Ansatz is based on the fact that $\widetilde{W}_{irr}$ diverges in the thermodynamic limit as $\widetilde{W}_{irr} \sim |K - K_c|^{-\kappa}$, while for finite-size systems at $K = K_c$ it increases algebraically with the system size as in (17.8). In order to deal with the divergence more conveniently at the critical point we define a normalized function as

$$W_{nor} = (\widetilde{W}^m_{irr} - \widetilde{W}_{irr})/\widetilde{W}^m_{irr}. \tag{17.10}$$

Using the Ansatz of (17.9) one can show that

$$W_{nor} = g(N^{\lambda/\kappa}|K - K_c|), \tag{17.11}$$

where $g(x)$ is a scaling function which can be determined numerically. In order to evaluate the exponent κ we search for the value of κ such that the values of W_{nor} as

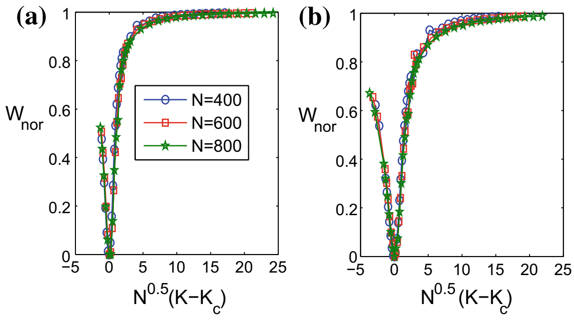

Fig. 17.3 Finite-size scaling. The finite-size scaling of W_{nor} according to the Ansatz of (17.11) for: **a** $J' = 0.4$; **b** $J' = 0.5$. From [38]

a function of $N^{\lambda/\kappa}|K - K_c|$, for various system sizes N, collapse on each other, as shown in Fig. 17.3a, b for two different impurity couplings $J' = 0.4$ and $J' = 0.5$ respectively. As is evident from the figure, using the predetermined exponent $\lambda = 0.4$, one finds that $\kappa = 0.8$.

The irreversible work has been measured in quantum mechanical setups using various methods [13, 14]. Here we follow a different route, showing that, for the present system and for small quenches, one can rely on measuring only the two-impurity correlation function $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle$ with respect to the ground state. The SU(2) symmetry of the Hamiltonian (17.1) implies that the reduced density matrix of the two impurities is always a Werner state

$$\rho_{1_L,1_R} = \frac{3 + \langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle}{12} I_4 - \frac{\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle}{3} |\psi^-\rangle\langle\psi^-|, \tag{17.12}$$

where $|\psi^-\rangle$ is the singlet state, I_4 represents the 4×4 identity matrix and $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle$ is the two-point correlation function of the impurity spins with respect to the ground state. It is immediate to see that the two-point correlation functions determine all the properties of the two impurities [58], including their entanglement (measured by concurrence [59]) which becomes

$$C = \max\left\{ -\frac{1 + \langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle}{2}, 0 \right\}. \tag{17.13}$$

By expanding (17.5) for small ΔK we obtain

$$\widetilde{W}_{irr} = -\frac{1}{2} \frac{\partial \langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle}{\partial K}. \tag{17.14}$$

The divergence of $\widetilde{W}_{irr}$ at the critical point and (17.14) suggest that the two-point impurity correlator $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle$ mimics the behavior of an order parameter, capturing the quantum criticality and showing scaling behavior near the transition. In Fig. 17.4a, b we plot the spin correlator $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle$ versus the coupling K for two impurity couplings

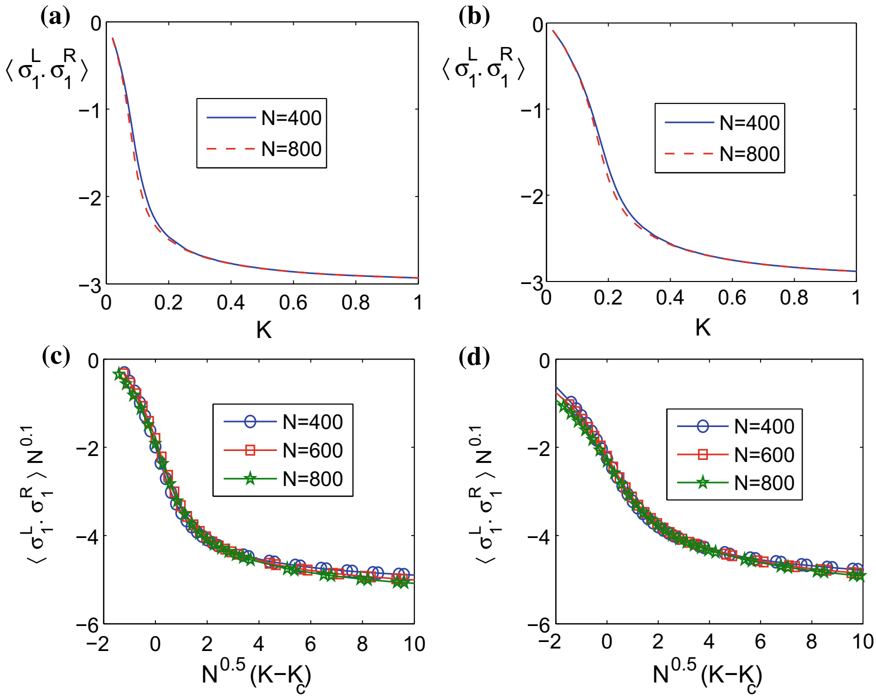

Fig. 17.4 Two-point impurity correlation function. Correlation function $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle$ of the two impurities versus RKKY coupling K in a chain with **a** $J' = 0.4$; **b** $J' = 0.5$. The finite-size scaling for $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle$ with **c** $J' = 0.4$; **d** $J' = 0.5$ [38]

$J' = 0.4$ and $J' = 0.5$ respectively. The correlator varies from 0 (for $K = 0$) in the Kondo regime to $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle = -3$ (for very large K) deep in the RKKY phase. To extract its scaling properties, we make the finite-size-scaling Ansatz

$$\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle = N^{-\beta/\nu} f(N^{1/\nu}|K - K_c|), \tag{17.15}$$

where, in the limit $N \to \infty$, β characterizes scaling of the correlator near criticality, $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle \sim |K - K_c|^{\beta}$, ν is the exponent governing the divergence of the crossover scale $\xi \sim |K - K_c|^{-\nu}$ [42, 46], and $f(x)$ is a scaling function. In order to determine these critical exponents we identify the values of β and ν such that the plots of $\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle N^{\beta/\nu}$ as a function of $N^{1/\nu}|K - K_c|$ collapse to a single curve for arbitrary system sizes, as shown in Fig. 17.4c, d. The best data collapse is achieved by choosing $\beta = 0.2$ and $\nu = 2$, which are in excellent agreement with the ones found from the analysis of the Schmidt gap [35].

Furthermore, as an alternative way of computing the scaling of the irreversible work $\widetilde{W}_{irr}$, one may directly differentiate both sides of (17.15) with respect to the RKKY coupling K to get

$$\widetilde{W}_{irr} \sim \partial_K \langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \rangle \sim N^{(1-\beta)/\nu} f'(N^{1/\nu}|K - K_c|), \tag{17.16}$$

where $f'(x) = \mathrm{d}f/\mathrm{d}x$. The finite-size scaling of (17.16) implies that $\widetilde{W}_{irr} \sim |K - K_c|^{\beta-1}$, which then leads to

$$\kappa = 1 - \beta. \tag{17.17}$$

Moreover, comparing (17.16) and (17.11), we obtain another constraint between the exponents as

$$\kappa = \lambda\nu. \tag{17.18}$$

Equation (17.17) and (17.18) are indeed satisfied for the values found in our numerical analysis as $\lambda = 0.4$, $\nu = 2$, $\beta = 0.2$ and $\kappa = 0.8$, confirming our scaling Ansätze.

It is worth emphasizing that in our local quench problem the energy change, for every finite quench, is always finite and, for an infinitesimal quench ΔK, the irreversible work can be approximated by $W_{irr} \simeq -\Delta K \Delta \left\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \right\rangle /2$. Since $\left\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \right\rangle$ varies between 0 and 3, then $W_{irr} \leq -3\Delta K/2$, which vanishes for $\Delta K \to 0$. As a consequence, the un-rescaled irreversible work W_{irr} shows no divergences even as $N \to \infty$.

17.5 Variance Analysis of Work

The variance of work is another important non-equilibrium quantity which is defined as

$$\Delta W^2 = \left\langle W^2 \right\rangle - \langle W \rangle^2 \ . \tag{17.19}$$

For convenience, we also rescale the variance as $\Delta\widetilde{W}^2 = \Delta W^2/\Delta K^2$. For a sudden quench one can show that

$$\Delta\widetilde{W}^2 = 3 - 2\left\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \right\rangle - \left\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \right\rangle^2 . \tag{17.20}$$

The derivative of the rescaled variance with respect to K becomes

$$\partial_K(\Delta\widetilde{W}^2) = 4\left(1 + \left\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \right\rangle\right) \widetilde{W}_{irr}. \tag{17.21}$$

Since the correlation function $\left\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \right\rangle$ is always finite, both $\widetilde{W}_{irr}$ and $\partial_K(\Delta\widetilde{W}^2)$ diverge at the critical point in the thermodynamic limit. Moreover, $\Delta\widetilde{W}^2$ takes its maximum for values of K slightly smaller than K_c where $\left\langle \boldsymbol{\sigma}_1^L \cdot \boldsymbol{\sigma}_1^R \right\rangle = -1$, i.e. the minimum value of K at which the two impurities are entangled [6].

17.6 Out-of-Equilibrium Features

We should emphasise the fact that both the irreversible work and the variance of work are truly out-of-equilibrium quantum thermodynamic quantities, although evaluated at equilibrium due to the sudden small-quench approximation. In fact, for quasi-static processes, the irreversible work would result identically null as the work equals the free energy difference, and the work PDF would be a delta function peaked at the energy difference between the pre- and post-quenched ground states, resulting in zero variance. In the sudden quench case, however, both quantities give certain measures of irreversibility [10, 27]. Moreover, as another feature of non-equilibrium, we should point out that whereas a temperature can be associated to the initial state (which is $T = 0$ in our analysis), the same does not hold after the quench has been performed.

17.7 Summary

In this paper, we have numerically shown that both irreversible work and work variance, as non-equilibrium quantities, signal the impurity quantum phase transition between the Kondo and RKKY regimes in the TIKM. Both quantities exhibit scaling at the quantum critical point, and allow for known equilibrium critical exponents to be extracted. In addition, a new critical exponent κ, governing the behavior of the rescaled irreversible work at the phase transition, is brought to light. Importantly, all out-of-equilibrium quantities considered are amenable to experimental observation in solid-state nanostructures or ultra cold atoms, since ultimately it is sufficient to measure a two-point spin correlation function.

References

1. C. Jayprakash, H.R. Krishna-murthy, J.W. Wilkins, Two-impurity kondo problem. Phys. Rev. Lett. **47**, 737 (1981)
2. B.A. Jones, C.M. Varma, J.W. Wilkins, Low- temperature properties of the two-impurity Kondo Hamiltonian. Phys. Rev. Lett. **61**, 125 (1988)
3. J. Bork, Y.-H. Zhang, L. Diekhöner, Lázló Borda, P. Simon, J. Kroha, P. Wahl, K. Kern, A tunable two-impurity Kondo system in an atomic point contact. Nat. Phys. **7**, 901 (2011)
4. J. Mravlje, A. Ramsak, T. Rejec, Conductance of a molecule with a center of mass motion. Phys. Rev. B **74**, 205320 (2006)
5. S.Y. Cho, R.H. McKenzie, Quantum entanglement in the two-impurity Kondo model. Phys. Rev. A **73**, 012109 (2006)
6. A. Bayat, S. Bose, P. Sodano, H. Johannesson, Entanglement probe of two-impurity Kondo physics in a spin chain. Phys. Rev. Lett. **109**, 066403 (2012)
7. A. Bayat, S. Bose, H. Johannesson, P. Sodano, Universal single-frequency oscillations in a quantum impurity system after a local quench. Phys. Rev. B **92**, 155141 (2015)
8. A. Bayat, Scaling of Tripartite Entanglement at Impurity Quantum Phase Transitions. Phys. Rev. Lett. **118**, 036102 (2017)
9. A. Polkovnikov, K. Sengupta, A. Silva, M. Vengalattore, Colloquium: Nonequilibrium dynamics of closed interacting quantum systems. Rev. Mod. Phys. **83**, 863 (2011)

10. C. Jarzynski, Nonequilibrium equality for free energy differences. Phys. Rev. Lett. **78**, 2690 (1997)
11. S. Toyabe, T. Sagawa, M. Ueda, E. Muneyuki, M. Sano, Experimental Demonstrations of Information-to-Energy Conversion and Validation of the Generalized Jarzynski Equality. Nat. Phys. **6**, 988 (2010)
12. J.V. Koski, V.F. Maisi, J.P. Pekola, D.V. Averin, Experimental realization of a Szilard engine with a single electron. Proc. Natl. Acad. Sci. U.S.A. **111**, 13786 (2014)
13. T.S. Batalhao, A.M. Souza, L. Mazzola, R. Auccaise, R.S. Sarthour, I.S. Oliveira, J. Goold, G. De Chiara, M. Paternostro, R.M. Serra, Experimental reconstruction of work distribution and study of fluctuation relations in a closed quantum system. Phys. Rev. Lett. **113**, 140601 (2014)
14. S. An, J.-N. Zhang, M. Um, D. Lv, Y. Lu, J. Zhang, Z. Yin, H.T. Quan, K. Kim, Experimental test of quantum Jarzynski equality with a trapped ion system. Nat. Phys. **11**, 193 (2015)
15. O. Fialko, D.W. Hallwood, Isolated quantum heat engine. Phys. Rev. Lett. **108**, 085303 (2012)
16. O. Abah, J. Rossnagel, G. Jacob, S. Deffner, F. Schmidt-Kaler, K. Singer, E. Lutz, Single-ion heat engine at maximum power. Phys. Rev. Lett. **109**, 203006 (2012)
17. J. Roßnagel, S.T. Dawkins, K.N. Tolazzi, O. Abah, E. Lutz, F. Schmidt-Kaler, K. Singer, A single-atom heat engine. Science **352**, 325 (2016)
18. G. Maslennikov, S. Ding, R. Habltzel, J. Gan, A. Roulet, S. Nimmrichter, D. Matsukevich, Quantum absorption refrigerator with trapped ions. Nat. Commun. **10**, 202 (2019)
19. J. Eisert, M. Friesdorf, C. Gogolin, Quantum many-body systems out of equilibrium. Nat. Phys. **11**, 124 (2015)
20. M. Campisi, P. Hänggi, P. Talkner, Colloquium: quantum fluctuation relations: foundations and applications. Rev. Mod. Phys. **83**, 771 (2011)
21. J. Goold, M. Huber, A. Riera, L. del Rio, P. Skrzypczyk, The role of quantum information in thermodynamics—a topical review, J. Phys. A: Math. Theor. **49**, 143001 (2016)
22. M.T. Mitchison, *Quantum thermal absorption machines: refrigerators, engines and clocks*, arxiv:1902.02672
23. P. Talkner, E. Lutz, P. Hänggi, Fluctuation theorems: work is not an observable. Phys. Rev. E **75**, 050102(R) (2007)
24. A. Silva, Statistics of the work done on a quantum critical system by quenching a control parameter. Phys. Rev. Lett. **101**, 120603 (2008)
25. R. Dorner, J. Goold, C. Cormick, M. Paternostro, V. Vedral, Emergent thermodynamics in a quenched quantum many-body system. Phys. Rev. Lett. **109**, 160601 (2012)
26. L. Fusco, S. Pigeon, T.J.G. Apollaro, A. Xuereb, L. Mazzola, M. Campisi, A. Ferraro, M. Paternostro, G. De Chiara, Assessing the nonequilibrium thermodynamics in a quenched quantum many-body system via single projective measurements. Phys. Rev. X **4**, 031029 (2014)
27. F. Plastina, A. Alecce, T. J. G. Apollaro, G. Falcone, G. Francica, F. Galve, N. Lo Gullo, R. Zambrini, Irreversible work and inner friction in quantum thermodynamic processes. Phys. Rev. Lett. **113**, 260601 (2014)
28. E. Mascarenhas, H. Bragança, R. Dorner, M. França, Santos, V. Vedral, K. Modi, J. Goold, Work and quantum phase transitions: quantum latency. Phys. Rev. E **89**, 250602 (2014)
29. A. Sindona, J. Goold, N. Lo Gullo, F. Plastina, Statistics of the work distribution for a quenched fermi gas. New J. Phys. **16**, 045013 (2014)
30. S. Paganelli, T.J.G. Apollaro, Irreversible work versus fidelity susceptibility for infinitesimal quenches. Int. J. Mod. Phys. B **31**, 1750065 (2017)
31. F. Cosco, M. Borrelli, P. Silvi, S. Maniscalco, G. De Chiara, Non-equilibrium quantum thermodynamics in Coulomb crystals. Phys. Rev. A **95**, 063615 (2017)
32. T.J.G. Apollaro, G. Francica, M. Paternostro, M. Campisi, *Work Statistics, Irreversible Heat and Correlations Build-up in Joining Two Spin Chains* (2014), arXiv:1406.0648
33. D. Nigro, D. Rossini, E. Vicari, *Scaling properties of work fluctuations after quenches at quantum transitions*, arxiv:1810.04614
34. M. Vojta, Impurity quantum phase transitions. Philos. Mag. **86**, 1807 (2006)
35. A. Bayat, H. Johannesson, S. Bose, P. Sodano, An order parameter for impurity systems at quantum criticality. Nat. Commun. **5**, 3784 (2014)

36. L. Wang, H. Shinaoka, M. Troyer, *Fate of the Kondo Effect and Impurity Quantum Phase Transitions Through the Lens of Fidelity Susceptibility* (2015), arXiv:1507.06991
37. S. Lorenzo, J. Marino, F. Plastina, G. M. Palma, T.J.G. Apollaro, Quantum critical scaling under periodic driving. Sci. Rep. **7**, 5672 (2017)
38. A. Bayat, T.J.G. Apollaro, S. Paganelli, G. De Chiara, H. Johannesson, S. Bose, P. Sodano, Nonequilibrium critical scaling in quantum thermodynamics. Phys. Rev. B **93**, 201106(R) (2016)
39. C. Jayaprakash, H.-R. Krishnamurthy, J. Wilkins, Two-impurity Kondo problem. Phys. Rev. Lett. **47**, 737 (1981)
40. B.A. Jones, C.M. Varma, Critical point in the solution of the two magnetic impurity problem. Phys. Rev. B **40**, 324 (1989)
41. I. Affleck, A.W.W. Ludwig, Exact critical theory of the two-impurity Kondo model. Phys. Rev. Lett. **68**, 1046 (1992)
42. I. Affleck, A.W.W. Ludwig, B.A. Jones, Conformal-field-theory approach to the two-impurity Kondo problem: comparison with numerical renormalization group results. Phys. Rev. B **52**, 9528 (1995)
43. C. Sire, C.M. Varma, H.R. Krishnamurthy, Theory of the non-Fermi-liquid transition point in the two-impurity Kondo model. Phys. Rev. B **48**, 13833 (1993)
44. J. Gan, Mapping the critical point of the two-impurity Kondo model to a two-channel problem. Phys. Rev. Lett. **74**, 2583 (1995)
45. G. Zaránd, C.-H. Chung, P. Simon, M. Vojta, Quantum criticality in a double quantum-dot system, Phys. Rev. Lett. **97**, 166802 (2006)
46. E. Sela, A.K. Mitchell, L. Fritz, Exact crossover Green function in the two-channel and two-impurity Kondo models. Phys. Rev. Lett. **106**, 147202 (2011)
47. A.K. Mitchell, E. Sela, D.E. Logan, Two-channel Kondo physics in two-impurity Kondo models. Phys. Rev. Lett. **108**, 086405 (2012)
48. R.-Q. He, J. Dai, Z.-Y. Lu, Natural orbitals renormalization group approach to the two-impurity Kondo critical point. Phys. Rev. B **91**, 155140 (2015)
49. S.J. Chorley, M.R. Galpin, F.W. Jayatilaka, C.G. Smith, D.E. Logan, M.R. Buitelaar, Tunable Kondo physics in a carbon nanotube double quantum dot. Phys. Rev. Lett. **109**, 156804 (2012)
50. A. Spinelli, M. Gerrits, R. Toskovic, B. Bryant, M. Ternes, A. F. Otte, *Full experimental realisation of the two-impurity Kondo problem*, arXiv:1411.4415v2
51. K. Okamoto, K. Nomura, Fluid-dimer critical point in $S = 1/2$ antiferromagnetic Heisenberg chain with next nearest neighbor interactions. Phys. Lett. A **169**, 433 (1992)
52. S. Eggert, Numerical evidence for multiplicative logarithmic corrections from marginal operators. Phys. Rev. B **54**, 9612 (1996)
53. S.R. White, Density matrix formulation for quantum renormalization groups. Phys. Rev. Lett. **69**, 2863 (1992)
54. U. Schollwöck, The density-matrix renormalization group. Rev. Mod. Phys. **77**, 259 (2005)
55. G. De Chiara, M. Rizzi, D. Rossini, S. Montangero, Density matrix renormalization group for dummies. J. Comput. Theor. Nanosci. **5**, 1277 (2008)
56. R. Dorner, S.R. Clark, L. Heaney, R. Fazio, J. Goold, V. Vedral, Extracting quantum work statistics and fluctuation theorems by single-qubit interferometry. Phys. Rev. Lett. **110**, 230601 (2013); L. Mazzola, G. De Chiara, M. Paternostro, Measuring the characteristic function of the work distribution. Phys. Rev. Lett. **110**, 230602 (2013)
57. A.J. Roncaglia, F. Cerisola, J.P. Paz, Work measurement as a generalized quantum measurement. Phys. Rev. Lett. **113**, 250601 (2014); G. De Chiara, A.J. Roncaglia, J.P. Paz, Measuring work and heat in ultracold quantum gases. New J. Phys. **17**, 035004 (2015)
58. S.Y. Cho, R.H. McKenzie, Quantum Entanglement in the two impurity kondo model. Phys. Rev. A **73**, 012109 (2006)
59. W.K. Wootters, Entanglement of formation of an arbitrary state of two qubits. Phys. Rev. Lett. **80**, 2245 (1998)