Suggested Session:
Simulation of Quantum Systems

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32f

Monte-Carlo Simulations of Fermions on Quasiperiodic Chains. P. M. GRANT,* Materials Institute (IIM), Nat. Auto. U. México (UNAM). — We have studied the statistical mechanics of the half-filled 1D spinless fermion model (or, equivalently, the spin-1/2 Heisenberg chain), and the half-filled 1D Hubbard model on a chain lattice where the nearest neighbor transfer integral is chosen to follow a Fibonacci sequence from site to site. The world line, or checkerboard, method was the computational basis of the simulation. We find qualitative behavior similar to earlier studies on random-exchange quantum spin chains,[1] and discuss in detail the effect of quasiperiodicity on long range correlations at low temperature.

*On sabbatical leave from IBM Almaden Research Center, San Jose, CA. USA.

[1] H.-B. Schüttler, D. J. Scalapino and P. M. Grant, Phys. Rev. B35, 3461 (1987).

Prefer Standard Session

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THE QUESTION

How do the properties of quantum chains with quasi–periodic coupling compare to those with random and purely periodic interactions?

$$|f(x+\tau_\varepsilon)-f(x)| \leqq \varepsilon$$
$$-\infty < x < \infty;\ \varepsilon \geqq 0$$

$$f(x) = \sum_n A_n e^{-i\lambda_n x}$$

where $\{\lambda_n\}$ are denumerable, with at least one member an irrational

Random exchange effects in antiferromagnetic quantum spin chains: A Monte Carlo study

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We have carried out Monte Carlo studies of a random-exchange antiferromagnetic spin-$\frac{1}{2}$ chain. For systems with XY-like (anisotropic) and with Heisenberg (isotropic) coupling, our results confirm the existence of a disorder-induced low-temperature (T) divergence in the long-wavelength S^z-S^z susceptibility χ which was previously predicted by real-space renormalization-group (RSRG) treatments. Over the finite temperature range studied, these results are consistent with a $1/(T\ln^2 T)$ behavior of χ, and hence in qualitative agreement with the RSRG results. As in the XY-Heisenberg regime, we also find a disorder-induced enhancement of the low-T susceptibility for a system with Ising-like exchange coupling which, over the finite temperature range studied, is again consistent with RSRG results. However, there are inconsistencies between the RSRG predictions in the Ising-like regime at very low temperatures, and the exact results for the random-exchange Ising chain and the low-temperature behavior of χ in the Ising-like regime may in fact be more complicated than predicted by RSRG. Finally, we also present results for the antiferromagnetic susceptibility and structure factor. For both Heisenberg and Ising-like systems, we find that disorder suppresses the long-range antiferromagnetic correlations at low T.

I. INTRODUCTION

During recent years, one-dimensional (1D) disordered spin systems have received a great deal of theoretical attention.[1–6] Experimentally, this was stimulated, in part, by the unusual magnetic properties of certain tetracyanoquinodimethane (TCNQ) compounds.[7–10] For example, quinolinium $(TCNQ)_2$ is found to exhibit at low temperatures T a power-law divergence in the magnetic susceptibility,[7,10]

$$\chi \propto 1/T^{\alpha} , \tag{1}$$

where α is typically less than but close to unity.

The magnetic behavior of this material is commonly described as that of a quantum spin-$\frac{1}{2}$ chain[10] with a random and possibly anisotropic antiferromagnetic exchange coupling as given by the Hamiltonian

$$H=\frac{1}{2}\sum_{1\le j\le N} J_j(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y+\gamma\sigma_j^z\sigma_{j+1}^z) . \tag{2}$$

Here, N denotes the number of lattice sites, σ_j^x, σ_j^y, and σ_j^z are the Pauli matrices for a spin at a lattice site j, J_j denotes the exchange coupling between spins at sites j and $j+1$, and γ is the (site-independent) exchange anisotropy ratio. The J_j's are assumed to be randomly and independently distributed according to some probability distribution $P(J)$ [where $P(J)\equiv 0$ for $J<0$].

Several real-space renormalization-group (RSRG) treatments of (1) have been proposed which indeed indicate the possibility of a *disorder-induced* low-T divergence of the long-wavelength magnetic susceptibility.[3–6] Namely, for the Heisenberg case[3–6] ($\gamma=1$) and in the XY-like regime,[5] $0\le\gamma<1$, the RSRG results predict that in the presence of disorder the susceptibility exhibits a divergence of the form (1), however, with an exponent α that is slowly temperature dependent. More specifically, it was suggested that for $0\le\gamma\le 1$ and $T\to 0$, χ (as obtained from numerical solution of the RSRG equation) can be represented as[5]

$$\chi=A/[T\ln^m(T/T_0)] , \tag{3}$$

where the exponent m is close to 2 and only weakly dependent on γ or the distribution of exchange coupling. These results are in contradiction to an earlier cluster approximation treatment of the Heisenberg case ($\gamma=1$),[1] which predicted that $\chi(T)$ diverges at $T=0$ only if the distribution $P(J)$ has a corresponding singularity at $J=0$. They are consistent, however, with exact solutions of the XY case ($\gamma=0$), where it can be shown that, for arbitrarily weak disorder in the J_j's, χ exhibits a low-T divergence of the form (3) with an exponent $m=2$,[11,12] even for nonsingular distributions $P(J)$. Based on these results, it has been conjectured[5] that the $1/(T\ln^2 T)$ law might be the universal $T\to 0$ behavior of χ for $0\le\gamma\le 1$ and for arbitrary nonsingular distributions $P(J)$. However, the RSRG treatments[3–5] involve uncontrolled approximations so that a test of their reliability by comparison to numerical Monte Carlo (MC) results is of interest.

Aside from the long-wavelength properties, the effects of randomness on the long- and short-range antiferromagnetic (AF) order are of interest. Exact solutions[13–15] show that in the absence of disorder, the Hamiltonian (1) in the XY Heisenberg regime ($0\le\gamma\le 1$) exhibits a gapless excitation spectrum and AF spin-spin correlations at

THE MODEL

Spinless Fermions on a Chain

$$H = \sum_i [t_i(c_i c^*_{i+1} + h.c.) + V_i(n_i - 1/2)(n_{i+1} - 1/2)]$$

or

Anisotropic Heisenberg Chain

$$H = 0.5 \sum_i J_i(\sigma^x_i \sigma^x_{i+1} + \sigma^y_i \sigma^y_{i+1} + \gamma_i \sigma^z_i \sigma^z_{i+1})$$

$$J_i = t_i, \quad \gamma_i = V_i/2t_i$$

MEASUREMENTS

$$\rho(l, \tau=0) = (2NL)^{-1} \sum_{j=1}^{2L} \sum_{i=1}^{N} n_{i,j}\, n_{i+l,j}$$

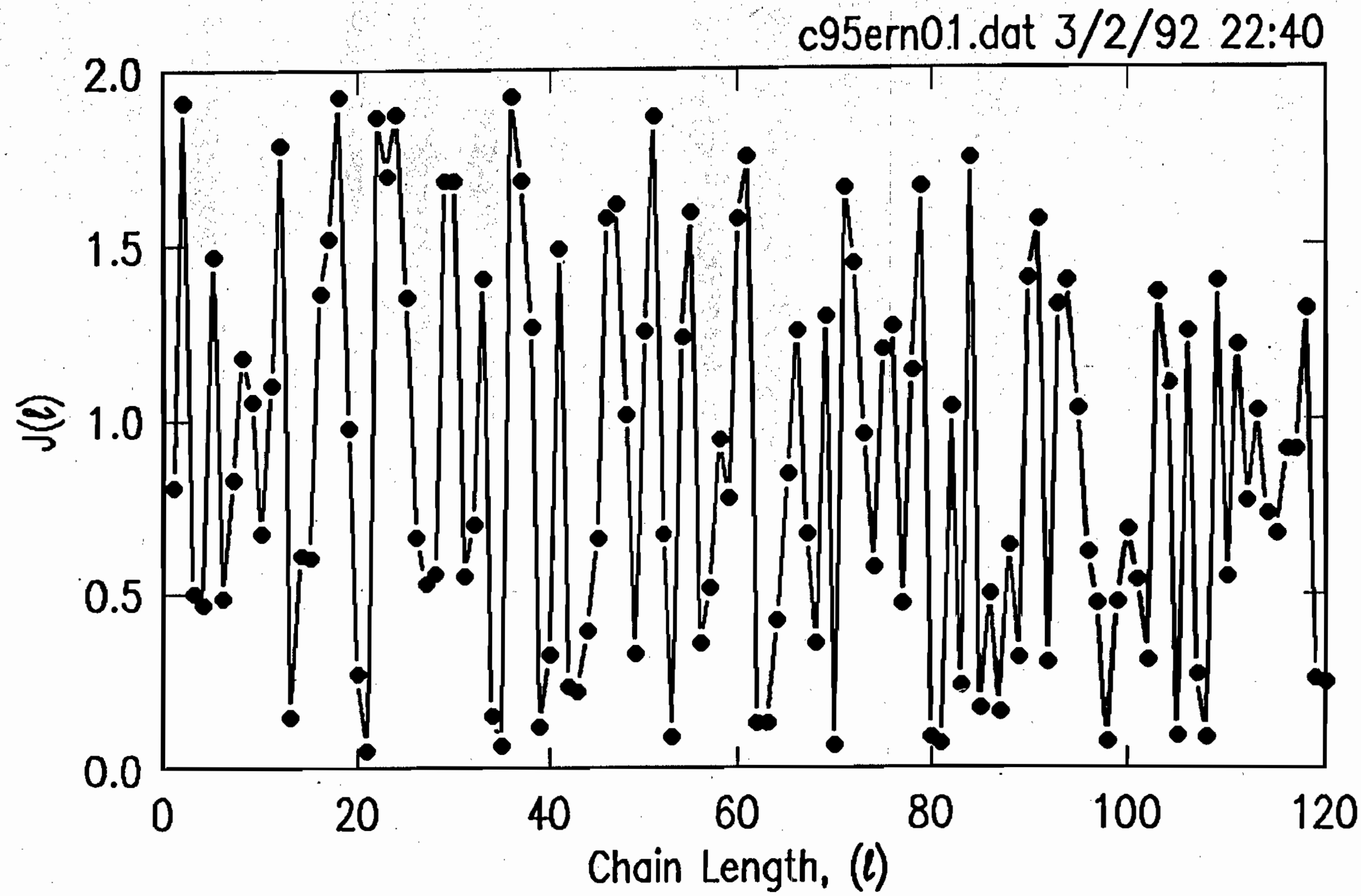
$$S(q, \tau=0) = \sum_{l} e^{-iql} \rho(l, \tau=0)$$

$$\langle J \rangle = 1$$

$$\gamma = 1$$

Monte–Carlo Parameters

- Chain Lengths: 4 – 378 sites
- Temperature: $\beta = 1/kT \geqq 12$
- I–time Slice: $\Delta\tau \leqq 0.1$
- $\rho(\ell,\tau=0)$, $S(q,\tau=0)$ measured as function of chain length
- 10,000 – 20,000 measurements, each separated by 5 equilibration passes
- Performed on UNAM Cray Y–MP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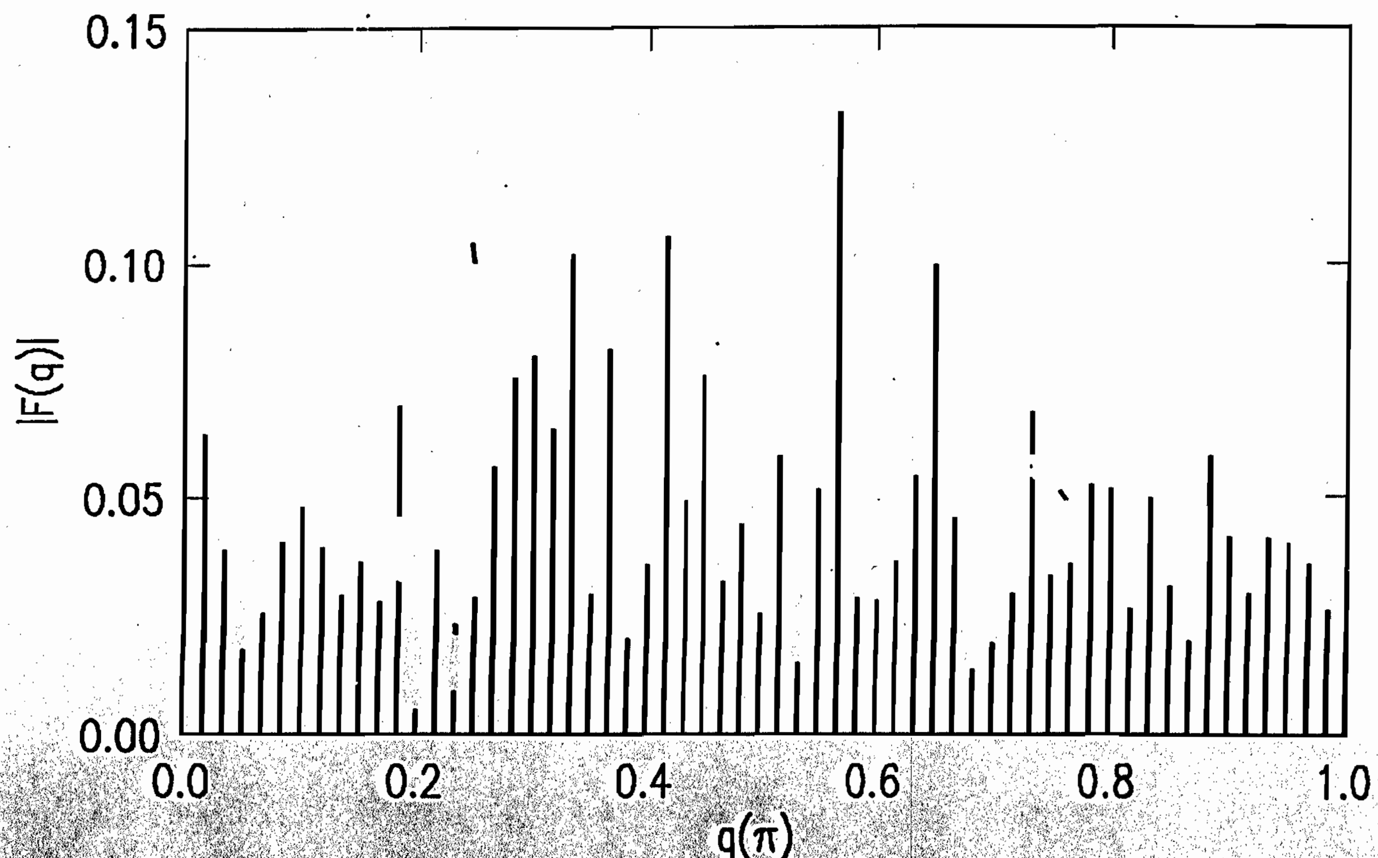
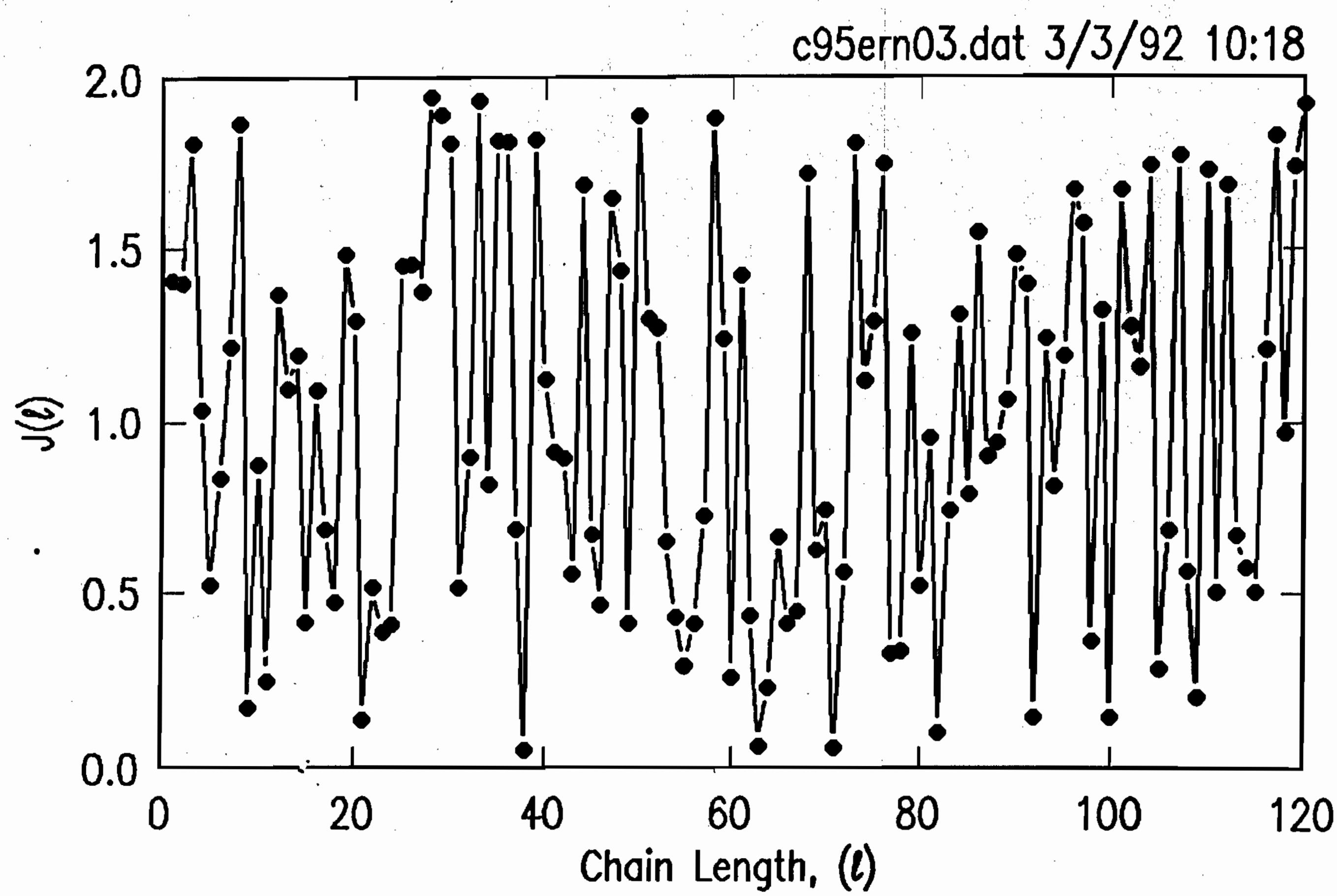
J(ℓ)
0
20
40
60
80
100
120
Chain Length, (ℓ)


0.15
0.10
0.05
0.00
|F(q)|
0.0
0.2
0.4
0.6
0.8
1.0
q(π)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J(ℓ)
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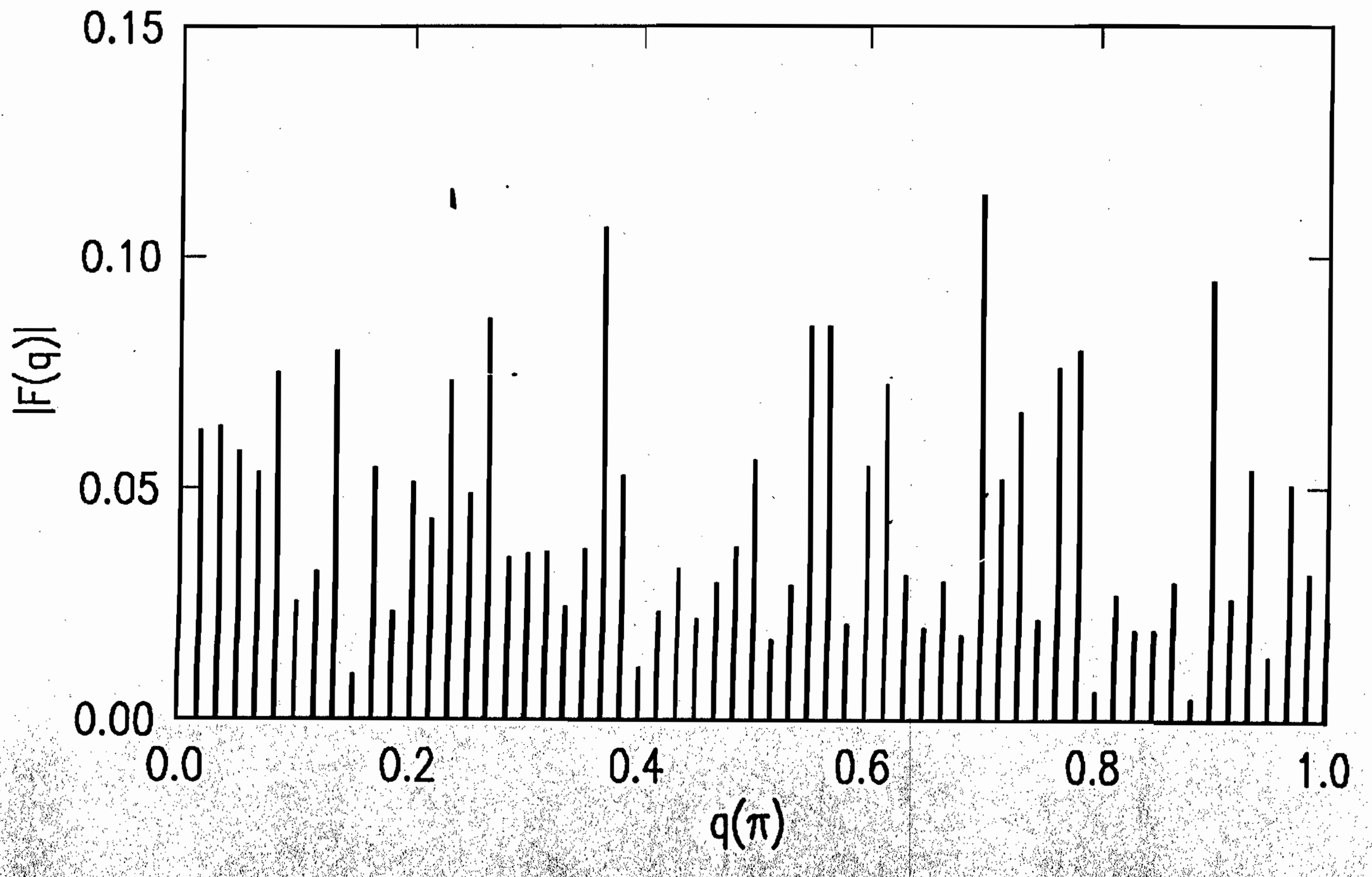
80
100
120
Chain Length, (ℓ)


0.15
0.10
0.05
0.00
|F(q)|
0.0
0.2
0.4
0.6
0.8
1.0
q(π)

Fibonacci Chains

Definition

$$G_n = G_{n-1}|G_{n-2}, \; n = 3,4,5,\ldots,\infty$$

Where $G_1 = a$, $G_2 = ab$

Ex. $G_6 = abaababaabaab$ $(N = 13)$

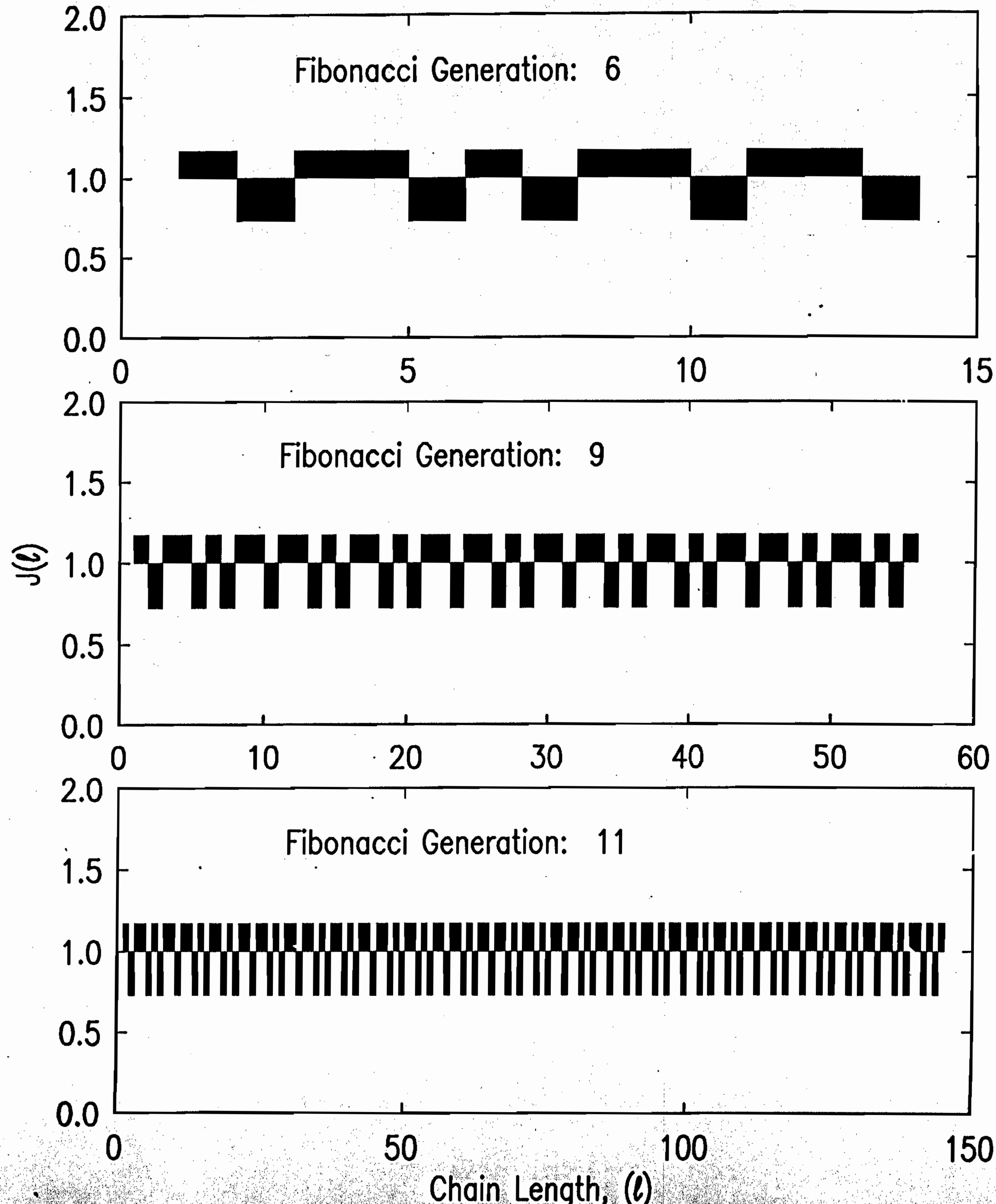
$$\lim_{n\to\infty} N_a(G_n)/N_b(G_n) = \tau = (1+\sqrt{5})/2 = 1.618\ldots$$

Choice of Exchange Constants

Take $J_a = c\tau J_b$, subject to $\langle J \rangle = J$,

Then $J_b = \tau J/[(1+c)\tau-1]$,

Where c is a "strength" parameter.


Fibonacci Generation: 6
Fibonacci Generation: 9
Fibonacci Generation: 11
J(ℓ)
Chain Length, (ℓ)
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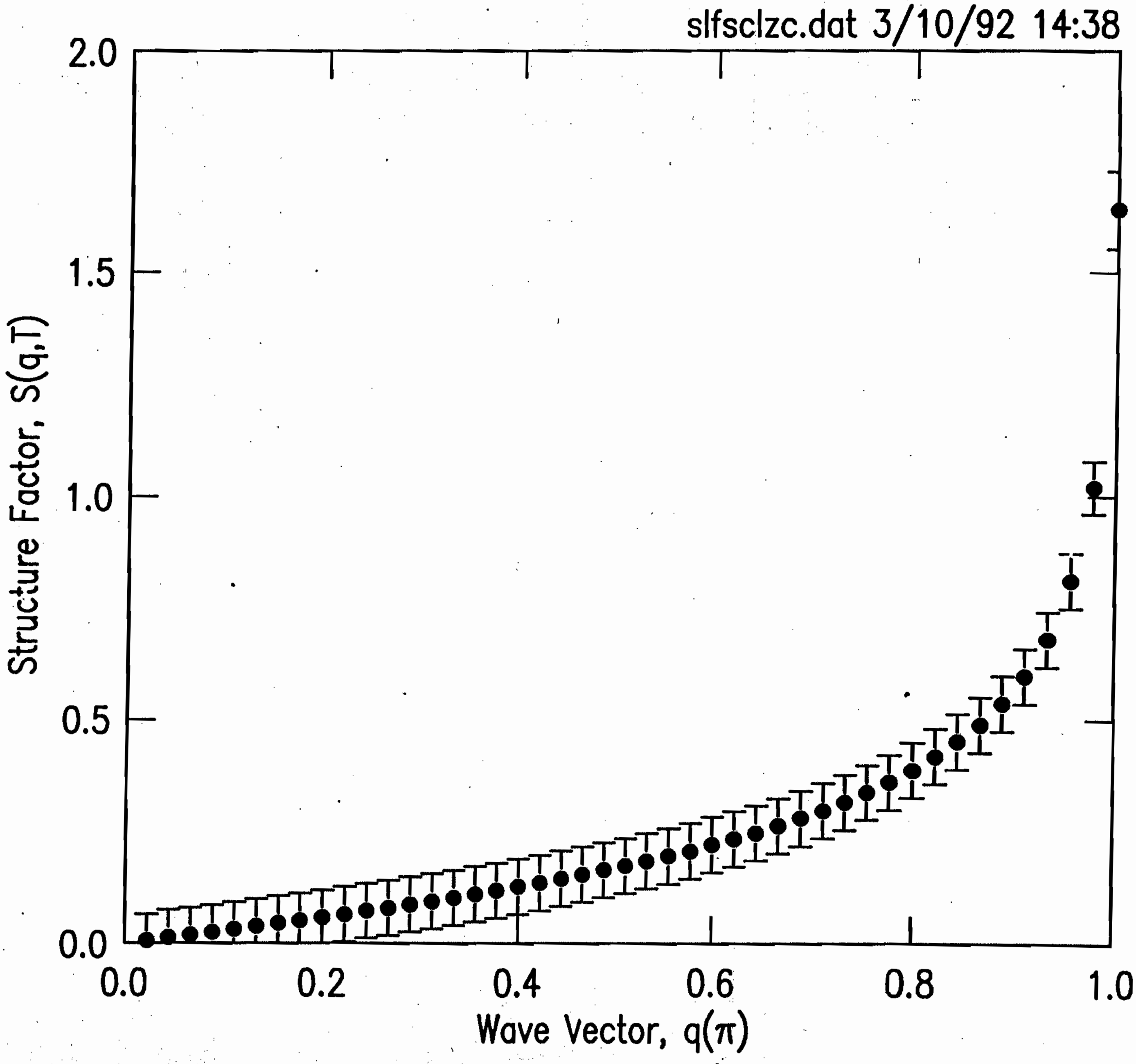
1.5
1.0
0.5
0.0
0
5
10
15
10
20
30
40
50
60
50
100
150

PERIODIC J

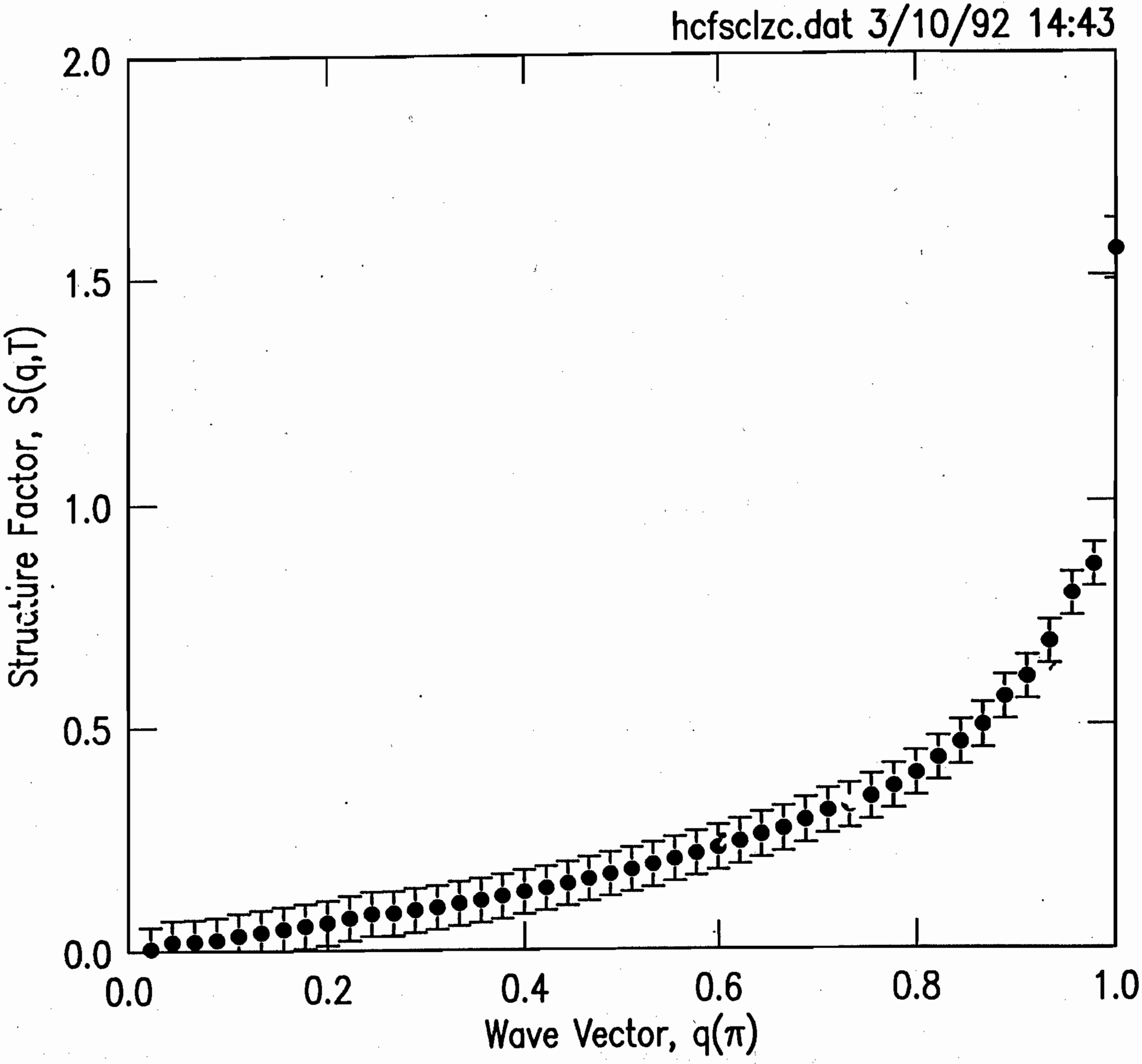
N = 90

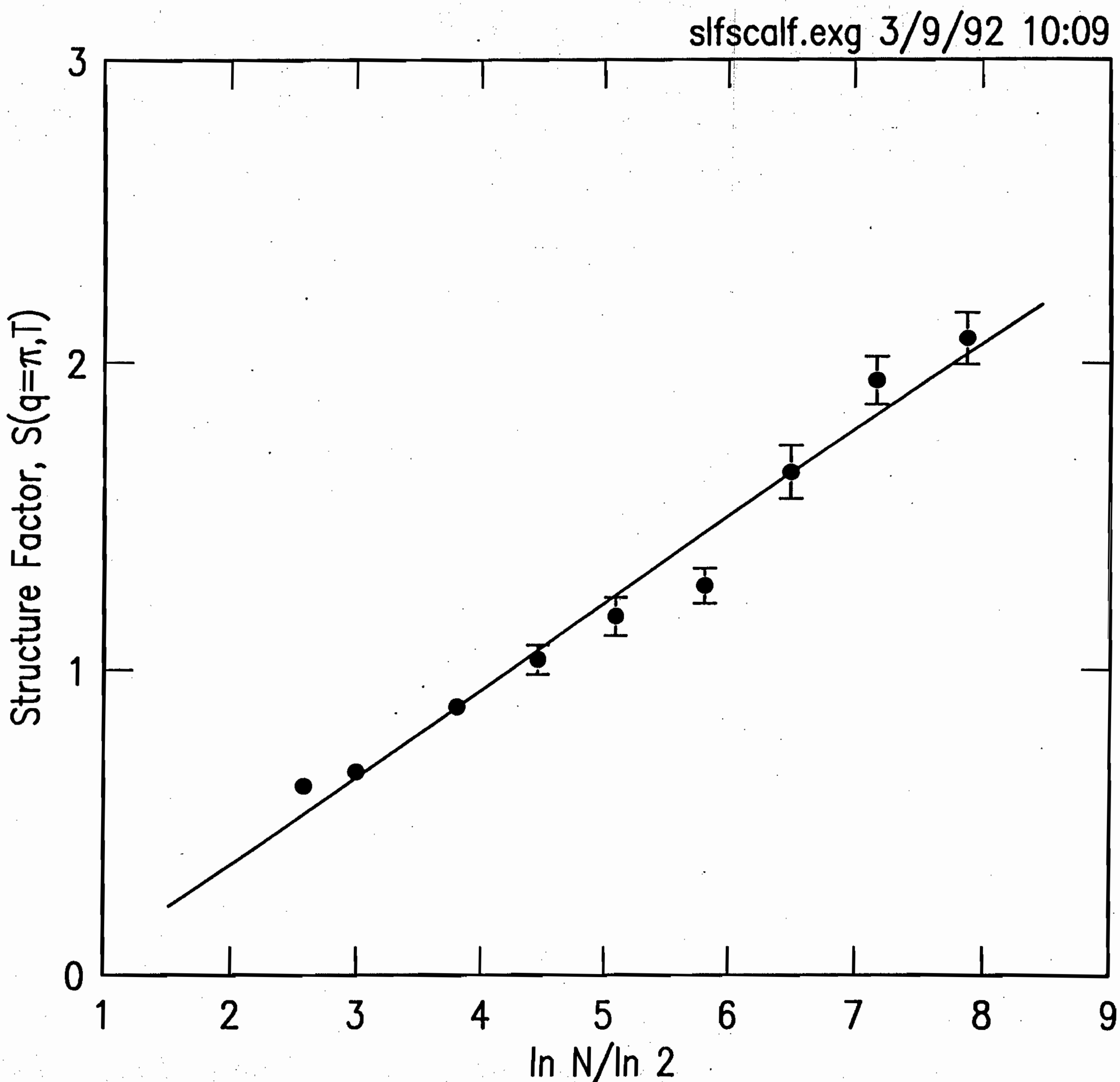


FIBONACCI J

$N_G = 10$

$N_{chain} = 90$





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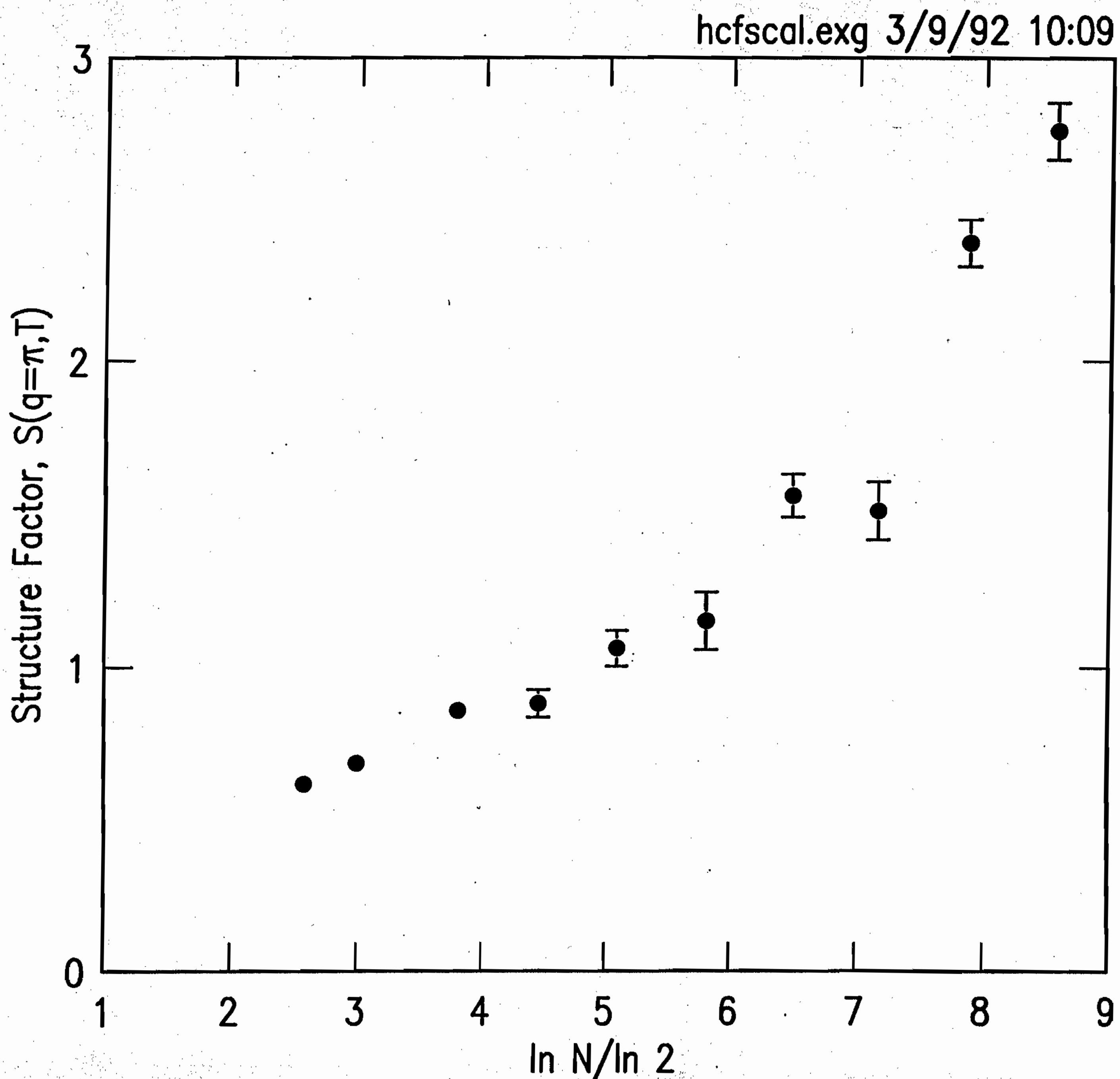
Structure Factor, S(q=π,T)
0
1
2
3
1
2
3
4
5
6
7
8
9
ln N/ln 2



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Structure Factor, S(q=π,T)
ln N/ln 2
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Summary

- Present Conclusions
  - LRO appears to exist in weakly quasi-periodic spin-1/2 isotropic Heisenberg chains.
- Future Agenda
  - Examine $\chi(q \to 0, T)$ for evidence of power law divergence.
  - Investigate strongly quasi-periodic case.