Sparse Polynomial Space Approach to dissipative quantum systems

Andreas Alvermann
Holger Fehske

Institut für Physik
Ernst-Moritz-Arndt Universität Greifswald

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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: $\binom{n+M}{M} \approx M^n$ states
    \[ \text{‘curse of dimension’} \]
  (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:

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

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

(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 \( \leftarrow \leftrightarrow \) \( n \)-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 \( \pm 1 \)

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 \( \forall \)

Instead: Use concepts from approximation theory \( \sim \) sparse grid
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 $\sum_{i=1}^{n} \lfloor \log_2(m_i + 1) \rfloor \leq N_g$
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 $\psi_n(\vec{\omega}) \leftrightarrow$ few parameters $\psi_{\vec{m}}$
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: \[ J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i) \propto \alpha \omega^s \quad \text{(for} \ 0 \leq \omega \leq \omega_c = 1) \]

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 $m = \langle \sigma_z \rangle \leftrightarrow$ 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

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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 $s < 0.5$

- 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