The Truncated Polynomial Expansion Method for Fermion Systems Coupled to Classical Fields

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Outline

• Introduction to “Spin-fermion” models
• Polynomial Expansion of the *Fermionic* Density of States Method
• Performance and Reliability
• Parallelization and Scalability
• Software Library and Optimizations
• Conclusions
Physical Systems

Some systems that have been described by models of fermions coupled to classical fields:

- **Manganites**, \([\text{local } t_{2g} \text{ spin, local lattice distortions (phonons)}]\)  

- **Diluted Magnetic Semiconductors** \([\text{local spin}]\)  

- **High Temperature Superconductors** \([\text{local magnetization, local superconducting order parameter}]\)  
  A. Moreo et al., PRL 84, 2690 (2000), G. Alvarez, cond-mat/0401474
Spin fermion: Manganese

\[ H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - J_H \sum_{i \alpha \beta} c_{i\alpha}^\dagger c_{i\beta} \vec{S}_i \cdot \vec{t}_{\alpha,\beta} \]

No approximations

Local spin

T \Delta

PM

AF

FM

0.0 0.5 1.0

\langle n \rangle

(electronic density)
Hamiltonian

General form:

\[ H = \sum_{i,\alpha,j,\beta} c_{i\alpha}^\dagger H[\phi_{i,\alpha,j\beta}] c_{j\beta} \]

Example: Manganites:

\[ H = -t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - J_H \sum_{i,\alpha} c_{i\alpha}^\dagger c_{i\beta} \vec{S}_i \cdot \vec{\tau}_{\alpha,\beta} \]

Partition Function

\[ Z = \int \mathcal{D}\phi \int \mathcal{D}c^\dagger \mathcal{D}c \exp(-\beta H[\phi]) \]

After integrating fermions:

\[ Z = \int \mathcal{D}\phi \prod_{\lambda} \left\{ 1 + \exp(-\beta \epsilon_{\lambda}[\phi]) \right\} \]
Diagonalization Method

- Hamiltonian is *quadratic* in fermion operators: $4^N$ Hilbert space but problem reduces to solve the “*one-particle*” Hilbert space ($2N$ states) and filling levels.
- Classical fields are integrated using classical Monte Carlo. Different “*Boltzmann Weight*” than Ising Model
- One diagonalization has a complexity of $O(N^3)$ but it must be repeated $\sim N$ times per Monte Carlo step $\Longrightarrow$ total complexity is $O(N^4)$
Polynomial Expansion of the Density of States

N. Furukawa and Y. Motome, 2001

\[ A(\phi) = \int_{-\infty}^{\infty} F(x)D(\phi, x)\,dx \]

Ex.: if A is number of particles:
\[ F(x) = \text{fermi function} \]

\[ F(x) = \sum_{m=0}^{\infty} f_m T_m(x) \]

\[ f_m = \int_{-1}^{1} \alpha_m F(x)T_m(x)/\left(\pi\sqrt{1-x^2}\right) \]

\[ A(\phi) = \sum_{m} f_m \mu_m(\phi) \]

\[ \mu_m(\phi) = \sum_{\nu=1}^{N_{\text{dim}}} \langle n|T_m(H(\phi))|n \rangle \]

A(\phi): Observable
\[ D(\phi, x) = \sum_{\nu} \delta(x-\varepsilon_{\nu}(\phi)) \]: Density of States or D.O.S.
\[ T_m(x) \]: Chebyshev polynomial of order m

Sum over m needs to be done only up to a cut-off M

Sparse matrix-vector product, e.g. in \[ T_m(H)|\nu \rangle \], yields a cost of \[ O(N^2) \] for each conf., i.e. \[ O(N^3) \] for each Monte Carlo step.
Truncating the Expansion: 1. Matrix-Vector Products

Define:

\[ \mu_m(\phi) = \sum_n < n | n; m > \]

\[ |n; m >= T_m(H) |n > \]

\[ |n; 0 >= |n >, |n; 1 >= H |n; 0 > \]

Recursion

\[ |n; m >= 2H |n; m - 1 > - |n; m - 2 > \]

moments of the density of states

N. Furukawa and Y. Motome 2003-2004
Truncating the Expansion: 1. Matrix-Vector Products

N. Motome, Y. Furukawa, cond-mat/0308298

Not only is the matrix sparse but the vectors \(|n;m>\) have very few non-zero/large entries.
Truncating the Expansion: 2. Action Difference

\[ \frac{P(\phi^{new})}{P(\phi^{old})} = \exp(-\Delta S_{eff}), \quad S_{eff}(\phi) = \int F^s(x) D(\phi, x) dx \]

\[ \Delta S_{eff} = S_{eff}(\phi^{new}) - S_{eff}(\phi^{old}) = \sum_m f^s_m \sum_n \Delta \mu_m \]

Complexities

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>ln;m&gt;</th>
<th>Trace</th>
<th>Delta S</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diag.</td>
<td>------</td>
<td>------</td>
<td>O(N^3)</td>
<td>O(N^4)</td>
</tr>
<tr>
<td>full-PEM</td>
<td>O(MN)</td>
<td>O(N)</td>
<td>O(MN^2)</td>
<td>O(MN^3)</td>
</tr>
<tr>
<td>T-PEM</td>
<td>O(M^{d+1})</td>
<td>O(M^d)</td>
<td>O(M^{2d+1})</td>
<td>O(M^{2d+1}N)</td>
</tr>
</tbody>
</table>
Performance and Reliability

G. Alvarez et al.
submitted to Computer Physics Communications
Parallelization and Scalability

\[ \mu_m(\phi) = \sum_{\nu=1}^{N_{\text{dim}}} \langle n | T_m(H(\phi)) | n \rangle \]

(Independent terms)

\[ N_{\text{dim}} = \text{(size of the lattice)} \times \text{(internal degrees of freedom)} \]

Algorithm Scales: CPU Time \( \sim \frac{N_{\text{dim}}}{N_{\text{proc}}} \)

Up to \( N_{\text{proc}} = N_{\text{dim}} \)

**DMS context:** concentration=5%, 500 spins, 3 bands + spin

\( (500 \times 100/5) \times 3 \times 2 = 60,000 \) processors

**Manganites (CMR problem):** 20\(^3\) lattice, 2 bands + spin:

\( (20^3) \times 2 \times 2 = 32,000 \) processors
Parallelization and Scalability

\[ T^{-1} \left( 10^{-3} \text{ s}^{-1} \right) \]

- \( M = 30 \)
- \( J = 3 \)
- \( N = 6^3 \)
- \( \varepsilon_{pr} = 10^{-5} \)
- \( \varepsilon_{tr} = 10^{-3} \)

100 iterations

Number of CPUs vs. \( T^{-1} \) for different numbers of CPUs.
Software Library in C

- Model independent library for T/PEM.
- Use of Compressed Row Storage (CRS) for matrix storage.
- Entries to perform most operations related to the algorithm.
- Serial and Parallel (MPI) algorithms.
- G. Alvarez et al., submitted to Computer Physics Communications
- http://www.ccs.ornl.gov/~gonzalo/software/tpem/

FUTURE WORK: Optimize the library (sparse matrix - vector product) for High performance supercomputers (IBM, Cray, etc)
Conclusions

• T/PEM allows for the simulation of “spin-fermion” models much more efficiently than the exact diagonalization technique: $O(N)$ vs. $O(N^4)$.
• Larger lattices: Better Statistics.
• More realistic models (many bands, etc.).
• Wide range of applicability in condensed matter physics.
• Scalable parallelization.

Collaborators:
JAPAN: N. Furukawa, N. Motome.