Sparse Polynomial Space Approach to dissipative quantum systems

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Motivation

Open quantum systems: coupling to (dissipative) baths or (particle) reservoirs

- spin-boson model: two-level system coupled to bath of harmonic oscillators

  Leggett et al., Rev. Mod. Phys. 59, 1 (1987)

$$H = \frac{\Delta}{2}\sigma_x + \sum_i \lambda_i (b_i^+ + b_i)\sigma_z + \sum_i \omega_i b_i^+ b_i$$

continuous bath: $J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i) \propto \omega^s$ for $(0 \leq \omega \leq \omega_c)$

- physics: dissipative spin dynamics, (sub)-ohmic ($s \leq 1$) quantum phase transition

  possible methods: NRG, TD-NRG, QMC, DMRG, perturbation theory
  issues: long-time stability, nature of QPT (discrepancy NRG vs. QMC)

▶ What about exact diagonalization? (Lanczos, Jacobi-Davidson, Chebyshev, ...)

The problem: How to represent continuous bath degrees of freedom with a finite-dimensional Hamiltonian matrix?

▶ New suggestion: Sparse Polynomial Space Representation (SPSR)

Polynomial expansions

Calculation of, e.g., spectral functions using polynomial expansions

- orthogonal polynomials P_m to weight $w(\omega)$: $\int d\omega\ w(\omega)\ P_l(\omega)P_m(\omega) = \delta_{lm}$
- expansion of spectral function $A(\omega) = \langle\psi|\delta[\omega - H]|\psi\rangle = w(\omega)\sum_m \mu_m P_m(\omega)$
  - ▶ function $A(\omega) \leftrightsquigarrow$ moments $\mu_m = \int d\omega A(\omega)P_m(\omega) = \langle\psi|P_m[H]|\psi\rangle$
- two-term recurrence $P_{m+1}(\omega) = (a_m\omega - b_m)P_m(\omega) - c_m P_{m-1}(\omega)$
  $\rightsquigarrow$ efficient recursive calculation of μ_m to given H

Hamiltonian → finite matrix → moments μ_m → spectral function $A(\omega)$

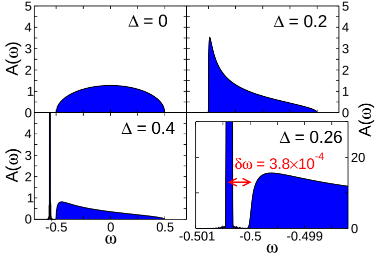
▶ 'best choice': Chebyshev polynomials with $w(\omega) \propto (1-\omega^2)^{-1/2}$

With Chebyshev polynomials: Kernel Polynomial Method (KPM)

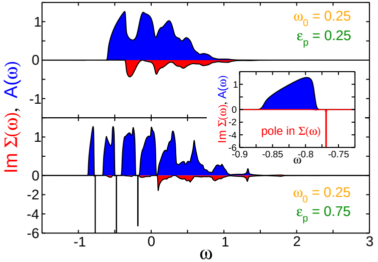
[review: Weiße, Wellein, Alvermann, Fehske, RMP 78, 275 (2006)]

- high resolution, fast convergence, absolute numerical stability even for discontinuous functions [no Gibbs phenomenon]

impurity in a host



Holstein polaron within DMFT



- efficient & general techniques for: static & dynamic correlations, zero & finite temperature, time-propagation

Prerequisite: represent quantum system by finite Hamiltonian matrix

Representation of continuous bath degrees of freedom

- traditional: discretization

(i) small number M of discrete energies replace continuous $J(\omega)$

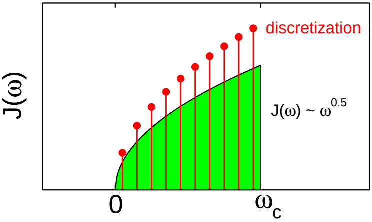
(ii) n bosons: $\binom{n+M}{M} \simeq M^n$ states

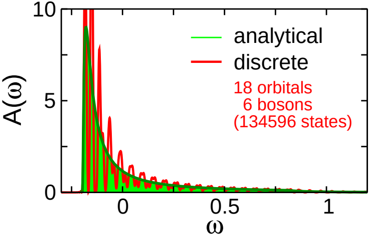
▶ 'curse of dimension'

(iii) small M results in

▶ discretization artefacts

example:
$A(\omega) = \langle \uparrow; \mathrm{vac} | \delta[\omega - H] | \uparrow; \mathrm{vac} \rangle$
for spin-boson model with $\Delta = 0$
[parameters: $s = 0.5, \alpha = 0.2$]





Instead of discretization: Construct polynomial function space

Sparse Polynomial Space Representation

Polynomial function space for multiple bosonic excitations

(i) n-boson state in first quantization: totally symmetric wavefunction

$$\psi_n : [0, \omega_c]^n \to \mathbb{C}$$
$$\vec{\omega} \mapsto \psi_n(\vec{\omega})$$

- $\psi_n(\vec{\omega})$: amplitude of bosons at energies $\vec{\omega} = (\omega_1, \dots, \omega_n)$

(ii) expansion in products of orthogonal polynomials

$$\psi_n(\vec{\omega}) = \sum_{\vec{m}} \psi_{\vec{m}} \prod_{i=1}^{n} P_{m_i}(\omega_i) \ ,$$

- n-dimensional function $\leftrightsquigarrow$ n-dimensional moments $\psi_{\vec{m}} \in \mathbb{C}^n$

(iii) operators $b^{(\dagger)}$: simple algebraic operations

- e.g. $H_B = \sum_i \omega_i b_i^\dagger b_i$ corresponds to multiplication $\psi_n(\vec{\omega}) \mapsto (\sum_i \omega_i)\psi_n(\vec{\omega})$
  i.e, using two-term recurrence for P_m, shifting indices of $\psi_{\vec{m}}$ by ± 1

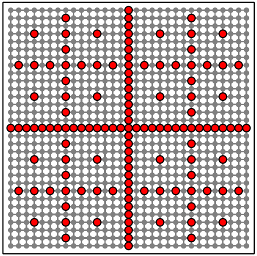
How to select finite subspace?

'naive': restrict degree of each P_{m_i}: $\quad m_i < M$
but: effort for M^n polynomials = effort for M^n discrete points ϟ

Instead: Use concepts from approximation theory $\rightsquigarrow$ sparse grid

Sparse Polynomial Space Representation

Sparse grids: Interpolation of multivariate functions



(i) Cartesian grid: M points along each axis
n-dim. function $\leftrightsquigarrow$ values at M^n points

(ii) Sparse grid: much less points
for interpolation with comparable accuracy
- n-dim. function $\leftrightsquigarrow$ values at *few* points

(iii) relevant for our purpose: sparse grid interpolation exact
for polynomials $P_{m_1} \cdots P_{m_n}$ with $\sum_{i=1}^{n} \lfloor \log_2(m_i + 1) \rfloor \leq N_g$
- this condition defines Sparse Polynomial Space to level N_g
- contains polynomials of high degree (up to $2^{N_g} - 1$) *and* only few in total

Sparse Polynomial Space Representation:

n-boson wavefunction $\psi_n(\vec{\omega}) \leftrightsquigarrow$ few parameters $\psi_{\vec{m}}$

Sparse Polynomial Space Representation

Sparse Polynomial Space Representation

continuous bath degrees of freedom
infinite bosonic Fock space

▼

n-dimensional complex functions

▼

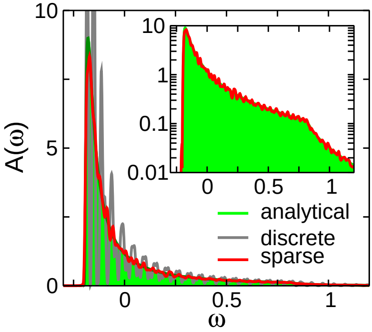
polynomial expansions

▼

sparse grid: sub-space selection

▼

sparse polynomial space



sparse grid with 129284 states
(less than discrete grid)

- intrinsic interpolation of sparse grid overcomes problems of discretization
- no discretization artefacts
- exact diagonalization techniques become applicable to open quantum systems

Results with excellent accuracy for moderate effort

Results for the spin-boson model

$$H = \frac{\Delta}{2}\sigma_x + \sum_i \lambda_i (b_i^+ + b_i)\sigma_z + \sum_i \omega_i b_i^+ b_i$$

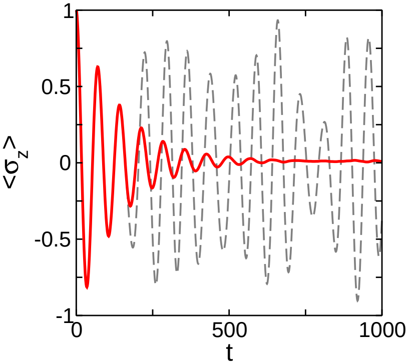
continuous bath: $J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i) \propto \alpha\,\omega^s$ (for $0 \leq \omega \leq \omega_c = 1$)

Spin dynamics

Sparse Polynomial Space + Chebyshev time propagation

initial state:
spin $|\uparrow\rangle$ + relaxed oscillator bath

- time evolution of a dissipative system with a finite hermitian matrix
- no (discretization) error
- dynamics on long time scales: transients & steady state
- no additional averaging or damping



for comparison:
discrete grid of comparable size

Results for spin-boson model

Sub-Ohmic ($s < 1$) quantum phase transition

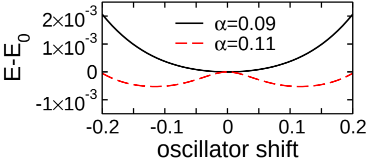
for coupling α above critical α_c: degenerate groundstate with magnetization $\neq 0$

our criterion: magnetization $m = \langle \sigma_z \rangle \leftrightsquigarrow$ oscillator shift $b_i \mapsto b_i - m\frac{\lambda_i}{\omega_i}$

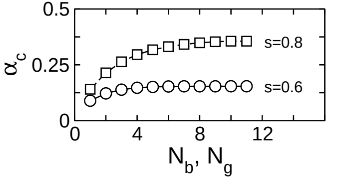
- groundstate energy E

(i) $\alpha < \alpha_c$: minimum at $m = 0$, shift $= 0$

(ii) $\alpha > \alpha_c$: minima at $m \neq 0$, shift $\neq 0$



- convergence of numerical α_c with
  N_b: number of boson
  N_g: sparse grid level



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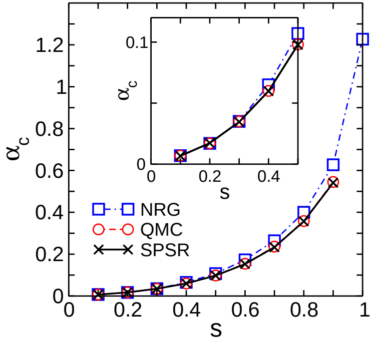
Phase diagram $(\Delta/\omega_c = 0.1)$

- direct approach
  (no scaling, no extrapolation)
- very accurate & efficient computations
- results agree with QMC and NRG
  (taking NRG discretization into account)

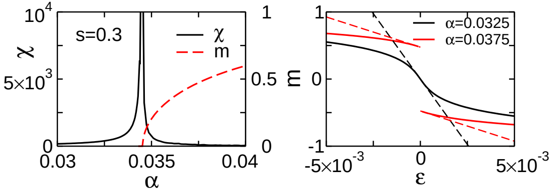


QMC/NRG data: Winter, Rieger, Vojta, Bulla, PRL 102, 030601 (2009)

Results for spin-boson model

Quantum phase transition: Critical behaviour for $s < 0.5$

- calculate magnetization $m = \langle \sigma_z \rangle$ directly in groundstate, susceptibility $\chi = -\partial m / \partial \epsilon$ with external field $\epsilon \sigma_z$



Of which type is the quantum phase transition for $s < 0.5$?

Results for spin-boson model

Quantum phase transition: Critical behaviour for $s < 0.5$

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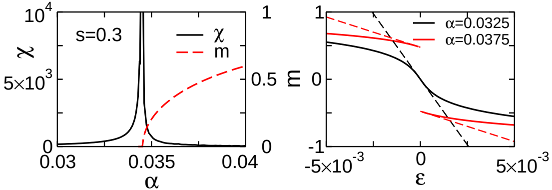
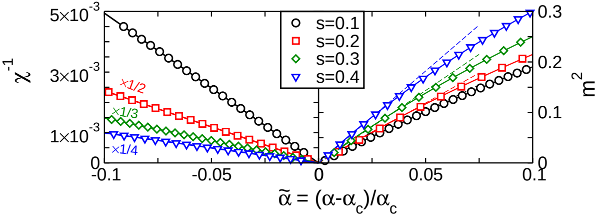


- critical behaviour: mean-field exponents $\chi \propto (\alpha_c - \alpha)^{-1}$, $m \propto (\alpha - \alpha_c)^{1/2}$
  in accordance with QMC, but in contradiction to NRG [cf. Winter et al.]



Conclusion & Outlook

Sparse Polynomial Space Representation

- new idea: combine polynomial expansions with sparse grids
  to represent continuous bath degrees of freedom without discretization
- Hilbert space techniques (Lanczos, Jacobi-Davidson, Chebyshev . . .)
  become applicable to open quantum systems
- no discretization error: results with excellent accuracy
  e.g. for time propagation on long time scales

For the spin-boson model:

- static & dynamic observables at weak & strong coupling
- quantum phase transition has mean-field character for $s < 0.5$

Applications & future development

- generalized spin-boson models
- fermionic reservoirs using anti-symmetrized functions
- non-equilibrium current and electron pumping in nanostructures

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KPM review: Weiße, Wellein, Alvermann, Fehske, Rev. Mod. Phys. 78, 275 (2006).
Chebyshev Space Method: A. Alvermann, H. Fehske, Phys. Rev. B 77, 045125 (2008).
Sparse Polynomial Space Approach: A. Alvermann, H. Fehske, arXiv:0812.2808.