Next Generation Multi-Scale Quantum Many-Body Simulation Software

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OUTLINE

• Complexity at the nanoscale
• Present Approach
  – Improved cluster solvers at short-length scales
• Multi-Scale Many-Body Approach
  – Separation of length scales
  – Diagrammatic methods at intermediate-length scales
• Summary
Complexity at the nanoscale

- Complex phase diagrams and new states of matter: e.g. Cuprates, manganites, ruthenates, DMSs...
- Proper understanding require simulations at long length scales

Present Approach

- A multi-scale approach
- Short length scales, within the cluster, treated explicitly.
- Long length scales treated within a mean field.

QMC Cluster Solver

\[ G^{-1} = \overline{G}^{-1} + \Sigma \]

\[ \Sigma = G^{-1} - G_c^{-1} \]

\[ \overline{G}(\mathbf{K}) = \sum_{\mathbf{k}} G(\mathbf{K} + \mathbf{k}) \]

QMC

G_c(\tau), \chi_c(\tau)

MEM

N(\omega), \chi(\omega)

Analysis Code

\[ \overline{\chi}(T), n(\mathbf{k}) \]

Effective Medium

• A QMC Algorithm for Non-local Corrections to the Dynamical Mean-Field Approximation, M. Jarrell, PRB 64, 195136/1-23 (2001).
Parallelization of the QMC solver

Serial

Perfectly Parallel

Hybrid Parallel (MPI+ OpenMP)
Improved QMC solvers at short length scales – Hybrid QMC
Multi-scale Many-Body formalism

- Appropriate method for each length scale
  - short = explicit
  - intermediate = perturbative
  - long = mean field
- Only MB processes from explicit calculation
  - $\Sigma$ and $\Lambda$ from QMC input to diagrammatic calculation
Intermediate length scale – Diagrammatic Approach

Parquet e.q.

\[ \Gamma_a(K, K', Q) = \Lambda(K, K', Q) + (\Gamma_b \chi^0 F)(-K', -K, K + K' + Q) \]

\[ \begin{bmatrix} \Gamma_a \\ \Lambda \end{bmatrix} = \begin{bmatrix} \Lambda \\ \chi^0 \end{bmatrix} + \begin{bmatrix} F \\ \Gamma_b \end{bmatrix} \]

Bethe-Salpeter e.q.

\[ F(K, K', Q) = \Gamma_a(K, K', Q) + (F \chi^0 \Gamma_a)(K, K', Q) \]

\[ \begin{bmatrix} F \\ \Gamma_a \chi^0 F \end{bmatrix} = \begin{bmatrix} \Gamma_a \\ \Gamma_a \end{bmatrix} \]

• Large cluster: solve parquet and Bethe-Salpeter equations self consistently.
• \( \Sigma, \Lambda \) from QMC
• \( \Gamma, F, \chi \) size nt >1600
• distribute data on Q

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Major Performance Bottlenecks

- **Computational Bottleneck**
  - Bethe-Salpeter Equation:
    - like 3D Matrix Multiplication
    - $O(nt^4)$ operations, so main loop is $O(nt^4)$
    - Dramatically limits size of computation
- **Communication Bottleneck**
  - Parquet Equations
    - Rotation of matrices:
      - Complex and Global message transferring pattern
      - Each Parquet Equation: $O(nt^3)$ messages
- Both are recalculated on each iteration
- No Minus sign problem
  - Algebraic rather than exponential scaling!
Summary

- Present methods cannot address multi-scale phenomena displayed by correlated materials
  - Minus sign problem
  - Complexity (number of correlated orbitals)
- MSMB method treats each length scale with an appropriate method
  - short = explicit
  - intermediate = diagrammatic
  - long = mean field
- Challenges, Outreach, Collaboration
  - MP QMC for measurements of Γ, F, etc.
  - Large matrix (tensor) algebra
  - Web distribution of codes (9/07)

http://scicompforge.org/petamat