Lectures on Quantum Monte Carlo Methods

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Progression of Lectures

1 Stochastic Integration

2 Random Numbers

3 Classical Statistical Mechanical Simulations

4 Cluster algorithms for classical models

5 Quantum Monte Carlo

6 The continuum limit

7 Observables and Estimators

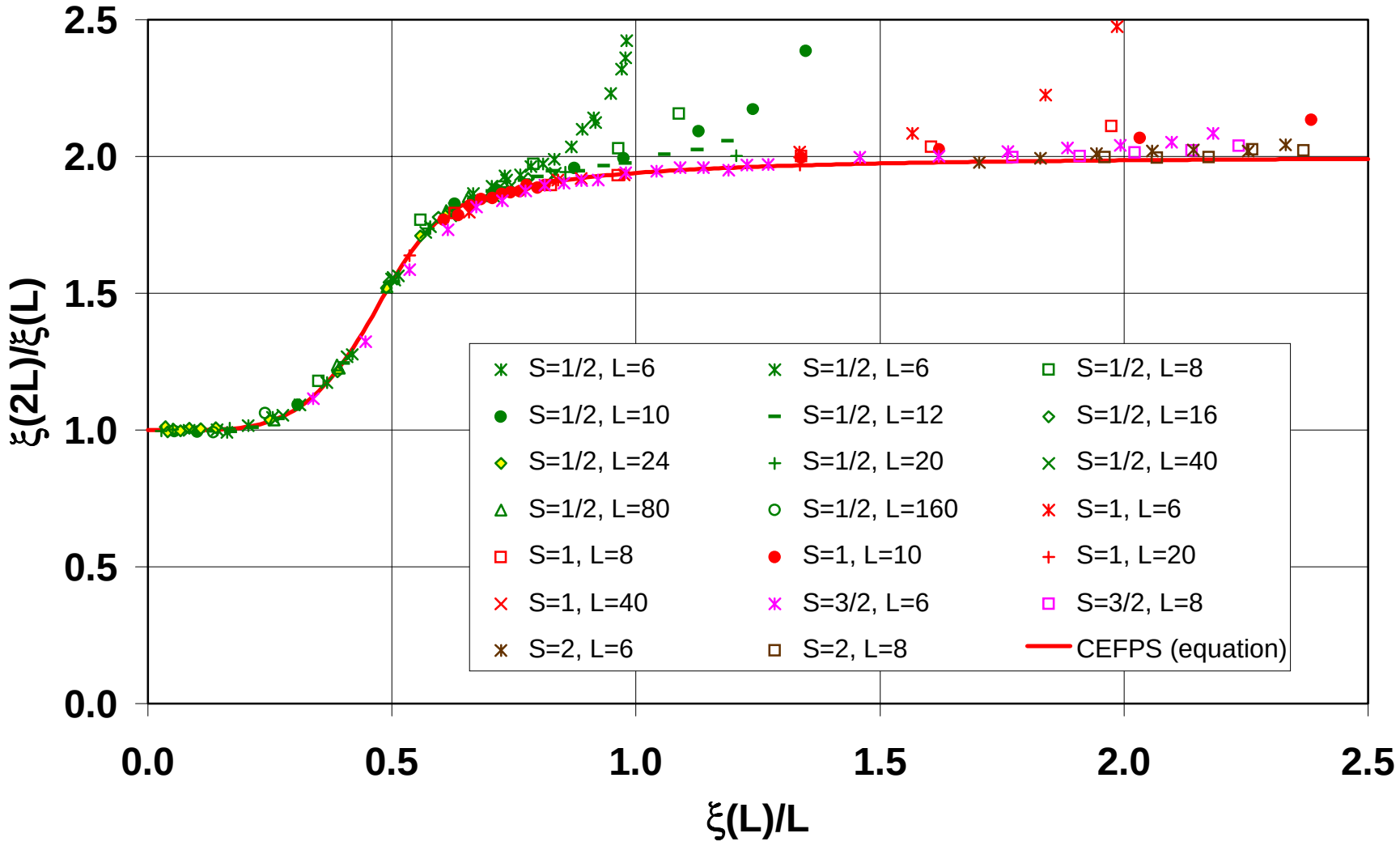
8 Finite-size scaling

9 More about the correlation length

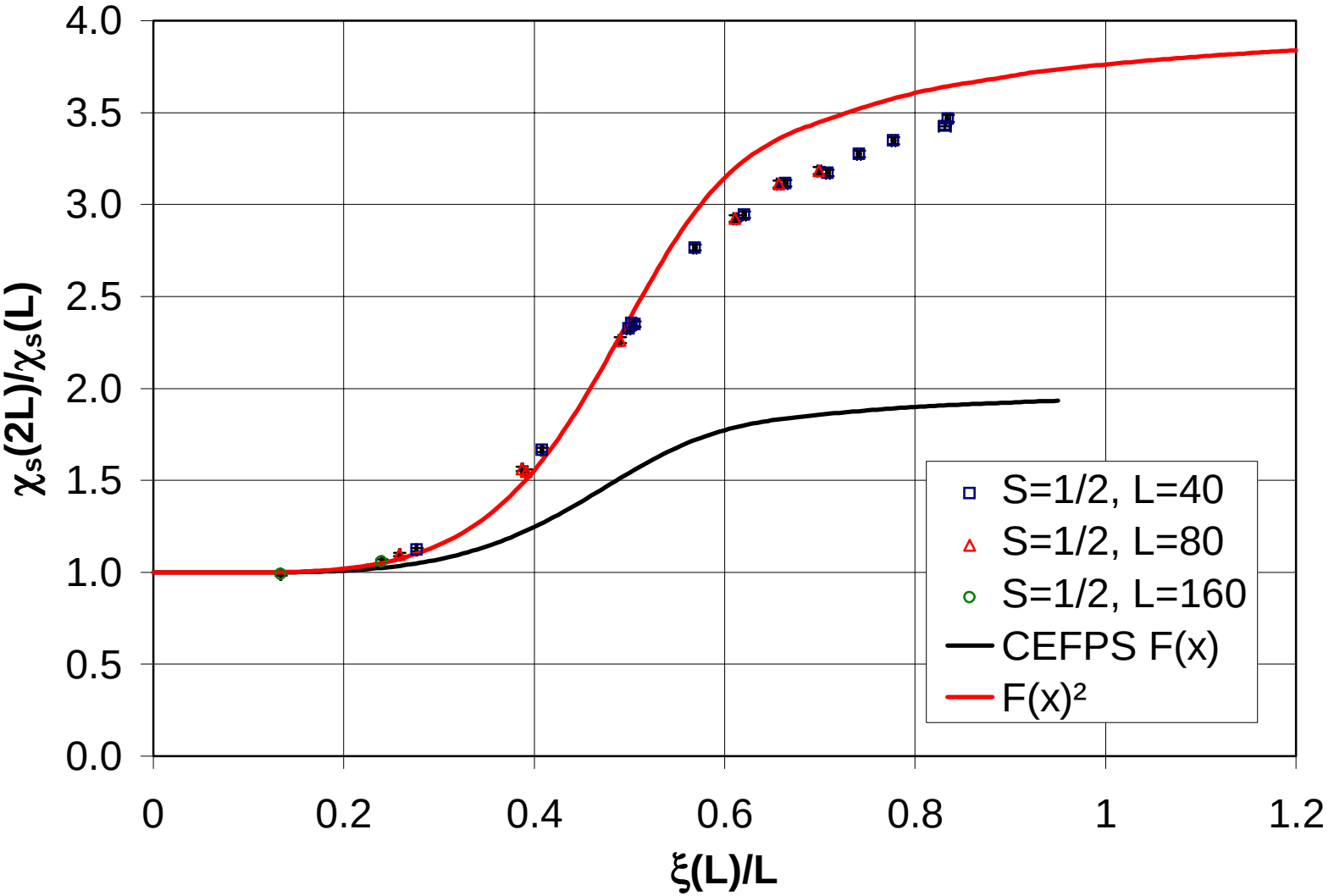
10 Survey of other applications

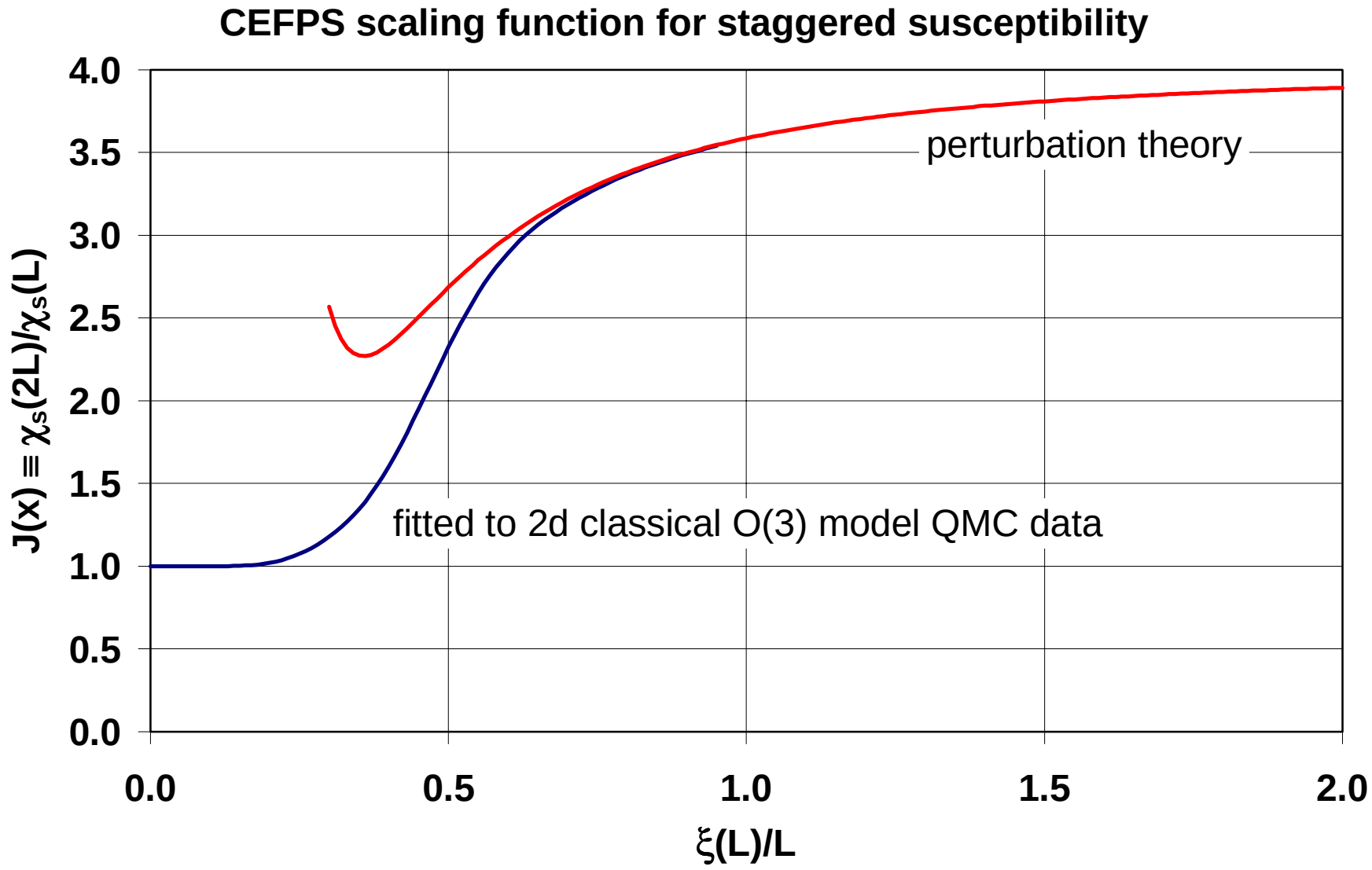
9. More about the correlation length

Or, the tale of the six blind men and the elephant.

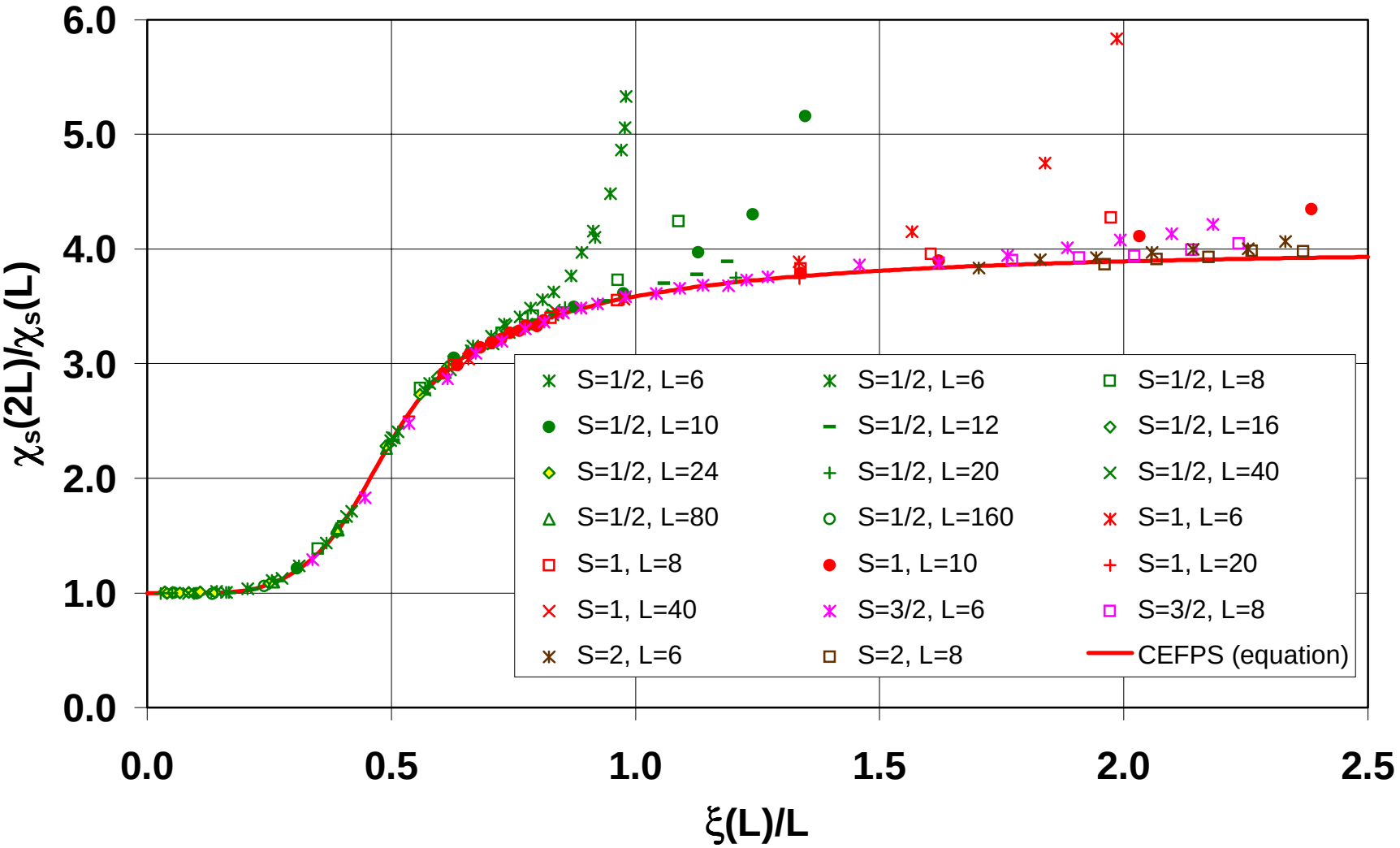

Scaling Chart for Correlation Length
2d Quantum AFHM, Varying S
ξ(2L)/ξ(L)
ξ(L)/L
0.0
0.5
1.0
1.5
2.0
2.5
S=1/2, L=6
S=1/2, L=6
S=1/2, L=8
S=1/2, L=10
S=1/2, L=12
S=1/2, L=16
S=1/2, L=24
S=1/2, L=20
S=1/2, L=40
S=1/2, L=80
S=1/2, L=160
S=1, L=6
S=1, L=8
S=1, L=10
S=1, L=20
S=1, L=40
S=3/2, L=6
S=3/2, L=8
S=2, L=6
S=2, L=8
CEFPS (equation)

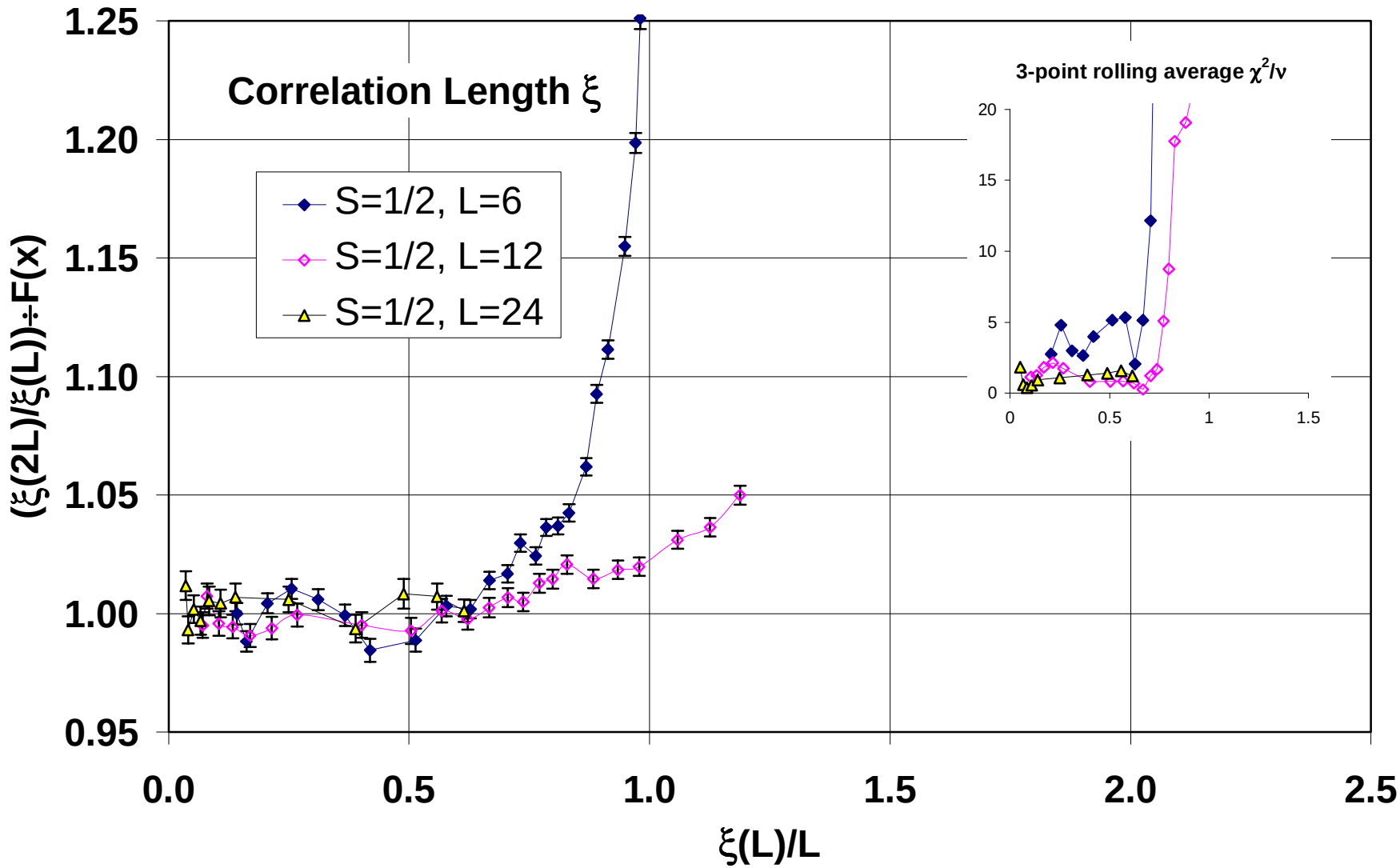
Preliminary Scaling Chart for Staggered Susceptibility

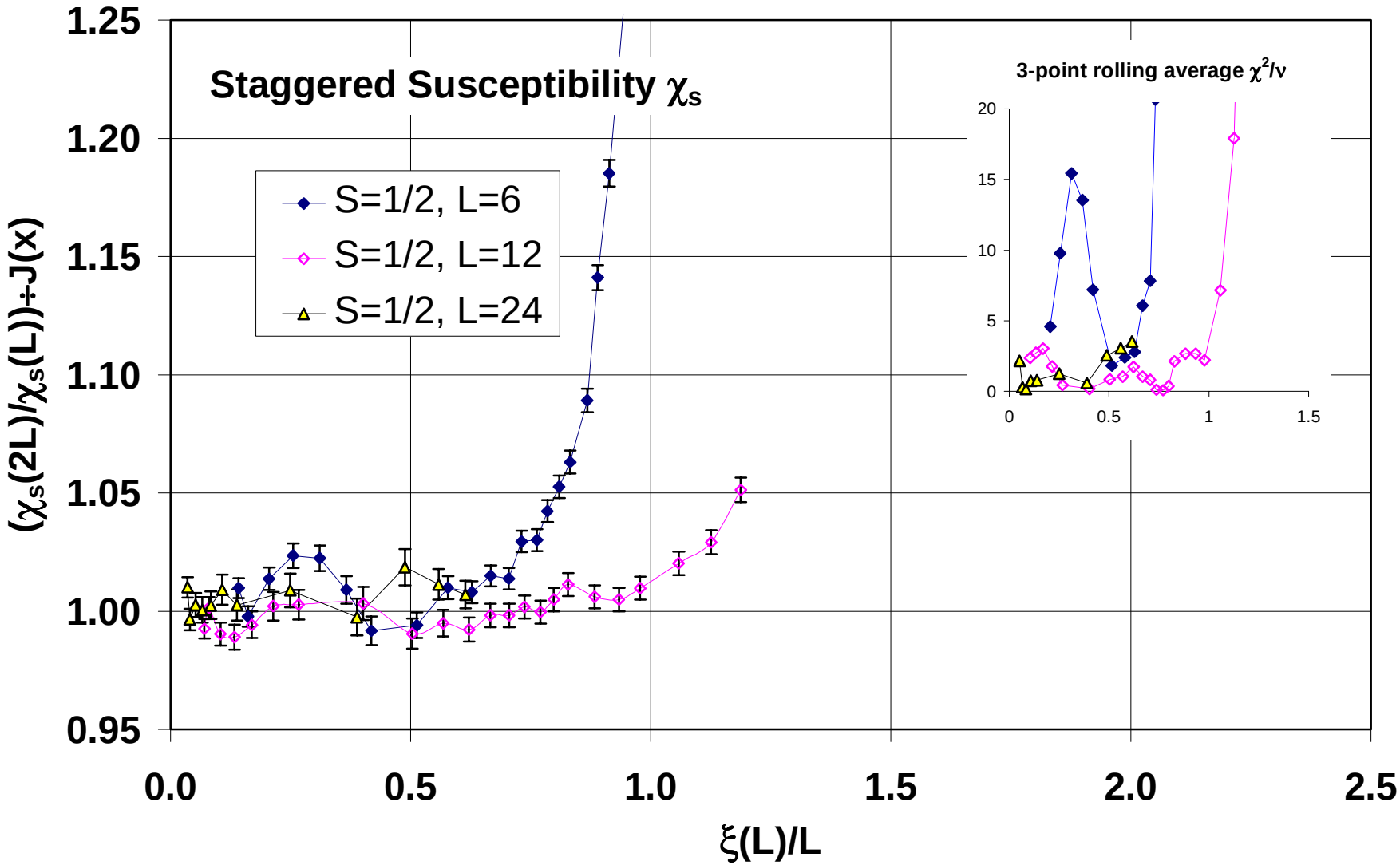


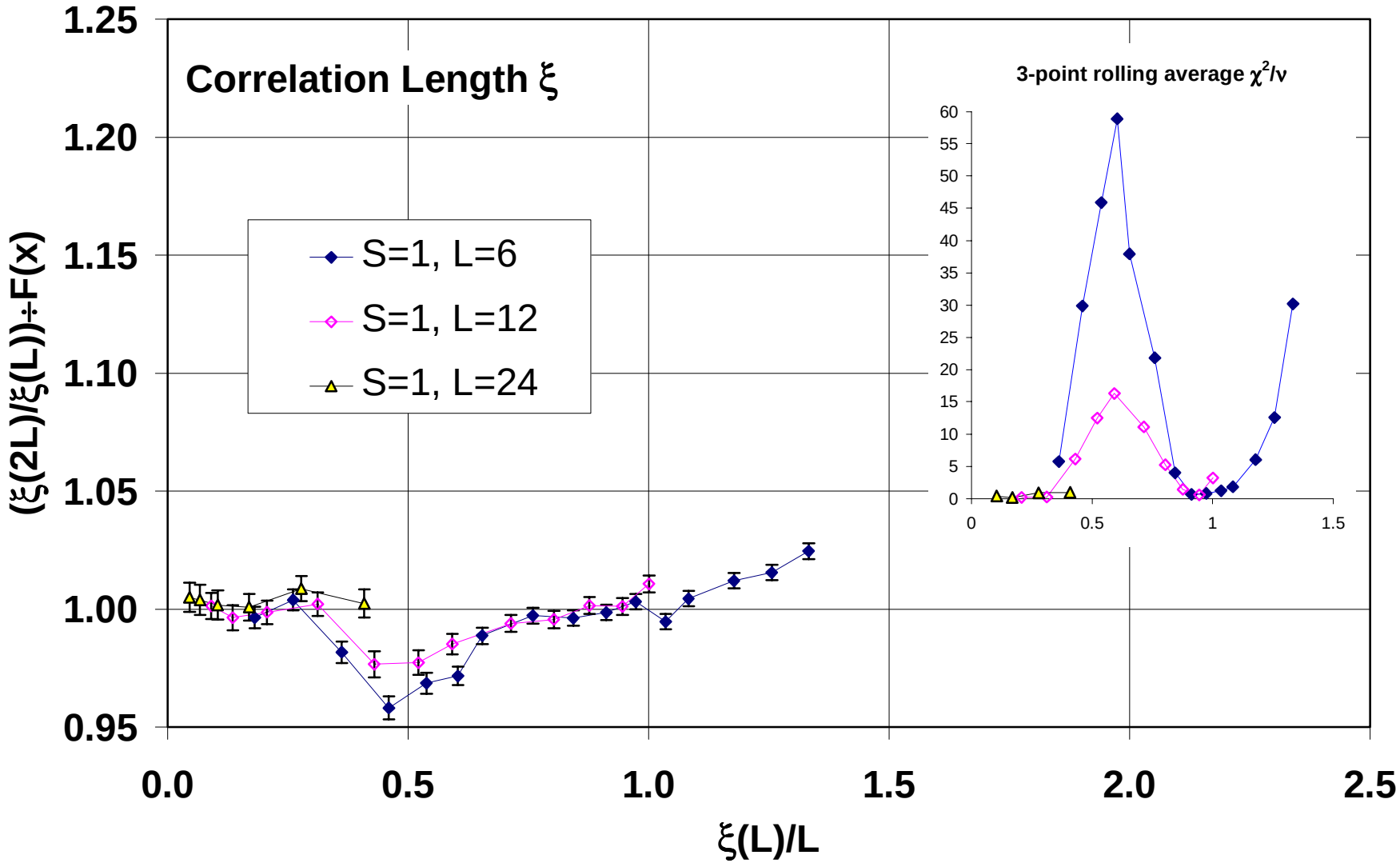

CEFPS scaling function for staggered susceptibility
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
J(x) ≡ χs(2L)/χs(L)
perturbation theory
fitted to 2d classical O(3) model QMC data
0.0
0.5
1.0
1.5
2.0
ξ(L)/L

Scaling Chart for Staggered Susceptibility
2d Quantum AFHM, Varying S




Correlation Length ξ
S=1/2, L=6
S=1/2, L=12
S=1/2, L=24
(ξ(2L)/ξ(L))÷F(x)
ξ(L)/L
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0.0
0.5
1.0
1.5
2.0
2.5
3-point rolling average χ²/ν
20
15
10
5
0
0
0.5
1
1.5


Staggered Susceptibility χ_s
S=1/2, L=6
S=1/2, L=12
S=1/2, L=24
$(\chi_s(2L)/\chi_s(L))\div J(x)$
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0.0
0.5
1.0
1.5
2.0
2.5
$\xi(L)/L$
3-point rolling average χ^2/ν
20
15
10
5
0
0
0.5
1
1.5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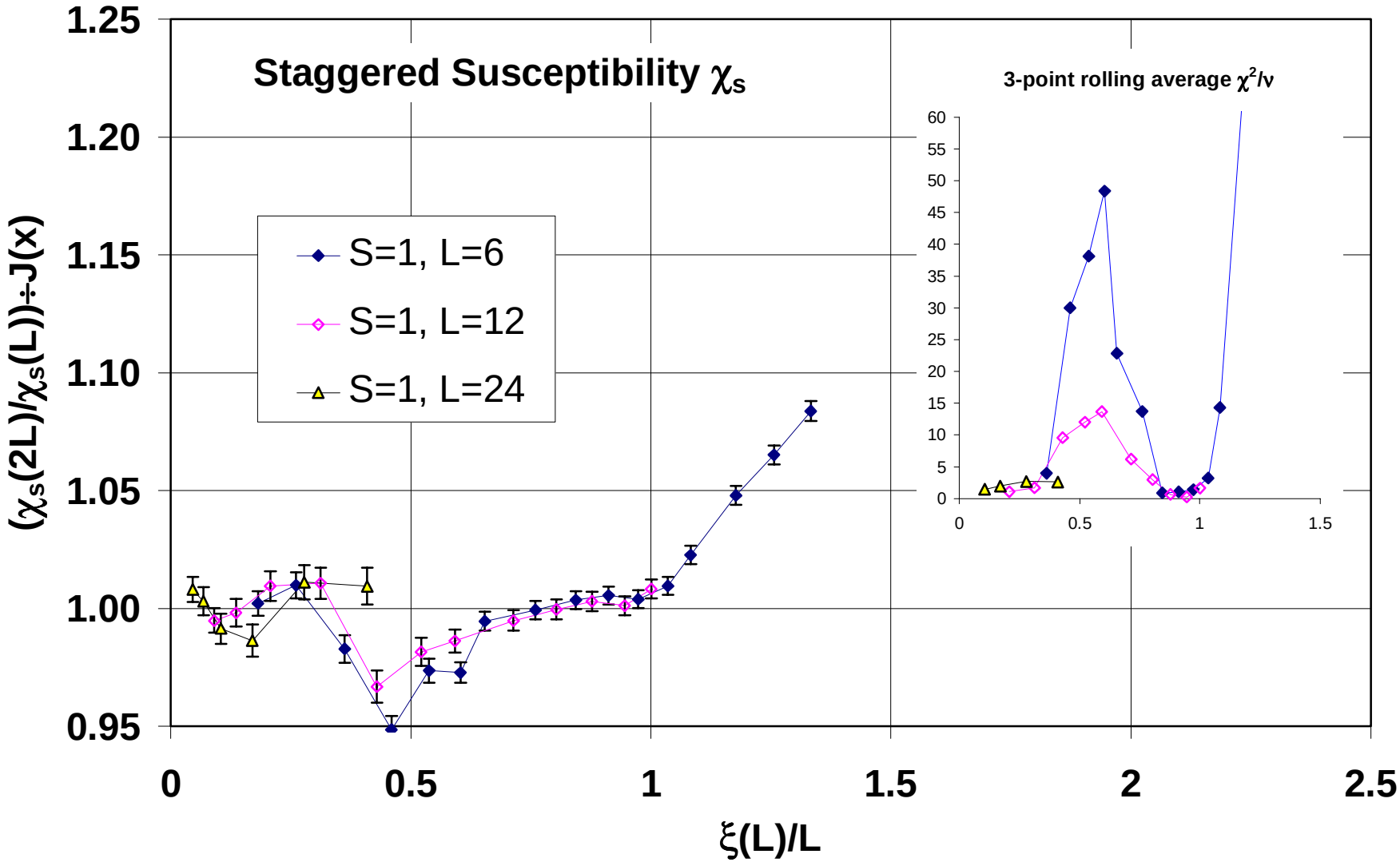
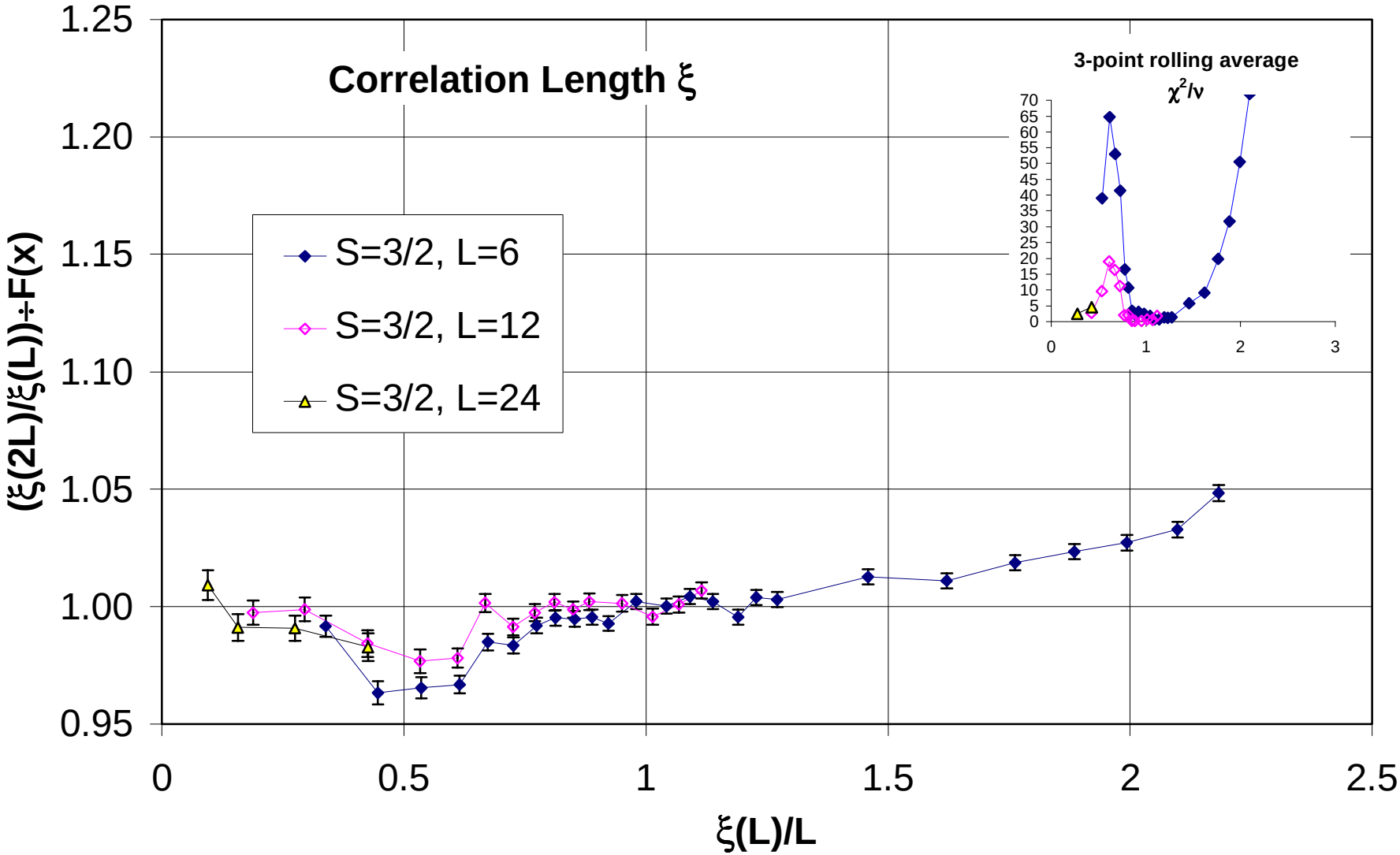
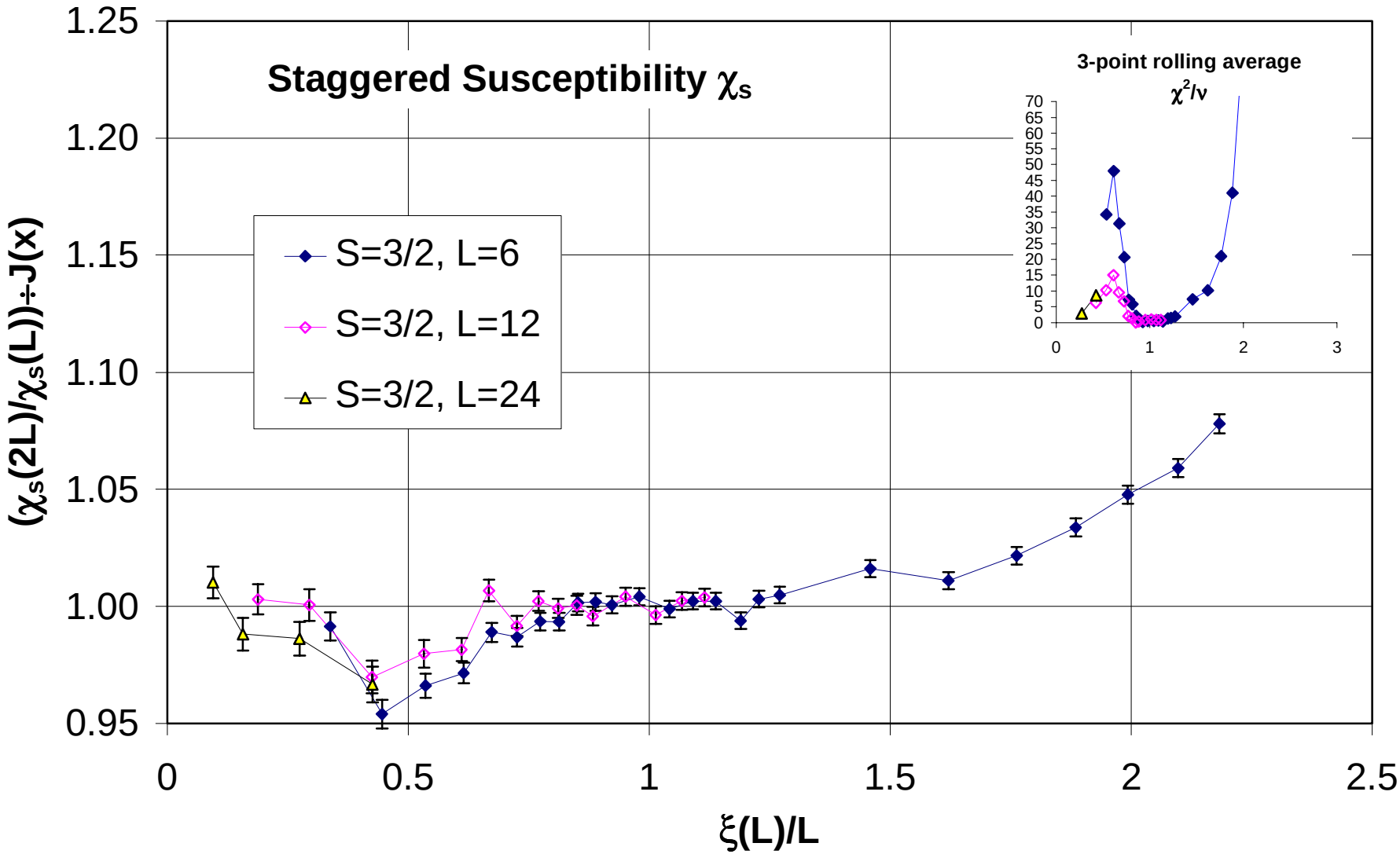
S=1, L=6
S=1, L=12
S=1, L=24
(ξ(2L)/ξ(L))÷F(x)
ξ(L)/L
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0.0
0.5
1.0
1.5
2.0
2.5
3-point rolling average χ²/ν
60
55
50
45
40
35
30
25
20
15
10
5
0
0
0.5
1
1.5


Staggered Susceptibility χ_s
3-point rolling average χ^2/ν
S=1, L=6
S=1, L=12
S=1, L=24
$(\chi_s(2L)/\chi_s(L))\div J(x)$
$\xi(L)/L$
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0
0.5
1
1.5
2
2.5
60
55
50
45
40
35
30
25
20
15
10
5
0
0
0.5
1
1.5


Correlation Length ξ
S=3/2, L=6
S=3/2, L=12
S=3/2, L=24
(ξ(2L)/ξ(L))÷F(x)
ξ(L)/L
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0
0.5
1
1.5
2
2.5
3-point rolling average
χ²/ν
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
0
1
2
3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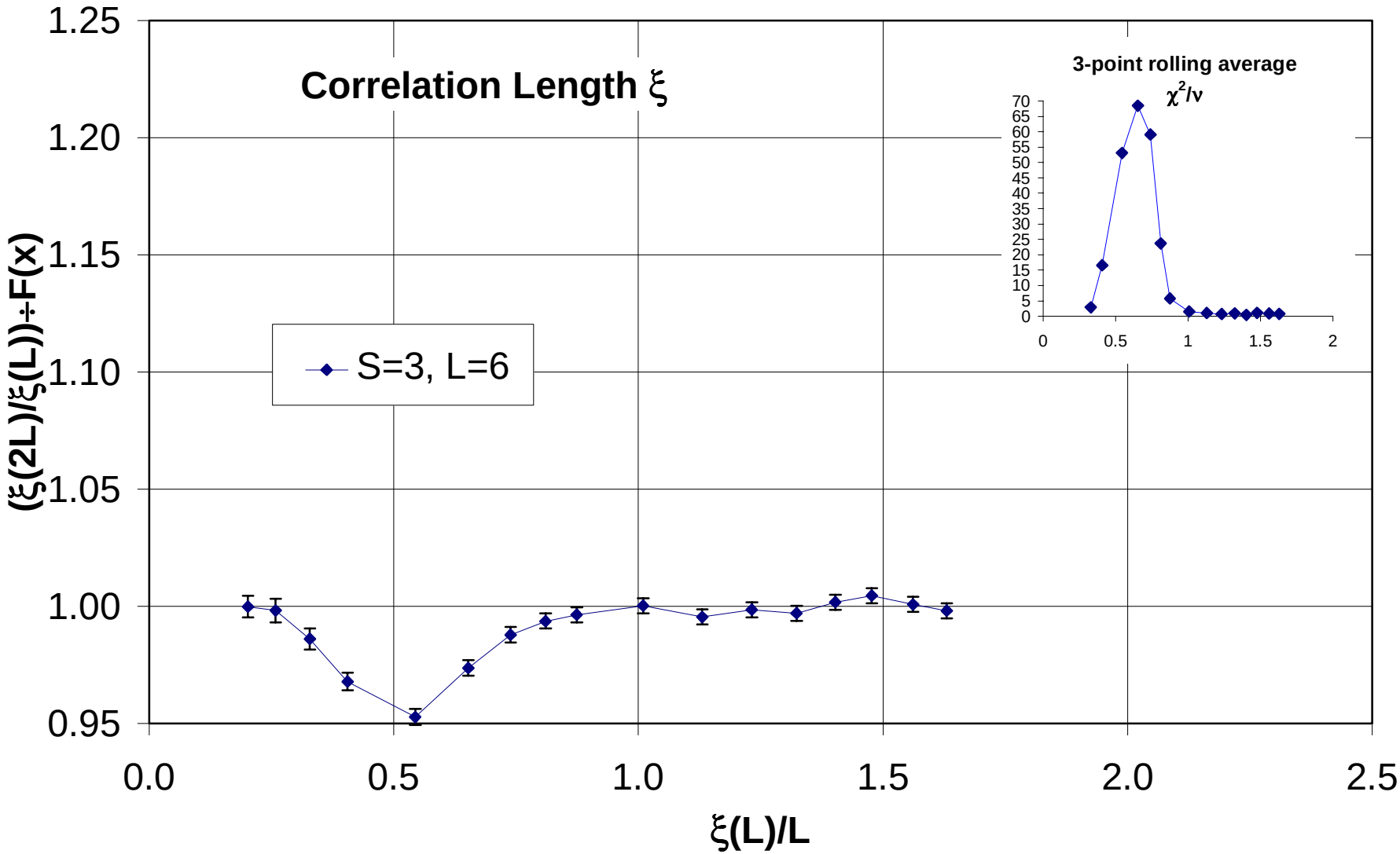
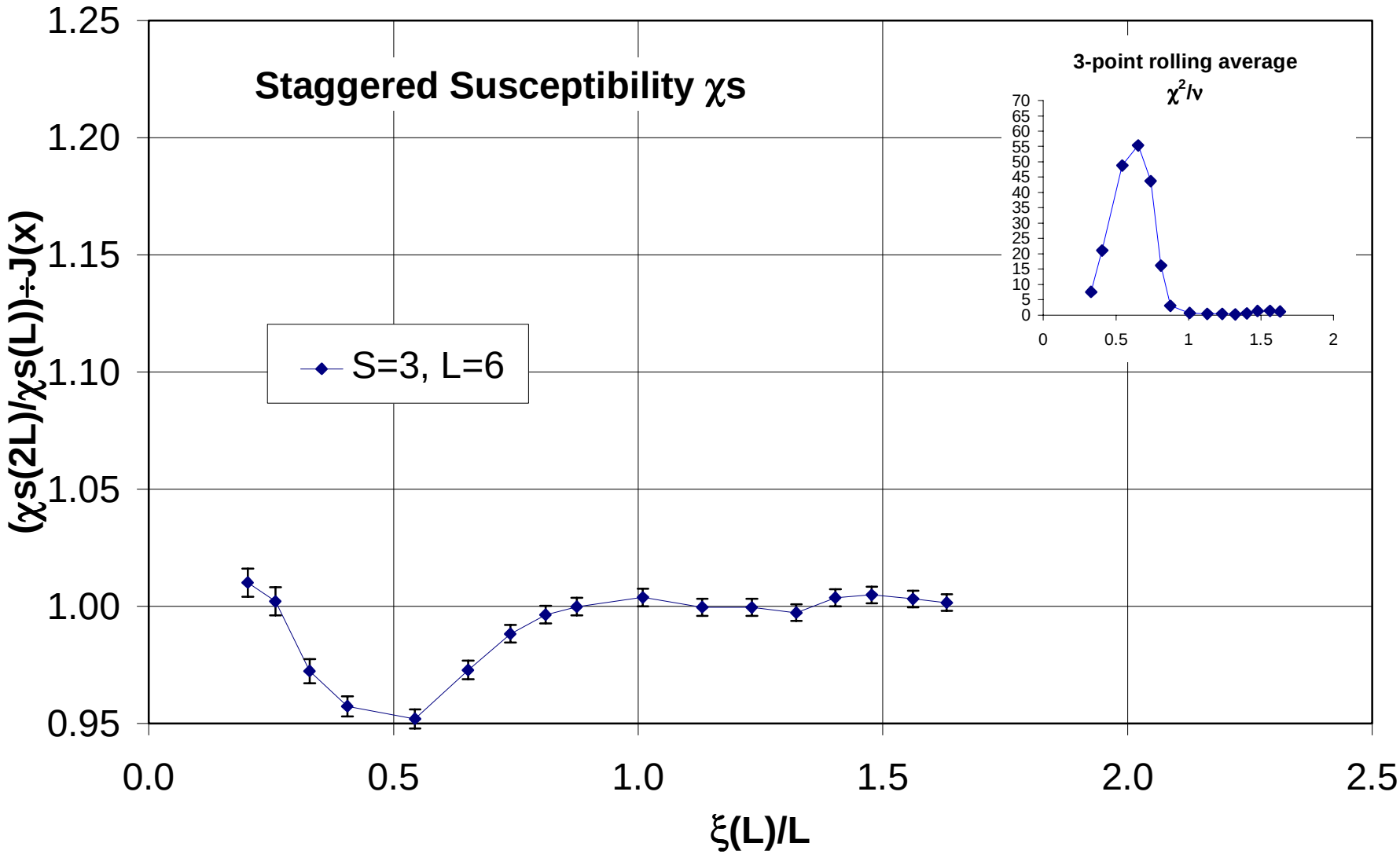
S=3/2, L=6
S=3/2, L=12
S=3/2, L=24
$(\chi_s(2L)/\chi_s(L))\div J(x)$
$\xi(L)/L$
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0
0.5
1
1.5
2
2.5
3-point rolling average
χ^2/ν
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
0
1
2
3

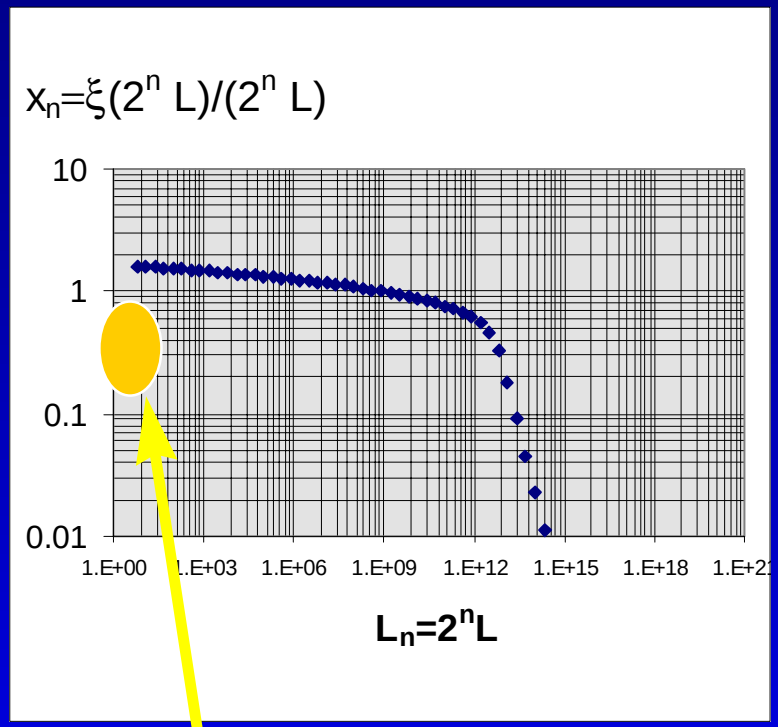

Correlation Length ξ
S=3, L=6
(ξ(2L)/ξ(L))÷F(x)
ξ(L)/L
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0.0
0.5
1.0
1.5
2.0
2.5
3-point rolling average
χ²/ν
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
0
0.5
1
1.5
2

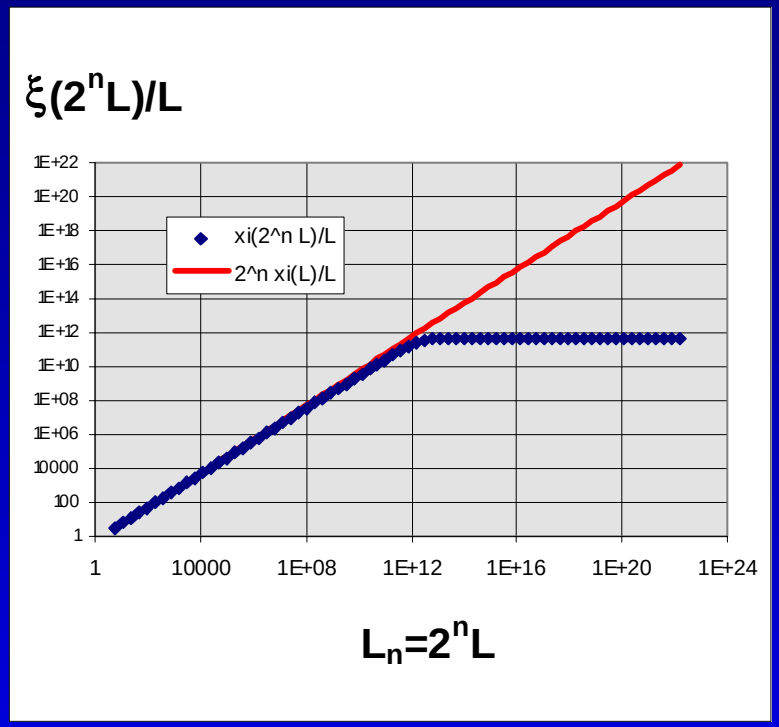

Staggered Susceptibility χs
S=3, L=6
(χs(2L)/χs(L))÷J(x)
ξ(L)/L
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0.0
0.5
1.0
1.5
2.0
2.5
3-point rolling average
χ²/ν
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
0
0.5
1
1.5
2

Extreme scaling

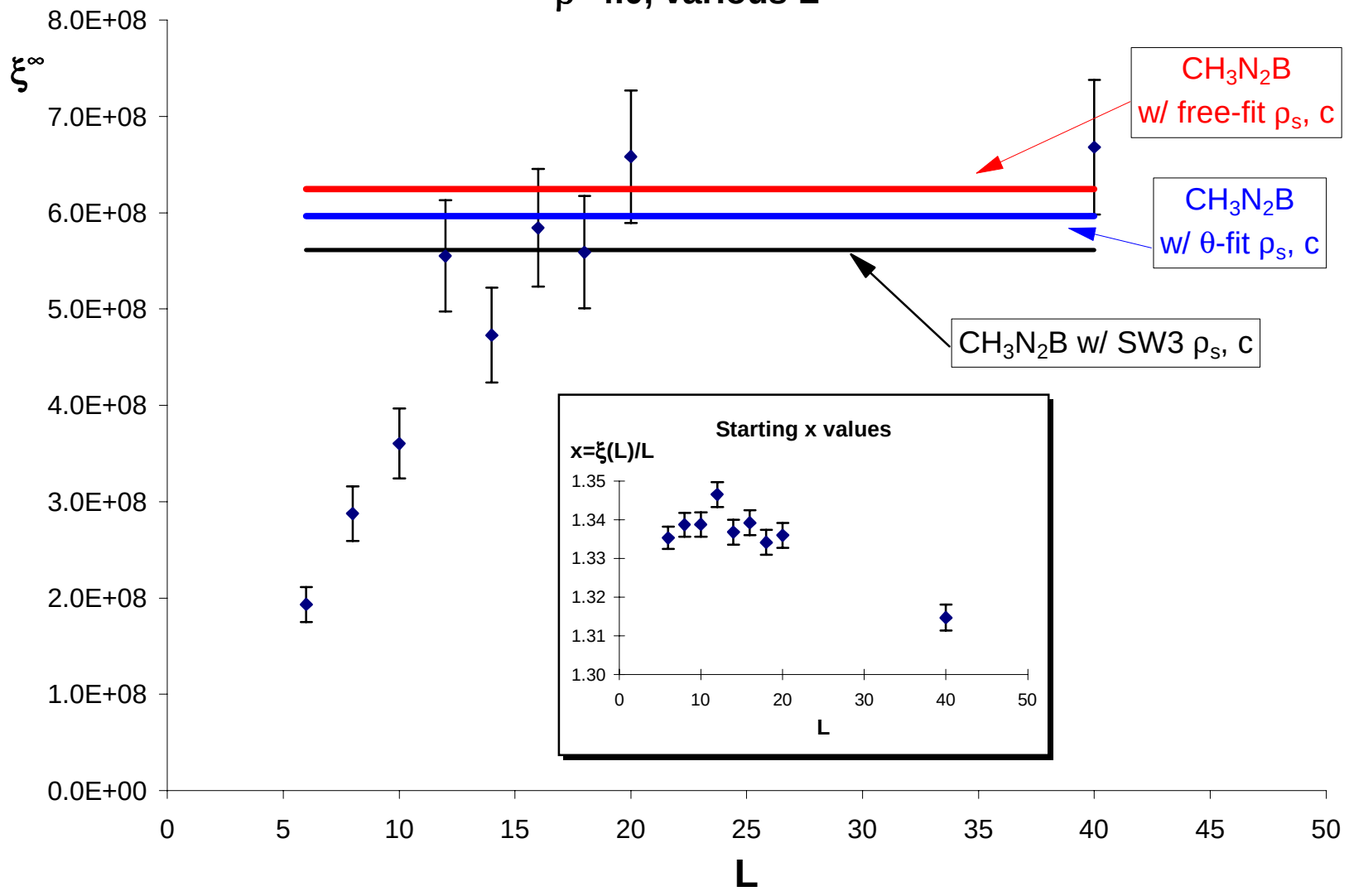
- Violations at high x get less severe with increasing spin S
- Iteration trajectory can avoid small-volume intermediate x regime
- Extrapolation to huge correlation lengths can be checked against CPT

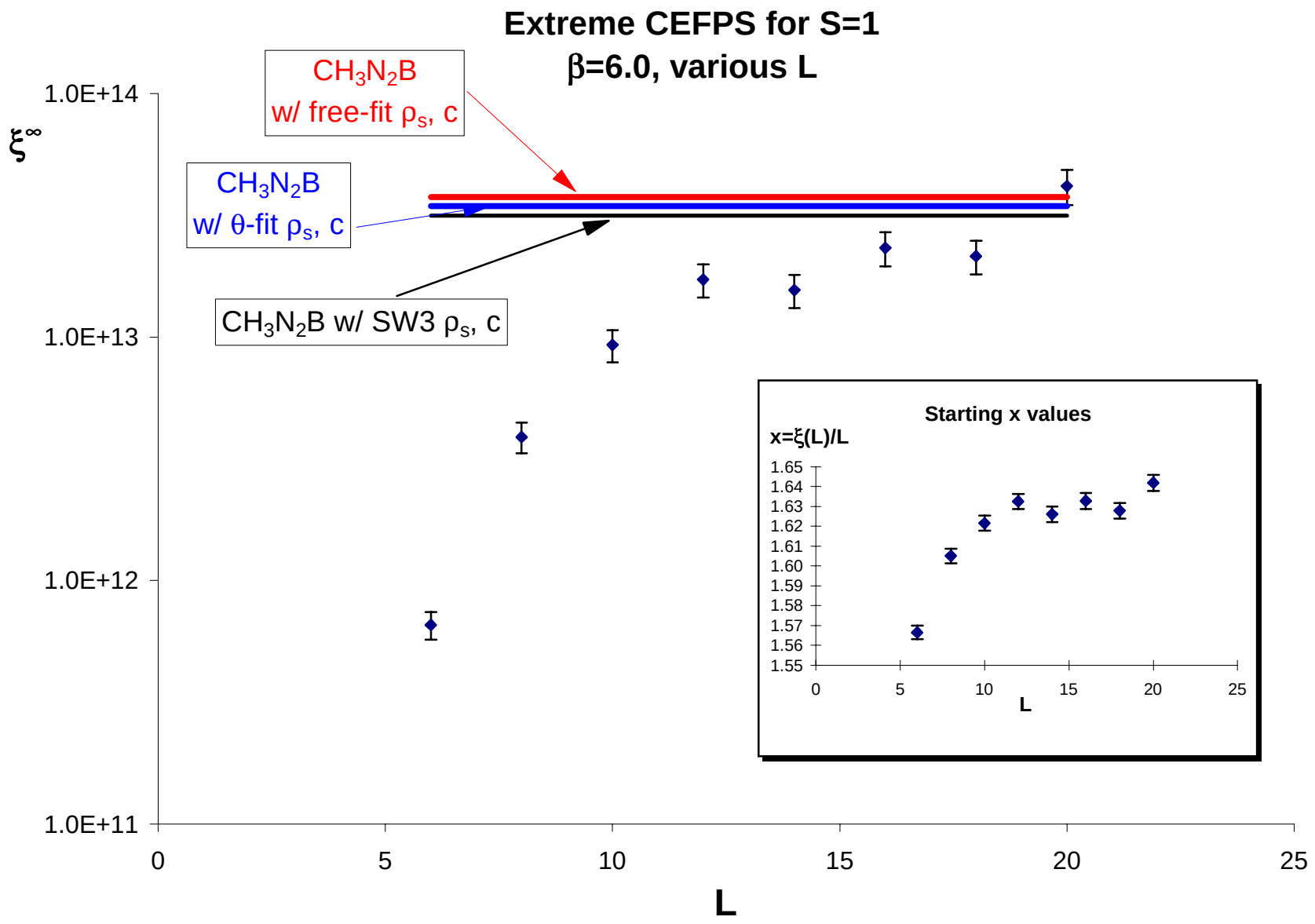
Trajectories for extreme scaling avoid violations

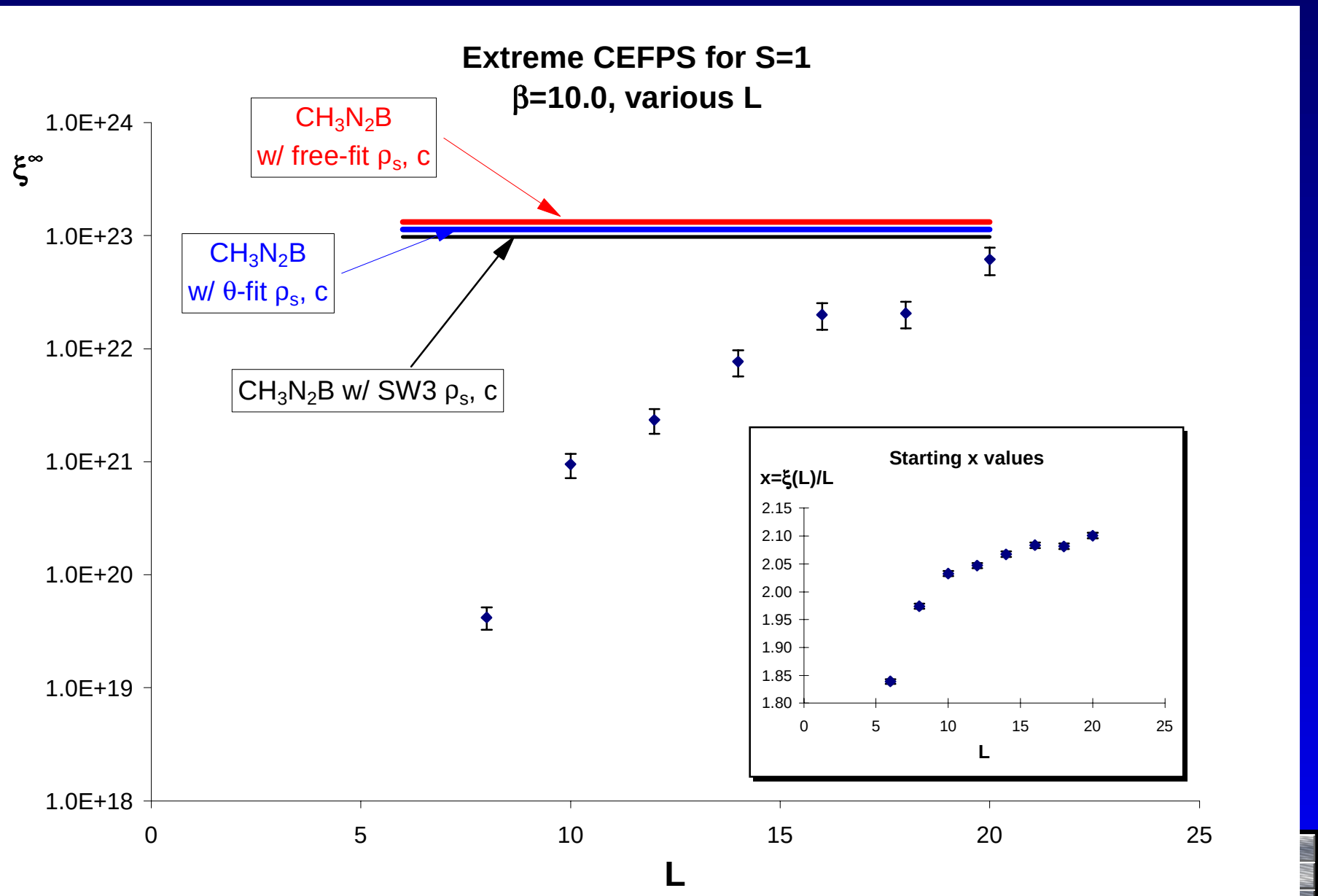




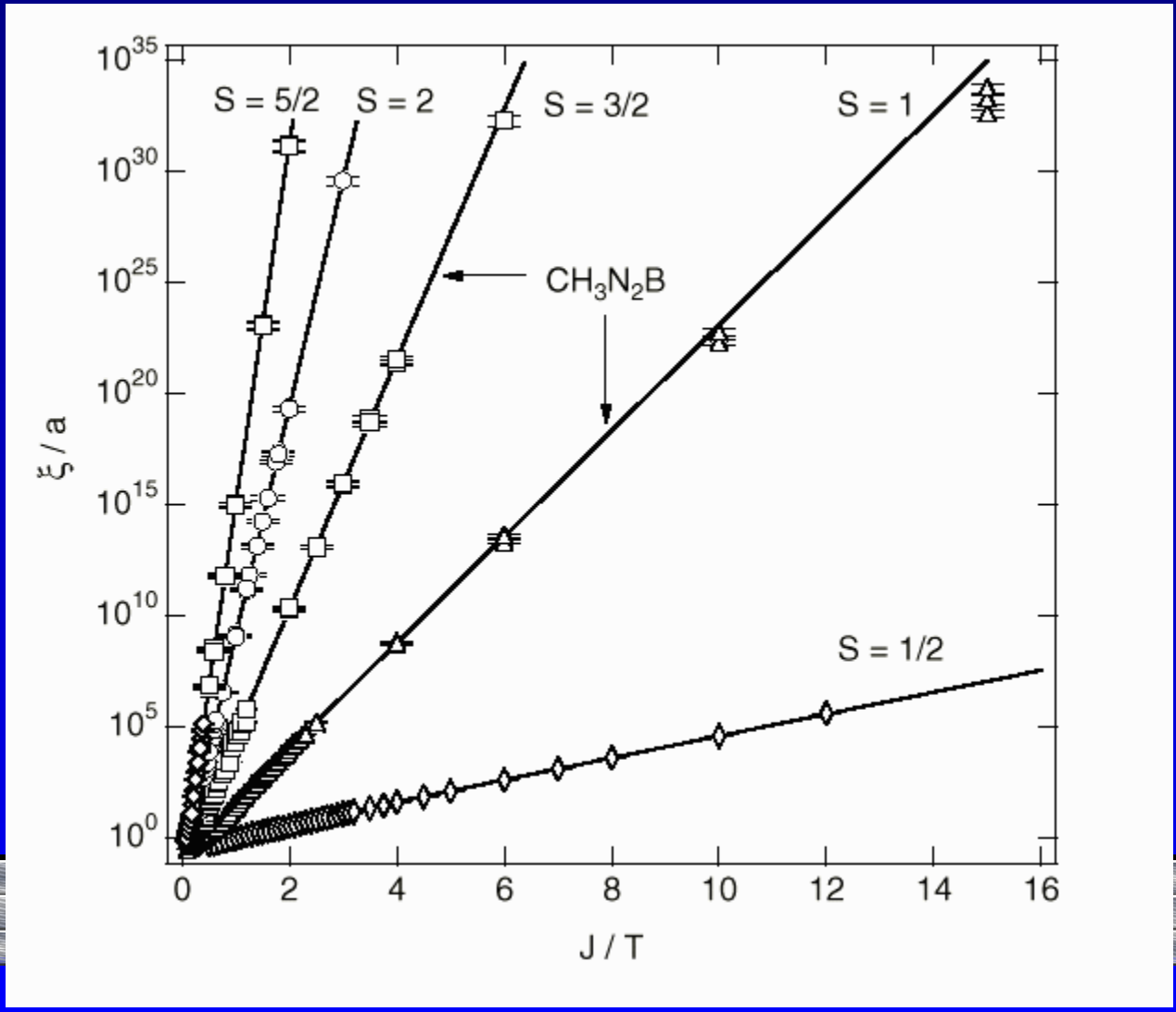
scaling violations at small volume, intermediate x


Extreme CEFPS for S=1
β=4.0, various L
ξ∞
8.0E+08
7.0E+08
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
0
5
10
15
20
25
30
35
40
45
50
L
CH3N2B
w/ free-fit ρs, c
CH3N2B
w/ θ-fit ρs, c
CH3N2B w/ SW3 ρs, c
Starting x values
x=ξ(L)/L
1.35
1.34
1.33
1.32
1.31
1.30
0
10
20
30
40
50
L


Extreme CEFPS for S=1
β=6.0, various L
CH3N2B
w/ free-fit ρs, c
CH3N2B
w/ θ-fit ρs, c
CH3N2B w/ SW3 ρs, c
ξ∞
1.0E+14
1.0E+13
1.0E+12
1.0E+11
0
5
10
15
20
25
L
Starting x values
x=ξ(L)/L
1.65
1.64
1.63
1.62
1.61
1.60
1.59
1.58
1.57
1.56
1.55
0
5
10
15
20
25
L


Extreme CEFPS for S=1
β=10.0, various L
CH3N2B
w/ free-fit ρs, c
CH3N2B
w/ θ-fit ρs, c
CH3N2B w/ SW3 ρs, c
ξ∞
1.0E+24
1.0E+23
1.0E+22
1.0E+21
1.0E+20
1.0E+19
1.0E+18
0
5
10
15
20
25
L
Starting x values
x=ξ(L)/L
2.15
2.10
2.05
2.00
1.95
1.90
1.85
1.80
0
5
10
15
20
25
L

Vanishing scaling violations enable extreme scaling

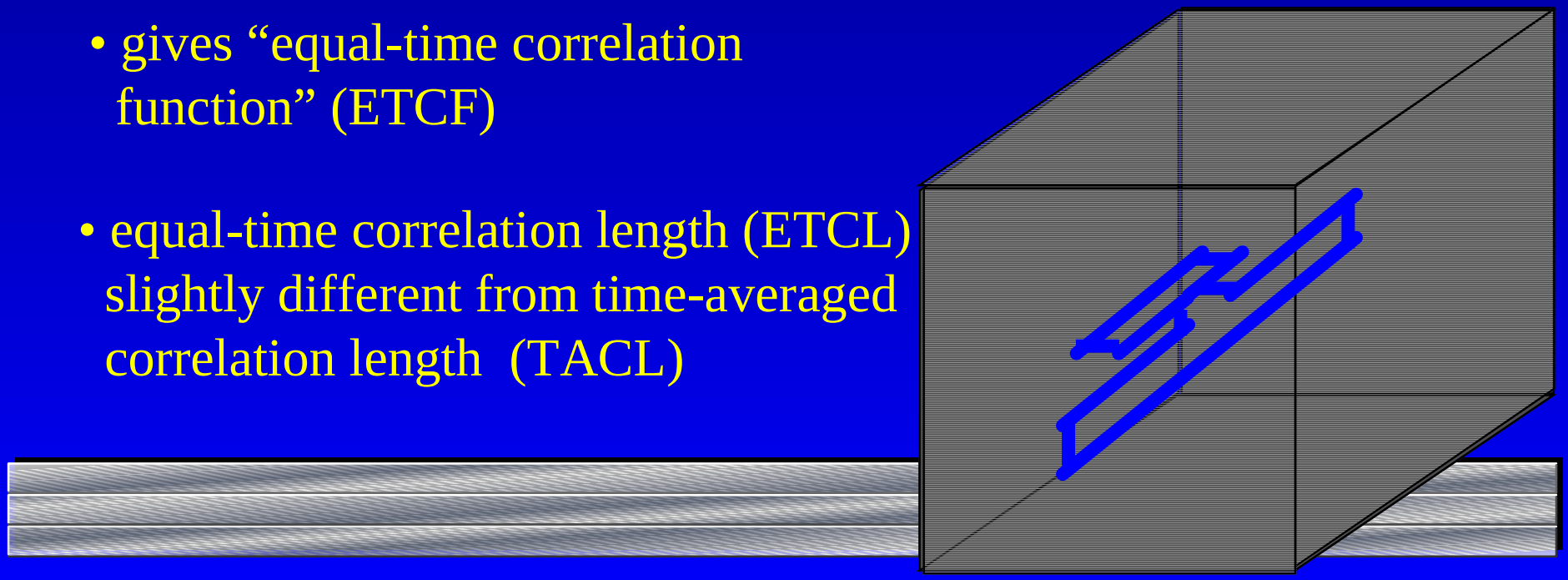


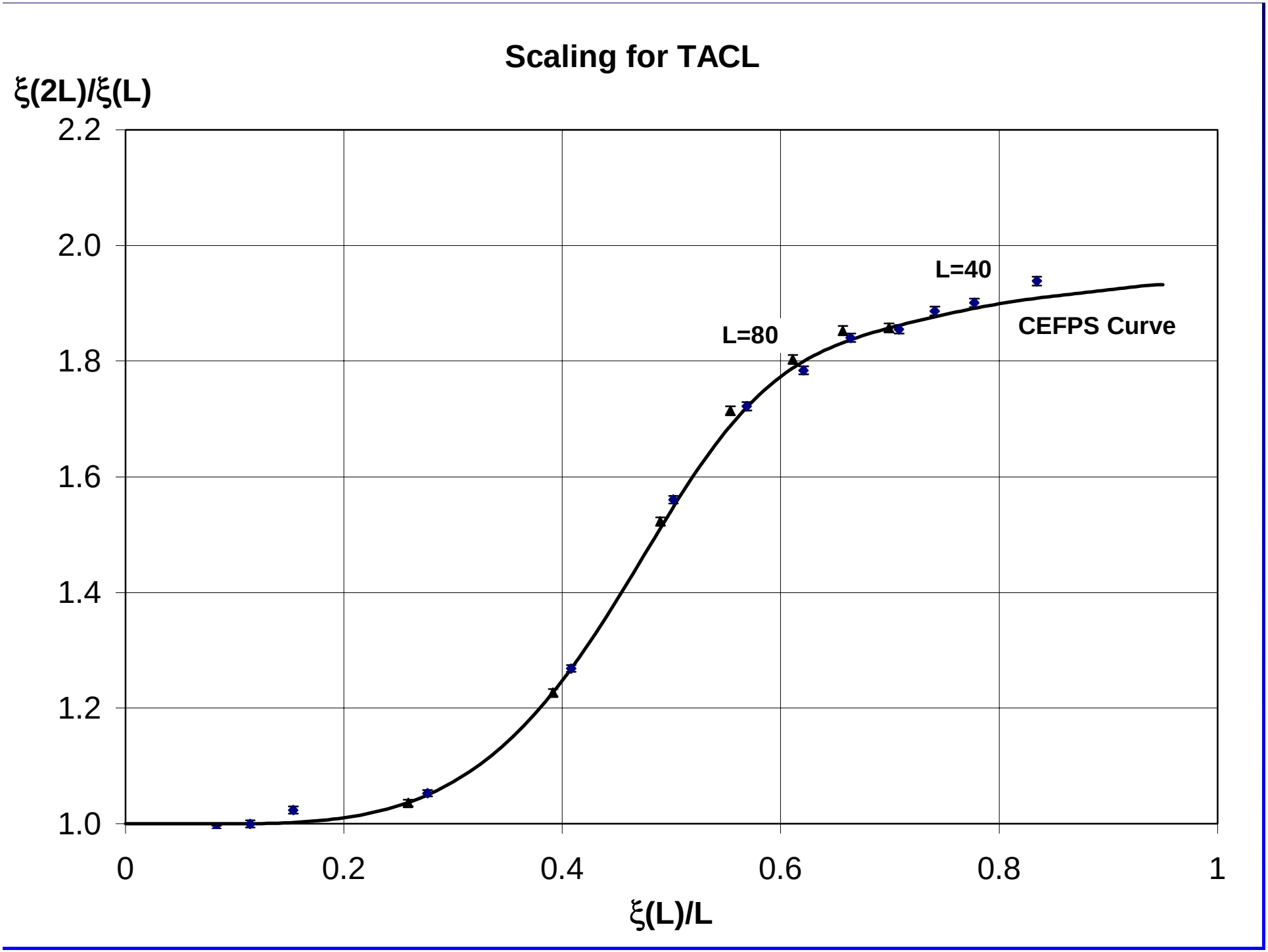
Alternative to TACF: measure correlations within a time slice

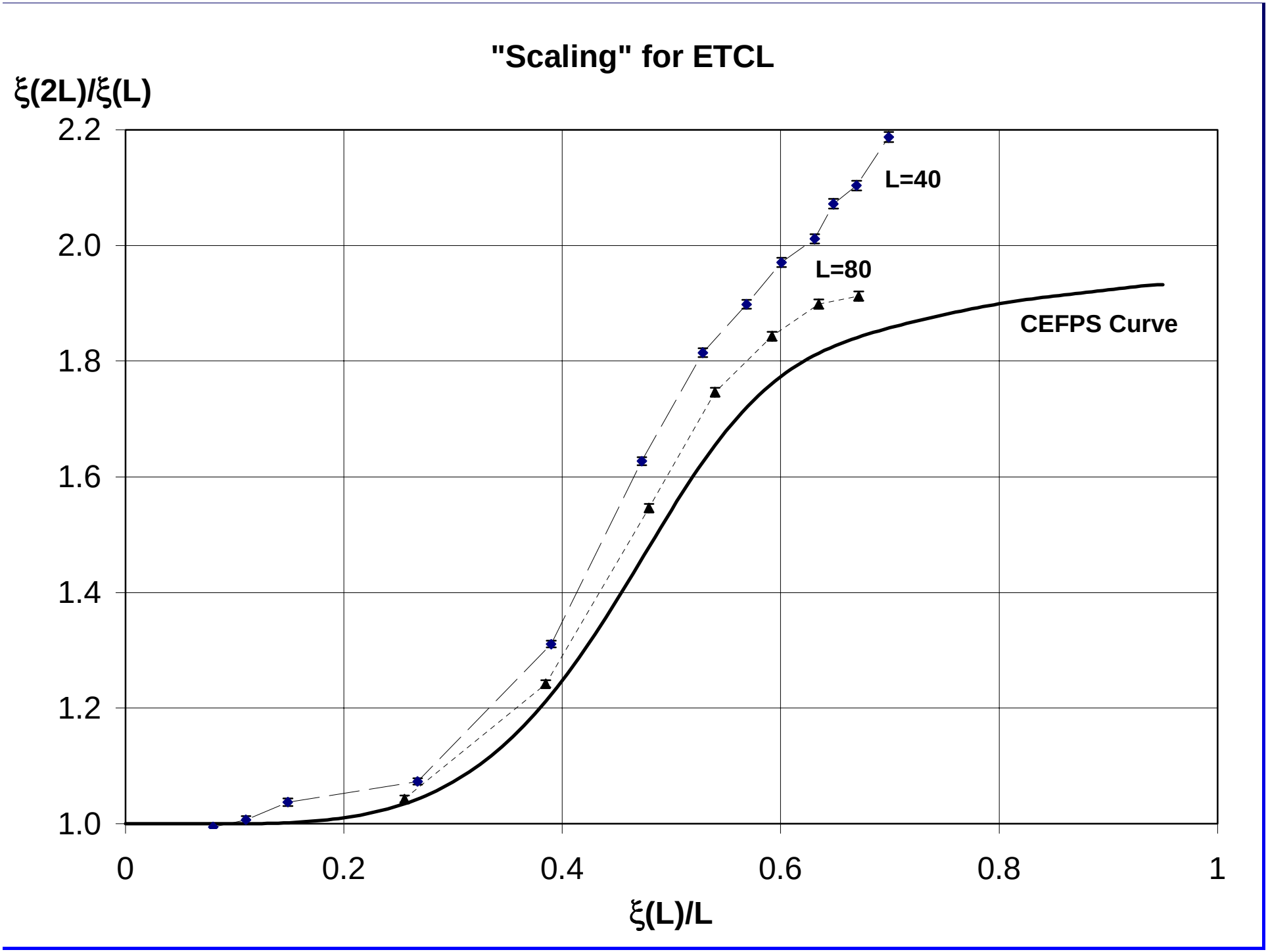
$$\widehat{G}_{\text{Wolff}}(r) = \frac{\frac{1}{|C|}\sum_{\vec{\mathbf{x}}\in\mathbf{C}}^{*} S_s^z(\vec{\mathbf{x}}) S_s^z(\vec{\mathbf{x}}+\vec{\mathbf{r}})}{|C|}$$

$* \leftrightarrow \vec{\mathbf{r}}\cdot\hat{\tau} = 0$ measure only within a time slice

- gives "equal-time correlation function" (ETCF)
- equal-time correlation length (ETCL) slightly different from time-averaged correlation length (TACL)




Scaling for TACL
ξ(2L)/ξ(L)
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0
0.2
0.4
0.6
0.8
1
ξ(L)/L
L=40
L=80
CEFPS Curve


"Scaling" for ETCL
ξ(2L)/ξ(L)
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0
0.2
0.4
0.6
0.8
1
ξ(L)/L
L=40
L=80
CEFPS Curve

Scaling enables extraordinary calculation

- Scaling violations appear in two regimes:
  - ⇨intermediate x : predicted in large N limit
  - ⇨high x: rapidly reduced as S increases
- Correlation length and susceptibility show similar trends
- High-S AFHM allows extreme scaling
- ETCL has large violations compared to TACL

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1 Stochastic Integration

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4 Cluster algorithms for classical models

5 Quantum Monte Carlo

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8 Finite-size scaling

9 More about the correlation length

10 Survey of other applications