TITLE

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I. INTRODUCTION

- Detail balance
- Ergodic
- Stochastic
- Entropy driven phase transitions
- Equations of state

II. METHODOLOGY

III. MODEL

Our simulated system consists of N number of particles enclosed in a cubic container of volume V. The potential energy between any two particles in the system is given by the Lennard-Jones potential, expressed in the reduced unit scheme as

$$U_{LJ} = 4\left(\frac{1}{r^{12}} - \frac{1}{r^6}\right) \tag{1}$$

where r is the reduced distance between the particles. The number of particles in the system was kept constant for every initial configuration and, as such, achieving a given reduced density required the container length to be varied. When applying perturbations to a particle in the system, the interaction potential was considered for every other particle in the system under periodic boundary conditions, or up to half the container length.

Virial equation and configuration energy per particle

The model and method were verified by direct comparison to Monte Carlo results at liquid and vapour-like densities along isotherms $T^* = 0.85, 0.90$ published by United States' National Institute of Standard and Technology (NIST). NIST's results were for 500 particles whose Lennard-Jones interaction had been truncated to 3σ and standard long range corrections had been applied. Their systems were equilibrated for 5.0e7 moves and quantities calculated over 2.5e8 moves. Figure 1 shows the configuration energy per particle, u^*, and virial pressure, $p^* = P - \rho kT$ for both our system and NIST's. Our results were obtained as described in section II. See appendix B for the values and their associated uncertainties of NIST's and our simulations.

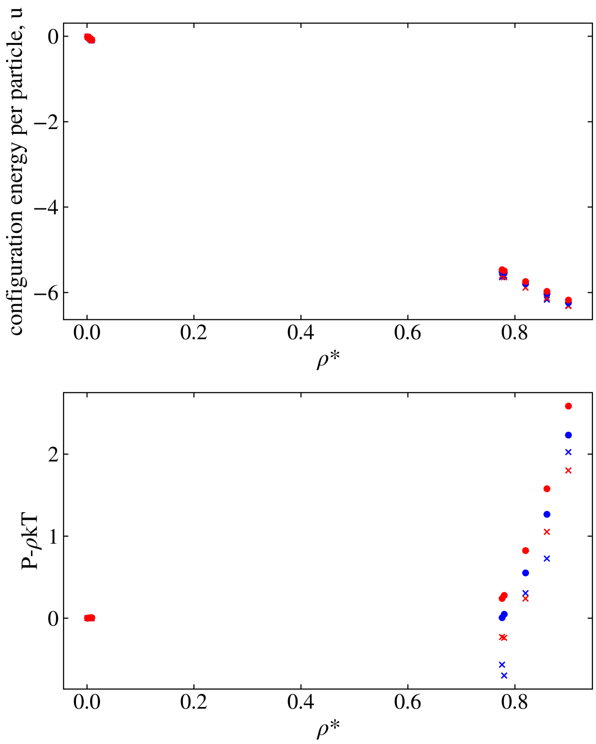

FIG. 1: Configuration energy per particle, u^*, and virial pressure, $p^* = P - \rho kT$ for NIST data (dots) and our model (crosses). The blue and red data are along isotherms $T^* = 0.85, 0.90$ respectively.

IV. RESULTS

The resulting reduced pressure and configuration energies as functions of the reduced density are shown in figures 2 (and...) respectively. Configuration energy can be seen to reduce from approximately 0 at $\rho^* = 0$ before reaching some local minimum value and increasing. The value of ρ^* at which this local minima is reached appears to vary as a function of the system temperature; the absolute value of the minima is decreased and occurs at smaller ρ^* at higher temperatures when compared to that of lower temperatures.

Interpretation - at lower densities we are essentially considering an ideal gas; compare to total energy u-config + u-kinetic

Reduced pressure can be seen to increase *exponentially* from approximately 0 at $\rho^* = 0$ with increasing ρ^*. The rate of increase can be seen to be greater at higher than

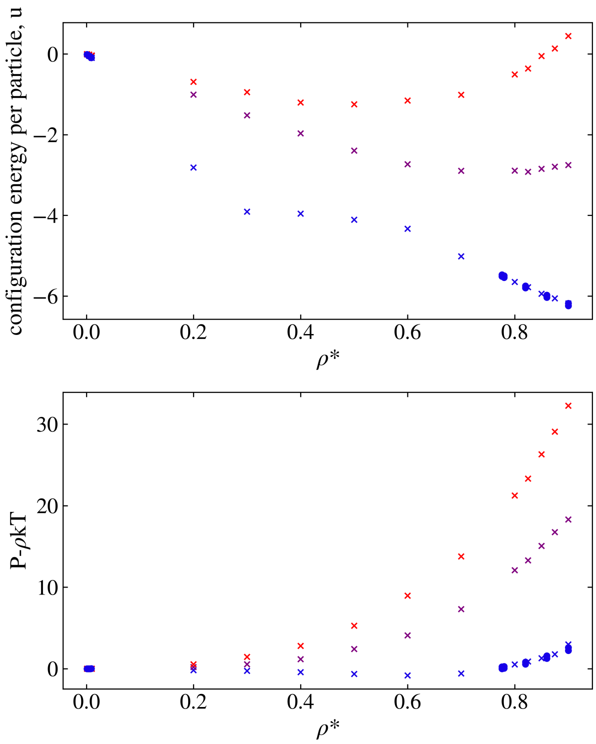

FIG. 2: Configuration energy per particle, u^*, and virial pressure, $p^* = P - \rho kT$ for NIST data (dots) and our model (crosses). The blue and red data are along isotherms $T^* = 0.85, 0.90$ respectively.

lower temperatures.

At very low ρ^* the system temperature is observed to have little impact on the configuration energy or pressure. However at larger ρ^* the difference between systems of different temperatures increases.

V. DISCUSSION

VI. CONCLUSIONS

References

[1] A. N. Other, Title of the Book, edition, publishers, place of publication (year of publication), p. 123.

[2] I. G. Hughes, T. P. A Hase, Measurements and their Uncertainties A Practical Guide to Modern Error Analysis, 1st, Oxford University Press, Oxford (2010)

APPENDIX A: ERROR ANALYSIS

All propagation of errors is performed as outlined in [2].

APPENDIX B: COMPARISON TO NIST DATA

T^*	ρ^*	U^*_{NIST}	$\pm$	U^*_{ours}	$\pm$	p^*_{NIST}	$\pm$	p^*_{ours}	$\pm$
0.85	1.00E-3	-1.0317E-2	2.34E-5	-9.968E-3	9.17E-5	8.4402E-4	4.66E-8	-5.288E-6	1.72E-7
	3.00E-3	-3.1019E-2	5.91E-5	-3.156E-2	2.87E-4	2.4965E-3	4.99E-7	-6.121E-5	1.48E-6
	5.00E-3	-5.1901E-2	7.53E-5	-5.485E-2	5 .07E-4	4.1003E-3	5.05E-7	-1.472E-4	4.75E-6
	7.00E-3	-7.2834E-2	1.34E-4	-7.499E-2	6.87E-4	5.6565E-3	7.96E-7	-2.854E-4	8.98E-6
	9.00E-3	-9.3973E-2	1.29E-4	-9.863E-2	9.18E-4	7.1641E-3	2.24E-6	-4.568E-4	1.51E-5
	7.76E-1	-5.5121	4.55E-4	-5.623	5.21E-2	6.7714E-3	1.77E-3	-5.577E-1	9.91E-2
	7.80E-1	-5.5386	7.26E-4	-5.611	5.14E-2	4.7924E-2	3.18E-3	-6.311E-1	9.88E-2
	8.20E-1	-5.7947	6.03E-4	-5.908	5.59E-2	5.5355E-1	4.13E-3	2.588E-1	1.25E-1
	8.60E-1	-6.0305	2.38E-3	-6.175	5.87E-2	1.2660	1.36E-2	4.973E-1	1.41E-1
	9.00E-1	-6.2391	5.27E-3	-6.346	6.17E-2	2.2314	2.72E-2	1.823	1.75E-1
0.90	1.00E-3	-9.9165E-3	1.89E-5	-9.989E-3	9.05E-5	8.9429E-4	2.48E-8	-6.475E-6	1.76E-7
	3.00E-3	-2.9787E-2	3.21E-5	-3.065E-2	2.79E-4	2.6485E-3	2.54E-7	-4.368E-5	1.70E-6
	5.00E-3	-4.9771E-2	3.80E-5	-5.226E-2	4.75E-4	4.3569E-3	2.19E-7	-1.426E-4	4.35E-6
	7.00E-3	-6.9805E-2	7.66E-5	7.179E-2	6.50E-4	6.0193E-3	1.02E-6	-3.075E-4	8.14E-6
	9.00E-3	-8.9936E-2	2.44E-5	-9.151E-2	8.33E-4	7.6363E-3	1.44E-6	-4.295E-4	1.41E-5
	7.76E-1	-5.4689	4.20E-4	-5.615	5.21E-2	2.4056E-1	2.74E-3	-2.486E-1	1.04E-1
	7.80E-1	-5.4956	7.86E-4	-5.627	5.20E-2	2.7851E-1	2.97E-3	-2.576E-1	1.06E-1
	8.20E-1	-5.7456	7.51E-4	-5.870	5.53E-2	8.2386E-1	2.85E-3	2.921E-1	1.25E-1
	8.60E-1	-5.9753	5.53E-4	-6.130	5.89E-2	1.5781	3.29E-3	1.193	1.53E-1
	9.00E-1	-6.1773	1.57E-3	-6.312	6.14E-2	2.5848	9.54E-3	1.871	1.75E-1