

Supporting information for: On the Equivalence of Schemes for Simulating Bilayers at Constant Surface Tension

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1 Full Histogram Data for $N_{lip}=256$

Figures S1 to S3 display both the probability density profiles as well as the deviations from the best estimate for V_{lip} , A_{lip} , and L_{\perp} with $N_{lip} = 256$ and $\gamma = 0.0$. Figures S4 to S6 display the same data for $N_{lip} = 256$ and $\gamma = 2.0$.

As discussed in Section 5 of the main paper,¹ the variation between all sampled histograms are reasonably within the calculated error bars.

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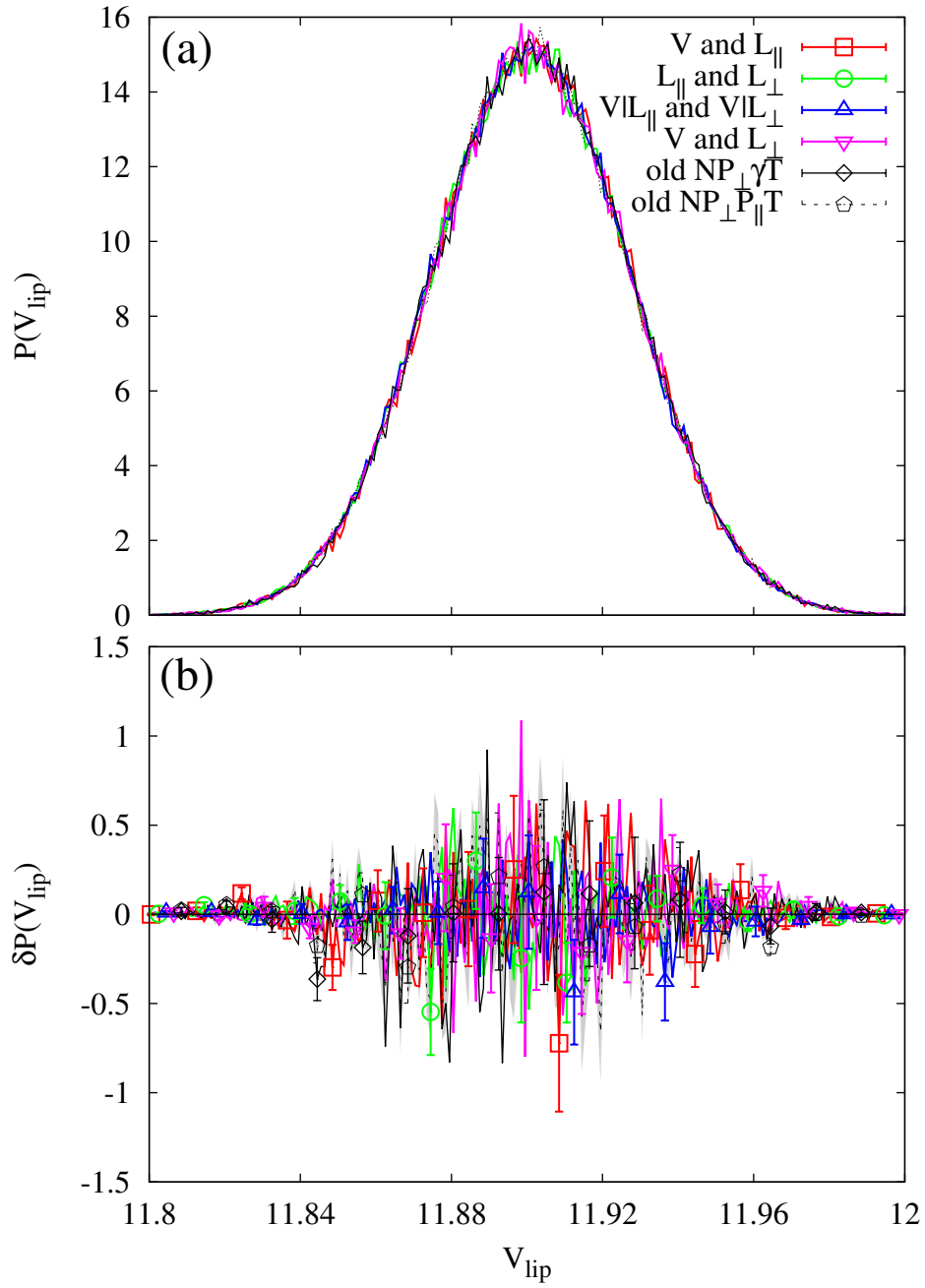


Figure S1: V_{lip} probability density and deviations for $N_{lip} = 256$ and $\gamma = 0.0$. Displayed data symbols are staggered across MC move sets and only shown every 12 points for readability.

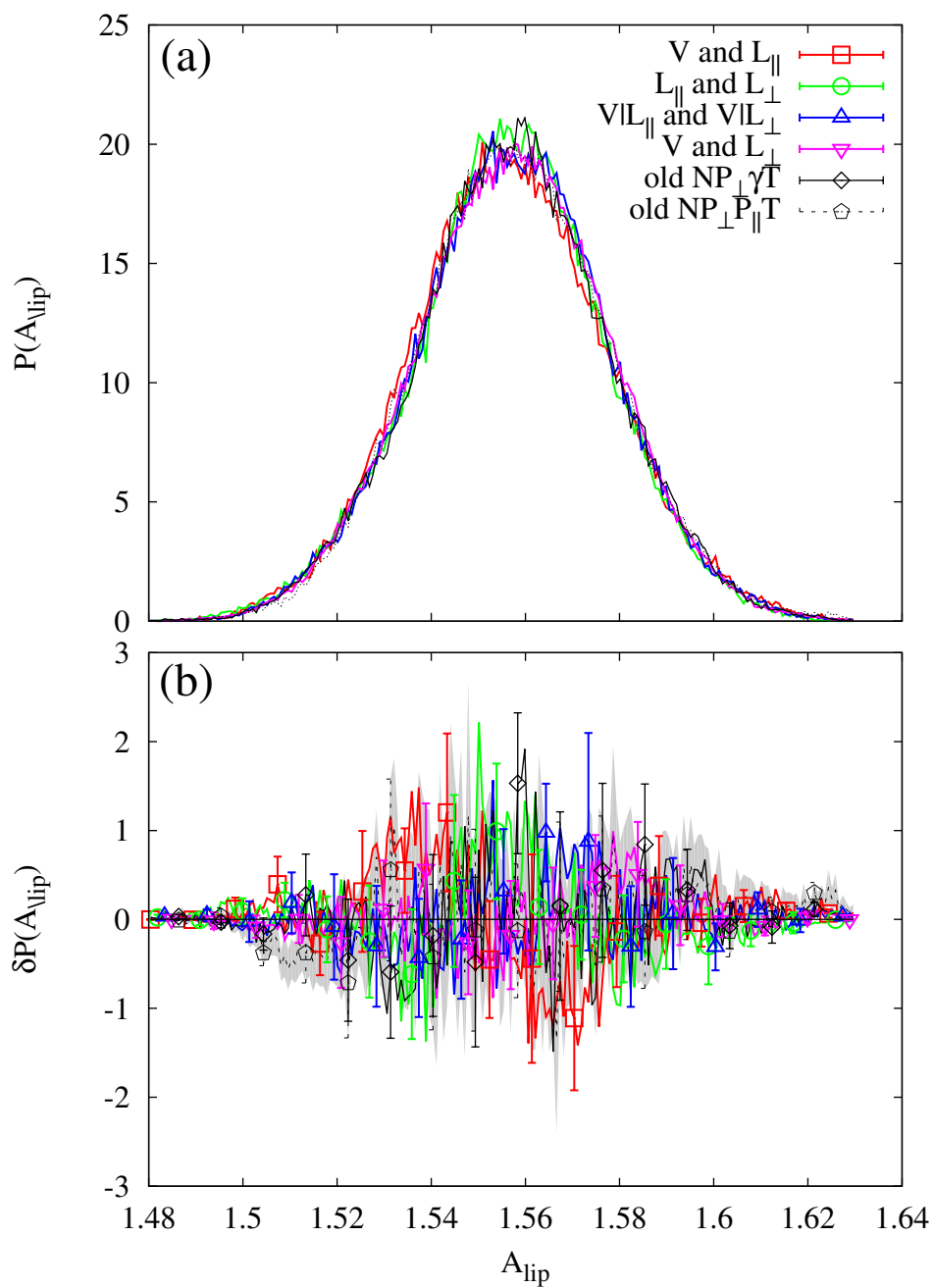


Figure S2: A_{lip} probability density and deviations for $N_{lip} = 256$ and $\gamma = 0.0$. Displayed data symbols are staggered across MC move sets and only shown every 12 points for readability.

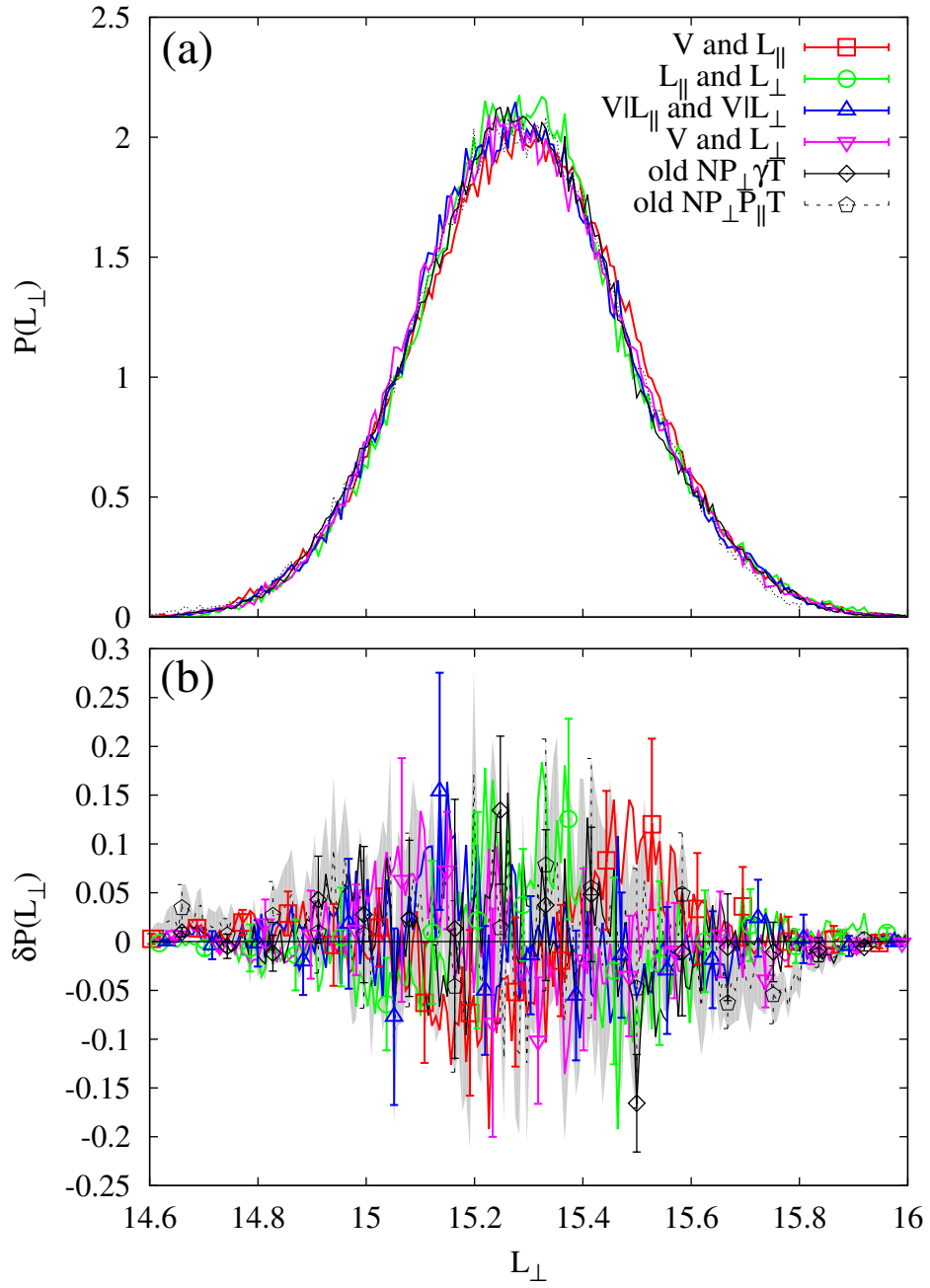


Figure S3: L_{\perp} probability density and deviations for $N_{\text{lip}} = 256$ and $\gamma = 0.0$. Displayed data symbols are staggered across MC move sets and only shown every 12 points for readability.

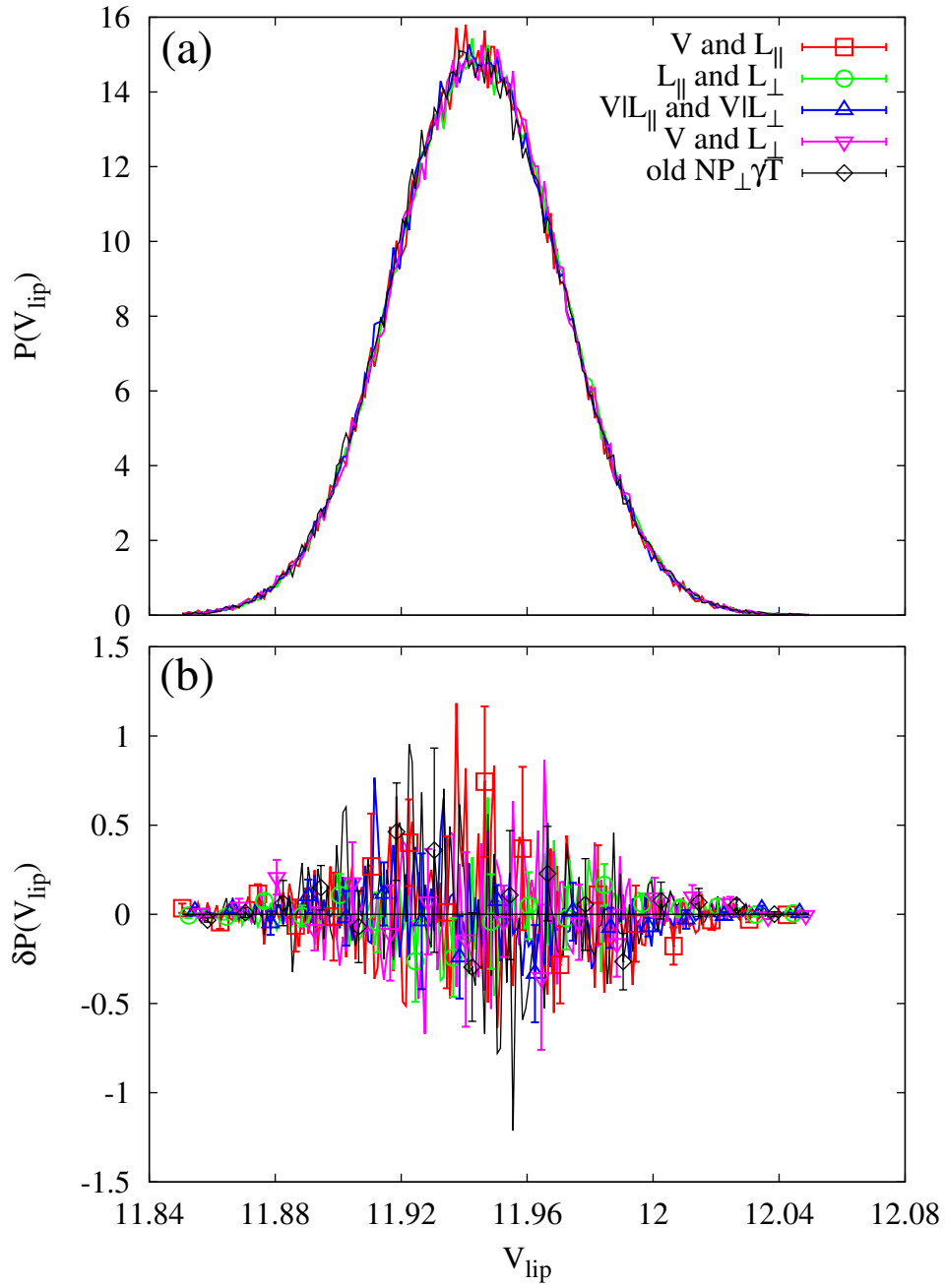


Figure S4: V_{lip} probability density and deviations for $N_{lip} = 256$ and $\gamma = 2.0$. Displayed data symbols are staggered across MC move sets and only shown every 12 points for readability.

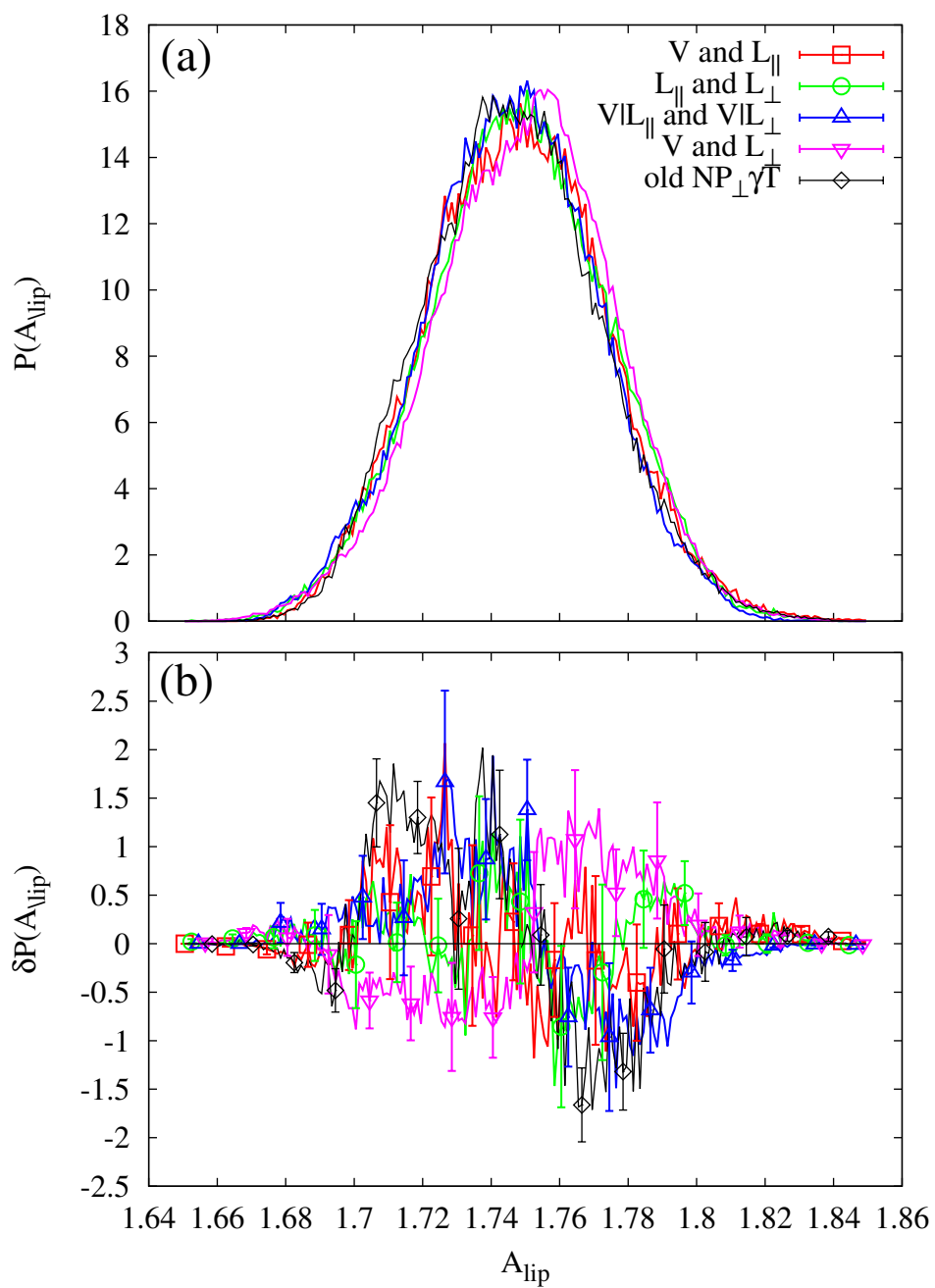


Figure S5: A_{lip} probability density and deviations for $N_{lip} = 256$ and $\gamma = 2.0$. Displayed data symbols are staggered across MC move sets and only shown every 12 points for readability.

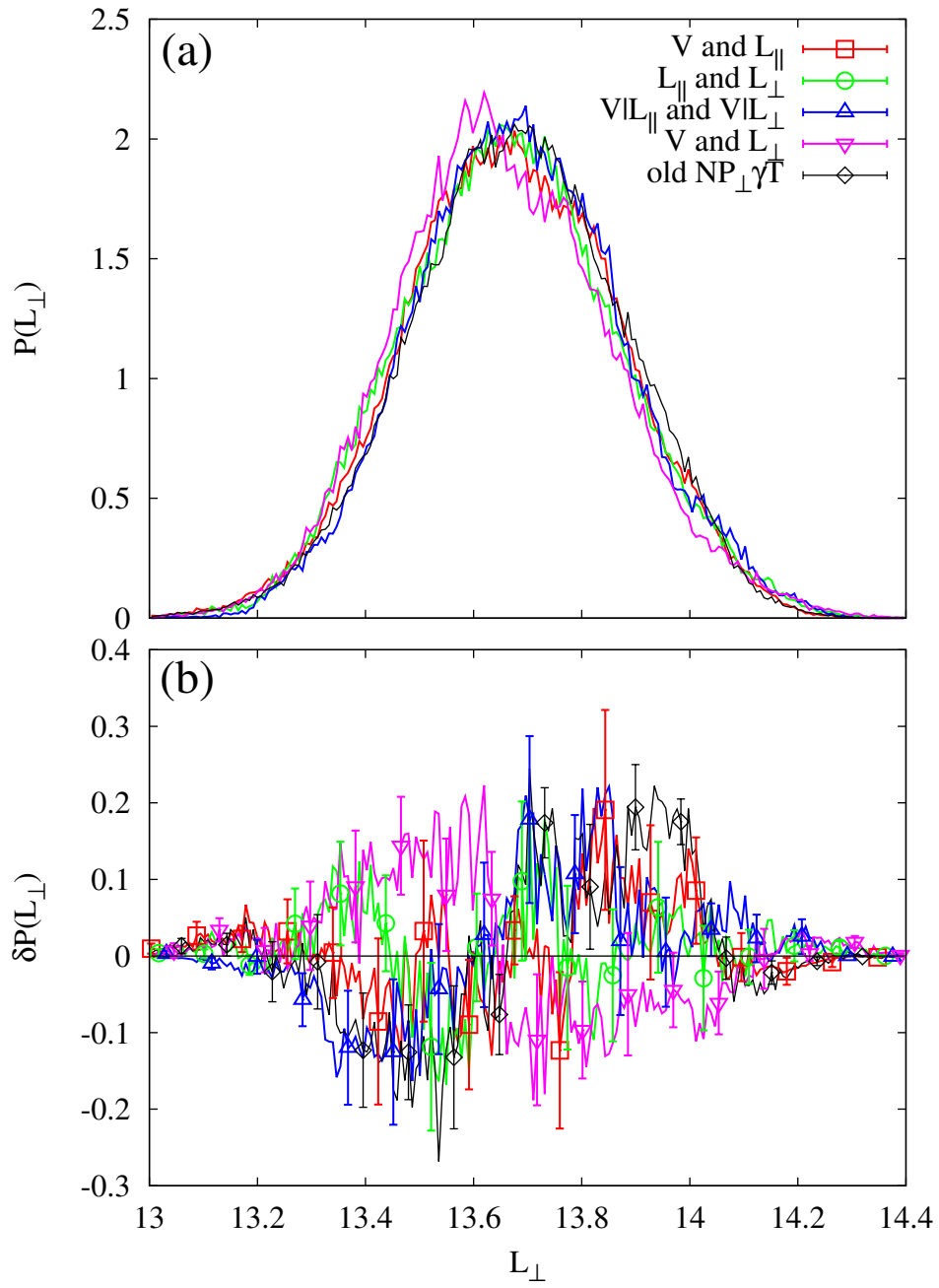


Figure S6: L_{\perp} probability density and deviations for $N_{\text{lip}} = 256$ and $\gamma = 2.0$. Displayed data symbols are staggered across MC move sets and only shown every 12 points for readability.

References

- (1) Rodgers, J. M.; Smit, B. *J. Chem. Theory Comput.* **2011**, *submitted*.