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Quantum phase transitions in the spin-boson model

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4. Summary

Ref. 1. S. He, L. W. Duan, and *QHC*, **PRB** 97, 115157 (2018)
2. Y. Z. Wang, S. He, L. W. Duan, and *QHC*, **PRB** 100, 115106 (2019)

1. Brief introduction to the spin-boson model

$$H = \frac{\varepsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^+ a_k + \sum_k \lambda_k \left(a_k^+ + a_k\right)\sigma_x$$

spin | bosonic bath | coupling

σ_i (i = x, y,z) are the Pauli matrices, Δ is the qubit (spin, two-level-system) frequency, a_k ($a^\dagger_k$) is the bosonic annihilation (creation) operator for a boson with frequency ω_k .

The coupling between spin and bath is described by spectral functions

$$J(\omega) = \pi \sum_k \lambda_k^{\ 2} \delta(\omega - \omega_k)$$

sub-ohmic	s<1
Ohmic	s=1
Super-ohmic	s>1

$$J(\omega) = 2\pi\alpha\omega_c^{\ 1-s}\omega^s, 0 < \omega < \omega_c,$$

α is coupling strength

Single-mode: **quantum Rabi model** $H = \frac{\varepsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \omega a^+ a + g\left(a^+ + a\right)\sigma_x$

Quantum phase transtions in the sub-Ohmic SBM （$\varepsilon=0$）

Mapping (***not exactly***) to Local Φ^4 theory, a long range interaction in imaginary time

$$\frac{1}{2}S^z(\tau)\chi_0^{-1}(\tau-\tau')S^z(\tau'), \chi_0^{-1}(\tau-\tau') \propto \frac{1}{(\tau-\tau')^{1+s}}$$

1D Ising model with long range interaction: M. E. Fisher, PRL29, 917 (1972)

Quantum-to-classical correspondence (QCC)：

$0 < s < \frac{1}{2}$ Gaussian critical fixed point and classical exponents, above the upper critical dimension

$\frac{1}{2} < s < 1$ **Interacting** critical fixed point and non classical exponents below the upper critical dimension

Classical model, E. Luijten and H. Blöte, PRB 56, 8945 (1997).

But

Initial NRG: R. Bulla et al, PRL 91, 170601 (2003); 94, 070604 (2005)

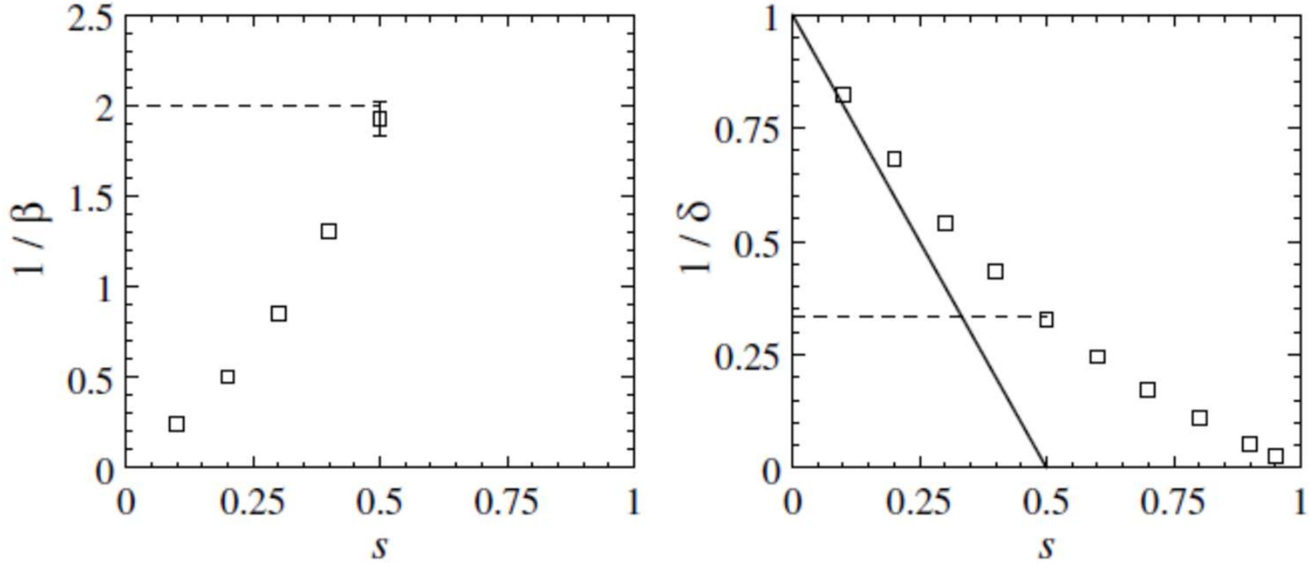
Critical fixed points are interacting and non classical exponents for 0<s<1/2

Failure of QCC:

Conventional NRG before 2009， Anders, Bulla, and Vojta, PRL 98, 210402 (2007)

Failure of quantum-classical mapping

$m \propto (\alpha - \alpha_c)^{\beta}$ $m(\alpha = \alpha_c) \propto \varepsilon^{1/\delta}$



But 3 papers in 2009 and 2010 suggested mean-field behavior for 0< s <1/2

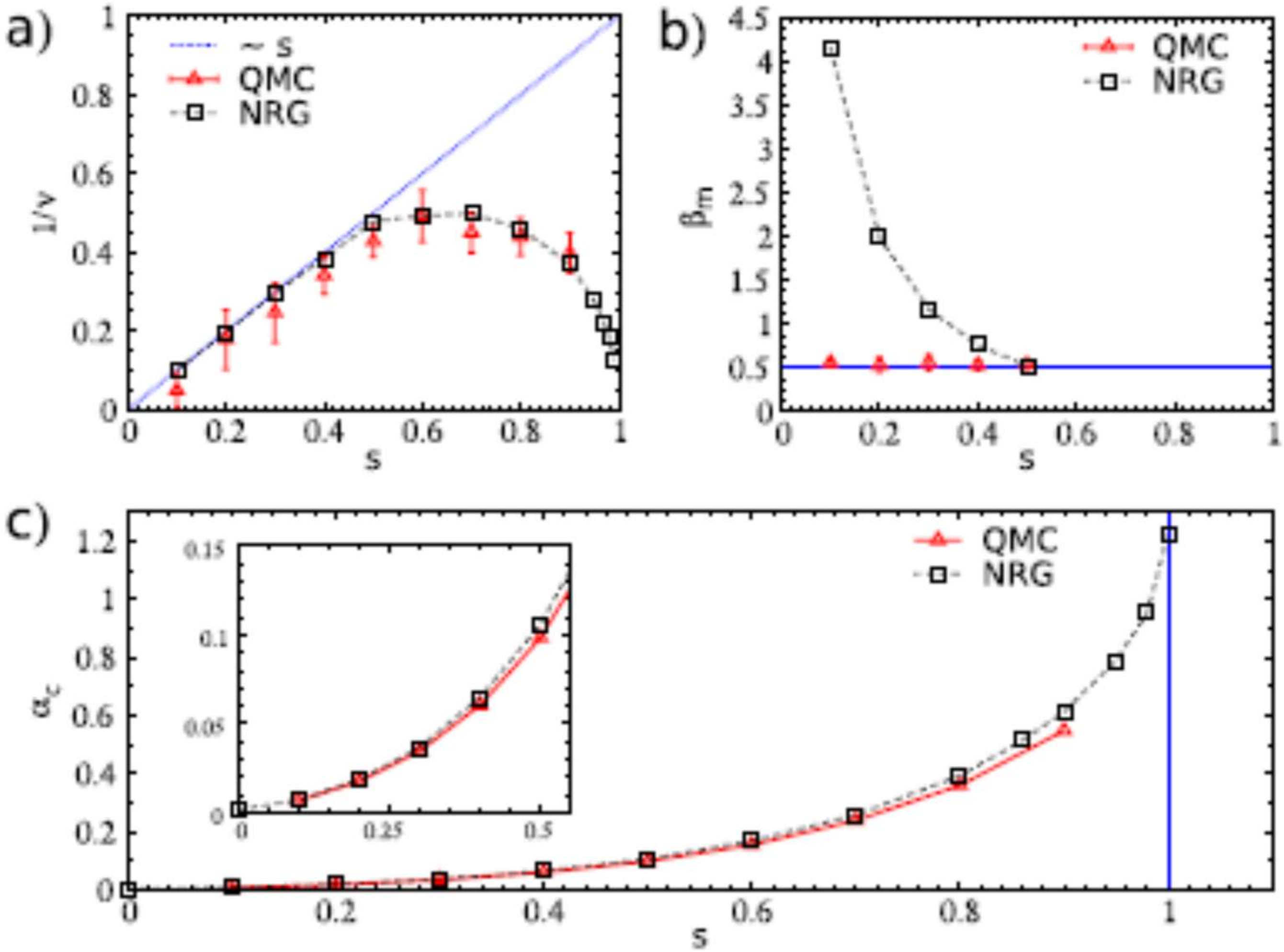
Vojta et al., PRB 81, 075122(2010), PRB 85, 115113

Two errors

(1) Boson-state truncation error. effects on exponents β and δ

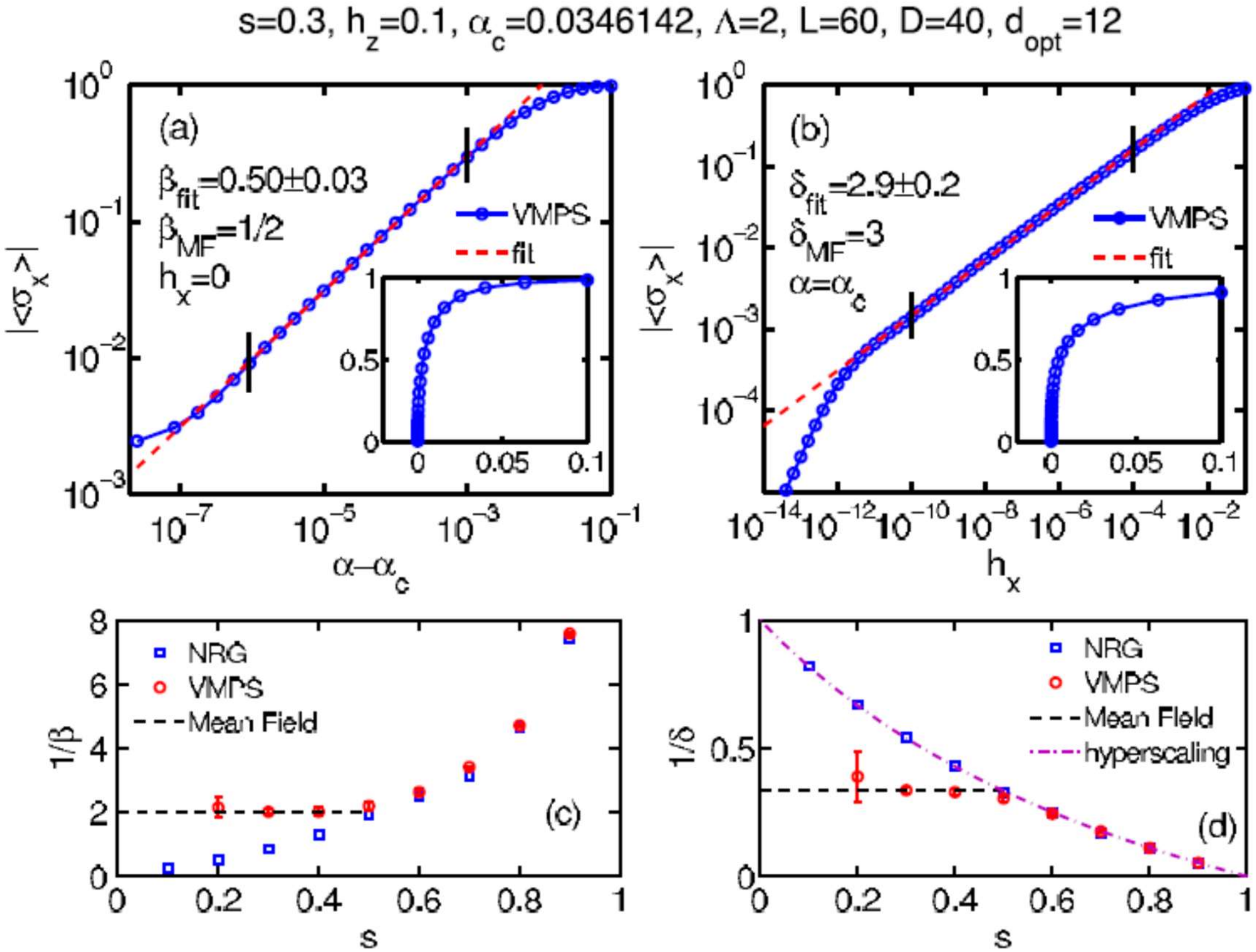
(2) Mass-flow error: x

Quantum Monte Carlo study, A. Winter et al., **PRL** 102, 030601 (2009)



β=1/2, γ=1, mean-field like, for 0< s <1/2

Variational **matrix product state** (MPS) approach involving an optimized boson basis.
C. Guo, A. Weichselbaum, J. V. Delft, and M. Vojta, **PRL** 108, 160401 (2012).



$$m = \langle \sigma_x \rangle \propto (\alpha - \alpha_c)^{\beta}$$

$$m(\alpha = \alpha_c) \propto \varepsilon^{1/\delta}$$

Silbey-Harris ansatz, i.e. polaron ansatz: many applications

R. Silbey and R. A. Harris, **J. Chem. Phys**. 80, 2615 (1984)

$$|\Psi\rangle_{SH} \propto \begin{pmatrix} A\exp\left[\sum_k \alpha(k) a_k^\dagger\right] \\ A\exp\left[-\sum_k \alpha(k) a_k^\dagger\right] \end{pmatrix} |0\rangle$$

◇ A. W. Chin et al, **PRL** 107, 160601 (2011)

$$|\Psi\rangle_{GSH} \propto \begin{pmatrix} A\exp\left[\sum_k \alpha(k) a_k^\dagger\right] \\ B\exp\left[-\sum_k \beta(k) a_k^\dagger\right] \end{pmatrix} |0\rangle$$

◇ S. Bera et al., **PRB** 89, 121108 (R) (2014); **PRB** 90, 075110 (2014).

Superposing many nonorthogonal coherent states on the equal footing

$$\Psi = \begin{pmatrix} \left\{A_1\exp\left[\sum_k \alpha_1(k) a_k^\dagger\right] + A_2\exp\left[\sum_k \alpha_2(k) a_k^\dagger\right] + \ldots\right\} |0> \\ \left\{B_1\exp\left[-\sum_k \beta_1(k) a_k^\dagger\right] + B_2\exp\left[-\sum_k \beta_2(k) a_k^\dagger\right] + \ldots\right\} |0> \end{pmatrix} +$$

2. Orthogonal displaced Fock states approach and applications to the spin boson model

S. He, L. W. Duan, and *QHC*, **Phys. Rev. B** 97, 115157 (2018)

$$H=\begin{pmatrix} \sum_k \omega_k a_k^+ a_k + \frac{1}{2}\sum_k g_k (a_k^+ + a_k) & -\frac{\Delta}{2} \\ -\frac{\Delta}{2} & \sum_k \omega_k a_k^+ a_k - \frac{1}{2}\sum_k g_k (a_k^+ + a_k) \end{pmatrix}$$

Parity conservation $[\Pi, H]=0$

$$\Pi = -\sigma_z \exp\left(i\pi N\right)$$

$$N=\sum_k a_k^\dagger a_k$$

Expanding in complete orthogonal basis and *no parity symmetry breaking*

$$\left|\Psi\right\rangle = \begin{pmatrix} \left[1+\sum_k u_k a_k^\dagger + \sum_{k_1k_2} v_{k_1k_2} a_{k_1}^\dagger a_{k_2}^\dagger + \sum_{k_1k_2k_3} w_{k_1k_2k_3} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger + \ldots\right]\left|0\right\rangle \\ \left[1-\sum_k u_k a_k^\dagger + \sum_{k_1k_2} v_{k_1k_2} a_{k_1}^\dagger a_{k_2}^\dagger - \sum_{k_1k_2k_3} w_{k_1k_2k_3} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger + \ldots\right]\left|0\right\rangle \end{pmatrix}$$

Displaced operator $D[\mathrm{u}(k)] = \exp\left[\sum_k u(k)\left(a_k^\dagger - a_k\right)\right], D^\dagger[\mathrm{u}(k)] a_k^\dagger D[\mathrm{u}(k)] = a_k^\dagger + u(k)$

$$\left|\Psi\right\rangle = \begin{pmatrix} \left[1+\sum_{k_1k_2} b_{k_1k_2} a_{k_1}^\dagger a_{k_2}^\dagger + \sum_{k_1k_2k_3} c_{k_1k_2k_3} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger + \ldots\right] D\left[u_k\right]\left|0\right\rangle \\ \left[1+\sum_{k_1k_2} b_{k_1k_2} a_{k_1}^\dagger a_{k_2}^\dagger - \sum_{k_1k_2k_3} c_{k_1k_2k_3} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger + \ldots\right] D\left[-u_k\right]\left|0\right\rangle \end{pmatrix}$$

$$Sub-Ohmic$$

$$|\Psi\rangle = \begin{pmatrix} \left[1+\sum_{k_1k_2} b_{k_1k_2} a_{k_1}^{\dagger} a_{k_2}^{\dagger} + \sum_{k_1k_2k_3} c_{k_1k_2k_3} a_{k_1}^{\dagger} a_{k_2}^{\dagger} a_{k_3}^{\dagger} + \ldots\right] D[u_k]|0\rangle \\ \left[A+\sum_{k_1k_2} B_{k_1k_2} a_{k_1}^{\dagger} a_{k_2}^{\dagger} - \sum_{k_1k_2k_3} C_{k_1k_2k_3} a_{k_1}^{\dagger} a_{k_2}^{\dagger} a_{k_3}^{\dagger} + \ldots\right] D[-U_k]|0\rangle \end{pmatrix}$$

- Zeroth-order approximation: $\Psi_0 = \begin{pmatrix} D[\alpha(k)]|0\rangle \\ D^{\dagger}[\alpha(k)]|0\rangle \end{pmatrix}$

Projecting the Schroedinger Eq. onto the orthogonal states

$$\langle 0|D^{+}(\alpha_k), \langle 0|a_k D^{+}(\alpha_k), \ \ldots$$

$$E = \sum_k \omega_k \alpha_k^2 + \sum_k g_k \alpha_k - \frac{\Delta}{2} \exp\left[-2\sum_k \alpha_k^2\right]$$

$$\alpha_k = \frac{-\frac{1}{2} g_k}{\omega_k + \Delta \exp\left(-2\sum_k \alpha_k^2\right)},$$

Famous Silbey-Harris ansatz comes out naturally

◇ second-order approximation: (two-particle correlations are fully considered)

$$\Psi_2 = \left(\begin{array}{c} \left(1+\sum_{k_1k_2} b(k_1k_2)a_{k_1}^{\dagger}a_{k_2}^{\dagger}\right) D[\alpha(k)]|0\rangle \\ \left(1+\sum_{k_1k_2} b(k_1k_2)a_{k_1}^{\dagger}a_{k_2}^{\dagger}\right) D^{\dagger}[\alpha(k)]|0\rangle \end{array} \right) \qquad D[\alpha(k)] = \exp\left[\sum_k \alpha(k)\left(a_k^{\dagger} - a_k\right)\right]$$

$$\sum_k \left[\omega_k \alpha^2(k) + g_k \alpha(k)\right] - \frac{\Delta}{2}\eta\left[1+4\sum_k B_k^{(O)}\alpha(k)\right] = E \qquad (1)$$

$$0 = \left[\omega_k \alpha(k) + \frac{g_k}{2}\right] + 2\sum_{k'} b(k,k')\left[\omega_{k'}\alpha(k') + \frac{g_{k'}}{2}\right] - 2\Delta\eta B_k^{(O)} + \Delta\eta\alpha(k)\left[1+4\sum_k B_k^{(O)}\alpha(k)\right] \qquad (2)$$

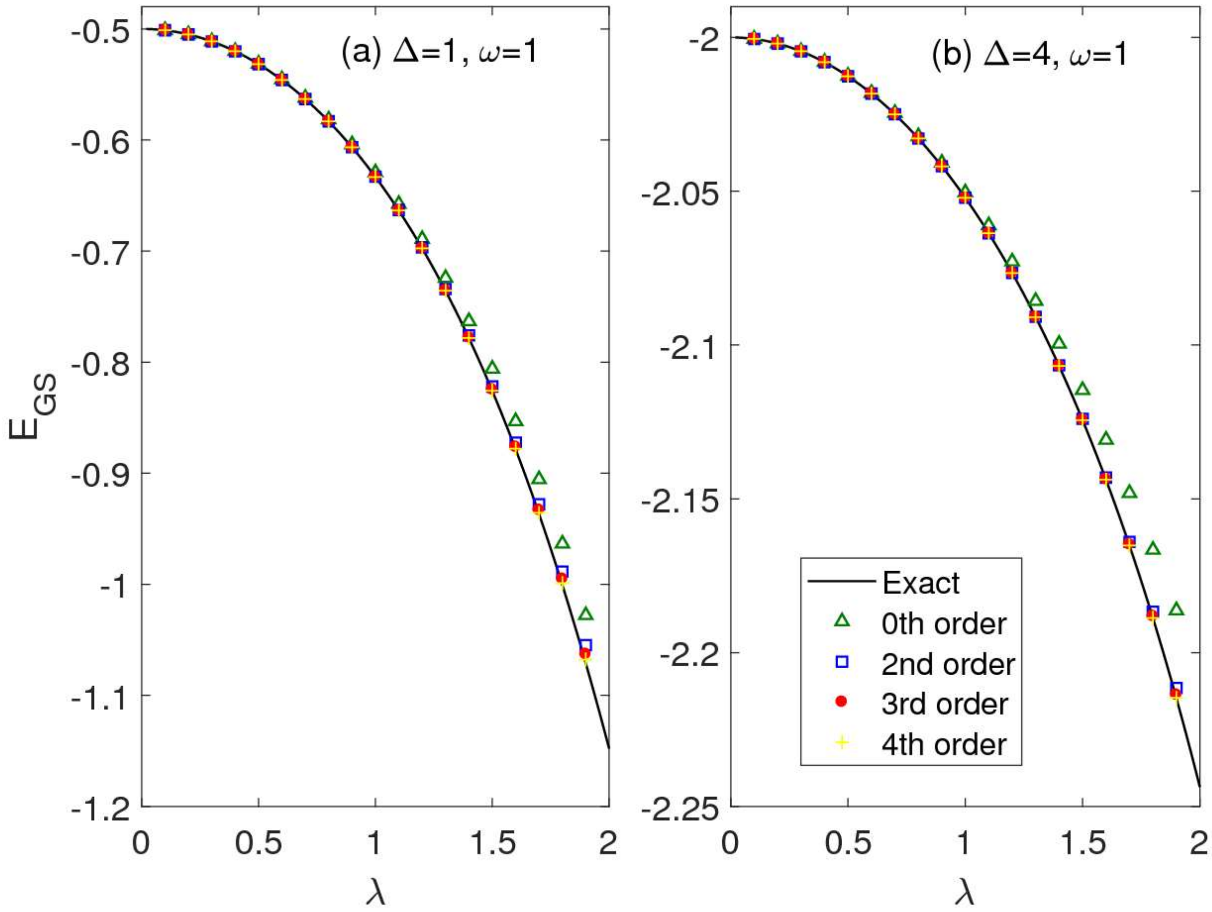
$$\begin{aligned} 0 \ =\ & b(k_1,k_2)\left(\omega_{k_1}+\omega_{k_2}\right) + \frac{\Delta}{2} b(k_1,k_2)\eta\left[1+4\sum_k B_k^{(O)}\alpha(k)\right] \\ & -\frac{\Delta}{2}\eta b(k_1,k_2) + \Delta\eta\left[B_{k_1}^{(O)}\alpha(k_2) + B_{k_2}^{(O)}\alpha(k_1)\right] - \Delta\eta\alpha(k_1)\alpha(k_2)\left[1+4\sum_k B_k^{(O)}\alpha(k)\right] \end{aligned} \qquad (3)$$

Three coupled equations can be solved self-consistently

◇ Further projection on the orthogonal displaced Fock states can be performed straightforwardly, and the solution within any desired accuracy could be achieved.

Applications to the single-mode Quantum Rabi model

$$H = \frac{\Delta}{2}\sigma_z + \omega a^{+}a + g\left(a^{+} + a\right)\sigma_x$$



The results in the 4th order is almost exact

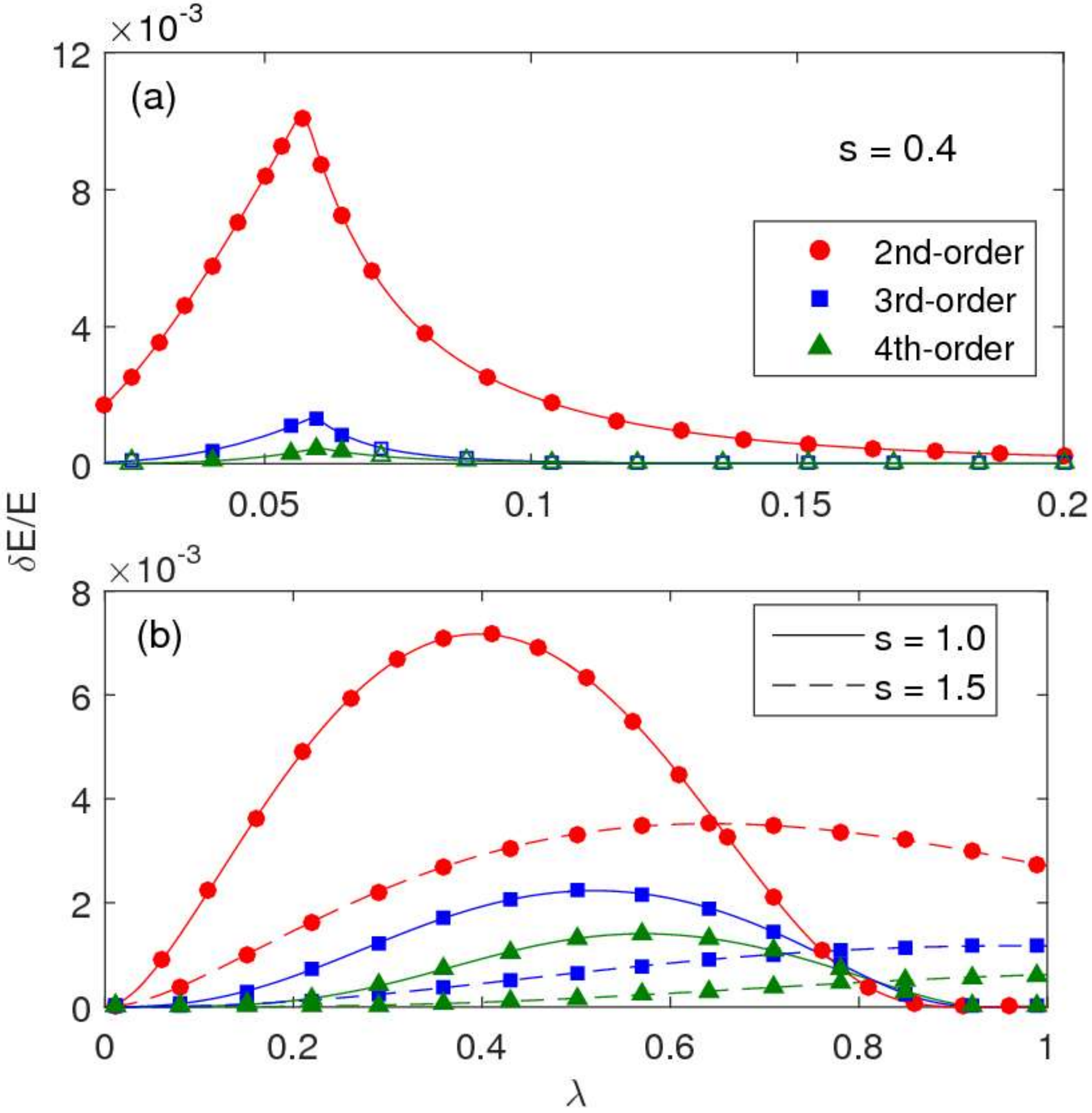
Applications to the spin-bosn model

Relative difference of the ground-state energy in the successive order for all typical baths

sub-Ohmic $s<1$

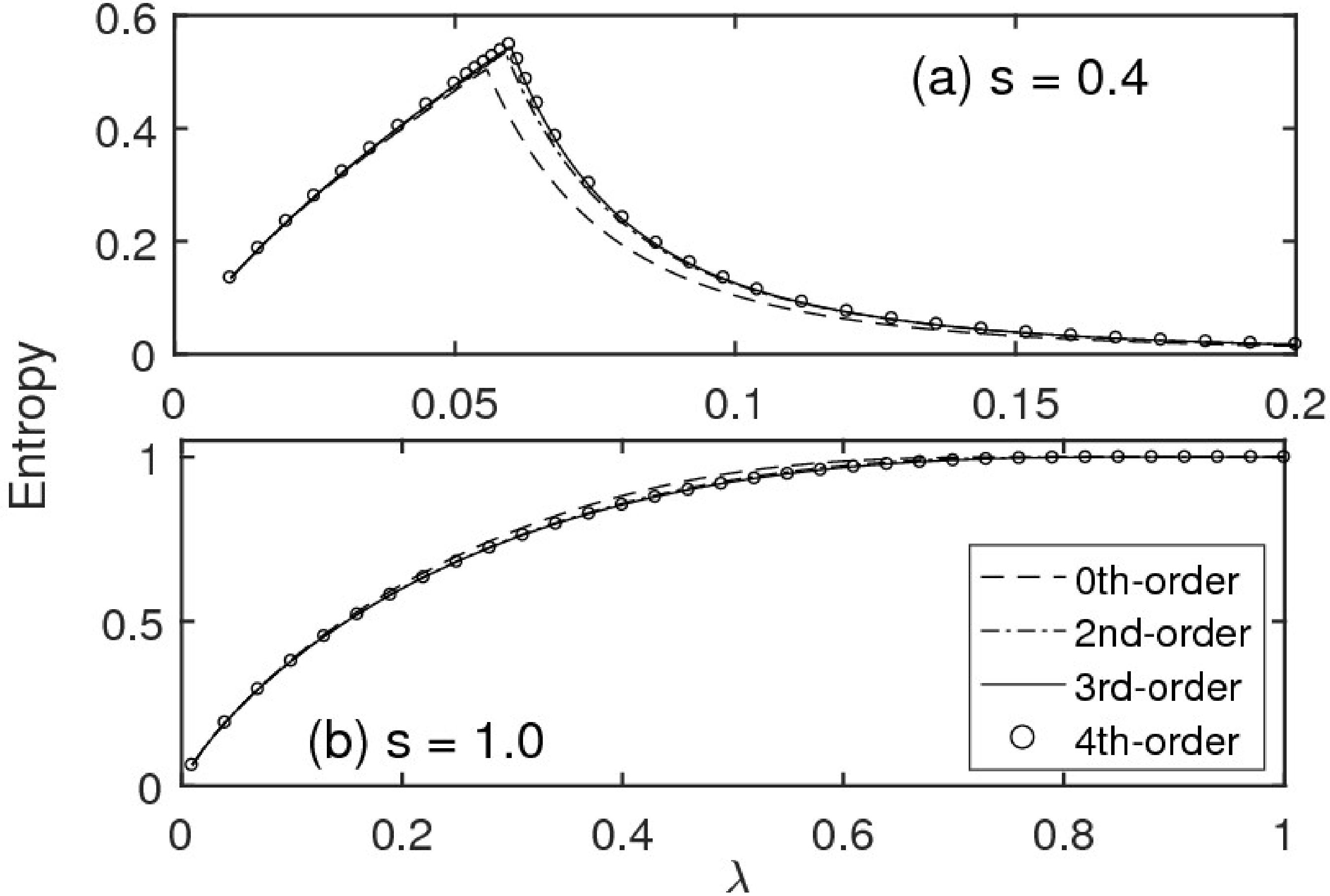
Ohmic $s=1$

super-Ohmic $s>1$

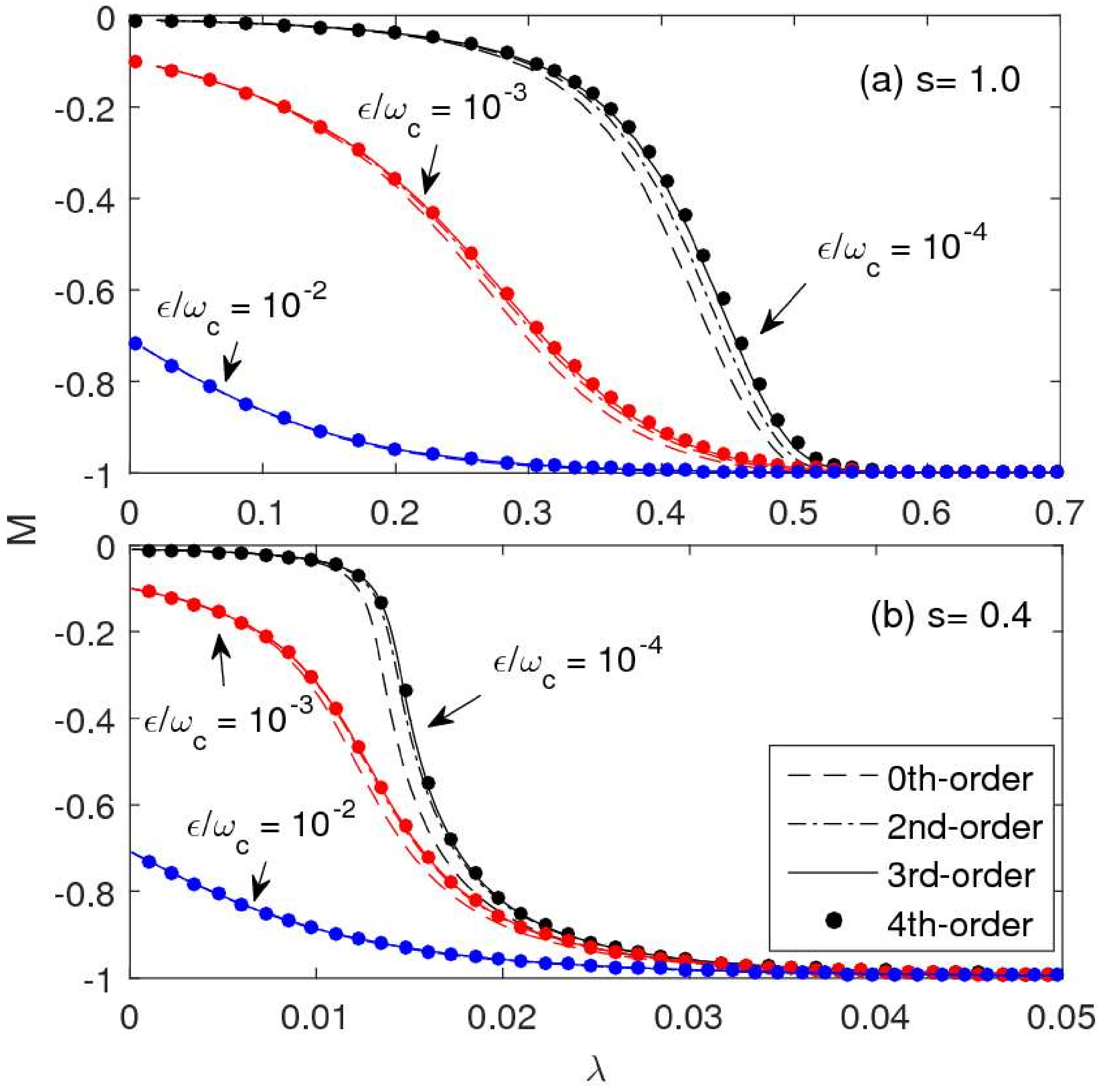


Entanglement entropy

$$S = -p_+ \log_2 p_+ - p_- \log_2 p_- \quad p_\pm = \left(1 \pm \sqrt{\langle\sigma_x\rangle^2 + \langle\sigma_z\rangle^2}\right)/2$$



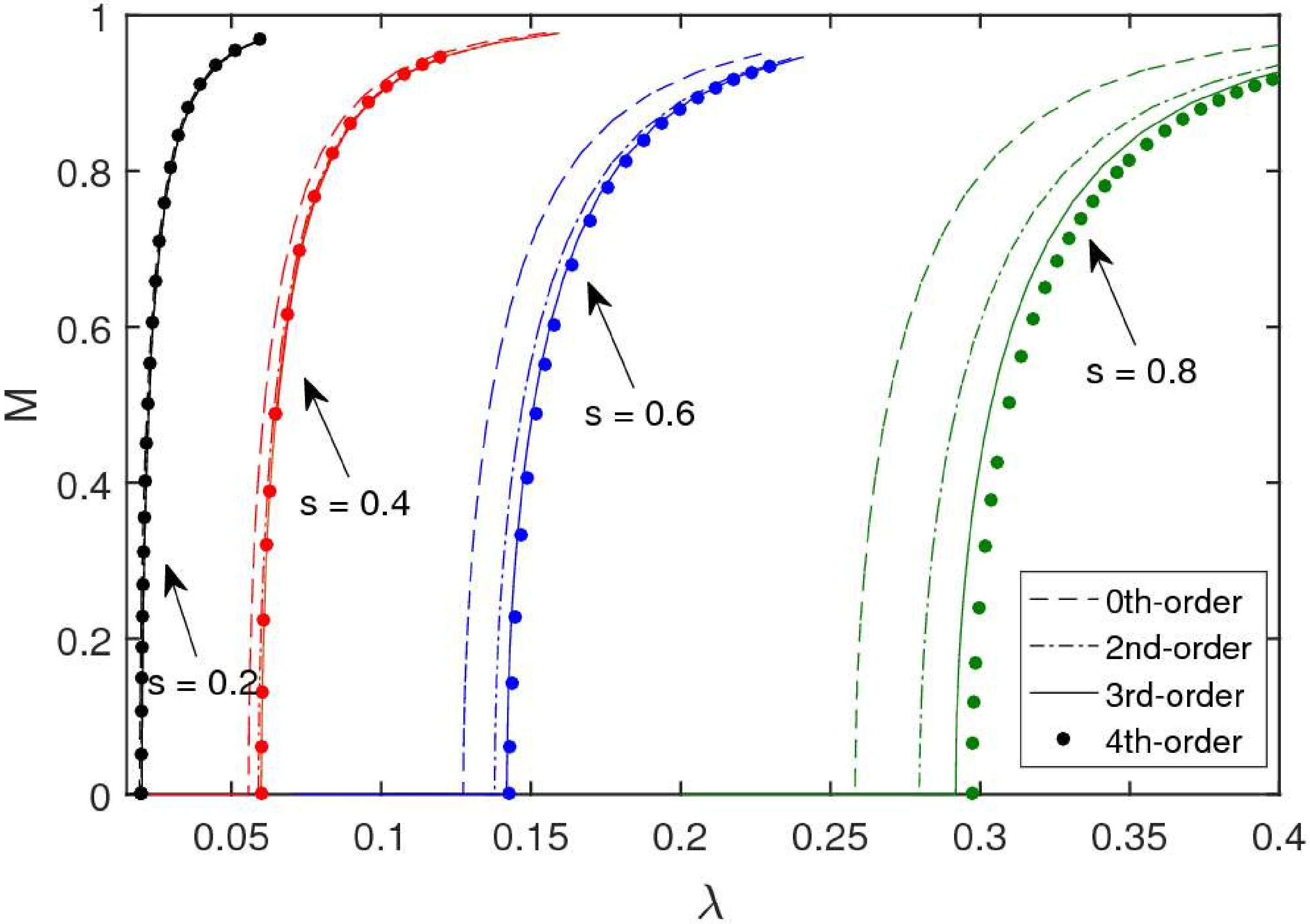
In excellent agreement with the Bethe ansatz solutions for Ohmic baths
A. Kopp and K. Le Hur, PRL 98, 220401(2007)



(a) s= 1.0
ϵ/ω_c = 10^-3
ϵ/ω_c = 10^-4
ϵ/ω_c = 10^-2
(b) s= 0.4
ϵ/ω_c = 10^-4
ϵ/ω_c = 10^-3
ϵ/ω_c = 10^-2
0th-order
2nd-order
3rd-order
4th-order
M
λ
0
-0.2
-0.4
-0.6
-0.8
-1
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.01
0.02
0.03
0.04
0.05

Quantun phase transitions in the sub-Ohmic boson model

$M = \langle \sigma_z \rangle$ Order parameter



The magnetization $\langle\sigma_z\rangle$ as a function of the coupling strength within different finite-order corrections *for s=0.2, 0.4,0.6,* and 0.8. $\Delta/\omega_c=0.1$

TABLE I: The critical coupling strengths within different approaches. The results by the present three order approximations are given in the second, third, and the fourth columns. The fifth column presents those by quantum Monte Carlo simulations [19], the sixth by the NRG results[15], the last column by the results from MPS[24].

ABLE I: The critical coupling strengths within different order approximations are collected. The sixth column pres
y quantum Monte Carlo simulations [21].

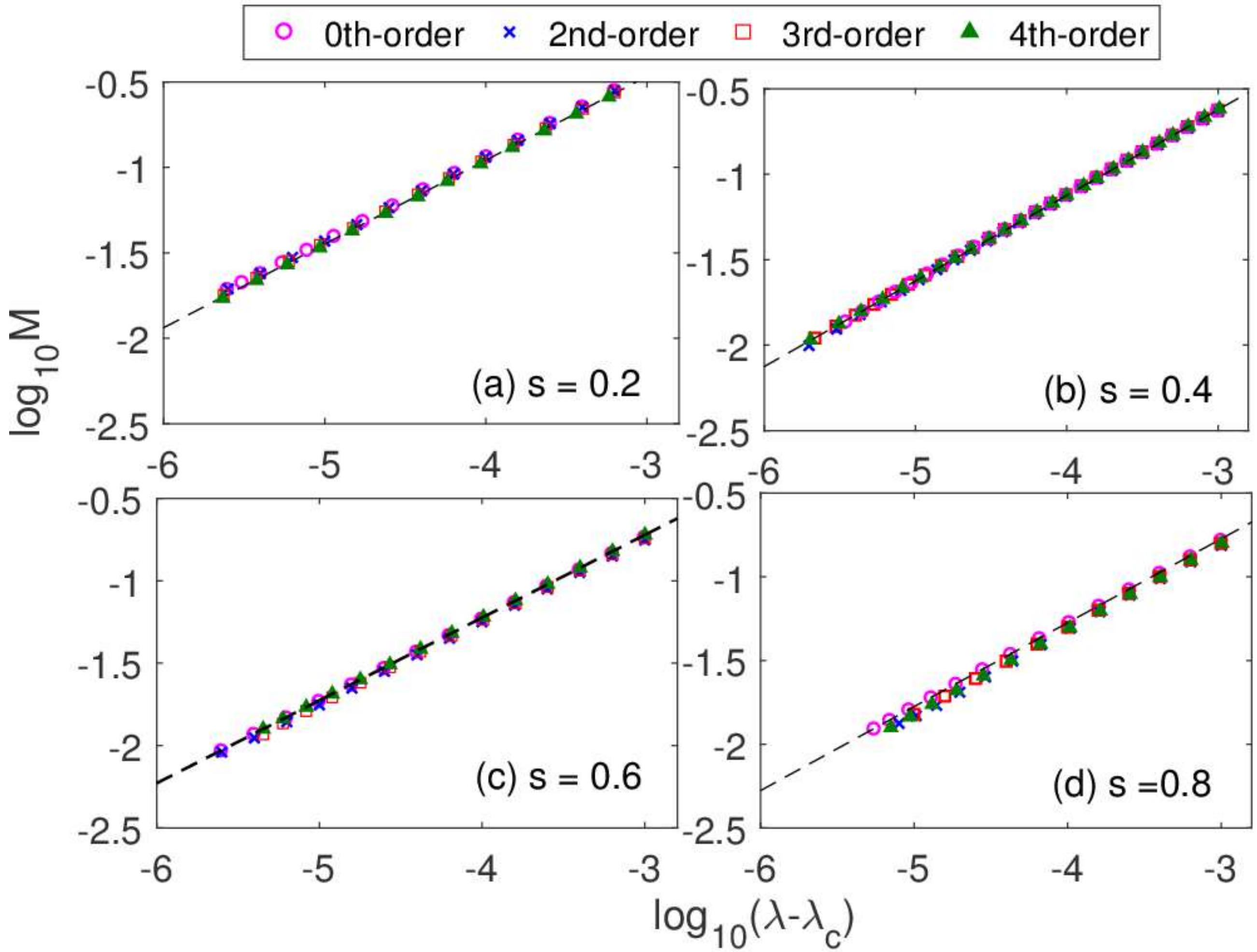
s	$0th$	$2nd$	$3rd$	$4th$	$QMC^{Ref.[21]}$
0.2	0.0195	0.02005	0.02013	0.02014	0.0175
0.4	0.0557	0.0590	0.0599	0.0600	0.0601
0.6	0.127	0.138	0.142	0.143	0.155
0.8	0.258	0.280	0.292	0.297	0.359

λ_c for $s=0.4$ in our third-order DFS is very close to that in the Quantum Monte Carlo simulations

λ_c for $s=0.2$ unlikely converges to the QMC value due to the trend of convergence. The statistical error in QMC simulations may account for this slight

Our results for 0<s<1/2 can be regarded as benchmark because of no approximation and convergence

Order parameter exponent up to the fourth-order approximations



$$m = \langle \sigma_z \rangle \propto (\alpha - \alpha_c)^{\beta}$$

The log-log plot of the magnetization *M* as a function the α-α_c , Δ/ω_c=0.1.
Power law curves with β≈0.5 are also observed for all values of $s<1$.

3. Quantum phase transitions in the sub-Ohmic spin boson model in the RWA

Y. Z. Wang, S. He, L. W. Duan, and *QHC*, **Phys. Rev. B** 100, 115106 (2019)

$$H = \frac{\Delta}{2}\sigma_z + \sum_k \omega_k a_k^+ a_k + \frac{1+\lambda}{2}\sum_k g_k (a_k^+ \sigma_- + a_k \sigma_+) + \frac{1-\lambda}{2}\sum_k g_k (a_k^+ \sigma_+ + a_k \sigma_-)$$

rotating terms counter-rotating terms

$$H = \frac{\Delta}{2}\sigma_z + \sum_k \omega_k a_k^+ a_k + \frac{1}{2}\sum_k g_k (a_k^+ + a_k)\sigma_x + \frac{\lambda}{2}\sum_k g_k (a_k - a_k^+) \mathrm{i}\sigma_y$$

$\lambda = 0 \rightarrow$ full spin-boson model

$\lambda = 1 \rightarrow$ spin-boson model in the RWA

The spectral density : Sub-Ohmic (0 < s < 1)

$$J(\omega) = \pi \sum_k g_k^2 \delta(\omega - \omega_k) = 2\pi\alpha\omega_c^{1-s}\omega^s \Theta(\omega_c - \omega) \qquad \omega_c = 10\Delta$$

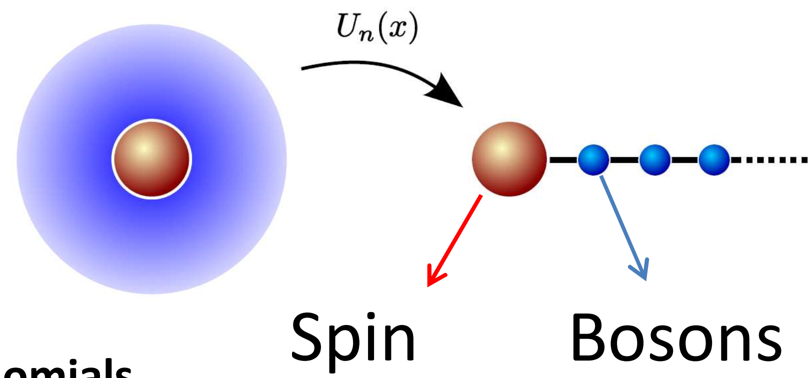
Based on discrete logarithm
$\Lambda = 2$

$$g_k^2 = \int_{\Lambda^{-(k+1)}\omega_c}^{\Lambda^{-k}\omega_c} J(\omega)\, d\omega \quad \omega_k = g_k^{-2} \int_{\Lambda^{-(k+1)}\omega_c}^{\Lambda^{-k}\omega_c} J(\omega)\, \omega\, d\omega$$

The Variational Matrix Product State Approach (VMPS) :

➢ 1: Mapping the model into 1D semi-infinite chain

$$H=\frac{\Delta}{2}\sigma_z+\frac{1}{2}c_0\left(b_0+b_0^{+}\right)\sigma_x+\frac{\lambda}{2}c_0\left(b_0-b_0^{+}\right)i\sigma_y$$
$$+\sum_{n=0}^{L-2}\varepsilon_n b_n^{+}b_n+t_n\left(b_{n+1}^{+}b_n+b_n^{+}b_{n+1}\right)$$



by orthogonal polynomials

Spin-boson model ➡ 1D semi-infinite chain with nearest neighbor interaction

➢ 2: Optimize M through sweeping the 1D chain iteratively

$$|\psi\rangle=\sum_{\{N_n\}=1}^{d_n}M[N_1]\ldots M[N_L]|N_1,\ldots N_L\rangle$$

N_n is the physical dimension of each site *n* with truncation d_n, and D_n is the bond dimension for matrix *M* with the open boundary condition, bounding the maximal entanglement in each subspace. We can optimize M iteratively by variational approach to obtain the ground state.

Exact Diagonalization In Truncated Hilbert Space (NED) :

$\lambda = 1$ $\Rightarrow$ $H = \frac{\Delta}{2}\sigma_z + \sum_k \omega_k a_k^{+} a_k + \sum_k g_k (a_k^{+}\sigma_- + a_k \sigma_+)$

U(1) Symmetry: $[H, N] = 0 \;\; with \;\; N = \sum_k \sigma_+\sigma_- + a_k^{+} a_k$

We can separate the Hilbert space into several subspaces with different excitation numbers l = 0, 1, 2...N . The wave function in l-subspace $|\psi_l\rangle$can be written explicitly with l excitations

$$|\psi_0\rangle = |\downarrow\rangle|0\rangle$$

$$|\psi_1\rangle = c|0\rangle|\uparrow\rangle + \sum_k d_k a_k^{\dagger}|0\rangle|\downarrow\rangle$$

$$|\psi_2\rangle = \sum_k e_k a_k^{\dagger}|0\rangle|\uparrow\rangle + \sum_{kk'} f_{kk'} a_k^{\dagger} a_{k'}^{\dagger}|0\rangle|\downarrow\rangle$$

$$|\psi_3\rangle = \sum_{kk'} p_{kk'} a_k^{\dagger} a_{k'}^{\dagger}|0\rangle|\uparrow\rangle + \sum_{kk'k''} q_{kk'k''} a_k^{\dagger} a_{k'}^{\dagger} a_{k''}^{\dagger}|0\rangle|\downarrow\rangle$$

$|\psi\rangle^{\leq N} = \sum_{l=0}^{N} |\psi_l\rangle$ $\Rightarrow$ **Truncated Hilbert space**

$$N = 3$$

The Multi-Coherent States Ansatz (MCS) :

Rotate the model around the y-axis by an angle $\pi/2$

$$H^T = -\frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^{+} a_k + \frac{1}{2}\sum_k g_k (a_k^{+} + a_k)\sigma_z + \frac{\lambda}{2}\sum_k g_k (a_k - a_k^{+})\mathrm{i}\sigma_y$$

$$|\psi^T\rangle = \begin{pmatrix} \sum_{n=1}^{N_c} A_n \exp\left[\sum_{k=1}^{L} f_{n,k}\left(a_k^{\dagger} - a_k\right)\right]|0\rangle \\ \sum_{n=1}^{N_c} B_n \exp\left[\sum_{k=1}^{L} h_{n,k}\left(a_k^{\dagger} - a_k\right)\right]|0\rangle \end{pmatrix}$$

Trial State

$$N_c = 6$$

To minimize the energy expectation value by the variational approach

$$\frac{\partial E}{\partial A_n} = \frac{\partial E}{\partial B_n} = \frac{\partial E}{\partial f_{ij}} = \frac{\partial E}{\partial h_{ij}} = 0 \qquad E = \frac{\langle \psi^T | H^T | \psi^T \rangle}{\langle \psi^T | \psi^T \rangle}$$

$$\sum_n \left(2A_n F_{i,n}\left(\alpha_{i,n} - E\right) - \Gamma_{i,n} B_n \gamma_{i,n}\right) = 0$$

$$\sum_n \left(2B_n G_{i,n}\left(\beta_{i,n} - E\right) - \Gamma_{n,i} A_n \gamma_{n,i}\right) = 0$$

$$\sum_n \{-\Gamma_{i,n} B_n \left(h_{n,j}\gamma_{i,n} + \lambda g_j\right) + A_n F_{i,n}\left[2\left(\alpha_{i,n} + \omega_j - E\right) f_{n,j} + g_j\right]\} = 0$$

$$\sum_n \{-\Gamma_{n,i} A_n \left(f_{n,j}\gamma_{n,i} - \lambda g_j\right) + B_n G_{i,n}\left[2\left(\beta_{i,n} + \omega_j - E\right) h_{n,j} - g_j\right]\} = 0$$

$$F_{m,n} = \exp\left[-\frac{1}{2}\sum_k \left(f_{m,k} - f_{n,k}\right)^2\right]$$

$$G_{m,n} = \exp\left[-\frac{1}{2}\sum_k \left(h_{m,k} - h_{n,k}\right)^2\right]$$

$$\Gamma_{m,n} = \exp\left[-\frac{1}{2}\sum_k \left(f_{m,k} - h_{n,k}\right)^2\right]$$

$$\alpha_{m,n} = \sum_k \left[\omega_k f_{m,k} f_{n,k} + \frac{g_k}{2}\left(f_{m,k} + f_{n,k}\right)\right]$$

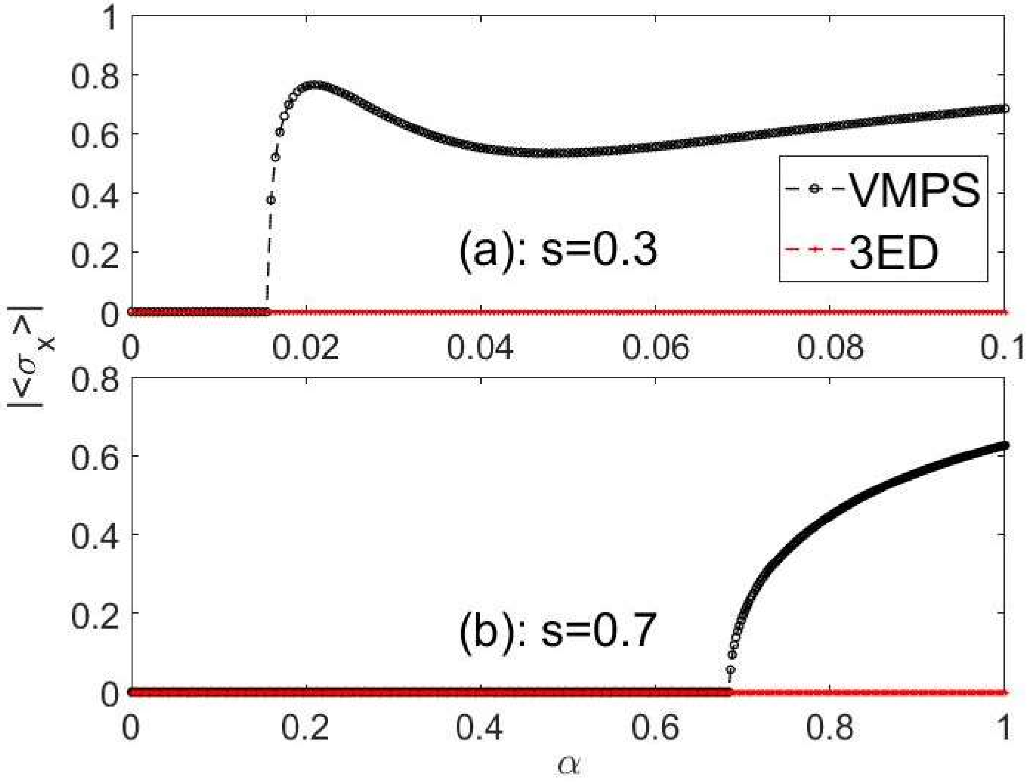
$$\beta_{m,n} = \sum_k \left[\omega_k h_{m,k} h_{n,k} - \frac{g_k}{2}\left(h_{m,k} + h_{n,k}\right)\right]$$

$$\gamma_{m,n} = \left[\Delta + \lambda \sum_k g_k \left(f_{m,k} - h_{n,k}\right)\right]$$

The second-order QPT in Spin-Boson model in the RWA has never been observed before! But we found that it can really occur

The Order Parameter $|\langle \sigma_x \rangle|$:

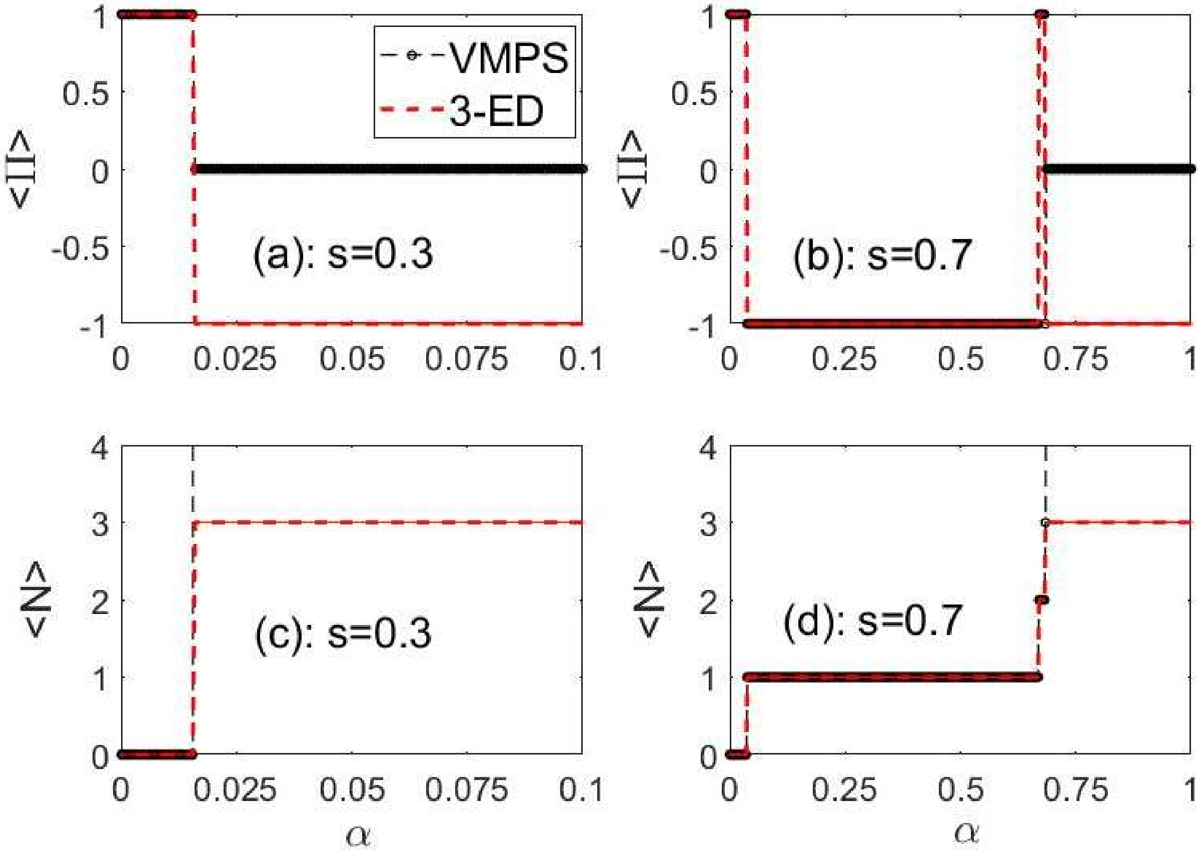
$\lambda = 1$



1. VMPS : $|\langle \boldsymbol{\sigma_x} \rangle|$ changes from zero to nonzero at α_c
2. NED : $|\langle \boldsymbol{\sigma_x} \rangle|$ remains zero where U(1) symmetry is preserved.

The parity symmetry breaking

$\lambda = 1$



$$\Pi = \exp(i\pi N)$$

Eigenvalues: ± 1

$$N = \sum_k \sigma_+ \sigma_- + a_k^\dagger a_k$$

Eigenvalues: $N = 0, 1, 2, 3 \ldots$

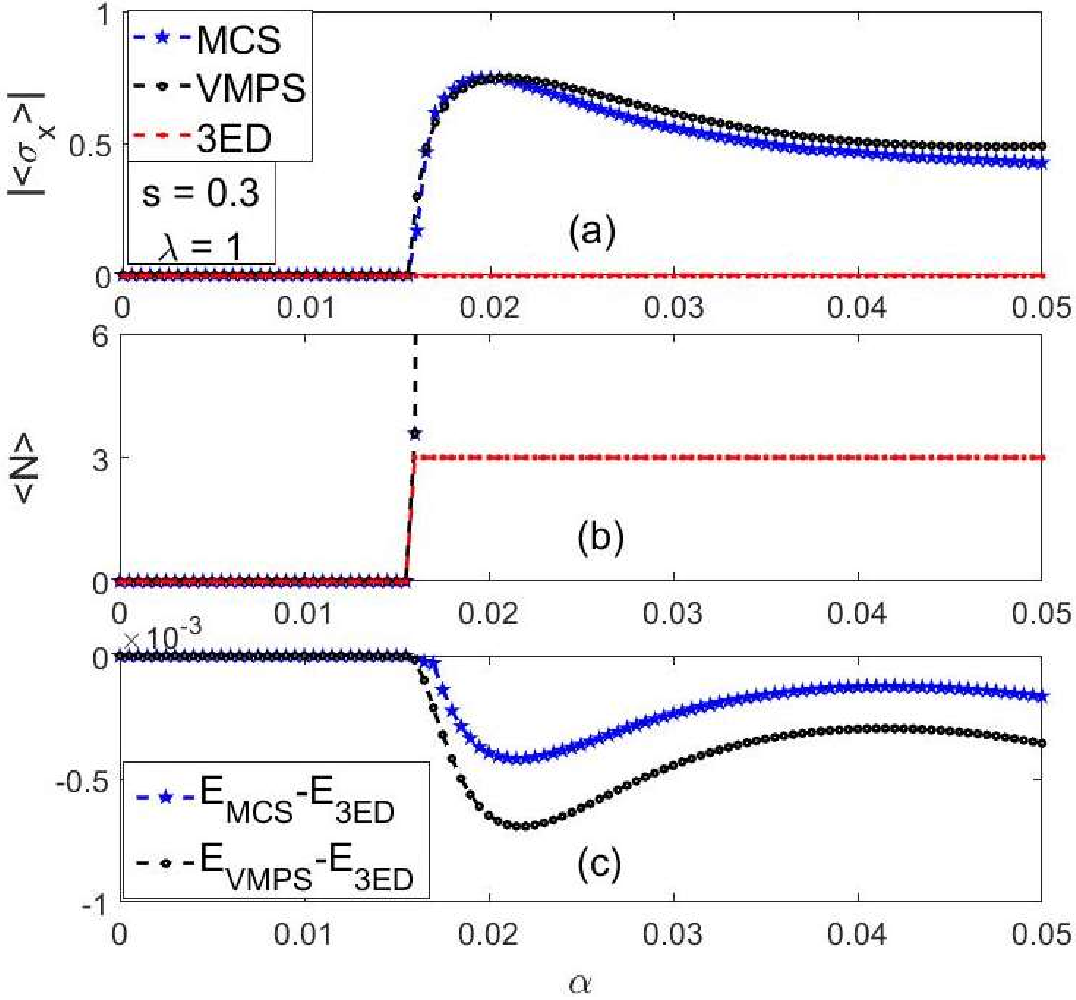
1、 The jump of ⟨N⟩ can account for the back and forth of the parity from 1 and −1.

2、 The instability of ⟨N⟩ before α_c → the 1st-order QPT.

3、 ⟨N⟩ by VMPS increases abruptly and ⟨Π⟩ becomes zero → the 2nd -order QPT.

U(1) Symmetry Breaking Z_2 Symmetry Breaking

Evidence for the 2nd -Order QPT by MCS Variational Studies

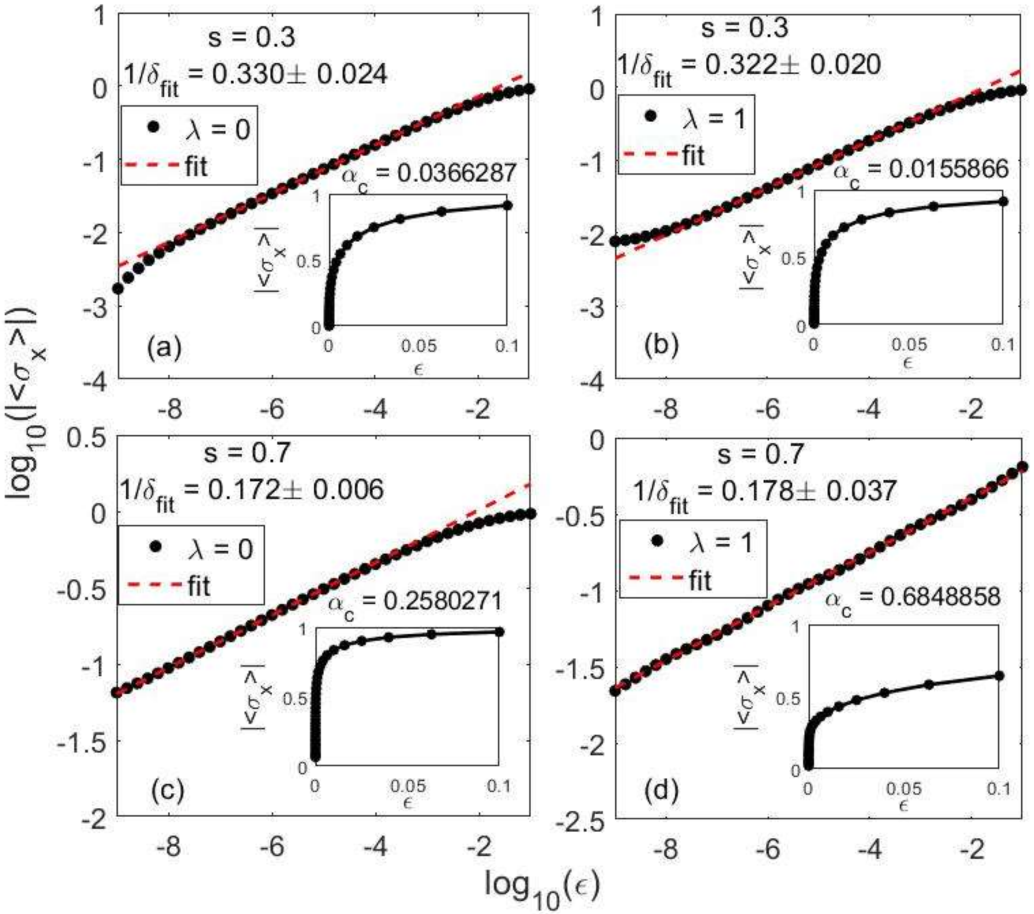


$\lambda = 1$

$N_c = 6$

The MCS further confirm the existence of the 2nd-order QPT qualitatively, but not precise location of the critical points.

The Critical Exponent δ



$$H_{bias} = H + \frac{\varepsilon}{2}\sigma_x$$

$$\langle \sigma_x \rangle \sim \varepsilon^{1/\delta}$$

$$0 < s < 1/2 \quad \rightarrow \quad 1/\delta = 1/3$$

$$1/2 < s < 1 \quad \rightarrow \quad 1/\delta = (1-s)/(1+s)$$

Within the statistical error, the counter rotating terms would have no effects on critical exponent δ in the spin-boson model.

4. Summary

◇ New effective analytical approach for the spin-boson model is proposed. It may paves the track to the true analytical solution to this famous model.

◇ The second-order QPT is observed in the sub-Ohmic spin-model in the RWA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China proverb: Hangzhou, Paradise on earth
West Lake @ Hangzhou
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Thank you!