Esercizio simulazione Monte-Carlo

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Monte-Carlo for adsorbate configurations

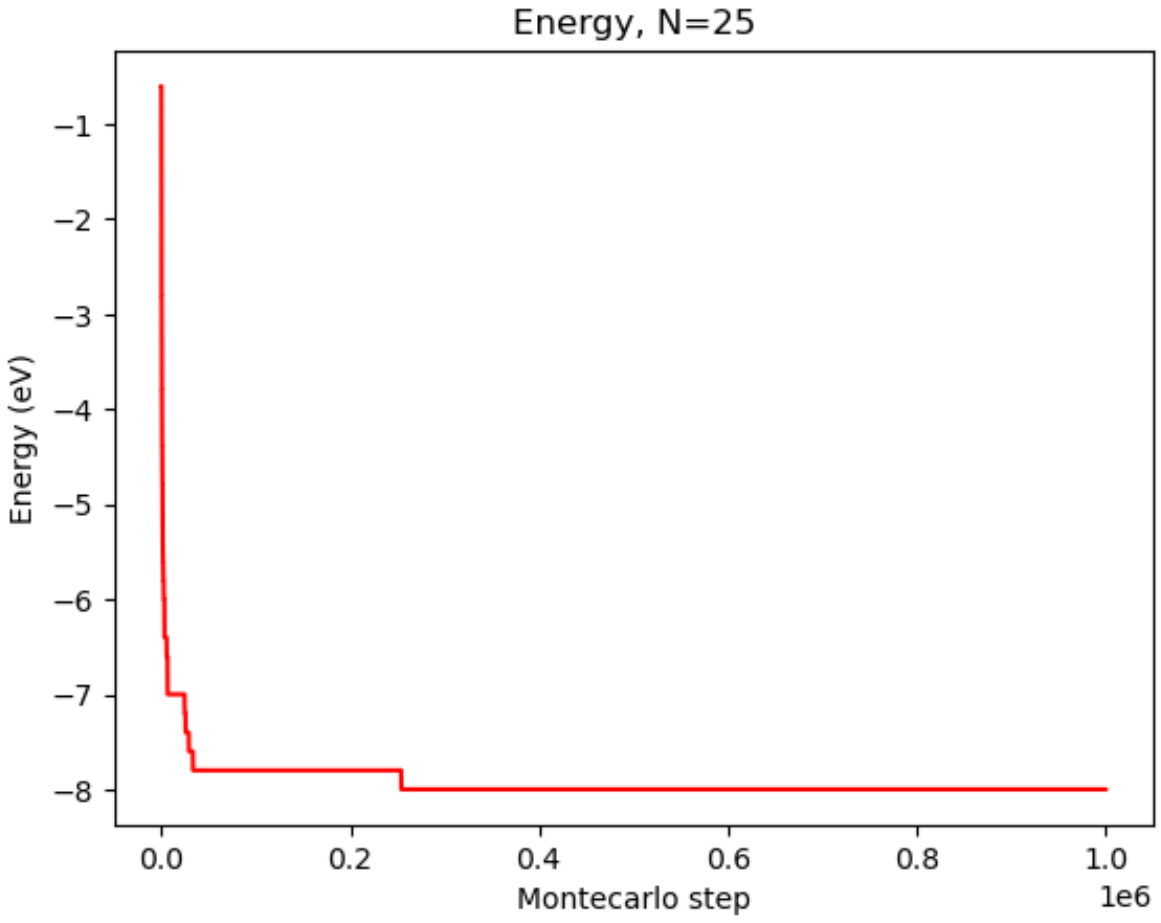
Study a system of adsorbate atom with Monte-Carlo

The energy is

$$H = \frac{1}{2} \sum_{i=0}^{N-1} n_1(i) J_1$$

Zero temperature MC, minimum energy configuration

$$N = 25, E_{min} = -8\,eV$$



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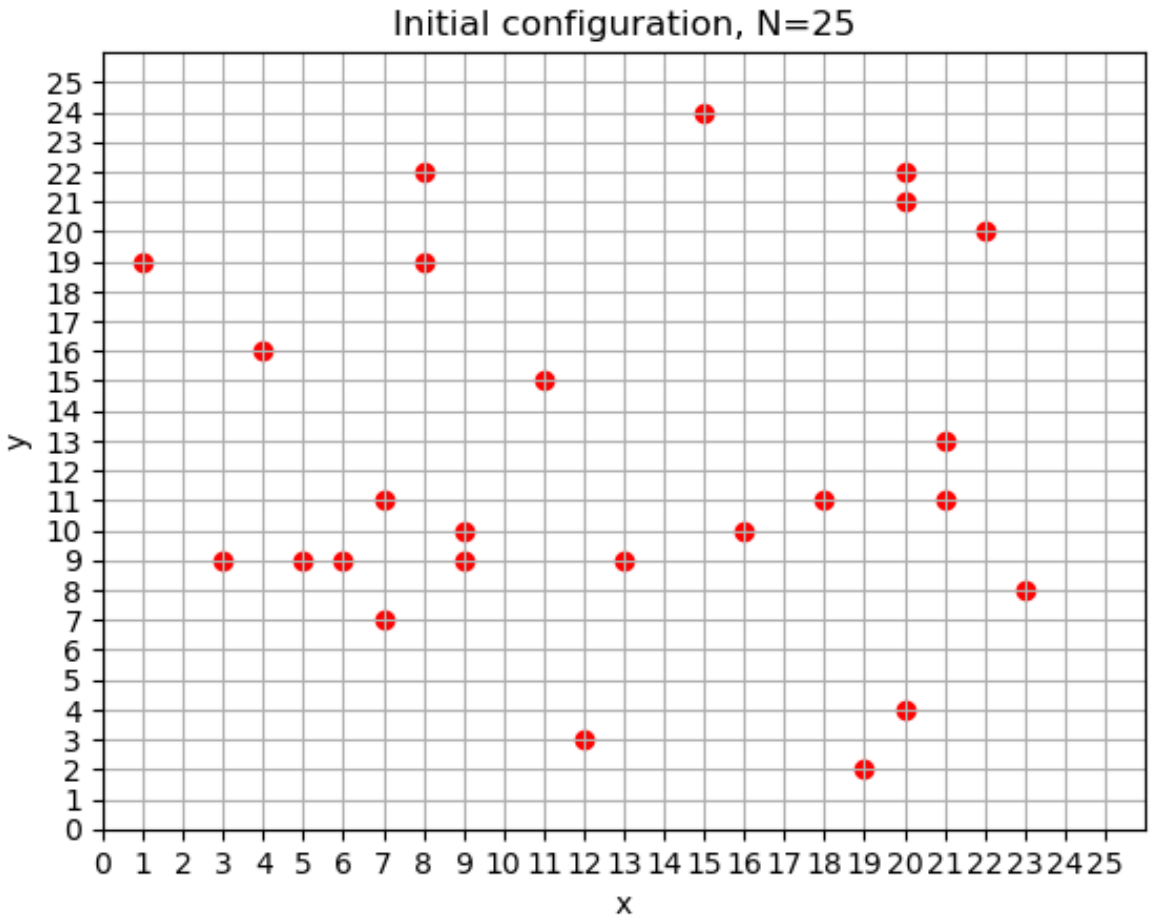

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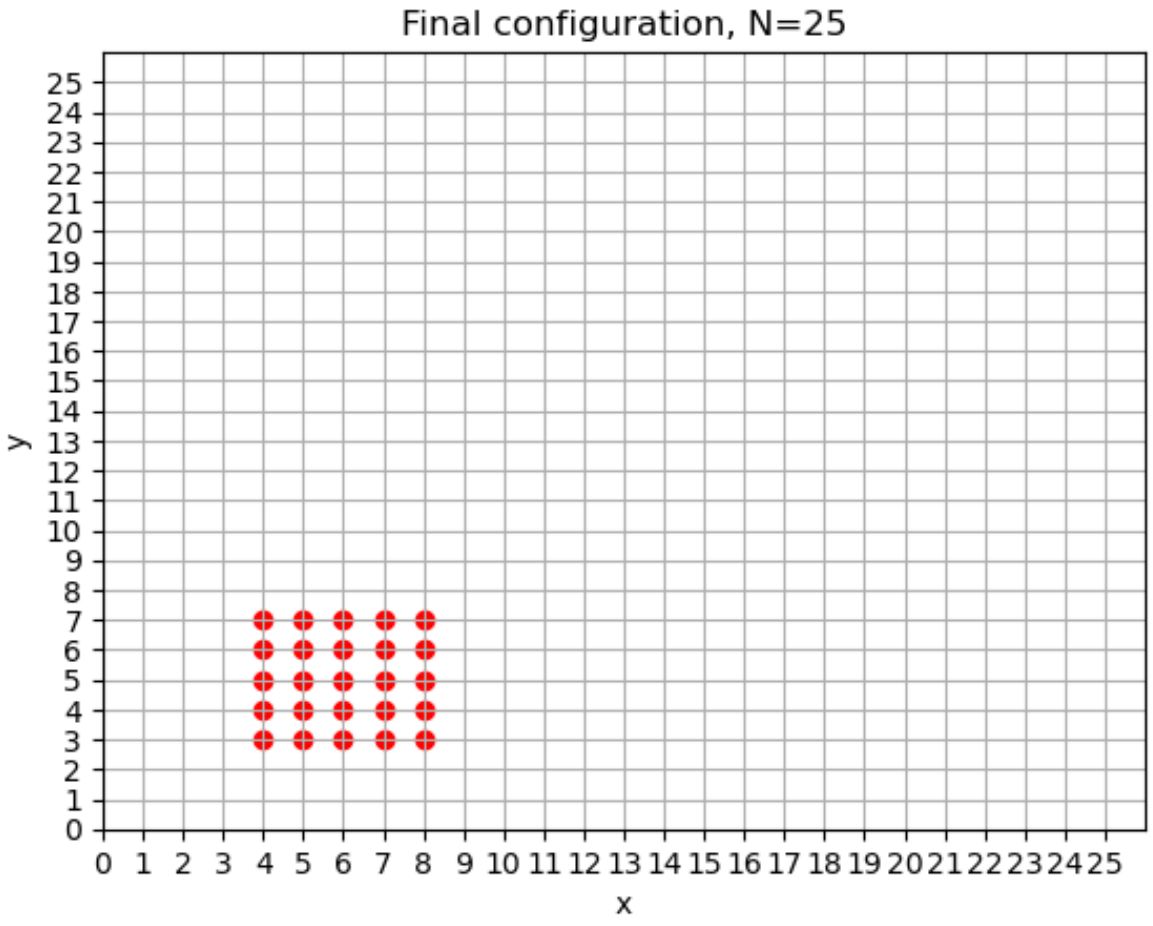
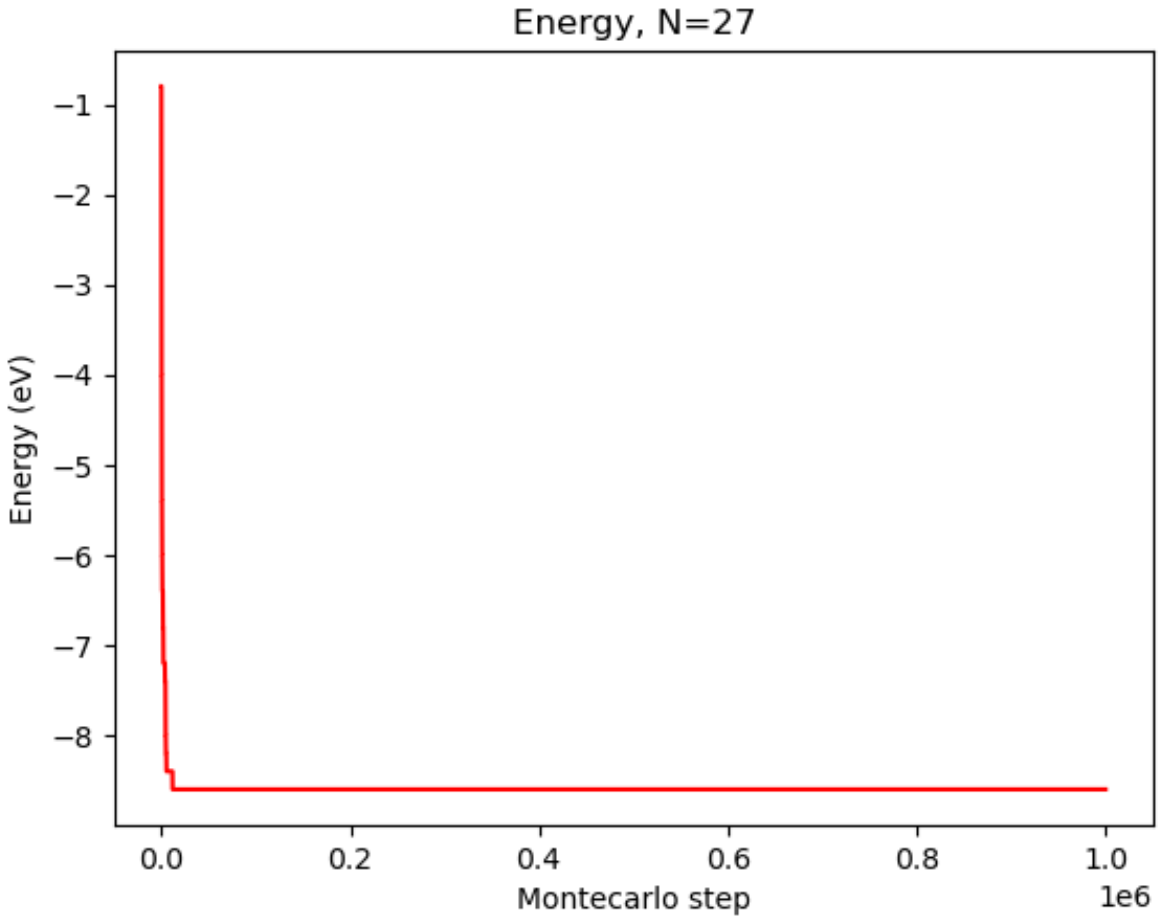


Zero temperature MC, minimum energy configuration

$$N = 27, E_{min} = -8.6\, eV$$



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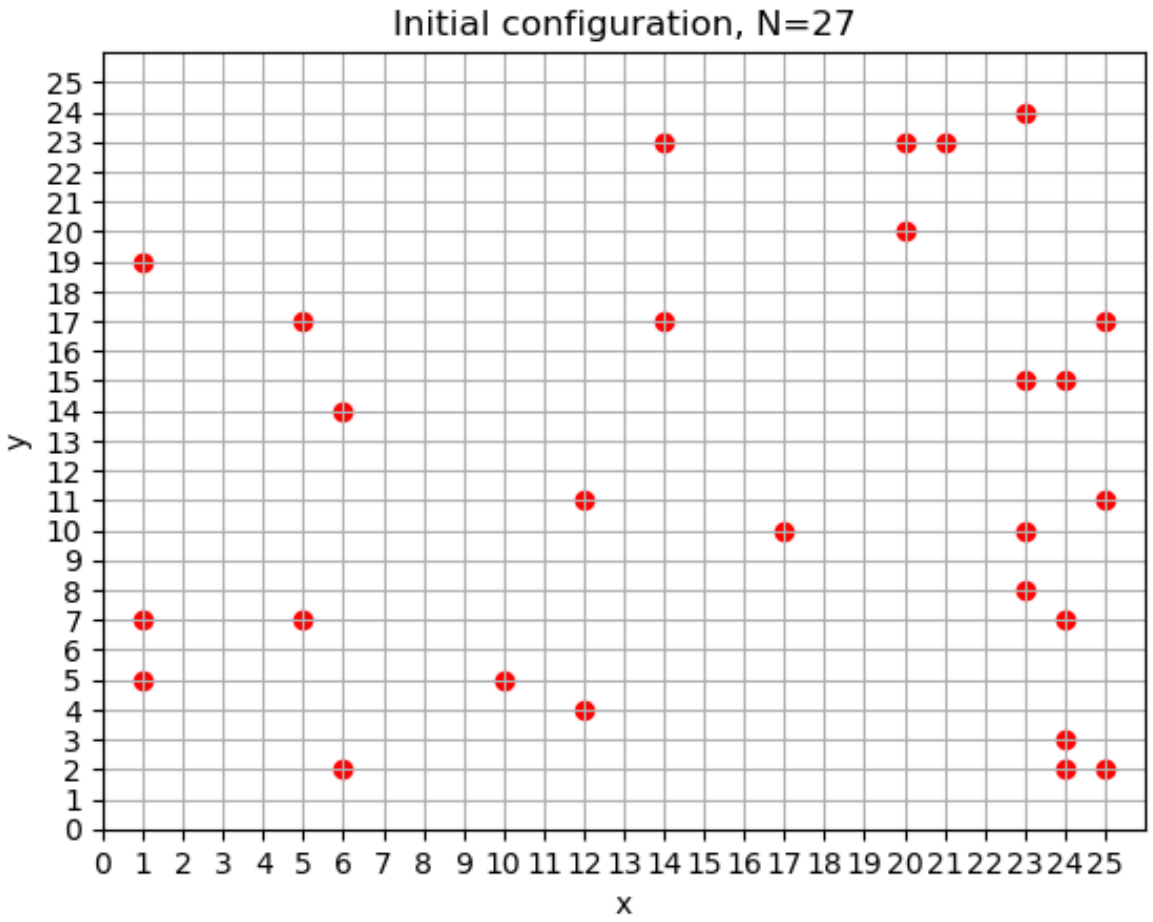

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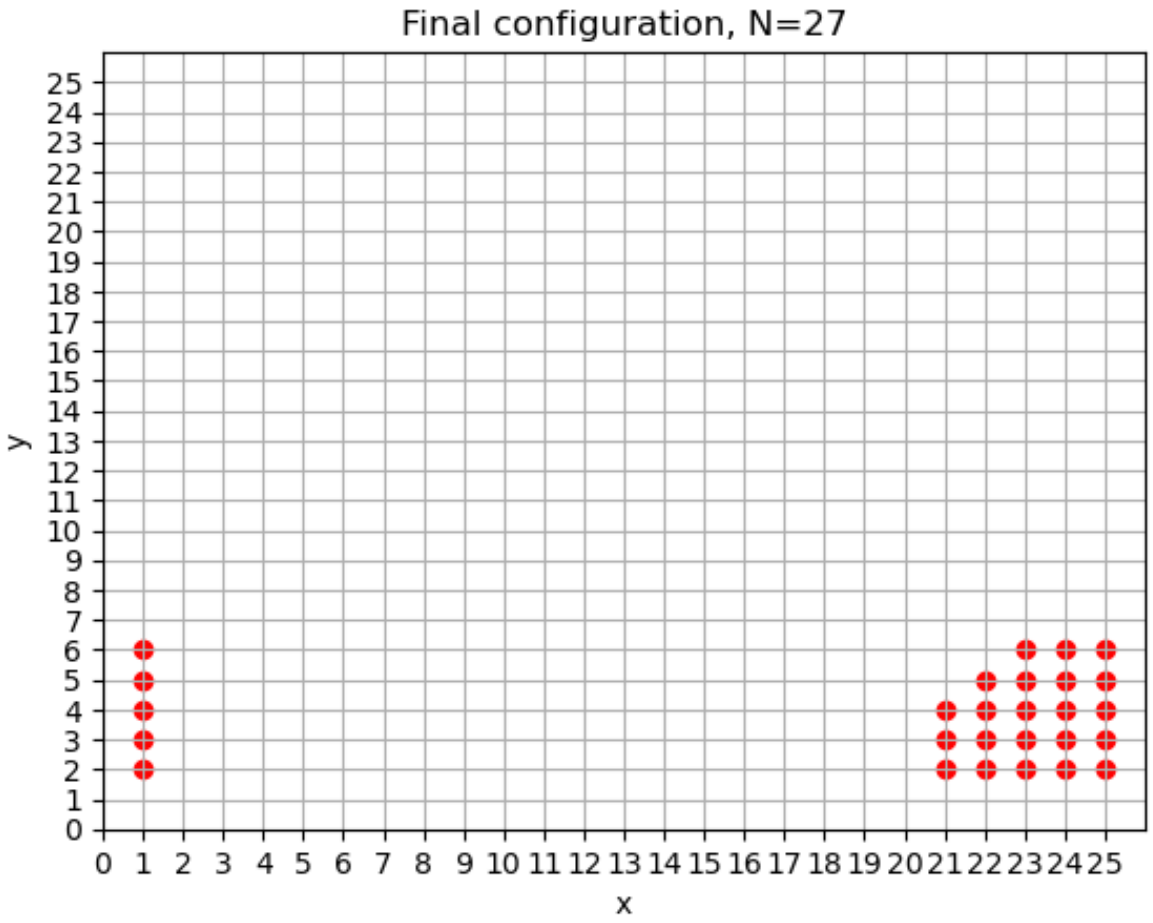
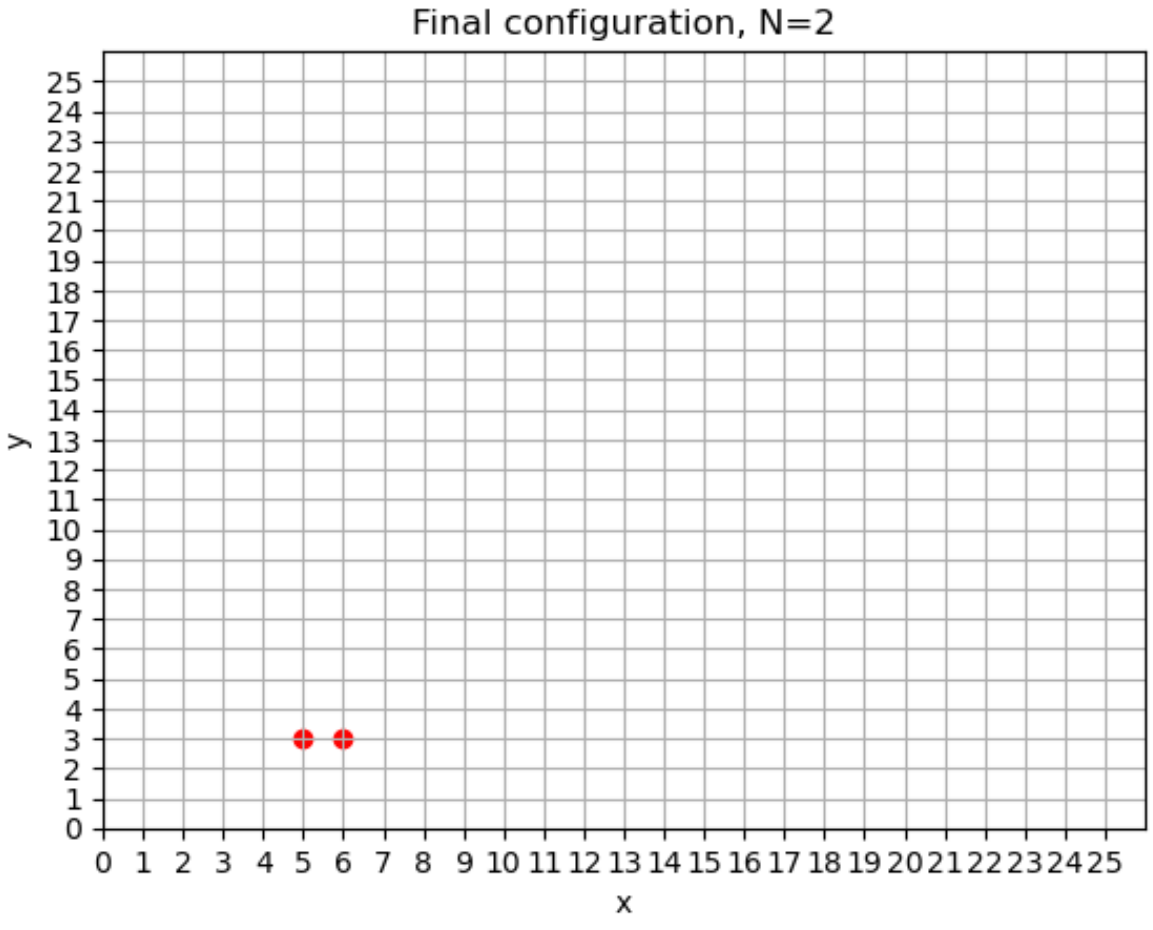


Zero temperature MC, minimum energy configuration

Obtain minimum energy configuration for different values of N



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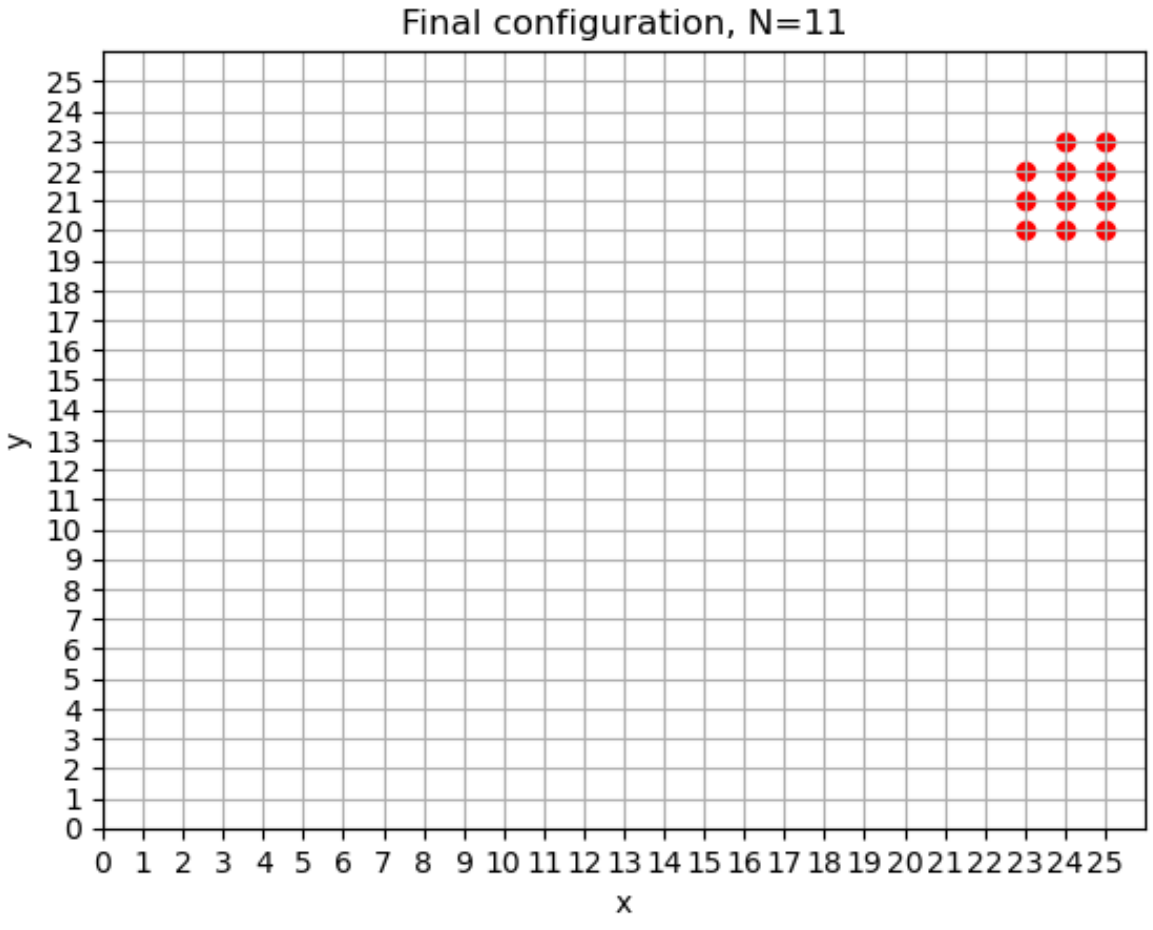

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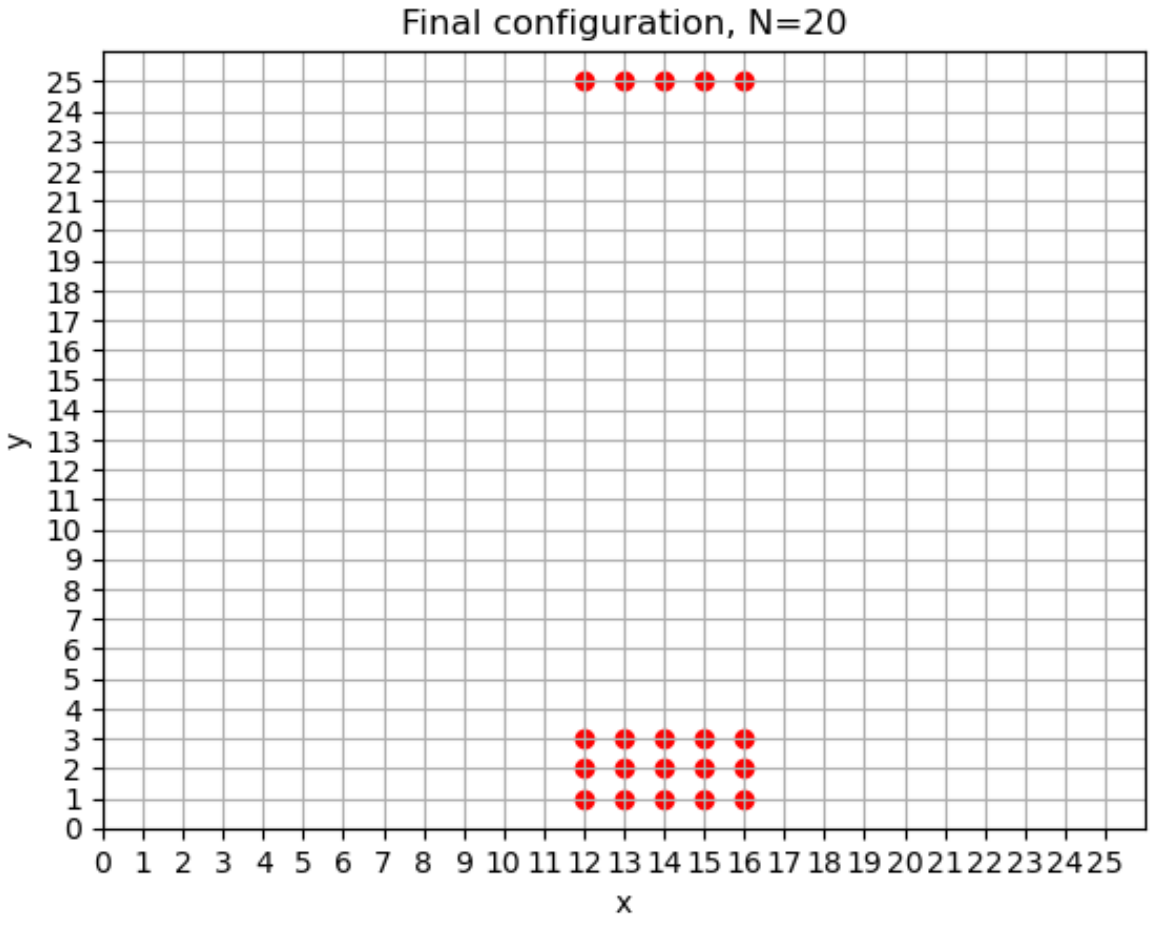
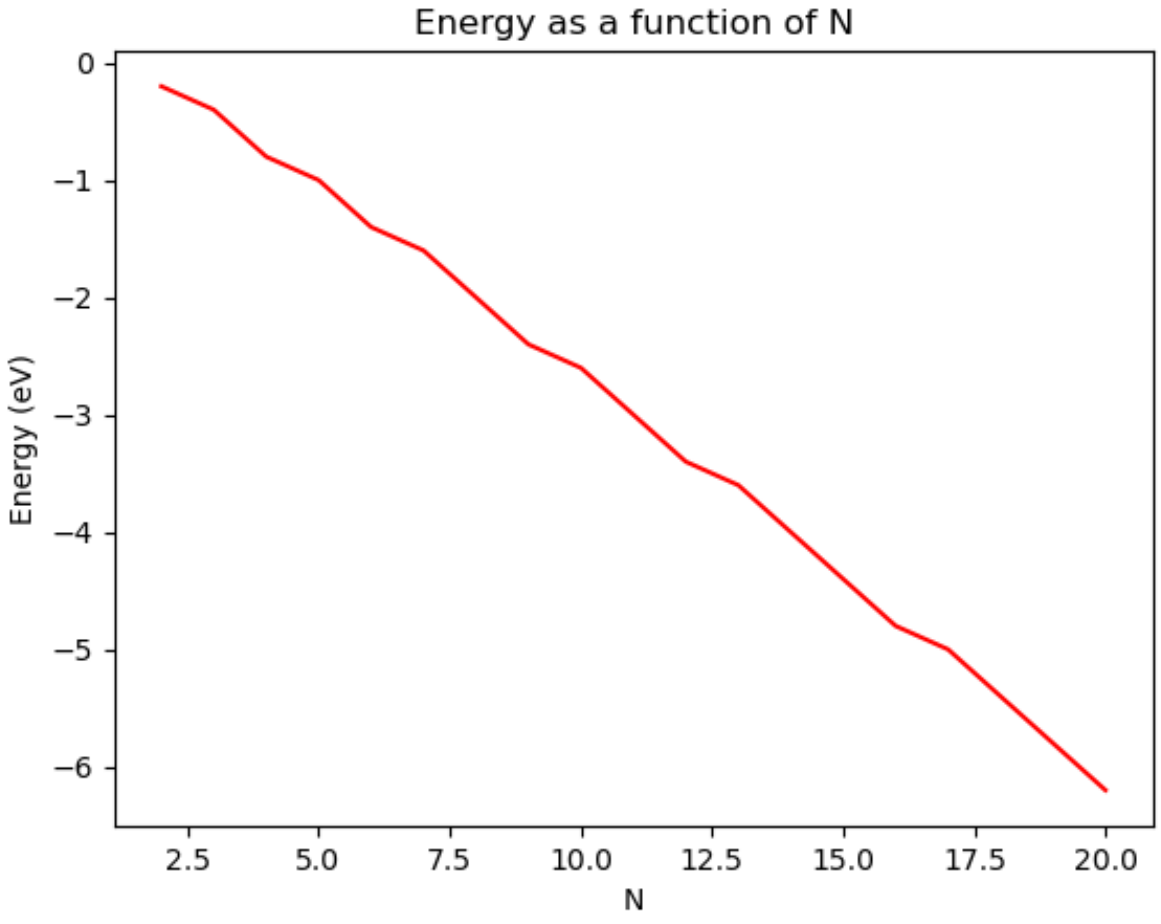
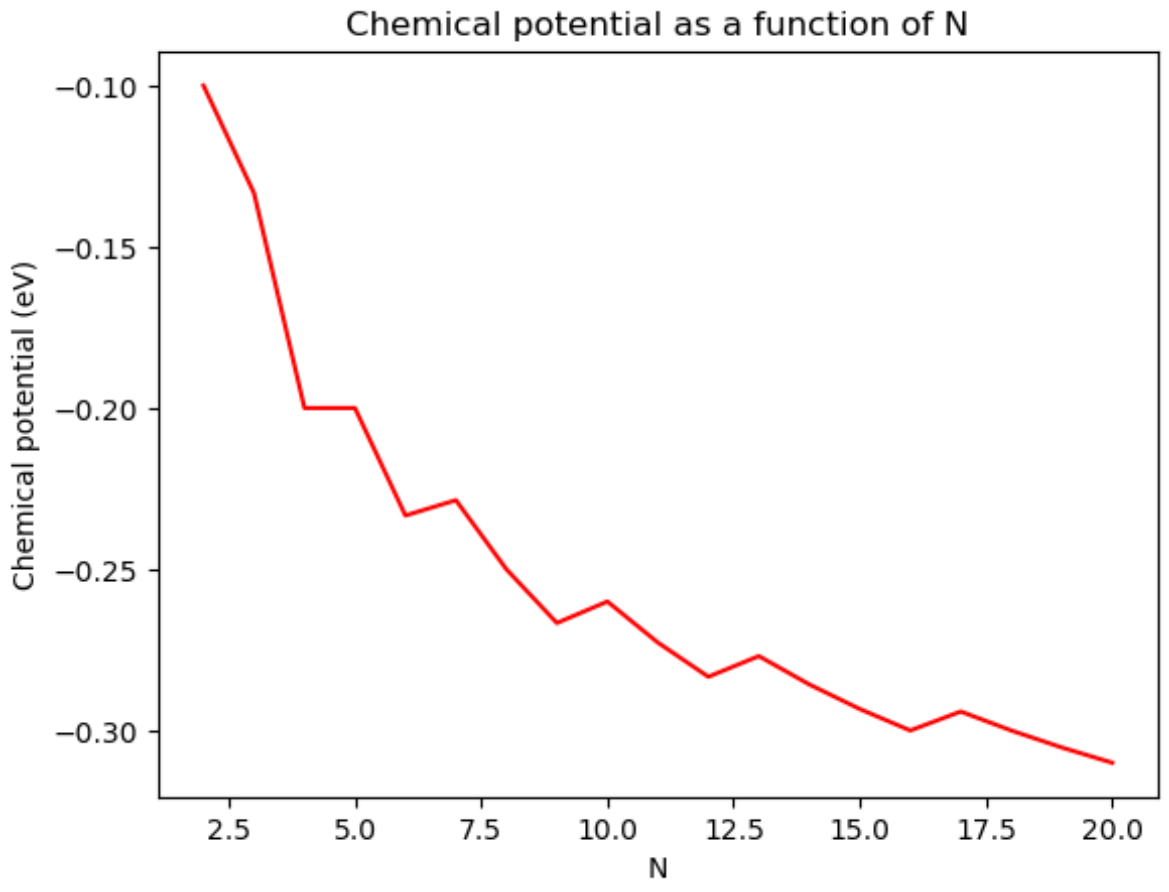


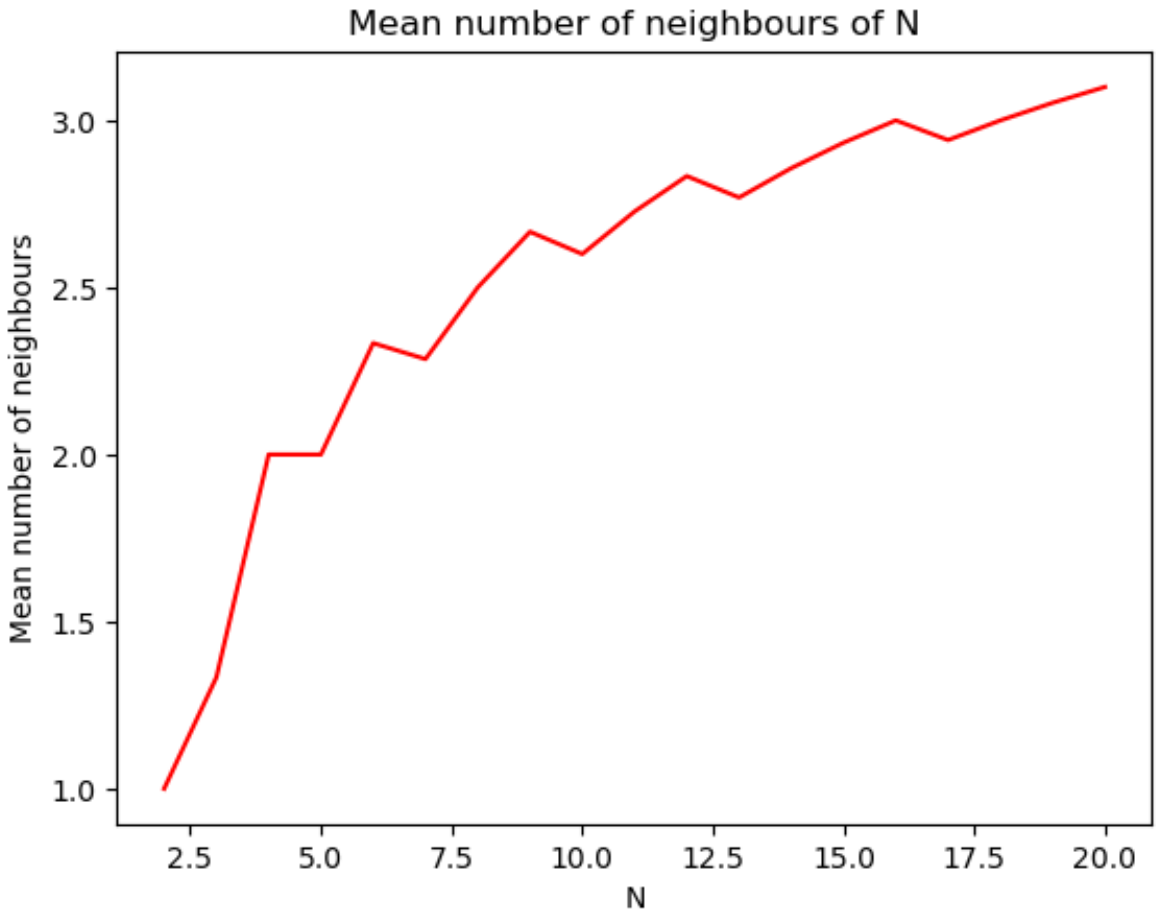
Zero temperature MC, energy variation with N



Zero temperature MC, μ variation with N

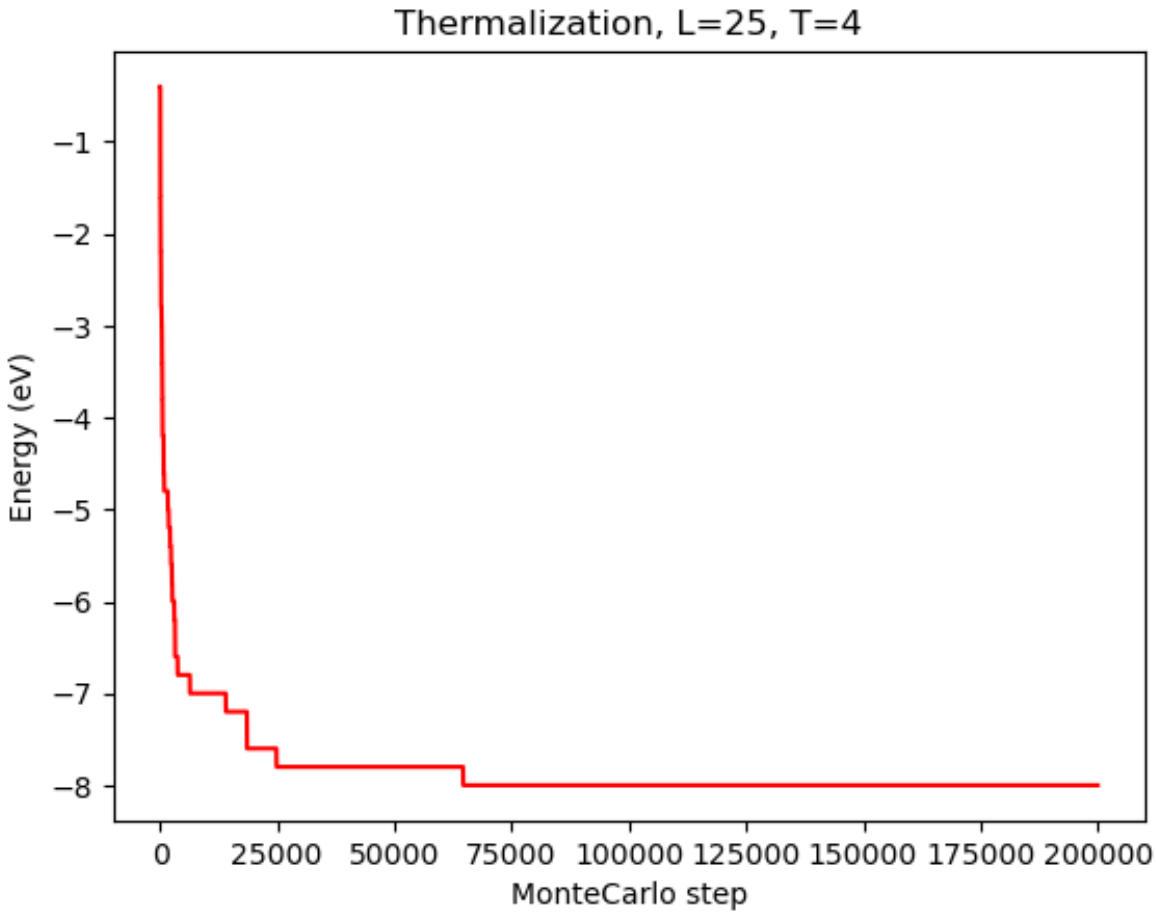


Zero temperature MC, number of neighbours variation with N



Finite temperature MC, $L = 25$

$$T = 4\,K$$



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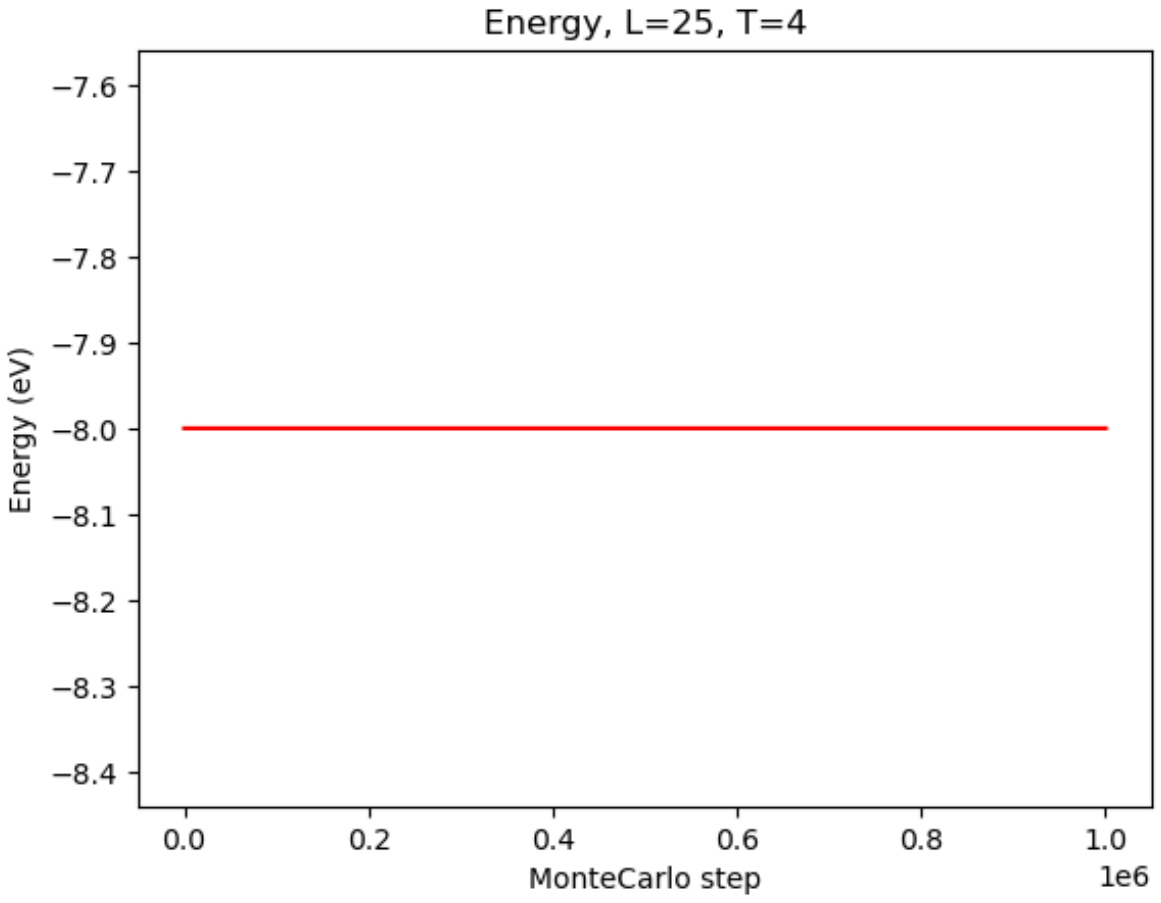
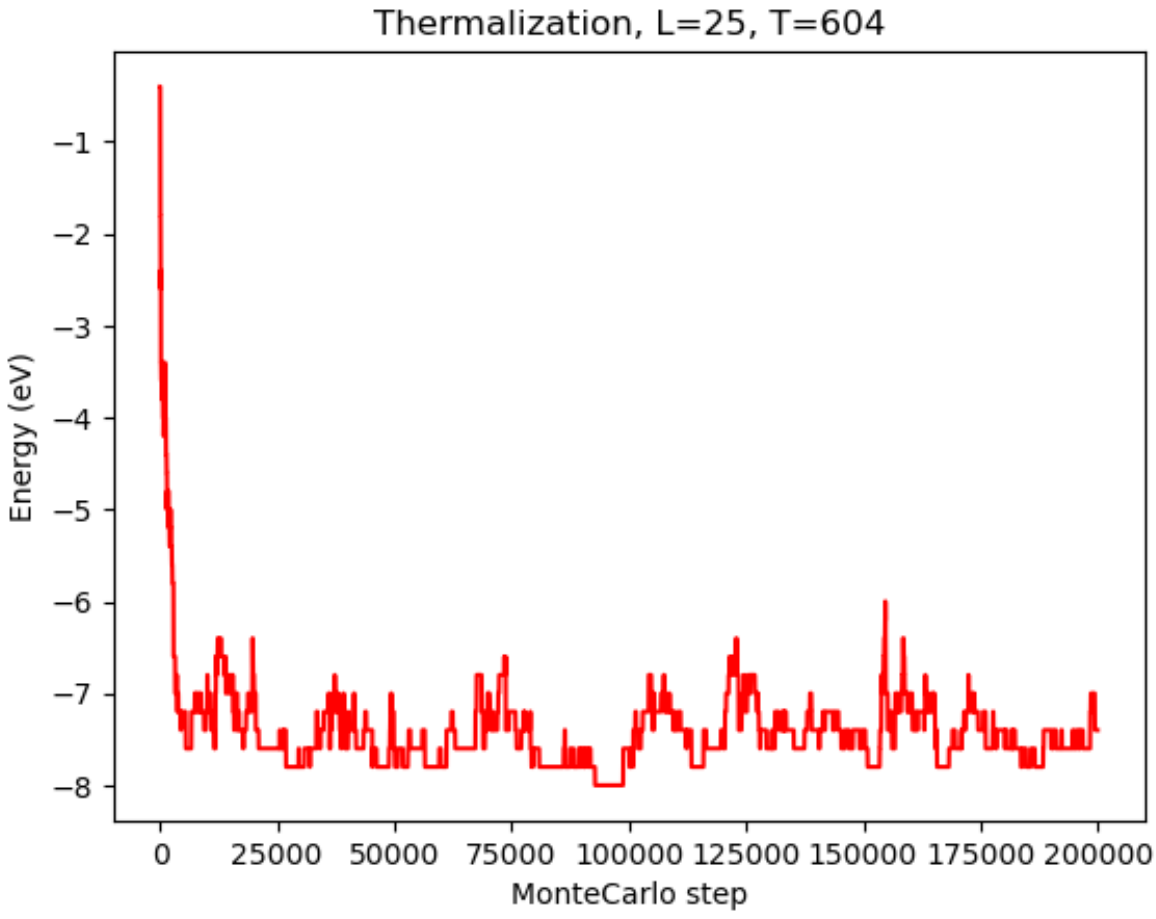


Finite temperature MC, $L = 25$

$$T = 604\,K$$



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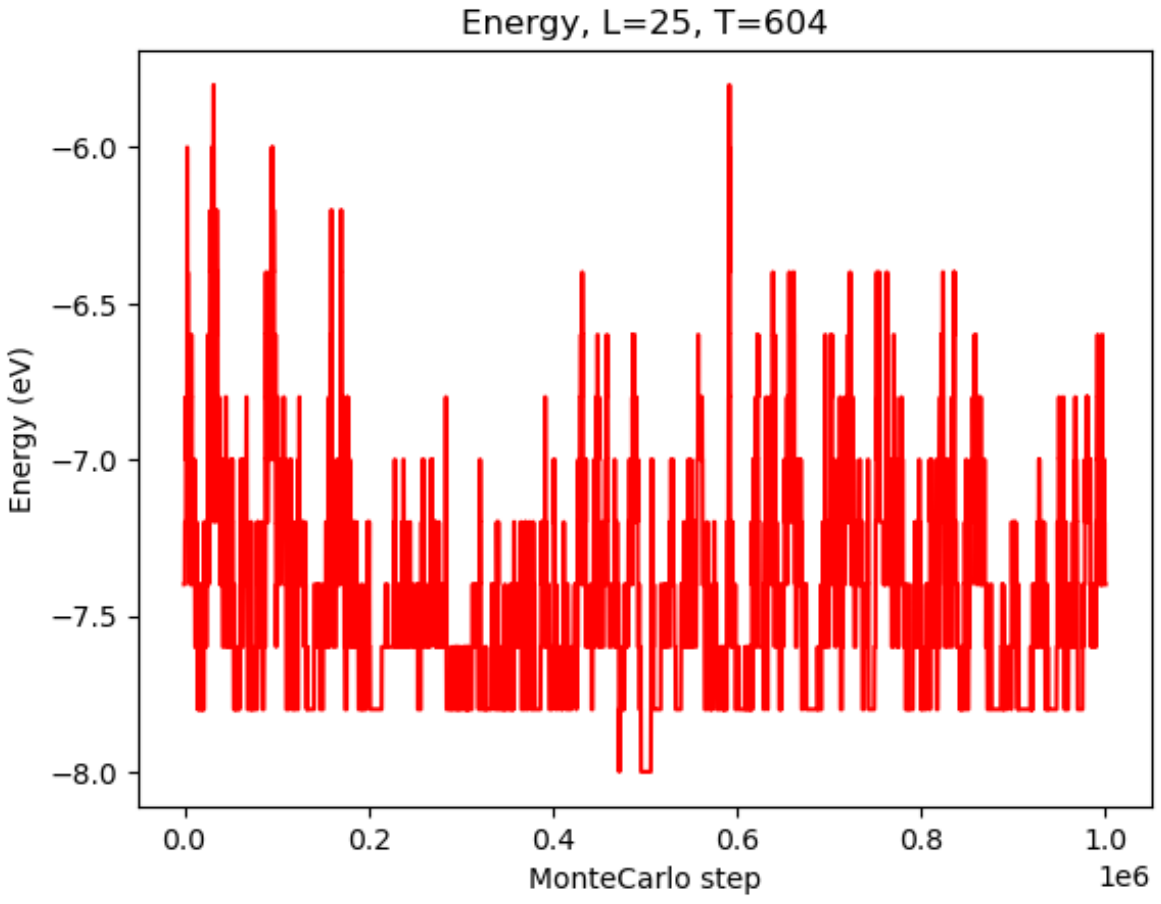
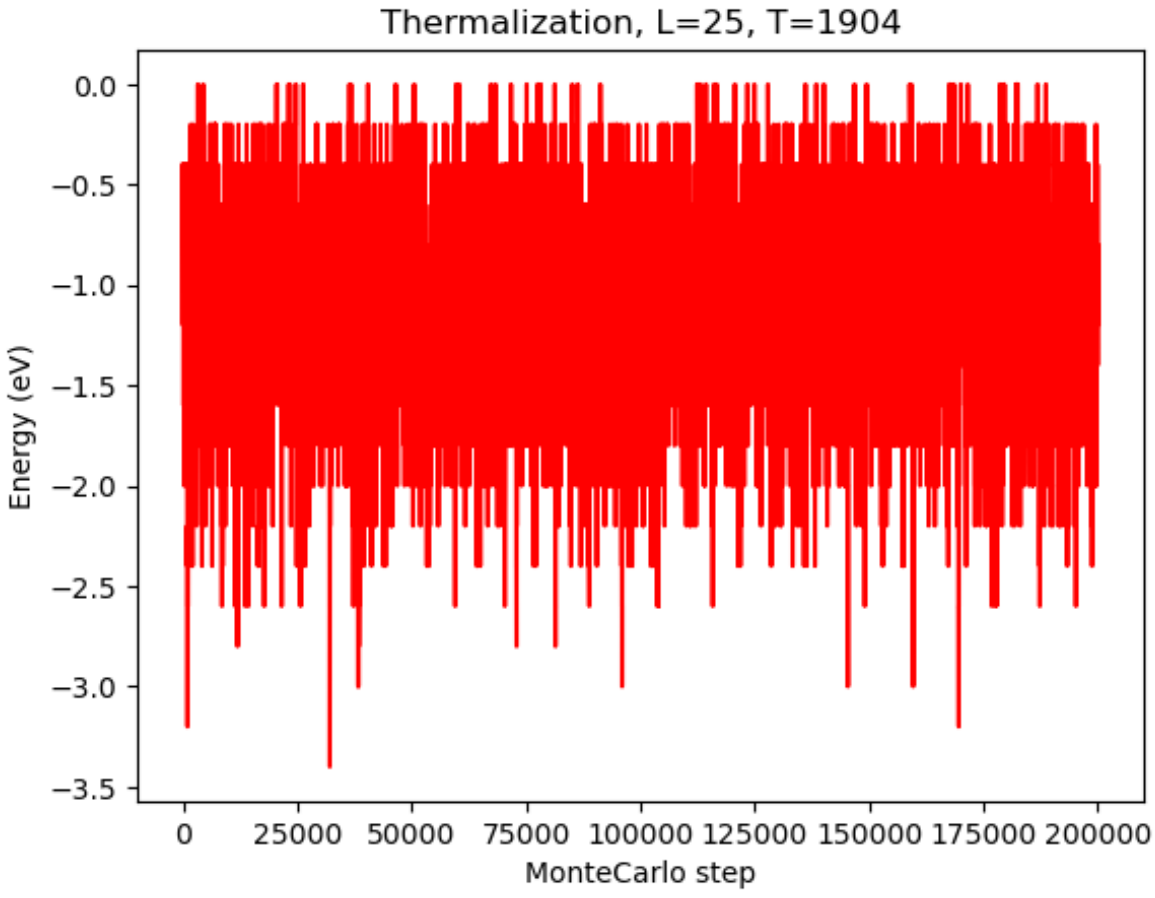


Finite temperature MC, $L = 25$

$$T = 1904\,K$$



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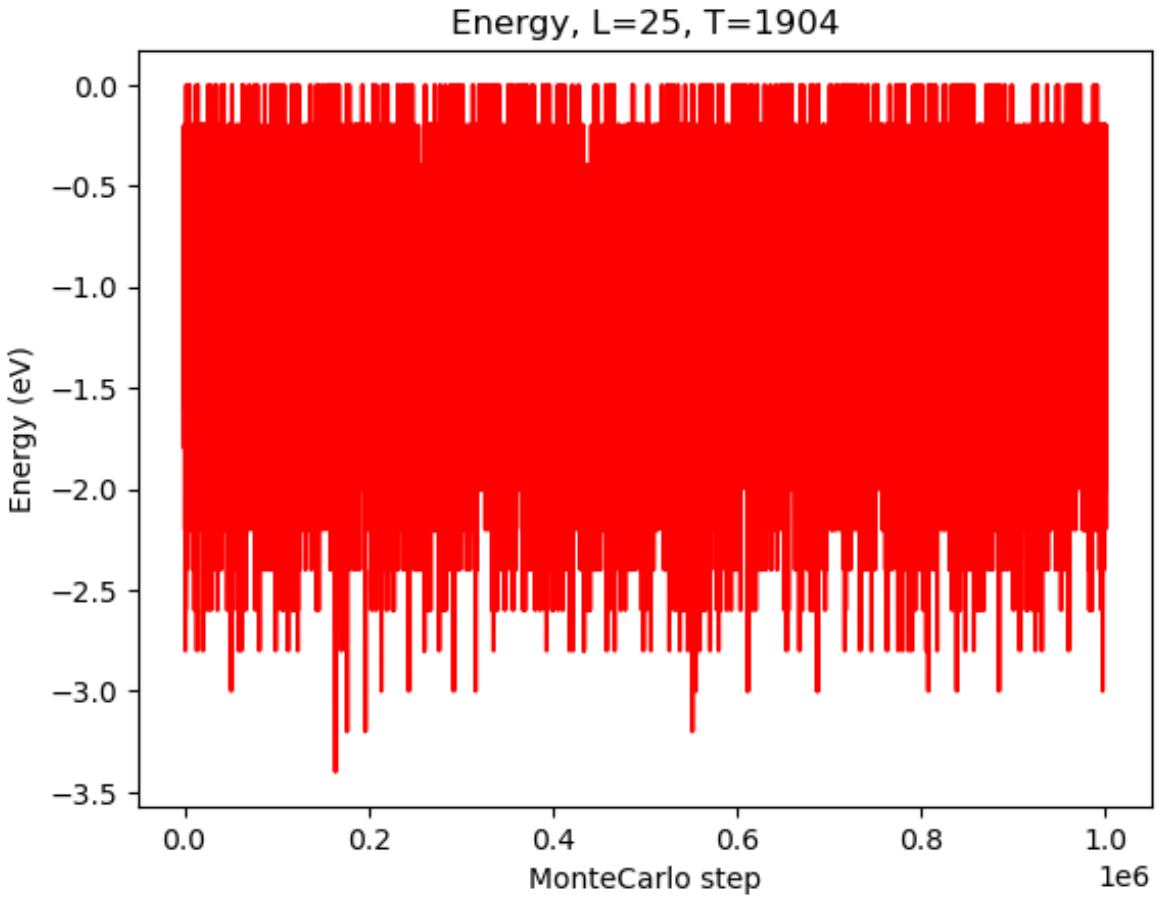
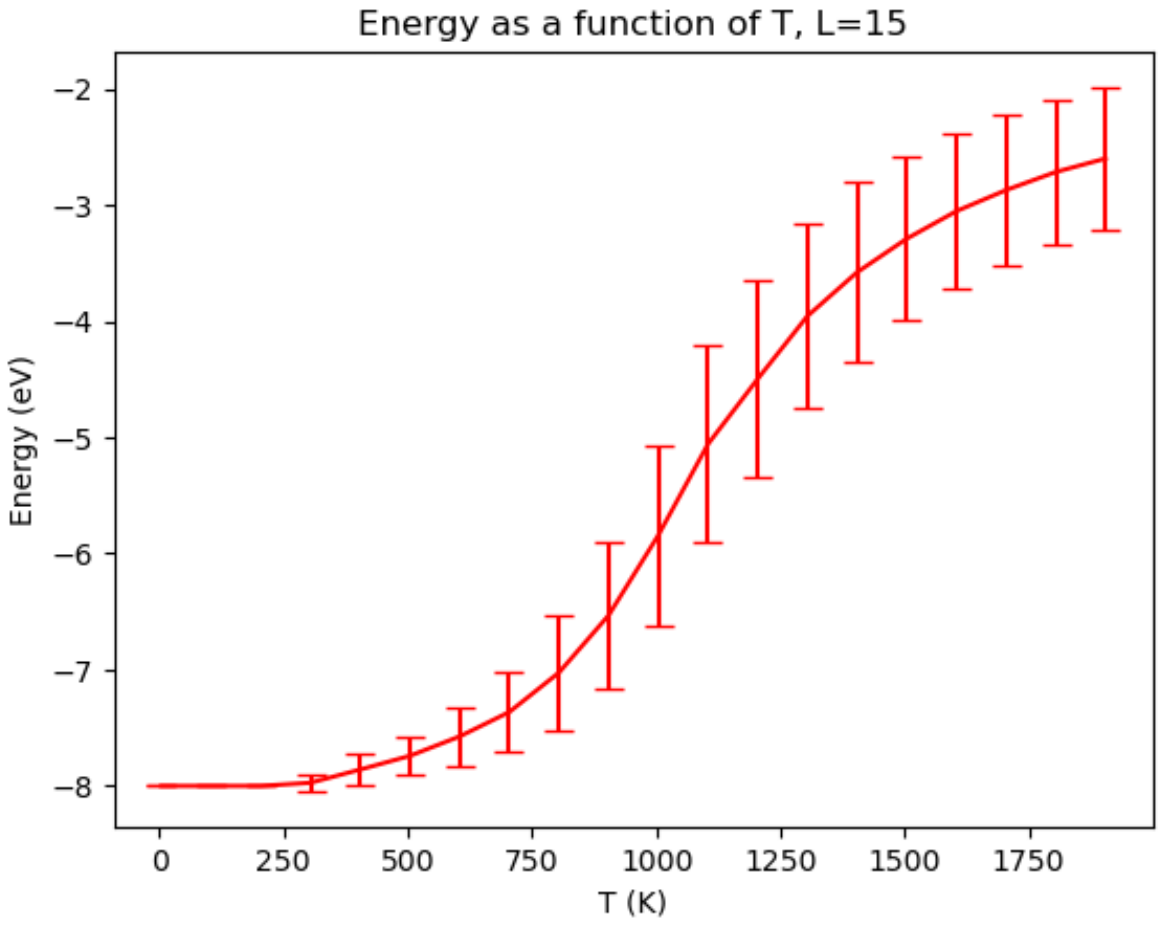


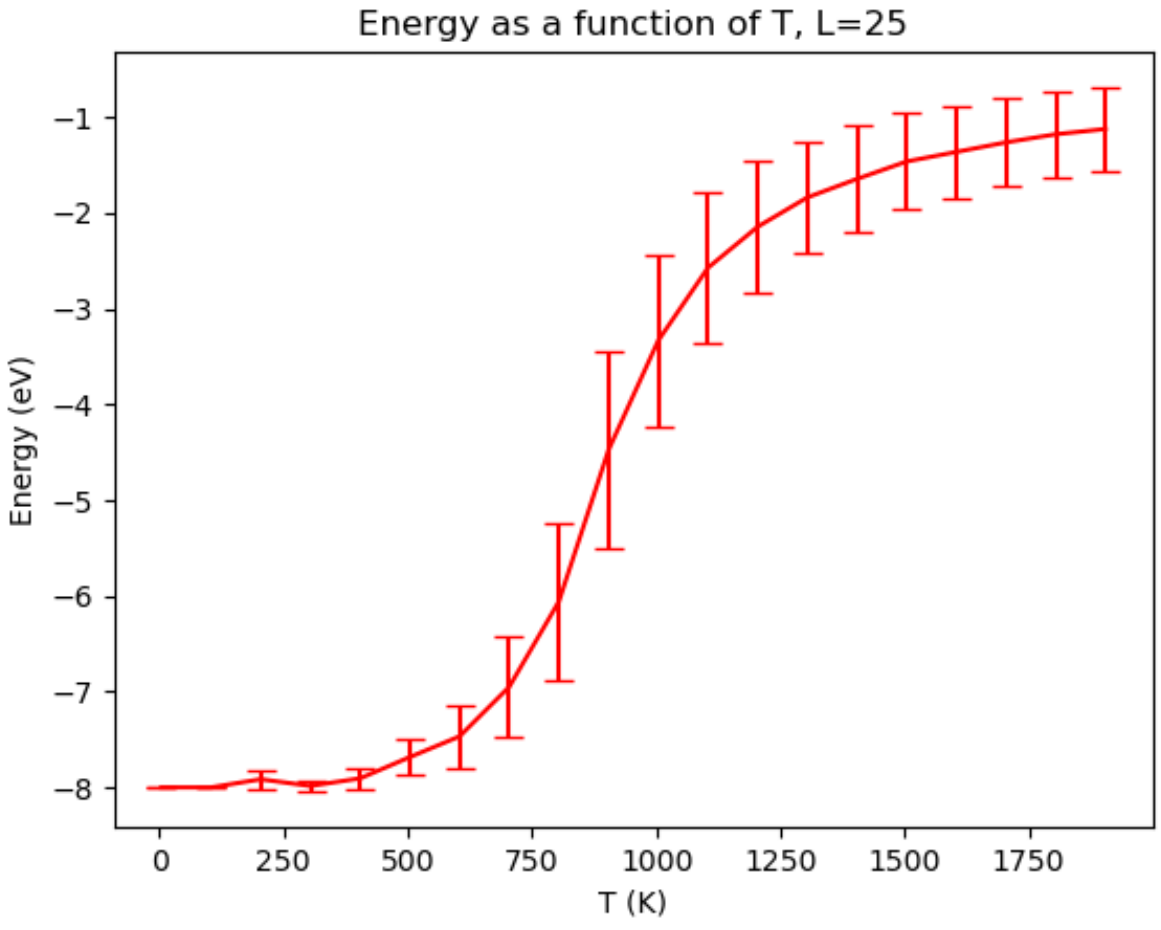
Finite temperature MC, $L = 15$

Mean energy variation with temperature



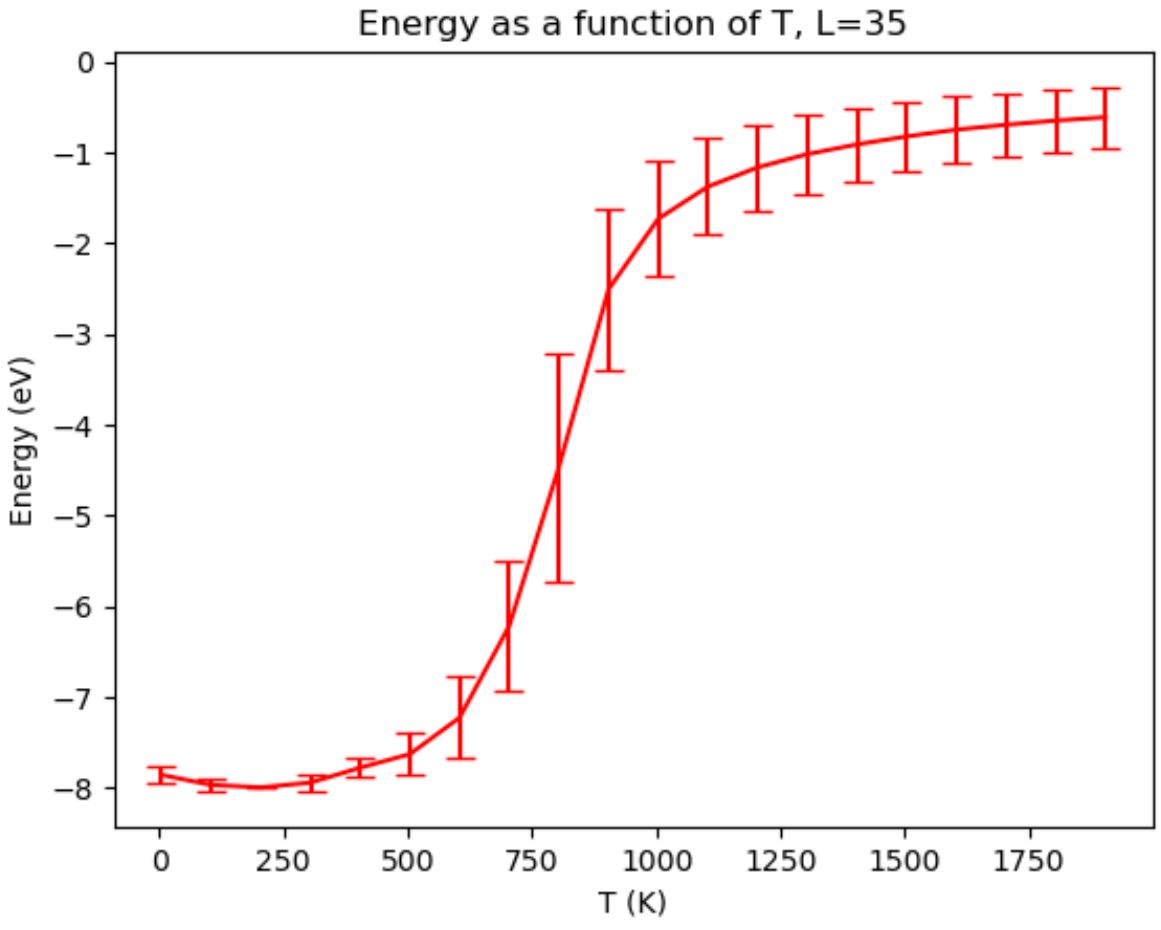
Finite temperature MC, $L = 25$

Mean energy variation with temperature



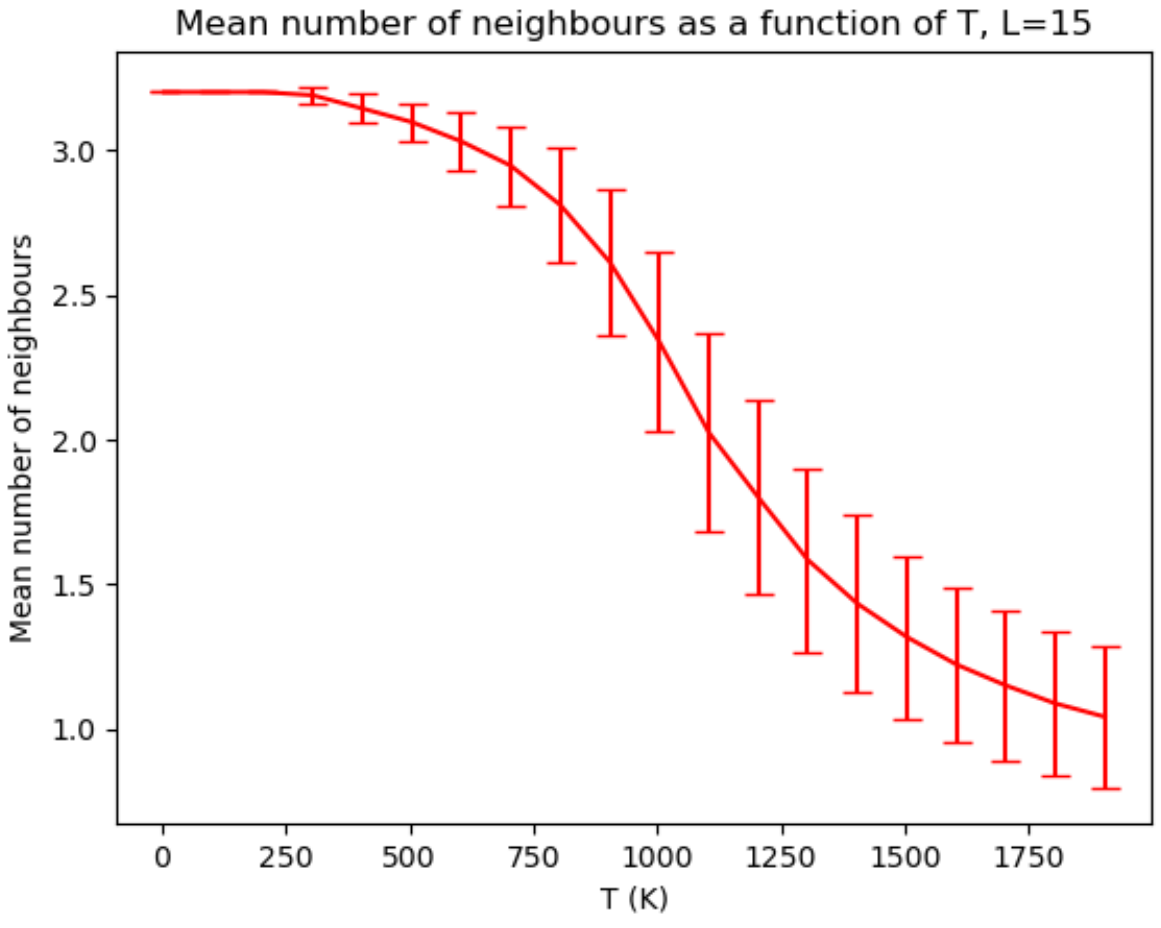
Finite temperature MC, $L = 35$

Mean energy variation with temperature



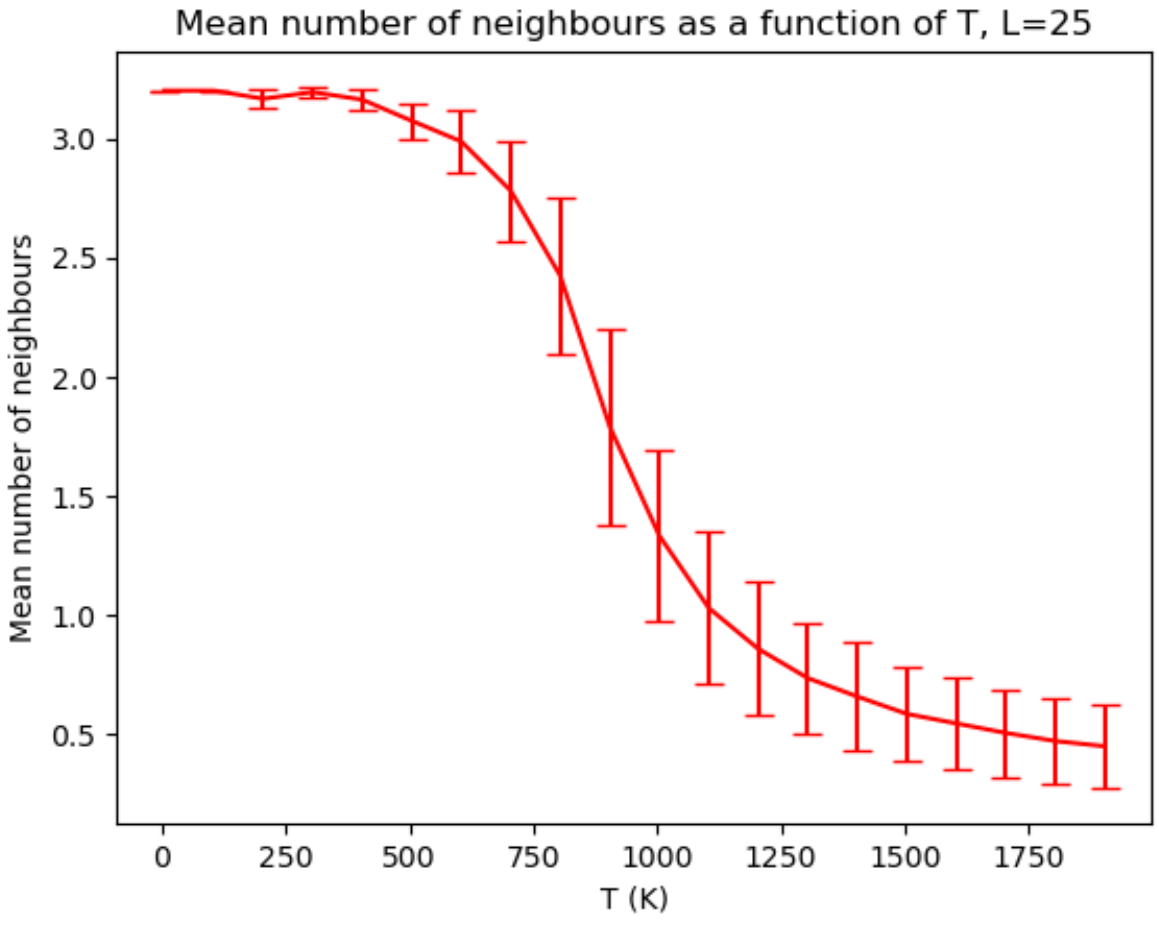
Finite temperature MC, $L = 15$

Mean number of neighbours variation with temperature



Finite temperature MC, $L = 25$

Mean number of neighbours variation with temperature



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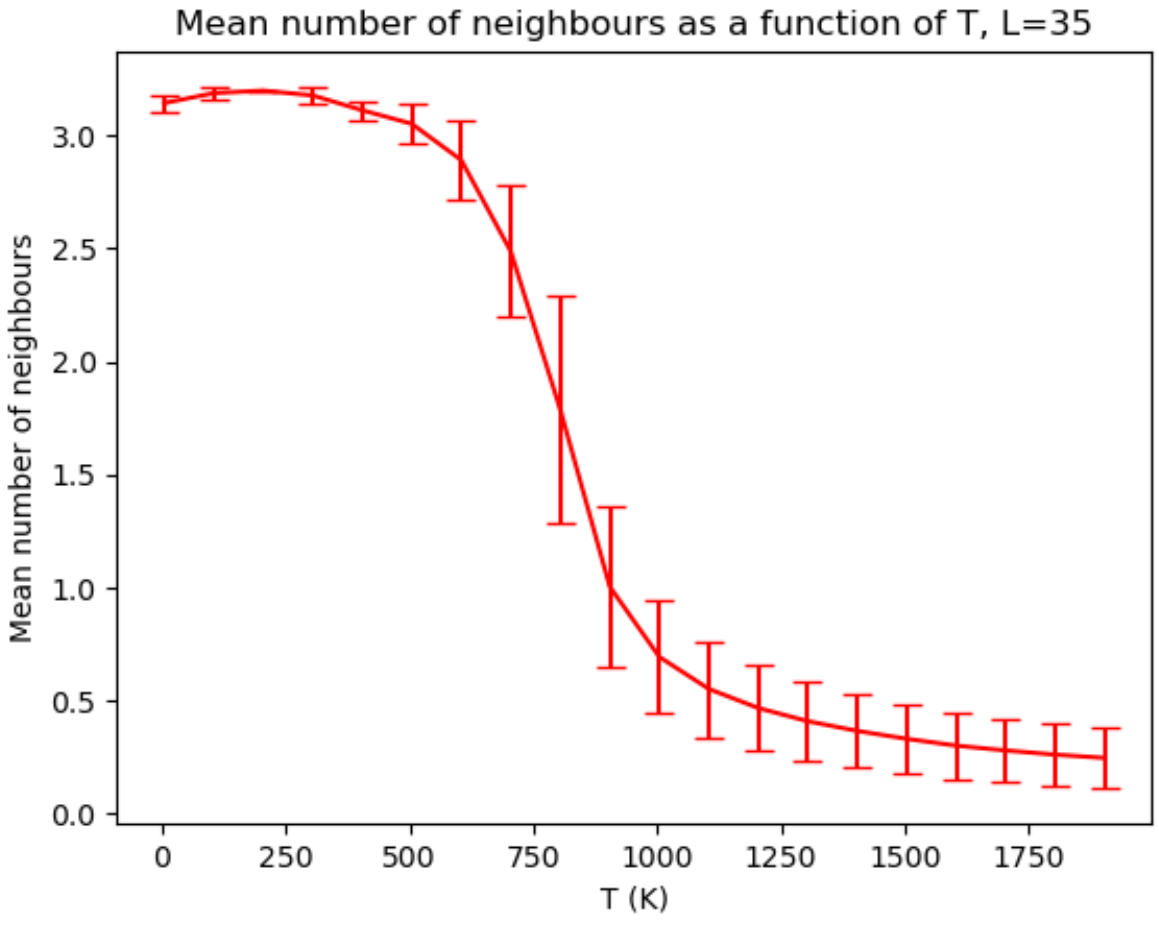
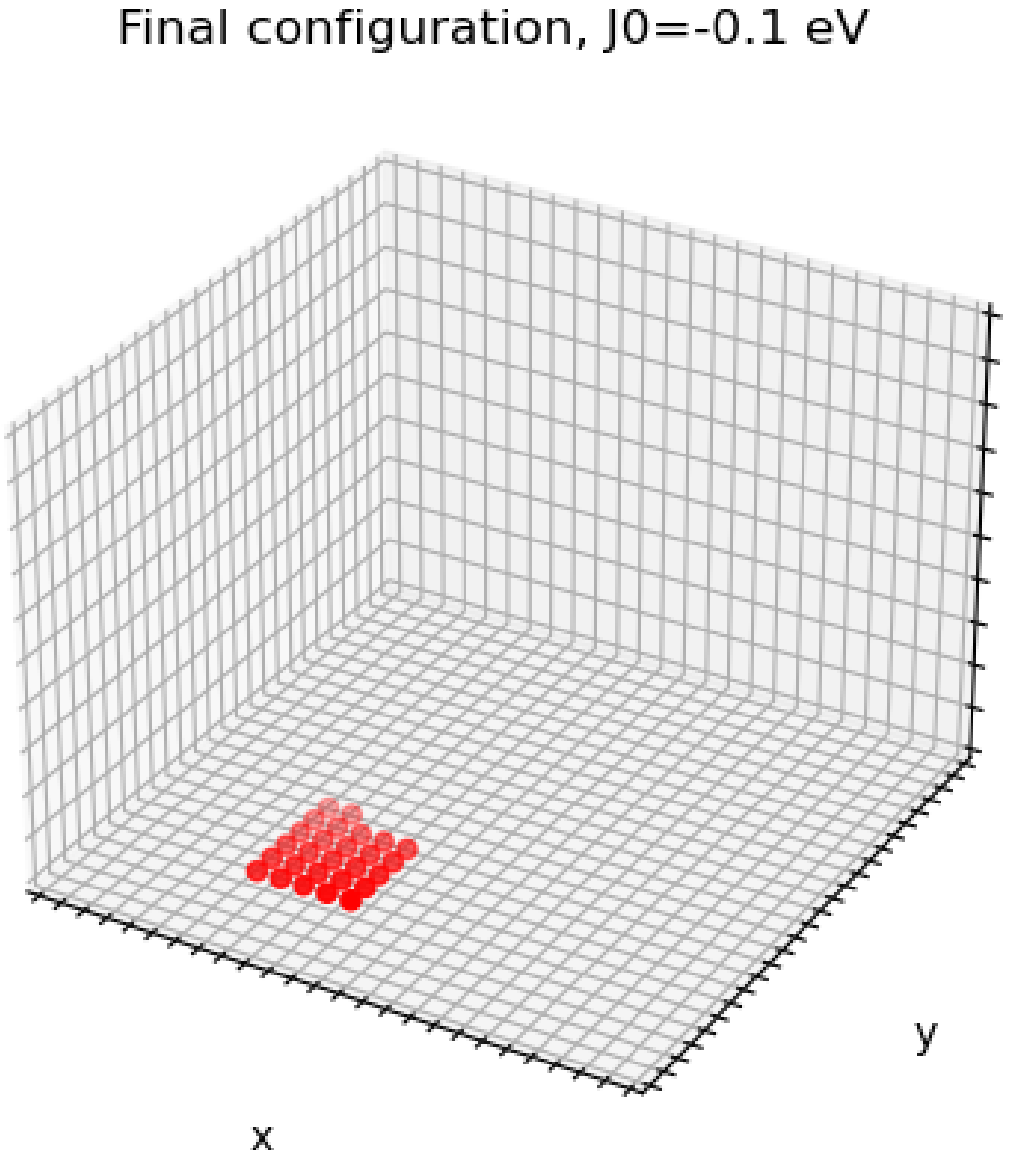


3 dimensional MC, $T = 0\,K$



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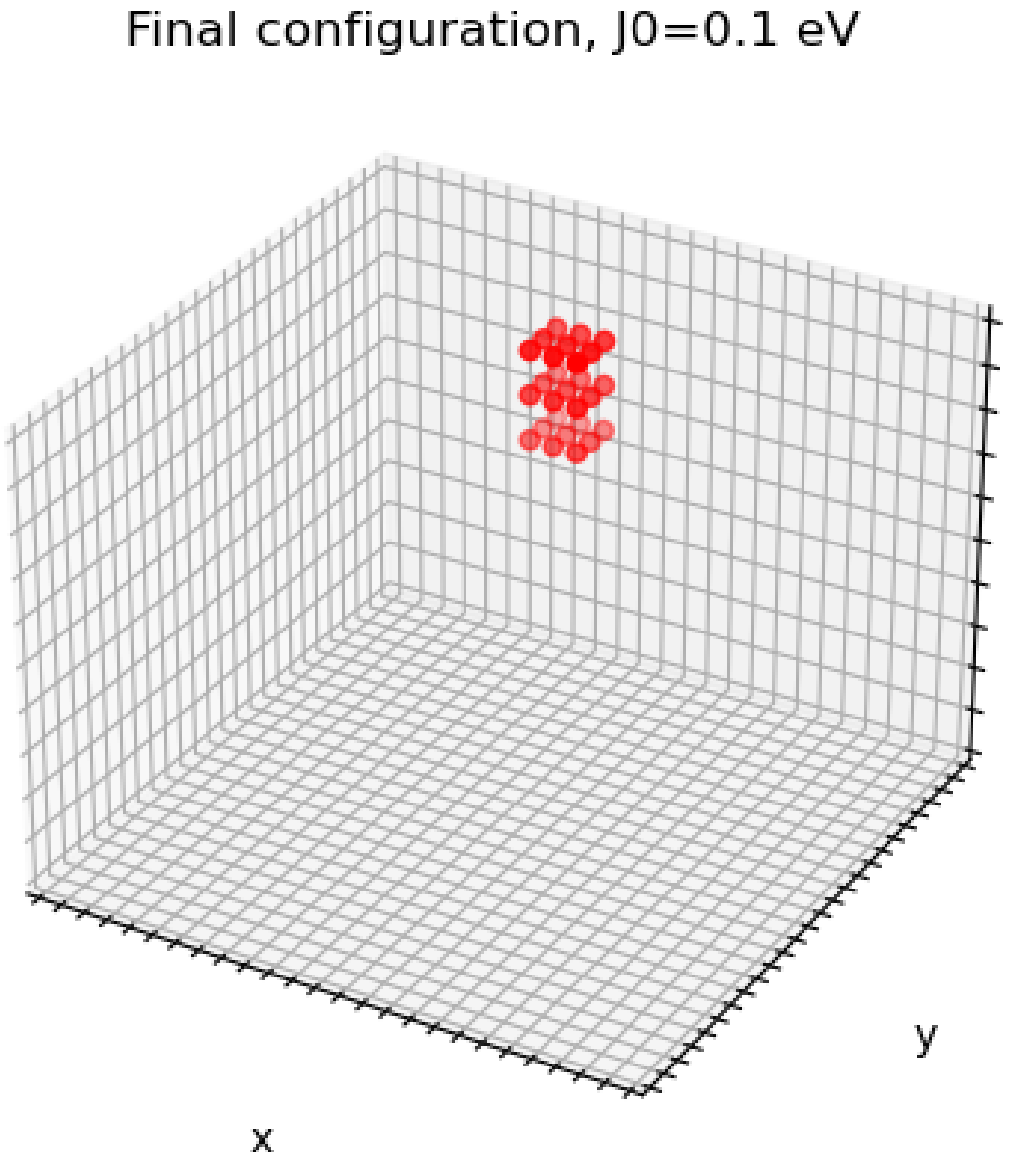
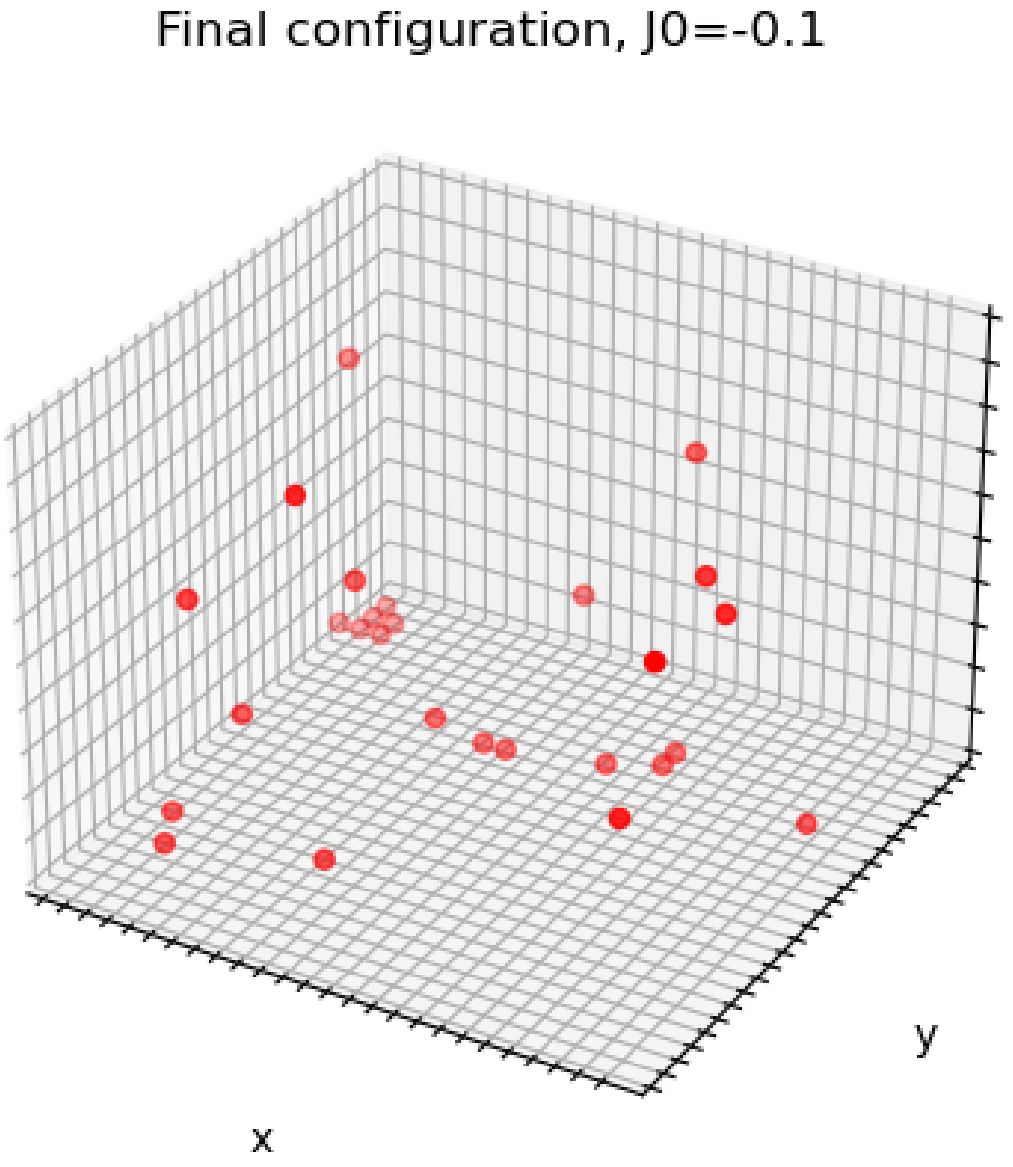
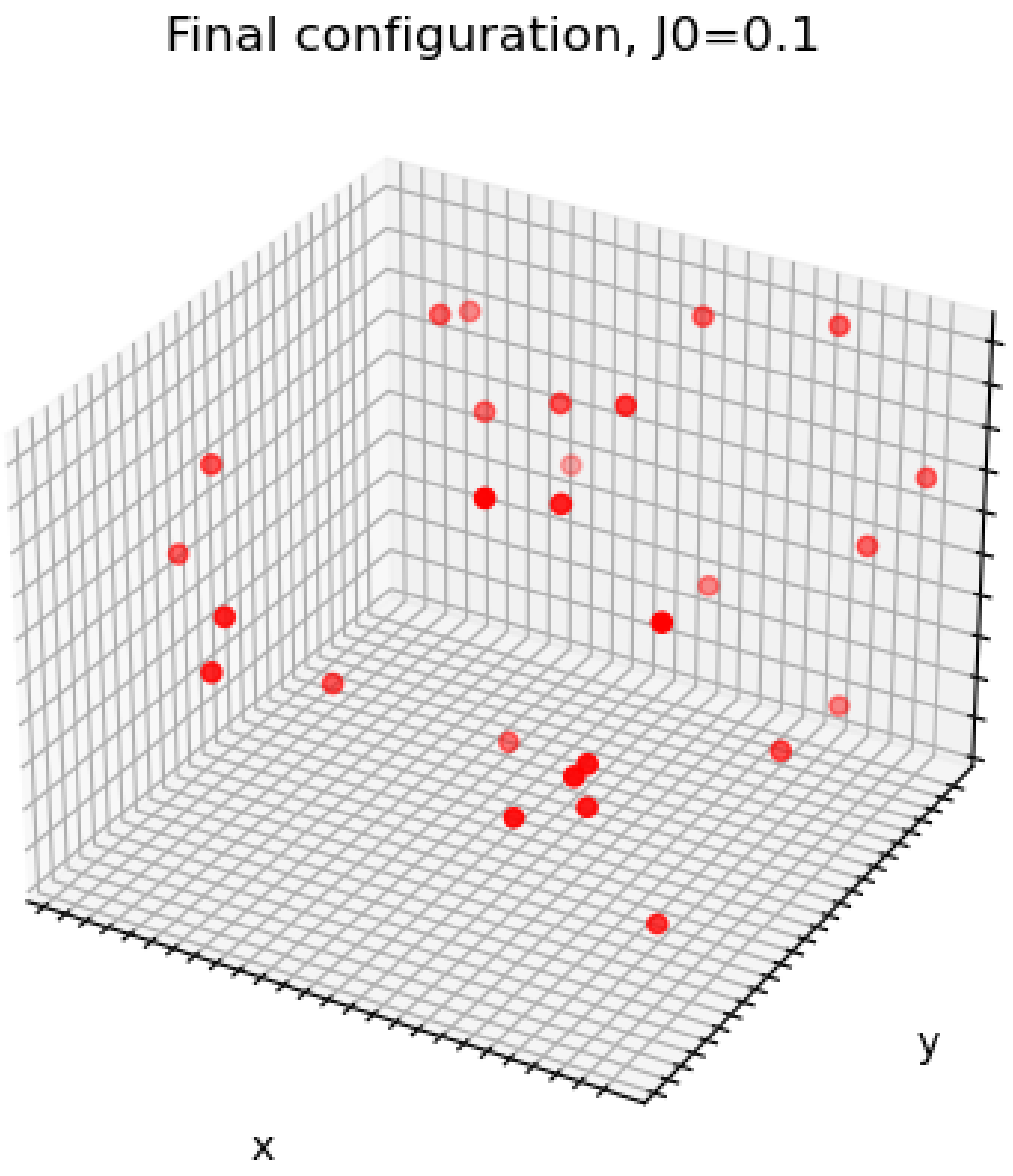


3 dimensional MC, $T = 1000\,K$

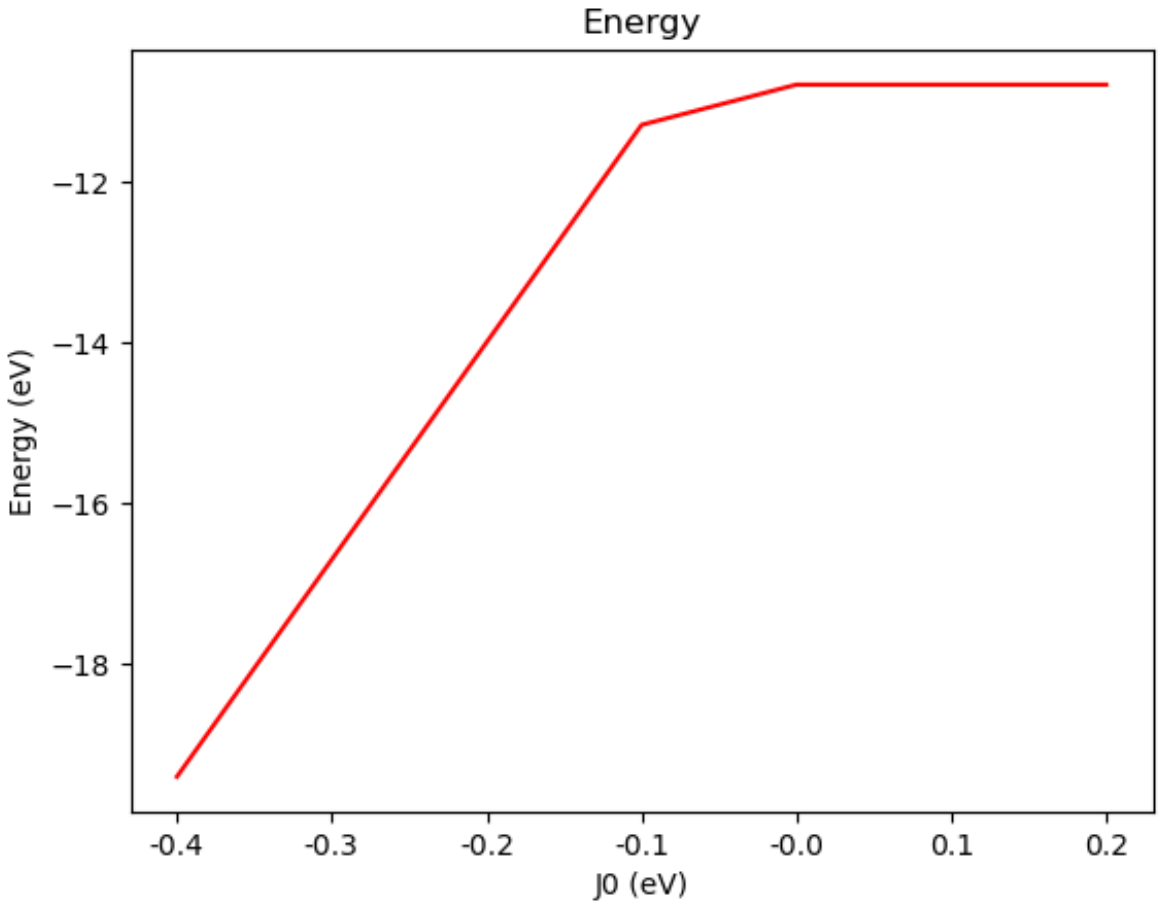


3 dimensional MC, $T = 1000\,K$



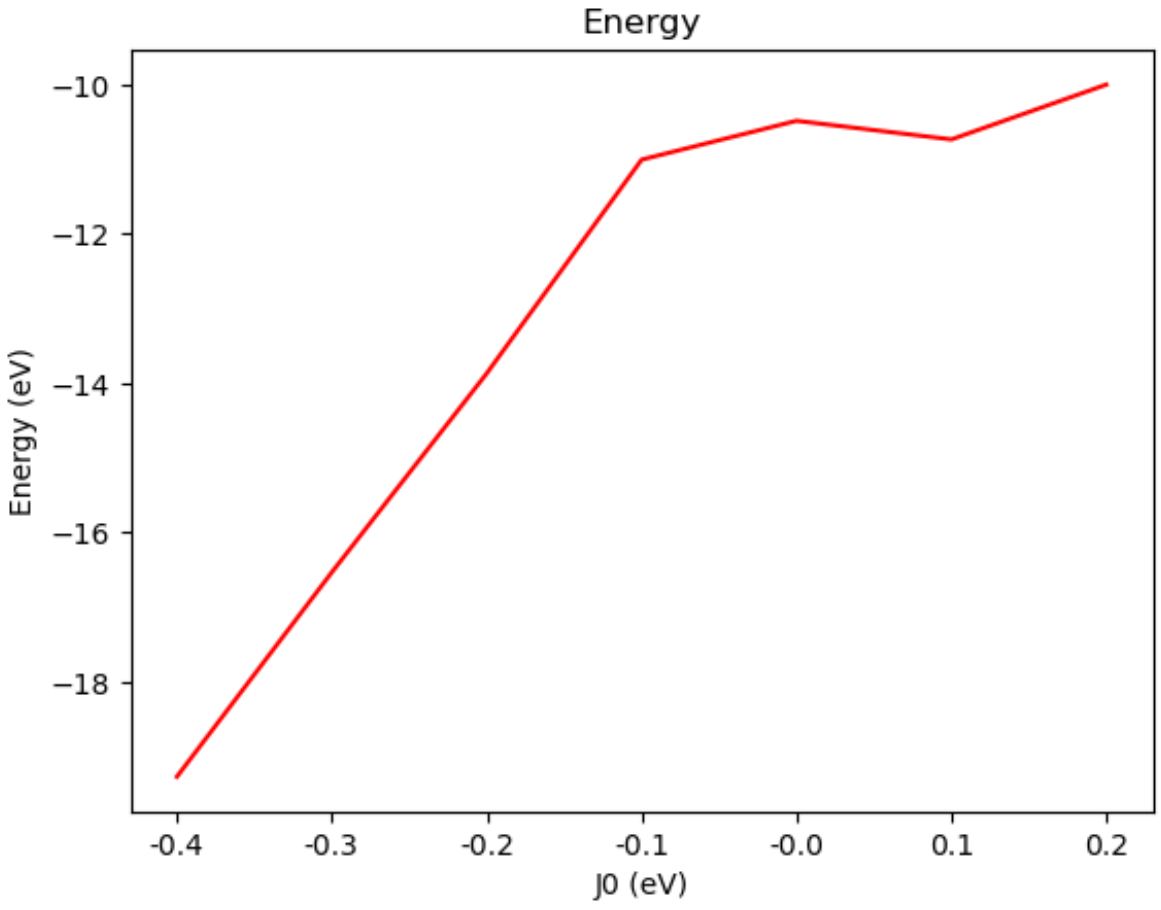
3 dimensional MC, $N = 27$

Energy @ $T = 0\,K$



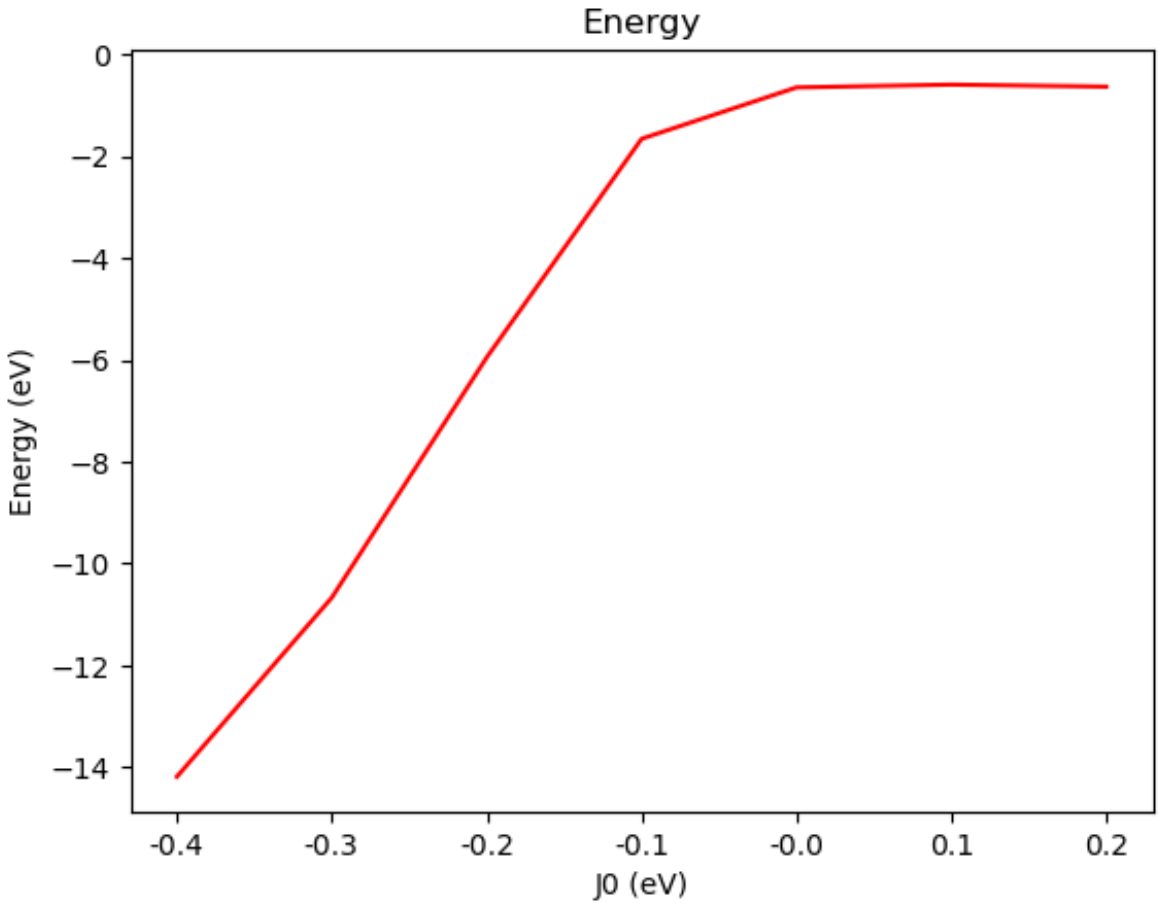
3 dimensional MC, $N = 27$

Energy @ $T = 500\,K$



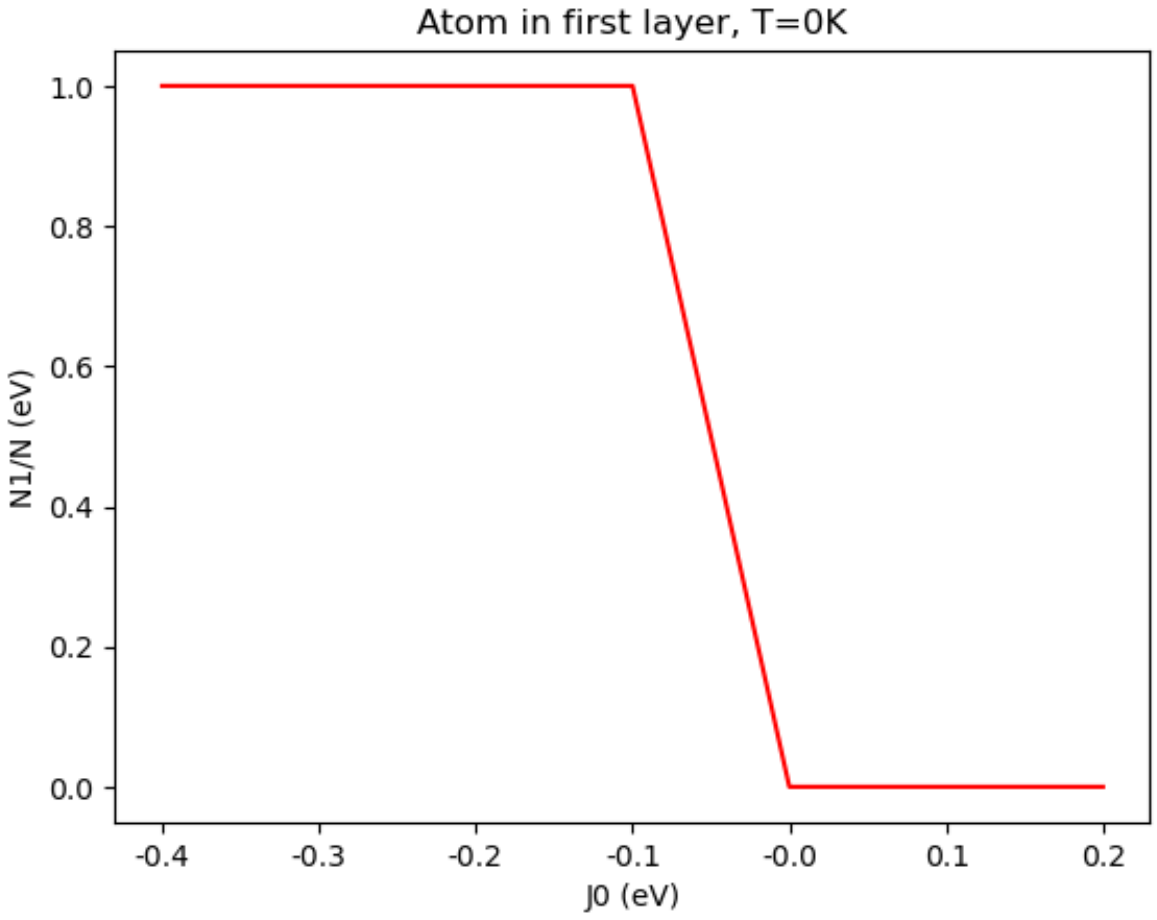
3 dimensional MC, $N = 27$

Energy @ $T = 1000\,K$



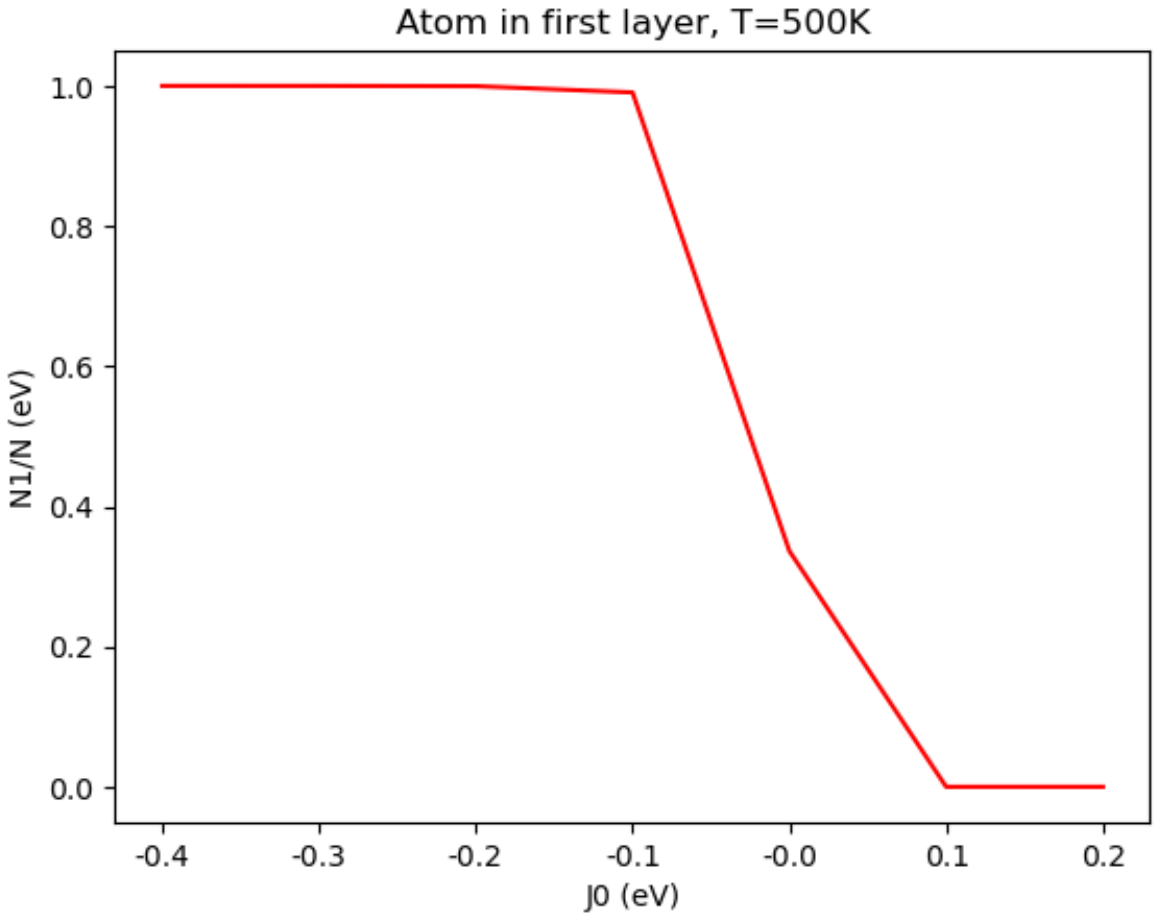
3 dimensional MC, $N = 27$

$$N_1/N \,@\, T = 0\,K$$



3 dimensional MC, $N = 27$

$$N_1/N \,@\, T = 500\,K$$



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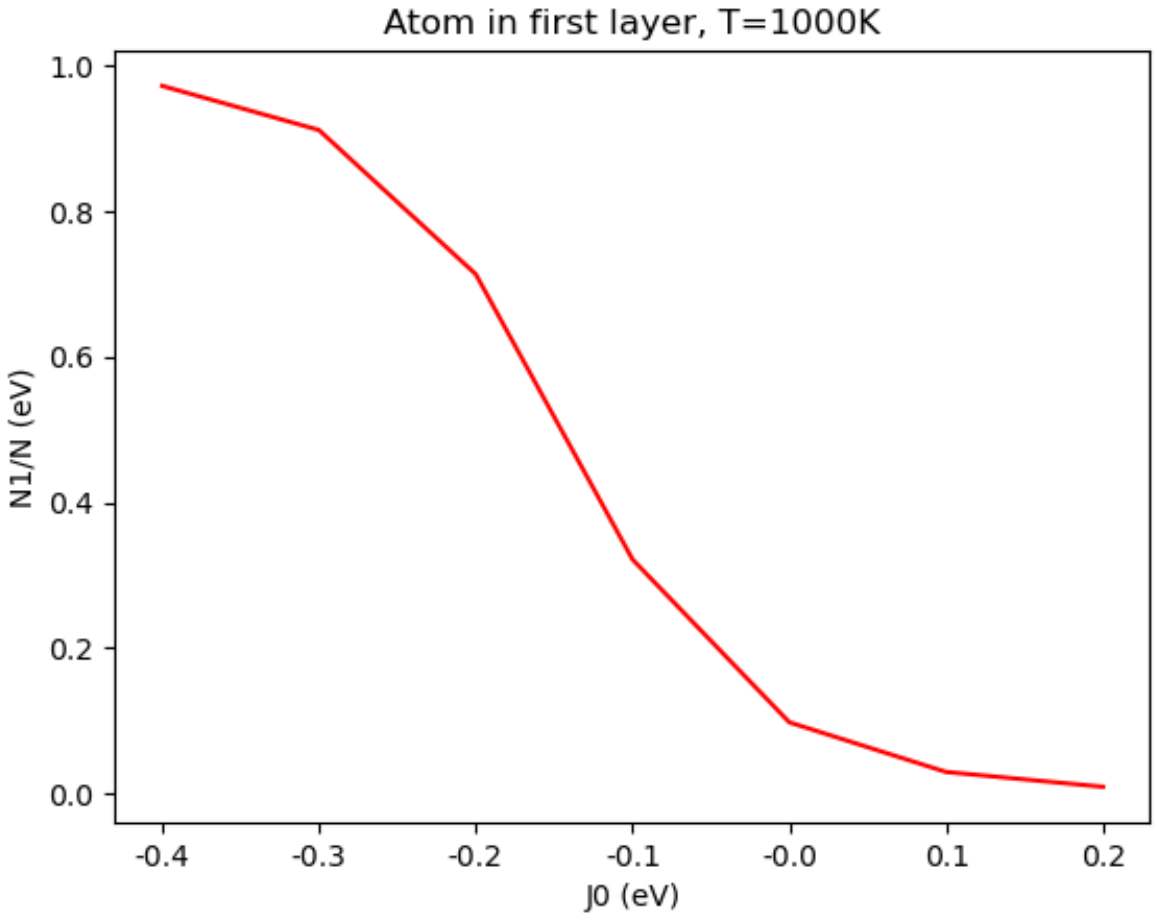
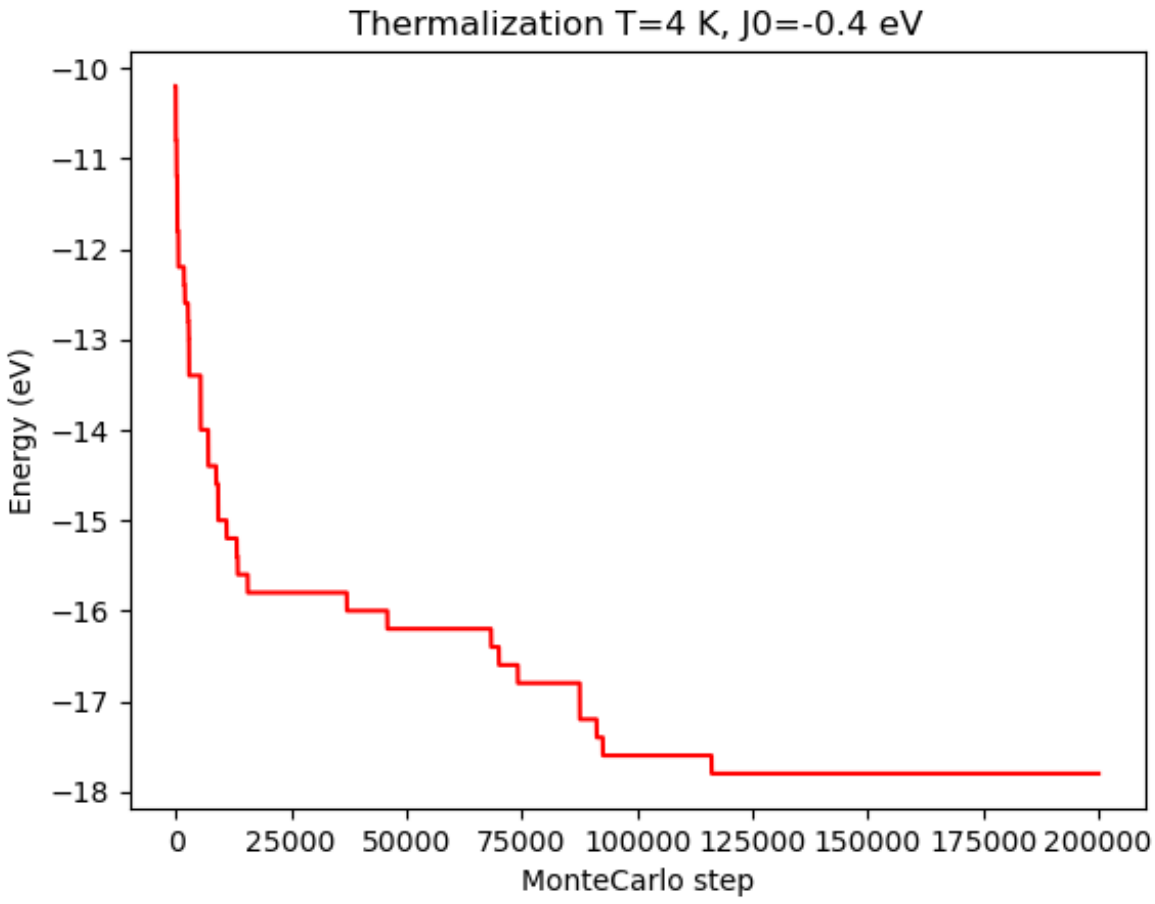


Monolayer distribution

Low temperature, negative coupling



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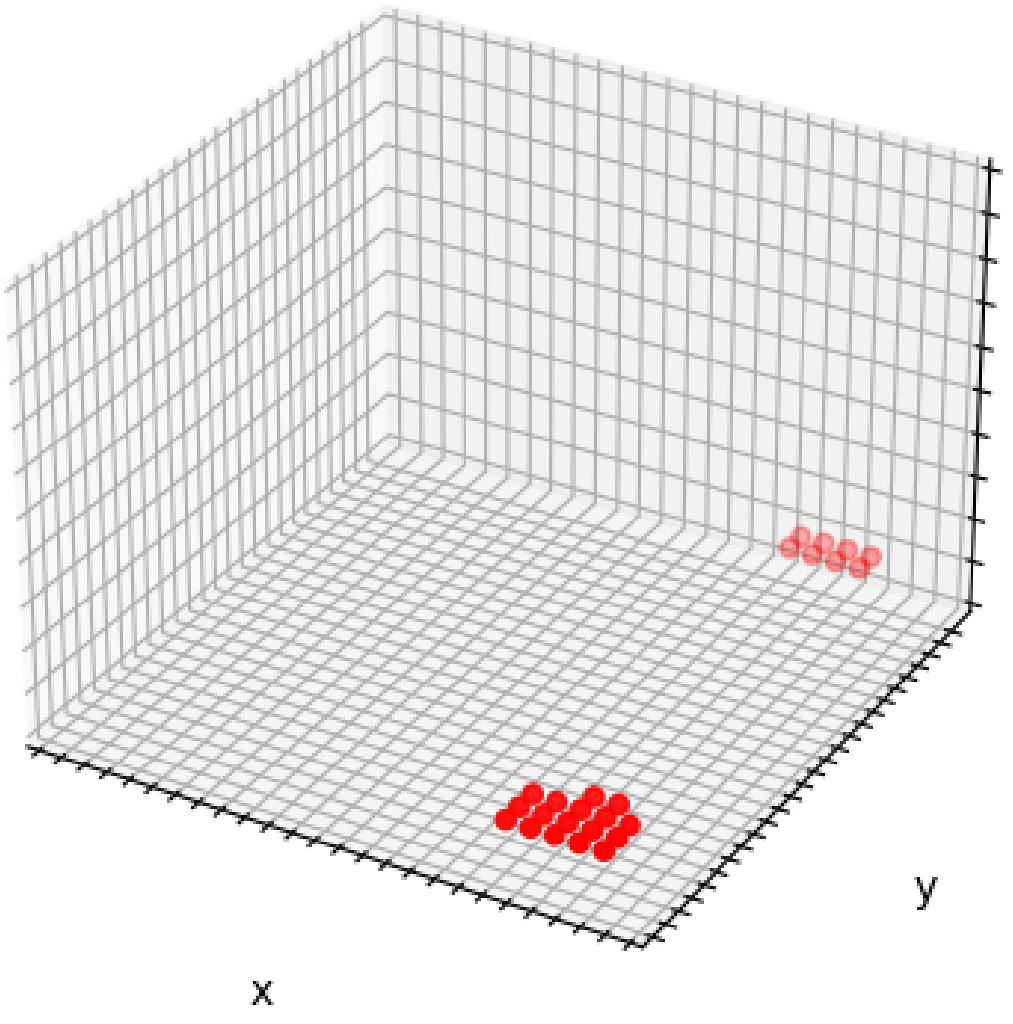

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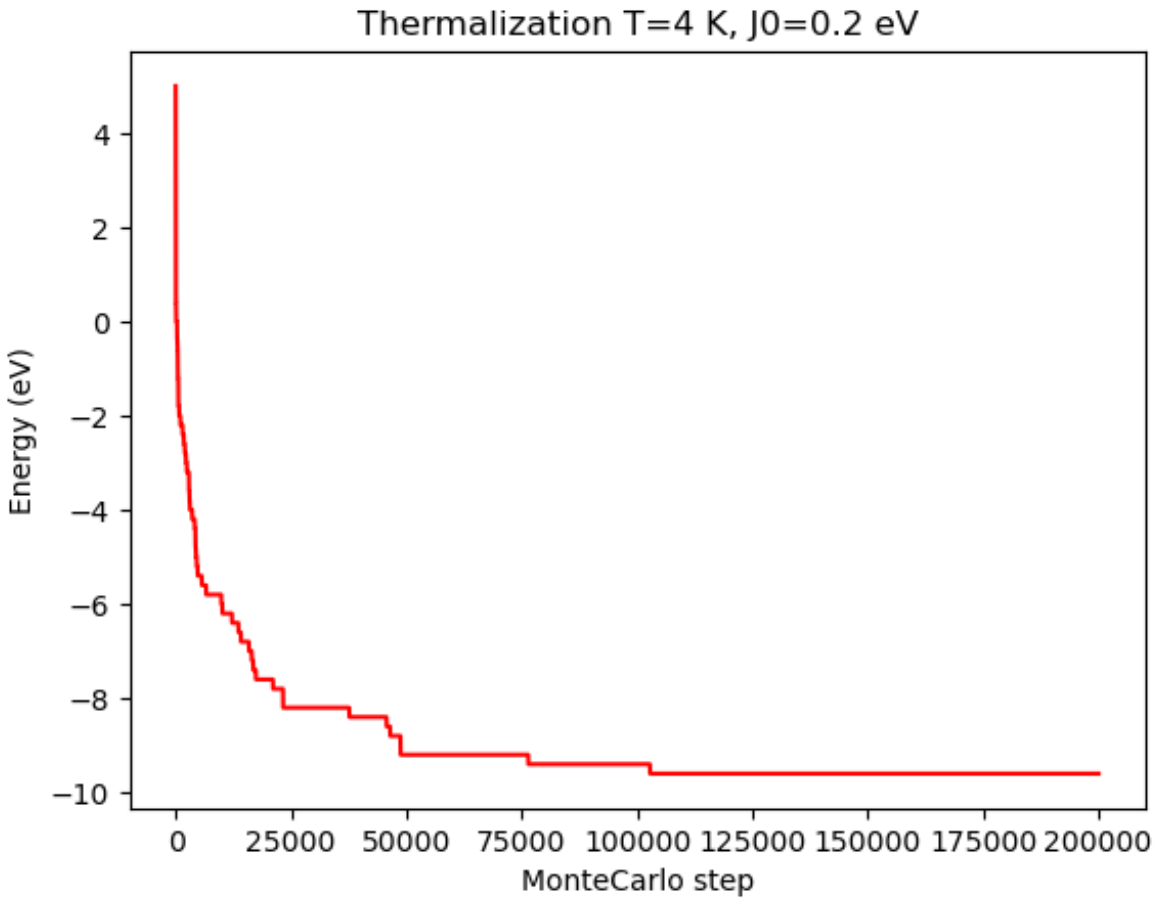

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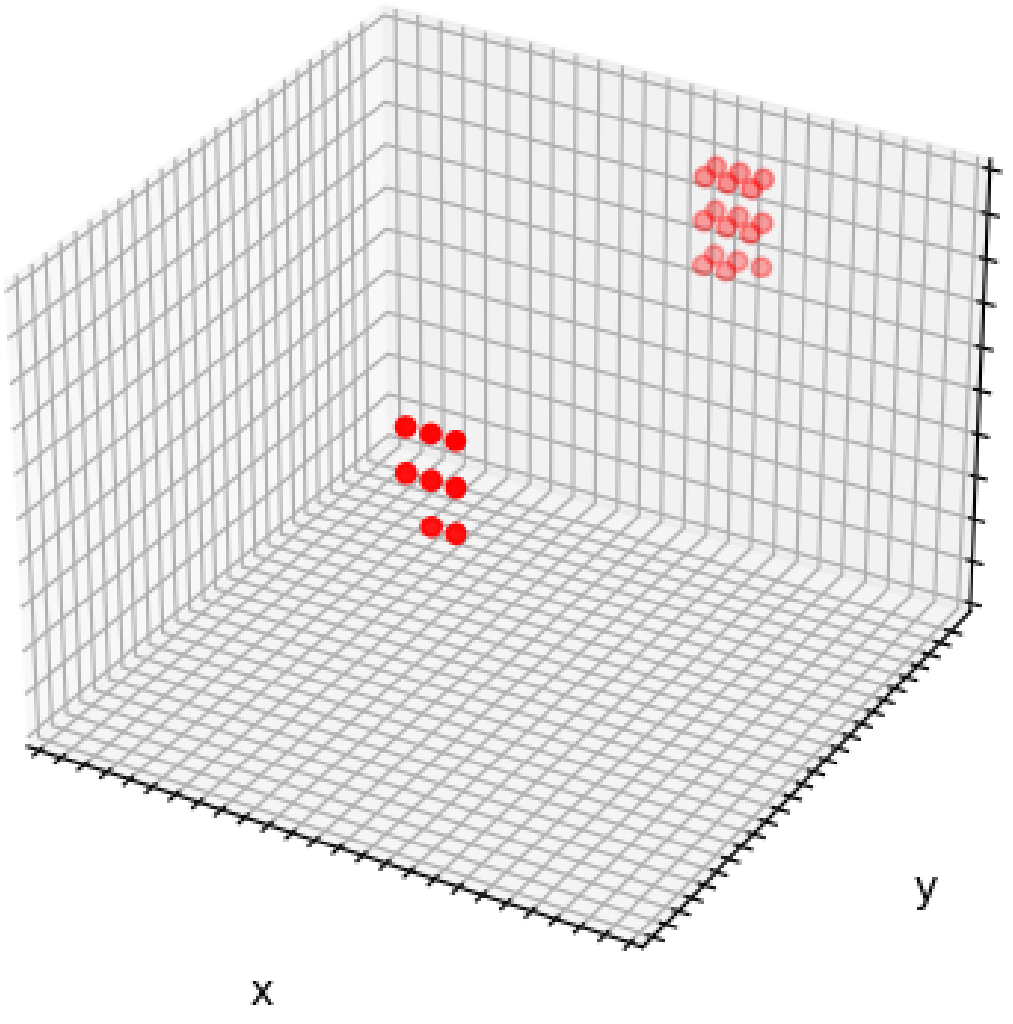

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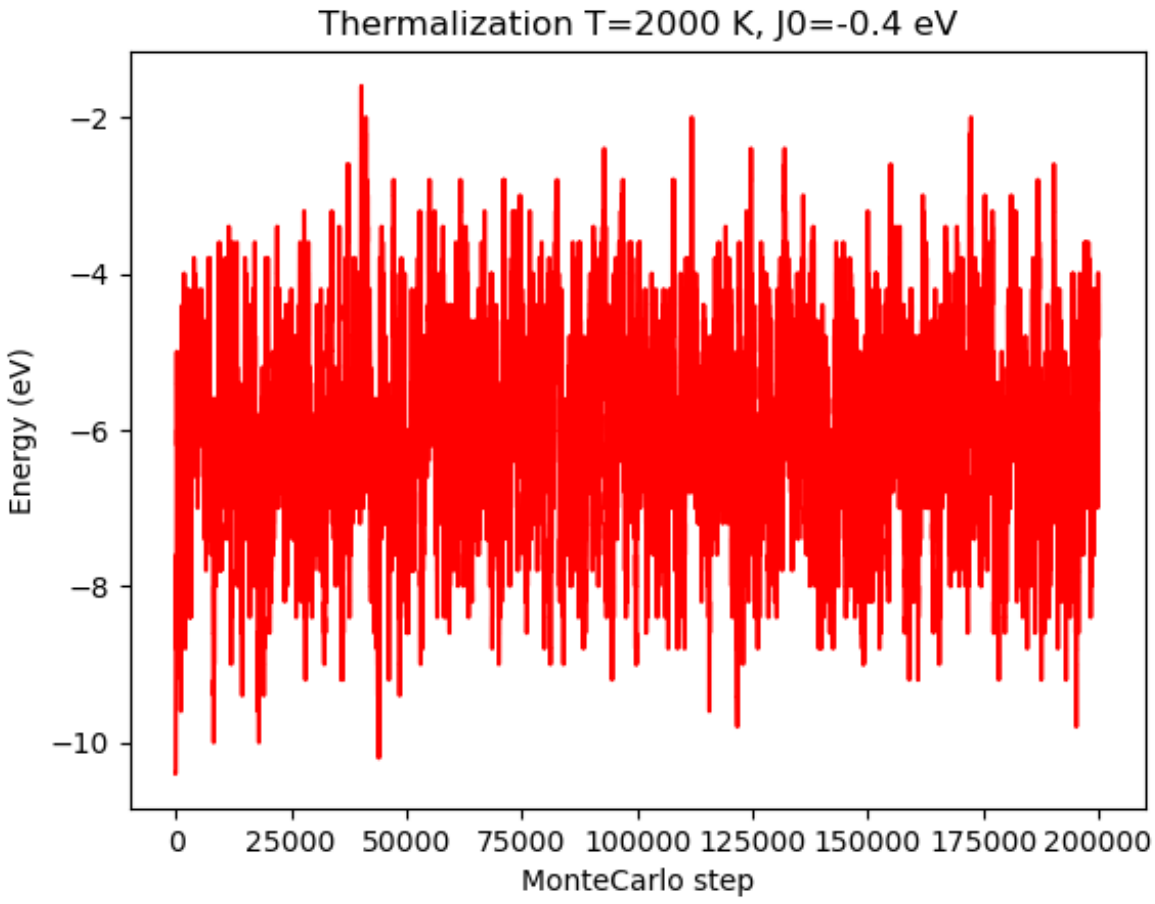

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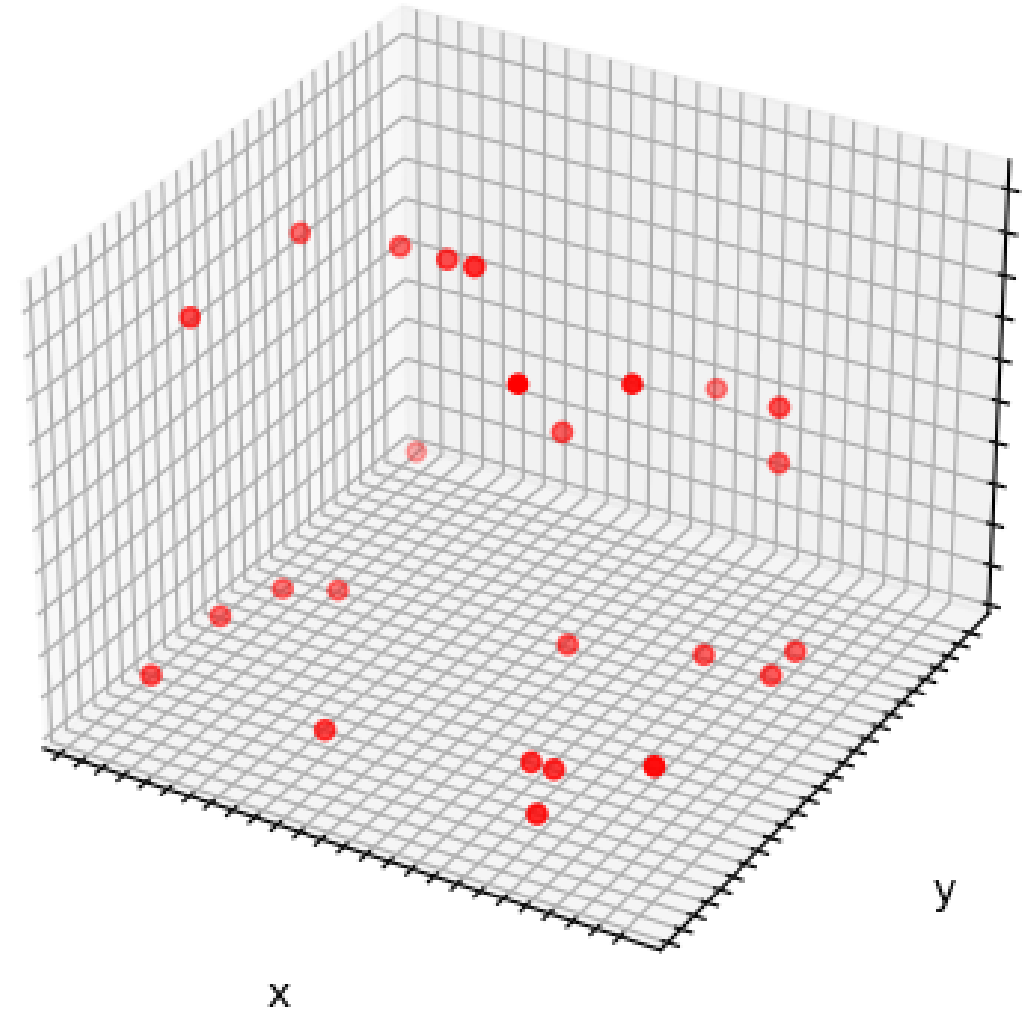

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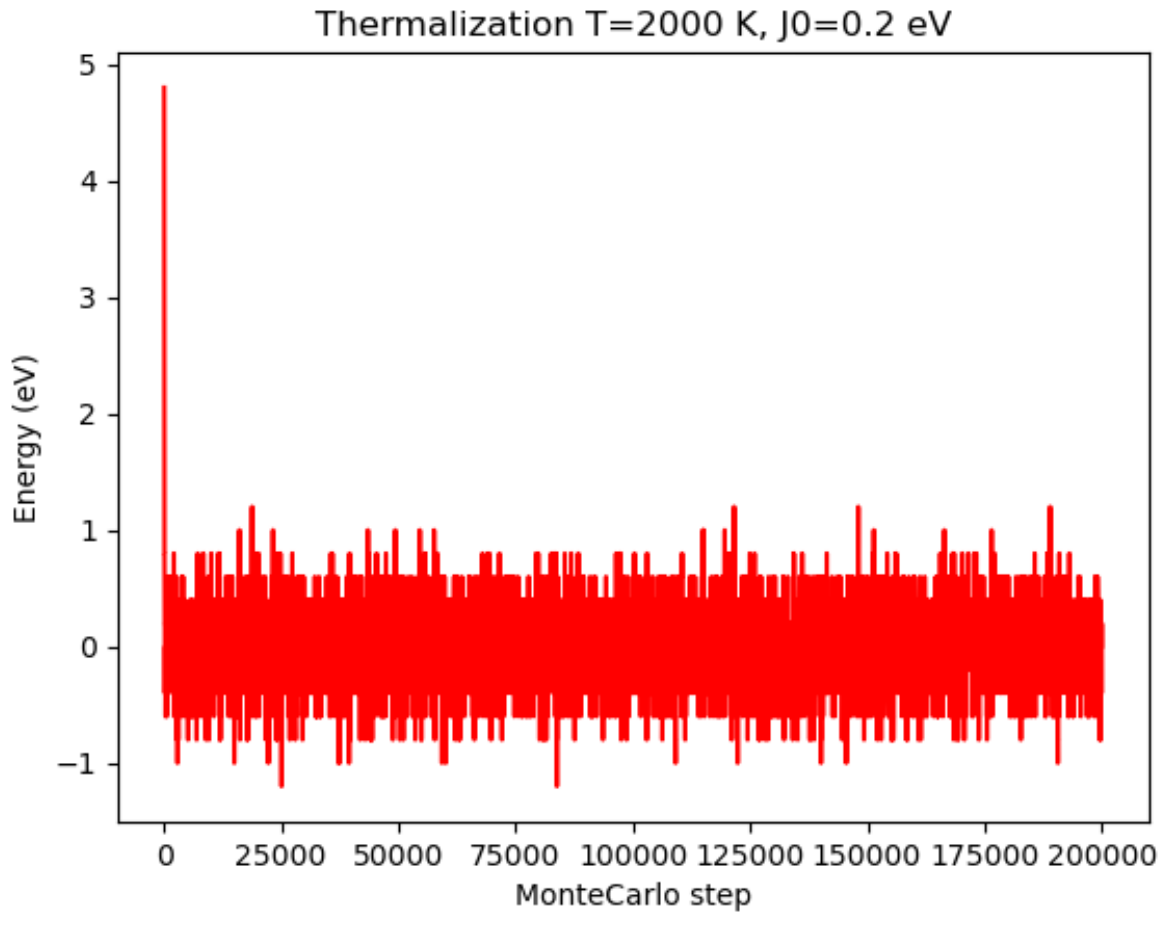

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