Holographic principle in thermodynamics

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NMR experiments (USTC)

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Outline

I. Introduction

– thermodynamics on the complex plane

II. Thermodynamic holography

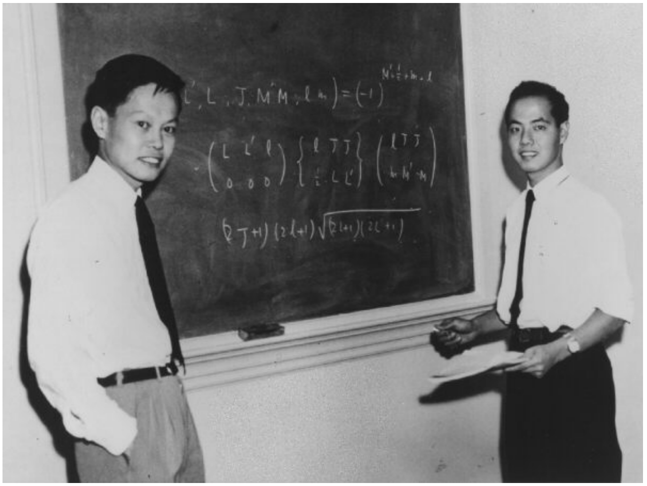
The imaginary number

A key step in mathematics $i = \sqrt{-1}$

A key step in physics $i\hbar \frac{\partial}{\partial t}\psi = \hat{H}\psi$

A key step in thermodynamics

$$\exp(-2\beta\mu) \Rightarrow z \in \mathbb{C}$$



C. N. Yang & T. D. Lee (1952)

Lee-Yang Theorem (1952)

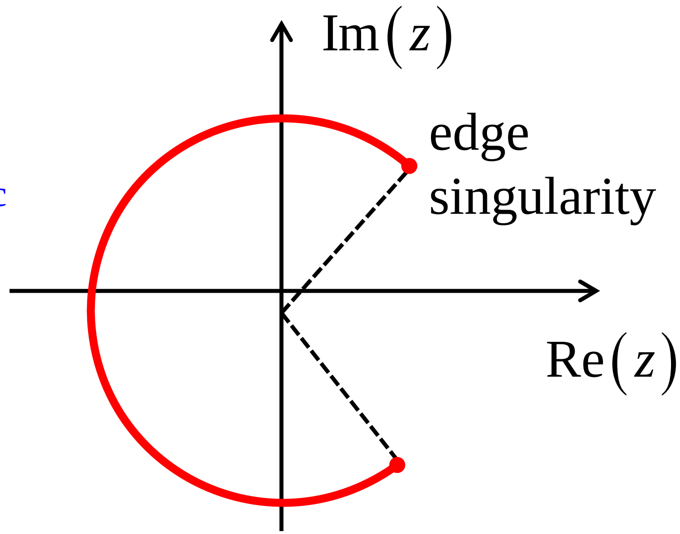
$$H = -\sum J_{ij}\sigma_i\sigma_j - h\sum \sigma_j$$

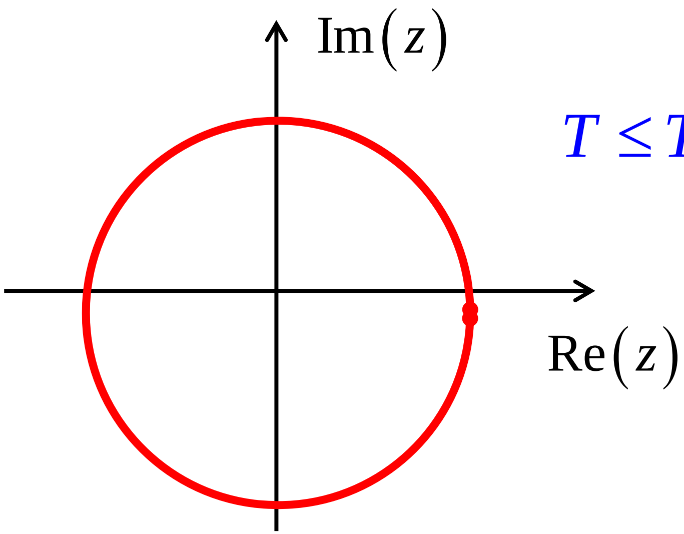
$$Z = \mathrm{Tr}\left[\exp\left(-\beta H\right)\right] = \exp\left(\beta N h\right)\sum_{n=0}^{N} p_n z^n = \exp\left(\beta N h\right)\prod_{n=1}^{N}\left(z - z_n\right)$$

$$z = \exp\left(-2\beta h\right)$$

Lee-Yang zeros on unit circle

$T > T_c$

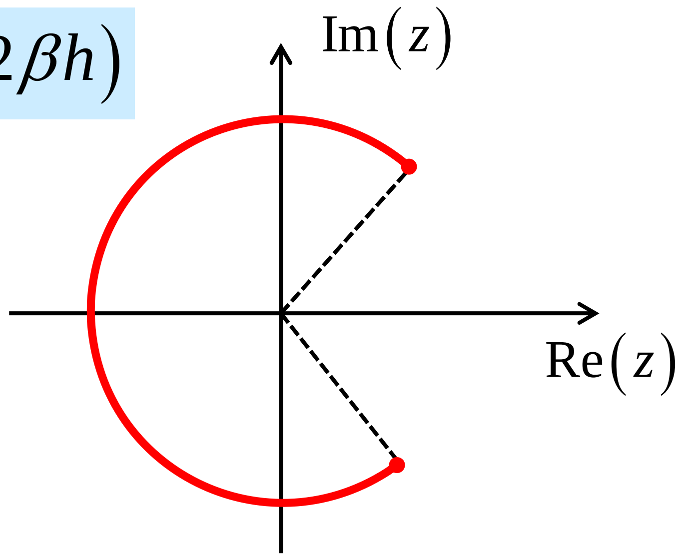




$T \leq T_c$

Observation of Lee-Yang zeros?

$$z = \exp(-2\beta h)$$



Lee-Yang zeros @ complex field or temperature, which are unphysical.

Make of a complex parameter

Boltzmann & Schrodinger

probability: $\exp(-\beta H)$ probability amplitude: $\exp(-itH)$

Quantum evolution → complex parameter

$$L(t) = \mathrm{Tr}\left[\exp\left(-\beta H - itH_I\right)\right]$$

$$H = \sum \lambda_k H_k \qquad \text{If } H_I = H_k, \text{ then } \lambda_k \Rightarrow \lambda_k + it/\beta$$

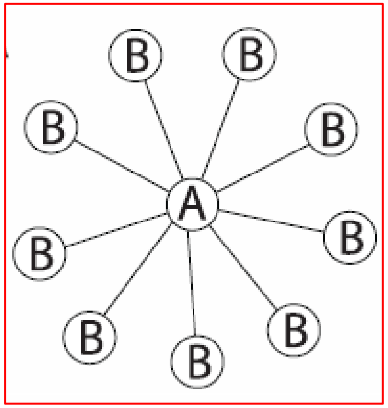
Examples [B.B. Wei et al, Scientific Reports 4, 5202 (2014)]:

If $H_I = \sum s_j^z$, magnetic field continuated (Lee-Yang zeros)

If $H_I = H$, temperature continuated (Fisher zeros)

If $H_I = \sum s_j^x s_{j+1}^x$, coupling continuated (??? zeros), ...

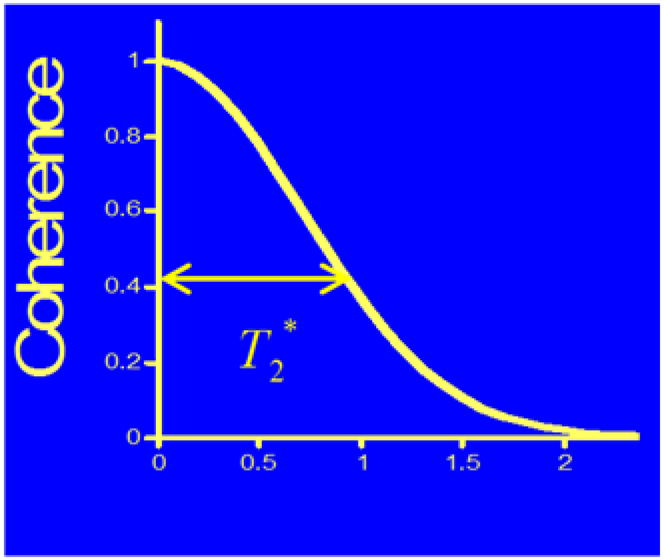
Physical make of a complex parameter



central spin decoherence:

$$H_{\text{total}} = H + S_z B$$

$$|\downarrow\rangle + |\uparrow\rangle \xrightarrow[\text{evolution}]{\text{noise } B} |\downarrow\rangle + e^{-i\int_0^t B dt} |\uparrow\rangle$$



$$\langle S_x + iS_y \rangle = \langle e^{-iBt} \rangle = \frac{\mathrm{Tr}\left[e^{-\beta H - iBt}\right]}{\mathrm{Tr}\left[e^{-\beta H}\right]}$$

Probe coherence ⇔ partition function

Time-domain study by a probe spin

arbitrary Ising model: $H(h) = -\sum J_{ij}\sigma_i\sigma_j - h\sum \sigma_j$

probe-bath coupling: $H_I = -\lambda S_z \sum \sigma_j \equiv -\lambda S_z H_1 = -S_z B$

probe spin coherence

$$\langle S_x \rangle + i\langle S_y \rangle = \langle \exp(iBt) \rangle = Z^{-1}\mathrm{Tr}\left[e^{-\beta H} e^{i\lambda H_1 t}\right]$$

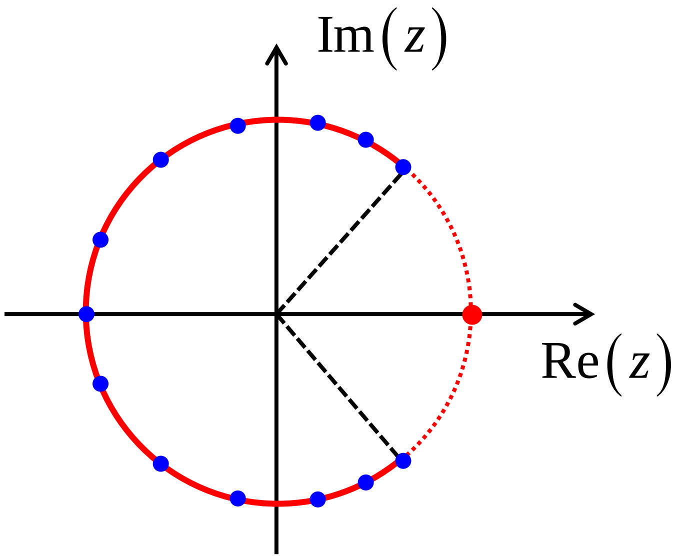
$$= Z(\beta, h - it\lambda/\beta)/Z(\beta, h)$$

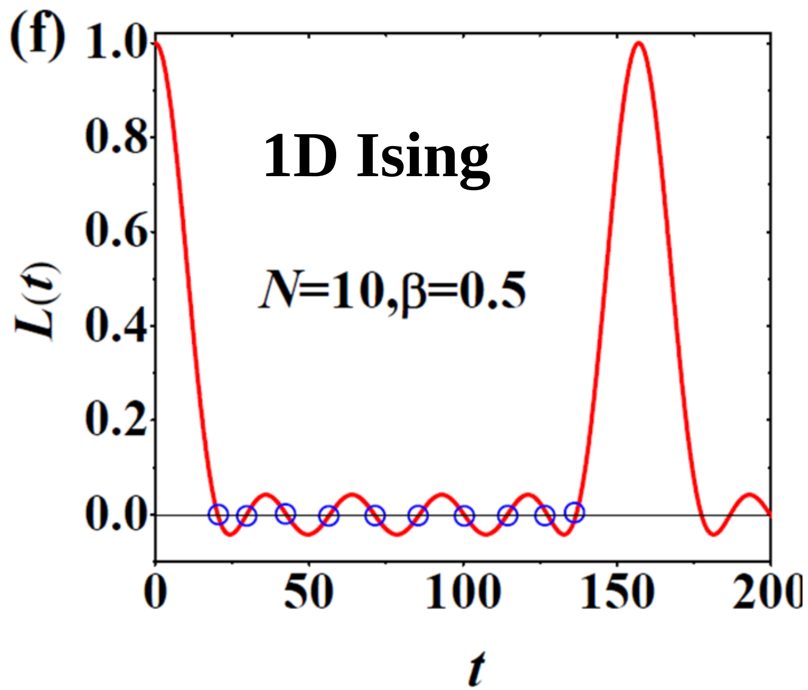
$$= e^{i4N\lambda t} \frac{\prod_{n=1}^{N}\left(e^{-2\beta h + 2i\lambda t} - z_n\right)}{\prod_{n=1}^{N}\left(e^{-2\beta h} - z_n\right)}$$

BB Wei & RBL, PRL **109**, 185701 (2012)

Time-domain study by a probe spin

probe spin coherence $\langle S_x + iS_y \rangle = e^{i4N\lambda t} \prod_{n=1}^{N} \left(e^{2i\lambda t} - z_n\right) \Big/ \prod_{n=1}^{N} (1 - z_n)$

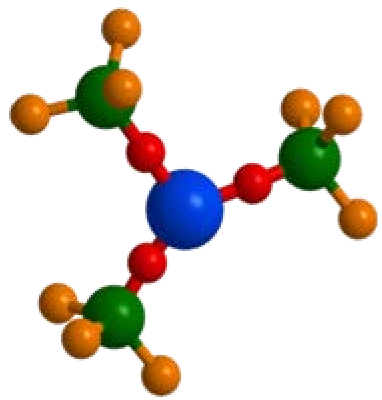


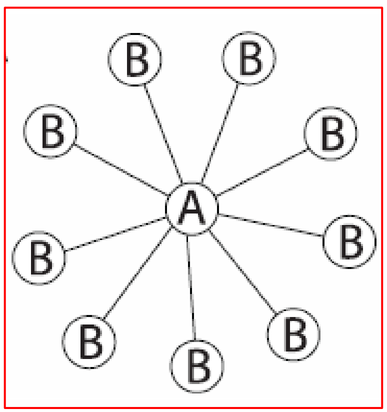


Coherence zeros @ Lee-Yang zeros $2\lambda t_n = \arg(z_n)$

BB Wei & RBL, PRL **109**, 185701 (2012)

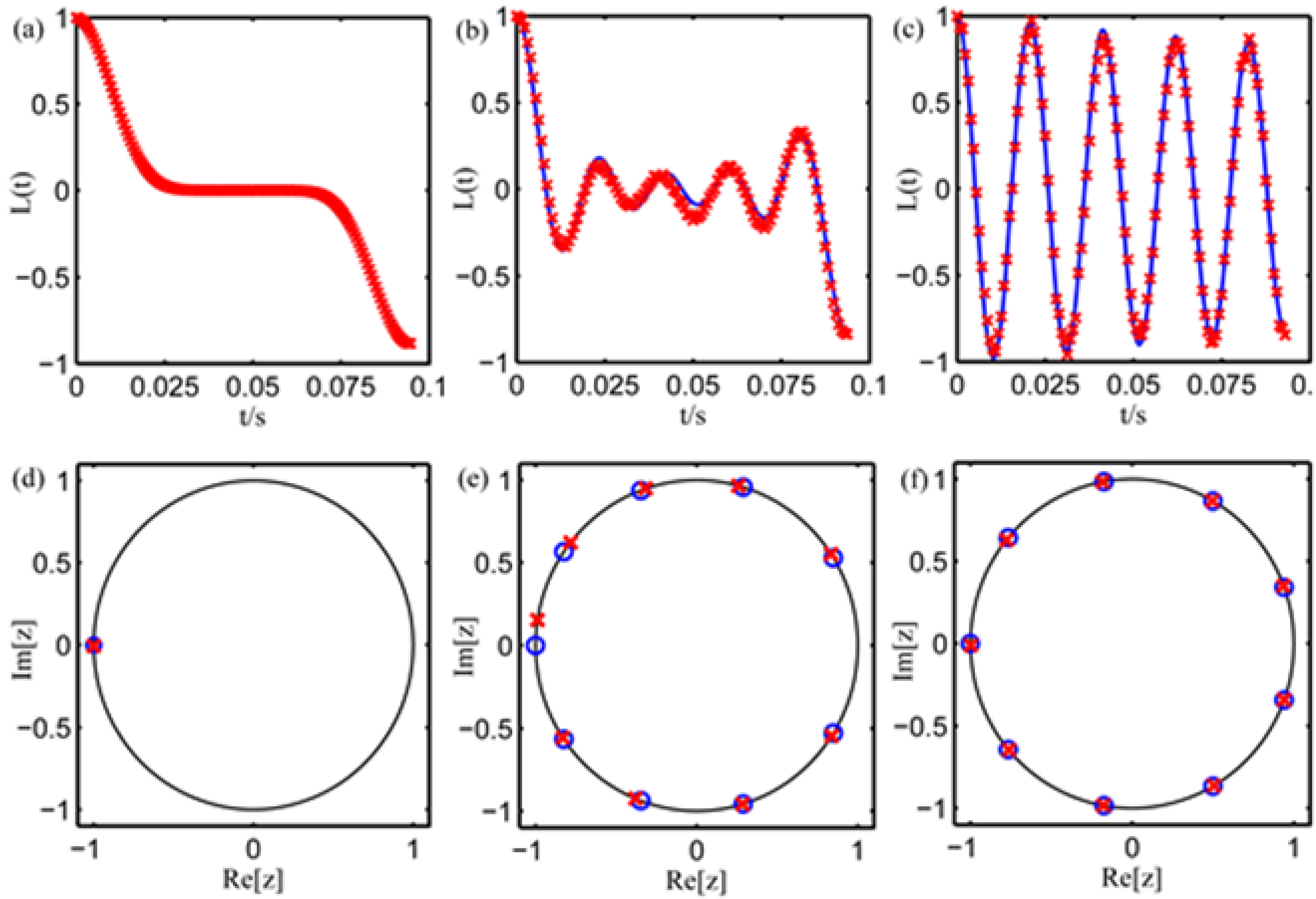
Liquid NMR Observation of Lee-Yang zeros





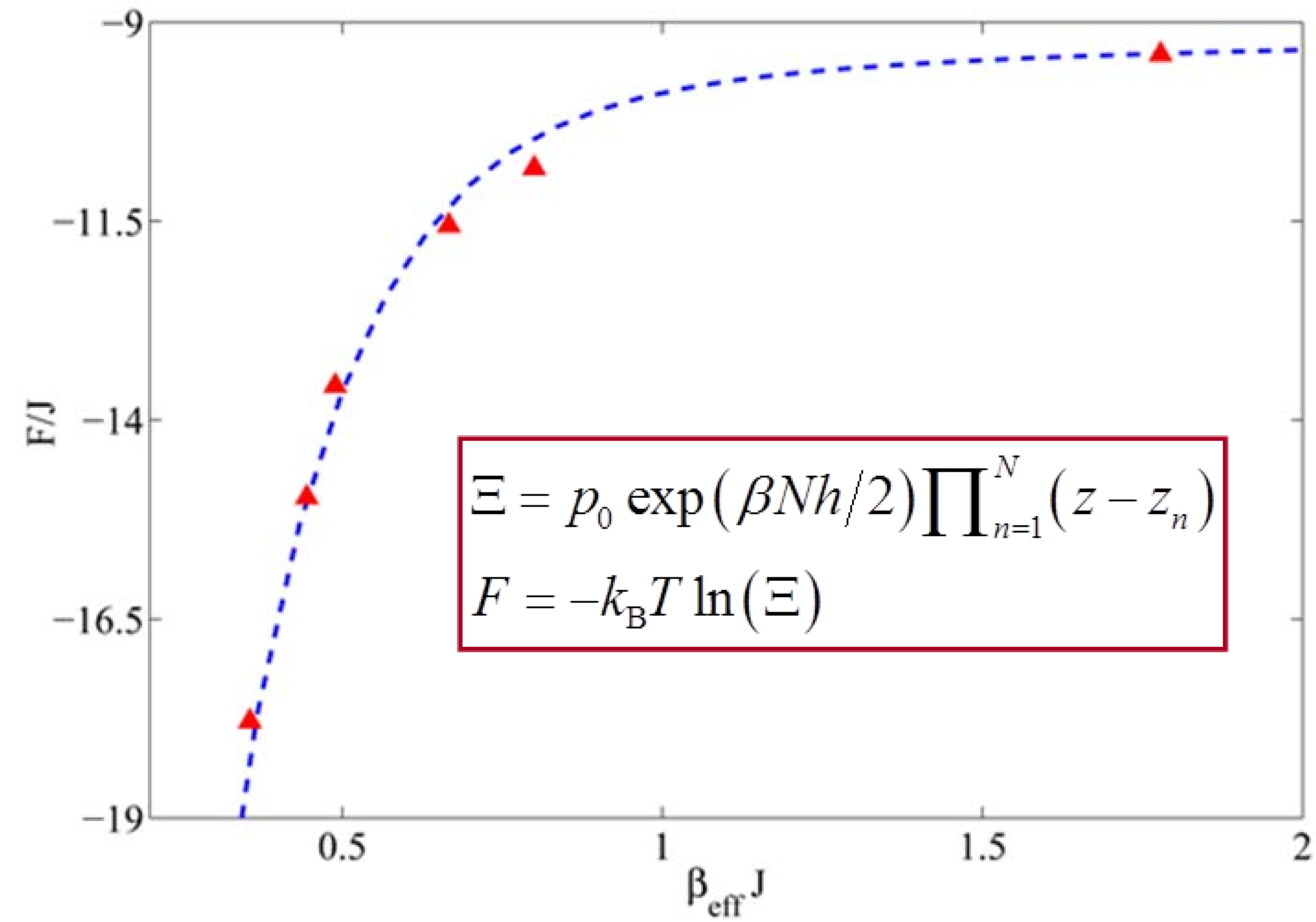
$$H_{\text{eff}} = -J\mathbf{s}_i \cdot \mathbf{s}_j$$

$$T_{\text{eff}} = \infty \qquad T_{\text{eff}} = \frac{15}{8}J > T_C \qquad T_{\text{eff}} = \frac{9}{40}J << T_C$$



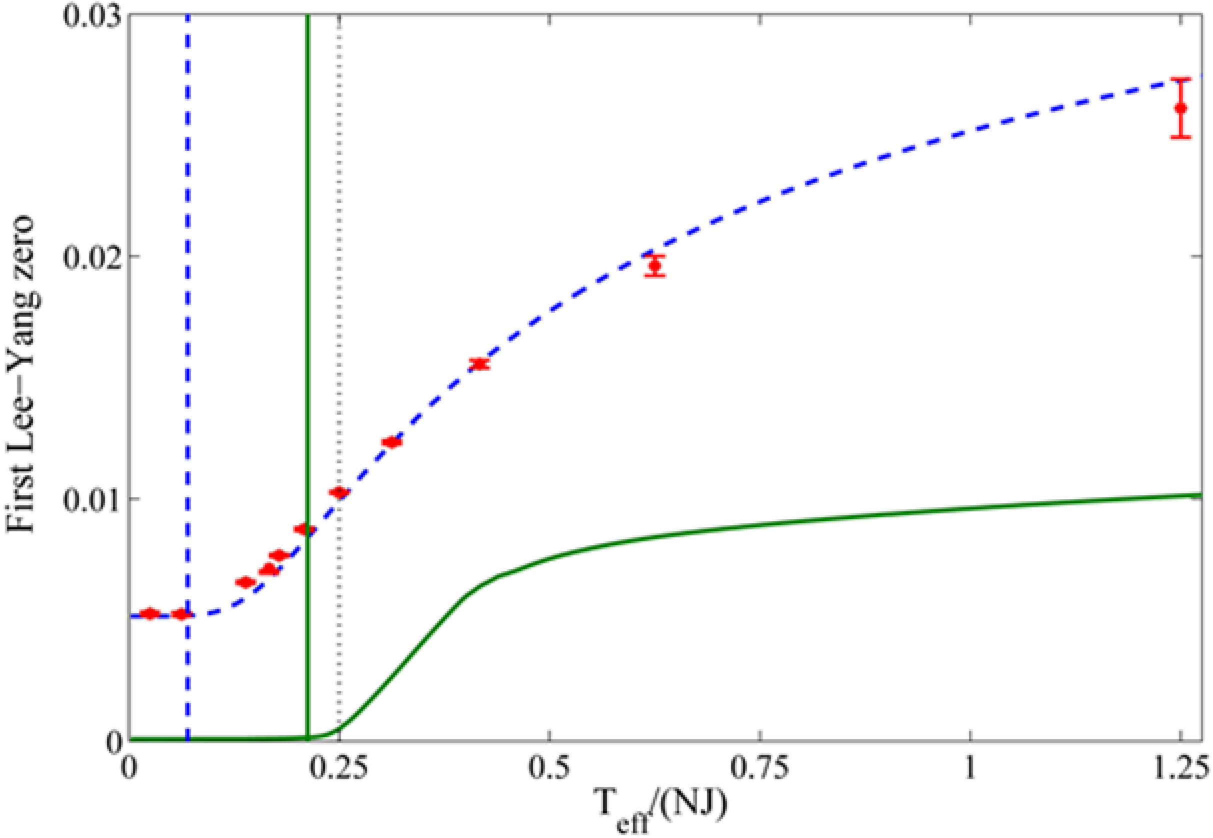
X. H. Peng et al, arXiv:1403.5383; PRL (in press)

Reconstruction of free energy using LY zeros



X. H. Peng et al, arXiv:1403.5383; PRL (in press)

Determination of phase transitions by LY zero



$$T_C = NJ/4 \text{ for } N \to \infty$$

X. H. Peng et al, arXiv:1403.5383; PRL (in press)

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B. B. Wei, Z. F. Jiang & RBL, arXiv: 1411.6342

Holography in Physics

- Optical hologram
- Unique theorem in electrostatics
- DFT: $n_0(\mathbf{r})$ ➔ full properties of ground states (Kohn, Hohenberg, Sham)
- Holographic principle in quantum gravity & string theory (t'Hooft, Susskind)
- ... …

Analyticity of partition function

For $H(\lambda) = H_0 + \lambda H_1$

$$\Xi(\beta,\lambda) = \mathrm{Tr}\left[\exp(-\beta H)\right]$$
$$= \mathrm{Tr}\left[1 - \beta H + \frac{1}{2!}(\beta H)^2 - \frac{1}{3!}(\beta H)^3 + \cdots + \frac{(-1)^N}{N!}(\beta H)^N + O(\varepsilon)\right]$$

Lemma 1. The partition function of a quantum system that has a finite number of basis states (e.g., spins and/or fermions on lattices) is analytic in the whole complex plane of λ.

For unbounded systems, such as bosons, however, it may not be the case

$$\Xi(\beta,\lambda) = \mathrm{Tr}\left[\exp\left(-\beta\omega a^\dagger a\right)\right] = \frac{1}{1-\exp(-\beta\omega)}$$

Continuation of partition function – general cases

Assumption: Quantization in a large box – discrete states

By Hölder's inequality (for finite-dimensional matrices):

$$\left|\mathrm{Tr}[A^\dagger B]\right| \le \sqrt{\mathrm{Tr}[A^\dagger A]}\sqrt{\mathrm{Tr}[B^\dagger B]}$$

For any basis state, $\left|\left\langle k \left| e^{-\beta H + i\lambda_I H_I} \right| k \right\rangle\right| \le \left\langle k \left| e^{-\beta H/2 + i\lambda_I H_I/2} e^{-\beta H/2 - i\lambda_I H_I/2} \right| k \right\rangle$

By Bernstein inequality: $\mathrm{Tr}[e^{A^\dagger} e^{A}] \le \mathrm{Tr}[e^{A^\dagger + A}]$

> *Lemma 2*. For any basis state, $\left|\left\langle k \left| e^{-\beta H + i\lambda_I H_I} \right| k \right\rangle\right| \le \left\langle k \left| e^{-\beta H} \right| k \right\rangle$,
>
> and hence $\left|\mathrm{Tr}\left(e^{-\beta H + i\lambda_I H_I}\right)\right| \le \mathrm{Tr}\left(e^{-\beta H}\right)$

Meaning: partition function maximizes on the real axis.

Analyticity of partition function – general cases

If the partition function is bounded for a real parameter in a range,

$$\Xi(\lambda_{\mathrm{R}}) \le \Xi_{\max}$$

We can choose a basis $\{|0\rangle, |1\rangle, |2\rangle, \ldots, |\mathrm{K}\rangle\}$ such that

$\Xi_K(\lambda) = \sum_{k=0}^{K} \langle k | e^{-\beta H(\lambda)} | k \rangle$ uniformly converges to $\Xi(\lambda)$, i.e.,

there exists a K_ε such that $\left|\Xi_{K>K_\varepsilon}(\lambda_{\mathrm{R}}) - \Xi(\lambda_{\mathrm{R}})\right| < \varepsilon$ for any small ε.

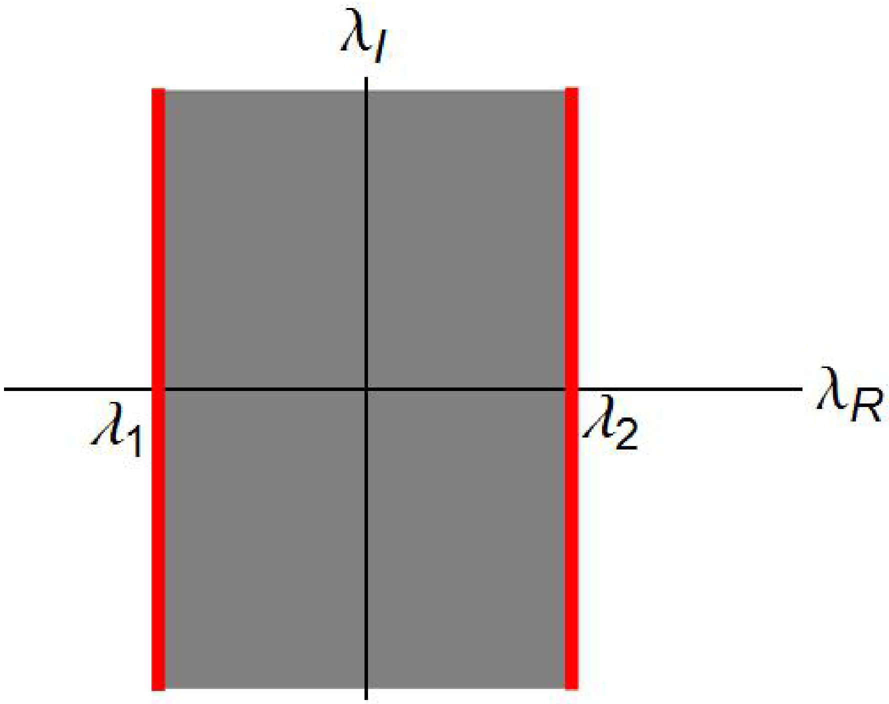
Using Lemma 2, we get,

$$\left|\sum_{k>K_\varepsilon}^{\infty} \langle k | \exp\left[-\beta H(\lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}})\right] | k \rangle\right| < \varepsilon,$$

i.e., $\Xi_K(\lambda_{\mathrm{R}} + i\lambda_{\mathrm{I}})$ uniformly converges.

Analyticity of partition function – general cases

Theorem For a system with discrete energy spectrum (quantized in a large box), if its parition function $\mathrm{Tr}\left[e^{-\beta(H+\lambda H_1)}\right]$ exists for real $\lambda \in (\lambda_1, \lambda_2)$, then $\mathrm{Tr}\left[e^{-\beta(H+\lambda H_1)}\right]$ is analytic for complex λ where $\mathrm{Re}(\lambda) \in (\lambda_1, \lambda_2)$.

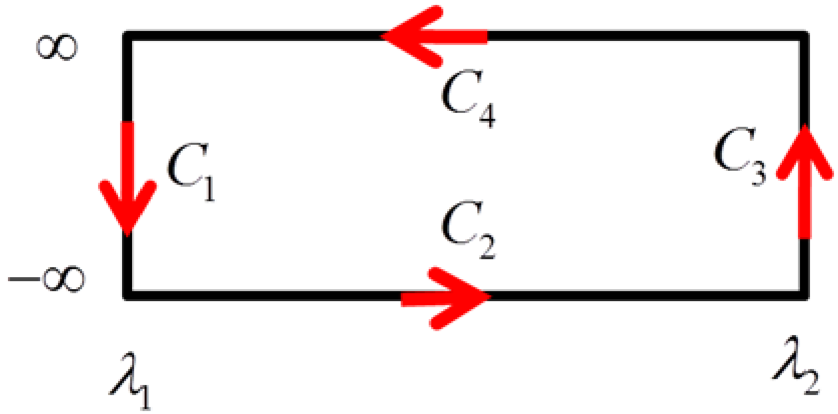


Applicable to fermions, spins, and/or bosons, on lattices or in continuum

Holography of partition function

Cauchy's theorem

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

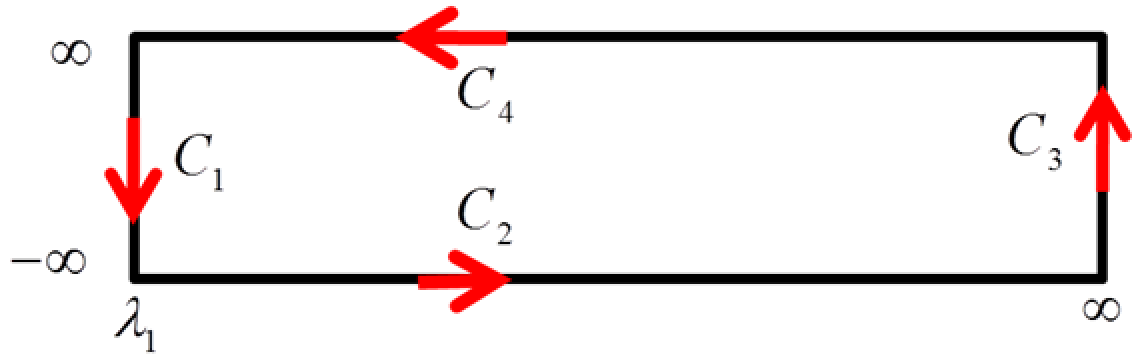


$$C_2 + C_4 \xrightarrow{\lambda_I\to\infty} 0$$

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

Reduction to one integration

let $\lambda_2 \to \infty$



$$M \le \min\left\{\langle n|\, H_j \,|n\rangle\right\}$$

Rescaling: $e^{\beta\lambda M}\,\Xi(\beta,\lambda)$

$$\Xi(\beta,\lambda') = -\int_{-\infty}^{\infty} \frac{e^{\beta(\lambda_1+i\lambda_I-\lambda')M}\,\Xi(\beta,\lambda_1+i\lambda_I)}{\lambda_1+i\lambda_I-\lambda'}\frac{d\lambda_I}{2\pi}$$

Thermodynamic holography via probe coherence

Partition function & probe spin decoherence

$$H(\lambda_1,\ldots,\lambda_k)=\sum_j \lambda_j H_j \quad \& \quad H_{SB}=-S_z\otimes H_I$$

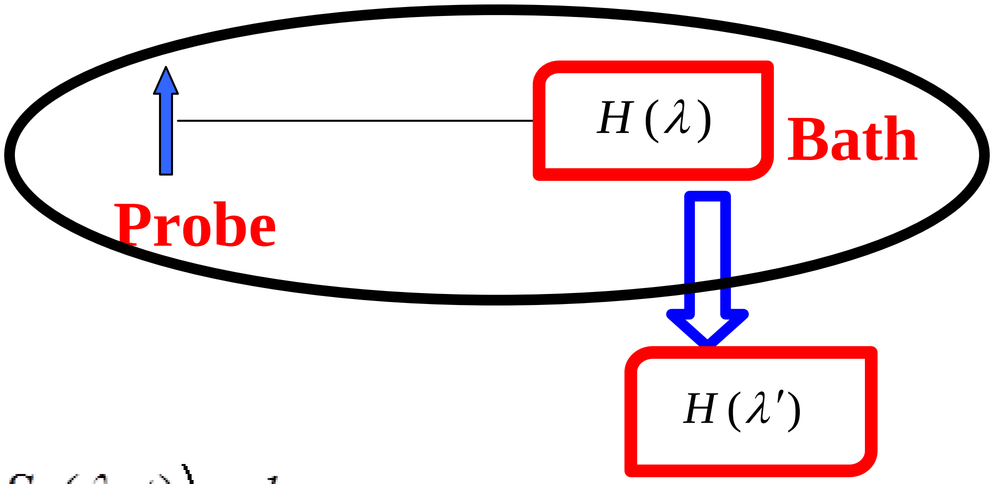
$$\langle S_+(\lambda,t)\rangle=\frac{\Xi(\beta,\lambda+it/\beta)}{\Xi(\beta,\lambda)}.$$

B. B. Wei & RBL, PRL,**109**,185701(2012).

$$\lambda\to\lambda+it/\beta$$

$$\Xi(\beta,\lambda')=-\Xi(\beta,\lambda_1)\int_{-\infty}^{\infty}\frac{e^{\beta(\lambda_1+it/\beta-\lambda')M}\langle S_+(\lambda_2,t)\rangle}{\lambda_1+it/\beta-\lambda'}\frac{dt}{2\pi\beta}$$

Application 1: Free energy difference



$$\exp(-\beta\Delta F) = \frac{\Xi(\beta,\lambda')}{\Xi(\beta,\lambda)}$$

$$= \int_{-\infty}^{\infty} \frac{e^{\beta(\lambda+it/\beta-\lambda')M}\left\langle S_+(\lambda,t)\right\rangle}{\lambda+it/\beta-\lambda'}\frac{dt}{2\pi\beta}$$

c.f. Jarzynski equality: $\exp(-\beta\Delta F) = \left\langle \exp\left(-\beta\Delta W\right)\right\rangle_{\lambda\to\lambda'}$

C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997)

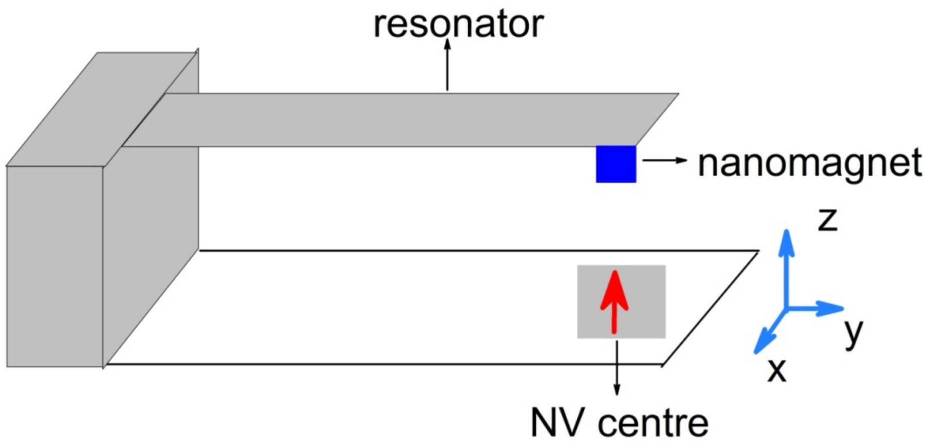
Application 2: Holography of spin coherence

$$\lambda' \to \lambda' + it'/\beta$$

$$\left\langle S_+(\lambda',t')\right\rangle = \frac{\int_{-\infty}^{\infty} \frac{e^{\beta(\lambda+it/\beta-\lambda'-it'/\beta)M}\left\langle S_+(\lambda,t)\right\rangle}{\lambda+it/\beta-\lambda'-it'/\beta}dt}{\int_{-\infty}^{\infty} \frac{e^{\beta(\lambda+it/\beta-\lambda')M}\left\langle S_+(\lambda,t)\right\rangle}{\lambda+it/\beta-\lambda'}dt},$$

Extract probe spin decoherence for arbitrary parameters by measurement for just one value of the parameter.

NV center + oscillator (~ spin + phonon in ion trap)



$$H = \Delta S_z^2 + \omega a^+ a + \delta S_z (a^+ + a)$$

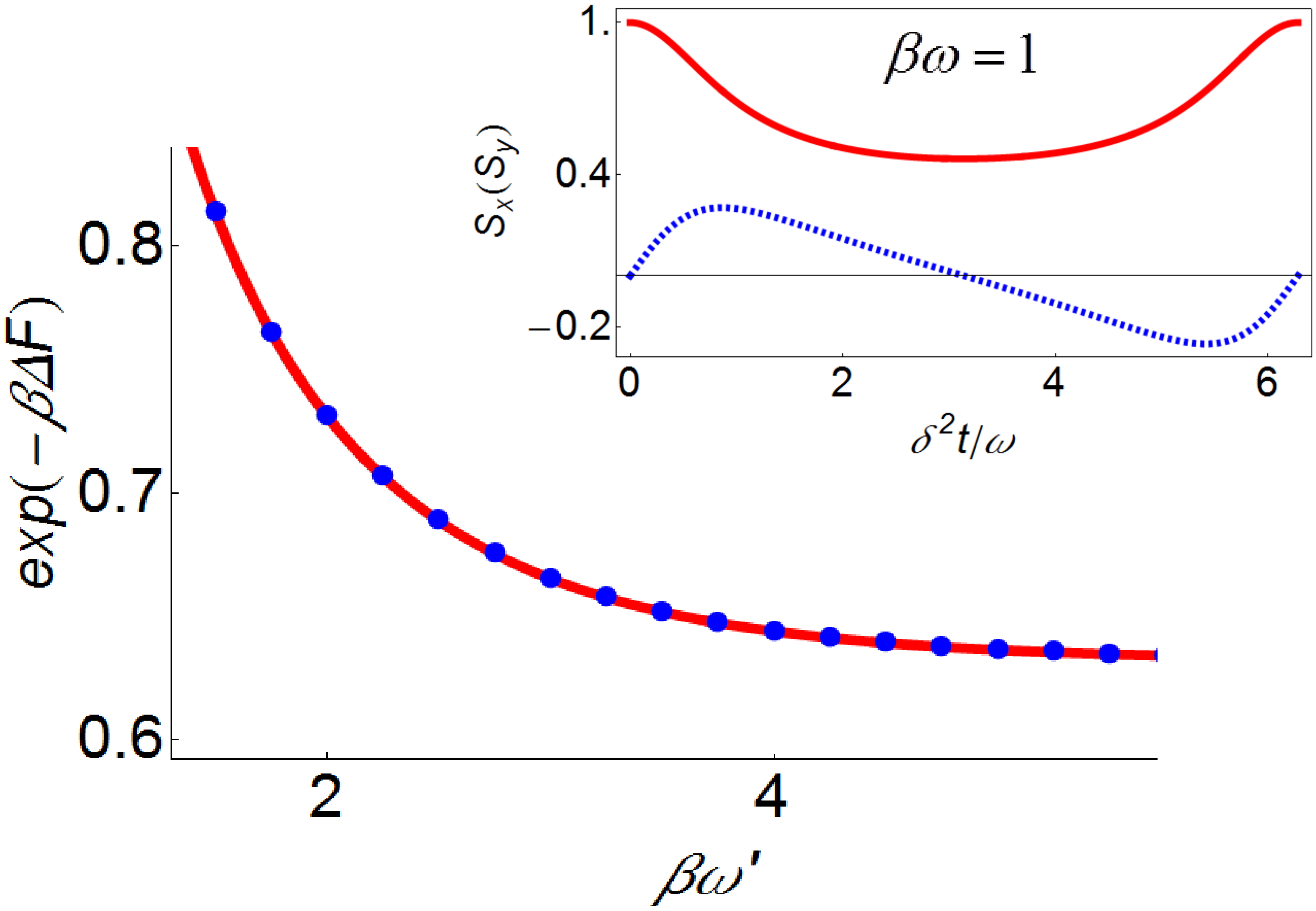
$$\delta(\sim 100 \text{ kHz}) << \omega(\sim \text{MHz})$$

$$H \xrightarrow[\text{perturbation}]{\text{2nd order}} \Delta S_z^2 + \omega a^+ a + \frac{\delta^2}{\omega} S_z \otimes a^+ a$$

Probe: NV center spin; **System:** Oscillator

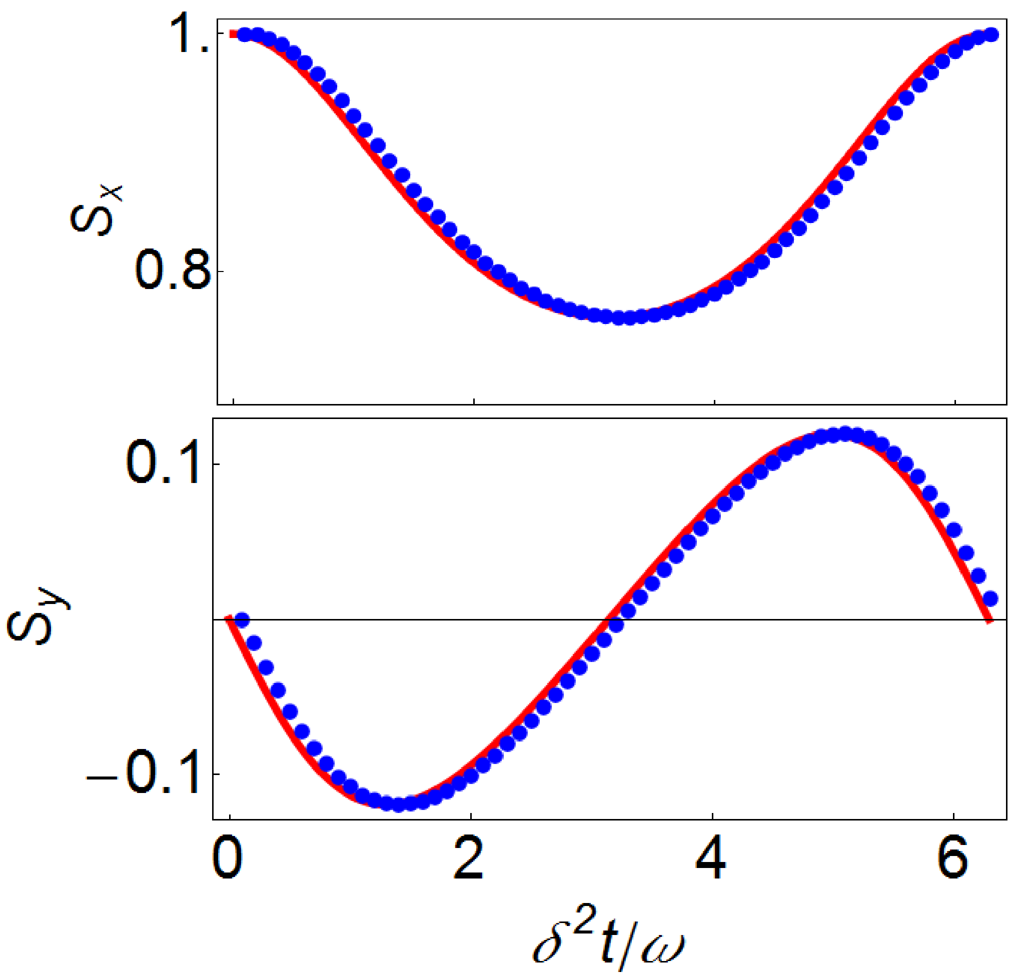
Rabl, P. *et al*. *Phys. Rev. B* **79**, 041302 (2009).
Arcizet, O. *et al*. *Nature Phys*. **7**, 879 (2011).
Kolkowitz, S. *et al*. *Science* **335**, 1063 (2012).

Spin decoherence → free energy of oscillator



Spin decoherence for h → that for h'

$\beta\omega' = 2$



Application 3: duality for many-body physics?

Strong correlation – weak correlation

duality?

Summary

- Central spin decoherence as an approach to thermodynamic on the complex plane
- Thermodynamic holography – a new approach to many-body physics?