Water in Nanotubes: A New Phase of Water?

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A Very Useful Theorem

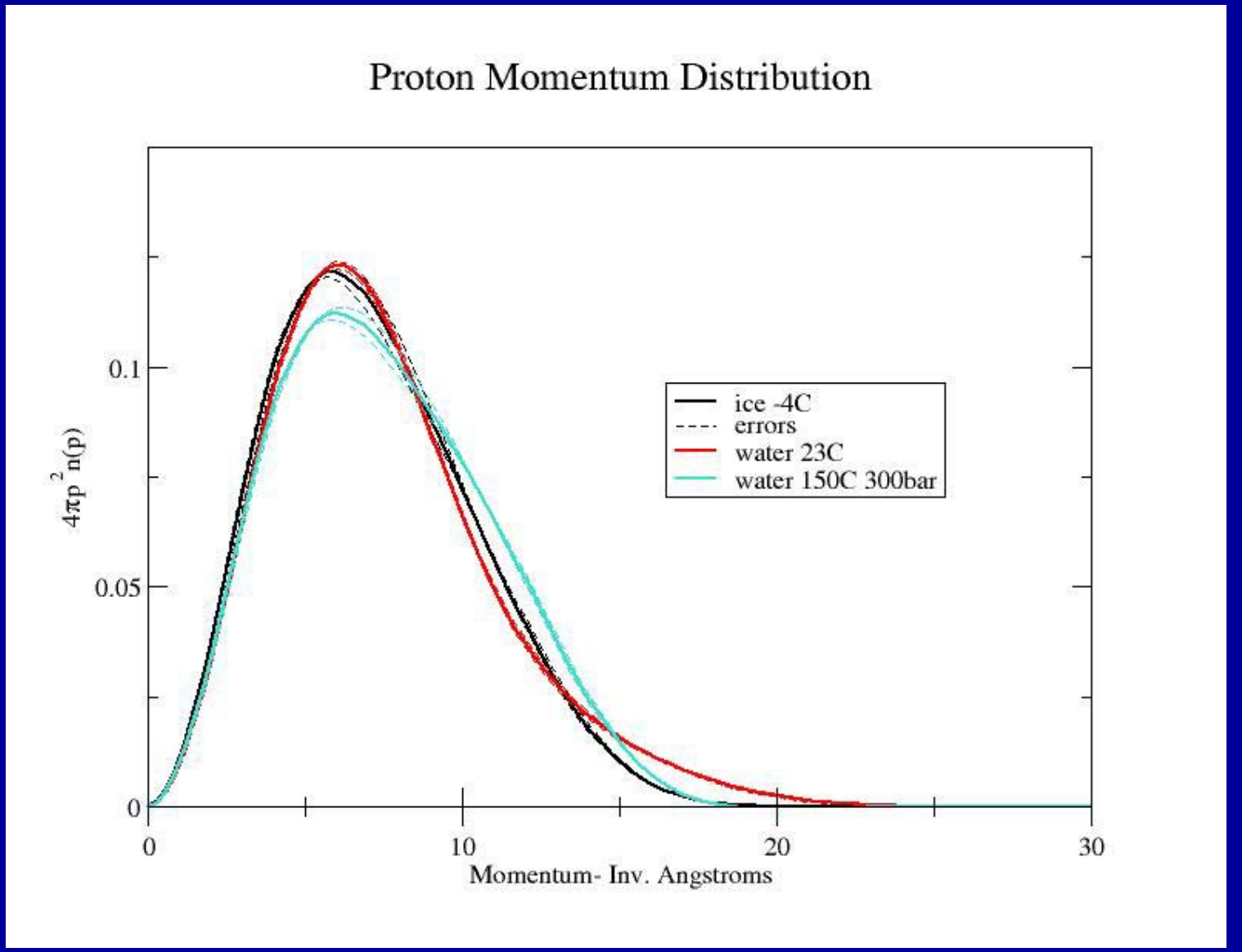
$$\frac{M}{q} J(y, \hat{q}) = \frac{M}{q} \int n(\vec{p}) \delta(y - \vec{p}.\hat{q}) d\vec{p}$$

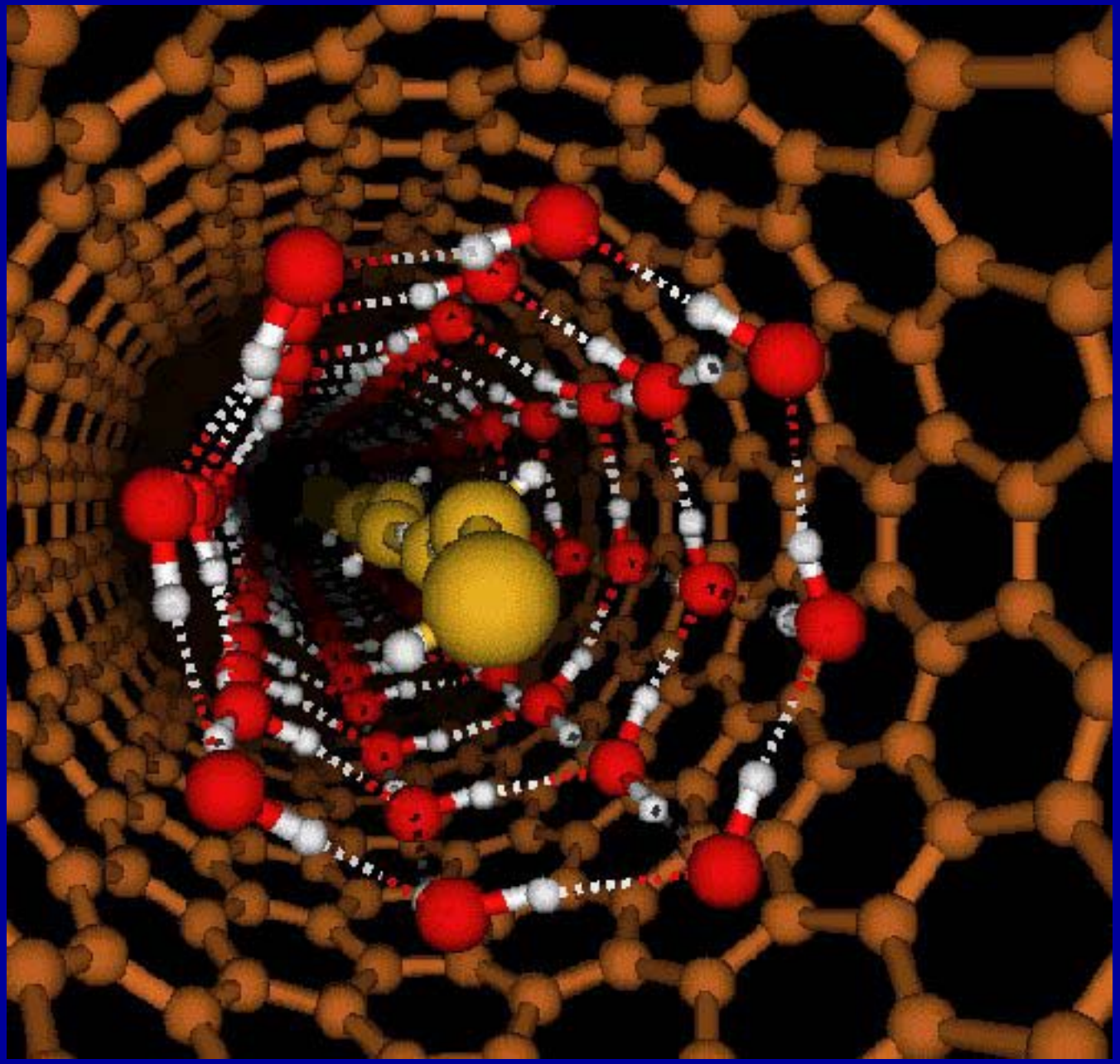
If

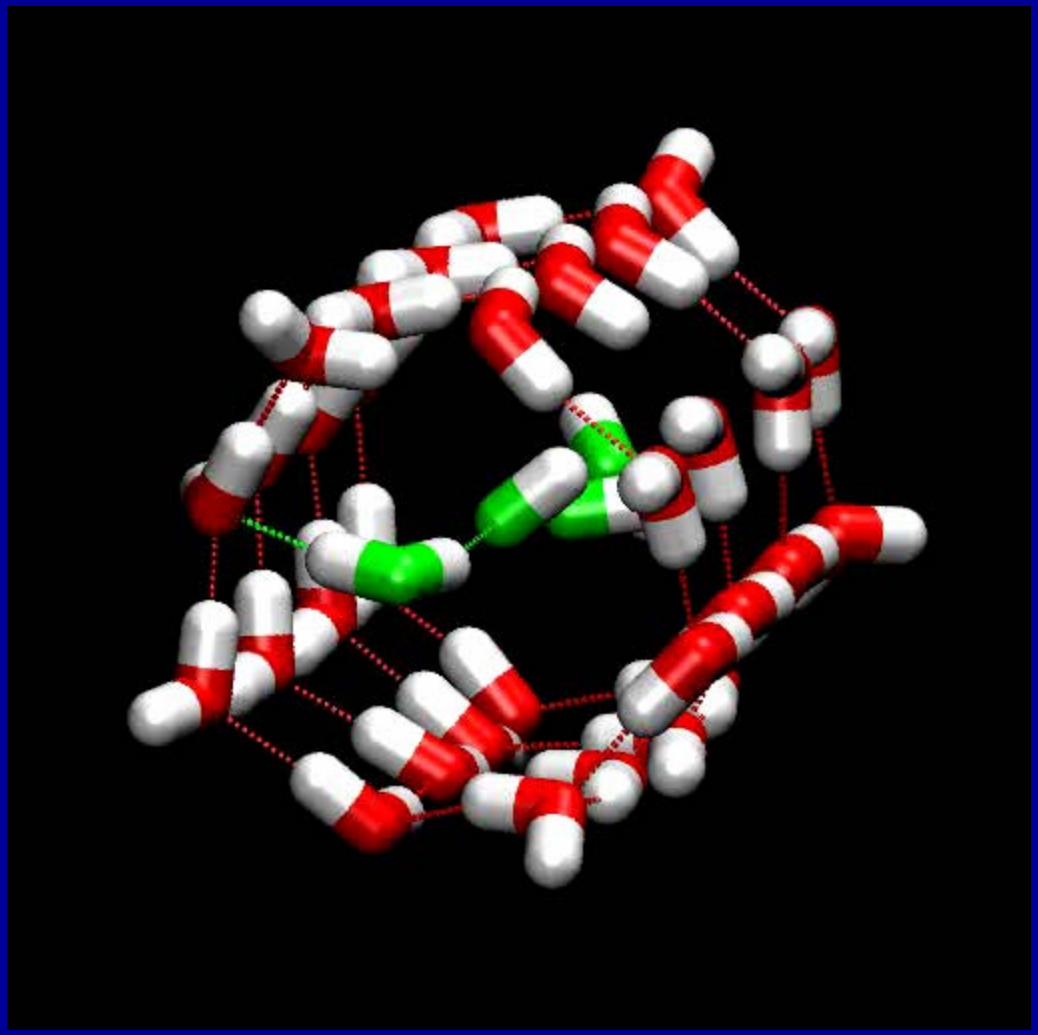
$$J(y, \hat{\mathbf{q}}) = \sum_{l,m,n} \frac{e^{-y^2}}{\sqrt{\pi}} a_{l,m,n} H_{2n+l}(y) Y_{l,m}(\hat{\mathbf{q}})$$

then

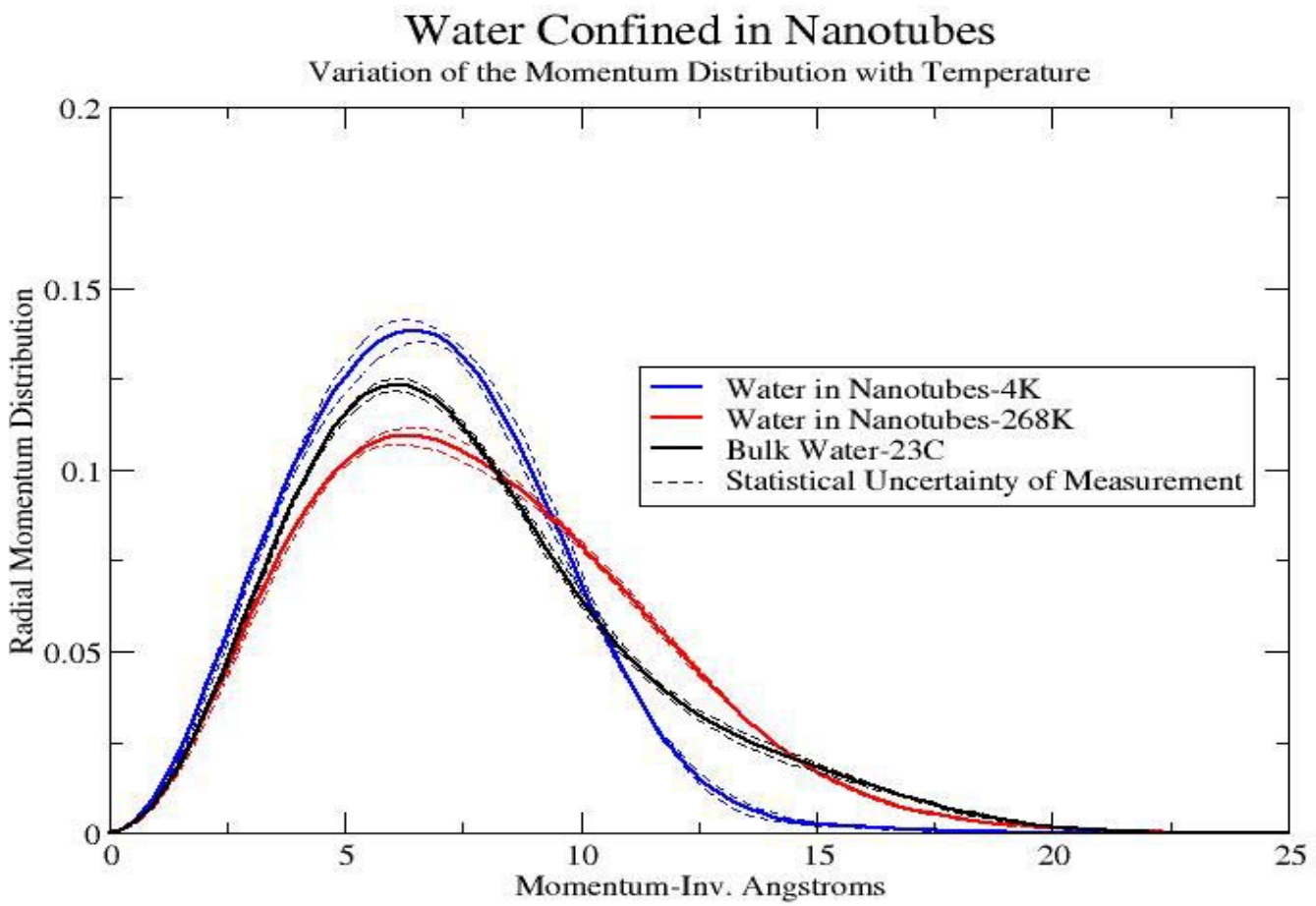
$$n(\mathbf{p}) = \sum_{l,m,n} \frac{e^{-p^2}}{\pi^{\frac{3}{2}}} a_{l,m,n} n! 2^{2n+l} (-1)^n p^{2l} L_n^{l+\frac{1}{2}}(p^2) Y_{l,m}(\hat{\mathbf{q}})$$


Proton Momentum Distribution
0.1
0.05
0
$4\pi p^2 n(p)$
0
10
20
30
Momentum- Inv. Angstroms
ice -4C
errors
water 23C
water 150C 300bar





Measured n(p)


Water Confined in Nanotubes
Variation of the Momentum Distribution with Temperature
Radial Momentum Distribution
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
Momentum-Inv. Angstroms
Water in Nanotubes-4K
Water in Nanotubes-268K
Bulk Water-23C
Statistical Uncertainty of Measurement

PIMD calculation of n(p) of shell-chain model