

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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December 5, 2018

Task N ^o	Points	Avail. points
Σ		

Introduction

....

Task 1: mean field theory

Fits: we obtained $\alpha \approx 0.494$

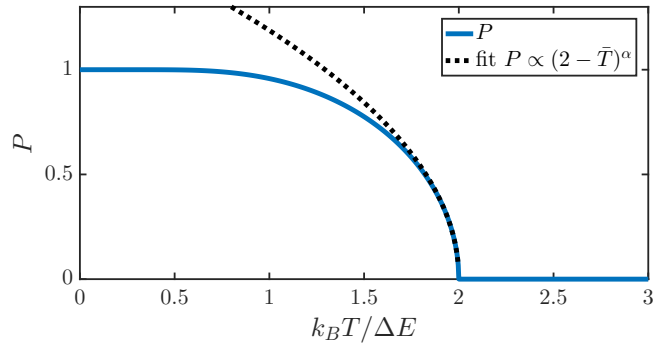


Figure 1:

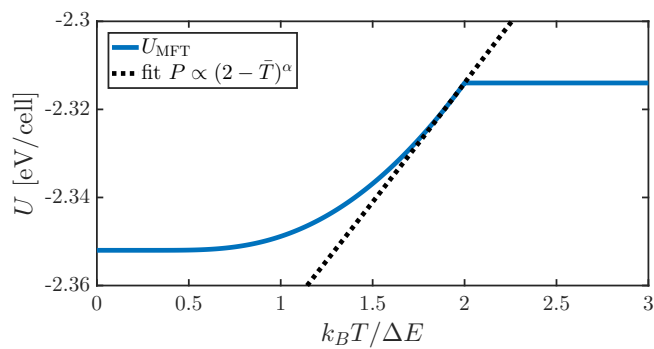


Figure 2:

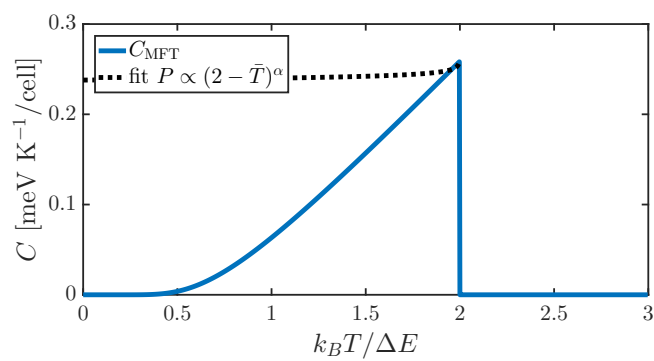


Figure 3:

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.

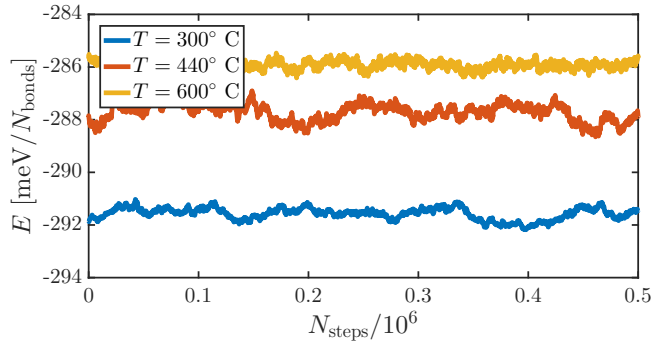


Figure 4: ...

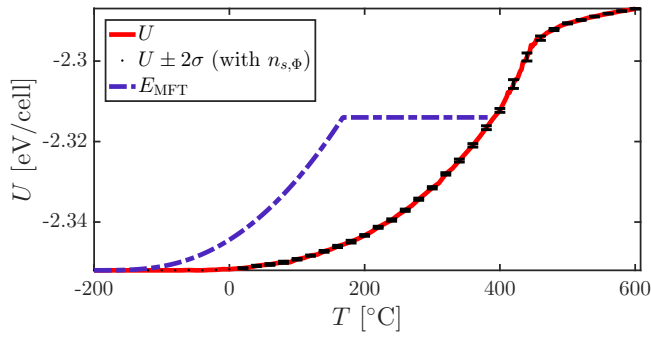


Figure 5: ...

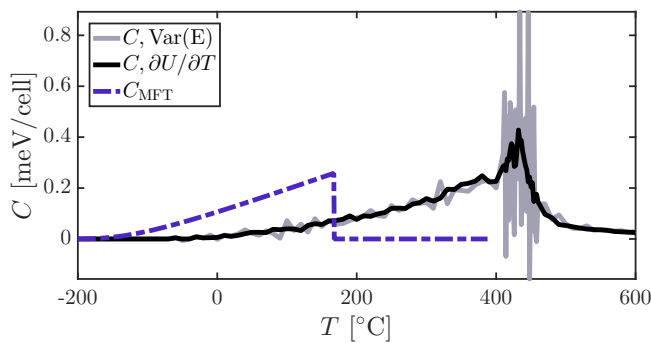


Figure 6: ...

0.1 Statistical inefficiency

Figures 9 and 10 show the statistical inefficiency at three temperatures, calculated with the correlation function and block average respectively.

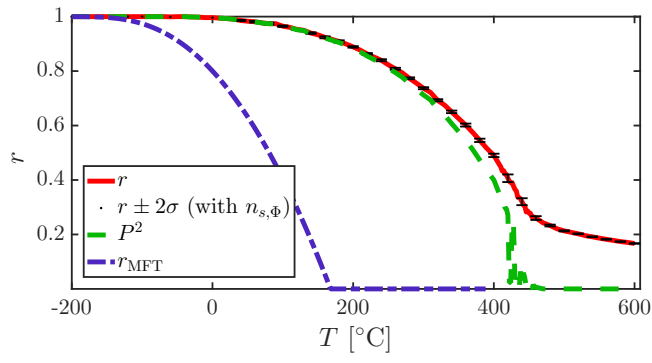


Figure 7: ...

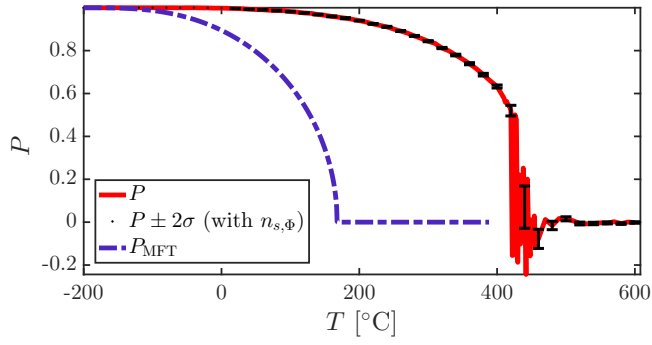


Figure 8: ...

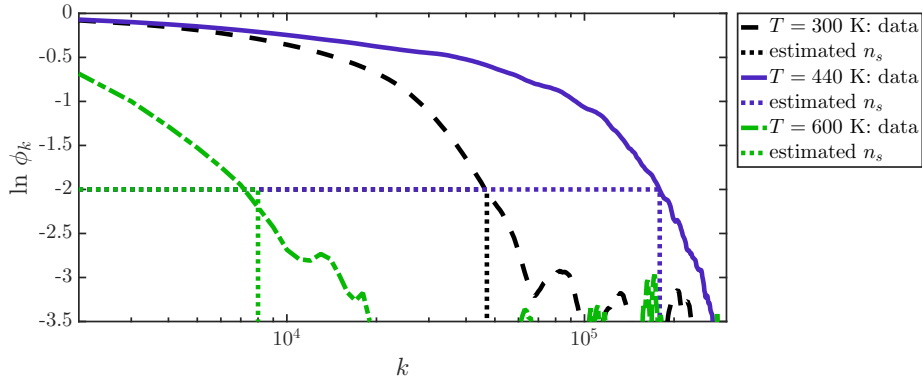


Figure 9: ...

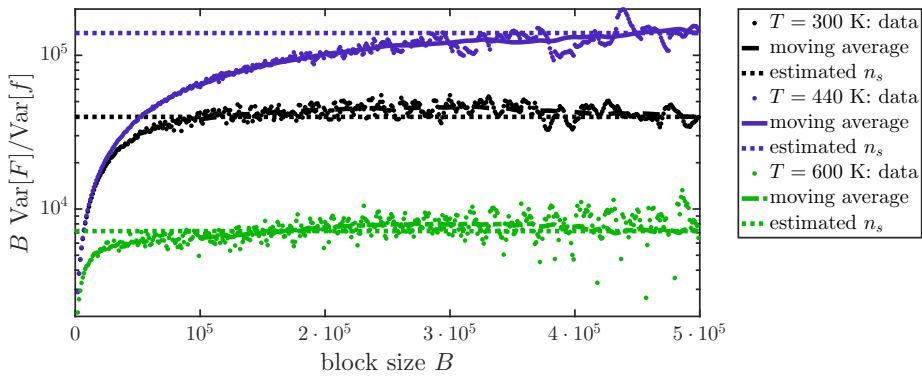


Figure 10: ...

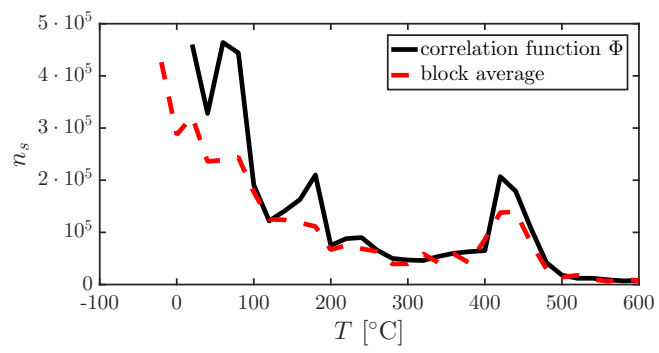


Figure 11: ...

Concluding discussion

...

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:
    
$$\phi_k = (\langle f_{i+k} f_i \rangle - \langle f_i \rangle^2) / (\langle f_i^2 \rangle - \langle f_i \rangle^2)$$

    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 = 0;
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/1e6, 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('$N_{\rm steps}/10^6$')
111 ImproveFigureCompPhys(1)
112
113 figure(3); clf;figure(2); clf;
114 [ns_Phi,ns_block] = deal(nan(size(Ts)));
115 Nskip = 10;
116 for i=1:numel(Ts)
117     data = load(sprintf('../data/stat_inefficiency-T%d.tsv',Ts(i)));
118     k = data(:,1);
119     block_size = k+Nskip;
120     phi = data(:,2);
121     VarF_norm = data(:,3);
122     kstar = k(find(log(phi)<-2, 1, 'first'));
123     if ~isempty(kstar)
124         ns_Phi(i) = kstar;
125     end
126     N_avg = 100;
127     filtereddata = movmean(VarF_norm,N_avg);
128     ns_block(i) = filtereddata(end);
129
130     if any(Ts(i) == TsToPlot)
131         figure(2)
132
133         semilogx(k, log(phi));hold on;
134         plot([0.1 kstar kstar], [-2 -2 -6],':k')
135
136         figure(3)
137         semilogy(block_size, VarF_norm, '.'); hold on;
138         plot(block_size(N_avg:end), filtereddata(N_avg:end));
139         plot(block_size, filtereddata(end)*ones(size(block_size)), ':k');
140
141     end
142 end
143
144 figure(4); clf;
145 plot(Ts, ns_Phi, 'k',Ts, ns_block, '--r')
146 ax = gca;
147 ax.YTickLabel = {'0', '$10^5$', '$2\cdot 10^5$', '$3\cdot 10^5$', '$4\cdot 10^5$',
148     '$5\cdot 10^5$'};
149 ylabel('$n_s$');
150 legend('correlation function $\Phi_k$', 'block average');
151 xlabel('$TS$ [\circ$C]');
152 ImproveFigureCompPhys(gcf)
153
154 legs_Phi = cell(6,1);
155 legs_block = cell(9,1);
156 for i = 1:numel(TsToPlot)
157     tt = ['$T=' num2str(TsToPlot(i)) '$ K: '];
158     legs_Phi{1 + 2*(i-1)} = [tt 'data'];
159     legs_Phi{2 + 2*(i-1)} = 'estimated $n_s$';
160     legs_block{1 + 3*(i-1)} = [tt 'data'];
161     legs_block{2 + 3*(i-1)} = 'moving average';
162     legs_block{3 + 3*(i-1)} = 'estimated $n_s$';
163 end
164
165 figure(2);
166
167 legend(legs_Phi, 'location', 'northeastoutside');
168 xlabel('$k$'); ylabel('ln $\phi_k$');
169 ylim([-3.5 0]);
170 xlim([2e3 3e5])
171 %ax = gca; ax.XTick = [3e3 1e4 3e4 1e5 3e5];

```

```

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

```

```

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