ABSTRACT SUBMITTED
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1D Systems -- Theory

Effect of Impurities and Disorder on 1D Spinless Fermions. **P. M. GRANT**, IBM Research Laboratories, San Jose-- Using Monte Carlo simulation techniques[1] applied to a 1D system of interacting spinless fermions, we have measured the effect of impurities and disorder on the density-density correlation function and associated structure factor for this model. We varied both the nearest neighbor Coulomb repulsion, V, and the hopping energy, t, randomly from site to site up to values ±0.5 about their mean. We report results in the parameter space $V \geq 2t$, where charge density wave formation is known to occur for 1D spinless fermions on a half-filled lattice with uniform V and t and show how the $q = 2k_F$ divergence in the unperturbed structure factor is modified by disorder.

[1] J. E. Hirsch, R. L. Sugar, D. J. Scalapino and R. Blankenbecler, Phys. Rev. B26, 5033 (1982).

(X) Prefer Standard Session

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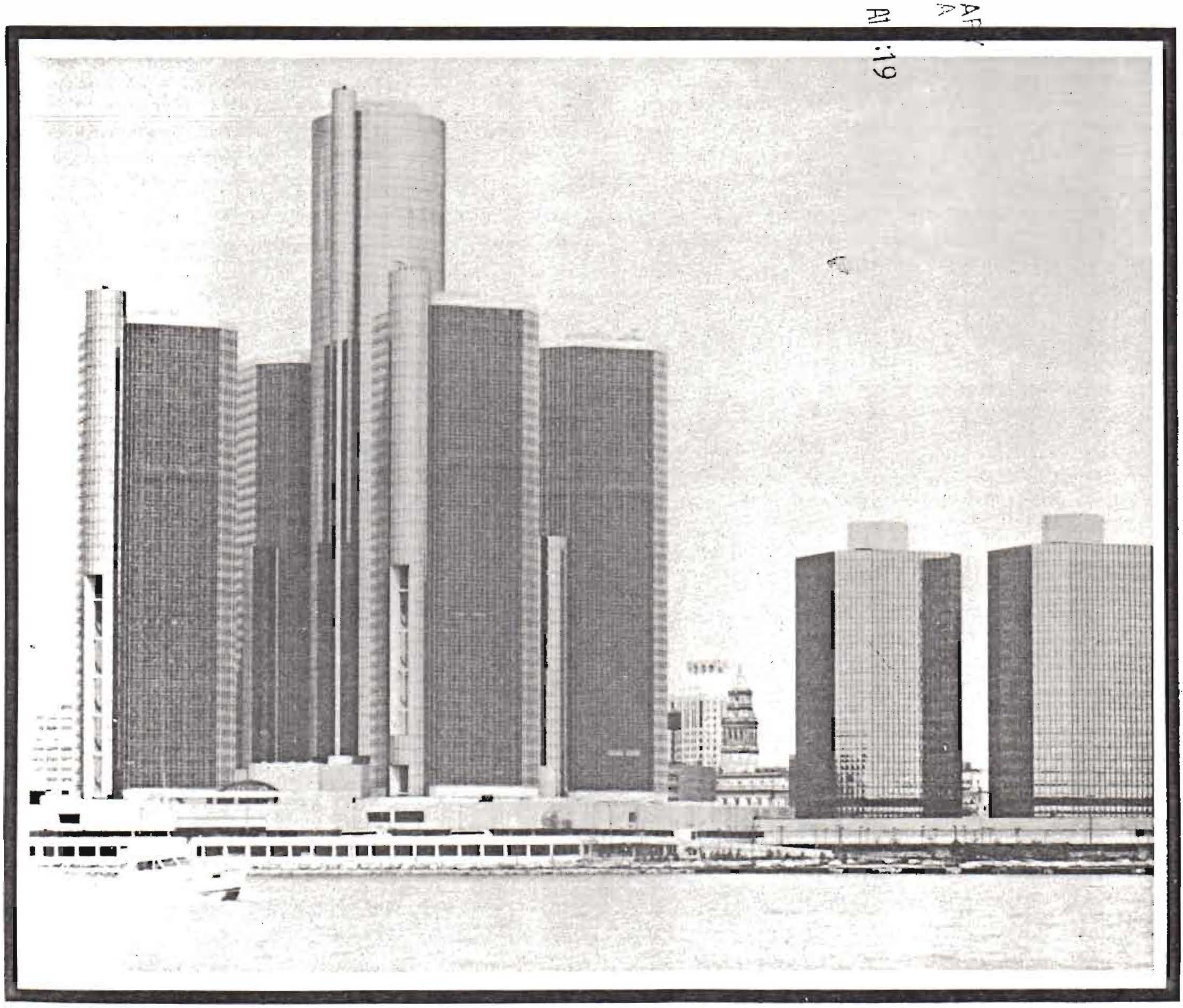

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lattice scattering is dominant as expected, and that the Q1D mobility may be larger than bulk mobilities if the transverse dimensions are large enough. The limitations of the model and the implications of the results will be discussed.

14:48

EH 3 Physical Properties of Ultrathin Pt Wires,* A.C. SACHAROFF and R.M. WESTERVELT, Harvard U. -- A systematic investigation of the structural and electrical properties of ultrathin, drawn, single Pt wires and multifilamentary Pt yarn with filament diameters to 10 nm is reported. Single ultrathin wires produced by the same drawing process were studied for possible effects of electronic localization and interaction on their electronic transport at low temperatures.[1,2] Our principle conclusions are: 1) The drawing process does not introduce quantities $\gtrsim 3\%$ of the Ag matrix or of other metallic impurities into Pt filaments. 2) Ultrathin Pt filaments remain polycrystalline at the smallest diameter <100 nm with very small grain size ~ 10 nm. 3) Unusually large values of resistivity $\rho > 100\ \mu\Omega$-cm found in Pt filaments are produced by structural disorder rather than by atomic impurities.

*Supported by NSF grant no. DMR81-21563.

[1] A.C. Sacharoff, R.M. Westervelt, and J. Bevk, Phys. Rev. B26, 5976 (1982).

[2] A.C. Sacharoff, R.M. Westervelt, and J. Bevk, Phys. Rev. B, to be published.

15:00

EH 4 Quantum Freeze-out of Carriers in Semimetallic and Semiconducting Thin Wires. V.K. ARORA, King Saud Univ. and H.N. SPECTOR, I.I.T.--A semimetal-semiconductor transition is predicted to take place due to the quantum freeze-out of carriers in semimetallic thin wires. In cylindrical wires, the onset of semiconducting behavior is expected to occur at a critical radious $R^* = 2.405\,\hbar/(2M\Delta)^{\frac{1}{2}}$ where M is the reduced mass of the electron-hole system and Δ is the overlap of the conduction and valence bands. For wires of radii smaller than R*, the electrical conductivity of the thin wire will decrease exponentially with temperature because of the presence of an effective energy gap arising from the size quantization of the electron and hole energies in the wire.

15:12

EH 5 Hydrogenic Impurity States in a Quantum Well Wire. H.N. SPECTOR, I.I.T. and J. LEE, GTE. - We have performed a variational calculation of hydrogenic-like impurity binding energies in quantum well wires. The binding energy of the hydrogenic impurity has been calculated as a function of the transverse dimensions of the wire. It is found that the binding energy of the hydrogenic impurity increases as the ratio of the Bohr radius of the impurity in a bulk semiconductor to the transverse dimensions of the wire increases. To test the sensitivit of the binding energies to the trial wave function we have used in our calculations, we use a wave function of the same type to calculate the binding energies of hydrogenic impurities confined in a quasi-two dimensional quantum well as a function of well width and compare our results to those obtained by Bastard.[1].

1. G. Bastard, Phys. Rev. B24, 4714 (1981).

15:24

EH 6 Interband Optical Absorption in Thin Semiconducting Quantum Well Wires. H.H. HASSAN and H.N. SPECTOR, I.I.T. - We have calculated the optical absorption due to interband transitions between quantized subbands in the valence and conduction bands of thin semiconducting quantum well wires having a direct band gap Eg. The model used in the calculation assumes electron wave functions of the particle in a box type for motion perpendicular to the axis of the thin semiconducting wire. The threshold for the start of optical absorption due to interband transitions is shifted to shorter wave lengths as the cross-sectional area of the wire decreases. Above the threshold, the absorption is an oscillatory function of the photon energy for fixed transverse dimensions of the wire. The selection rules allows transitions only between those subbands in the conduction and valence bands which have the same set of quantum numbers. The absorption has peaks whenever the photon energy is such that transitions can take place between new pairs of subbands. This behavior is due to the energy dependence of the 1D density of states of the electron gas.

15:36

EH 7 Effect of Impurities and Disorder on 1D Spinless Fermions. P. M. GRANT, IBM Research Laboratories, San Jose-- Using Monte Carlo simulation techniques[1] applied to a 1D system of interacting spinless fermions, we have measured the effect of impurities and disorder on the density-density correlation function and associated structure factor for this model. We varied both the nearest neighbor Coulomb repulsion, V, and the hopping energy, t, randomly from site to site up to values ±0.5 about their mean. We report results in the parameter space $V \geq 2t$, where charge density wave formation is known to occur for 1D spinless fermions on a half-filled lattice with uniform V and t and show how the $q = 2k_F$ divergence in the unperturbed structure factor is modified by disorder.

[1] J. E. Hirsch, R. L. Sugar, D. J. Scalapino and R. Blankenbecler, Phys. Rev. B26, 5033 (1982).

15:48

EH 8 Hydrogenic Impurity States in Quantum Well Wires.* GARNETT W. BRYANT, McDonnell Douglas Research Laboratories, St. Louis, MO 63166.--The binding energies for the bound states of a hydrogenic impurity placed on the axis of a quantum well wire (QWW) are calculated using variational solutions to the effective mass equation. The QWW is a cylinder of GaAs surrounded by $Ga_{1-x}Al_xAs$. In a small wire the electrons leak out of the wire and behave as three-dimensional electrons in $Ga_{1-x}Al_xAs$. An abrupt crossover to one-dimensional behavior occurs when the wire radius becomes greater than the radial spread of the bound state. In this regime the binding energies are greatly enhanced and the wave functions are squeezed radially to fit the wire. In a large wire the bound electrons no longer interact with the wire boundary and they act as three-dimensional electrons in GaAs. Implications of the enhanced binding in QWW for recent calculations of the effect of ionized impurity scattering on electron mobility in QWW are considered.

*Research conducted under the McDonnell Douglas Independent Research and Development program.

16:00

EH 9 Electron Wave Functions in a 1-D Disordered System A. Hartstein, R. A. Webb, A. B. Fowler and J. J. Wainer IBM - T. J. Watson Research Center-- Extensive measurements have been made in the strong localization regime of narrow pinched accumulation layer MOSFET samples. The conductance behaves as $\sigma = \sigma_0 \exp\text{-}(T_0/T)^{-n}$, with n = 1/2 for low gate voltages and n = 1/3 for high gate voltages. This is interpreted as 1-D variable range hopping at low gate voltages and 2-D variable range hopping at high gate voltages. In both ranges the parameter T_0 varies exponentially with gate voltage. This is interpreted in terms of an exponential variation of the decay length of the localized wave functions with Fermi energy. It is shown that this can be understood in terms of a "weak localization" model. In addition to explaining the strong localization behavior, the model predicts the crossover between "weak" and "strong" localization.

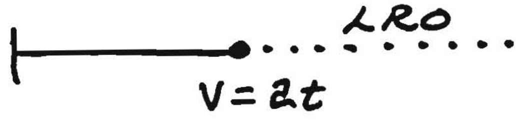
16:12

EH 10 Dimensional Resonances in the Laterally Confined 2-Dimensional Electron Gas. S. J. ALLEN, JR.*, F. DEROSA*, H. STORMER, A. R. TRETOLA, G. J. DOLAN, and

DISORDERED SPINLESS FERMIONS

- $H = \sum_{l} -t_l \left(c_{l+1}^{+} c_l + c_l^{+} c_{l+1} \right) + V_l n_l n_{l+1}$

- For a half-filled band, and $V \geq 2t$, CDW state is estabished



- study effect of randomly varying t_l and/or V_l on the singularity in structure factor $S(q)$ at $q = 2k_F$

SIMULATION PARAMETERS

- $\beta = 4$
  48 site lattice, half-occupied
  18 $\Delta\tau$- slices ($\Delta\tau = 0.222$)
  500 Warm-up Passes
  3 Passes per measurement
  5000 Measurements

- Uniform Probability Distribution Function for Choosing V_i, t_i Constrained to give $\langle v \rangle = 2 \langle t \rangle$

- Range of variation of V_i, t_i kept within $\langle v \rangle \pm V_a$, $\langle t \rangle \pm t_a$

MEASUREMENTS

- Density-Density Correlation Function

$$\rho(\ell) = \langle n_{i+\ell}\, n_i \rangle$$

For CDW state, $\rho(\ell) \sim \dfrac{(-1)^{\ell}}{\ell}$ $\left\{ \begin{array}{l} \text{AF Heis.} \\ \text{Luther,} \\ \text{Peschel} \end{array} \right.$

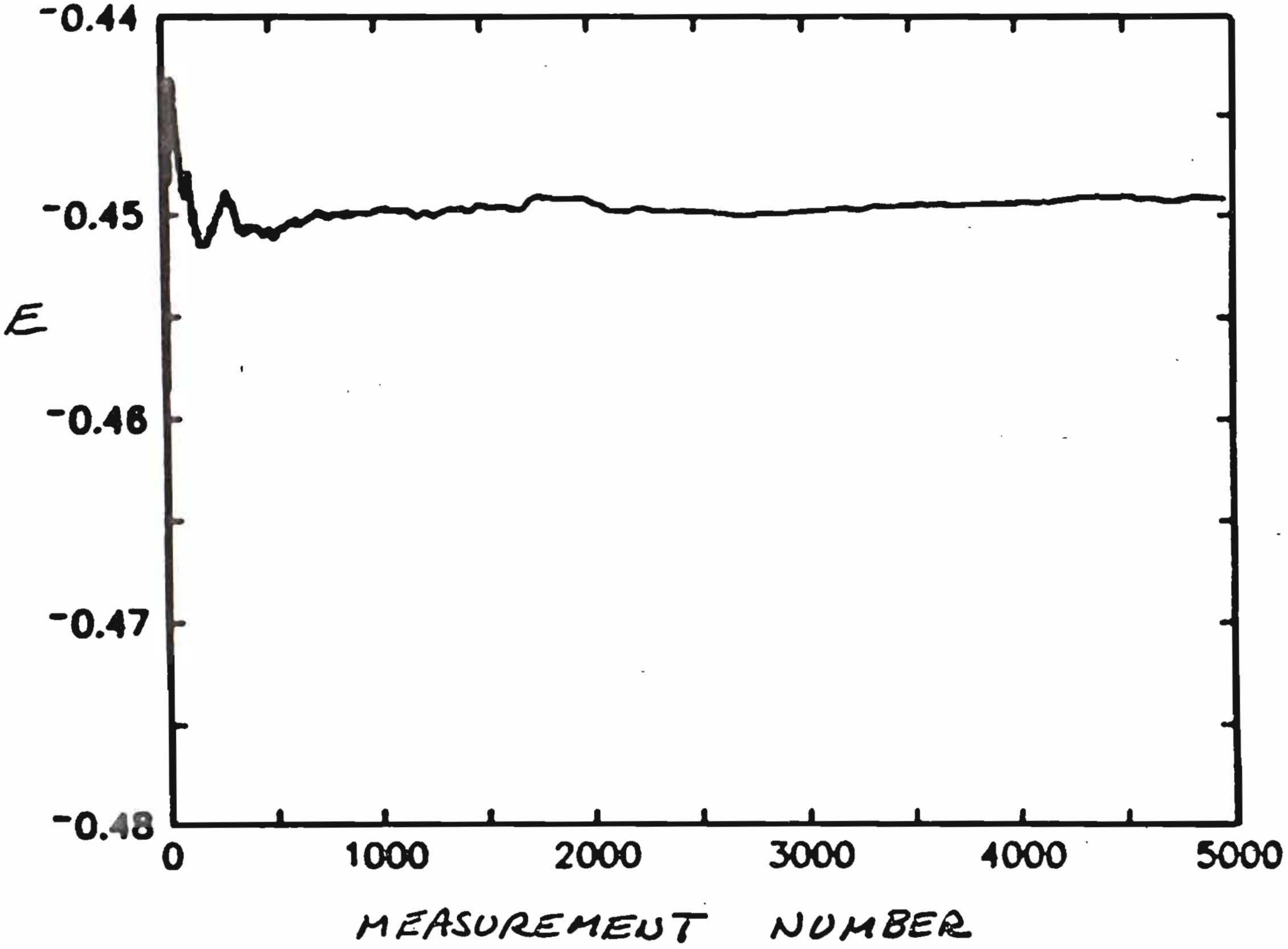
- Structure Factor

$$S(q) = \frac{1}{N} \sum_{\ell} e^{iq\ell} \left(\rho(\ell) - \langle n \rangle^2 \right)$$

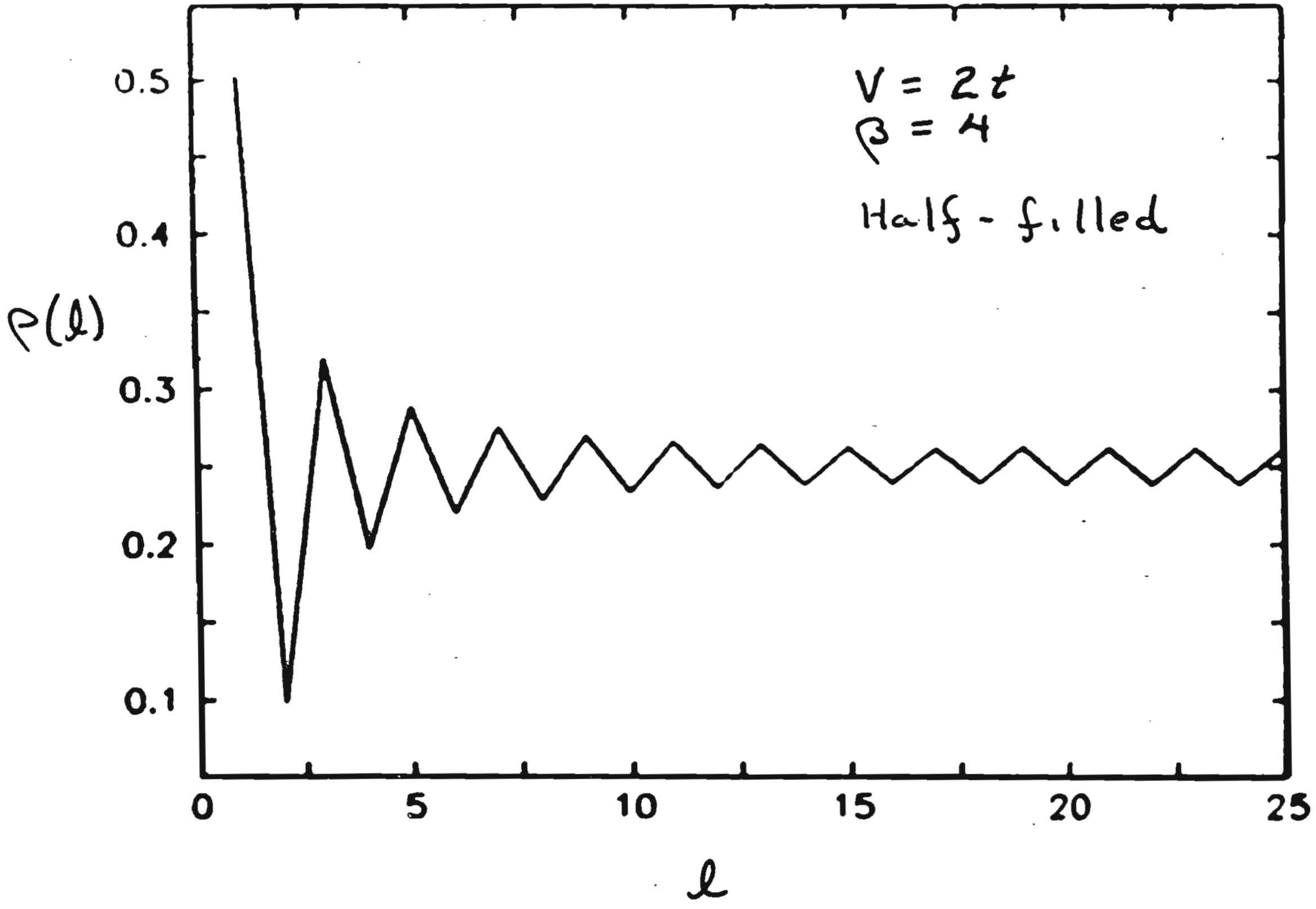
For CDW state, at $q = 2k_F = \pi$

$$S(\pi) \sim \ln N$$

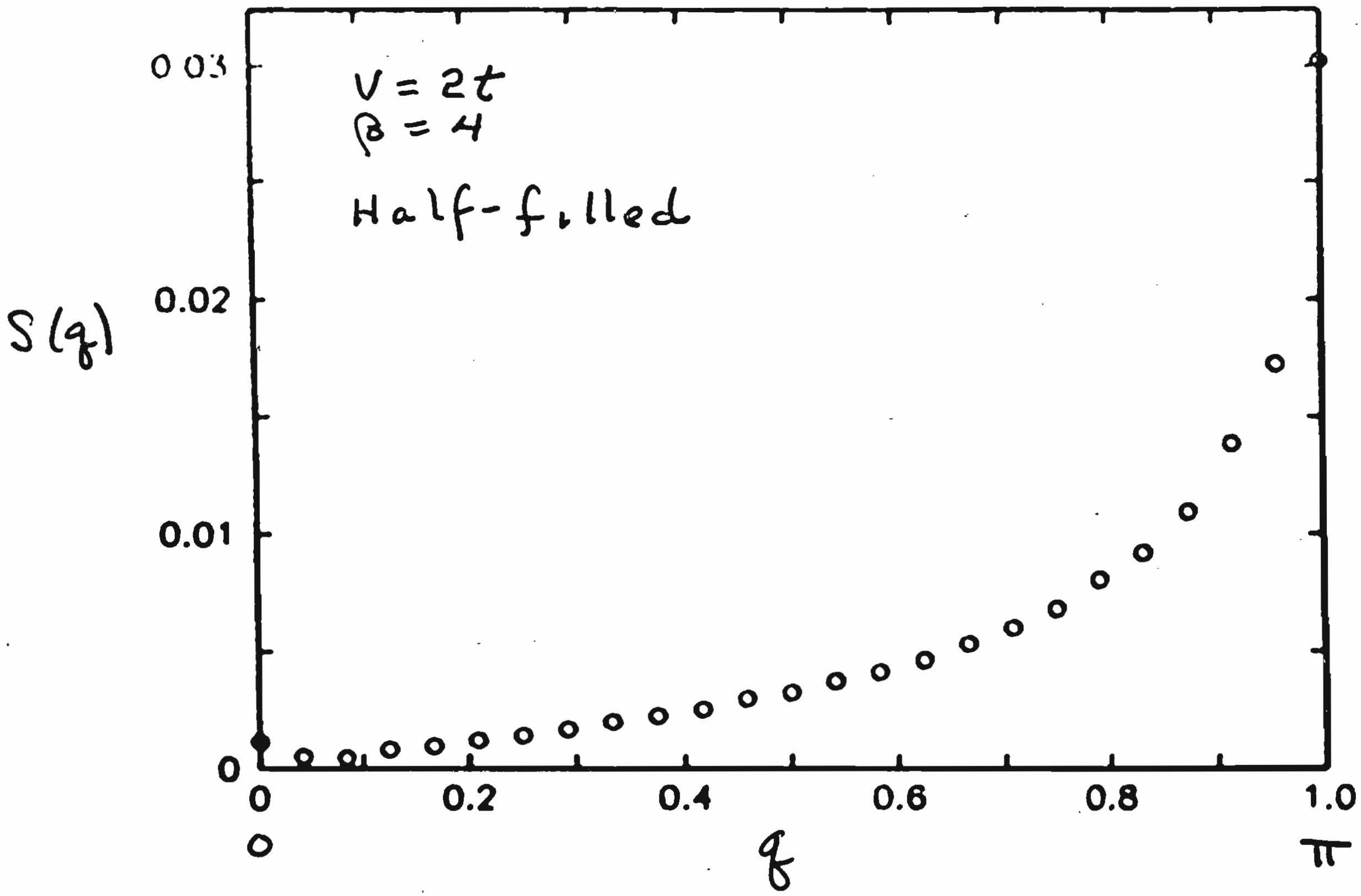
RUNNING AVERAGE OF ENERGY/UNIT CELL



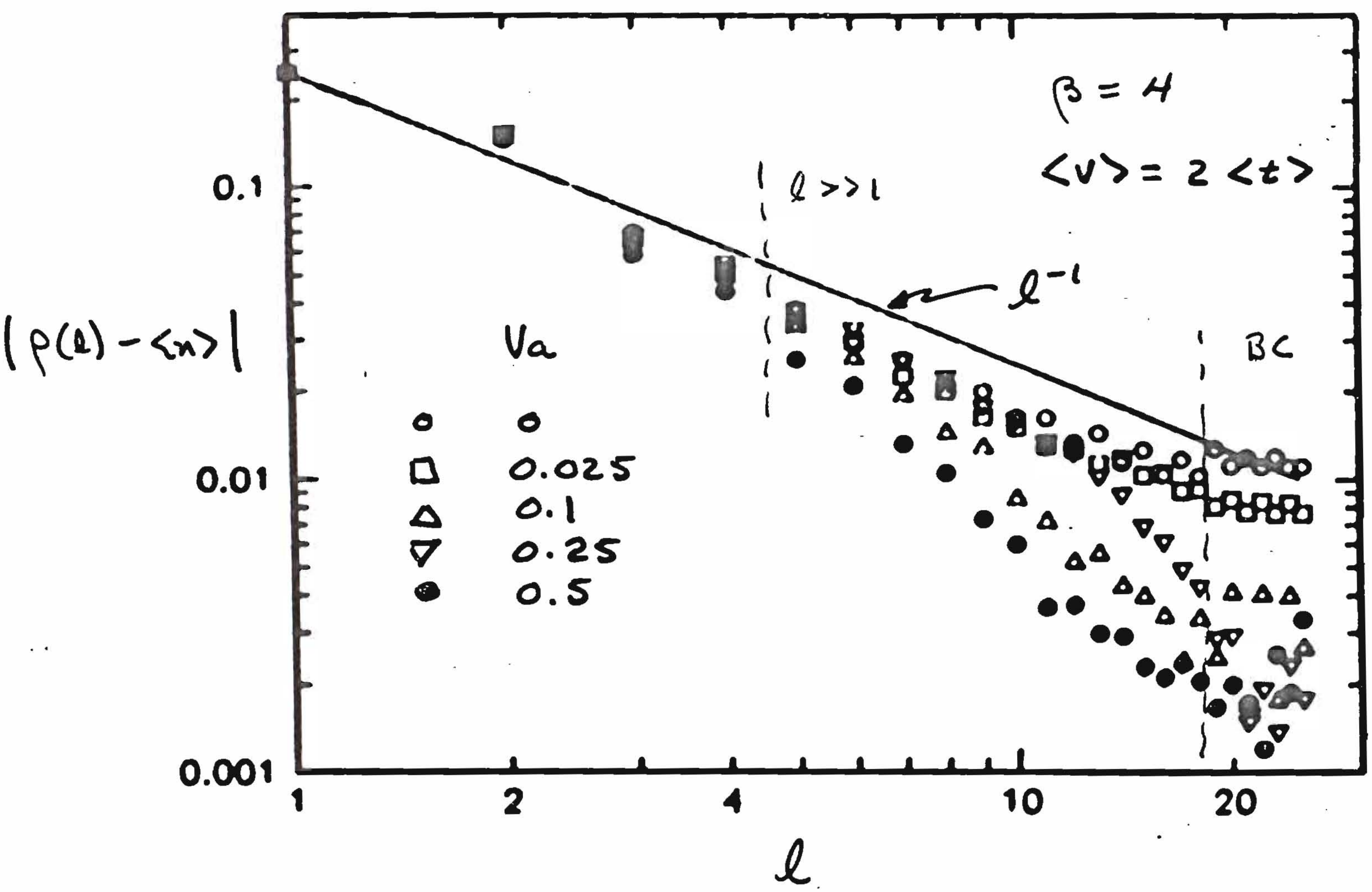
Density - Density Correlation



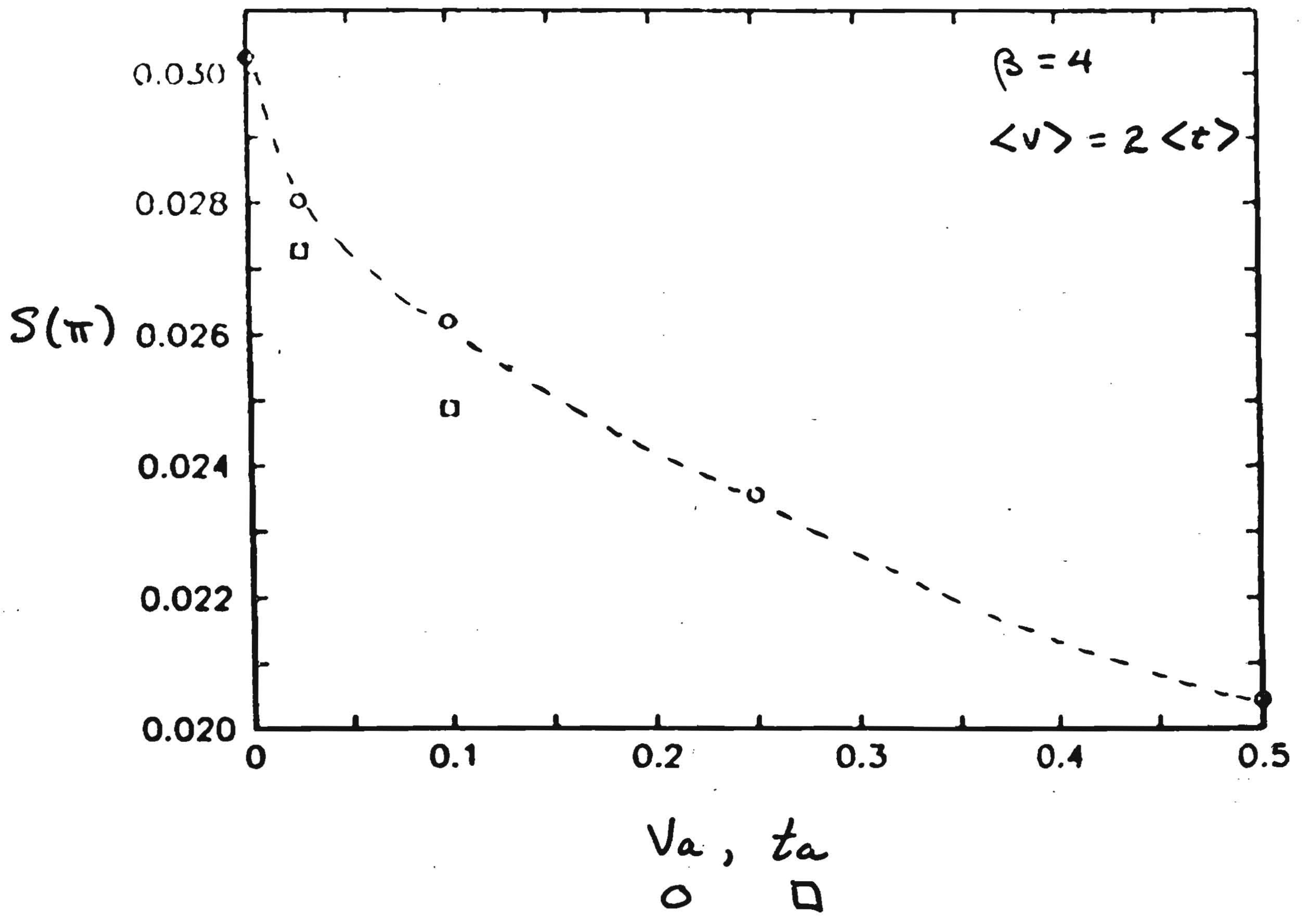
Structure Factor



ρ(ℓ) for Random V



S(π) vs Va, ta



STATUS

- At $V = 2t$, disorder strongly suppressed CDW LRO

- More work need on:
  - Scaling
  - $V > 2t$
  - Effect of distribution function
  - Extended Hubbard Model