Quantum Cluster Simulations of Low D Systems

Electronic Correlations on Many Length Scales

M. Jarrell, University of Cincinnati

- High Perf. QMC
  - SP Sep. in 1D
- Hybrid Method
  - SP Sep. in 1D
- NEW MEM
  - 2-Chain Spectra
- Other Projects
Collaborators and References

- J. Hague
- S. Doluweera
- O. González
- A. Macridin
- Th. Maier
- Th. Pruschke
- C. Slezak
- Th. Schulthess
- D. Johnson

Papers, talks, and example codes
- www.physics.uc.edu/~jarrell/
- www.physics.uc.edu/~jarrell/TALKS/
- xxx.lanl.gov
Vertically coupled GaAs/AlGaAs quantum wires

Non-perturbative physics
- correlations over all length scales
- very low temperatures

J. Mintmire, PRL 68, 631

Carbon Nanotubes

H. Smolinski, PRL 80, 5164

M. Weckworth, Superlattices and Microstruct 20, 561
Effective Medium

Periodic Lattice

Dynamical Cluster Approximation

Effective Medium
DCA Mapping to Cluster: Coarse Graining

\[ \Delta = N \delta_{k_1 + k_2, k_3} \]

\[ N_c \delta_{M(k_1) + M(k_2), M(k_3)} \]
The Nature of Cluster Approximations

x=0

screening cloud $\Sigma(r)$

$x=0$

<table>
<thead>
<tr>
<th></th>
<th>Self Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>DMFA</td>
<td>Local</td>
</tr>
<tr>
<td>DCA</td>
<td>Short Ranged</td>
</tr>
</tbody>
</table>
Problems Simulating 1D Systems

- QMC requires significant computer power
- Correlations over many length scales
- QMC minus sign problem—spectra
Problems Simulating 1D Systems

- QMC requires significant computer power
- Correlations of many length scales
- QMC minus sign problem—spectra
We Solve The Cluster Problem with QMC

ORNLCES and
OSC CRAY X1

ORNLIIBM
p690 (cheetah)
Quantum Monte Carlo Cluster Solver

Serial

$G_0$

QMC Cluster Solver on one processor

QMC time

warmup

sample

Perfectly Parallel

$G_0$

QMC Cluster Solver on one processor

QMC Cluster Solver on one processor

QMC Cluster Solver on one processor

QMC Cluster Solver on one processor

QMC time

warmup

sample
Performance of Concurrent DGERS

\[ G' = G + a* b^T \quad N = 4480 \]

Note the log scale.

![Graph showing performance of Concurrent DGERS](image)
Hybrid Parallel QMC

Perfectly parallel array of cpu's

Hybrid parallel array of cpu's

QMC Cluster Solver on many processors

G
G
G
G
G
G
G
G

G
G
G
G

G
G
G
G

G
G
G
G

OpenMP
PBLAS

QMC Cluster Solver on many processors

G_0

G

G

G

warmup
sample
QMC time
Performance of threaded DGERs

X1 eliminates the need for hybrid parallelization
Velocities fit to Luttinger Liquid form (Zacher, PRB 57, 6370)
Problems Simulating 1D Systems

- QMC requires significant computer power
- **Correlations over many length scales**
- QMC minus sign problem—spectra
Hybrid, Multiple Embedding

Length scales within the small cluster are treated explicitly.

Length scales between the large and small cluster are treated perturbatively.

Length scales beyond the large cluster are treated with a mean field.

K. Aryanpour, PRB, 2003
Ingredients of the Hybrid Approach

- Dynamical Cluster Approximation
  - glue

- Quantum Monte Carlo
  - small cluster

- FLEX perturbation theory
  - large cluster

N.E. Bickers, 1989
The Fluctuation-Exchange Approximation

An infinite geometric resummation of certain classes of pp and ph graphs.

N.E. Bickers, 1989
1D Hubbard Model

J. Hague, PRB 69, 165113

Lieb and Wu, PRL 1968
Spin-Charge Separation with Hybrid FLEX

C. Slezak

Hybrid FLEX-QMC Velocities

QMC $N_c=8$, FLEX $N_c'=8-32$, $U=W$, $n=0.75$

$N_c=8$ Hybrid result, roughly $= N_c=20$ QMC Result, saving a factor of 16
$U=W$, $n=0.75$, $\beta=31$, QMC $N_c=8$, FLEX $N'_c=32$
Problems Simulating 1D Systems

- QMC requires significant computer power
- Correlations over many length scales
- QMC minus sign problem—spectra
The "minus sign problem" happens when the QMC sampling weight is not positive definite.

In this case, we associate the sign with the measurement, so M.E.M recalculates the analytic continuation problem.

\[ P(A|G) = \frac{P(G|A)P(A)}{\langle G \rangle} \] where \[ \langle G \rangle = \langle G_s \rangle \mid W \rangle \langle s \rangle \mid W \rangle \]

A. Macridin, preprint
Spectra of 2-chain model

Carbon Nanotubes

J. Mintmire
PRL 68, 631

vertically coupled GaAs/AlGaAs quantum wires

NaV$_2$O$_5$

H. Smolinski PRL 80, 5164

M. Weckworth, Superlattices and Microstruct 20, 561
S. Doluweera

DOS and A(k,w) Spectra of Two chain Hubbard model
at half filling, $\beta = 54.6$

t_{perp}=t=0.25, U=4t=1, N_c=8, N=1

$A[(\omega, k)] = A[(\pi - k, \pi)]$

Endres PRB 53 5530
2-chain Hubbard model, $t_{\text{leg}}=t_{\text{rug}}=0.25$ eV, $U=1$ eV
filling = 0.75 %, $T=0.018$ eV
Other Projects

- Spectra of 1D Hubbard model
- Thermodynamics of 2-chain model
- More Accurate Hybrid Method
- First-Principles simulations of disorder
  - D. Johnson, W. Shelton
Configurational Correlations in Binary Alloys

M. Jarrell, D. Johnson, ... preprint
More Accurate Hybrid Approach

\[ G_0 \xrightarrow{} \text{QMC Cluster Solver} \]

\[ G \xrightarrow{} \Sigma \xrightarrow{} \Gamma \]

\[ F = \Gamma + \Gamma \]

\[ k, i\omega_n, \sigma \xrightarrow{} k+q, i\omega_n + iv, \sigma \xrightarrow{} -\sigma \xrightarrow{} k, i\omega_n, \sigma \]
Conclusions

• QMC + MEM allow us to study 1D systems
  – spin-charge separation
  – coupled chains
• Improved efficiency with hybrid approach.
• New MEM much greater frequency resolution
• Improved formalism for alloys