Finding Optimal Window Size to Calculate Integrated Autocorrelation Time for Lattice QCD Ensembles

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Introduction

What is Autocorrelation time?

Introduction

- Autocorrelation time (τ) measures the timescale over which a signal or process correlates with itself. It quantifies how quickly, values in a time series become uncorrelated as the time lag between them increases. In this report, we discuss the definition, calculation methods, and applications of autocorrelation time in lattice QCD simulations.

Introduction

- Calculation of Autocorrelation Time

Introduction

The autocorrelation function C(t) can be calculated directly from a time series x(t) using:

$$C(t) = \frac{1}{N-t}\sum_{n=1}^{N-t}(x(n)-\bar{x})(x(n+t)-\bar{x})$$

where N is the total number of data points, t is the lag, and x_bar is the mean of the time series.

Introduction

The integrated autocorrelation time is defined as:

$$\tau_{\text{int}} = \frac{1}{2} + \sum_{t=1}^{T} \frac{C(t)}{C(0)}$$

This approximation provides a practical way to estimate the integrated autocorrelation time from the autocorrelation function up to a certain lag T

SU(3) WILSON GAUGE THEORY

lattice formulation of Quantum Chromodynamics (QCD), describing interactions between quarks and gluons.

SU(3) WILSON GAUGE THEORY

The Wilson action for SU(3) lattice gauge theory is given by:

$$S_W = \beta \sum_{\text{plaquettes}} \left(1 - \frac{1}{3}\mathrm{Re}\,\mathrm{Tr}(U_p)\right)$$

Autocorrelation Time in Lattice QCD

Quantifies the rate at which fluctuations in the lattice gauge fields decorrelate as the Markov chain evolves, affecting the statistical accuracy of observables computed from the configurations.

Significance of Autocorrelation Time in Lattice QCD

- Efficient Sampling:

Understanding autocorrelation time is crucial for optimizing the performance of MCMC algorithms in lattice QCD simulations. It helps determine appropriate step sizes and decorrelation strategies to enhance the efficiency of sampling configurations.

Significance of Autocorrelation Time in Lattice QCD

- Algorithm Optimization:

Autocorrelation time guides the development and optimization of algorithms tailored for lattice QCD simulations, aiming to minimize computational costs and improve sampling efficiency.

- Error Estimation:

Longer autocorrelation times lead to larger error bars, affecting the precision of computed observables.

IMPORTANCE OF LAG IN CALCULATING INTEGRATED AUTOCORRELATION TIME

$$\tau_{\text{int}} = \frac{1}{2} + \sum_{t=1}^{T} \frac{C(t)}{C(0)}$$

Lag plays a critical role in determining the accuracy and reliability of the calculation.

The lag parameter determines the range of temporal separations over which correlations between successive measurements are examined.

IMPORTANCE OF LAG IN CALCULATING INTEGRATED AUTOCORRELATION TIME

- Balance between Bias and Variance
- Efficiency of Sampling
- Convergence of Autocorrelation
- Trade-off with Computational Resources

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AUTOMATIC WINDOWING ALGORITHM

- designed to select an optimal window size W or lag
- based on the hypothesis that the autocorrelation time, τ, is approximately a certain factor, S, times the integrated autocorrelation time, τ_{int}
- the algorithm aims to find a self-consistently close to optimal summation window, ensuring that the chosen value exhibits a plateau in the statistical errors of the autocorrelation function.

AUTOMATIC WINDOWING ALGORITHM

- The algorithm involves the following steps:
- Plateau Verification: Ensure that τint(W) exhibits a plateau around the chosen W value. If not, adjust S accordingly.

1. **Initial Hypothesis**: Assume $\tau \approx S \cdot \tau_{\text{int}}$, with S typically set between 1 and 2.
2. **Estimator Calculation**: Compute the estimator $\bar{\tau}(W)$ using the formula:

$$\bar{\tau}(W) = \frac{1}{\ln(2\bar{\tau}_{\text{int}}(W) + 1)}$$

   If $\bar{\tau}_{\text{int}} \leq \frac{1}{2}$, set $\bar{\tau}(W)$ to a small positive value.
3. **Window Selection**: For $W = 1, 2, \ldots$, calculate:

$$g(W) = \exp\left[-\frac{W}{\bar{\tau}(W)}\right] - \frac{\bar{\tau}(W)}{\sqrt{WN}}$$

   The first value of W where $g(W)$ is negative is chosen as the window size.

EXPERIMENTS AND RESULTS

Lattice configuration data

- Lattice Dimensions: $24 \times 24 \times 24 \times 4$
- Data was taken for ten values of lattice gauge coupling β varied non-linearly from β = 5.6 till β =5.9.
- For each β, 1000 lattice configurations were generated.
- The observable used is the norm of the value of Polyakov loop, and autocorrelations were calculated on them for each value of lattice gauge coupling.

EXPERIMENTS AND RESULTS

Data visualisation

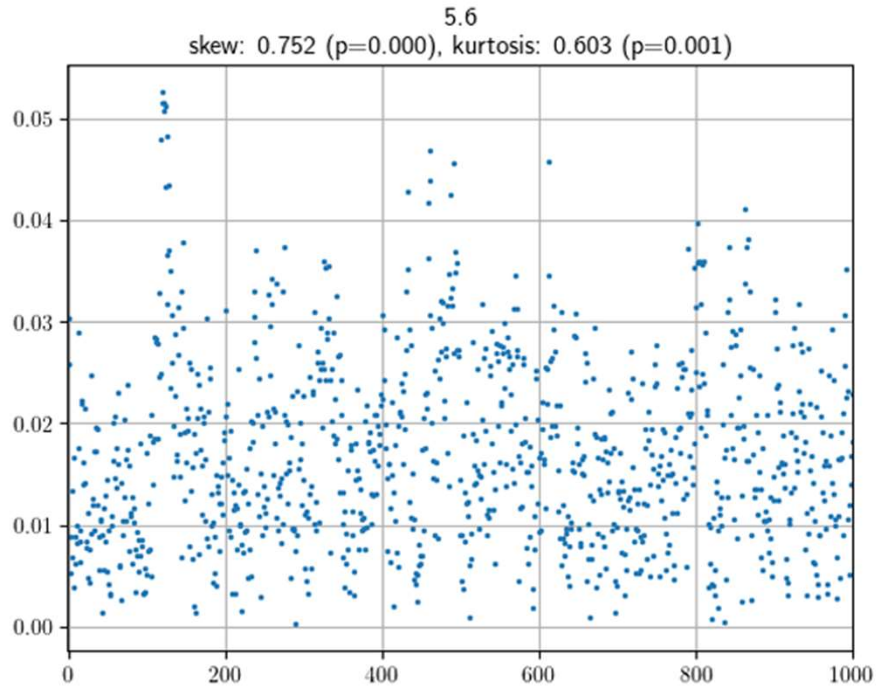

FIG. 1. for $\beta = 5.6$

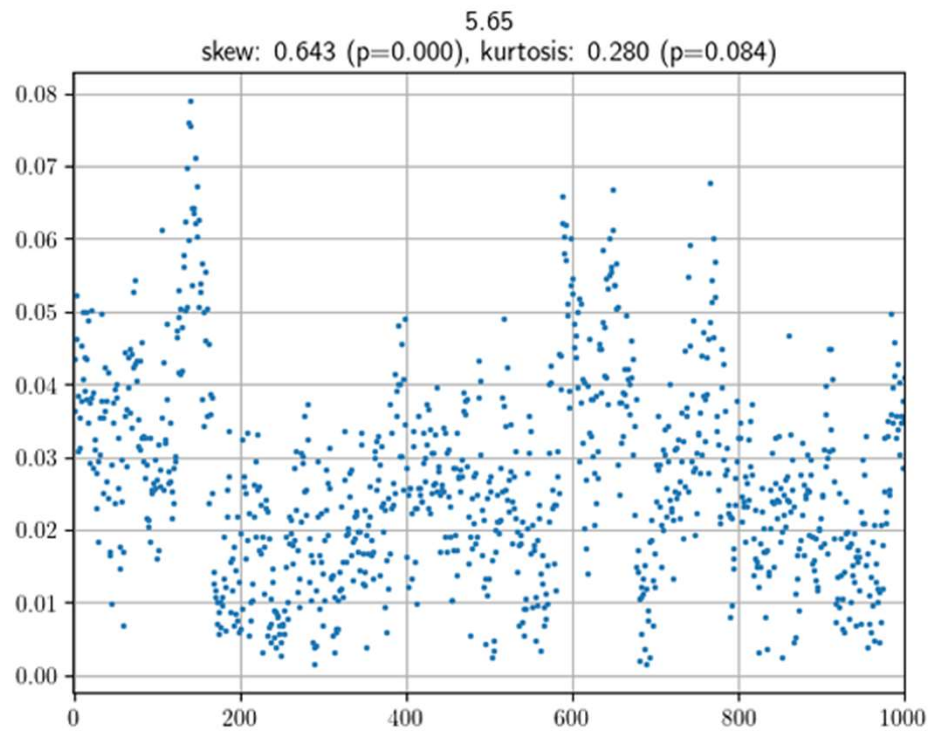

FIG. 2. for $\beta = 5.65$

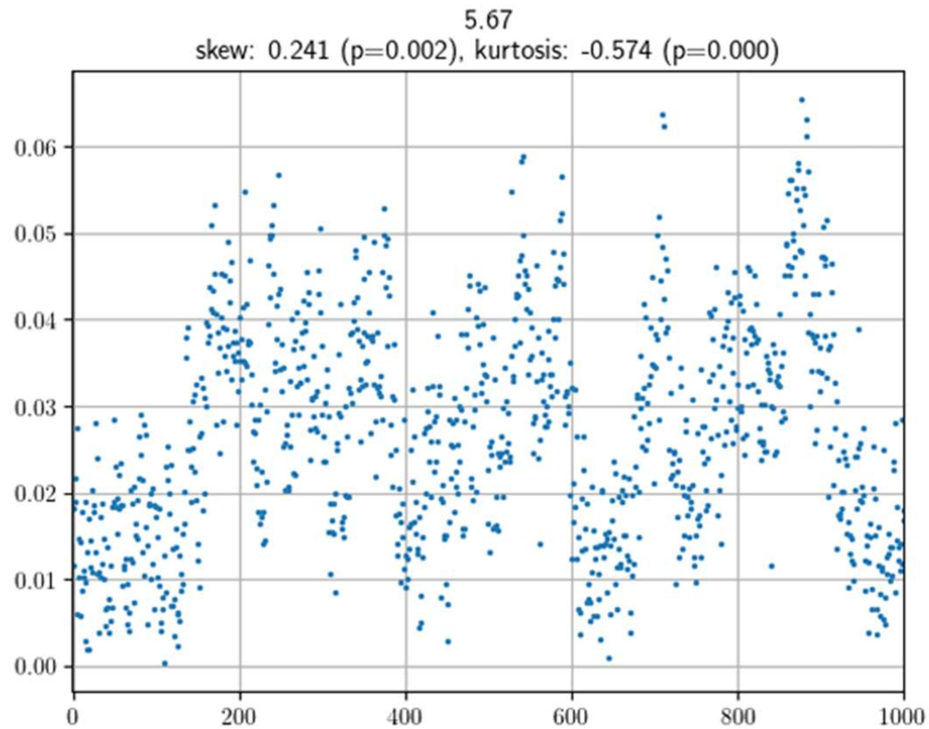

FIG. 3. for $\beta = 5.67$

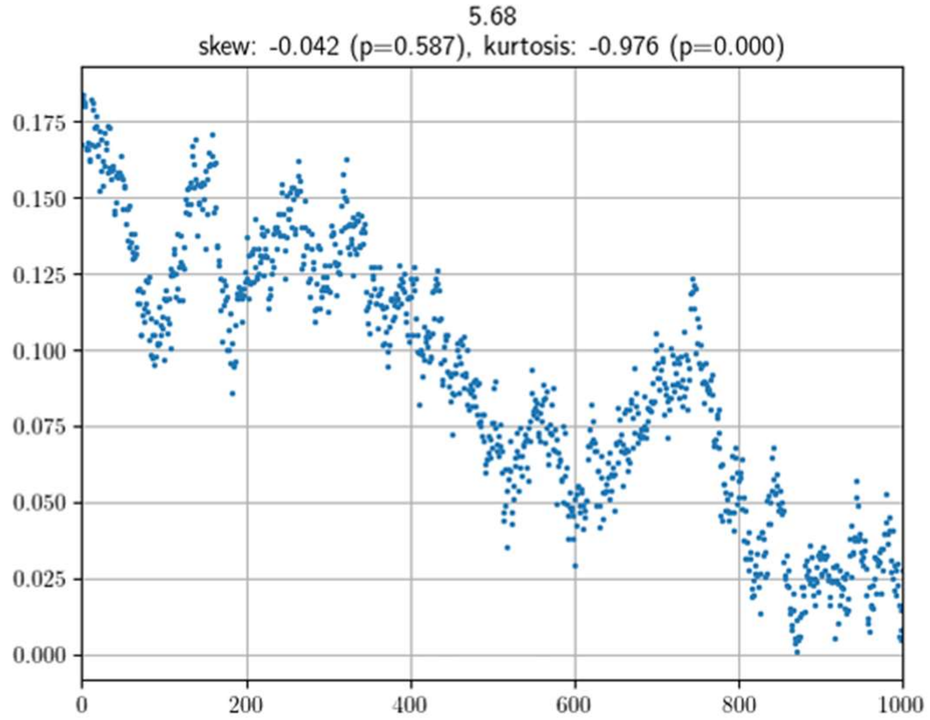

FIG. 4. for $\beta = 5.68$

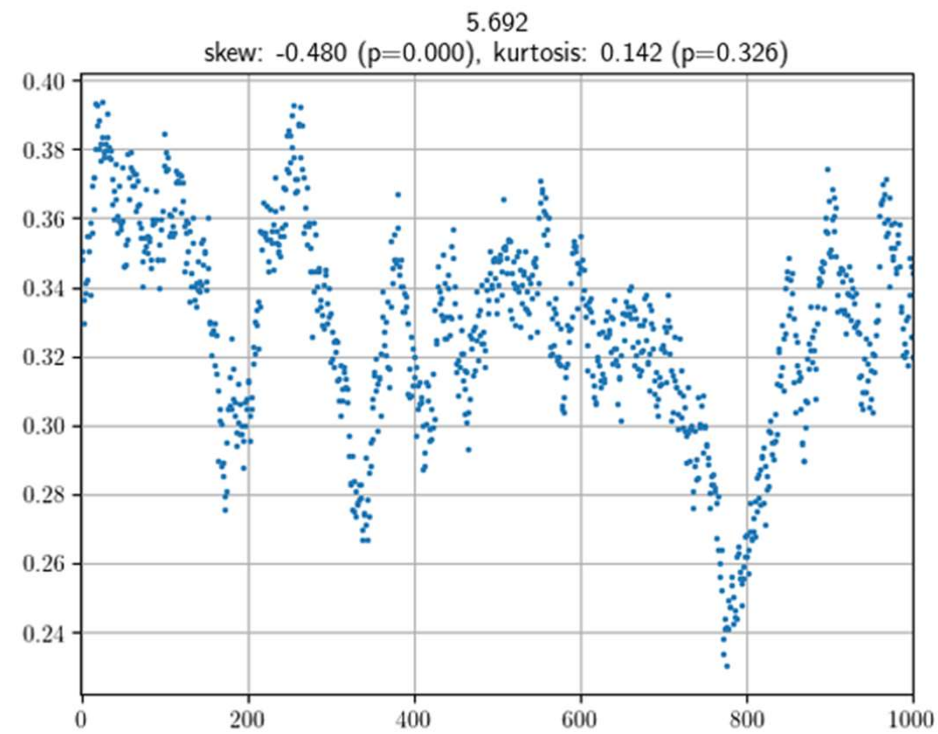

FIG. 5. for $\beta = 5.692$

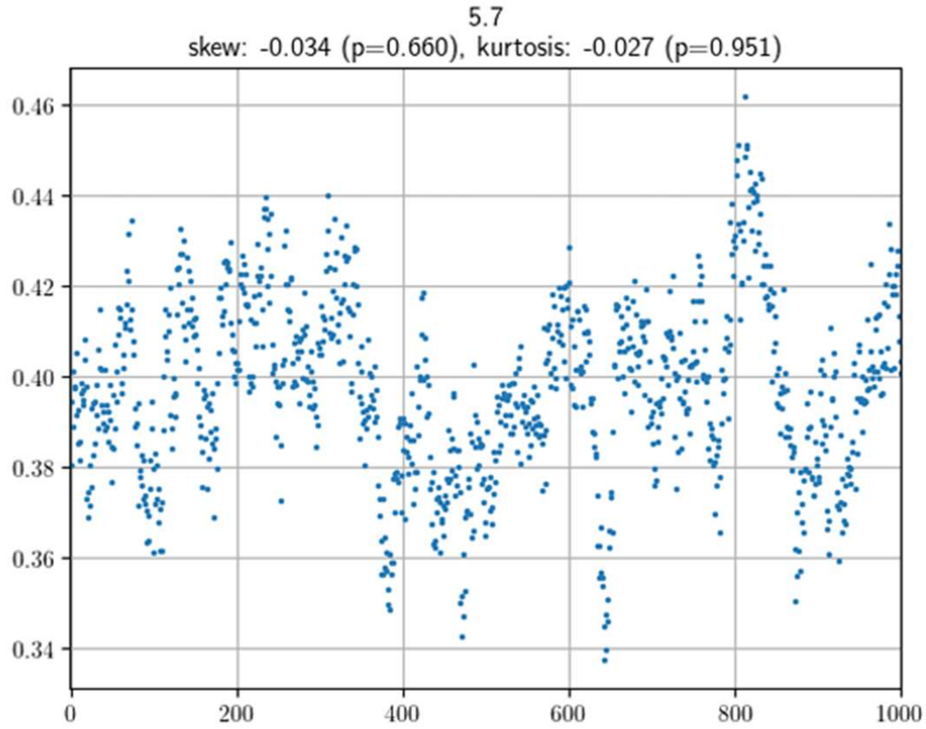

FIG. 6. for $\beta = 5.7$

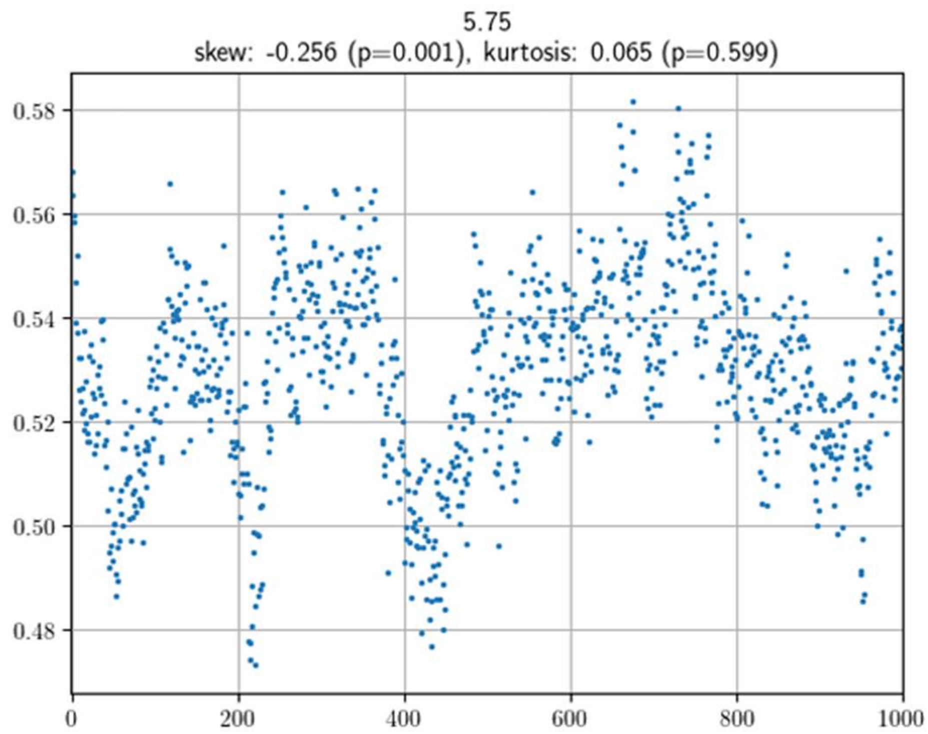

FIG. 7. for $\beta = 5.75$

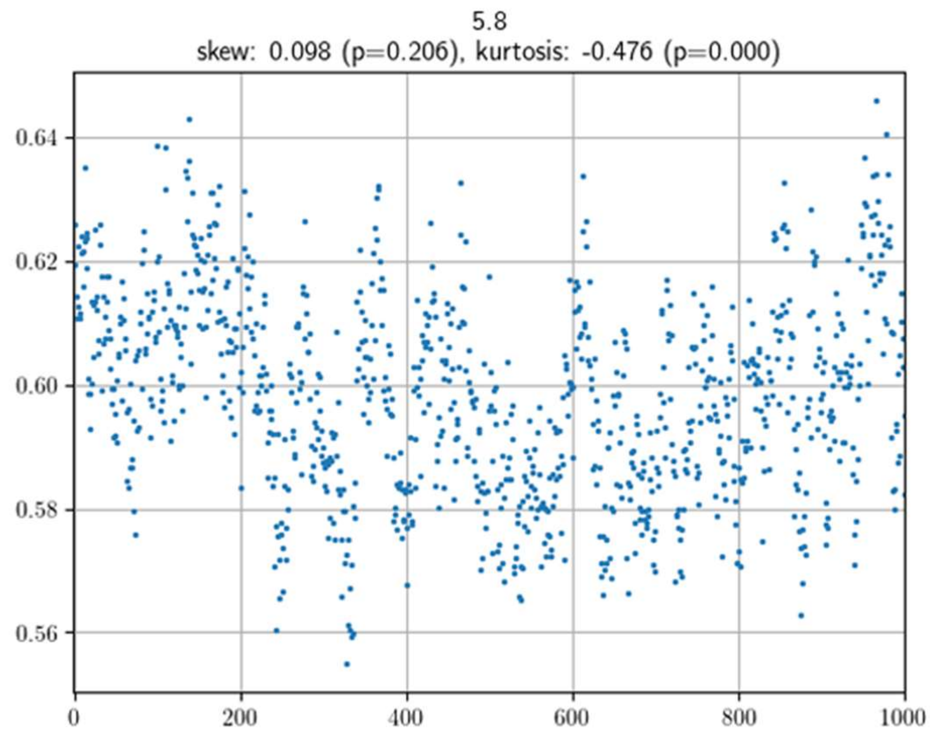

FIG. 8. for $\beta = 5.8$

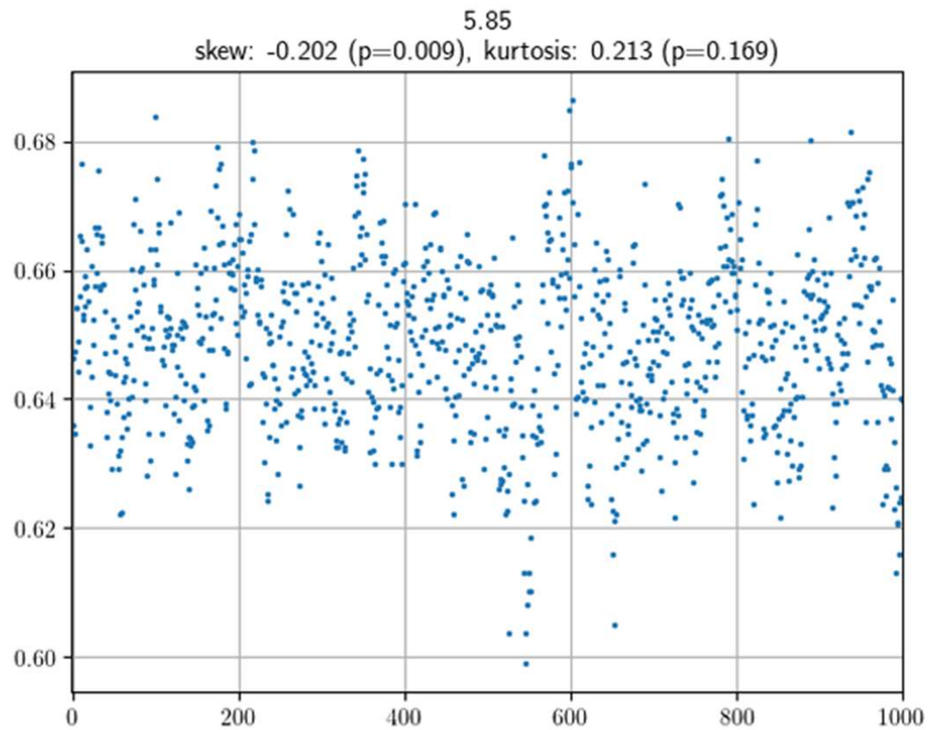

FIG. 9. for $\beta = 5.85$

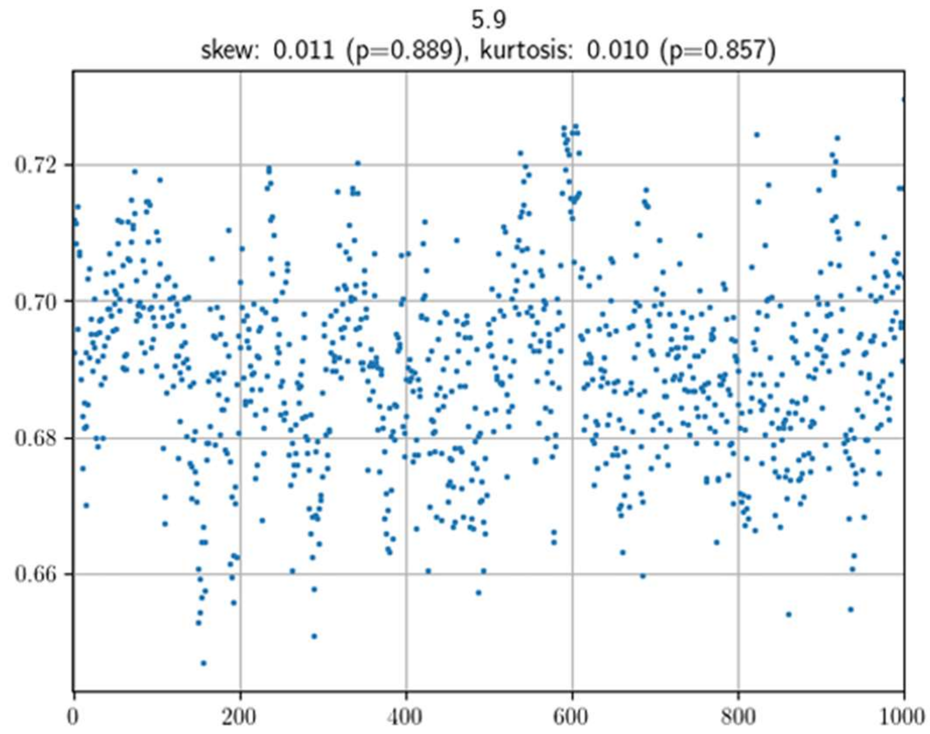

FIG. 10. for $\beta = 5.9$

EXPERIMENTS AND RESULTS

Results obtained from automatic windowing and their corresponding integrated τ values

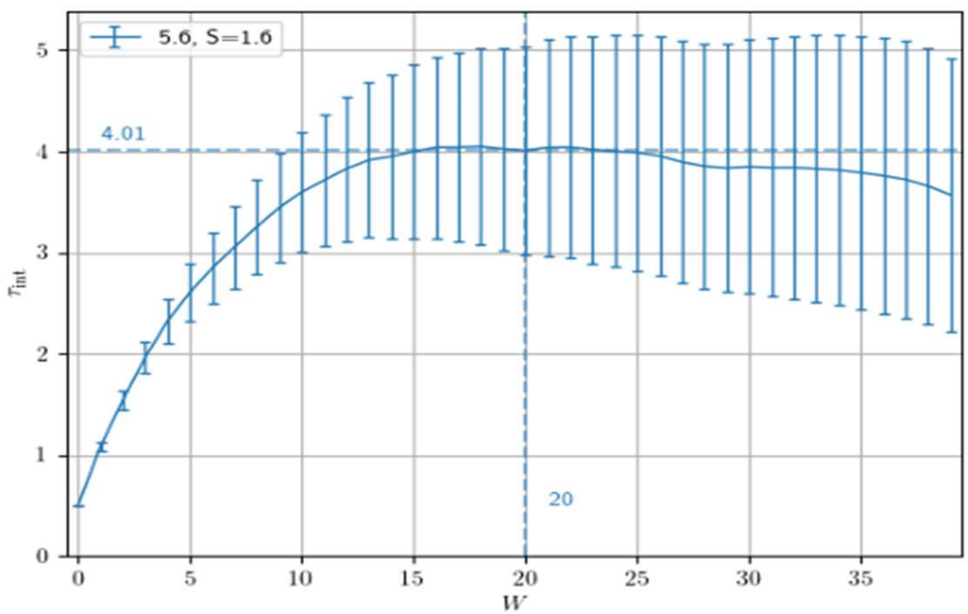

FIG. 11. $\tau_{\rm int}$ vs W for $\beta = 5.6$

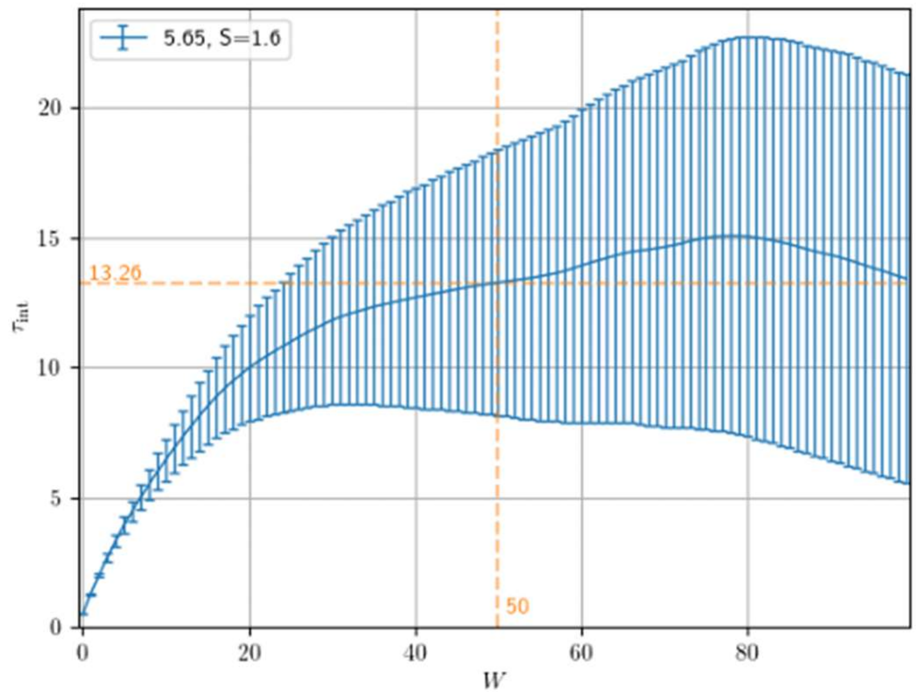

FIG. 12. $\tau_{\rm int}$ vs W for $\beta = 5.65$

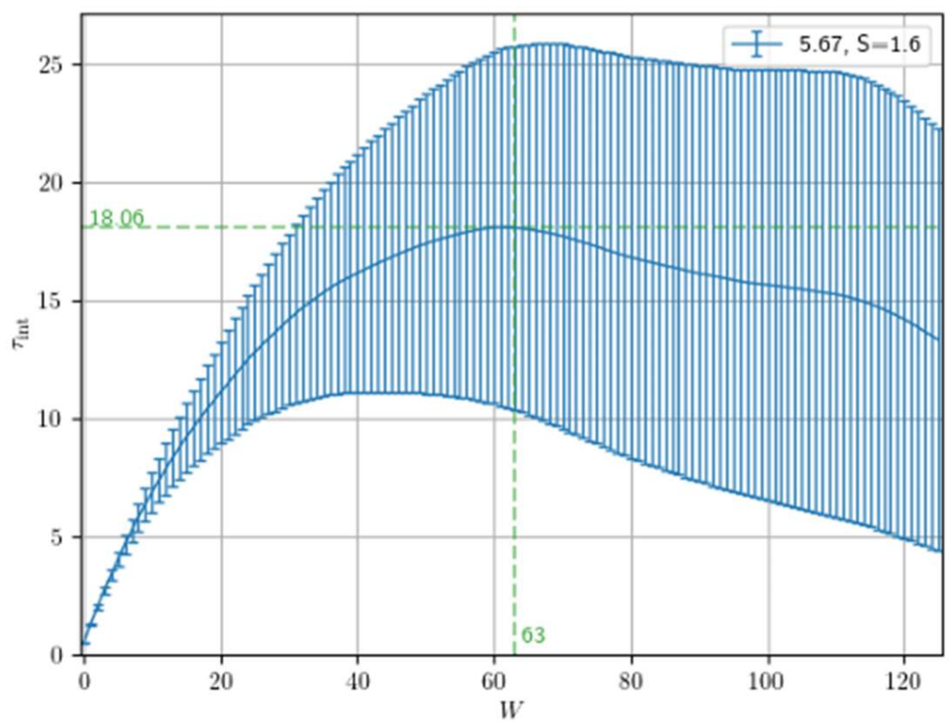

FIG. 13. τ_{int} vs W for $\beta = 5.67$

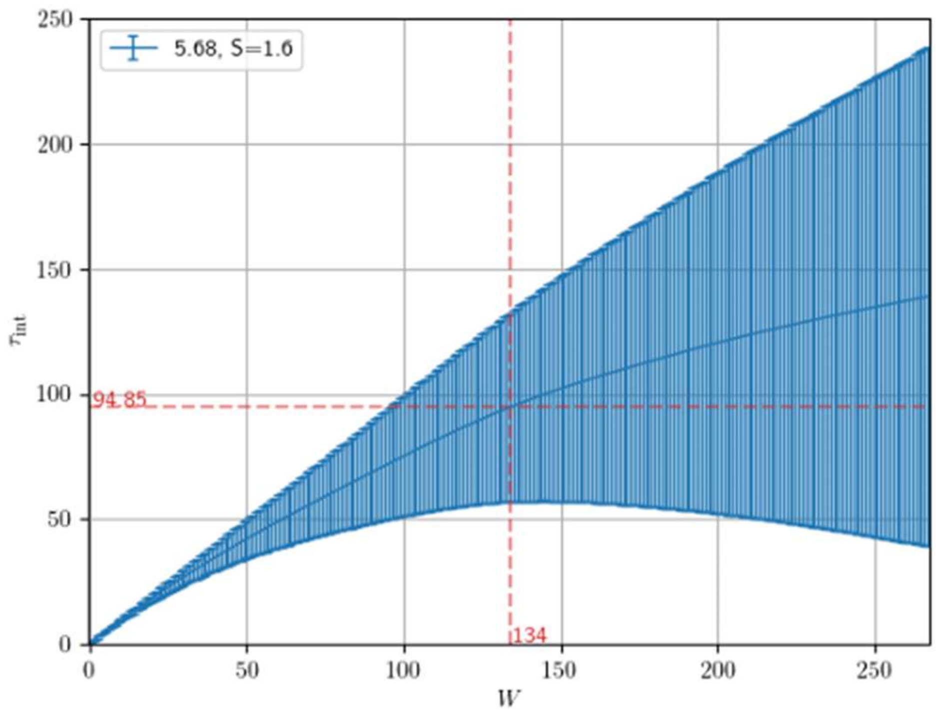

FIG. 14. τ_{int} vs W for $\beta = 5.68$

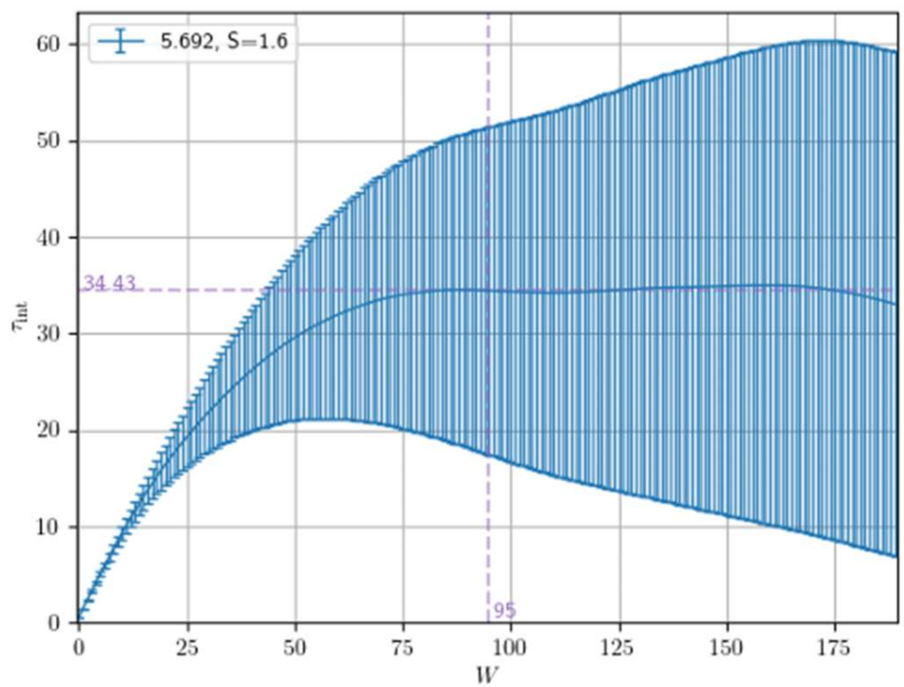

FIG. 15. $\tau_{\rm int}$ vs W for $\beta = 5.692$

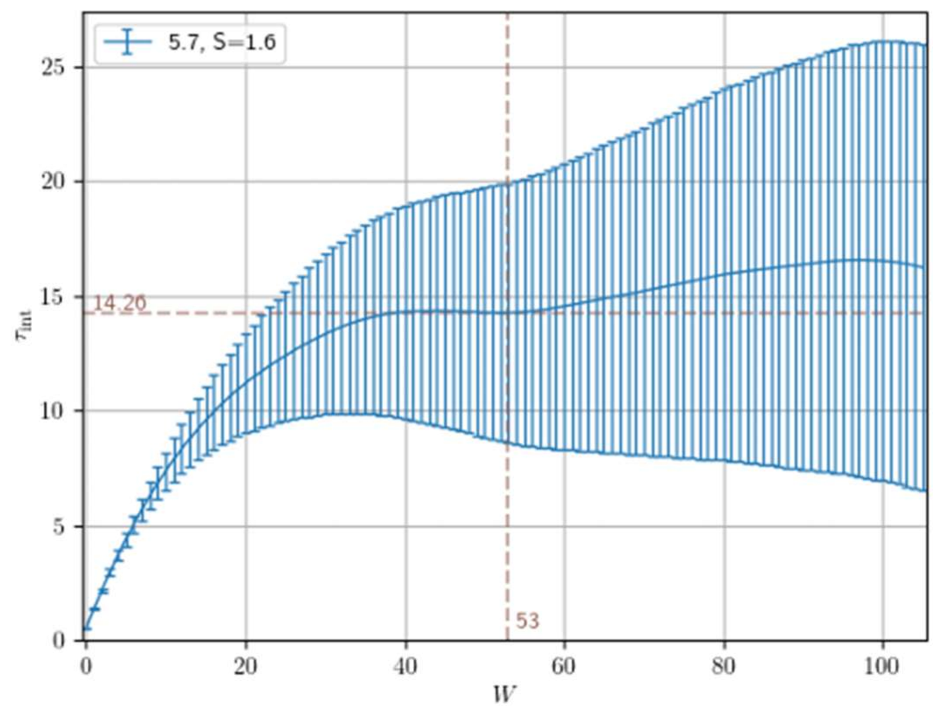

FIG. 16. τ_{int} vs W for $\beta = 5.7$

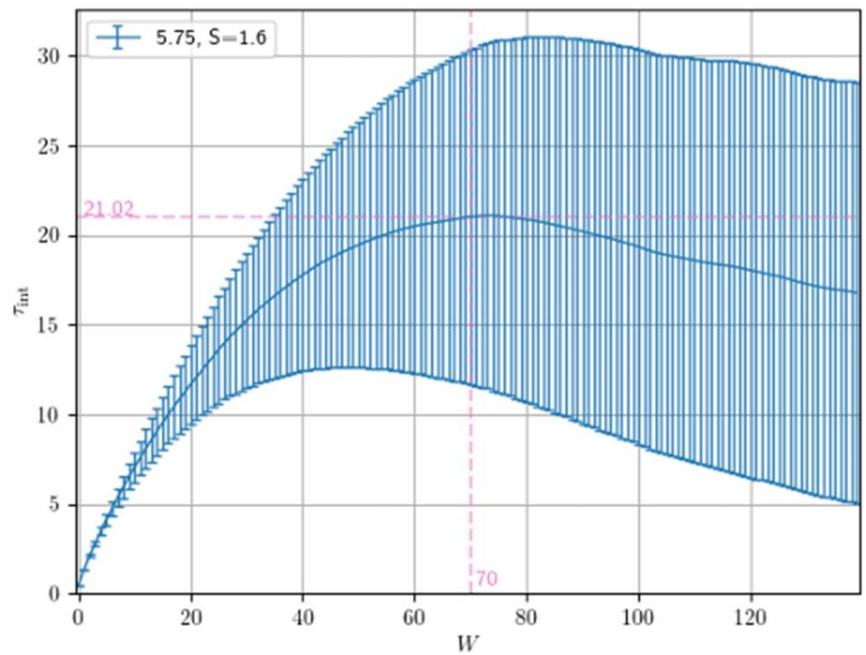

FIG. 17. τ_{int} vs W for $\beta = 5.75$

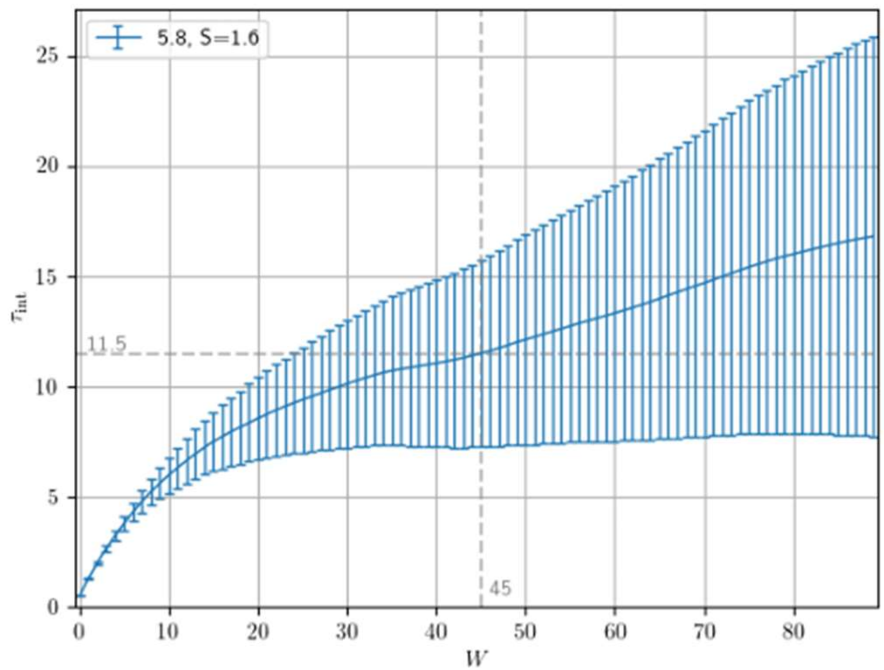

FIG. 18. $\tau_{\rm int}$ vs W for $\beta = 5.8$

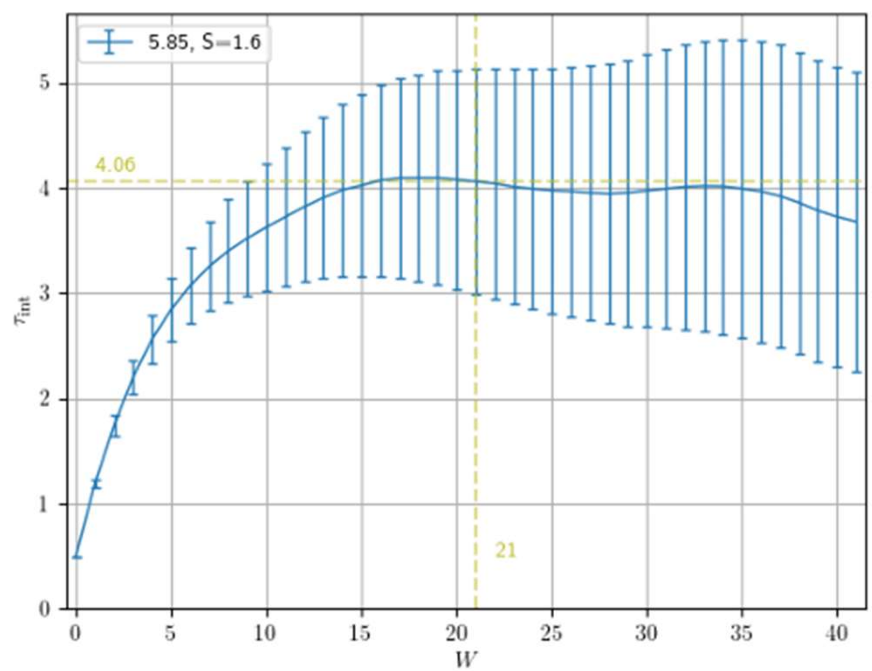

FIG. 19. $\tau_{\rm int}$ vs W for $\beta = 5.85$

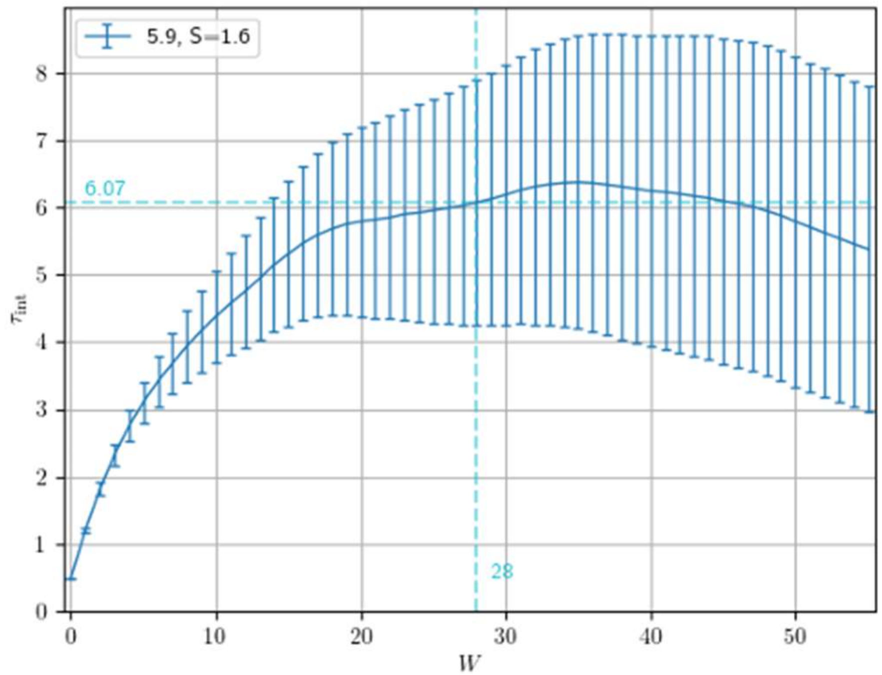

FIG. 20. $\tau_{\rm int}$ vs W for $\beta = 5.9$

EXPERIMENTS AND RESULTS

Results:

- Figures [11-20] are plotted for integrated autocorrelation time vs window size used for each value of β.
- As discussed above, the optimal window size was calculated using an automatic windowing algorithm implemented in Python.
- The vertical and horizontal dashed line marks the value of optimal window size (or lag) and the corresponding value of τ_{int} respectively.
- We have chosen the value of our hypothesis param eter S as 1.6, as τ_{int} reaches a plateau around the chosen W value for all the lattice gauge coupling values.

References:

[1] Wolff, U. (2006). Monte Carlo errors with less errors *arXiv:hep-lat/0306017*. Retrieved from `https://doi.org/10.48550/arXiv.hep-lat/0306017`

[2] Madras, N & Sokal, AD 1988, 'The pivot algorithm: A highly efficient Monte Carlo method for the self-avoiding walk *Journal of Statistical Physics, vol. 50, no. 1-2, pp. 109-186*. Retrieved from `https://doi.org/10.1007/BF01022990`