1) Run Ising model simulations for T=[1.75,2.00,2.25,2.50,2.75] for a 4x4 and an 8x8 grid of spins. Plot $< E >$ vs T, C_v vs T, and $< |M| >$ vs T for each grid and discuss the critical point and critical exponent.

The plots for the Ising model are shown below. Extra points were included for T=[2.10,2.20,2.30,2.40] to show the differences from the number of spins and plots for a 20x20 grid are included as well. The simulations had 100,000 equilibration steps and 1,000,000 steps for the statistics (values recorded every 1000 steps for 1000 data points).

The critical temperature for the 4x4 and 8x8 grids is between 2.25 and 2.50, but the exact value is hard to estimate even when the extra points are included in the plots. The critical exponent calculated by fitting

$$ln(< |M| >) = \alpha ln(2.269 - T) + C$$

was 0.100 for the 4x4 grid and 0.0636 for the 8x8 grid. These values do not compare well to $\alpha = 0.125$, but the systems are small.

For the 20x20 grid that was included for completeness, the C_v shows a sharp peak around T=2.25, and the critical temperature is more clearly shown. The critical exponent calculated using this simulation was 0.111 which is in much better agreement with the correct value.

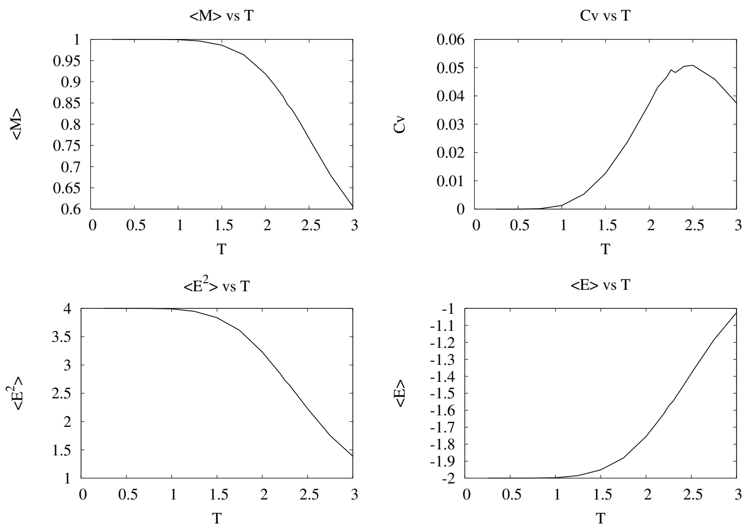

Figure 1: Results for the 4x4 grid of spins.

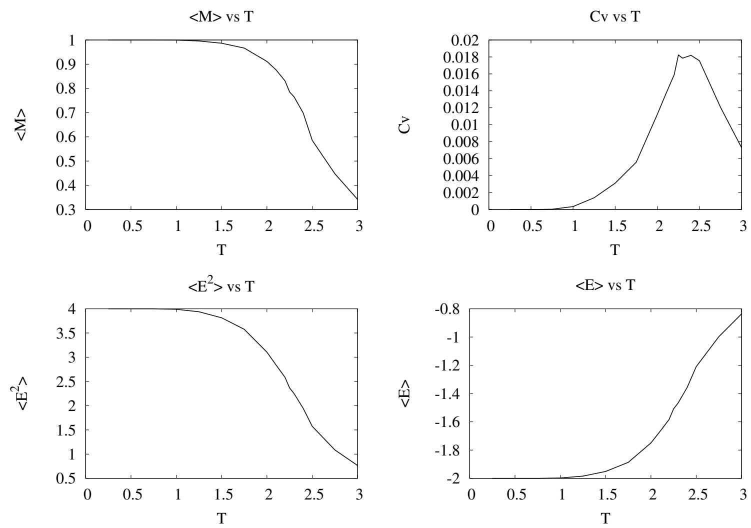

Figure 2: Results for the 8x8 grid of spins.

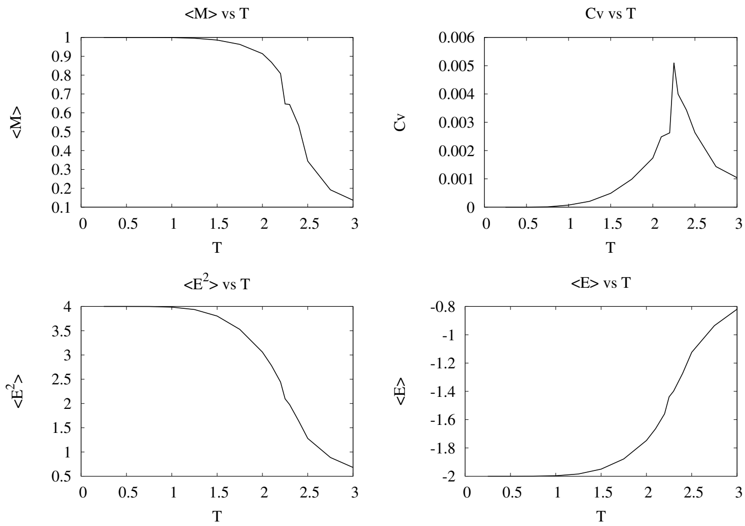

Figure 3: Results for the 20x20 grid of spins.

2) Find the second Virial coefficient and the Boyle Temperature for the Berthelot equation of state. (McQuarrie 12-4)

The Virial equation represents pressure as a power series in terms of ρ

$$P = kT\rho + B_2\rho^2 + B_3\rho^3 \cdots$$

The Berthelot EOS is

$$(P + \frac{N^2A}{V^2T})(V - NB) = NkT$$

$$P(V - NB) + \frac{N^2A}{VT} - \frac{N^3AB}{V^2T} = NkT$$

$$P(1 - \rho B) + \frac{A}{T}\rho^2 - \frac{AB}{T}\rho^3 = kT\rho$$

$$P = \frac{1}{1 - \rho B}(kT\rho - \frac{A}{T}\rho^2 + \frac{AB}{T}\rho^3)$$

let

$$x = \rho B$$

and use

$$\frac{1}{1 - x} = 1 + x + x^2 \cdots$$

The EOS then becomes (truncating at the second term)

$$P = kT\rho + kTx\rho - \frac{A}{T}\rho^2 - \frac{Ax}{T}\rho^2 + \frac{AB}{T}\rho^3 + \frac{ABx}{T}\rho^3$$

$$P = kT\rho + kTB\rho^2 - \frac{A}{T}\rho^2 - \frac{AB}{T}\rho^3 + \frac{AB}{T}\rho^3 + \frac{AB^2}{T}\rho^4$$

$$B_2 = kTB - \frac{A}{T}$$

$$B_3 = \frac{AB}{T} + \frac{AB}{T} = \frac{2AB}{T}$$

The Boyle temperature is the temperature where $B_2 = 0$

$$kT_bB = \frac{A}{T_b}$$

$$T_b^2 = \frac{A}{kB}$$

$$T_b = \sqrt{\frac{A}{kB}}$$