SCIENTIFIC REPORTS

OPEN

Thermodynamic holography

Bo-Bo Wei[1], Zhan-Feng Jiang[1] & Ren-Bao Liu[1,2]

Received: 30 November 2014
Accepted: 15 September 2015
Published: 19 October 2015

The holographic principle states that the information about a volume of a system is encoded on the boundary surface of the volume. Holography appears in many branches of physics, such as optics, electromagnetism, many-body physics, quantum gravity, and string theory. Here we show that holography is also an underlying principle in thermodynamics, a most important foundation of physics. The thermodynamics of a system is fully determined by its partition function. We prove that the partition function of a finite but arbitrarily large system is an analytic function on the complex plane of physical parameters, and therefore the partition function in a region on the complex plane is uniquely determined by its values along the boundary. The thermodynamic holography has applications in studying thermodynamics of nano-scale systems (such as molecule engines, nano-generators and macromolecules) and provides a new approach to many-body physics.

The most famous example of holography is probably the optical hologram, where the three-dimensional view of an object is recorded in a two-dimensional graph[1]. The holographic principle indeed has profound implications in many branches of physics. In electromagnetism, for instance, the electrostatic potential in a volume is uniquely determined by its values at the surface boundary[2]. Density functional theory[3,4], which is the foundation of quantum chemistry and first-principle calculations[4], may be viewed as a holography that maps the full ground-state wave function of a many-electron system (a complex function in an enormously high-dimensional space) to the ground state single-particle density (a real function in three-dimensional space). The holographic principle has also been shown relevant in quantum gravity[5] and string theory[6,7]. Recently, the holographic approach has been employed to tackle strongly-correlated systems in condensed matter physics[8].

The physical properties of a system at thermodynamic equilibrium are fully determined by the partition function $\Xi(\beta, \lambda_1, \lambda_2, \ldots, \lambda_K)$ as a function of coupling parameters $\left\{\lambda_j \middle| j = 1, 2, \ldots, K\right\}$ and the temperature T (or the inverse temperature $\beta \equiv 1/T$). In this paper we set the Boltzmann constant k_B and the Planck constant $\hbar$ to be unity. The partition function is the summation of the Boltzmann factor $e^{-\beta H(\lambda_1, \lambda_2, \ldots, \lambda_K)}$ over all energy eigen states, i.e., $\Xi = \mathrm{Tr}[e^{-\beta H(\lambda_1, \lambda_2, \ldots, \lambda_K)}]$, where the Hamiltonian $H = \sum_j \lambda_j H_j$ is characterized by a set of coupling parameters $\{\lambda_j\}$ (e.g., in spin models the magnetic field $h = \lambda_1$, the nearest neighbor coupling $J = \lambda_2$, and the next nearest neighbor coupling $J' = \lambda_3$, etc.). The normalized Boltzmann factor $\Xi^{-1}\exp(-\beta H)$ is the probability of the system in a state with energy H. In the following we consider one of the physical parameters of the system, $\lambda \in \{\lambda_1, \lambda_2, \ldots, \lambda_K\}$ and suppress the other parameters for the simplicity of notation. We assume that the Hamiltonian is a linear function of the parameter, but the main results (the theorems and the corollaries) in this paper apply to Hamiltonians that are general analytic functions of the parameters (see Methods for discussion).

In this article, we establish that the holographic principle holds in thermodynamics, for a finite but arbitrarily large system. We prove that the partition function of a finite physical system is an analytic function of all the physical parameters on the complex plane, and, according to Cauchy theorem[9], the partition function in any region on the complex plane of a physical parameter is uniquely determined by its values along the boundary. Since the partition function with a complex parameter is equivalent to the coherence of a quantum probe[10–12], it is physically feasible to determine the whole thermodynamic properties of a system by measuring the probe spin coherence for just one value of the parameter. We theoretically study an experimentally realizable system, namely, a nitrogen-vacancy centre coupled to a mechanical resonator, to demonstrate that the free energy of the resonator is fully determined by the

[1]Department of Physics and Centre for Quantum Coherence, The Chinese University of Hong Kong, Hong Kong, China. [2]Institute of Theoretical Physics, The Chinese University of Hong Kong, Hong Kong, China. Correspondence and requests for materials should be addressed to R.-B.L. (email: rbliu@phy.cuhk.edu.hk)

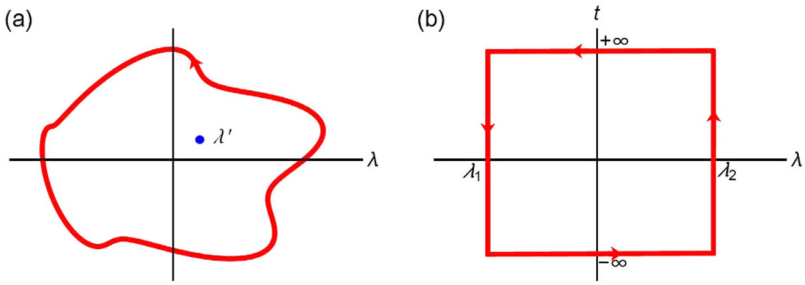

Figure 1. Holography of partition function in the complex plane of a physical parameter. (**a**) Integration contour in the complex plane of λ. The red solid curve is the integration contour and λ' is a point inside the analytic domain. (**b**) A rectangular integration contour in the complex plane of a physical parameter λ with t being the imaginary part. Two vertical straight lines are parallel to the t-axis, with real parts being λ_1 and λ_2, and imaginary parts extended from $-\infty$ to $+\infty$. The other two segments are parallel to the real axis with imaginary parts at $-\infty$ or $+\infty$.

nitrogen-vacancy centre spin decoherence for just one setting of parameters. The holographic principle is applicable for any finite systems of fermions and spins. Because the system size can be arbitrarily large, the physics in systems that approach the thermodynamic limit can be captured. For bosons, however, the validity of theory is verified only in some special cases.

Results

Holography of partition function. The thermodynamic holography states that the partition function of a finite physical system in an area of the complex plane of a physical parameter is uniquely determined by its values along the boundary. This stems from the Cauchy theorem in complex analysis[9] for analytic functions. The analyticity of partition functions is based on the following Theorem (see Fig. 1a for illustration).

Theorem 1. The partition function $\Xi(\lambda)$ of a finite physical system is analytic in the whole complex plane of a physical parameter λ.

The proof is based on the fact that the partition function of a finite system can be expanded into Taylor's series in terms of the Hamiltonian and the Taylor's series, being polynomial functions of the parameter λ, are all analytic and converge uniformly (see details in Methods). Here by "finite physical system" we mean that the system has a finite number of discrete basis states. For a finite (but arbitrarily large) system of spins and fermions on lattices, the partition function is analytic in the whole complex plane of physical parameters. For bosons, the partition function can be non-analytical in certain regions[13,14] (e.g., the partition functions of free bosons have singularities along the imaginary axis of frequencies, and for coupled bosons the system can become unstable when the coupling is too strong). The theorem can be generalized to infinite-dimensional systems that satisfy certain conditions (see Methods). However, infinite systems in general cases still need further study.

Here comes the main result of this paper. According to Cauchy theorem and Theorem 1, the partition function satisfies

$$\Xi(\beta,\, \lambda') = \frac{1}{2\pi i}\oint_C \frac{\Xi(\beta,\, \lambda)}{\lambda - \lambda'} d\lambda, \tag{1}$$

where λ' is a complex parameter enclosed by the integration contour C in the complex plane of λ where the partition function is analytic (see Fig. 1a). A convenient choice of the boundary (the integration contour) can be a rectangular path (see Fig. 1b) that consists of two straight lines perpendicular to the real axis, whose real parts $\lambda_{\Re}$ are respectively λ_1 and λ_2, and two segments parallel to the real axis, whose imaginary parts are respectively $-\infty$ and $+\infty$. The contributions from the two segments at infinity vanish based on the inequality $|\mathrm{Tr}(e^{A+iB})| \le \mathrm{Tr}(e^{A})$ for finite-dimensional Hermitian operators A and B (see Lemma 1 in Methods for details). Thus we have the following theorem.

Theorem 2. The partition function of a finite physical system along two vertical lines in the complex plane of a physical parameter where the partition function is analytic uniquely determines the partition function at any complex parameter between these two vertical lines, that is,

$$\Xi(\beta,\, \lambda') = \int_{-\infty}^{\infty} \frac{\Xi(\beta,\, \lambda_2 + i\lambda_{\mathrm{I}})}{\lambda_2 + i\lambda_{\mathrm{I}} - \lambda'}\frac{d\lambda_{\mathrm{I}}}{2\pi} - \int_{-\infty}^{\infty} \frac{\Xi(\beta,\, \lambda_1 + i\lambda_{\mathrm{I}})}{\lambda_1 + i\lambda_{\mathrm{I}} - \lambda'}\frac{d\lambda_{\mathrm{I}}}{2\pi}, \tag{2}$$

for $\lambda_1 < \Re(\lambda') < \lambda_2$.

Theorem 2 can be simplified by introducing a constant M_- less than the minimum eigenvalue of $\partial_\lambda H$ (which is just H_I for $H = H_0 + \lambda H_\mathrm{I}$) to ensure $e^{\beta\lambda M_-}\Xi(\beta, \lambda)$ vanishes as $\Re(\lambda) \to +\infty$. That leads to

Corollary 1. If the partition function is analytic on the half complex plane ($\Re(\lambda) \geq \lambda_1$) of a physical parameter, the partition function along this line uniquely determines the partition function on that half complex plane, that is,

$$\Xi(\beta, \lambda') = -\int_{-\infty}^{\infty} \frac{e^{\beta(\lambda_1 + i\lambda_\mathrm{I} - \lambda')M_-}\Xi(\beta, \lambda_1 + i\lambda_\mathrm{I})}{\lambda_1 + i\lambda_\mathrm{I} - \lambda'} \frac{d\lambda_\mathrm{I}}{2\pi}, \tag{3}$$

for any complex parameter λ' satisfying $\lambda_1 < \Re(\lambda') < \infty$.

Similarly, by introducing a constant M_+ greater than the maximum eigenvalue of $\partial_\lambda H$ to ensure $e^{\beta\lambda M_+}\Xi(\beta, \lambda)$ vanishes as $\Re(\lambda) \to -\infty$, we have

Corollary 2. If the partition function is analytic on the half complex plane ($\Re(\lambda) \leq \lambda_2$) of a physical parameter, the partition function along this line uniquely determines the partition function on that half complex plane, that is,

$$\Xi(\beta, \lambda') = \int_{-\infty}^{\infty} \frac{e^{\beta(\lambda_2 + i\lambda_\mathrm{I} - \lambda')M_+}\Xi(\beta, \lambda_2 + i\lambda_\mathrm{I})}{\lambda_2 + i\lambda_\mathrm{I} - \lambda'} \frac{d\lambda_\mathrm{I}}{2\pi}, \tag{4}$$

for any complex parameter λ' satisfying $-\infty < \Re(\lambda') < \lambda_2$.

Corollaries 1 and 2 are particularly usefully for boson systems, where the partition functions may not be analytic on the whole complex plane of a parameter. For example, the partition function of free bosons has singularity points along the imaginary axis.

Equations (2–4) establish the holographic principle for partition functions. In practical application, one can make use of the partition functions of weakly interacting systems, which can be easy to calculate, to derive the partition functions of strongly interacting systems, which are usually difficult to calculate since the perturbation method may fail in absence of small parameters.

Possible experimental realization of thermodynamic holography. Recently our group discovered that the partition function of a system with a complex parameter is equivalent to the quantum coherence of a probe spin coupled to the system[10–12]. One can use a probe spin-1/2 ($S_z \equiv (|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)/2$) coupled to a system (bath) with bath Hamiltonian $H(\lambda)$ and probe-bath interaction $H' = -\eta S_z \otimes H_\mathrm{I}$, where η is a small coupling constant and $H_\mathrm{I} = \partial_\lambda H$. If the probe spin is initialized in the superposition state $|\psi\rangle = |\uparrow\rangle + |\downarrow\rangle$ and the system in the thermal equilibrium with density matrix $\Xi^{-1}\exp(-\beta H)$, the quantum coherence of the probe spin is quantified by the spin polarization $\langle S_x(t)\rangle + i\langle S_y(t)\rangle = \mathrm{Tr}[|\psi\rangle\langle\psi|e^{-\beta H}e^{i(H+H')t}|\uparrow\rangle\langle\downarrow|e^{-i(H+H')t}]/\Xi(\beta, \lambda)$. When $[H, H_\mathrm{I}] = 0$, the probe spin coherence has an intriguing form as[10]

$$\langle S_+(\lambda, t)\rangle \equiv \langle S_x(\lambda, t)\rangle + i\left\langle S_y(\lambda, t)\right\rangle = \frac{\Xi(\beta, \lambda + it\eta/\beta)}{\Xi(\beta, \lambda)}, \tag{5}$$

which is equivalent to the partition function with a complex parameter, $\lambda + it\eta/\beta$. Now the evolution time serves as the imaginary part of the physical parameter. Recently, Lee-Yang zeros have been observed via such a measurement[12]. In more general cases ($[H, H_I] \neq 0$), it is possible to engineer the probe-bath interaction so that the probe spin coherence still has the form in equation (5)[11]. In terms of the probe spin coherence, equation (2) can be rewritten as

$$\Xi(\beta, \lambda') = \Xi(\beta, \lambda_2)\int_{-\infty}^{\infty} \frac{\langle S_+(\lambda_2, t)\rangle}{\lambda_2 + i\eta t/\beta - \lambda'} \frac{\eta dt}{2\pi\beta} - \Xi(\beta, \lambda_1)\int_{-\infty}^{\infty} \frac{\langle S_+(\lambda_1, t)\rangle}{\lambda_1 + i\eta t/\beta - \lambda'} \frac{\eta dt}{2\pi\beta}. \tag{6}$$

Similarly, equation (3) can be rewritten as

$$\Xi(\beta, \lambda') = -\Xi(\beta, \lambda_1)\int_{-\infty}^{\infty} \frac{e^{\beta(\lambda_1 + i\eta t/\beta - \lambda')M_-}\langle S_+(\lambda_1, t)\rangle}{\lambda_1 + i\eta t/\beta - \lambda'} \frac{\eta dt}{2\pi\beta}, \tag{7}$$

and equation (4) as

$$\Xi(\beta, \lambda') = \Xi(\beta, \lambda_2)\int_{-\infty}^{\infty} \frac{e^{\beta(\lambda_2 + i\eta t/\beta - \lambda')M_+}\langle S_+(\lambda_2, t)\rangle}{\lambda_2 + i\eta t/\beta - \lambda'} \frac{\eta dt}{2\pi\beta}. \tag{8}$$

Note that the probe spin coherence resembles the form of quantum quenches[15]. Therefore the quantum quench dynamics may also be studied using the thermodynamic holography.

Equations (6–8) establish an experimentally implementable holographic approach to thermodynamics. For an arbitrary real parameter λ', we can determine the free energy $F = -\beta^{-1}\ln(\Xi)$ by

$$e^{-\beta[F(\lambda')-F(\lambda)]} = \mathrm{sgn}(\lambda - \lambda') \int_{-\infty}^{\infty} \frac{e^{\beta(\lambda + i\eta t/\beta - \lambda')M_{\mathrm{sgn}(\lambda-\lambda')}} \langle S_+(\lambda, t)\rangle}{\lambda + i\eta t/\beta - \lambda'} \frac{\eta dt}{2\pi\beta}. \tag{9}$$

Thus we can extract the full thermodynamic properties of the system from the probe spin coherence measurement for just a single value of the physical parameter. Note that previously the free energy difference (ΔF) has been related to the work (ΔW) in a non-equilibrium physical process by the Jarzynski equality $\exp(-\beta\Delta F) = \langle \exp(-\beta\Delta W)\rangle$[16]. The Jarzynski equality is particularly useful for determining free energy differences for small thermodynamic systems such as quantum engines and biomolecular systems[17–19]. Using the thermodynamic holography and the Jarzynski equality, we establish a general relation between the probe spin coherence, the work done on small systems, and the free energy changes. This general relation is indeed the foundation of two recent proposals for experimental measurement of the characteristic function of the work distributions[20,21], which plays a central role in the fluctuation relations in quantum quenches[15] and more generally in non-equilibrium thermodynamics[22]. The power of the thermodynamic holography is that one can obtain free energy change for any parameters using the probe spin coherence measurement for just one value of the parameter instead of quenching the system to various parameters[17–19].

The thermodynamic holography can also be used to determine the probe spin coherence for an arbitrary parameter by the coherence measurement for just one value of the parameter. Choosing a complex parameter $\lambda' + it'\eta/\beta$, we have the probe spin coherence

$$\langle S_+(\lambda', t')\rangle = \frac{\int_{-\infty}^{\infty} dt \frac{e^{\beta(\lambda + i\eta t/\beta - \lambda' - i\eta t'/\beta)M_{\mathrm{sgn}(\lambda-\lambda')}}\langle S_+(\lambda, t)\rangle}{\lambda + i\eta t/\beta - \lambda' - i\eta t'/\beta}}{\int_{-\infty}^{\infty} \frac{e^{\beta(\lambda + i\eta t/\beta - \lambda')M_{\mathrm{sgn}(\lambda-\lambda')}}\langle S_+(\lambda, t)\rangle}{\lambda + i\eta t/\beta - \lambda'} dt}. \tag{10}$$

The holographic method can be further simplified in many cases. Since the partition function, $\Xi = \mathrm{Tr}[\exp(-\beta H)]$, is the sum of exponential function of the Hamiltonian, the probe spin coherence would be a periodic function of time if the energy level differences of a system are quantized in some unit, such as in the spin Ising models[10]. Then in such cases one does not need to measure the probe spin coherence as a function of time from $-\infty$ to $+\infty$. Instead, the probe spin coherence in one period of time, from 0 to $2\pi/\eta$, is sufficient to produce the full information of the partition function. In such cases, equation (9) becomes

$$\exp(-\beta\Delta F) = \mathrm{sgn}(\lambda - \lambda') \int_0^{2\pi/\eta} \frac{e^{\beta(\lambda + i\eta t/\beta - \lambda')M_{\mathrm{sgn}(\lambda-\lambda')}}\langle S_+(\lambda, t)\rangle}{\tanh[(\beta\lambda + i\eta t - \beta\lambda')/2]} \frac{\eta dt}{4\pi}, \tag{11}$$

and equation (10) becomes

$$\langle S_+(\lambda', \eta t')\rangle = \frac{\int_0^{2\pi/\eta} \frac{e^{(\beta\lambda + i\eta t - \beta\lambda' - i\eta t')M_{\mathrm{sgn}(\lambda-\lambda')}}\langle S_+(\lambda, t)\rangle}{\tanh[(\beta\lambda + i\eta t - \beta\lambda' - i\eta t')/2]} dt}{\int_0^{2\pi/\eta} \frac{e^{(\beta\lambda + i\eta t - \beta\lambda')M_{\mathrm{sgn}(\lambda-\lambda')}}\langle S_+(\lambda, t)\rangle}{\tanh[(\beta\lambda + i\eta t - \beta\lambda')/2]} dt}. \tag{12}$$

Discussion

Thermodynamic holography of a mechanical resonator coupled to a probe spin. To demonstrate the idea of thermodynamic holography, we study an experimentally realizable system as the model example, namely, a nitrogen-vacancy (NV) centre spin coupled to a nano-mechanical resonator[23,24] (see Fig. 2a). This model may also be realized in a superconducting resonator[25]. The NV centre has a spin triplet ground state ($S = 1$) with a large zero field splitting $\Delta = 2.87$ GHz. The mechanical resonator, with frequency $\omega \sim 3$ GHz, is assumed to have a magnetic tip. The NV centre is placed right under the tip. The oscillation of the mechanical resonator generates a time dependent magnetic field on the NV centre spin with an interaction Hamiltonian $V = g(a^+ + a) \otimes S_x$. Under realistic conditions, the coupling g can reach 1 MHz for a magnetic tip with size of 100 nm and an NV centre located about 25 nm under the tip[26]. The Hamiltonian of coupled mechanical resonator and the NV center is $H = \Delta S_z^2 + \omega a^+ a + g S_x(a^+ + a)$. We make use of the spin states $|+1\rangle$ and $|0\rangle$ as a probe and define $\sigma_z \equiv |+1\rangle\langle +1| - |0\rangle\langle 0|$ and the corresponding spin flip operators $\sigma^+ \equiv |+1\rangle\langle 0|$ and $\sigma^- \equiv |0\rangle\langle +1|$. Since the coupling g ($\leq$1MHz) $\ll \omega$ (~3GHz) & Δ(~2.87 GHz), the perturbation theory (see Methods for details) gives an effective Hamiltonian

$$H_{\mathrm{eff}} \approx \Delta\sigma_z + \omega a^+ a + \eta\sigma_z \otimes a^+ a, \tag{13}$$

with $\eta = 4g^2\omega/(\Delta^2 - \omega^2)$. The NV center acts as a probe spin and the mechanical resonator as a system (bath). The partition function $\Xi(\beta, \omega) = (1 - e^{-\beta\omega})^{-1}$ of the oscillator has an infinite number of singularity points $\omega = i2n\pi/\beta$ (where n is an arbitrary integer) along the imaginary axis of the frequency.

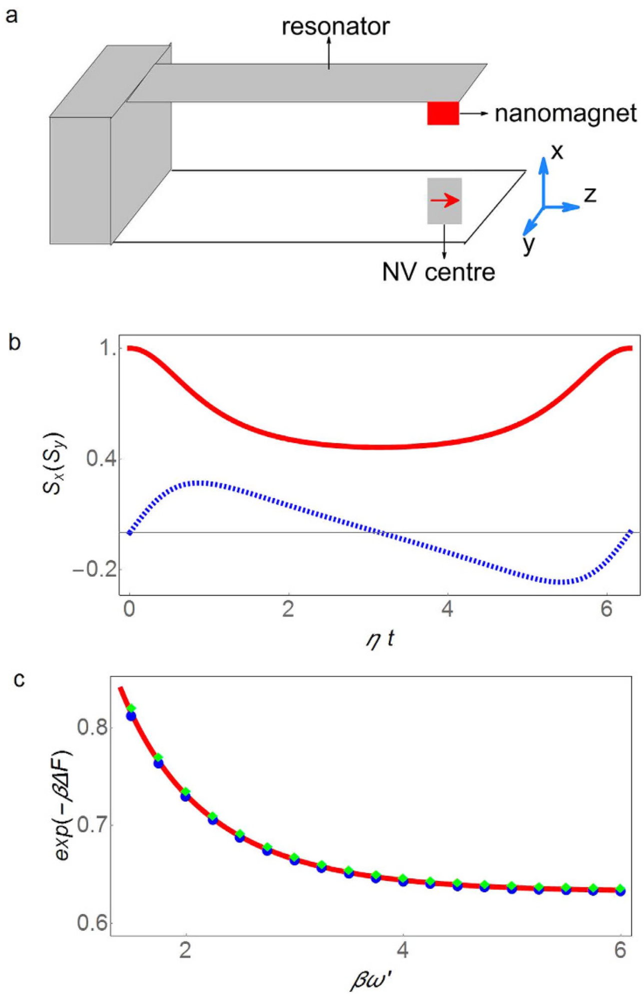

Figure 2. Extracting free energy difference of an oscillator from the probe spin coherence measurement. (**a**) Schematic plot of an NV centre coupled to a mechanical resonator. The mechanical resonator has a magnetic tip attached at the end. An NV centre is placed right under the magnetic tip. The oscillation of the mechanical resonator generates a time-dependent magnetic field on the NV centre spin. (**b**) The spin coherence of the NV center as a function of scaled time, ηt with $\eta = 4g^2\omega/(\Delta^2 - \omega^2)$, at temperature $\beta\omega = 1$. The red solid line presents S_x and the dashed blue line shows S_y. (**c**) The free energy difference for the mechanical resonator obtained from the probe spin coherence. The solid red line is the direct solution. The symbols are obtained by the holographic method using spin decoherence at $\beta\omega = 1$. For the green diamonds (blue dots), 63 (157) evenly spaced data points in one period of time have been used in the numerical integration.

But the partition function is analytic on the half complex plane of frequency with positive real part (See Methods). Hence the holographic principle applies. We shall demonstrate that the free energy difference can be extracted from the probe spin coherence measurement of the NV center. We assume that the NV center is initialized in the superposition state $|1\rangle + |0\rangle$ and the mechanical resonator in the thermal equilibrium. Note that in the current case the probe spin coherence is a periodic function of time since the energy levels of the oscillator are equally spaced. So the probe spin coherence in one period of time, from 0 to $2\pi/\eta$, is sufficient to yield the full information of the partition function. The measurement time of the NV center spin coherence is ~$2\pi/\eta \approx 100$ μs, which is within the spin coherence time of an NV centre in an isotopically purified diamond[27].

Figure 2b presents the real (red solid line) and imaginary (blue dashed line) parts of the NV centre spin coherence as functions of time for the resonator at temperature 150 mK ($\beta\omega = 1$). From the spin coherence we can obtain the free energy (relative to the value at $\beta\omega = 1$) for arbitrary $\beta\omega$. Figure 2c shows the exponentiated free energy difference (green squares and blue dots) constructed via equation (11) from the NV center spin coherence shown in Fig. 2b. The green squares are obtained with numerical integration of 63 evenly separated data points of the NV center spin coherence during one period of evolution at $\beta\omega = 1$. The error in the numerical integration is $\sim(2\pi)^3 f''(x)/(12 \times 63^2) \leq 0.01$, where

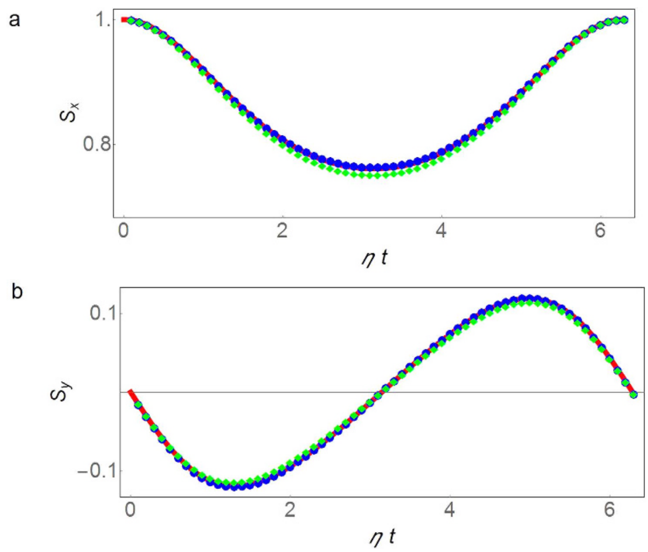

Figure 3. Probe spin coherence by thermodynamic holography. (**a**) The real part of the probe spin coherence at $\beta\omega = 2$ as a function of scaled time, ηt with $\eta = 4g^2\omega/(\Delta^2 - \omega^2)$. The symbols are obtained by the holographic method using spin decoherence at $\beta\omega = 1$. For the green diamonds (blue dots), 63 (157) evenly spaced data points in one period of time have been used in the numerical integration. (**b**) The same as (**a**) but for the imaginary part of the spin coherence.

$f''(x)$ is the second order derivative of the integrand and $0 \le x \le 2\pi$. The blue dots are obtained by numerical integration of 157 evenly separated data points with numerical error $\sim(2\pi)^3 f''(x)/(12 \times 157^2) \le 0.001$. The results obtained by the holographic method agree with the direct calculation of the free energy (the solid red line in Fig. 2c) within the numerical errors.

The holographic approach can also be used to determine the probe spin coherence for arbitrary $\beta\omega$. The real and imaginary parts of the constructed spin coherence for $\beta\omega = 2$ as functions of time are presented respectively in Fig. 3a,b. The green squares are obtained by equation (12) with numerical integration of 63 evenly spaced data points of the NV center spin coherence at $\beta\omega = 1$ during one period of time. The error in the numerical integration is $\sim(2\pi)^3 f''(x)/(12 \times 63^2) \le 0.02$. The blue dots are obtained by numerical integration of 157 evenly spaced data points with numerical error $\sim(2\pi)^3 f''(x)/(12 \times 157^2) \le 0.002$. The results agree with the direct solution within numerical errors.

Summary

In this work we have established the concept of thermodynamic holography. We prove that the partition function of a finite physical system in an area of the complex plane of a physical parameter is uniquely determined by its values along the boundary. Since the partition function with a complex parameter is equivalent to the probe spin coherence, one can experimentally implement the thermodynamic holography through probe spin coherence measurement for just one physical parameter. Thermodynamic holography may have applications in studying thermodynamics of nano-scale systems (such as molecule engines[28], nano-generators[29] and macromolecules[17,30]) and provide a new approach to many-body physics.

Methods

Proof of Theorem 1. The system has a finite number (K) of basis states. We define a series of functions $\Xi^{(N)}(\lambda) = \sum_{n=0}^{N} \frac{1}{n!} \mathrm{Tr}[-\beta H(\lambda)]^n$, which are sums of a finite number of polynomial functions of λ. Obviously, all these functions are analytic in the whole complex plane of λ. Considering the parameter in the range $|\lambda| \le \Lambda$, for an arbitrarily small quantity ε, there exists an integer N_ε such that $\sum_{n=N_\varepsilon+1}^{\infty} \frac{h^n}{n!} < \varepsilon$, where h is the maximum of $|\mathrm{Tr}[-\beta H(\lambda)]|$ for $|\lambda| \le \Lambda$. Therefore $|\Xi^{(N)}(\lambda) - \Xi(\lambda)| < \varepsilon$ for $N > N_\varepsilon$, i.e., the function series uniformly converge to the partition function in the parameter range $|\lambda| \le \Lambda$. According to the uniform convergence theorem of analytic functions[9], the partition function is analytic for $|\lambda| \le \Lambda$. Since Λ can be chosen to be arbitrarily large, Theorem 1 is proved.

A trace inequality. *Lemma 1*. Two Hermitian operators A and B satisfy the trace inequality $|\mathrm{Tr}(e^{A+iB})| \le \mathrm{Tr}(e^{A})$ for a system that has a finite number of basis states, or for a system that has an infinite number of discrete basis states if B, $[A,B]$, $[A,[A,B]]$, … commute with each other.

Proof. For a system with a finite number of basis states, both A and B are finite dimensional matrices. By Hölder's inequality for finite-dimensional matrices[31], $|\mathrm{Tr}\,[U^\dagger V]| \le \sqrt{\mathrm{Tr}\,[U^\dagger U]}\sqrt{\mathrm{Tr}\,[V^\dagger V]}$ for operators U and V, we have $|\mathrm{Tr}\,(e^{A+iB})| = |\mathrm{Tr}\,(e^{(A+iB)/2}e^{(A+iB)/2})| \le |\mathrm{Tr}\,(e^{(A+iB)/2}e^{(A-iB)/2})|$. Then according to Bernstein inequality[32], $|\mathrm{Tr}\,(e^{M}e^{M^\dagger})| \le \mathrm{Tr}\,(e^{M+M^\dagger})$ for an operator M, we have $|\mathrm{Tr}\,(e^{(A+iB)/2}e^{(A-iB)/2})| \le \mathrm{Tr}\,(e^{A})$ and hence $|\mathrm{Tr}\,(e^{A+iB})| \le \mathrm{Tr}\,(e^{A})$.

We now consider infinite-dimensional systems. We define $\tilde{B}(s) = \exp(-sA)\,B\,\exp(sA)$. If B, $[A, B]$, $[A, [A, B]]$, … commute with each other, $[\tilde{B}(s_2), \tilde{B}(s_1)] = 0$ for arbitrary real numbers s_1 and s_2. Thus we have[33] $\mathrm{Tr}\,[e^{A+iB}] = \mathrm{Tr}\left[e^{A/2}\exp\left(i\int_{-1/2}^{+1/2}\tilde{B}(s)\,ds\right)e^{A/2}\right] = \mathrm{Tr}\,[\exp(A)\exp(iB')]$, where $B' \equiv \int_{-1/2}^{+1/2}\tilde{B}(s)\,ds$ is Hermitian. By Cauchy Schwarz inequality[31], we have $|\mathrm{Tr}\,[e^{A+iB}]| = |\mathrm{Tr}\,[e^{A}e^{iB'}]| \le \mathrm{Tr}\,[e^{A}]$.

Thus Lemma 1 is proved.

For more general cases of infinite-dimensional operators, however, we have not been able to prove the trace inequality $|\mathrm{Tr}\,[e^{A+iB}]| \le \mathrm{Tr}\,[e^{A}]$. It needs further study.

Generalization of Theorem 1 to certain infinite-dimensional systems. For a physical system with an infinite number of basis states (such as bosons), we assume that the basis states are discrete (countable), which is always possible since we can confine the system using a sufficiently large box.

We can generalize Theorem 1 to infinite-dimensional Hamiltonians that satisfy the specified condition for Lemma 1 (i.e., H_{I}, $[H, H_{\mathrm{I}}]$, $[H, [H, H_{\mathrm{I}}]]$, … commute with each other). We choose the eigenstates of H as the discrete basis states denoted by $\{|0\rangle, |1\rangle, |2\rangle, \ldots\}$ in the ascending order of eigenvalues and define a truncated series of partition functions $\tilde{\Xi}_K(\lambda) = \sum_{k=0}^{K}\langle k|e^{-\beta H(\lambda)}|k\rangle$ in a finite subspace $\{|0\rangle, |1\rangle, |2\rangle, \ldots, |\mathrm{K}\rangle\}$, which are of course analytic functions of λ. If we can prove that these truncated partition functions $\tilde{\Xi}_1(\lambda), \tilde{\Xi}_2(\lambda), \tilde{\Xi}_3(\lambda), \cdots\cdots$ approach to $\Xi(\lambda)$ uniformly, then according to the uniform convergence theorem of analytic functions[9], the partition function $\Xi(\lambda)$ is analytic. If the partition function $\Xi(\lambda)$ exists in a close segment on the real axis $\lambda_{\mathrm{R}} \in [\lambda_{\min}, \lambda_{\max}]$, there always exists an integer K_ε for an arbitrary small positive number ε such that $\sum_{k>K_\varepsilon}\langle k|e^{-\beta H(\lambda_{\mathrm{R}})}|k\rangle < \varepsilon$ for $\lambda_{\mathrm{R}} \in [\lambda_{\min}, \lambda_{\max}]$. According to Lemma 1, $|\sum_{k>K_\varepsilon}\langle k|e^{-\beta H(\lambda_{\mathrm{R}}) - i\beta\lambda_{\mathrm{I}}H_{\mathrm{I}}}|k\rangle| < \sum_{k>K_\varepsilon}\langle k|e^{-\beta H(\lambda_{\mathrm{R}})}|k\rangle < \varepsilon$ if H_{I}, $[H, H_{\mathrm{I}}]$, $[H, [H, H_{\mathrm{I}}]]$, … commute with each other. So the series of analytic functions $\tilde{\Xi}_1(\lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}}), \tilde{\Xi}_2(\lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}}), \tilde{\Xi}_3(\lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}}), \ldots$ uniformly converge to $\Xi(\lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}})$ for $\lambda_{\mathrm{R}} \in [\lambda_{\min}, \lambda_{\max}]$. According to the uniform convergence theorem of analytic functions[9], the partition function $\Xi(\lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}})$ is analytic for $\lambda_{\mathrm{R}} \in [\lambda_{\min}, \lambda_{\max}]$. Thus Theorem 1 applies to infinite-dimensional systems if H_{I}, $[H, H_{\mathrm{I}}]$, $[H, [H, H_{\mathrm{I}}]]$, … commute with each other.

Proof of Theorem 2. We just need to show $\int_{\lambda_1}^{\lambda_2}\frac{\Xi(\beta, \lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}})}{\lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}} - \lambda'}\frac{d\lambda_{\mathrm{R}}}{2\pi} \to 0$ for $|\lambda_{\mathrm{I}}| \to \infty$. Suffices it to show that $\Xi(\beta, \lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}}) = \mathrm{Tr}\,[e^{-\beta H - i\beta\lambda_{\mathrm{I}}H_{\mathrm{I}}}]$ is bounded for $\lambda_{\mathrm{R}} \in [\lambda_{\min}, \lambda_{\max}]$. According to Lemma 1, $|\Xi(\beta, \lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}})| \le \Xi(\beta, \lambda_{\mathrm{R}})$. Since $\Xi(\lambda_{\mathrm{R}})$ is bounded for $\lambda_{\mathrm{R}} \in [\lambda_{\min}, \lambda_{\max}]$, $\Xi(\beta, \lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}})$ is bounded. Therefore Theorem 2 is proved.

Generalization to Hamiltonians that are general analytic functions of parameters. For Hamiltonians that are general analytic functions of the parameters, $H = H_0 + f(\lambda)H_{\mathrm{I}}$, then $\mathrm{Tr}\,[e^{-\beta H - i\beta\lambda_{\mathrm{I}}H_{\mathrm{I}}}]$ is be replaced by $\mathrm{Tr}\,[e^{-\beta H(f_{\mathrm{R}}) - i\beta f_{\mathrm{I}}H_{\mathrm{I}}}]$, where $f_{\mathrm{R}}(\lambda) = \Re[f(\lambda)]$ and $f_{\mathrm{I}}(\lambda) = \Im[f(\lambda)]$. Theorem 1 and 2 and Corollaries 1 and 2 still hold but the specific forms of Corollaries I and II depend on the specific forms of the Hamiltonians when the parameter is extended to positive and negative infinity.

Derivation of the effective Hamiltonian of a coupled spin-oscillator system. The coupling Hamiltonian for the pseudo spin and the oscillator is $H = \Delta\sigma_z + \omega a^+a + g\sigma_x(a^+ + a)$. Since $g \ll \omega$, Δ, we can treat $g\sigma_x(a^+ + a)$ as a perturbation. A unitary transformation defined by $U = \exp[2g\omega/(\Delta^2 - \omega^2)(\sigma^+a - \sigma^-a^+)]$ leads to $UHU^+ \approx \Delta\sigma_z + \omega a^+a + [4g^2\omega/(\Delta^2 - \omega^2)]\,\sigma_z \otimes a^+a + [g^2\omega/(\Delta^2 - \omega^2)]\,\sigma_z$. The last term can be dropped since it is only a small correction to the Zeeman energy of the spin. We therefore obtain equation (13).

Numerical method. In determining the free energies of the mechanical oscillator from the probe spin coherence through thermodynamic holography, we took equally spaced points of the NV centre spin coherence within one period $t \in [0, 2\pi/\eta]$ and then carried out numerical integrations by the trapezoidal rule.

References

1. Hecht, E. & Zajac, A. *Optics* (Addison-Wesley, 1974).
2. Griffiths, D. J. *Introduction to Electrodynamics* (Addison-Wesley, 2012).
3. Hohenberg, P. & Kohn, W. Inhomogenous electron gas. *Phys. Rev.* **136,** B864 (1964).
4. Kohn, W. & Sham, L. J. Self-consistent equations including exchange and correlation effects. *Phys. Rev.* **140,** A1133 (1965).

5. Stephens, C. R., 't Hooft, G. & Whiting, B. F. Black hole evaporation without information loss. *Class. Quantum Grav.* **11,** 621 (1994).
6. Susskind, L. The world as a hologram. *J. Math. Phys.* **36,** 6377 (1995).
7. Witten, E. Anti-de sitter space and holography. *Adv. Theor. Math. Phys*. **2,** 253 (1998).
8. Witczak-Krempa, W., Sørensen, E. S. & Sachdev, S. The dynamics of quantum criticality revealed by quantum Monte Carlo and holography, *Nature Phys.* **10,** 361–366 (2014).
9. Gamelin, T. W. *Complex Analysis*. (Springer-Verlag, New York, 2001).
10. Wei, B. B. & Liu, R. B. Lee-Yang zeros and critical times in decoherence of a probe spin coupled to a bath. *Phys. Rev. Lett.* **109,** 185701 (2012).
11. Wei, B. B., Chen, S. W., Po, H. C. & Liu, R. B. Phase transitions in the complex plane of physical parameters. *Sci. Rep.* **4,** 5202 (2014).
12. Peng, X. H. *et al.* Experimental observation of Lee-Yang zeros. *Phys. Rev. Lett.* **114,** 010601 (2015).
13. Wang, X. Z. Yang-Lee zeros of one-dimensional quantum many-body systems, *Phys. Rev. E* **59,** 222 (1999).
14. Wang, X. Z. Critical nature of ideal Bose-Einstein condensation: Similarity with Yang-Lee theory of phase transition, *Phys. Rev. E* **59,** 1242 (1999).
15. Polkovnikov, A., Sengupta, K., Silva, A. & Vengalattore, M. Nonequilibrium dynamics of closed interacting quantum systems. *Rev. Mod. Phys*. **83,** 863 (2011).
16. Jarzynski, C. Nonequilibrium equality for free energy differenece. *Phys. Rev. Lett.* **78,** 2690 (1997).
17. Collin, D. *et al.* Verification of the Crooks fluctuation theorem and recovery of RNA folding free energies. *Nature* **437,** 231–234 (2005).
18. Hummer, G. & Szabo, A. Free energy reconstruction from nonequilibrium single-molecule pulling experiments, *Proc. Natl. Acad. Sci.* **98,** 3658 (2002).
19. Liphardt, J., Dumont, S., Smith, S. B., Tinoco, I., Jr. & Bustamante, C. Equilibrium information from nonequilibrium measurements in an experimental test of Jarzynski's equality. *Science* **296,** 1832–1835 (2002).
20. Dorner, R. *et al.* Extracting quantum work statistics and fluctuation theorems by single-qubit interferometry. *Phys. Rev. Lett.* **110,** 230601 (2013).
21. Mazzola, L., Chiara, G. D. & Paternostro, M. M. Measuring the characteristic function of the work distribution. *Phys. Rev. Lett.* **110,** 230602 (2013).
22. Campisi, M., Hanggi, P. & Talkner, P. *Colloquium*: Quantum fluctuation relations: Foundations and applications. *Rev. Mod. Phys*. **83,** 771 (2011).
23. Rabl, P. *et al.* Strong magnetic coupling between an electronic spin qubit and a mechanical oscillator. *Phys. Rev. B* **79,** 041302 (2009).
24. Kolkowitz, S. *et al.* Coherent sensing of a mechanical resonator with a single-spin qubit. *Science* **335,** 1063–1606 (2012).
25. LaHaye, M. D., Suh, J., Echternach, P. M., Schwab, K. C. & Roukes, M. L. Nanomechanical measurements of a superconducting qubit. *Nature* **459,** 960–964 (2009).
26. Mamin, H. J., Poggio, M., Degen, C. L. & Rugar, D. Nuclear magnetic resonance imaging with 90-nm resolution. *Nature Nanotechnol*. **2,** 301–306 (2007).
27. Maurer, P. C. *et al.* Room-temperature quantum bit memory exceeding one second. *Science* **336,** 1283–1286 (2012).
28. Bockrath, M. W. A Single-molecule engine, *Science* **338,** 754–755 (2012).
29. Wang, Z. L. & Song, J. Piezoelectric nanogenerators based on zinc oxide nanowire arrays, *Science* **312,** 242–246 (2006).
30. Gratzer, W. *Giant Molecules: From nylon to nanotubes*. (Oxford University Press, 2011).
31. Horn, R. A. & Johnson, C. R. *Matrix Analysis* (Cambridge University Press, 2012).
32. Bernstein, D. S. Inequalities for the trace of matrix exponentials, *SIAM J. Matrix Anal. Appl.* **9,** 156 (1988).
33. Wilcox, R. M. Exponential operators and parameter differentiation in quantum physics. *J. Math. Phys.* **8,** 962 (1967).

Acknowledgements

This work was supported by Hong Kong Research Grants Council/General Research Fund 401413 and The Chinese University of Hong Kong Vice Chancellor's One-Off Discretionary Fund.

Author Contributions

R.B.L. conceived the idea, designed the project and formulated the theory. B.B.W. & R.B.L. designed the model. B.B.W. and R.B.L. carried out the research. Z.F.J. participated in the study in its initial stage. R.B.L. & B.B.W. wrote the paper.

Additional Information

Competing financial interests: The authors declare no competing financial interests.

How to cite this article: Wei, B.-B. *et al.* Thermodynamic holography. *Sci. Rep.* **5**, 15077; doi: 10.1038/srep15077 (2015).

This work is licensed under a Creative Commons Attribution 4.0 International License. The images or other third party material in this article are included in the article's Creative Commons license, unless indicated otherwise in the credit line; if the material is not included under the Creative Commons license, users will need to obtain permission from the license holder to reproduce the material. To view a copy of this license, visit http://creativecommons.org/licenses/by/4.0/