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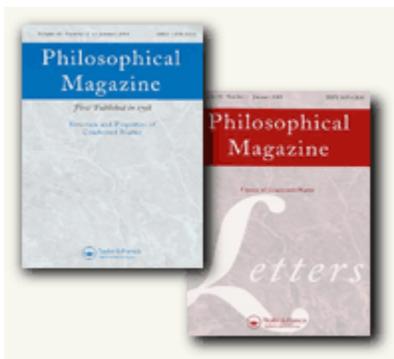
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Transition from quasicrystals to amorphous structures

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For the model structure the smooth transition from perfect quasicrystalline to amorphous structure has been observed and changes in the diffraction patterns has been investigated. It turned out that all dependencies can be easily handled by means of some well-defined probability distributions. Given these distributions one can perform an appropriate calculations in the average unit cell method and describe the transition in a simple and consistent way.

Keywords: Quasicrystals; Diffraction; Disordered materials

1. Introduction

The diffraction pattern of any structure can be obtained by the Fourier transformation of its atomic positions. Classical crystallographic approach, however is based on the concept of unit cell and reciprocal lattice, therefore its validity is constrained to the analysis of perfectly periodic crystals. If a given structure is not of this type, the unit cell doesn't exist and this approach fails. It has been shown [1] that diffraction pattern of such structures may be correctly described in the average unit cell approach based on the reference lattice concept. In this approach periodicity of real structure is not important, nevertheless when it holds, the average unit cell is fully equivalent to the classic unit cell. It is possible to construct probability distributions of positions of atoms (nodes) relative to the unit cell and then calculate Fourier transformation to get so-called envelope function correctly describing intensities for certain well-defined scattering vectors.

The diffraction pattern of perfect crystals consists of Bragg peaks corresponding to the points of the appropriate reciprocal lattice. Unfortunately, for all non-periodic even well-defined structures the classic crystallographic concepts of unit cell and reciprocal lattice are nearly useless. Although the diffraction pattern of perfect quasicrystals also consists of Bragg peaks, the reciprocal lattice of such structure does not exist. As an example, in this work Fibonacci chain and its modifications has been investigated.

Fibonacci chain is well-known and thoroughly analysed one-dimensional model of perfect quasicrystal [2]. It can be obtained for example by iterative substituting $L \rightarrow LS$ and $S \rightarrow L$, where S is the shorter distance between the nodes of the Fibonacci chain and L is τ times longer (golden number $\tau = (1+\sqrt{5})/2 \approx 1.618$). In this work S has been taken as the unity length. Another popular method of constructing the Fibonacci chain is the projection of the strip of two-dimensional square lattice onto certain well-defined direction.

The diffraction pattern of Fibonacci chain consists of main peaks and series of satellite peaks. We can construct the average unit cell of the length a equal to the average distance between nodes (given by $a=1+1/\tau^2 \approx 1.382$) and obtain probability distribution $P(u)$ in such average unit cell, where u is the shortest distance between positions of nodes of Fibonacci chain and nodes of the periodic reference lattice with period equal to a . Fourier transformation of such probability

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3 distribution gives an envelope function which shows correct intensities of all main reflections. By
4 creating separate average unit cell of the bigger length $b = a \cdot \tau$ and appropriate $P(v)$ distributions we
5 are able to describe correctly also intensities of all satellite peaks. In the (u, v) parameter space
6 probability distribution $P(u, v)$ proves to be only one line with the constant value on it and zero
7 elsewhere (fig.1).
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9

10 [Insert figure 1 about here]
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12 Exactly the same reasoning can be used to describe disordered structures. For example, the perfect
13 Fibonacci chain nodes positions F_n (where n is a node number) can be perturbed by adding to them
14 a random shift ε of the Gaussian distribution with the standard deviation σ . So, the new position of
15 the n -th node can be written as follows: $f_n = F_n + \varepsilon$. Small sigma parameter (relative to the length of
16 the average unit cell) in periodic systems leads to the well-known Debye-Waller factor describing
17 the thermal motions of the atoms.
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21 The scope of the work was to observe influence of the ε . value on the diffraction pattern. Changes
22 in the $P(u, v)$ distributions as a function of the σ parameter also has been investigated. The fact that
23 there are two well-defined extreme cases: for $\sigma = 0$ we have just pure Fibonacci chain (i.e. perfect
24 one-dimensional quasicrystal) and for $\sigma \rightarrow \infty$ the structure becomes completely random, proved to
25 be very helpful and allowed to control validity of calculations. Between these two extremes,
26 however, exist large variety of partially disordered structures and we can observe transition from
27 amorphous to the quasicrystalline state.
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31 Two distinct cases have been taken into consideration. First, the σ parameter has been set to
32 constant value throughout the whole structure, that is σ has been independent of node number n . In
33 the second case σ has been set to be linearly rising function of n . As the more interesting results has
34 been obtained in the second case, only this case will be described below.
35
36

37 2. The description of the model 38

39 The positions of the nodes of pure Fibonacci chain have been perturbed by adding to them a
40 random value ε of the Gaussian distribution with the standard deviation σ . But, σ parameter has
41 been set to be linear function of node number n , that is $\sigma(n) = \alpha n$, where α is arbitrary chosen
42 positive constant. Such dependency preserves short range order but makes the correlations vanish
43 with distance. What is very important, this dependency ($\sigma(n)$) has been taken into consideration
44 only inside clusters of relatively small size N (varied from about 5 to 200), and not in the entire,
45 virtually infinite chain. These clusters have been taken as a parts of Fibonacci chain modified in the
46 way described above. The calculations have been performed for a big number of separate clusters
47 and then average values have been obtained. This procedure helped to get rid of fluctuations
48 coming from random factors as well as relatively small cluster sizes. One should also note that
49 cluster size N has not been fixed to be constant but could fluctuate around chosen value in such a
50 way that average N has been preserved.
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55 First, the diffraction patterns for various cluster sizes and various α parameters has been calculated.
56 One can observe two distinct parts of the diffraction patterns: first consists of quite sharp Bragg
57 peaks (the width of these peaks reduces as the cluster size grows) and **continuous** part which is
58 constant if intensities are scaled by N and not N^2 as usual (fig.2).
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[Insert figure 2 about here]

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4 The intensity of the first main Bragg peak ($k \approx 4.546$) versus cluster size has been investigated
5 (fig.3). It's clearly visible that for large N Bragg peaks vanish and **belong to the continuous part**
6 **of the diffraction pattern.**
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9 [Insert figure 3 about here]
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11 Behaviour of probability distribution $P(u,v)$ as well as its projections onto different directions has
12 been observed. For pure Fibonacci chain $u(v)$ is just a straight line with constant probability on it
13 and zero elsewhere. This line turns out to diffuse in both directions - quite slowly along the line and
14 much faster in the perpendicular direction (fig.4).
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17 [Insert figure 4 about here]
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20 Projection onto u axis gives probability distribution $P(u)$ which is strictly correlated with the main
21 peaks intensities. The Fourier transformation of $P(u)$ distribution gives an envelope function
22 correctly describing intensities for all scattering vectors (or, in our one-dimensional case just
23 numbers) $k=nk_0$, where $n=1,2,3,\dots$ is a natural number and $k_0=2\pi/a$ is a basic scattering vector
24 (number) related with average distance between nodes of pure Fibonacci chain a . For small cluster
25 sizes and small α parameters, $P(u)$ is close to rectangular distributions as in pure Fibonacci chain.
26 For bigger N , however, $P(u)$ distributions become more flat and have nonzero value for the whole u
27 range (fig.5)
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30 [Insert figure 5 about here]
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33 3. Conclusions

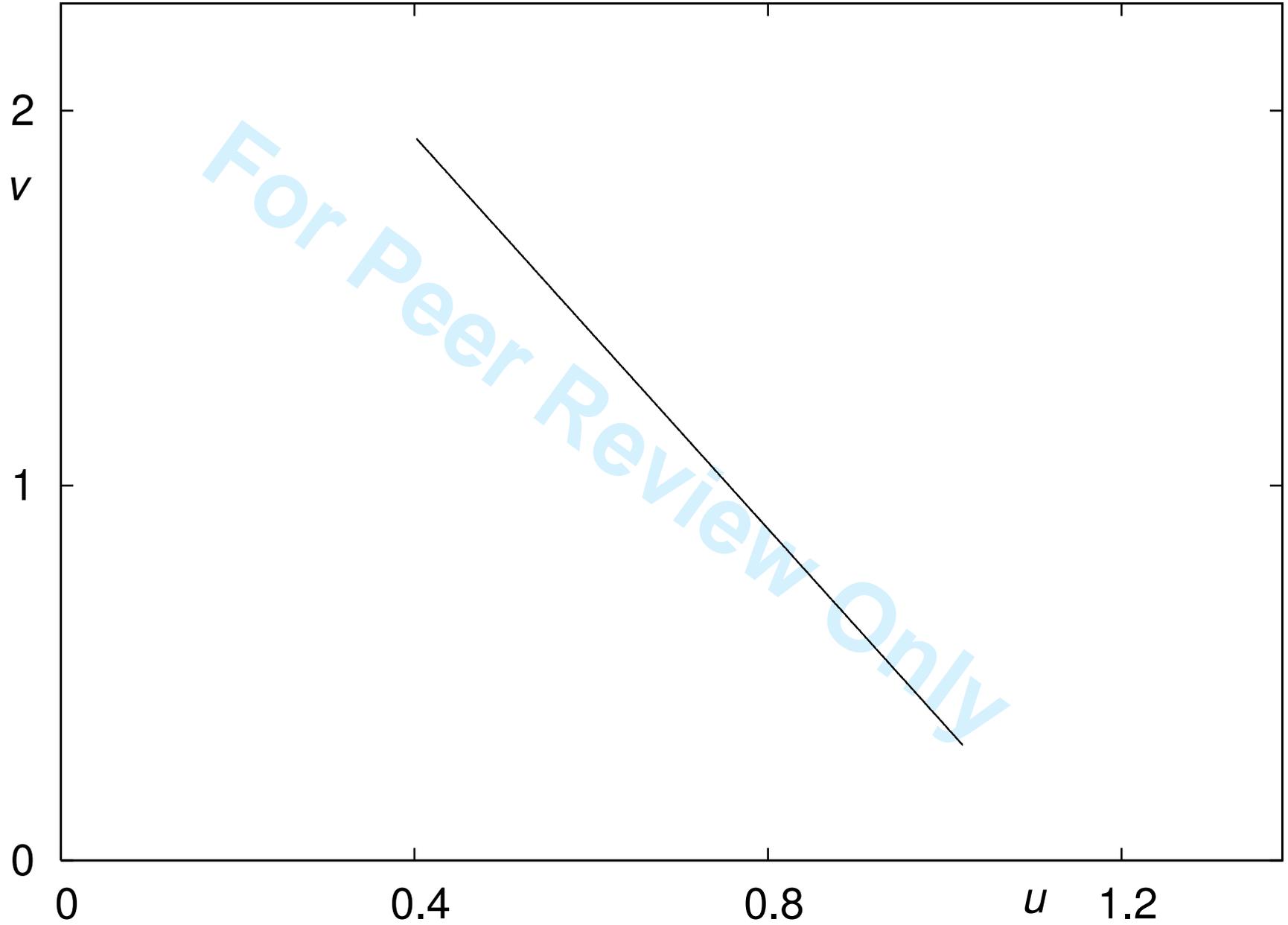
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35 In this model for the first time a smooth transition from perfect quasicrystal to the amorphous state
36 has been observed. In such a simple model one can easily investigate the behaviour of the
37 diffraction pattern depending on such things as a cluster size and its dispersion and parameter α
38 simulating vanishing correlations of atomic positions with regard to the perfect quasicrystalline
39 structure. All dependencies can be handled in simple way by means of probability distribution
40 $P(u,v)$ and its projections onto certain directions. Given probability distributions one can quickly
41 perform all appropriate calculations in the average unit cell method and this way one can describe
42 transition from quasicrystalline to amorphous state in consistent and well-defined way.
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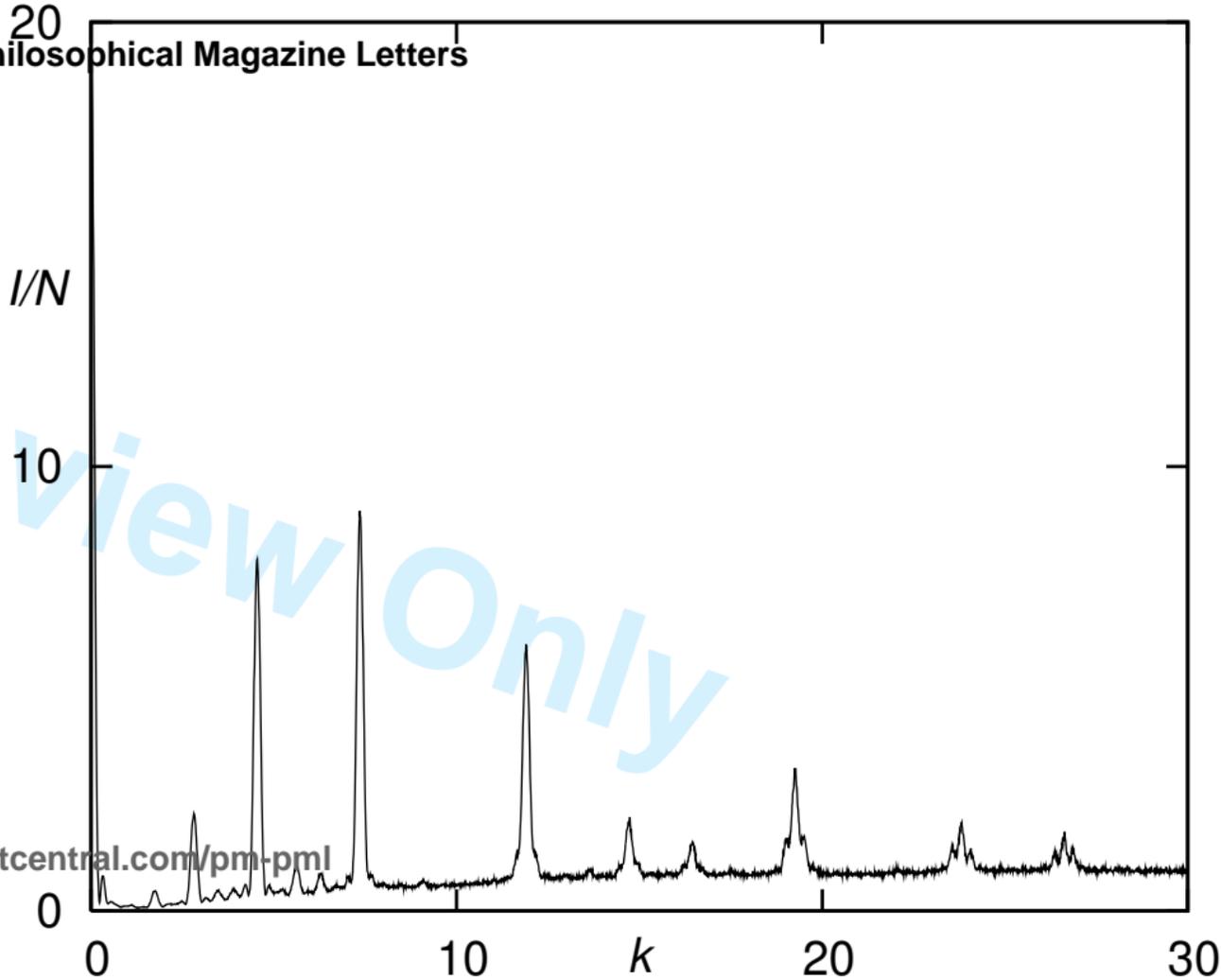
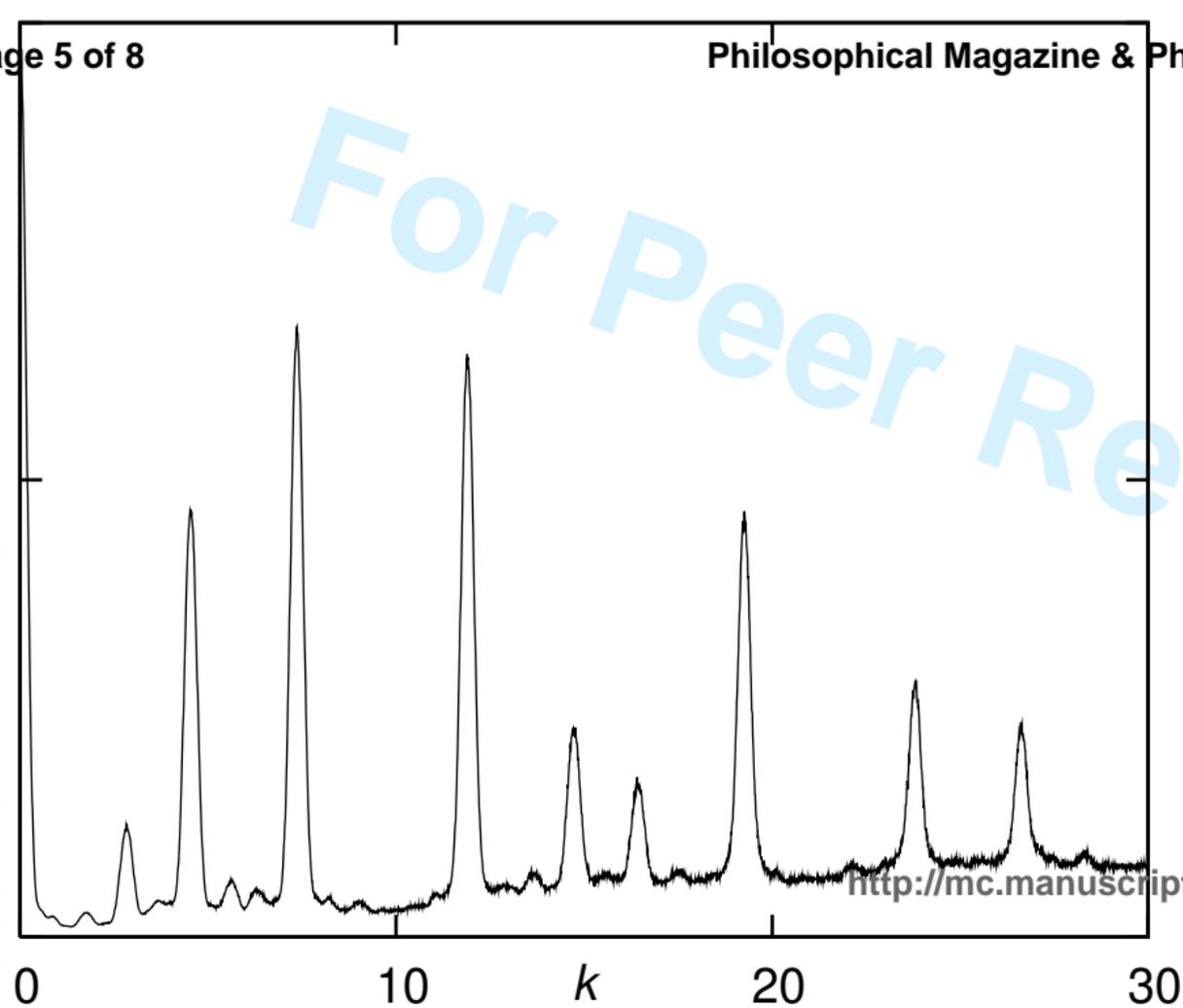
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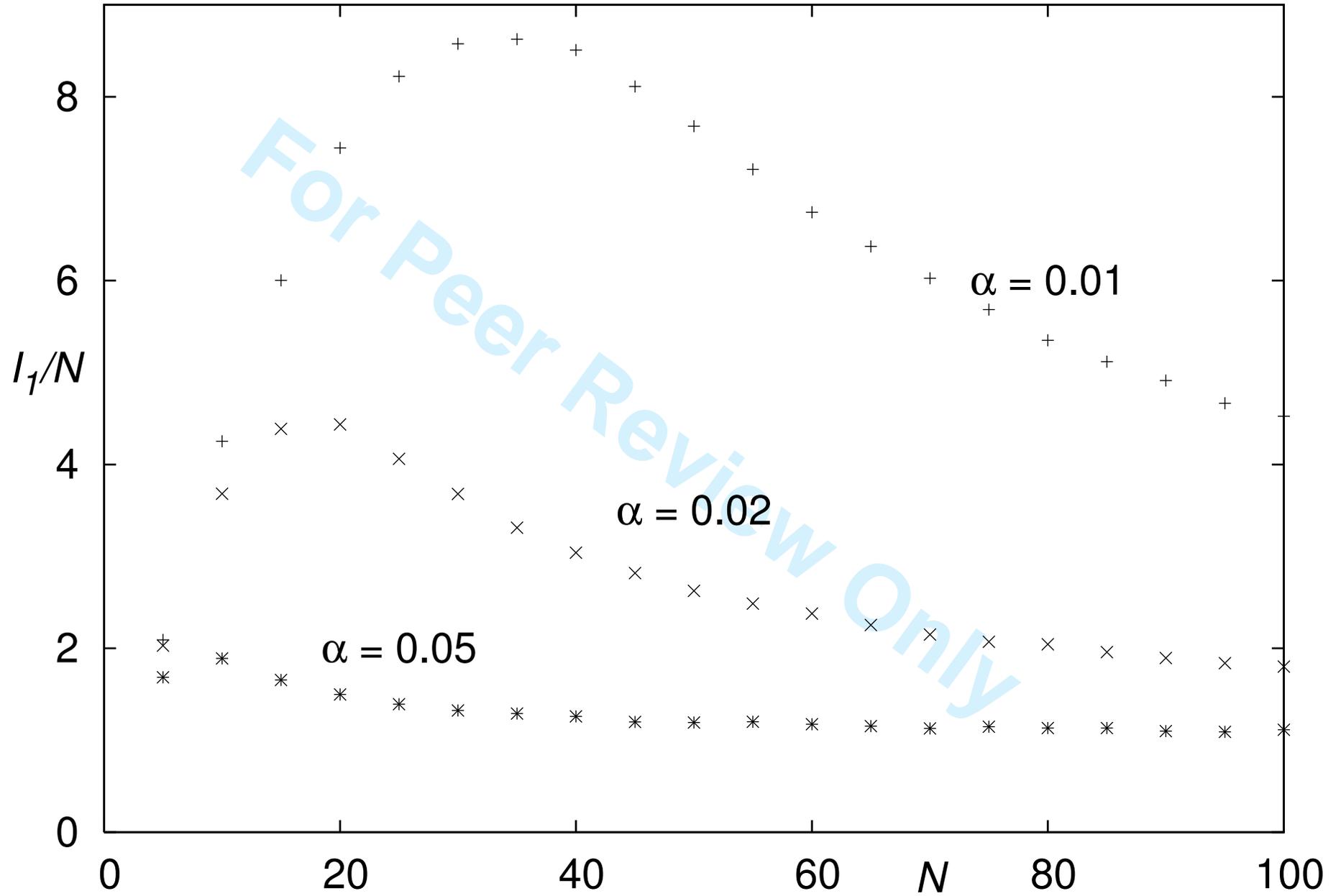
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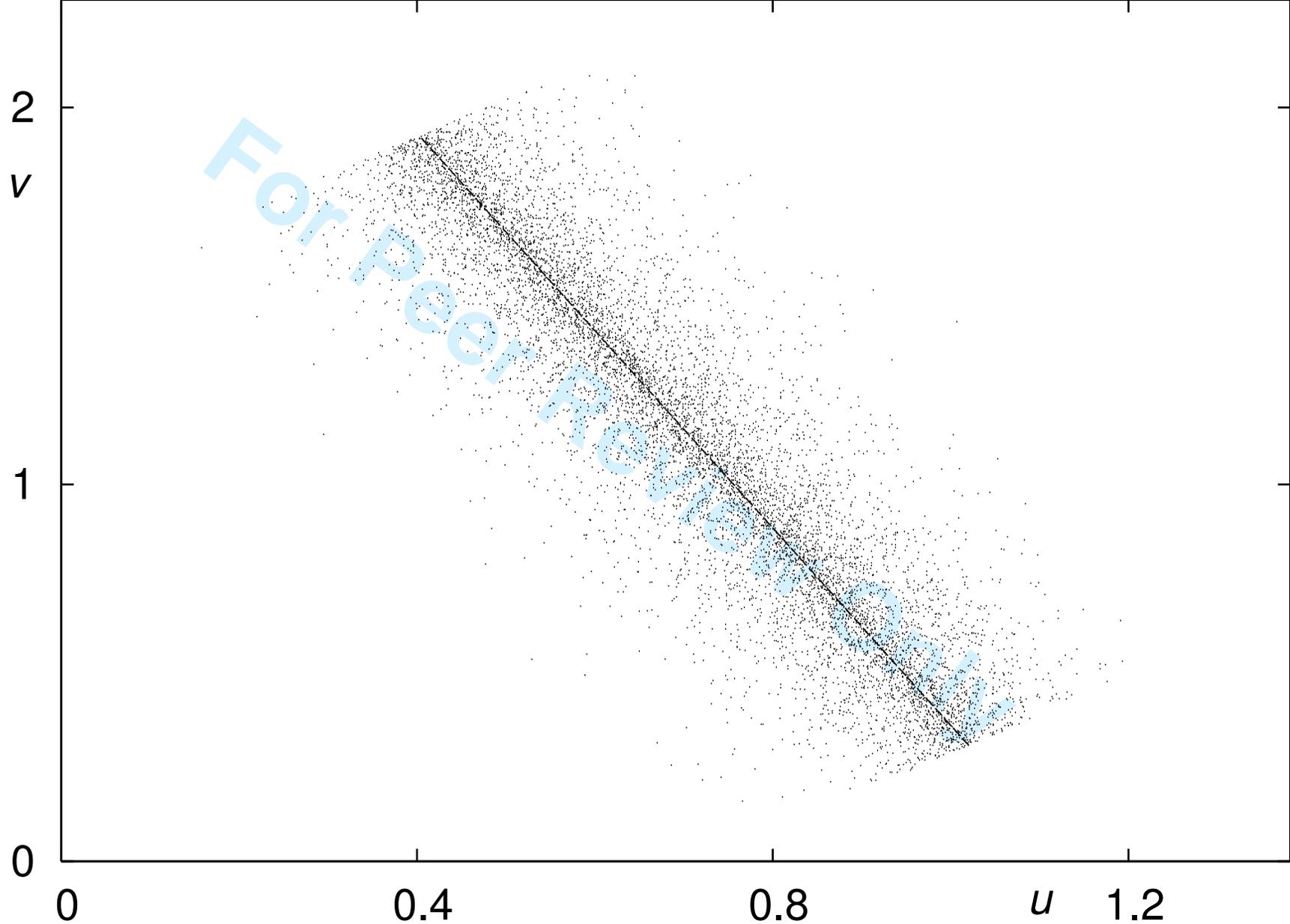
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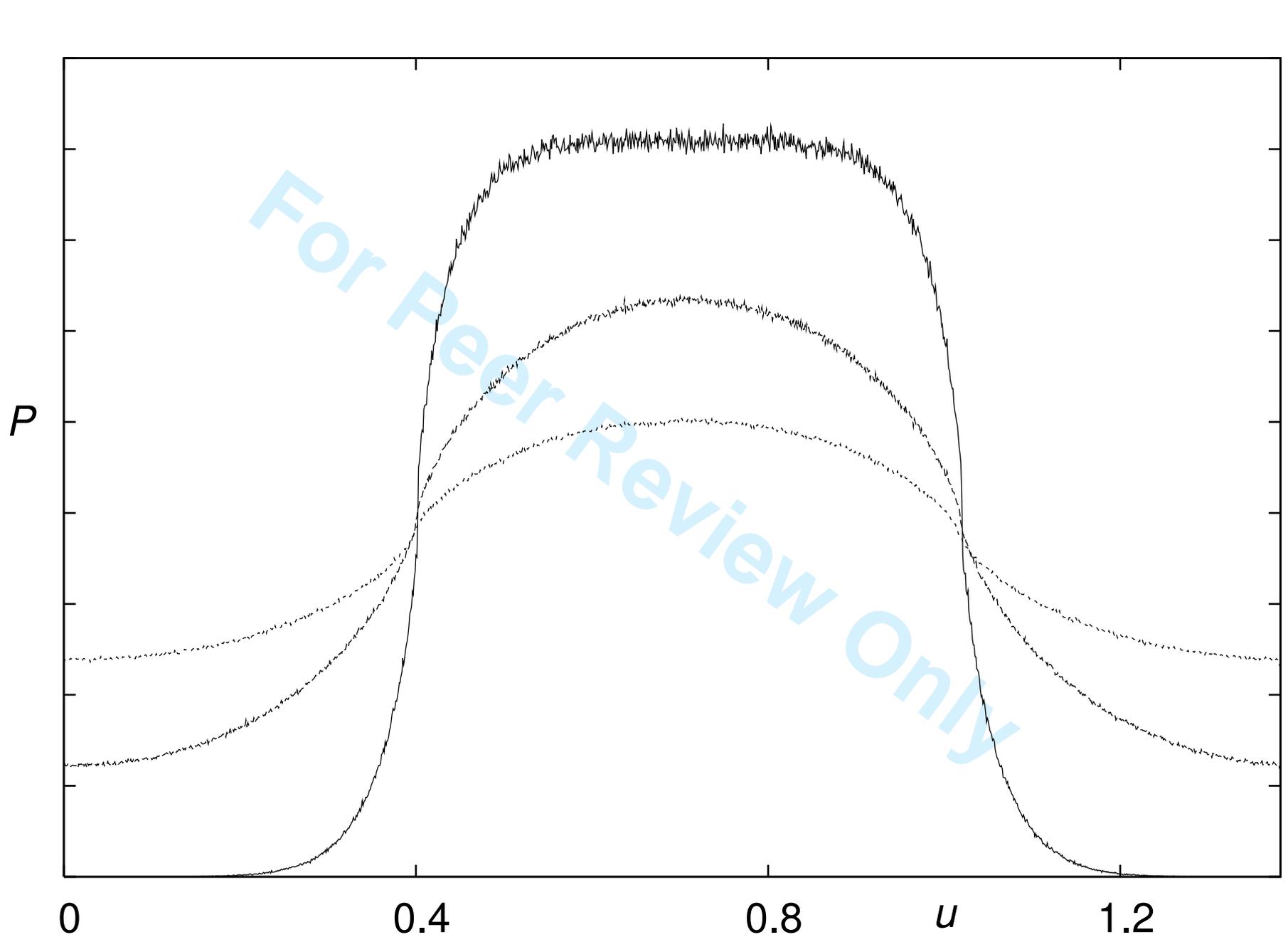
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