

NB: The graded, first version of the report must be returned if you hand in a second time!

H2a: Binary Alloy

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Task N ^o	Points	Avail. points
Σ		

Introduction

....

Task 1: mean field theory

Fits: we obtained $\alpha \approx 0.494$

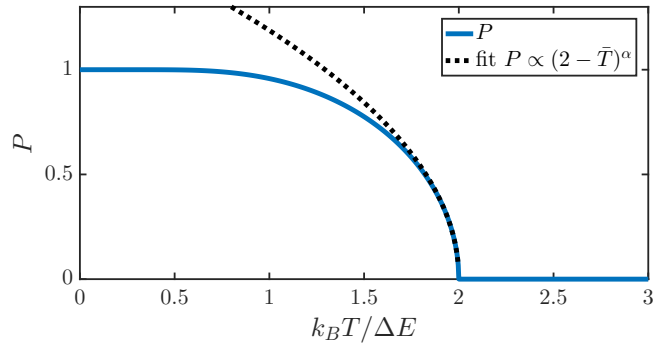


Figure 1:

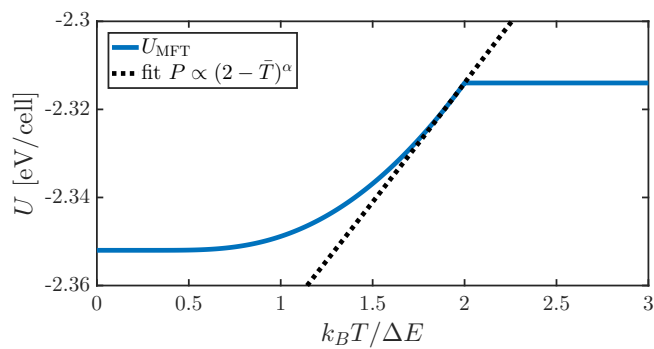


Figure 2:

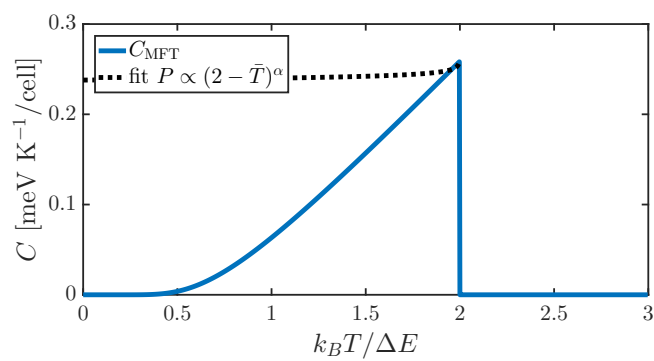


Figure 3:

Task 2: Ising model

$$E_{\text{CuZn}} = -294 \text{ meV} \quad (1)$$

$$E_{\text{CuCu}} = -436 \text{ meV} \quad (2)$$

$$E_{\text{ZnZn}} = -133 \text{ meV} \quad (3)$$

(4)

Figure 4 shows the equilibration at three different temperatures. We note that the energy per bond is in the range $E_{\text{CuZn}} \leq E \leq (E_{\text{CuCu}} + E_{\text{ZnZn}})/2 = 284.5 \text{ meV}$, which it should be.

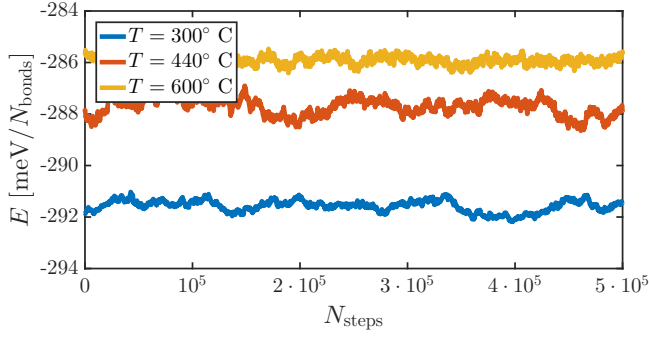


Figure 4: ...

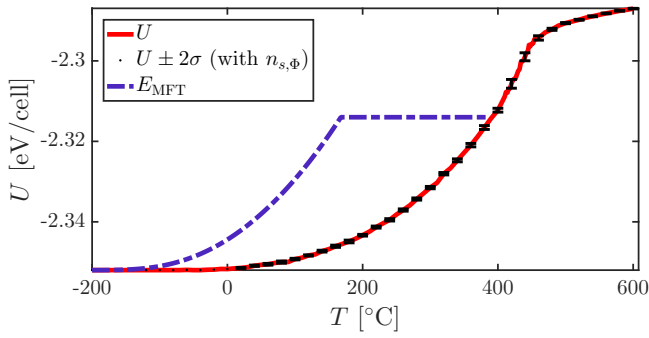


Figure 5: ...

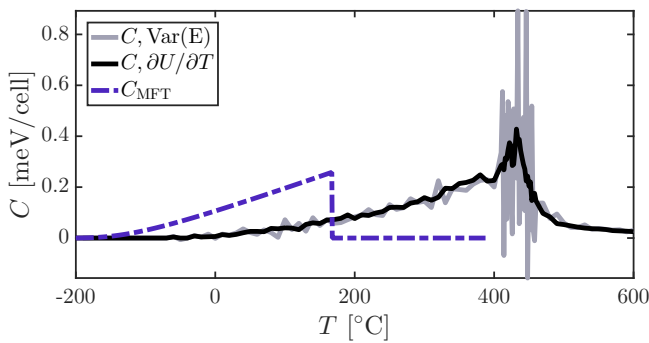


Figure 6: ...

Statistical inefficiency

As described in the Lecture notes, the statistical inefficiency can be used to obtain error estimates of correlated data.

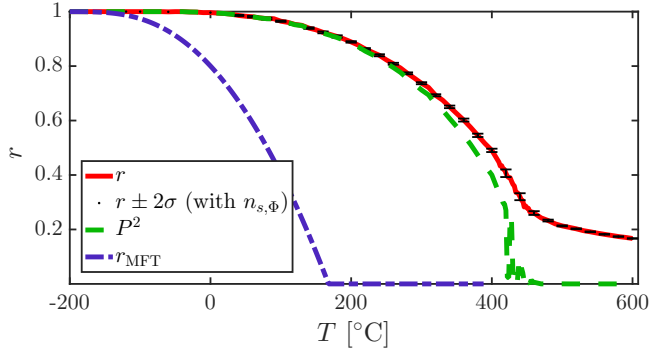


Figure 7: ...

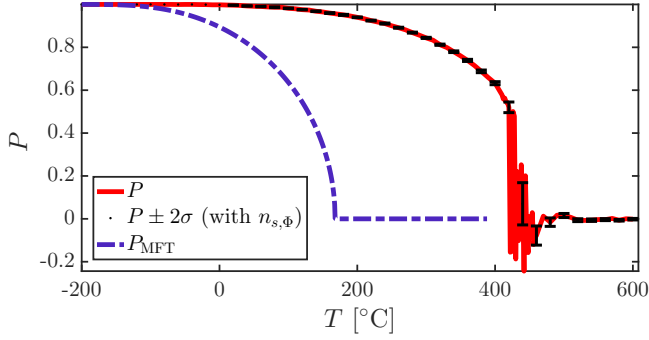


Figure 8: ...

Suppose we want to measure a quantity I , as an average of $N \gg 1$ measurements:

$$I = \langle f \rangle \equiv \frac{1}{N} \sum_{i=1}^N f_i. \quad (5)$$

The variance is then given by

$$\text{Var}[I] = \frac{n_s}{N} \text{Var}[f], \quad \text{Var}[f] = \langle f^2 \rangle - \langle f \rangle^2, \quad (6)$$

where n_s is the statistical inefficiency. The statistical inefficiency can be determined either from the decay of the correlation function,

$$\Phi_{k=n_s} = e^{-2} \approx 0.1, \quad \frac{\langle f_i f_{i+k} \rangle - \langle f \rangle^2}{\langle f^2 \rangle - \langle f \rangle^2}, \quad (7)$$

or from block averaging

$$n_s = \lim_{B \rightarrow \infty} \frac{B \text{Var}[F]}{\text{Var}[f]}, \quad F_j = \frac{1}{B} \sum_{i=1}^B f_{i+(j-1)B}, \quad j \in [1, N_{\text{blocks}}]. \quad (8)$$

The two methods in equations (7) and (8) should give similar estimates of n_s , which they do in the simulations here. The obtained statistical inefficiency is shown in figures 9 and 10 at three different temperatures, calculated with the correlation function and block average respectively.

In the case of block average, we used a moving average of 100 points, as the data become noisy when the block size become comparable to the total number of steps. Alternatively, we could have made more blocks of the largest sizes by also using shifted blocks of data, but the results obtained here were considered accurate enough.

Note in figures 9 and 10 that the statistical inefficiency is larger close to the phase transition at $T \approx 440^\circ\text{C}$ than at the lower and higher temperatures $T = 300^\circ\text{C}$ and $T = 600^\circ\text{C}$. We speculate that this is related to the diverging property of the correlation length close to the phase transition.

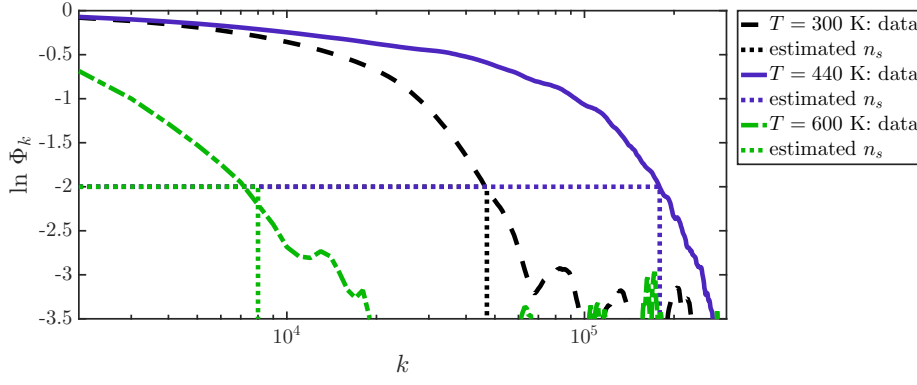


Figure 9: The logarithm of the correlation function $\Phi_k(k)$ for three different temperatures. Dotted lines mark the estimated value of $n_s = k(\ln \Phi_k = -2)$.

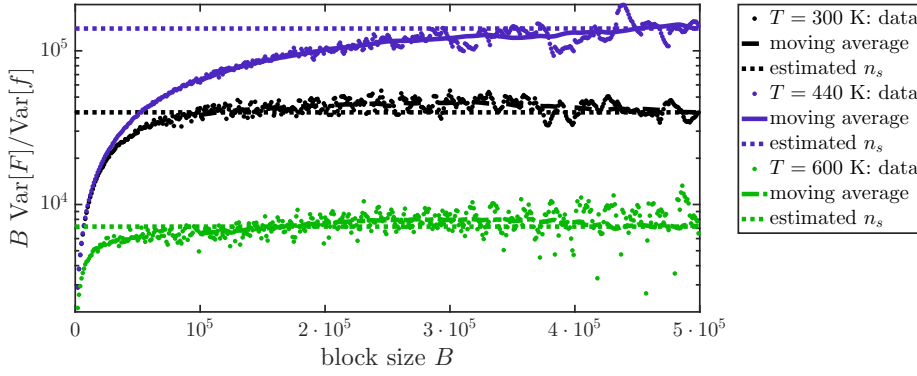


Figure 10: The statistical inefficiency determined with block averages for three different temperatures. Raw data is shown with dots, solid line show a moving average with 100 points, and the dotted lines show the estimated values of the statistical inefficiency.

This peak in the statistical inefficiency close to the phase transition can be clearly identified also in figure 11, where n_s is plotted as a function of temperature using the two methods described above. We note that both methods give similar estimates of n_s , but the correlation function give larger fluctuations than the block average method. Moreover, we note that the statistical inefficiency diverges as $T \rightarrow 0$ K. This is because very few changes in the lattice will be accepted at low temperatures, which give highly correlated data. At low temperatures, the equilibrium system is almost completely ordered, and we note that the uncertainty of the quantities U , P and r is still small at low temperatures as their variance decrease rapidly with decreasing temperature.

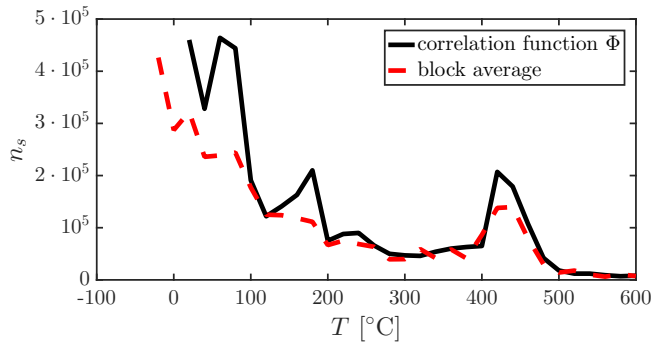


Figure 11: The statistical inefficiency n_s as a function of temperature using both the correlation function and block averages to determine n_s .

Concluding discussion

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A Source Code

A.1 Main program task 2: main.T2.c

```
1  /*
2   H2a, Task 2
3  */
4  #include <stdio.h>
5  #include <math.h>
6  #include <stdlib.h>
7
8  #include "funcs.h"
9
10 #define Nc 10 //number of cells
11 #define N_neigh 8
12 #define degC_to_K 273.15
13 #define kB 8.61733e-5
14
15 /* Main program */
16 int main(){
17     int N_Cu = Nc*Nc*Nc;
18     int N_atoms = 2*N_Cu;
19     int N_bonds = 8*N_Cu;
20     double Etot, E_Var, r, P; // Macro parameters
21     gsl_rng *q = init_random(); // initialize random number generator
22
23     /* done for all saved steps: */
24     int N_MCsteps = 1e7;
25     int N_eq = 1e6;
26     int N_eq_short = 5e5;
27     double *E_equilibration = malloc(sizeof(double[N_eq]));
28     double *P_equilibration = malloc(sizeof(double[N_eq]));
29     double *E_production = malloc(sizeof(double[N_MCsteps]));
30
31     /* statistical inefficiency */
32     int N_k = 500;
33     int N_skip = 1000; // k_Max = N_k * N_skip;
34     double *phi = malloc(sizeof(double[N_k]));
35     double *var_F = malloc(sizeof(double[N_k]));
36
37     /* set Temperature steps */
38     double beta;
39     double dT_small = 2;
40     double dT_large = 10;
41     double T_start = -200;
42     double T_end = 600;
43     double T_start_fine = 410;
44     double T_end_fine = 460;
45     int nT;
46     double *T_degC = init_temps(&nT, dT_small, dT_large, T_start, T_end,
47                                T_start_fine, T_end_fine);
48     // save equilibration data and stat inefficiency at T%20 =0
49     int T_save_step = 20;
50     /* done for all temps: */
51     double *E_mean = malloc(sizeof(double[nT]));
52     double *E_mean_approx = malloc(sizeof(double[nT]));
53     double *E_sq_mean = malloc(sizeof(double[nT]));
54     double *P_mean = malloc(sizeof(double[nT]));
55     double *P_sq_mean = malloc(sizeof(double[nT]));
56     double *r_mean = malloc(sizeof(double[nT]));
57     double *r_sq_mean = malloc(sizeof(double[nT]));
58
59     /* allocate and initialize lattice and nearest neighbors */
60     int *lattice = malloc(sizeof(int[N_atoms]));
61     init_ordered_lattice(N_atoms, N_Cu, lattice);
62     int (*nearest)[N_neigh] = malloc(sizeof(int[N_atoms][N_neigh]));
63     init_nearestneighbor(Nc, nearest);
64
65     /* initialize macro parameters */
66     Etot = get_Etot(lattice, N_Cu, nearest);
67     P = get_order_parameter(lattice, N_Cu);
68     r = get_short_range_order_parameter(lattice, nearest, N_Cu);
69
70
71     /* ***** start simulation ***** */
72     for (int iT=0; iT<nT; iT++){
73         /* Loop over all temperatures */
74         printf("Now running T = %.0f degC\n", T_degC[iT]);
75         beta = 1/(kB*(T_degC[iT] + degC_to_K));
76
77         /* ***** Equilibration run ***** */
78         if (iT!=0){// First run needs longer equilibration
79             N_eq=N_eq_short;
80         }
81         /* Do the Monte Carlo stepping */
82         for( int i=0; i<N_eq; i++){
83             MC_step(&Etot, &r, &P, q, lattice, nearest, beta, N_Cu);
```

```

84 // Save the energy `Etot` and orerparameter `P`
85 E_equilibration[i] = Etot;
86 P_equilibration[i]= P;
87 }
88 //Write the equilibration run to file
89 if ( ((int)T_degC[iT]) % T_save_step==0){
90     write_equil_to_file(T_degC[iT],
91         E_equilibration, N_bonds, P_equilibration, N_eq);
92 }
93
94 /* ***** Production run ***** */
95 /*
96 The saved energies are shifted by this (semi-arbitrary) amount.
97 This helps to increase the accuracy when calculating the
98 (needed for the heat capacity).
99 */
100 E_mean_approx[iT] = Etot;
101 /* initialize at temperature[iT] */
102 E_mean[iT] = 0; E_sq_mean[iT] = 0;
103 P_mean[iT] = 0; P_sq_mean[iT] = 0;
104 r_mean[iT] = 0; r_sq_mean[iT]=0;
105
106 /* Do the Monte Carlo stepping */
107 for( int i=0; i<N_MCsteps; i++){
108     MC_step( &Etot, &r, &P, q, lattice, nearest, beta, N_Cu);
109     E_production[i] = Etot- E_mean_approx[iT];
110     update_E_P_r(iT, Etot-E_mean_approx[iT], E_mean, E_sq_mean, P, P_mean,
111         P_sq_mean, r, r_mean,r_sq_mean, lattice, nearest, N_Cu);
112 }
113 /* Divide by number of Monte Carlo steps to get average */
114 E_mean[iT] *= 1/((double)N_MCsteps);
115 E_sq_mean[iT] *= 1/((double)N_MCsteps);
116 P_mean[iT] *= 1/((double)N_MCsteps);
117 P_sq_mean[iT] *= 1/((double)N_MCsteps);
118 r_mean[iT] *= 1/((double)N_MCsteps);
119 r_sq_mean[iT] *= 1/((double)N_MCsteps);
120
121 /*
122 We only calucluate the statistical inefficiency at some
123 temperatures to save on runtime.
124 */
125 if ( ((int)T_degC[iT]) % T_save_step==0 ){//calc stat ineff
126     // Calcualte the variance of the energy
127     E_Var = E_sq_mean[iT] - E_mean[iT]*E_mean[iT];
128
129     printf("Calculating statistical inefficiencies \n");
130     //Calcualte the auto-correlation
131     get_phi (phi, N_MCsteps, E_mean[iT], E_Var, E_production,N_k,N_skip);
132     //Calcualte the block-average variance
133     get_varF_block_average(var_F, N_MCsteps, E_mean[iT], E_Var,
134         E_production, N_k, N_skip);
135     //Write the stat ineff to file
136     write_stat_inefficiency_to_file(T_degC[iT], phi, var_F, N_k, N_skip);
137 }//END if calc stat ineff
138 }//END temp for
139
140 //Write the results of the production run to file
141 write_production(T_degC, nT, E_mean_approx, E_mean, E_sq_mean,
142     P_mean, P_sq_mean, r_mean, r_sq_mean);
143
144
145
146 //Don't forget to free all malloc's.
147 free(nearest); nearest = NULL;
148 free(lattice); lattice = NULL;
149 free(E_equilibration); E_equilibration = NULL;
150 free(P_equilibration); P_equilibration = NULL;
151 free(E_mean); E_mean = NULL;
152 free(E_mean_approx); E_mean_approx = NULL;
153 free(E_sq_mean); E_sq_mean = NULL;
154 free(P_mean); P_mean = NULL;
155 free(P_sq_mean); P_sq_mean = NULL;
156 free(r_mean); r_mean = NULL;
157 free(r_sq_mean); r_sq_mean = NULL;
158 free(E_production); E_production = NULL;
159 free(phi); phi = NULL;
160 free(var_F); var_F = NULL;
161 free(T_degC); T_degC = NULL;
162
163 gsl_rng_free(q); // deallocate rng
164 return 0;
165 }

```

A.2 Misc functions : funcs.c

```
1 #include "funcs.h"
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```

```

/***** get functions *****/
double get_bond_E(int site_1, int site_2){
    /*
    The bond can be one of three types: ZnZn, CuZn=ZnCu, or CuCu.
    With the lattice encoding Cu=1 and Zn=0, we get
    Zn+Zn = 0, Zn+Cu = Cu+Zn = 1, Cu+Cu = 2.
    Hence the switch over the three cases: 0, 1, and 2.
    */
    double Ebond=0;
    switch (site_1 + site_2){
    case 0:
        Ebond= -0.113;//E_ZnZn;
        break;
    case 1:
        Ebond= -0.294;//E_CuZn;
        break;
    case 2:
        Ebond= -0.436;//E_CuCu;
        break;
    }
    return Ebond;
}

double get_order_parameter(int *lattice, int N_Cu){
    /*
    The macro order parameter 'P' is given by the number of atoms in
    their respective sub-lattice (normalized and shifted to get a
    better physical interpretation), e.g. the number of Cu atoms in
    the Cu sub-lattice.
    */
    int N_Cu_in_Cu_lattice=0;
    for(int i=0;i<N_Cu;i++){
        /*
        Sum the atoms in the Cu sub-lattice (i=0,1,2,...,N_Cu-1), and
        with the encoding Cu=1 and Zn=0, we can simply add the values
        of the lattice encoding at each sub-lattice point.
        */
        N_Cu_in_Cu_lattice+=lattice[i];
    }
    return (double)N_Cu_in_Cu_lattice/N_Cu *2 -1;
}

double get_short_range_order_parameter(int *lattice, int(*nearest)[N_neigh],
    int N_Cu){
    /*
    The short range order parameter 'r' is given by the number of AB bonds
    (normalized and shifted to get a better physical interpretation).
    */
    int N_CuZnBonds=0;
    for(int i=0;i<N_Cu;i++){
        for( int j=0; j<N_neigh; j++){
            /*
            With the encoding Cu=1 and Zn=0, we know that in order for a
            bond to be a CuZn/ZnCu the sum of a lattice point with its
            neighbour must be 1 (see 'get_bond_E' for more detail).
            */
            N_CuZnBonds+= ((lattice[i] + lattice[nearest[i][j]]) == 1);
        }
    }
    return (double) N_CuZnBonds/(4*N_Cu)-1; // this is 'r'
}

double get_Etot(int *lattice, int N_Cu, int (*nearest)[N_neigh]){
    /*
    The total energy of the system is given by looping over every atom
    in one of the sub-lattices (Cu) and summing the energies of its
    bonds to every neighbour.
    We only need to sum over every atom in one sub-lattice since there
    are no bonds within a sub-lattice.
    */
    double Etot=0;
    for(int i=0; i<N_Cu; i++){ // loop over atoms
        for( int j=0; j<N_neigh; j++){ // loop over neighbours
            Etot+= get_bond_E(lattice[i], lattice[nearest[i][j]]);
        }
    }
    return Etot;
}

void get_phi (double *phi, int N_times, double f_mean,
    double f_var, double *data, int N_k, int N_skip){
    /*
    Function for calculating the auto-correlation in a data set. The
    rate at which the auto-correlation decay can be used to calculate
    the statistical inefficiency in the data set.
    Formula:
    phi_k = (<f_{i+k}f_i> - <f_i>^2) / (<f_i>^2 - <f_i>^2)
    Note that, by definition, phi_0 = 1.
    */

```

```

93 int N_terms_in_avg; // helper variable
94 for (int k=0; k<N_k; k++){
95     /*
96     We loop over `k` in the formula above to get the auto-correlation
97     at the different times.
98     `phi[k]` is used to hold intermediary values, and only becomes the
99     auto-correlation at the last step in this loop.
100    */
101    phi[k] = 0;
102
103    /*
104    The number of terms in the sum to get  $\langle f_{i+k} f_i \rangle$  must be such
105    that i fulfills the relation:
106    `(i+k)*N_skip < N_times`,
107    which is equivalent to saying that
108    `i < N_times/N_skip - k`.
109    */
110    N_terms_in_avg = N_times/N_skip - k;
111    for (int i=0; i<N_terms_in_avg; i++){
112        /*
113        Add the products of the off-setted data points to get:
114        sum_{i} f_{i+k}f_{i}
115        */
116        phi[k] += data[i*N_skip]*data[(i+k)*N_skip];
117    }
118    /*
119    First:
120     $\langle f_{i+k} f_i \rangle = (1/N\_avg) \sum_{i} \{N\_avg\} f_{i+k} f_i$ ,
121    then we get the auto-correlation by subtracting `f_mean`^2
122    and dividing by the variance.
123    */
124    phi[k] = (phi[k]/N_terms_in_avg - f_mean*f_mean)/f_var;
125 }
126 }
127
128 void get_varF_block_average(double *var_F, int N_times, double f_mean,
129                             double f_var, double *data, int N_k, int N_skip){
130     /*
131     Function for calculating the variances of the blockaverages for `N_k`
132     different block sizes. This variance can then be used to calculate the
133     statistical inefficiency in the data set.
134     */
135     int block_size;
136     double Fj; // help variable, holding each block average
137     int number_of_blocks; // The number of blocks depends on the block size
138
139     for (int k=0; k<N_k; k++) { // block size loop
140         /*
141         For every block size, we need to loop over every block,
142         and every element in that block
143         */
144         block_size = N_skip * (k+1);
145         number_of_blocks = N_times/block_size;
146
147         var_F[k] = 0; // start
148         for (int j=0; j<number_of_blocks; j++) { // loop over all blocks
149             /* For every block, we loop over all elements in it to take average. */
150             Fj = 0; // reset to 0
151             for (int i=0; i<block_size; i++) { // internal block loop
152                 /* Adding all elems in the block to get the average */
153                 Fj += data[j*block_size + i];
154             }
155             Fj *= 1/(double)block_size; // divide by block size to get average
156             var_F[k] += Fj*Fj; // will become the variance soon
157         }
158         /*
159         To get the variance of F we use:
160          $Var[F] = \langle F^2 \rangle - \langle F \rangle^2 = \langle F^2 \rangle - \langle f \rangle^2$ ,
161         where f is the data set the block averages were taken from.
162         */
163         var_F[k] = var_F[k]/number_of_blocks - f_mean*f_mean;
164         var_F[k] *= block_size/f_var;
165     } // end block size loop
166 }
167
168 /***** Monte Carlo step functions *****/
169 void MC_step( double *Etot, double *r, double *P, gsl_rng *q,
170              int *lattice, int (*nearest)[N_neigh], double beta, int N_Cu){
171     /*
172     Function that takes a Monte Carlo step and updates the lattice points,
173     `Etot`, `r`, and `P` accordingly.
174     It is important to utilize the _chage_ in energy, `r` and `P` when
175     updating them as to not have to do a costly full calculation of either
176     every step in the Monte Carlo loop.
177     */
178     // Picks two random sites in the whole lattice.
179     int i1 = (int)(2*N_Cu*gsl_rng_uniform(q));
180     int i2 = (int)(2*N_Cu*gsl_rng_uniform(q));
181     // saves the original values
182     int old_1 = lattice[i1];
183     int old_2 = lattice[i2];

```

```

184 // Used to calculate the change in `Etot` and `r`
185 double dr = 0;
186 double dE = 0;
187 // We only need to do something if the two atoms are different
188 if (old_1 != old_2){
189     for( int j=0; j<N_neigh; j++){
190         /*
191          The change in `Etot` and `r` are first _minus_ the old energies and `r`
192          contributions.
193          */
194         dE -= get_bond_E(lattice[i1], lattice[nearest[i1][j]])
195             + get_bond_E(lattice[i2], lattice[nearest[i2][j]]);
196
197         dr -= ((lattice[i1] + lattice[nearest[i1][j]]) == 1)
198             + ((lattice[i2] + lattice[nearest[i2][j]]) == 1);
199     }
200     /* Then we do the change of the two atoms */
201     lattice[i1] = old_2;
202     lattice[i2] = old_1;
203     for( int j=0; j<N_neigh; j++){
204         /*
205          And _add_ the contributions to `Etot` and `r` from the updated lattice.
206          */
207         dE += +get_bond_E(lattice[i1], lattice[nearest[i1][j]])
208             + get_bond_E(lattice[i2], lattice[nearest[i2][j]]);
209
210         dr += ((lattice[i1] + lattice[nearest[i1][j]]) == 1)
211             + ((lattice[i2] + lattice[nearest[i2][j]]) == 1);
212     }
213
214     if ( (dE<=0) || (exp(-beta * dE) > gsl_rng_uniform(q)) ){
215         /*
216          The test is accepted if dE < 0 (accept immediately), OR
217          otherwise it's accepted with a probability of `exp(-beta * dE)`
218          */
219         // Updates P
220         if (i1 < N_Cu)
221             *P += (double)(lattice[i1] - old_1 )/N_Cu *2;
222         if (i2 < N_Cu)
223             *P += (double)(lattice[i2] - old_2 )/N_Cu *2;
224     }else{
225         /*
226          If the test failed, we change back to the old lattice configuration
227          and no change happens to `Etot` or `r`
228          */
229         lattice[i1] = old_1;
230         lattice[i2] = old_2;
231         dE = 0;
232         dr = 0;
233     } // end if step is accepted
234     *Etot += dE;
235     *r += dr/(4*N_Cu);
236 } // end if atoms are different
237 }
238
239 void update_E_P_r(int iT, double E_dev, double *E_mean, double *E_sq_mean,
240                 double P, double *P_mean, double *P_sq_mean,
241                 double r, double *r_mean, double *r_sq_mean,
242                 int *lattice, int (*nearest)[N_neigh], int N_Cu){
243     /*
244      Updates the macro parameters `E`, `P`, and `r`, as well as their squares.
245      Runs in every Monte Carlo step during the production run.
246      */
247     E_mean[iT] += E_dev;
248     E_sq_mean[iT] += E_dev * E_dev;
249
250     P_mean[iT] += P;
251     P_sq_mean[iT] += P*P;
252
253     r_mean[iT] += r;
254     r_sq_mean[iT] += r*r;
255 }
256
257 /***** initializing functions *****/
258 double * init_temps( int *nT, double dT_small, double dT_large,
259                     double T_start, double T_end, double T_start_fine,
260                     double T_end_fine){
261     /*
262      Creates an array `T_degC` with the temperatures to loop over in the main
263      function, given the fine temperature step range and the sizes of the
264      temperature steps.
265      */
266     *nT = (int) ((T_end_fine - T_start_fine)/dT_small
267                 + (T_start_fine-T_start + T_end-T_end_fine)/dT_large +1);
268     double *T_degC = malloc(sizeof(double)*nT);
269     T_degC[0] = T_start;
270     for (int iT=1; iT<*nT; iT++){ // loop over all temps
271         if (T_degC[iT-1]>=T_start_fine && T_degC[iT-1]<T_end_fine){
272             T_degC[iT] = T_degC[iT-1] + dT_small;
273         }else{
274             T_degC[iT] = T_degC[iT-1] + dT_large;

```

```

275     }
276 }
277 return T_degC;
278 }
279
280
281 void init_ordered_lattice(int N_atoms, int N_Cu, int *lattice){
282     /*
283      Initialize lattice with Cu atoms (1) in Cu lattice (i=0:N_Cu-1)
284      and Zn (0) in Zn lattice (i=N_Cu:N_atoms-1):
285     */
286     for( int i=0; i<N_Cu; i++){
287         lattice[i] = 1;
288     }
289     for( int i=N_Cu; i<N_atoms; i++){
290         lattice[i] = 0;
291     }
292 }
293
294 void init_random_lattice(int N_atoms, int N_Cu, int *lattice, gsl_rng *q){
295     /*
296      Initialize lattice with Cu and Zn atoms randomly distributed:
297     */
298     for( int i=0; i<N_Cu; i++){
299         lattice[i] = (int)(gsl_rng_uniform(q)+0.5);
300         lattice[i+N_Cu] = 1-lattice[i];
301     }
302 }
303
304
305 void init_nearestneighbor(int Nc, int (*nearest)[N_neigh]){
306     /*
307      Create a matrix `nearest[i][j]` with the index of the `j`th nearest
308      neighbors to site `i`.
309      N.B. Each site has `N_neigh` (8) nearest neighbors.
310     */
311     int i_atom;
312     int N_Cu = Nc*Nc*Nc;
313     for( int i=0; i<Nc; i++){
314         for( int j=0; j<Nc; j++){
315             for( int k=0; k<Nc; k++){
316                 i_atom = k + Nc*j + Nc*Nc*i;
317                 // k i j in one lattice <=> "k-0.5" "i-0.5" "j-0.5" in the other lattice
318                 // use mod to handle periodic boundary conditions
319                 nearest[i_atom][0] = k + Nc*j + Nc*Nc*i + N_Cu;
320                 nearest[i_atom][1] = k + Nc*j + Nc*Nc*((i+1)%Nc) + N_Cu;
321                 nearest[i_atom][2] = k + Nc*((j+1)%Nc) + Nc*Nc*i + N_Cu;
322                 nearest[i_atom][3] = k + Nc*((j+1)%Nc) + Nc*Nc*((i+1)%Nc) + N_Cu;
323                 nearest[i_atom][4] = (k+1)%Nc + Nc*j + Nc*Nc*i + N_Cu;
324                 nearest[i_atom][5] = (k+1)%Nc + Nc*j + Nc*Nc*((i+1)%Nc) + N_Cu;
325                 nearest[i_atom][6] = (k+1)%Nc + Nc*((j+1)%Nc) + Nc*Nc*i + N_Cu;
326                 nearest[i_atom][7] = (k+1)%Nc + Nc*((j+1)%Nc) + Nc*Nc*((i+1)%Nc) + N_Cu;
327
328                 // k i j in one lattice <=> "k+0.5" "i+0.5" "j+0.5" in the other lattice
329                 // use mod to handle periodic boundary conditions
330                 // note that mod([negative])<0 :
331                 i_atom += N_Cu;
332                 nearest[i_atom][0] = k + Nc*j + Nc*Nc*i;
333                 nearest[i_atom][1] = k + Nc*j + Nc*Nc*((i-1+Nc)%Nc)↵
334
335                 nearest[i_atom][2] = k + Nc*((j-1+Nc)%Nc) + Nc*Nc*i;
336                 nearest[i_atom][3] = k + Nc*((j-1+Nc)%Nc) + Nc*Nc*((i-1+Nc)%Nc)↵
337
338                 nearest[i_atom][4] = (k-1+Nc)%Nc + Nc*j + Nc*Nc*i;
339                 nearest[i_atom][5] = (k-1+Nc)%Nc + Nc*j + Nc*Nc*((i-1+Nc)%Nc)↵
340
341                 nearest[i_atom][6] = (k-1+Nc)%Nc + Nc*((j-1+Nc)%Nc) + Nc*Nc*i;
342                 nearest[i_atom][7] = (k-1+Nc)%Nc + Nc*((j-1+Nc)%Nc) + Nc*Nc*((i-1+Nc)%Nc)↵
343
344             }
345         }
346     }
347 }
348
349 gsl_rng* init_random(){
350     /*
351      Initializes a GSL random nubner generator, and returns the pointer.
352     */
353     gsl_rng *q;
354     const gsl_rng_type *rng_T; // static info about rngs
355     gsl_rng_env_setup(); // setup the rngs
356     rng_T = gsl_rng_default; // specify default rng
357     q = gsl_rng_alloc(rng_T); // allocate default rng
358     gsl_rng_set(q,time(NULL)); // Initialize rng
359     return q;
360 }
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```

```

362  /*
363   Writes the energy per bond `E_equilibration`/'N_bonds` and order
364   parameter `P`, at each Monte Carlo step during the equilibration runs.
365  */
366  FILE *file_pointer;
367  char file_name[256];
368  sprintf(file_name, "../data/E_equilibration-T%d.tsv", (int) T_degC);
369  file_pointer = fopen(file_name, "w");
370  for (int i=0; i<N_eq; i++){
371      fprintf(file_pointer, "%.8f\t%.8f \n", E_equilibration[i]/N_bonds, P[i]);
372  }
373  fclose(file_pointer);
374  }
375
376  void write_production(double *T_degC, int nT, double *E_mean_approx,
377                      double *E_mean, double *E_sq_mean,
378                      double *P_mean, double *P_sq_mean,
379                      double *r_mean, double *r_sq_mean){
380
381      /*
382       Writes the macro parameters `E_mean_approx`, `E_mean`, `E_sq_mean`,
383       `P_mean`, `P_sq_mean`, `r_mean`, and `r_sq_mean` for each temperature
384       to file.
385      */
386      FILE *file_pointer;
387      char file_name[256];
388      sprintf(file_name, "../data/E_production.tsv");
389      file_pointer = fopen(file_name, "w");
390      fprintf(file_pointer, "%s T[degC]\t E_approx\t<E-E_approx>\t<(E-E_approx)^2>\t<
391          tP\ttr\n");
392      for (int iT=0; iT<nT; iT++){
393          fprintf(file_pointer, "%.2f\t%.8e\t%.8e\t%.8e\t%.8f\t%.8f\t %.8f\t%.8f \n",
394                  T_degC[iT], E_mean_approx[iT], E_mean[iT], E_sq_mean[iT], P_mean[iT],
395                  P_sq_mean[iT], r_mean[iT], r_sq_mean[iT]);
396      }
397      fclose(file_pointer);
398  }
399
400  void write_stat_inefficiency_to_file(double T_degC, double *phi, double *var_F,
401                                      int N_k, int N_skip){
402
403      /*
404       Writes the auto-correlation `phi` and block varaiances `var_F` for each
405       tested temperature to file.
406      */
407      FILE *file_pointer;
408      char file_name[256];
409      sprintf(file_name, "../data/stat_inefficiency-T%d.tsv", (int) T_degC);
410      file_pointer = fopen(file_name, "w");
411      for (int i=0; i<N_k; i++){
412          fprintf(file_pointer, "%d\t%.8f\t%.8f \n", i*N_skip, phi[i], var_F[i]);
413      }
414      fclose(file_pointer);
415  }

```

B Auxiliary

B.1 Makefile

```

1
2  CC = gcc
3  CFLAGS = -O3 -Wall
4
5  LIBS = -lm -lgsl -lgslcblas
6
7  HEADERS = funcs.h
8  OBJECTS = funcs.o
9
10
11  %.o: %.c $(HEADERS)
12      $(CC) -c -o $@ $< $(CFLAGS)
13
14  all: Task2
15
16
17
18  Task2: $(OBJECTS) main_T2.c
19      $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
20
21  # $(PROGRAMS): $(OBJECTS) main_T1.c
22  # $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
23
24  clean:
25      rm -f *.o
26      touch *.c

```

C MATLAB scripts

C.1 Task 1 and analysis scripts for Task 2

```
1 %% initial
2
3 tmp = matlab.desktop.editor.getActive; %% cd to current path
4 cd(fileparts(tmp.Filename));
5 set(0,'DefaultFigureWindowStyle','docked');
6 warning('off','MATLAB:handle_graphics:exceptions:SceneNode'); % interpreter
7 GRAY = 0.7*[0.9 0.9 1];
8 kB = 8.61733e-5;
9 %% task 1: MFT
10 doSave = 0;
11 clc
12
13 Pmin = 0;
14 Pmax = 1;
15
16 E_CuCu = -.436;
17 E_ZnZn = -.133;
18 E_CuZn = -.294;
19
20 E0=2*(E_CuCu+E_ZnZn+2*E_CuZn);
21 Delta_E=(E_CuCu+E_ZnZn-2*E_CuZn);
22
23 E0_bar=E0/Delta_E;
24 E_MFT=@(P) E0 - 2*P.^2*Delta_E;
25 E_MFT_bar=@(P) E0_bar - 2*P.^2;
26 dE_MFTdP =@(P) - 4*P*Delta_E;
27
28 F_MFT = @(P,Tbar) E_MFT_bar(P) + Tbar*(-2*log(2) + (1+P).*log(1+P)+(1-P).*log(1-←
    P));
29 P_eq=@(Tbar) fminbnd(@(P)F_MFT(P, Tbar), Pmin, Pmax, optimset('TolX',1e-9));
30
31 Tbar = linspace(0,3,1000)';
32 T_MFT=Tbar*Delta_E/kB;
33 T_MFT_degC = T_MFT - 273.15;
34 Peq = zeros(size(Tbar));
35 for iT = 1:numel(Tbar)
36     Peq(iT) = P_eq(Tbar(iT));
37 end
38
39 % plot P(T) and make a fit
40 figure(1);clf
41 plot(Tbar, Peq);hold on
42
43 dT=2-Tbar(Tbar<2);
44 Peq_nonzero = Peq(Tbar<2);
45
46 I_good = (dT<0.1);
47 log_dT = log(dT(I_good));
48 log_P = log(Peq_nonzero(I_good));
49 A=[ones(size(log_dT)), log_dT]\log_P;
50 b = exp(A(1));
51 alpha = A(2);
52 fprintf('alpha = %.3f\n', alpha)
53
54 P_approx = @(alpha,b,Tbar) b*(2-Tbar).^alpha;
55 plot(Tbar(Tbar<2),P_approx(alpha,b,Tbar(Tbar<2)),'k:')
56 xlabel('$k_B T / \Delta E$')
57 ylabel('$P$')
58 legend('$P$', 'fit $P \propto (2-\bar{T})^\alpha$', 'location', '↵
    NorthWest');
59 ylim([0 1.3]);
60 if doSave; setFigureSize(gcf, 300, 600); end
61
62 % plot E_MFT and the fit
63 figure(2);clf
64 plot(Tbar,E_MFT(Peq)); hold on
65 plot(Tbar,E_MFT(P_approx(alpha,b,Tbar)),'k:')
66 xlabel('$k_B T / \Delta E$')
67 ylabel('$U$ [eV/cell]')
68 legend('$U_{\rm MFT}$', 'fit $P \propto (2-\bar{T})^\alpha$', 'location', '↵
    NorthWest');
69 ylim([-2.36 -2.3]);
70 if doSave; setFigureSize(gcf, 300, 600); end
71
72 figure(3);clf
73 C_MFT=diff(E_MFT(Peq))./diff(T_MFT);
74 plot(Tbar(1:end-1), C_MFT*1e3); hold on
75 C_approx=4*b^2*kB*alpha*(2-Tbar).^(2*alpha-1);
76 plot(Tbar(Tbar<2),1e3*C_approx(Tbar<2),'k:')
77 xlabel('$k_B T / \Delta E$')
78 ylabel('$C$ [meV K$^{-1}$]/cell]')
79 legend('$C_{\rm MFT}$', 'fit $P \propto (2-\bar{T})^\alpha$', 'location', '↵
    NorthWest');
80 ylim([0 0.3])
```

```

81 if doSave; setFigureSize(gcf, 300, 600); end
82
83 ImproveFigureCompPhys()
84 if doSave
85     saveas(1, '../figures/P_MFT.eps', 'epsc');
86     saveas(2, '../figures/E_MFT.eps', 'epsc');
87     saveas(3, '../figures/C_MFT.eps', 'epsc');
88 end
89
90
91 %% task 2: equilibration and statistical inefficiency
92 clc;
93 doSave = 1;
94 Ts = [-200:20:600]';
95 TsToPlot = [300 440 600]';
96 t_eq=0;
97
98 figure(1);clf;
99
100 for i=1:numel(TsToPlot)
101     data = load(sprintf('../data/E_equilibration-T%d.tsv',TsToPlot(i)));
102     E = data(:,1);
103     steps = 1:length(E);
104     %P = data(:,2);
105     plot(steps, E*1000); hold on
106 end
107 legstr = strcat({'$T='}, num2str(TsToPlot), '\circ C');
108 legend(legstr, 'location', 'NorthWest');
109 ylabel('$E$ [meV/$N_{\rm bonds}$]')
110 xlabel('$N_{\rm steps}$')
111 ax = gca;
112 ax.XTickLabel = {'0', '$10^5$', '$2\cdot 10^5$', '$3\cdot 10^5$', '$4\cdot 10^5$', '$5\cdot 10^5$'};
113
114 ImproveFigureCompPhys(1)
115
116 figure(3); clf; figure(2); clf;
117 [ns_Phi, ns_block] = deal(nan(size(Ts)));
118 Nskip = 10; % did not use all k's when calculating block averages
119 N_avg = 100; % moving average
120 for i=1:numel(Ts)
121     data = load(sprintf('../data/stat_inefficiency-T%d.tsv',Ts(i)));
122     k = data(:,1);
123     block_size = k+Nskip;
124     phi = data(:,2);
125     VarF_norm = data(:,3);
126     kstar = k(find(log(phi)<=-2, 1, 'first'));
127     if ~isempty(kstar)
128         ns_Phi(i) = kstar;
129     end
130
131     filtereddata = movmean(VarF_norm, N_avg);
132     ns_block(i) = filtereddata(end);
133
134     if any(Ts(i) == TsToPlot)
135         figure(2)
136
137         semilogx(k, log(phi));hold on;
138         plot([0.1 kstar kstar], [-2 -2 -6], ':k')
139
140         figure(3)
141         semilogy(block_size, VarF_norm, '.'); hold on;
142         plot(block_size(N_avg:end), filtereddata(N_avg:end));
143         plot(block_size, filtereddata(end)*ones(size(block_size)), ':k');
144
145     end
146 end
147
148 figure(4); clf;
149 plot(Ts, ns_Phi, 'k', Ts, ns_block, '--r')
150 ax = gca;
151 ax.YTickLabel = {'0', '$10^5$', '$2\cdot 10^5$', '$3\cdot 10^5$', '$4\cdot 10^5$', '$5\cdot 10^5$'};
152 ylabel('$n_s$');
153 legend('correlation function $\Phi$', 'block average');
154 xlabel('$T$ [$\circ C]$');
155 ImproveFigureCompPhys(gcf)
156
157 legs_Phi = cell(6,1);
158 legs_block = cell(9,1);
159 for i = 1:numel(TsToPlot)
160     tt = ['$T=' num2str(TsToPlot(i)) '$ K: '];
161     legs_Phi{1 + 2*(i-1)} = [tt 'data'];
162     legs_Phi{2 + 2*(i-1)} = 'estimated $n_s$';
163     legs_block{1 + 3*(i-1)} = [tt 'data'];
164     legs_block{2 + 3*(i-1)} = 'moving average';
165     legs_block{3 + 3*(i-1)} = 'estimated $n_s$';
166 end
167
168 figure(2);
169

```

```

170 legend(legs_Phi, 'location', 'northeastoutside');
171 xlabel('$k$'); ylabel('ln $\Phi_k$');
172 ylim([-3.5 0]);
173 xlim([2e3 3e5]);
174 %ax = gca; ax.XTick = [3e3 1e4 3e4 1e5 3e5];
175 %ax.XTickLabel = {'$3\cdot 10^3$', '$10^4$', '$3\cdot 10^4$', '$10^5$', '$3\cdot 10^5$'};
176 figure(3);
177 ax = gca;
178 [ax.Children(:).MarkerSize] = deal(12);
179 legend(legs_block, 'location', 'northeastOutside');
180 xlabel('block size $B$');
181 ylabel('$B$ Var[$F$]/Var[$f$]');
182 ylim([2e3 2e5]);
183 ax = gca;
184 ax.XTickLabel = {'0', '$10^5$', '$2\cdot 10^5$', '$3\cdot 10^5$', '$4\cdot 10^5$', '$5\cdot 10^5$'};
185
186 ImproveFigureCompPhys(2, 'LineColor', {'LINNEAGREEN', 'LINNEAGREEN', 'GERIBLUE', 'GERIBLUE', 'k', 'k'}, ...
187 'LineStyle', {':', '-.', ':', '-', ':', '--'})
188 ImproveFigureCompPhys(3, 'LineColor', {'LINNEAGREEN', 'LINNEAGREEN', 'LINNEAGREEN', 'GERIBLUE', 'GERIBLUE', 'GERIBLUE', 'k', 'k', 'k'}, ...
189 'LineStyle', {':', '-.', 'none', ':', '-', 'none', ':', '--', 'none'});
190
191 if doSave
192     figure(1);
193     setFigureSize(gcf, 300, 600);
194     saveas(gcf, '../figures/equilibration.eps', 'eps');
195     figure(2);
196     setFigureSize(gcf, 350, 900);
197     saveas(gcf, '../figures/stat_inefficiency_Phi.eps', 'eps');
198     figure(3);
199     setFigureSize(gcf, 350, 900);
200     saveas(gcf, '../figures/stat_inefficiency_block.eps', 'eps');
201     figure(4);
202     setFigureSize(gcf, 300, 600);
203     saveas(gcf, '../figures/stat_inefficiency_both.eps', 'eps');
204 end
205
206
207 %% task 2: U, C, P and r
208
209 doSave = 0;
210
211 data = load('../data/E_production.tsv');
212 T_degC = data(:,1);
213 N_Cu = 1e3;
214 N_timeSteps = 1e7;
215
216 Emean_approx = data(:,2)/N_Cu; % divide by N_Cu to get energy and Cv per cell
217 Emean_shifted = data(:,3)/N_Cu;
218 E_sq_mean_shifted = data(:,4)/N_Cu^2;
219
220 E_Var = (E_sq_mean_shifted - Emean_shifted.^2);
221
222 Cv = 1./(kB * (T_degC+273.15).^2).*E_Var*N_Cu;
223 U = (Emean_shifted + Emean_approx);
224 U_std = sqrt(E_Var/N_timeSteps);
225 P = data(:,5);
226 P_std = sqrt((data(:,6)-P.^2)/N_timeSteps); % without ns so far
227 r = data(:,7);
228 r_std = sqrt((data(:,8)- r.^2)/N_timeSteps);
229
230 ind = zeros(size(Ts));
231 for i = 1:numel(Ts)
232     ind(i) = find(Ts(i) == T_degC);
233 end
234
235 figure(1); clf;
236 plot(T_degC, U); hold on;
237 errorbar(Ts, U(ind), 2*U_std(ind).*sqrt(ns_Phi), 'k', 'linewidth', 2.5); hold on;
238 plot(T_MFT_degC, E_MFT(Peq), '-.'); hold on
239 ImproveFigureCompPhys(gcf, 'LineColor', {'GERIBLUE', 'r'});
240 legend('$US$', '$U\pm 2 \sigma$ (with $n_{s, \rm \Phi}$)', '$E_{\rm MFT}$', 'Location', 'NorthWest');
241 ylabel('$US$ [eV/cell]')
242
243 figure(2); clf;
244 plot(T_degC(2:end), 1e3*diff(U)./diff(T_degC)); hold on;
245 plot(T_degC, 1e3*Cv);
246 plot(T_MFT_degC(1:end-1), 1e3*C_MFT, '-.');
247 ImproveFigureCompPhys(gcf, 'LineColor', {'GERIBLUE', 'k', GRAY});
248 legend('$C$, {\rm Var(E)}$', '$C$, {\partial U / \partial T}$', '$C_{\rm MFT}$', 'Location', 'NorthWest');
249 ylabel('$C$ [meV/cell]')
250
251 figure(3); clf;
252 plot(T_degC, P, 'r'); hold on;

```



```

253 errorbar(Ts, P(ind), 2*P_std(ind).*sqrt(ns_Phi), '.k', 'linewidth', 2.5); hold ←
    on;
254 plot(T_MFT_degC, Peq, '-.k');
255 ImproveFigureCompPhys(gcf, 'LineColor', {'GERIBLUE', 'r'}');
256 legend('$P$', '$P\pm 2 \sigma$ (with $n_{s, \rm \Phi}$)', '$P_{\rm MFT}$', '←
    Location', 'SouthWest');
257 ylabel('$P$ ')
258
259
260 figure(4);clf;
261 plot(T_degC, r, 'r');hold on;
262 errorbar(Ts, r(ind), 2*r_std(ind).*sqrt(ns_Phi), '.k','linewidth', 1.5);hold on;
263 plot(T_degC, P.^2, '--', T_MFT_degC, Peq.^2, '-.');
264 ImproveFigureCompPhys(gcf, 'LineColor', {'GERIBLUE', 'LINNEAGREEN', 'r'}');
265 legend('$r$', '$r\pm 2 \sigma$ (with $n_{s, \rm \Phi}$)', '$P^2$', '$r_{\rm MFT}$'←
    ', 'Location', 'SouthWest');
266 ylabel('$r$ ')
267
268 ImproveFigureCompPhys((2:4), 'linewidth', 2)
269
270 if doSave
271     for ifig = 1:4;
272         figure(ifig)
273         setFigureSize(gcf, 300, 600);
274         xlabel('$T$ [$^\circ\text{C}$]');
275         axis tight
276         xlim([-200 Inf])
277     end
278     ImproveFigureCompPhys(1:4);
279     saveas(1, '../figures/U.eps', 'eps');
280     saveas(2, '../figures/C.eps', 'eps');
281     saveas(3, '../figures/P.eps', 'eps');
282     saveas(4, '../figures/r.eps', 'eps');
283 end

```

C.2 Improve figure appearance: ImproveFigureCompPhys.m

```

1 function ImproveFigureCompPhys(varargin)
2 %ImproveFigureCompPhys Improves the figures of supplied handles
3 % Input:
4 % - none (improve all figures) or handles to figures to improve
5 % - optional:
6 %     LineWidth int
7 %     LineStyle column vector cell, e.g. {'-','--'}',
8 %     LineColor column vector cell, e.g. {'k',[0 1 1], 'MYBLUE'}'
9 %             colors: MYBLUE,MYORANGE,MYGREEN,MYPURPLE, MYYELLOW,
10 %             MYLIGHTBLUE, MYRED
11 %     Marker column vector cell, e.g. {'.', 'o', 'x'}'
12
13 % ImproveFigure was originally written by Adam Stahl, but has been heavily
14 % modified by Linnea Hesslow
15
16
17 %%% Handle inputs
18 % If no inputs or if the first argument is a string (a property rather than
19 % a handle), use all open figures
20 if nargin == 0 || ischar(varargin{1})
21     %Get all open figures
22     figHs = findobj('Type','figure');
23     nFigs = length(figHs);
24 else
25     % Check the supplied figure handles
26     figHs = varargin{1};
27     figHs = figHs(ishandle(figHs) == 1); %Keep only those handles that are ←
        proper graphics handles
28     nFigs = length(figHs);
29 end
30
31 % Define desired properties
32 titleSize = 24;
33 interpreter = 'latex';
34 lineWidth = 4;
35 axesWidth = 1.5;
36 labelSize = 22;
37 textSize = 20;
38 legTextSize = 18;
39 tickLabelSize = 18;
40 LineColor = {};
41 LineStyle = {};
42 Marker = {};
43
44 % define colors
45 co = [ 0      0.4470    0.7410
46       0.8500    0.3250    0.0980
47       0.9290    0.6940    0.1250
48       0.4940    0.1840    0.5560

```

```

49     0.4660    0.6740    0.1880
50     0.3010    0.7450    0.9330
51     0.6350    0.0780    0.1840 ];
52 colors = struct('MYBLUE', co(1,:),...
53 'MYORANGE', co(2,:),...
54 'MYYELLOW', co(3,:),...
55 'MYPURPLE', co(4,:),...
56 'MYGREEN', co(5,:),...
57 'MYLIGHTBLUE', co(6,:),...
58 'MYRED',co(7,:),...
59 'GERIBLUE', [0.3000    0.1500    0.7500],...
60 'GERIRED', [1.0000    0.2500    0.1500],...
61 'GERIYELLOW', [0.9000    0.7500    0.1000],...
62 'LIGHTGREEN', [0.4    0.85    0.4],...
63 'LINNEAGREEN', [7 184 4]/255);
64
65 % Loop through the supplied arguments and check for properties to set.
66 for i = 1:nargin
67     if ischar(varargin{i})
68         switch lower(varargin{i}) %Compare lower case strings
69             case 'linewidth'
70                 lineWidth = varargin{i+1};
71             case 'linestyle'
72                 LineStyle = varargin{i+1};
73             case 'linecolor'
74                 LineColor = varargin{i+1};
75                 for iLineColor = 1:numel(LineColor)
76                     if isfield(colors, LineColor{iLineColor})
77                         LineColor{iLineColor} = colors.(LineColor{iLineColor});
78                     end
79                 end
80             case 'marker'
81                 Marker = varargin{i+1};
82         end
83     end
84 end
85 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
86
87 %%% Improve the figure(s)
88
89 for iFig = 1:nFigs
90     fig = figHs(iFig);
91
92     lineObjects = findall(fig, 'Type', 'line');
93     textObjects = findall(fig, 'Type', 'text');
94     axesObjects = findall(fig, 'Type', 'axes');
95     legObjects = findall(fig, 'Type', 'legend');
96     contourObjects = findall(fig, 'Type', 'contour'); % not counted as lines
97
98     %%% TEXT APPEARANCE: first set all to textSize and then change the ones
99     %%% that need to be changed again
100
101     %Change size of any text objects in the plot
102     set(textObjects, 'FontSize', textSize);
103     set(legObjects, 'FontSize', legTextSize);
104
105     %%% FIX LINESTYLE, COLOR ETC. FOR EACH PLOT SEPARATELY
106     for iAx = 1:numel(axesObjects)
107         lineObjInAx = findall(axesObjects(iAx), 'Type', 'line');
108
109         %set line style and color style (only works if all figs have some
110         %number of line plots..)
111         if ~isempty(LineStyle)
112             set(lineObjInAx, {'LineStyle'}, LineStyle)
113             set(contourObjects, {'LineStyle'}, LineStyle); %%%%%%%%%
114         end
115         if ~isempty(LineColor)
116             set(lineObjInAx, {'Color'}, LineColor)
117             set(contourObjects, {'LineColor'}, LineColor); %%%%%%%%%
118         end
119         if ~isempty(Marker)
120             set(lineObjInAx, {'Marker'}, Marker)
121             set(lineObjInAx, {'Markersize'}, num2cell(10+22*strcmp(Marker, '.'))←
122             )
123         end
124
125         %%% change font sizes.
126         % Tick label size
127         xLim = axesObjects(iAx).XLim;
128         axesObjects(iAx).FontSize = tickLabelSize;
129         axesObjects(iAx).XLim = xLim;
130         %Change label size
131         axesObjects(iAx).XLabel.FontSize = labelSize;
132         axesObjects(iAx).YLabel.FontSize = labelSize;
133
134         %Change title size
135         axesObjects(iAx).Title.FontSize = titleSize;
136     end
137
138     %%% LINE APPEARANCE

```

```
139 %Change line thicknesses
140 set(lineObjects,'LineWidth',lineWidth);
141 set(contourObjects, 'LineWidth', lineWidth);
142 set(axesObjects, 'LineWidth',axesWidth)
143
144 % set interpreter: latex or tex
145 set(textObjects, 'interpreter', interpreter)
146 set(legObjects, 'Interpreter', interpreter)
147 set(axesObjects, 'TickLabelInterpreter', interpreter);
148 end
149 end
```

C.3 Change size of figures: setFigureSize.m

```
1 function [ fig ] = setFigureSize( fig, H, W )
2 fig.Units = 'points';
3 fig.WindowStyle = 'normal'; % undock
4 fig.Position(3:4) = [W H];
5 end
```