Sparse Polynomial Space Approach
to dissipative quantum systems

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

- spin-boson model: two-level system coupled to bath of harmonic oscillators
  
  \[ H = \frac{\Delta}{2} \sigma_x + \sum_i \lambda_i (b_i^+ + b_i) \sigma_z + \sum_i \omega_i b_i^+ b_i \]
  
  continuous bath: \[ J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i) \propto \omega^s \quad \text{for} \quad (0 \leq \omega \leq \omega_c) \]

- 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 $A(\omega) \leftrightarrow$ moments $\mu_m = \int d\omega A(\omega) P_m(\omega) = \langle \psi | P_m[H] | \psi \rangle$
- two-term recurrence $P_{m+1}(\omega) = (a_m \omega - b_m) P_m(\omega) - c_m P_{m-1}(\omega)$

  $\leadsto$ efficient recursive calculation of $\mu_m$ to given $H$

Hamiltonian $\rightarrow$ finite matrix $\rightarrow$ moments $\mu_m \rightarrow$ spectral function $A(\omega)$

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

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
Continuous bath degrees of freedom

Representation of continuous bath degrees of freedom

- traditional: discretization
  
  (i) small number $M$ of discrete energies replace continuous $J(\omega)$
  
  (ii) $n$ bosons: \((n+M)_M \approx M^n\) states
    - ‘curse of dimension’
  
  (iii) small $M$ results in discretization artefacts
    - example:
      $$A(\omega) = \langle \uparrow; \text{vac} | \delta[\omega - H] | \uparrow; \text{vac} \rangle$$
      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:
\[
\psi_n : [0, \omega_c]^n \rightarrow \mathbb{C}
\]
totally symmetric wavefunction
\[
\bar{\omega} \mapsto \psi_n(\bar{\omega})
\]
\( \psi_n(\bar{\omega}) \): amplitude of bosons at energies \( \bar{\omega} = (\omega_1, \ldots, \omega_n) \)

(ii) expansion in products of orthogonal polynomials
\[
\psi_n(\bar{\omega}) = \sum_{\bar{m}} \psi_{\bar{m}} \prod_{i=1}^{n} P_{m_i}(\omega_i),
\]
\( \psi_{\bar{m}} \): \( n \)-dimensional function \( \leftrightarrow \) \( n \)-dimensional moments \( \psi_{\bar{m}} \in \mathbb{C}^n \)

(iii) operators \( b_i(\dagger) \): simple algebraic operations
\( H_B = \sum_i \omega_i b_i^\dagger b_i \) corresponds to multiplication \( \psi_n(\bar{\omega}) \mapsto (\sum_i \omega_i) \psi_n(\bar{\omega}) \)
i.e., using two-term recurrence for \( P_m \), shifting indices of \( \psi_{\bar{m}} \) by \( \pm 1 \)

How to select finite subspace?

‘naive’: restrict degree of each \( P_{m_i} : m_i < M \)
but: effort for \( M^n \) polynomials = effort for \( M^n \) discrete points \( \nless \)

Instead: Use concepts from approximation theory \( \sim \) sparse grid
Sparse Polynomial Space Representation

Sparse grids: Interpolation of multivariate functions

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

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

(iii) relevant for our purpose: sparse grid interpolation exact
for polynomials \( P_{m_1} \cdots P_{m_n} \) with
\[ \sum_{i=1}^{n} \left\lfloor \log_2 (m_i + 1) \right\rfloor \leq N_g \]
\( n \)-dim. function \( \leftrightarrow \) values at few points
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 \( \psi_n(\vec{\omega}) \) \( \leftrightarrow \) few parameters \( \psi_{\vec{m}} \)
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

- 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 $\alpha$ above critical $\alpha_c$: degenerate groundstate with magnetization $\neq 0$

our criterion: magnetization $m = \langle \sigma_z \rangle \leadsto$ 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 $\alpha_c$ with
  - $N_b$: number of boson
  - $N_g$: sparse grid level
Sub-Ohmic ($s < 1$) quantum phase transition for coupling $\alpha$ above critical $\alpha_c$: degenerate groundstate with magnetization $\neq 0$

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

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 $\epsilon \sigma_z$

![Graph showing magnetization and susceptibility](image)

Of which type is the quantum phase transition for $s < 0.5$?
Results for spin-boson model

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

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

- 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

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.