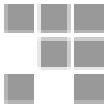
# Quantum Cluster Simulations of Low D Systems

## *Electronic Correlations on Many Length Scales*

M. Jarrell, University of Cincinnati

UNIVERSITY OF Cincinnati

OSC

OAK RIDGE NATIONAL LABORATORY

CCS The Center for Computational Sciences

*DOE High Performance Computing Research Center*

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

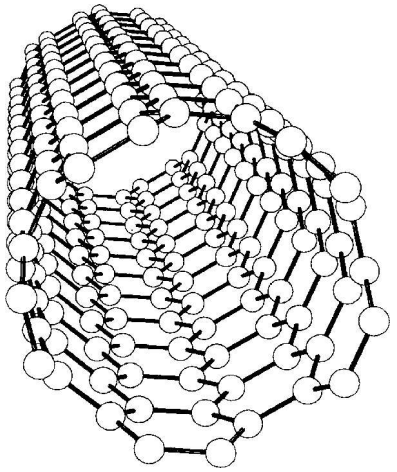
# Collaborators and References

- J. Hague
- S. Doluweera
- O. Gonazalez
- 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

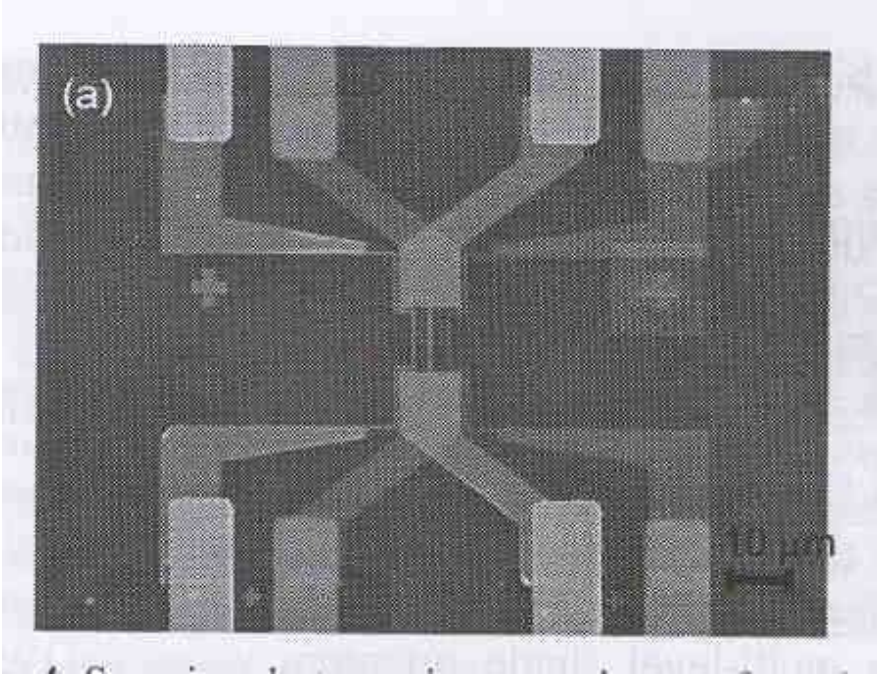
# Purpose

Carbon Nanotubes



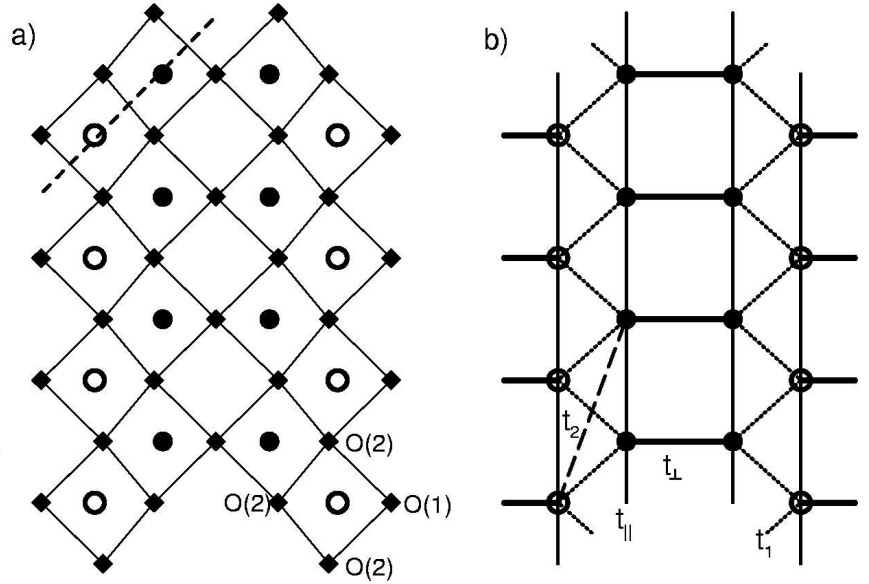
J. Mintmire
PRL 68, 631

**vertically coupled GaAs/AlGaAs quantum wires**




M. Weckworth, Superlattices and Microstruct 20, 561

$NaV_2O_5$

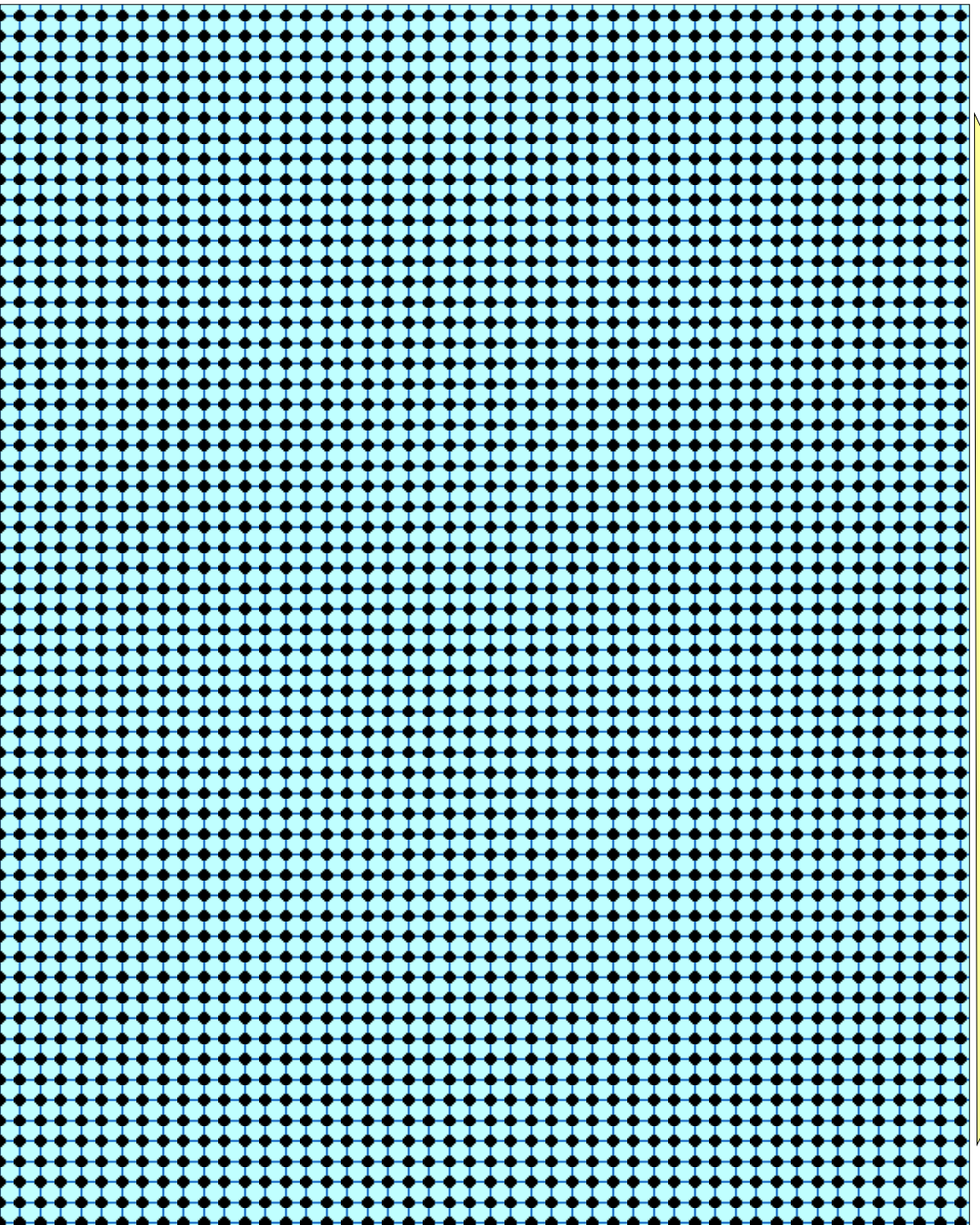



H. Smolinski PRL 80, 5164

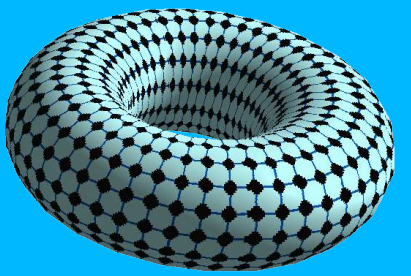
- Non-perturbative physics
- correlations over all length scales
- very low temperatures

Periodic Lattice

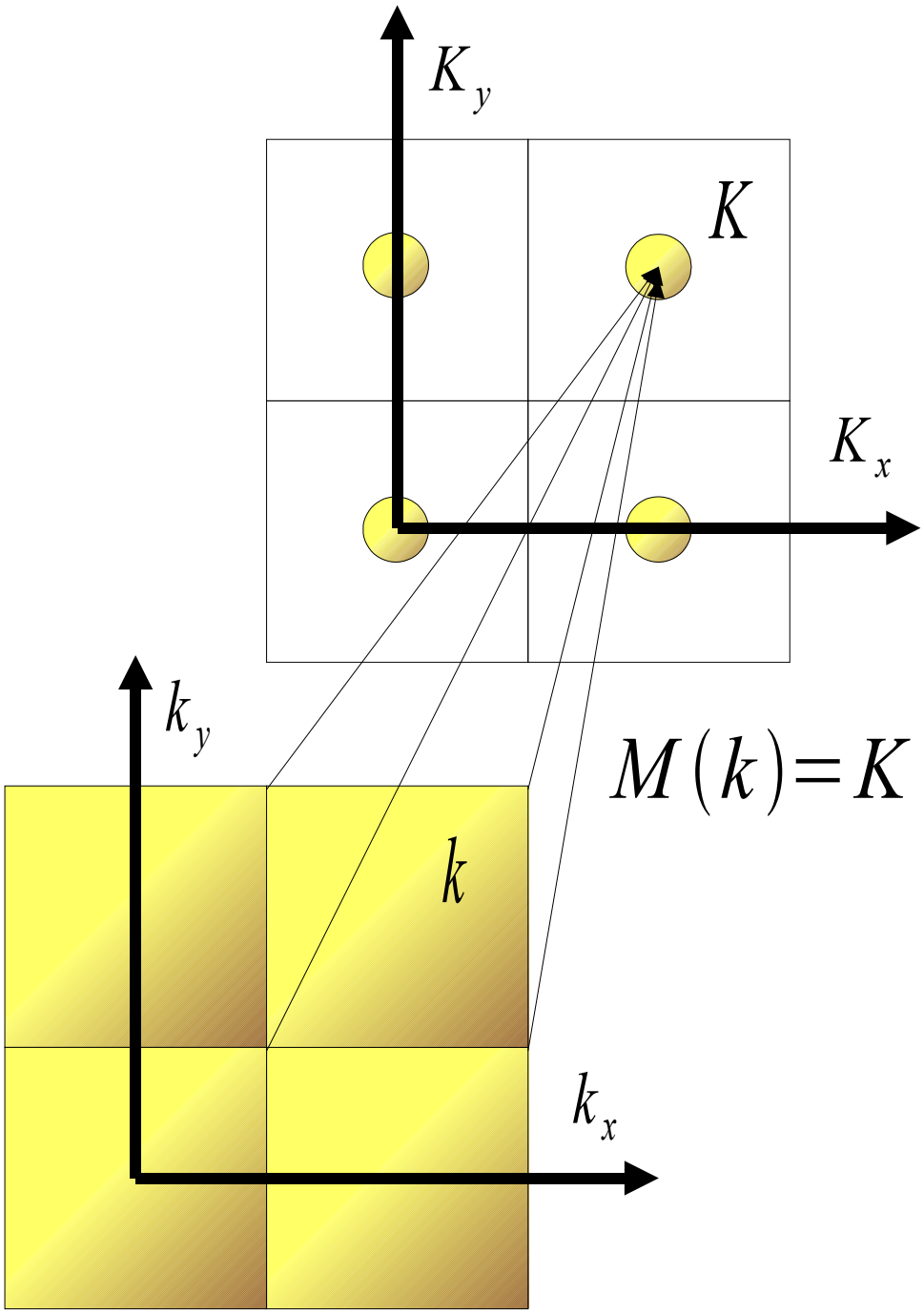
Dynamical Cluster Approximation



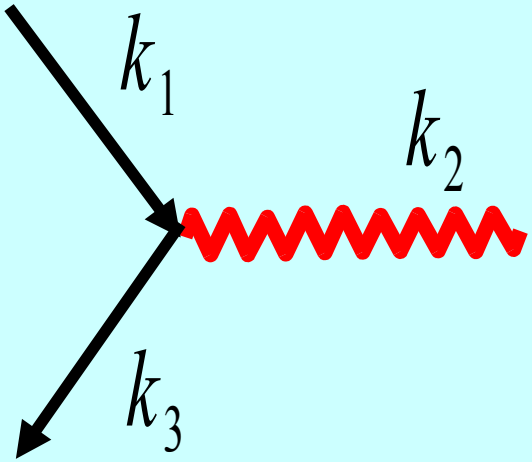
Effective Medium



# DCA Mapping to Cluster: Coarse Graining



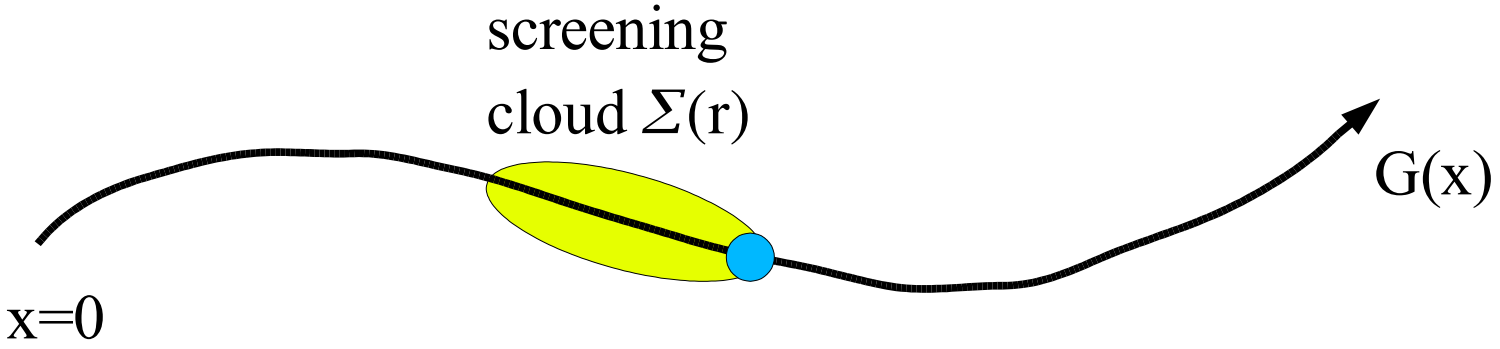

$$M(k) = K$$




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

$$N_c\,\delta_{M(k_1)+M(k_2),\,M(k_3)}$$

# The Nature of Cluster Approximations




| | Self Energy | |
|---|---|---|
| DMFA | Local | $\Sigma(k,\omega) \approx \Sigma(\omega)$ |
| DCA | Short Ranged | $\Sigma(k,\omega) \approx \Sigma(K,\omega)$ few K |

# Problems Simulating 1D Systems

- QMC requires significant computer power
- Correlations over many length scales
- QMC minus sign problem—spectra

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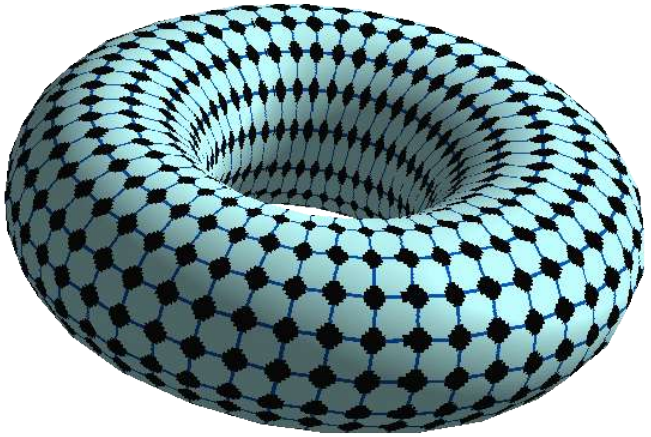
# We Solve The Cluster Problem with QMC

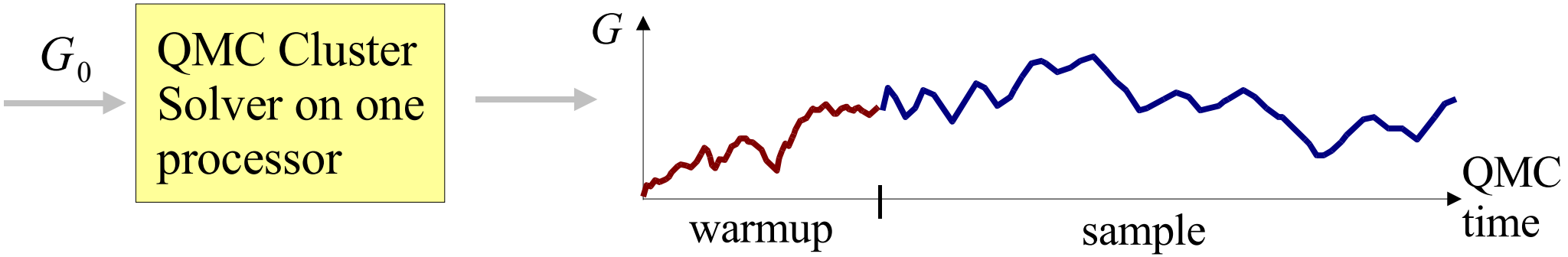
ORNL/CES and
OSC CRAY X1



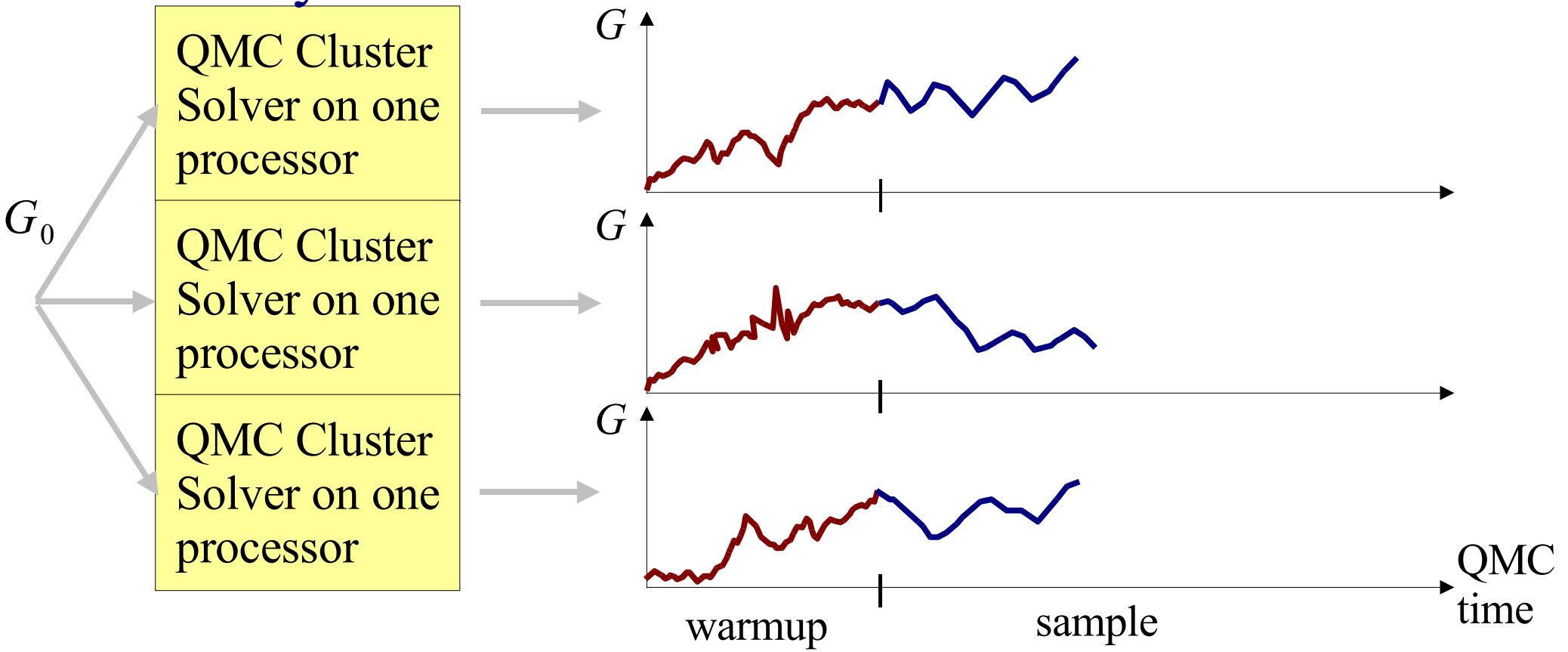
ORNL IBM
p690 (cheetah)

# Quantum Monte Carlo Cluster Solver

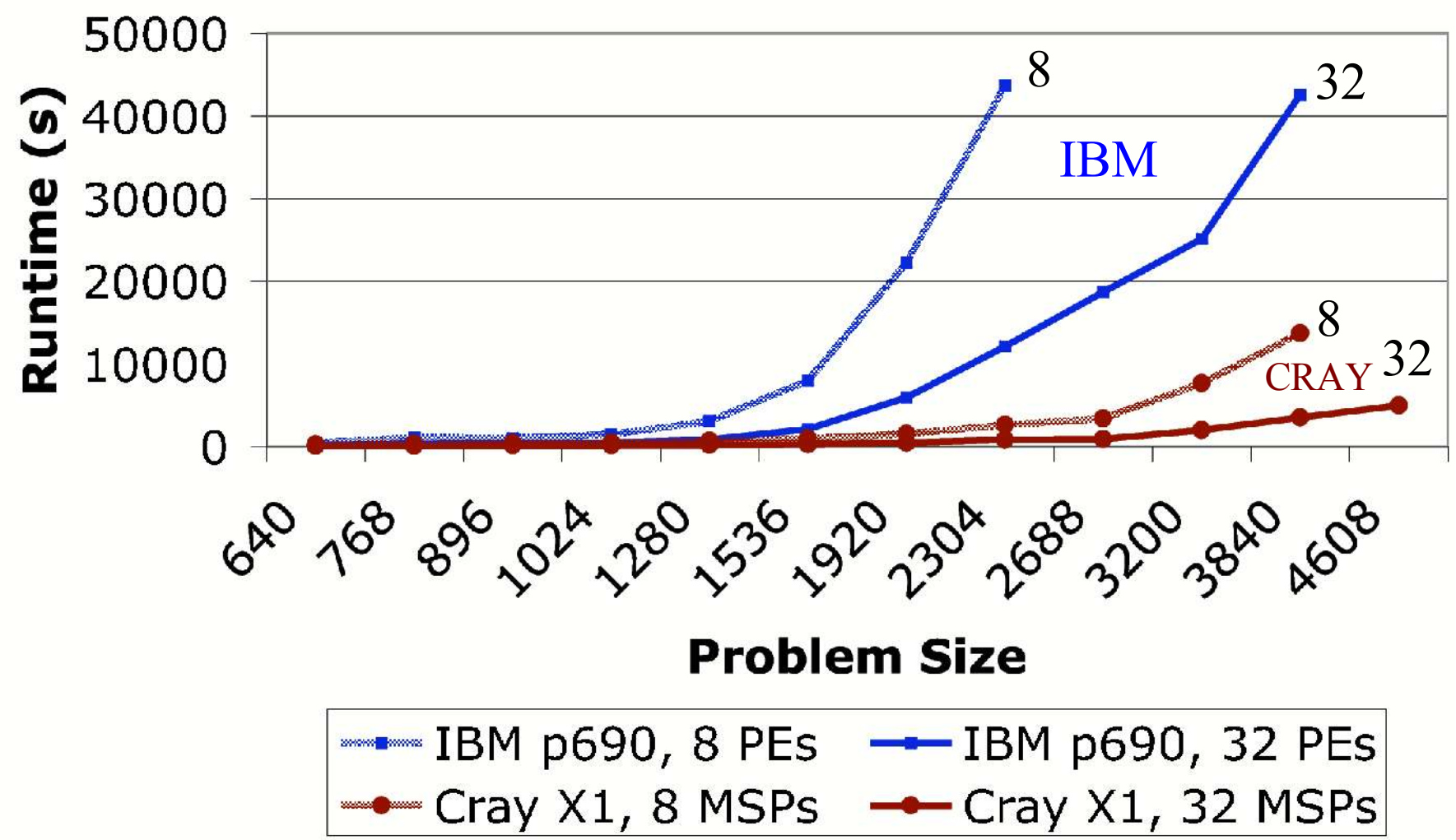
## Serial




## Perfectly Parallel



# DCA-QMC Runtime

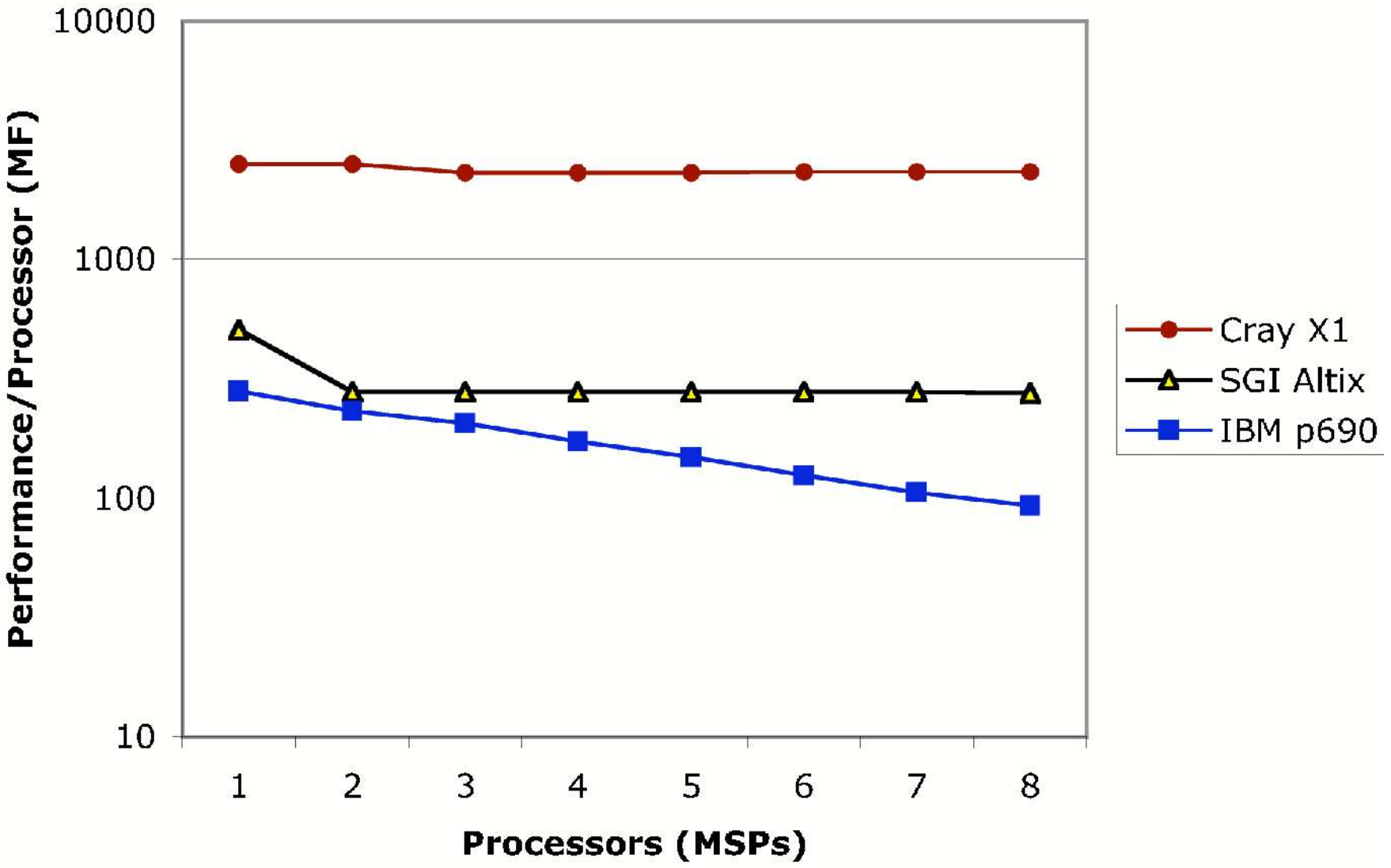



T. Maier, www.cray.com

# Performance of Concurrent DGERs

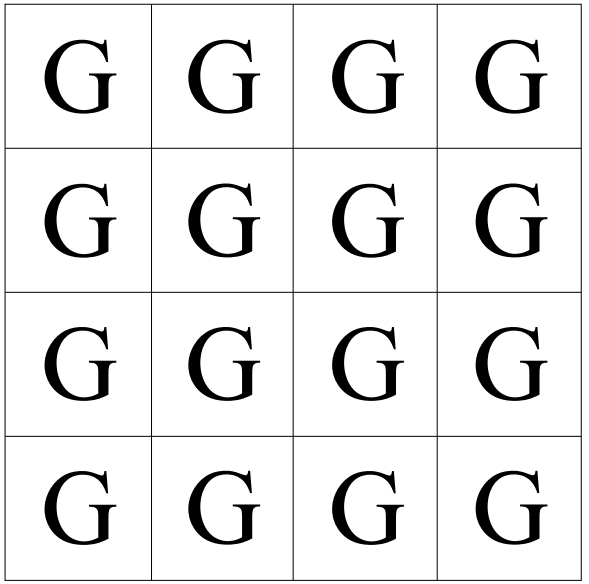
note the log scale

$$G' = G + a * b^T \quad \text{N=4480}$$

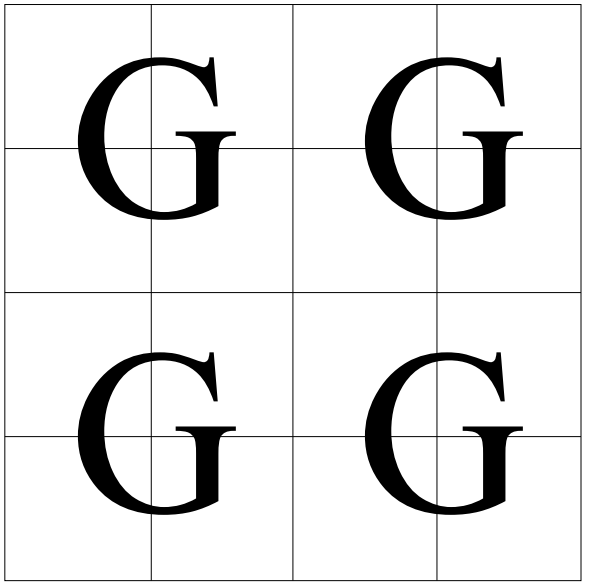


# Hybrid Parallel QMC

Perfectly parallel array of cpu's

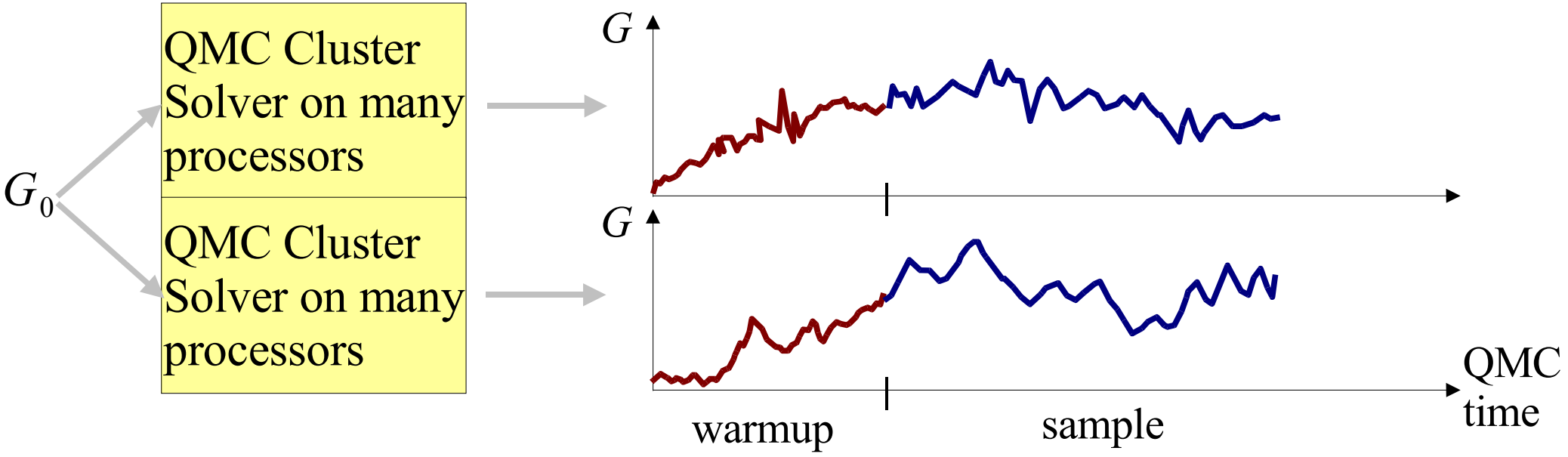



Hybrid parallel array of cpu's



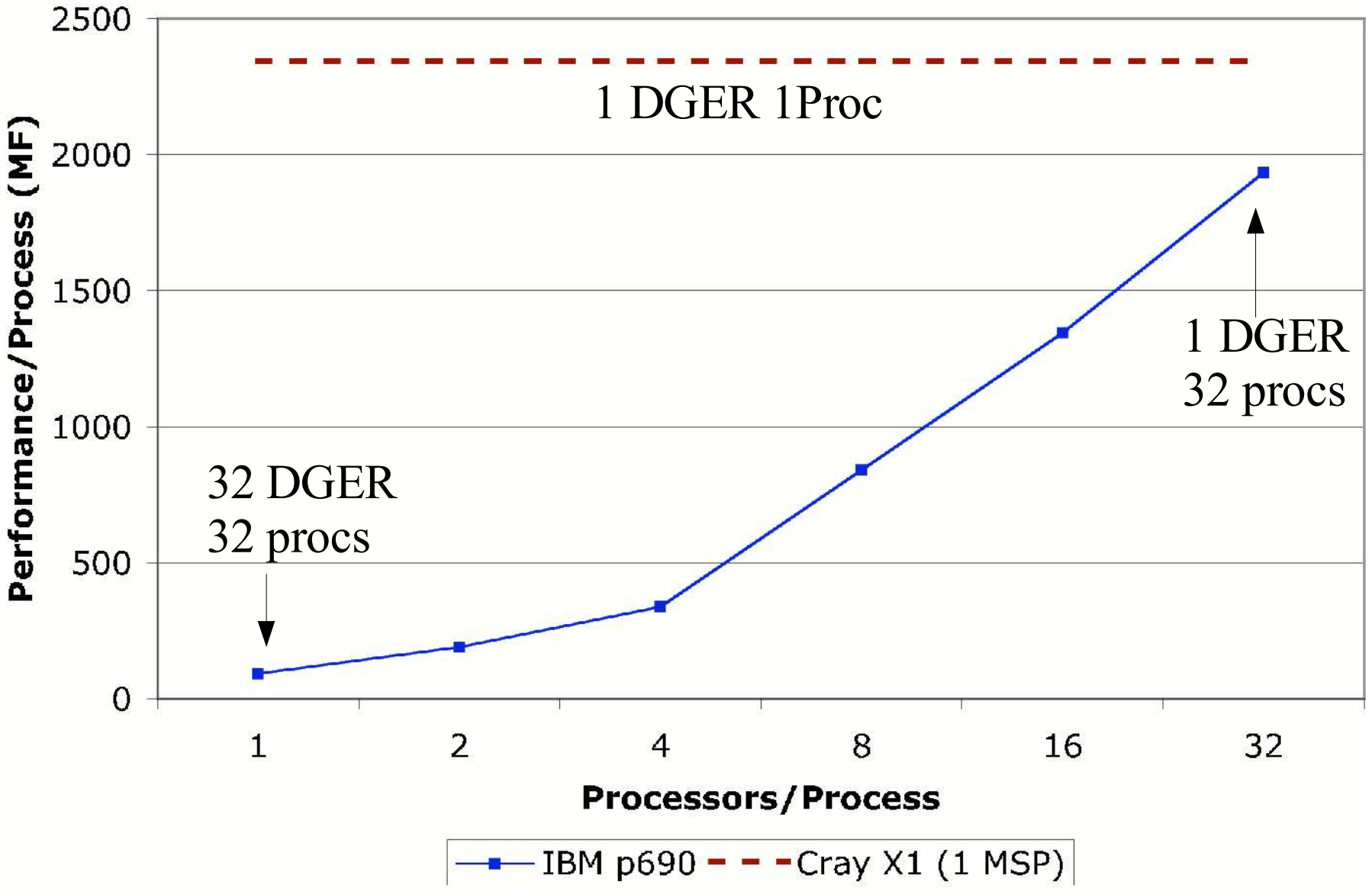

OpenMP

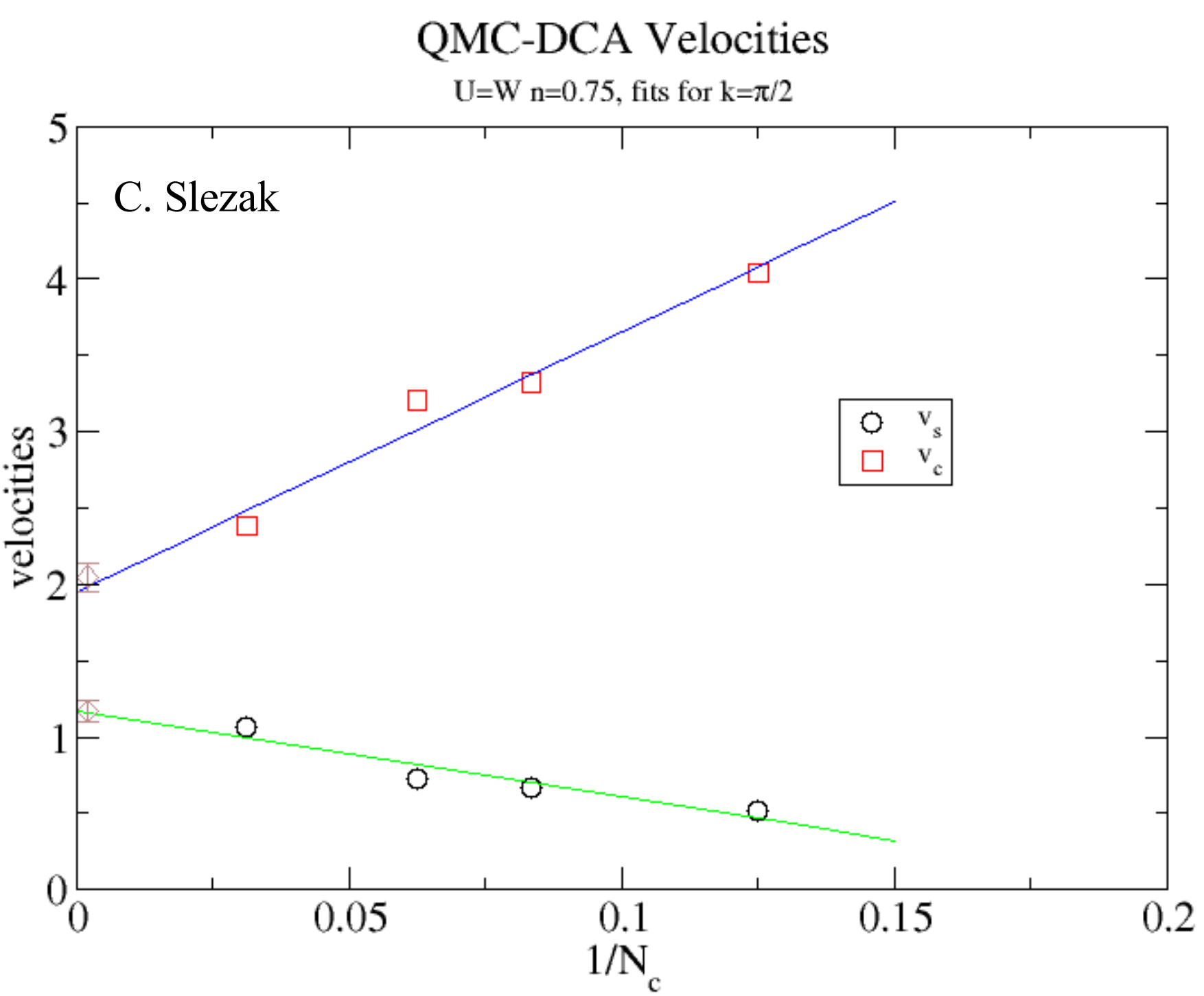
PBLAS



# 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
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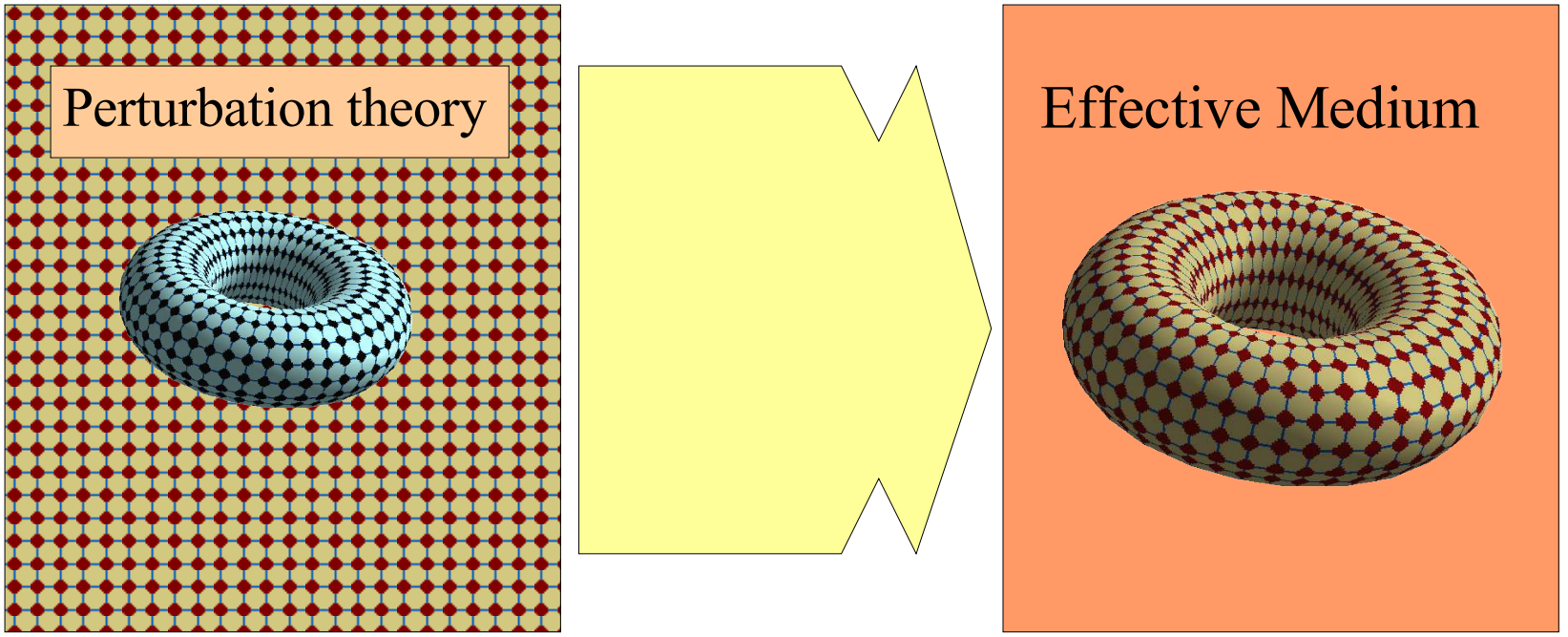
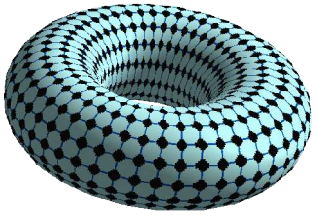
# Hybrid, Multiple Embedding

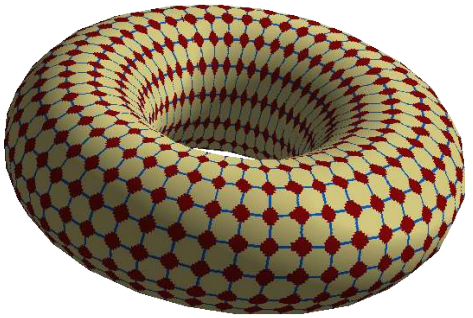



Length scales within the small cluster are treated explicitly

Length scales between the large and small cluster are treated perturbatively

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





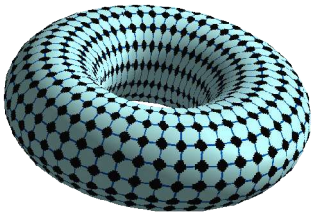
Effective Medium

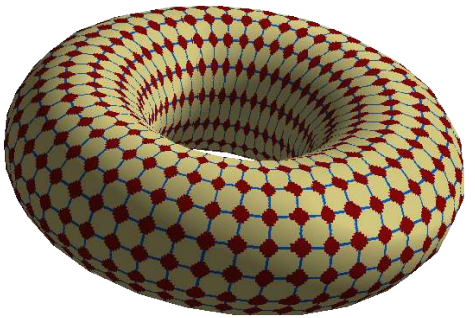
K. Aryanpour, PRB, 2003

# Ingredients of the Hybrid Approach

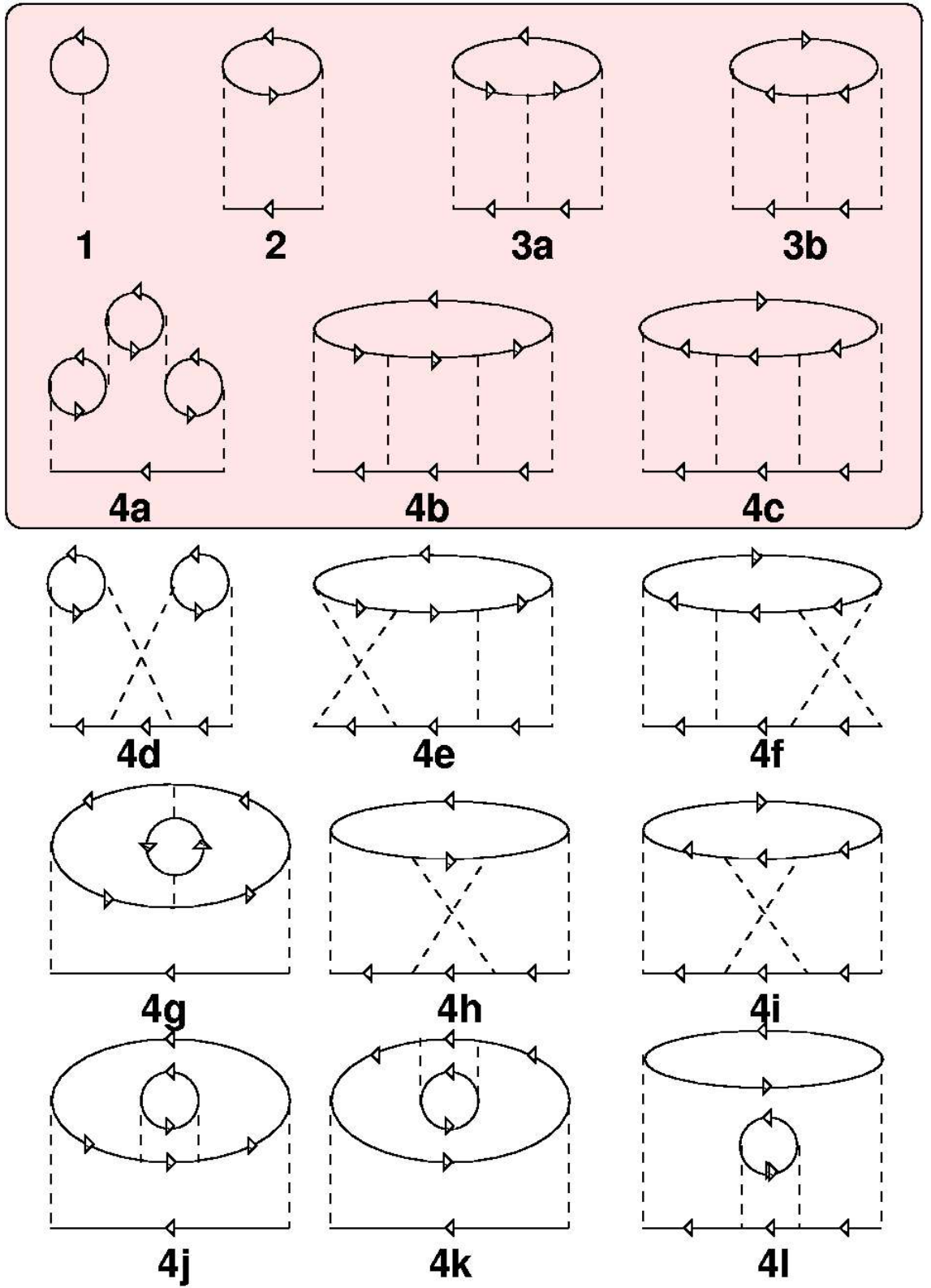
- Dynamical Cluster Approximation
  - glue
- Quantum Monte Carlo
  - small cluster
- FLEX perturbation theory
  - large cluster

Effective Medium





N.E. Bickers, 1989

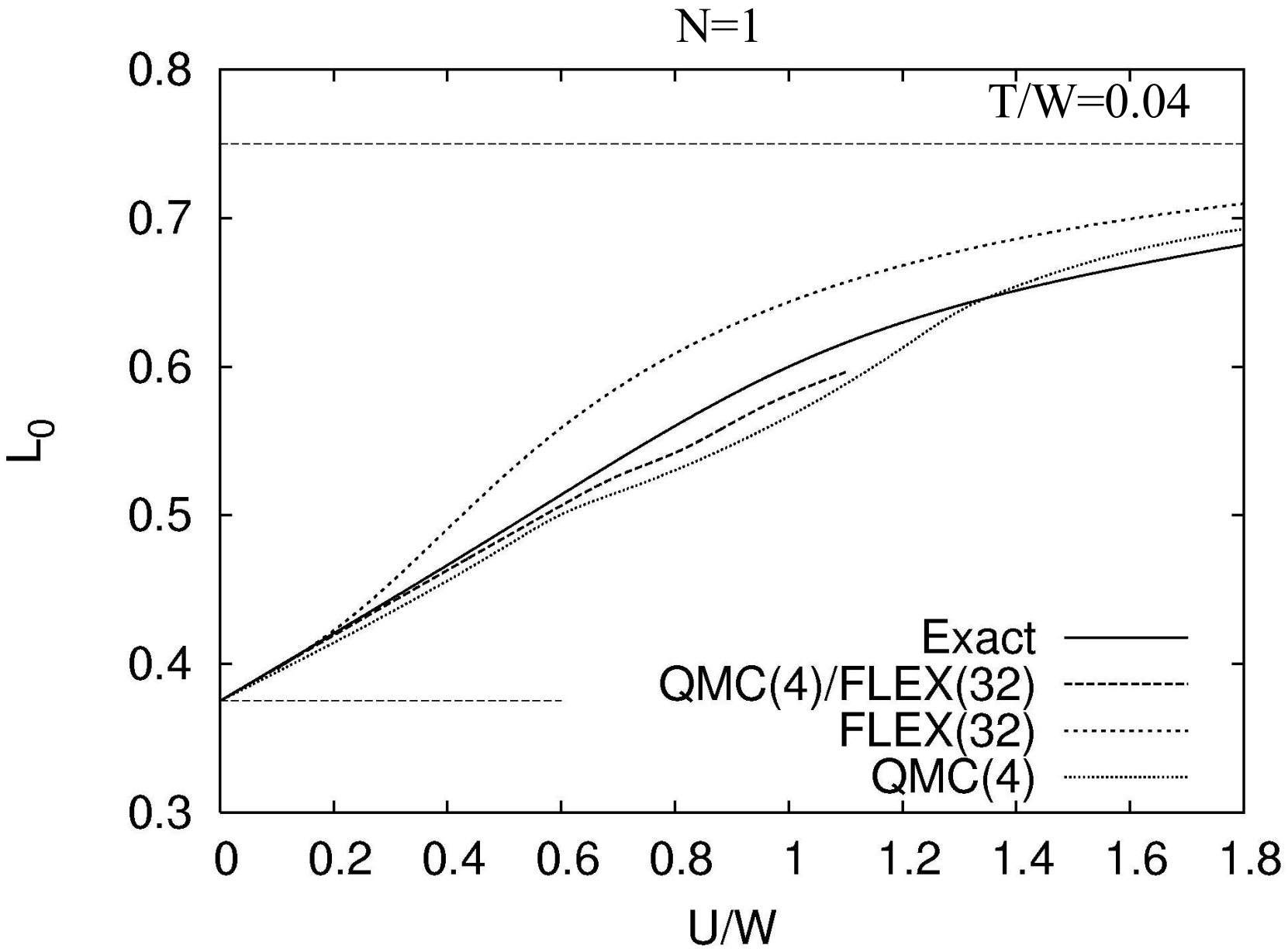



# The Fluctuation-Exchange Approximation

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

N.E. Bickers, 1989

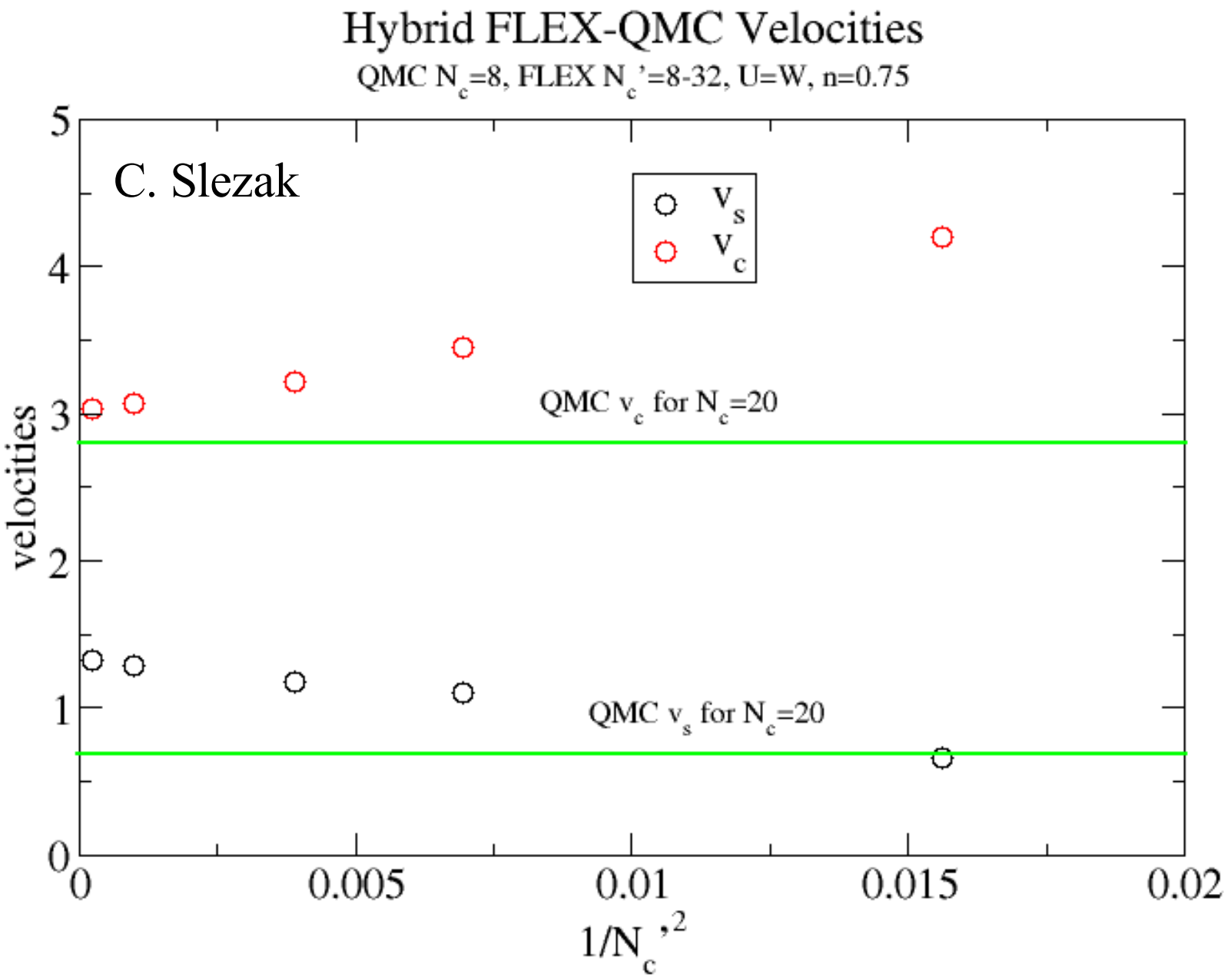
# 1D Hubbard Model



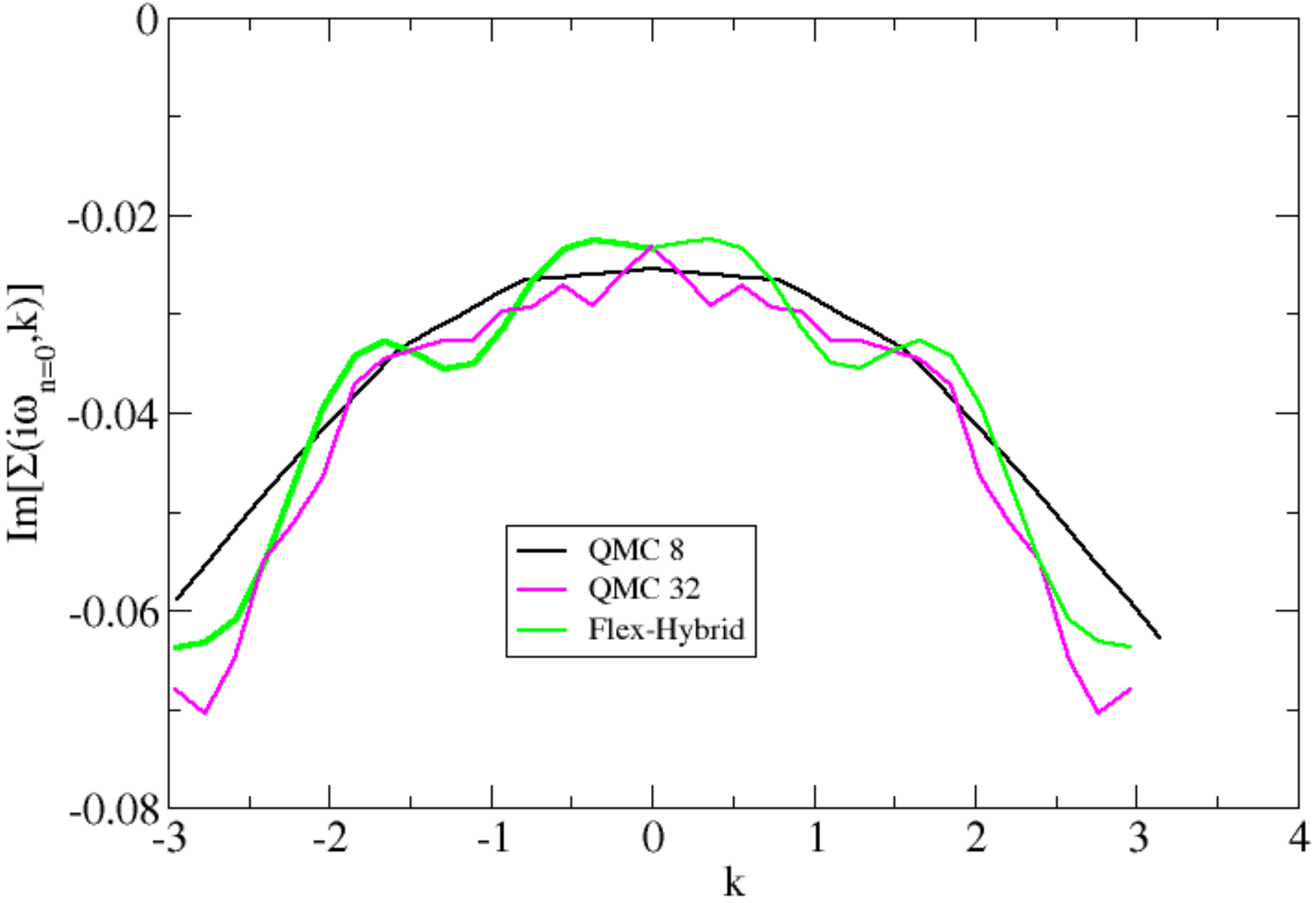

J. Hague, PRB 69, 165113

Lieb and Wu, PRL 1968

# Spin-Charge Separation with Hybrid FLEX




Nc=8 Hybrid result, roughly = Nc=20 QMC Result, saving a factor of 16


U=W, n=0.75, beta=31, QMC N_c=8, FLEX N_c'=32
0
-0.02
-0.04
-0.06
-0.08
Im[Σ(iω_n=0,k)]
-3
-2
-1
0
1
2
3
4
k
QMC 8
QMC 32
Flex-Hybrid

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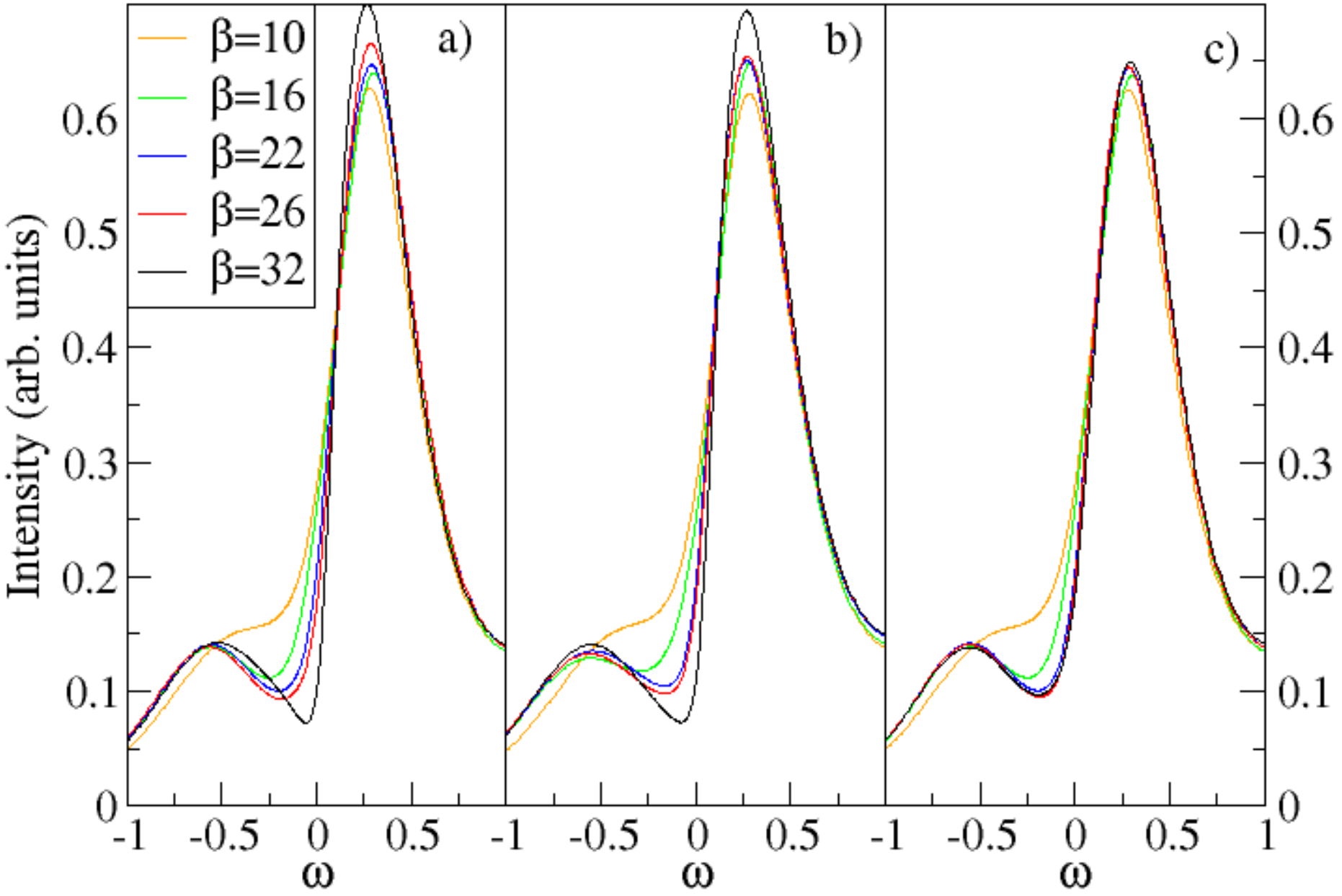
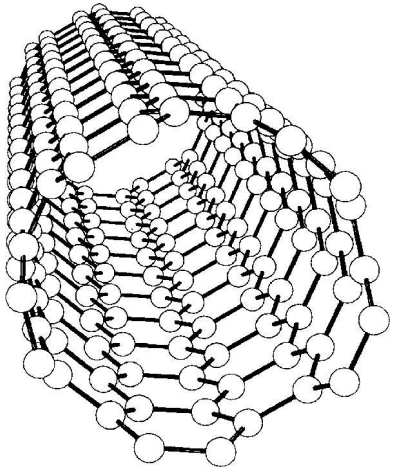



A. Macridin, preprint

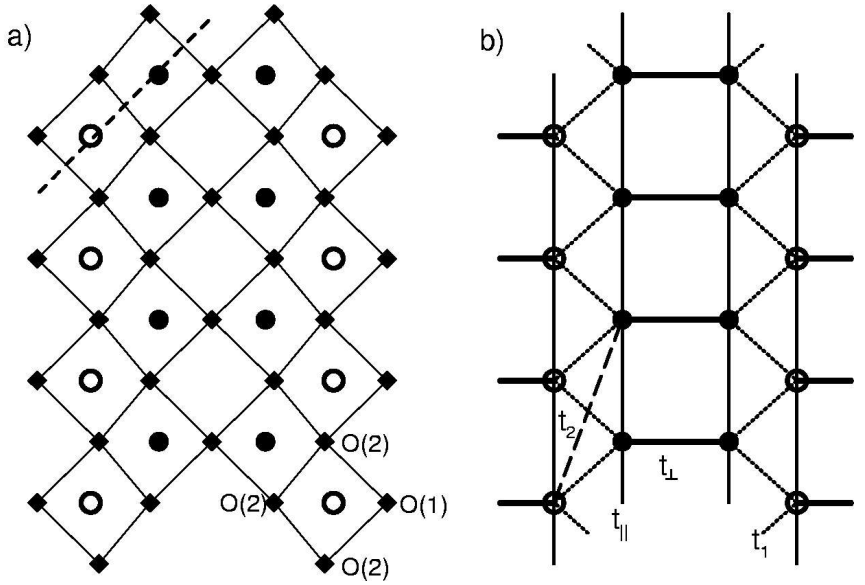
# Spectra of 2-chain model

Carbon Nanotubes



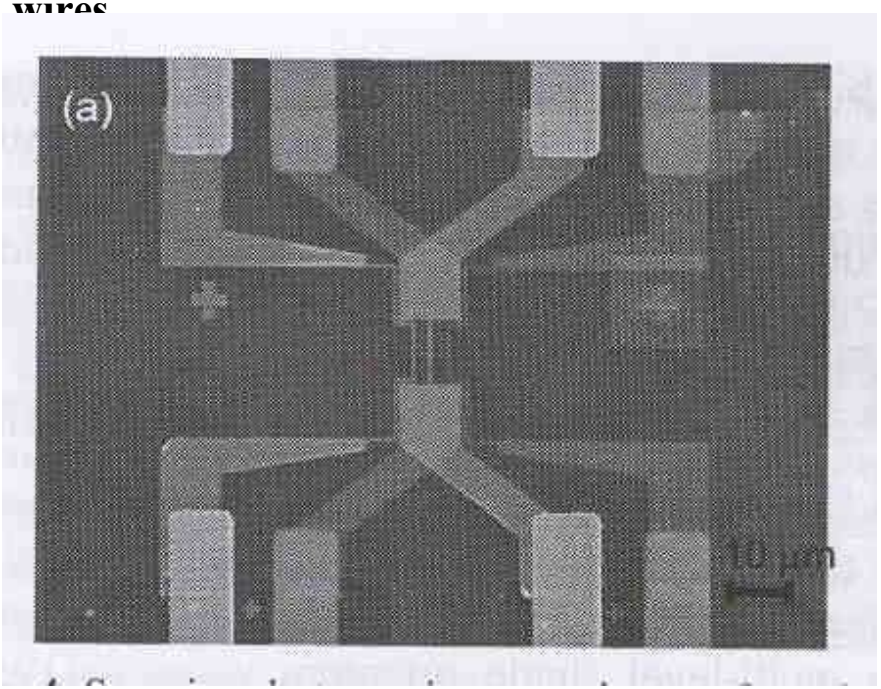
J. Mintmire
PRL 68, 631

$NaV_2O_5$



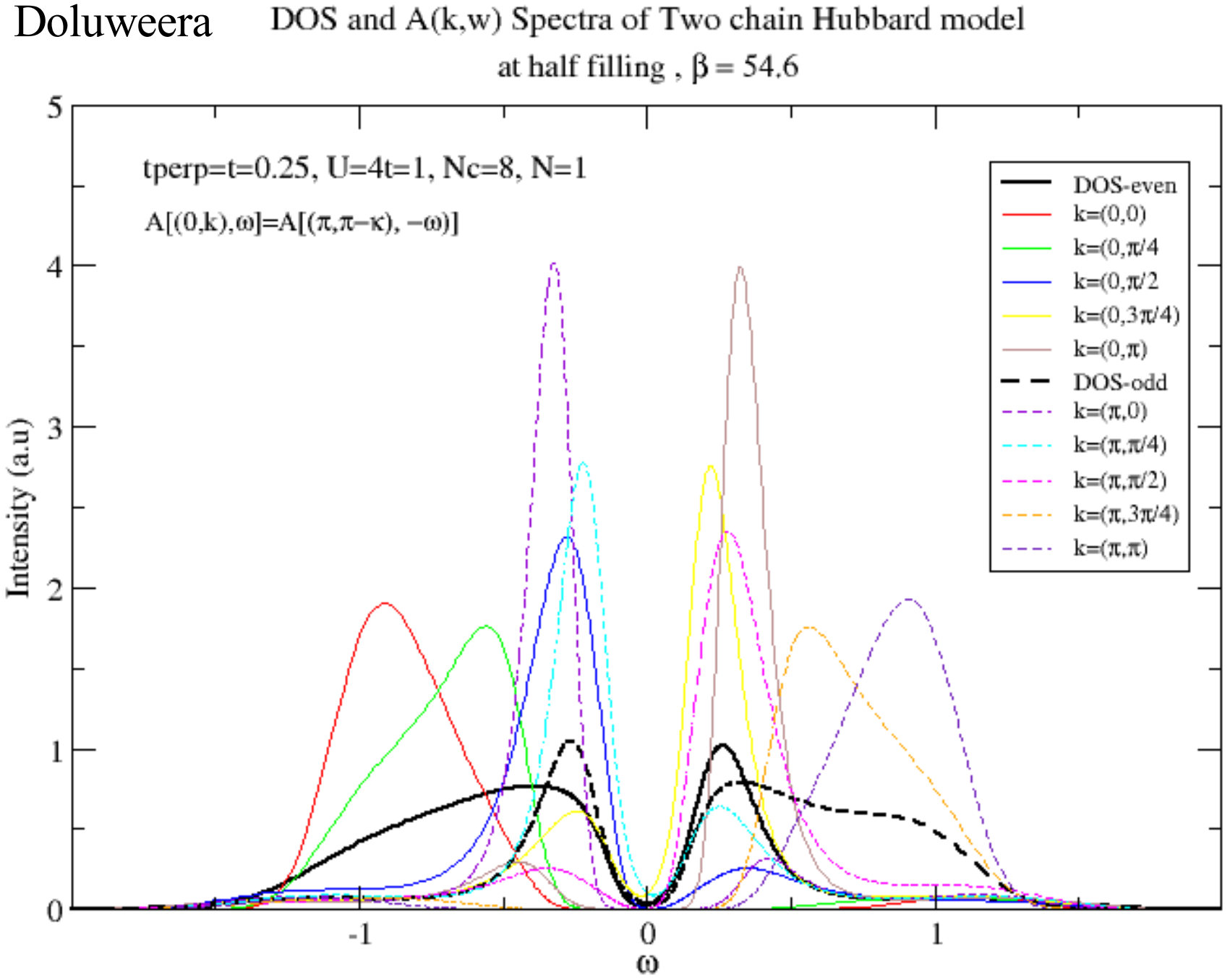

H. Smolinski PRL 80, 5164

**vertically coupled GaAs/AlGaAs quantum wires**

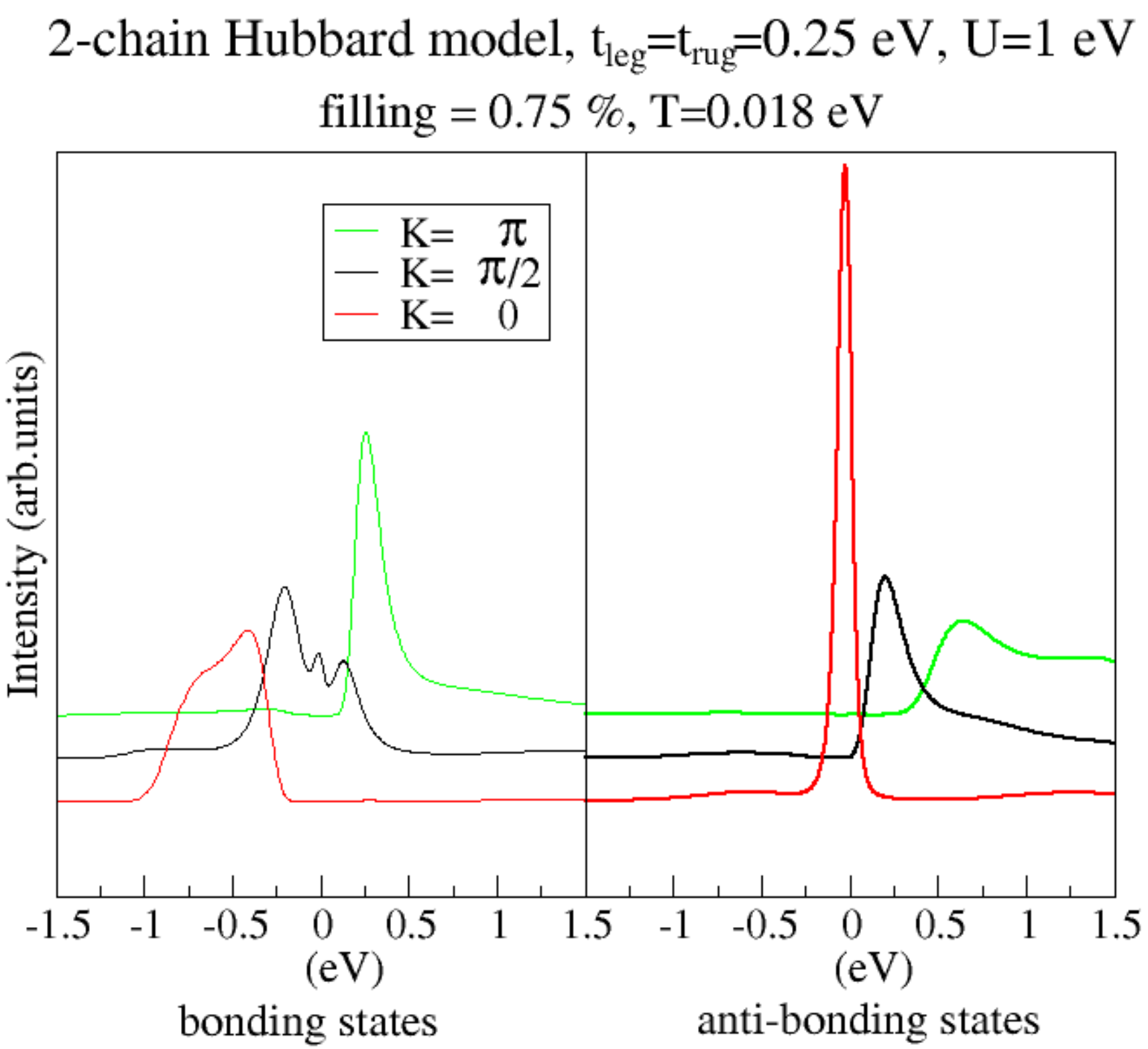



M. Weckworth, Superlattices and Microstruct 20, 561

S. Doluweera



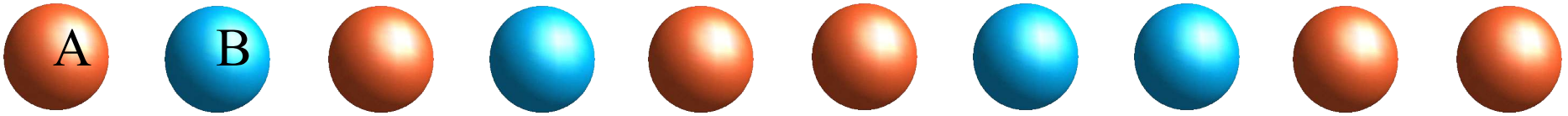

Endres PRB 53 5530

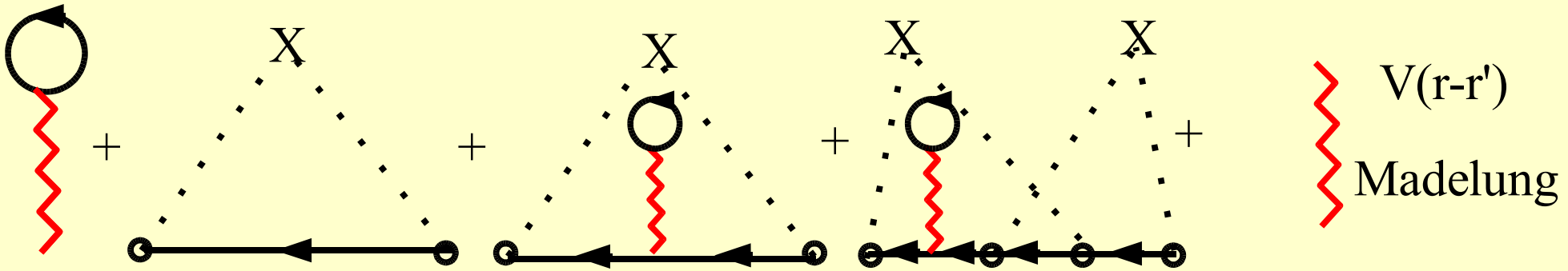

2-chain Hubbard model, $t_{leg}$=$t_{rug}$=0.25 eV, U=1 eV
filling = 0.75 %, T=0.018 eV
K= π
K= π/2
K= 0
Intensity (arb.units)
-1.5
-1
-0.5
0
0.5
1
1.5
(eV)
bonding states
anti-bonding states

# 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

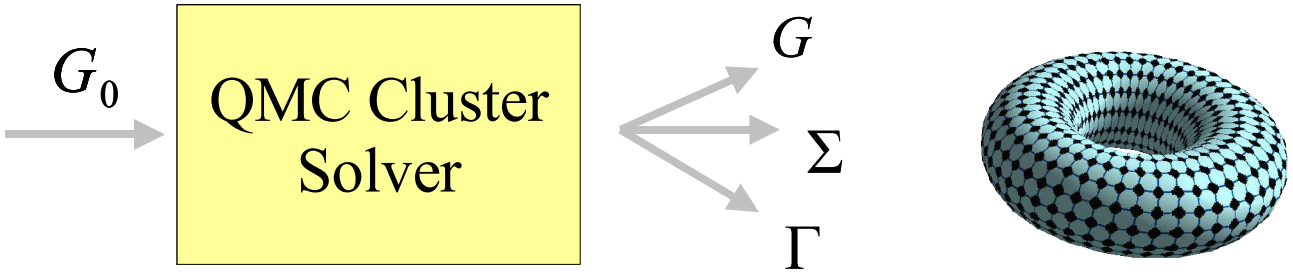
# Configurational Correlations in Binary Alloys

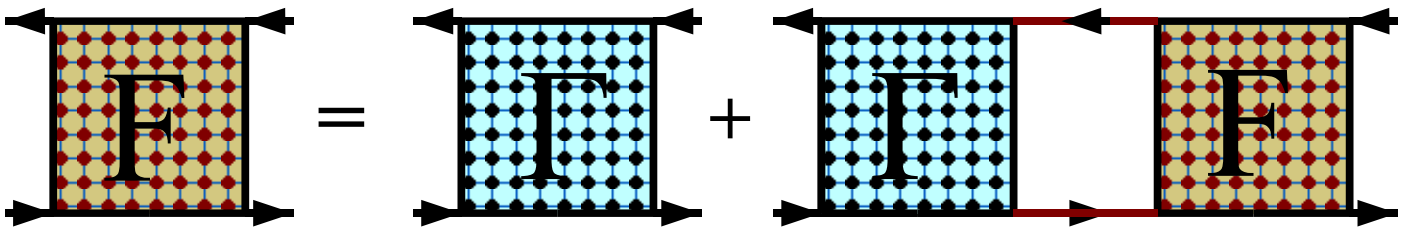


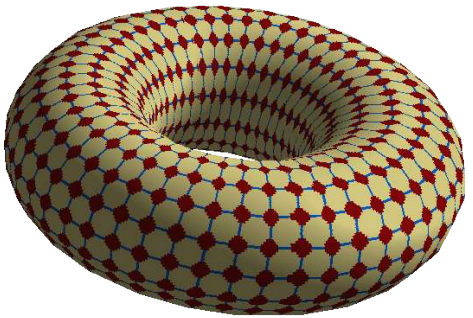



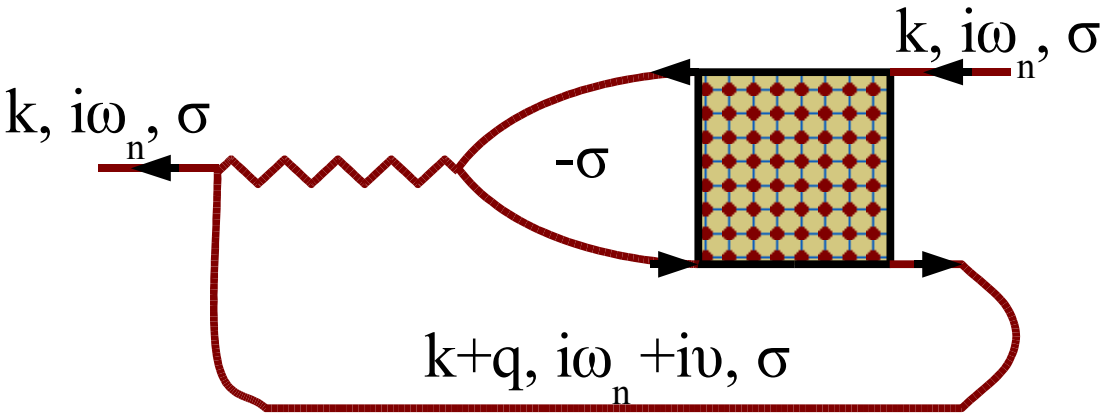

M. Jarrell, D. Johnson, ... preprint

# More Accurate Hybrid Approach





# 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