

Modelling Ordering Phenomena in Substitutional Binary Alloys Using a Spin-1 Ising Model

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Introduction

- Order-disorder phase transitions in 2D binary substitutional alloys A_xB_{1-x} , following the prototype of β -brass, are studied.
- Effects of finite vacancy concentration in thermal equilibrium properties are studied by means of a Spin-1 Ising Model.
- Critical curves on composition-temperature and chemical potential-temperature are studied in the context of the grand canonical ensemble.
- Critical phenomena is studied both from mean field approximations and Markov Chain Monte Carlo (MCMC) simulations.
- Results are compared to those of the Spin-1/2 Ising Model reported by Porta and Castán [7].
- Methodology follows the outline posed by Ibarra and others [4].

Background - Introducing the Physical System

Brass is a type of alloy composed by Cu and Zn. For low concentrations of Zn, the lattice structure of the solid is FCC, as in the pure solid form of Cu. Near stoichiometric proportions 1 : 1, the lattice structure is BCC [2].

The Physical System

In what follows, it is to be assumed that the system discussed is a binary alloy, with a bipartite lattice symmetry and non stoichiometric proportions: A_xB_{1-x} .

Interaction energy depends mainly on atom bonds, and thus the following Hamiltonian is defined [6, 5, 8]:

$$H = \frac{1}{2}(\epsilon_{AA}V_{AA} + \epsilon_{AB}V_{BB} + \epsilon_{BB}V_{BB}) \quad (1)$$

Where $\epsilon_{\alpha\beta}$ is the bond energy between atoms of species α and β , and $V_{\alpha\beta}$ is the number of (ordered) nearest neighbour (nn) pairs of bonds involving atoms of species α and β .

Background - Modelling via a Spin-1/2 Ising Hamiltonian

In terms a lattice variable with explicit definition

$$s_i = \begin{cases} 1, & \text{if lattice point } i \text{ is occupied by an atom of species A} \\ -1, & \text{if lattice point } i \text{ is occupied by an atom of species B} \end{cases}$$

It is possible to show that the lattice Hamiltonian can be written as [5, 8]

$$H = E_0 - J_{AB} \sum_{\langle ij \rangle} s_i s_j - h_{AB} \sum_i s_i \quad (2)$$

With the identifications:

$$E_0 = \frac{N_Z}{4} (\epsilon_{AA} + 2\epsilon_{AB} + \epsilon_{BB}) \quad (3)$$

$$J_{AB} = \frac{1}{4} (2\epsilon_{AB} - \epsilon_{AA} - \epsilon_{BB}) \quad (4)$$

$$h_{AB} = \frac{Z}{2} (\epsilon_{BB} - \epsilon_{AA}) \quad (5)$$

Atom Redistribution at Low temperatures

At high temperatures, all lattice points are indistinguishable in that the probability that an atom of Cu occupies a site is equal to the probability that it be occupied by an atom of Zn. However, when the system is at temperatures bellow a critical one ($T_c \approx 733K$), atoms of each species tend to occupy one of the two inter-crossing SC structures [5, 6, 8, 9].

Ordering in Bipartite Lattices

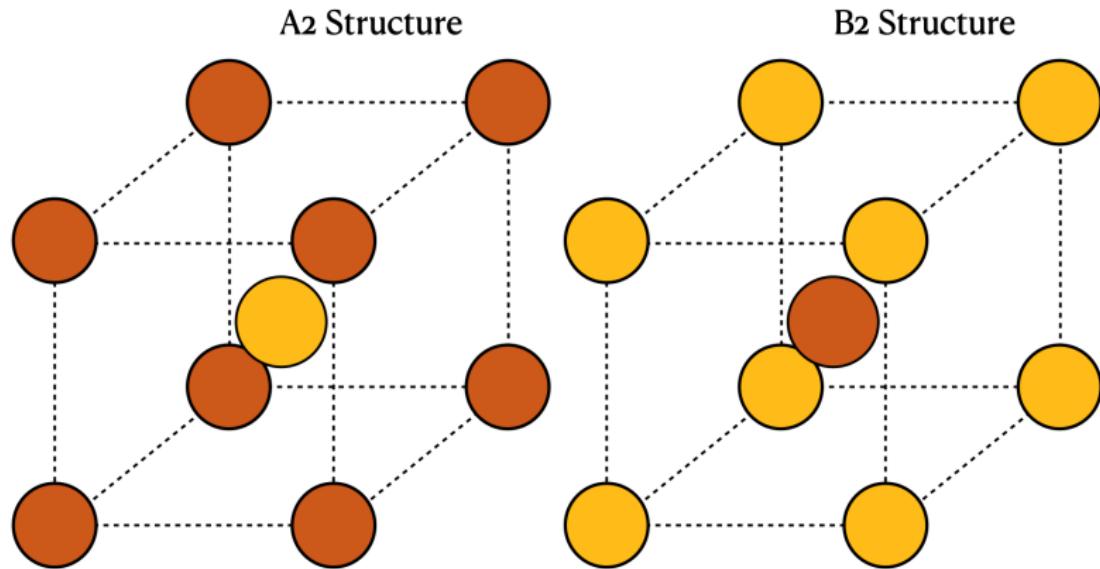


Figure: Intercrossing SC structures after BCC symmetry breaking in binary alloys. While m_α defines the concentration of orange atoms in the A₂ structure, m_β defines the concentration of yellow atoms in the B₂ structure [8].

Background - Fundamentals of Second Order Transitions

Ordering such as those of binary alloys is characterised by an **order parameter**. The order parameter reflects the symmetry breaking below the critical point. In the case of binary alloys, the symmetry of the BCC lattice is broken, leading to a SC symmetry [6]. For this particular system, the following order parameter is defined, see fig. 1 [8]:

$$\eta = \frac{m_\alpha - m_\beta}{2} \quad (6)$$

Continuous Ordering Transitions

Above a critical temperature T_C , order parameter is zero, whereas below critical temperature, order parameter increases rapidly until saturation occurs. Thermodynamic quantities vary **continuously** past transition point, while their derivatives vary discontinuously.

Divergence of derivatives of thermodynamic potentials is characterised by **critical exponents**. The specific heat (c_H) and order parameter derivative (χ_H) follow the laws [4]

$$c_H \sim |1 - T/T_c|^{-\alpha} \quad (7)$$

$$\chi_H \sim |1 - T/T_c|^{-\gamma} \quad (8)$$

Important: Ordering phenomena occurs due to long range correlation between interacting components of the system.

Main Features of Ordering Phenomena

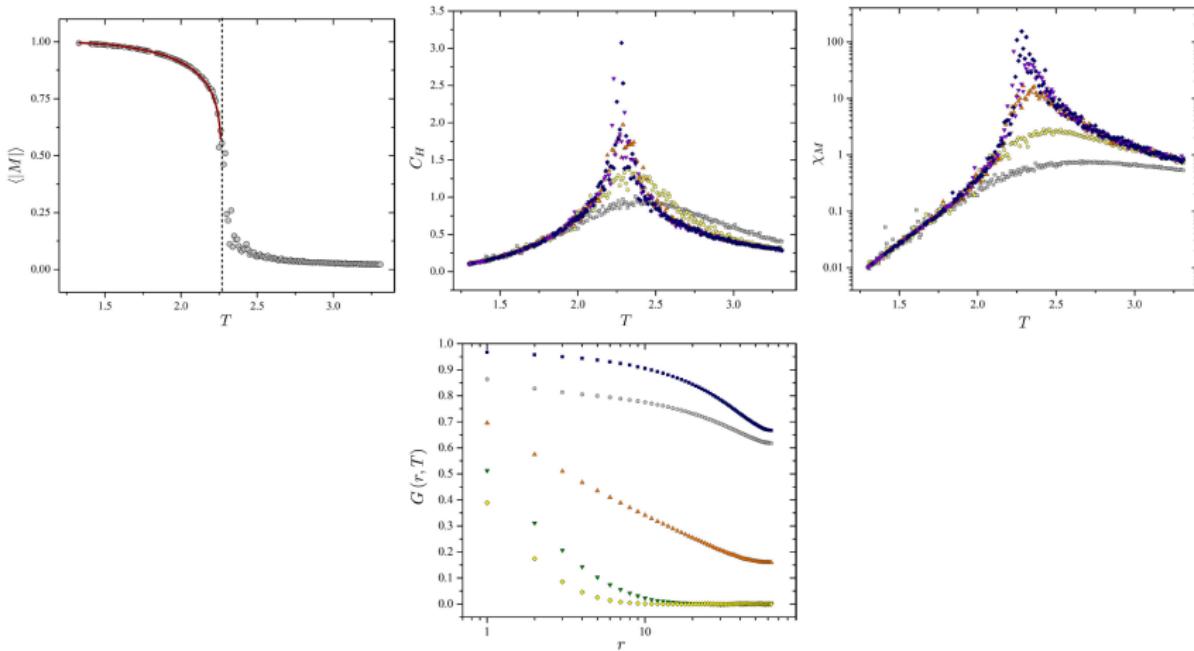


Figure: From left to right. (1) Magnetisation as a function of temperature, notice sudden increase below critical temperature. (2) and (3) specific heat and susceptibility as function of temperature, notice divergence near critical temperature. (4) Correlation function for temperatures below critical point (blue squares and gray dots) and above critical point (the rest), notice that at low temperatures the correlation length is quite large [4].

Background - Nuances of The Model

Necessity of Statistical Study in Gran Canonical Ensemble

A very important remark need be made regarding the summations involved in Hamiltonian 2. For fixed concentration of species A, x, lattice variables are constrained to

$$\frac{1}{N} \sum_i s_i = \sum_i (2C_i - 1) = 2x - 1 \quad (9)$$

As a result, statistical analysis is easier on the grand canonical ensemble. This is equivalent to performing a Legendre transform [7, 8]

$$\hat{H} = H - \zeta N_A \quad (10)$$

Where ζ is the **chemical potential difference** between atoms of types A and b.

Nature of Diffusion Processes in Substitutional Alloys

As pointed out by Porta and Vives [7], diffusion dynamics is drastically influenced by the presence of **vacant lattice sites**. This influences critically the ordering process of a binary Alloy.

Important: Neither Porta and Vives[7] nor Porta and Castán [8] consider the influence of both atom and vacancy concentration in ordering phase transitions of binary alloys. The first work only considers properties of stoichiometric alloys, the former does not consider influence of vacant lattice sites at all.

Diffusion Process in Substitutional Alloys

The reference example, CuZn, is a substitutional alloy in which vacancy diffusion is critical for ordering processes [2, 3].

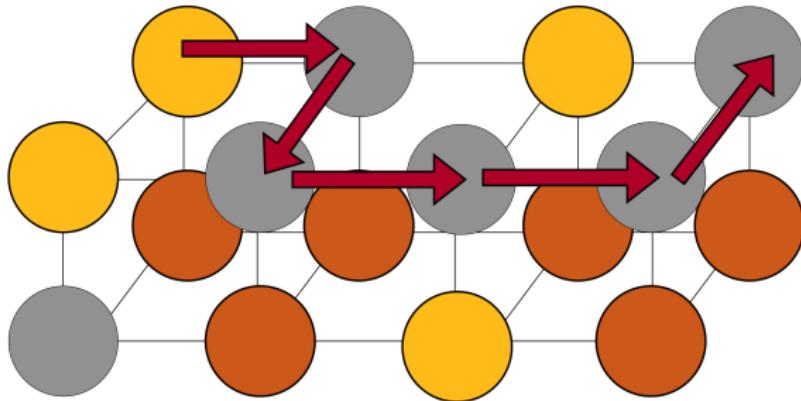


Figure: Cartoon of vacancy assisted diffusion in substitutional alloys. Atoms correspond to coloured sites, whereas vacancies correspond to gray sites

Statement of the Problem

Motivation of the Problem

Porta and Castan perform a study of the effects of non-stoichiometric concentration proportions in binary alloys by studying the system via a Spin-1/2 Ising Model in the grand canonical ensemble [8]. They present their results mainly on **composition-temperature** and **chemical potential-temperature** planes. Ibarra and others present a bird's eye view of the study of ordering phase transitions in the context of the 2D Ising Model [4]. Modelling of vacancy assisted diffusion ordering processes in **stoichiometric alloys** has been performed by Porta and Vives [7], using a Spin-1 Model

$$H = -J \sum_{\langle ij \rangle} S_i S_j - K \sum_{\langle ij \rangle} S_i^2 S_j^2 \quad (11)$$

Original Component

The problem of this project is to study the effects of vacancy assisted diffusion in ordering phase transitions of **non-stoichiometric alloys**, using a Spin-1 Model, in the context of the grand canonical ensemble. This amounts to a Legendre transform of Hamiltonian 11

$$\hat{H} = H - \mu N_V - \zeta N_A \quad (12)$$

This work aims at generalising results derived in [8] and [7], by considering variations on both atom and vacancy concentrations. It also extends the techniques presented by Ibarra and others [4] to non magnetic systems.

Objectives of the Project

General Objective

To study the effects of vacancy-assisted order-disorder transitions in binary alloys A_xB_{1-x} forming a bipartite lattice, on $x - T$ and $\zeta - T$ phase space projections, by using the BEG model Hamiltonian 11; both from a mean field approximation, and Monte Carlo Simulations.

Specific Objectives

- ① To demonstrate the pertinence and limitations of the BEG Model for describing atomic interaction in a binary alloy by correlating microscopic degrees of freedom and magnetic-related parameters to corresponding quantities in the system of interest.
- ② To apply Landau theory in a suitable mean field approximation of the BEG hamiltonian to compute critical curves in $x - T$ phase space projection, using the appropriate grand partition function, and rough estimates of mentioned critical exponents.
- ③ To compute specific heat, internal energy and order parameters, as a function of temperature, for different values of ζ as statistical averages obtained from Markov Chain Monte Carlo simulations.
- ④ To identify and locate in $\zeta - T$ projection of phase space critical points using Monte Carlo simulations and compare to results obtained via mean field approximation.

Bibliographic resources

- Google Scholar Database
- Azure for Students Account granted by Microsoft
- Arxiv Database
- American Physical Society Resources
- American Chemical Society Resources
- Other web resources provided by SINAB from Universidad Nacional de Colombia.

Computational resources

- Mac pc with Quad-Core intel Core i5 (3.4 GHz) processor and graphics board Radeon Pro 560 (4 GB).
- Ubuntu 18.06 Server with 8GB RAM and 2 vcpus, hosted by Microsoft Azure Services
- Free Google Colaboratory account with access to NVIDIA graphics board
- Python 3.x.

SO1 - Derivation of Alloy Hamiltonian

Given that the aim of the project is to study the influence of vacant lattice sites on the equilibrium properties of a binary alloy, the following interaction Hamiltonian is considered

$$H = \epsilon_{AA}N_{AA} + \epsilon_{BB}N_{BB} + \epsilon_{AB}N_{AB} + \epsilon_{AV}N_{AV} + \epsilon_{BV}N_{BV} \quad (13)$$

Since the lattice to be considered is assumed to be bipartite, there exist two sublattices whose sites are nearest neighbours to one another. Those sublattice are notated by A_2 and B_2 . Lattice variables are defined, on each sublattice, on equation 14. These set of variables allows description of the alloy in terms of a ferromagnetic BEG Hamiltonian.

$$S_i^{(A_2)} = \begin{cases} 1 & \text{if site } i \text{ is occupied by an A-type atom} \\ 0 & \text{if site } i \text{ is vacant} \\ -1 & \text{if site } i \text{ is occupied by a B-type atom} \end{cases} \quad (14)$$

$$S_i^{(B_2)} = \begin{cases} 1 & \text{if site } i \text{ is occupied by an B-type atom} \\ 0 & \text{if site } i \text{ is vacant} \\ -1 & \text{if site } i \text{ is occupied by a A-type atom} \end{cases} \quad (15)$$

SO1 - Derivation of Alloy Hamiltonian

In the appendix exact calculation of the Hamiltonian 13 in terms of lattice variables is performed. The result is quoted on equation 16, in the particular case when the atom vacancy interaction is independent of the atom type.

$$H = -\frac{J}{2} \sum_{\langle i_{A_2}, j_{B_2} \rangle} S_{i_{A_2}} S_{j_{B_2}} + \frac{K}{2} \sum_{\langle i_{A_2}, j_{B_2} \rangle} S_{i_{A_2}}^2 S_{j_{B_2}}^2 + D \sum_i S_i^2 \quad (16)$$

And

$$J = \frac{1}{4}(\epsilon_{AA} + \epsilon_{BB} - 2\epsilon_{AB})$$

Since the aim of the project is study of order-disorder transitions in a binary alloy, first order transitions will not be considered in this project. Second order transitions for Hamiltonian 16 are characterised by the order parameter

$$m = \langle S_{i_{A_2}} \rangle + \langle S_{i_{B_2}} \rangle \quad (17)$$

SO1 - Derivation of Alloy Hamiltonian

Study in grand canonical ensemble amounts to performing a Legendre transformation of the Hamiltonian of the form

$$H \rightarrow H - (\mu_V - \mu_B)N_V - (\mu_A - \mu_B)N_A \quad (18)$$

The transformation leads to a Hamiltonian of the form

$$H = H = -\frac{J}{2} \sum_{\langle i_{A_2}, j_{B_2} \rangle} S_{i_{A_2}} S_{j_{B_2}} + \frac{K}{2} \sum_{\langle i_{A_2}, j_{B_2} \rangle} S_{i_{A_2}}^2 S_{j_{B_2}}^2 + \mu \sum_i S_i^2 + h \sum_{i_B} S_{i_B} - h \sum_{i_A} S_{i_A} \quad (19)$$

Although Porta, Frontera and others [7] emphasize that the condition $K = 0$ alters significantly the kinetics of domain formation in binary alloys; as a first approximation, only the case $K = 0$ is considered in the present project:

$$H = -\frac{J}{2} \sum_{\langle i_{A_2}, j_{B_2} \rangle} S_{i_{A_2}} S_{j_{B_2}} + \mu \sum_i S_i^2 + h \sum_{i_B} S_{i_B} - h \sum_{i_A} S_{i_A} \quad (20)$$

SO2 - Landau Theory of BEG Hamiltonian

Consider Hamiltonian 20 defined on a bipartite lattice. The following variational Hamiltonian is proposed

$$\hat{H} = -\gamma_A \sum_{i_{A_2}} S_{i_{A_2}} - \gamma_B \sum_{i_{B_2}} S_{i_{B_2}} + \mu \sum_i S_i^2 \quad (21)$$

The partition function for the variational Hamiltonian 21 is

$$\hat{Z} = Z_{A_2}^{N/2} Z_{B_2}^{N/2} \quad (22)$$

With

$$Z_{A_2} = 1 + 2e^{-\beta\mu} \cosh(\beta\gamma_A) \quad (23)$$

$$Z_{B_2} = 1 + 2e^{-\beta\mu} \cosh(\beta\gamma_B) \quad (24)$$

Variational free energy is computed easily. By defining $m_A = \langle S_{i_A} \rangle$ and $m_B = \langle S_{i_B} \rangle$, it is straight forward to note that variational free energy, according to GBF method, is

$$\frac{\hat{F}}{N} = m_A \left[\frac{\gamma_A}{2} - \frac{Jz}{4} m_B - \frac{h}{2} \right] + m_B \left[\frac{\gamma_B}{2} - \frac{Jz}{4} m_A + \frac{h}{2} \right] - \frac{1}{2\beta} \ln Z_{A_2} - \frac{1}{2\beta} \ln Z_{B_2} \quad (25)$$

SO2 - Landau Theory of BEG Hamiltonian

Also

$$m_A = \frac{1}{\beta} \frac{\partial \gamma_A}{\partial \ln Z_A} \quad (26)$$

$$m_B = \frac{1}{\beta} \frac{\partial \gamma_B}{\partial \ln Z_B} \quad (27)$$

Minimisation of variational free energy with respect to parameters γ_A and γ_B thus lead to the conditions

$$\gamma_A = Jz m_B + h \quad (28)$$

$$\gamma_B = Jz m_A - h \quad (29)$$

For simplicity, the unit of energy is chosen as Jz , z being the coordination number of the lattice, and the unit of entropy is taken as k_B . The system of equations 27 may be rewritten as

$$m_A = f(m_B + h) \quad (30)$$

$$m_B = f(m_A - h) \quad (31)$$

With

$$f(u) = \frac{2 \sinh(\beta u)}{e^{\beta \mu} + 2 \cosh(\beta u)} \quad (32)$$

SO2 - Landau Theory of BEG Hamiltonian

Notice that the order parameter of the transitions

$$m = m_A + m_B$$

The following change of variables is made

$$m_A = m + n$$

$$m_B = m - n$$

And thus the system of equations 31 amounts to

$$m + n = f(m + (h - n)) \quad (33)$$

$$m - n = f(m - (h - n)) \quad (34)$$

In general, the system of equations 34 amounts to

$$m = \frac{1}{2} \left[f(m + (h - n)) + f(m - (h - n)) \right] \quad (35)$$

$$n = \frac{1}{2} \left[f(m + (h - n)) - f(m - (h - n)) \right] \quad (36)$$

$$(37)$$

SO2 - Landau Theory of BEG Hamiltonian

A rather simple solution is readily seen

$$m = 0 \quad (38)$$

$$n = n_0 = f(h - n_0) \quad (39)$$

The simple solution presented before is valid in the disordered phase of the alloy. A solution with non zero order parameter corresponds to an ordered phase of the alloy. Near a critical point, approaching from the disordered phase, the first equation of system 37 is equivalent to

$$m = f'(h - n)|_{n=n_0} m + \mathcal{O}(m^2) \quad (40)$$

This equation has non trivial solution only if

$$f'(h - n)|_{n=n_0} > 1 \quad (41)$$

The boundary for second order transitions is thus given by

$$f'(h - n)|_{n=n_0} = 1 \quad (42)$$

SO2 - Landau Theory of BEG Hamiltonian

The limit $h = 0$ was studied by Blume, Emery and Griffiths [1]. They proved that, in the limit of very low vacancy concentration, the critical temperature is $T_c = 1$. Also, critical temperature is related to μ by

$$\mu_c = T_c \ln \left[2 \frac{1 - T_c}{T_c} \right] \quad (43)$$

On the other hand, at $T_c = 0$, the energy of the ground state is equal to

$$E_m = -\frac{N}{2} + \mu N$$

If the external field is such that $h = 1$, the staggered configuration, i.e. with A-B bonds, has an energy

$$E_m = -\frac{N}{2} + \mu N$$

And thus the lowest energy level is degenerate. At higher values of the external field, the staggered configuration has lower energy than the parallel-spin configuration. And then, at $h = 1$ there is a transition from parallel-spin configuration to staggered spin configuration. Therefore, this should be a critical point on the critical curve on $h - T$ plane for second order phase transitions.

Mean Field Magnetisation

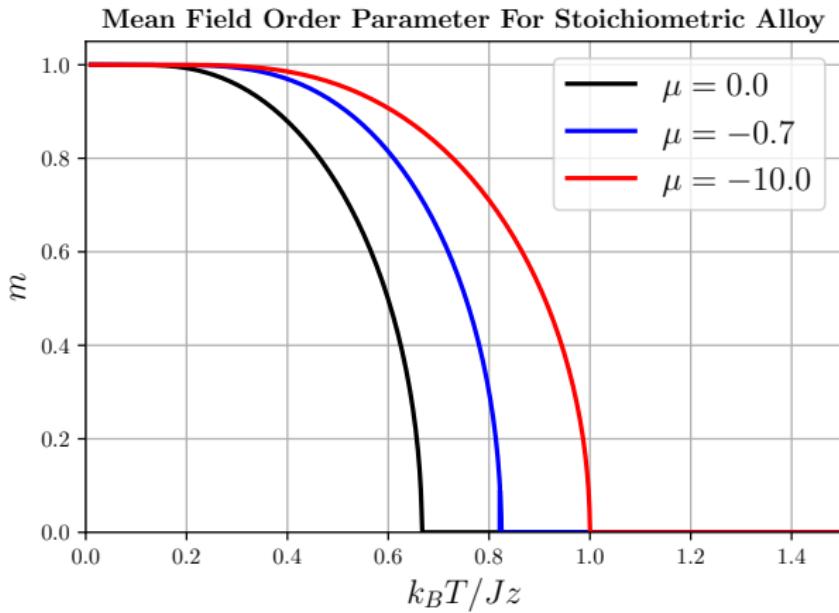


Figure: Temperature profile of order parameter, for a stoichiometric binary alloy, for different values of vacancy chemical potential. The more negative the chemical potential, the smaller the vacancy concentration.

Numerical Computation of Mean Field Curves on $h - T$ Plane

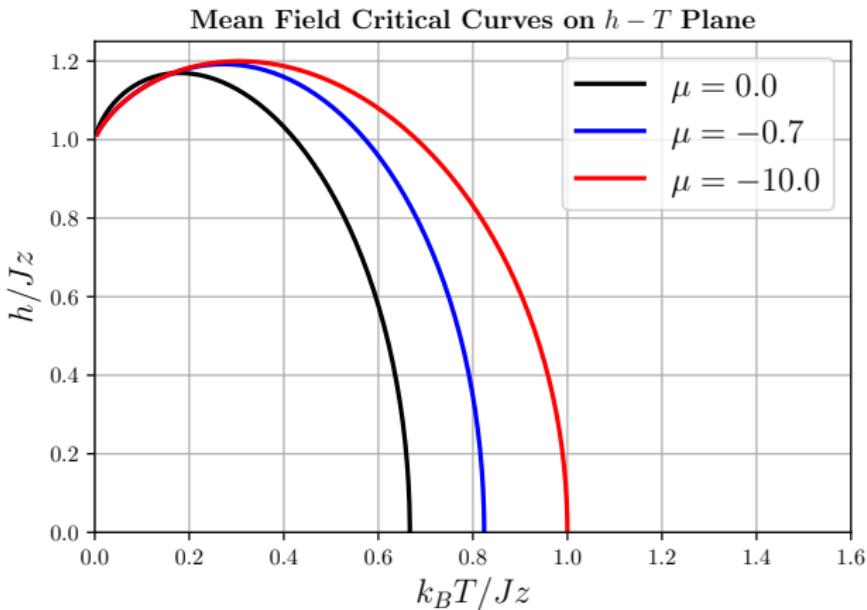


Figure: Critical curves on $h - T$ plane, in the mean field approximation. The more negative the chemical potential, the smaller the vacancy concentration.

Numerical Computation of Mean Field Curves on x – T Plane

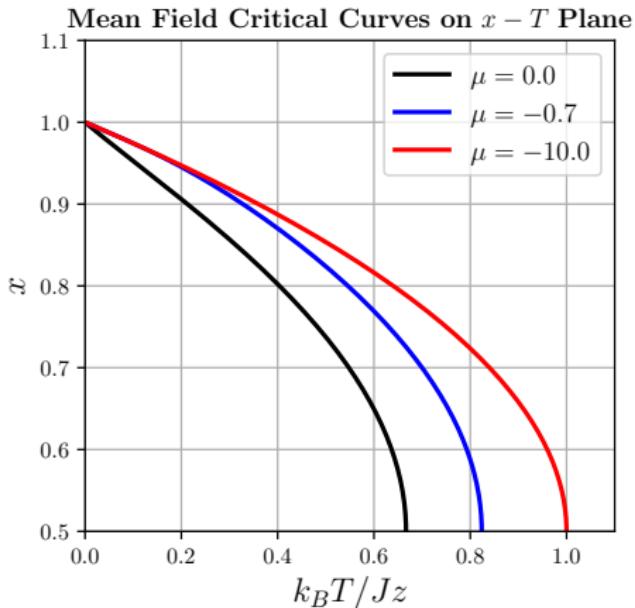


Figure: Critical curves on $x - T$ plane, in the mean field approximation. The more negative the chemical potential, the smaller the vacancy concentration.

Outline of the algorithm

- ① Propose a change of system configuration from $n \rightarrow m$.
- ② Compute the energy difference $\Delta H = H\{m\} - H\{n\}$.
- ③ Compute the acceptance probability $W = \min(1, \exp[-\beta \Delta H])$.
- ④ Select a random number κ between 0 and 1. If $\kappa \leq W$, m is accepted as a new configuration of the statistical ensemble. Otherwise, the configuration of the system remains as n

Details of Numerical Simulations

The Hamiltonian 20 was sampled using Metropolis Algorithm, thus following Glauber dynamics. The exchange integral $J = 1$, and units of entropy were taken as k_B . Due to time constraints, the following values for the external fields, related to chemical potential difference, were used:

$$\mu = 0.0, -1.7 \quad (44)$$

$$h = 0.0, 0.1, 0.3, 0.5 \quad (45)$$

Studied lattice sizes: $L = 55, 32, 16, 11, 8$.

SO3 - Markov Chain Monte Carlo Simulations

Listing 1: Function for computation of energy difference of flipping a spin variable.

```
def DeltaEnergy(self,next_spin,idx):
    dS = next_spin - self.Lattice[idx]
    s = next_spin + self.Lattice[idx]
    sig = -1 if idx >= self.LatticeSize**2 else 1
    return dS*(-0.5*sum(self.Lattice[k] for k in self.Neighbours[idx])+\
               self.h*sig + self.mu*s)
```

Listing 2: Function for updating configuration following Metropolis Algorithm.

```
def MCStep(self,beta):
    k = rd.randint(0,self.NumSpins-1)
    flip_idx = 1
    if rd.uniform(0.0,1.0) < 0.5:
        flip_idx = 0
    newspin = self.SpinflipKey[self.Lattice[k]][flip_idx]
    if rd.uniform(0.0,1.0) < np.exp(-beta*self.DeltaEnergy(newspin,k)):
        self.Lattice[k] = newspin
```

Computation of Thermodynamic Quantities for $\mu = 0.0$, $h = 0.0$

Binary Alloy Thermodynamic Quantites - MCMC Simulation
 $\mu = 0.0$, $h = 0.0$

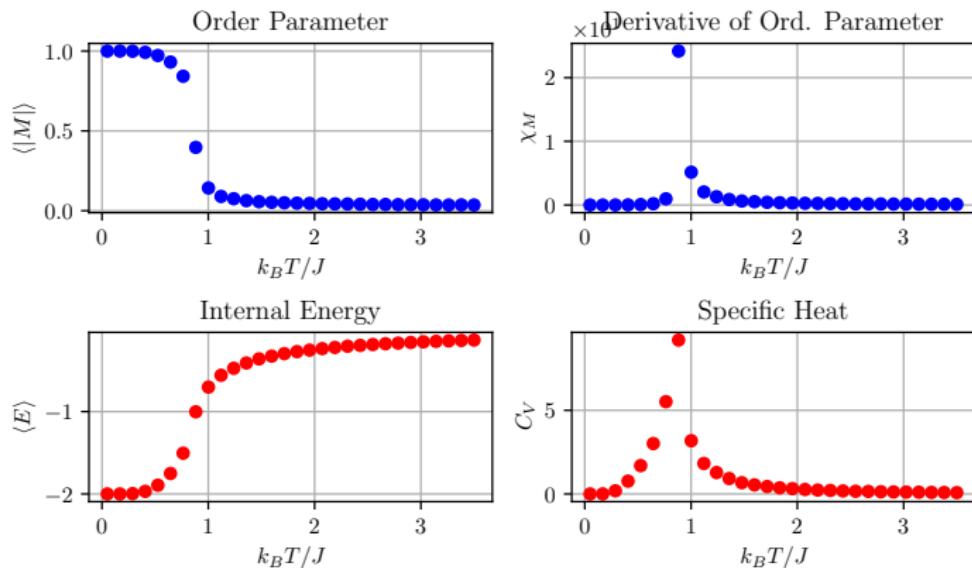


Figure: Thermodynamic quantities of Binary Alloy for a fixed vacancy chemical potential $\mu = 0.0$. Stoichiometric alloy, $h = 0.0$, presents a clearly visible critical point at $T_C = 0.809$. Non stoichiometric binary alloy, $h = 0.5$, does not present such a sharp transition; an inflection point, which coincides with maximum of order parameter derivative, is present at $T_C = 1.496$.

Computation of Thermodynamic Quantities for $\mu = 0.0$, $h = 0.5$

Binary Alloy Thermodynamic Quantites - MCMC Simulation
 $\mu = 0.0, h = 0.5$

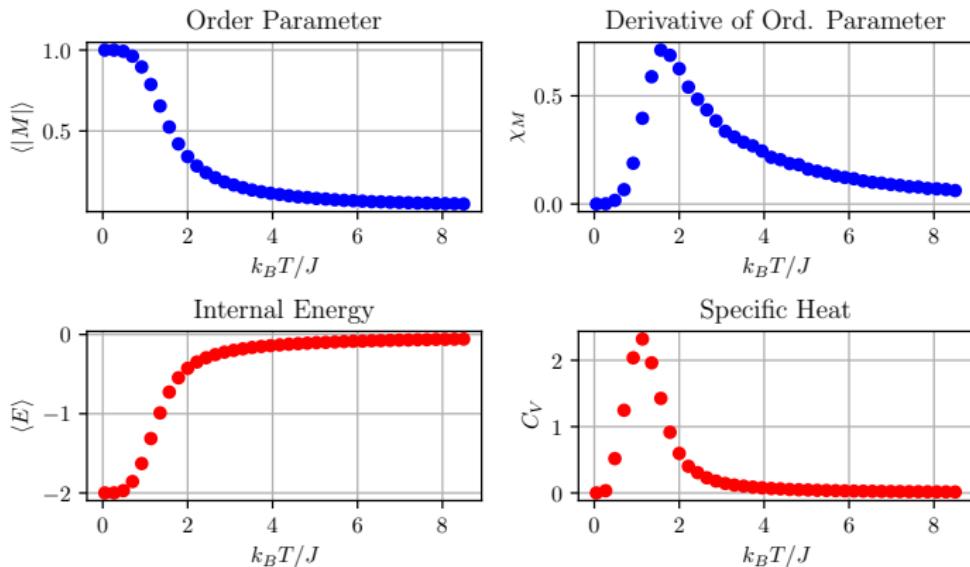


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Magnetisation Profiles with $\mu = 0.0$

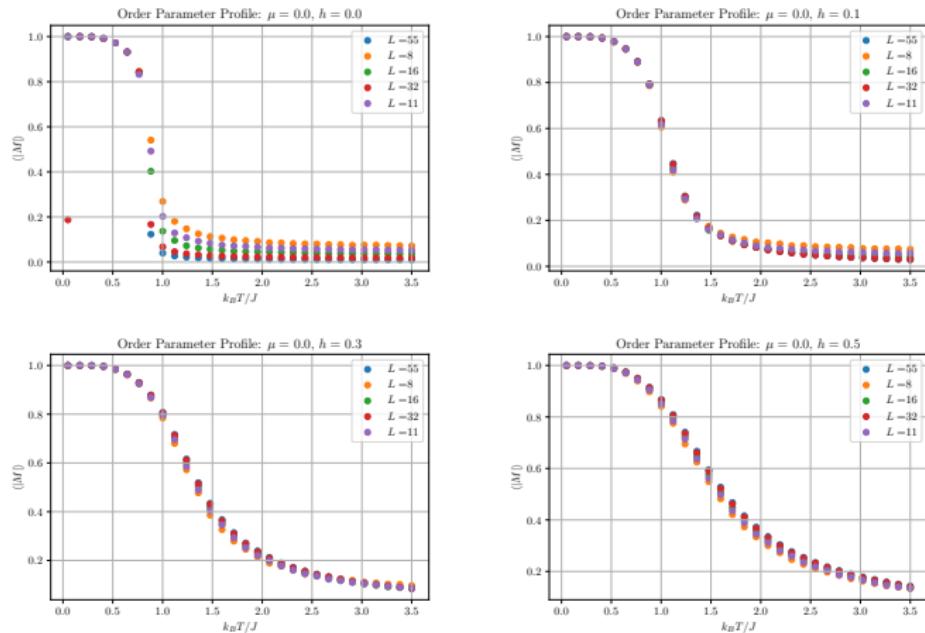


Figure: Order parameter profiles for several values of h and lattice sizes L , with $\mu = 0$. Notice how stoichiometric alloy has a different lattice size scaling than non-stoichiometric alloys. Critical temperature for stoichiometric alloy, and inflection temperature for non-stoichiometric alloys, are determined using the method posed by Ibarra and others [4].

Magnetisation Profiles with $\mu = -1.7$

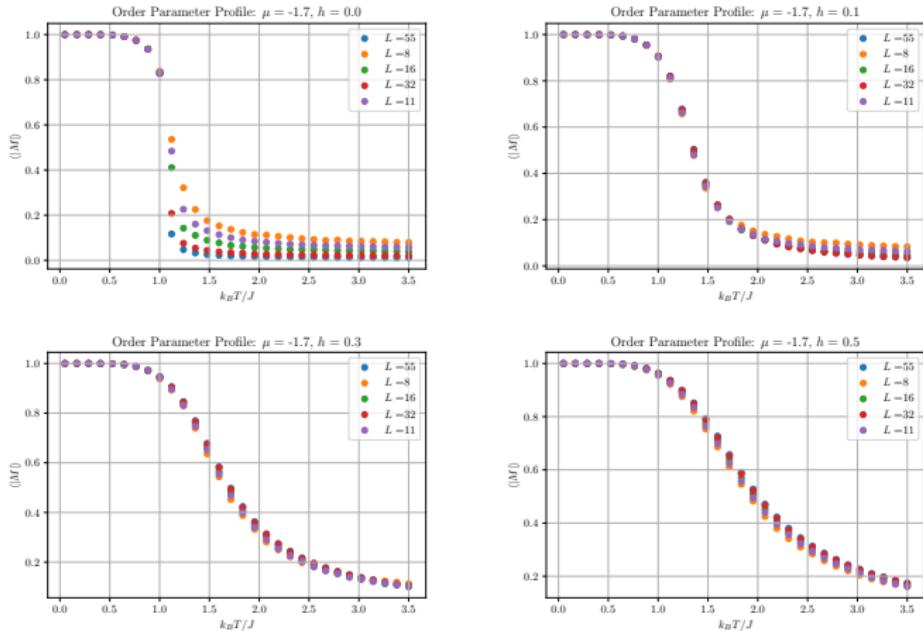


Figure: Order parameter profiles for several values of h and lattice sizes L , with $\mu = -1.7$. Notice how stoichiometric alloy has a different lattice size scaling than non-stoichiometric alloys. Critical temperature for stoichiometric alloy, and inflection temperature for non-stoichiometric alloys, are determined using the method posed by Ibarra and others [4].

SO4 - Computation of Critical Points on h – T plane

Unfortunately, not enough inflection points were computed in order to be able to interpolate a critical curve on h – T plane

h/J	$k_B T_C/J$
0.0	0.809
0.1	1.083
0.2	1.317
0.3	1.496

Table: Inflection temperatures for $\mu = 0.0$. Notice that inflection temperature increases with h , i.e. when atom concentration favours either type A or type B atoms.

h/J	$k_B T_C/J$
0.0	1.044
0.1	1.362
0.2	1.644
0.3	1.844

Table: Inflection temperatures for $\mu = 0.0$. Notice that inflection temperature increases with h , i.e. when atom concentration favours either type A or type B atoms. Also notice that inflection temperatures are higher than those obtained by setting $\mu = 0.0$.

Finite Size Scaling According to Ibarra and others [4]

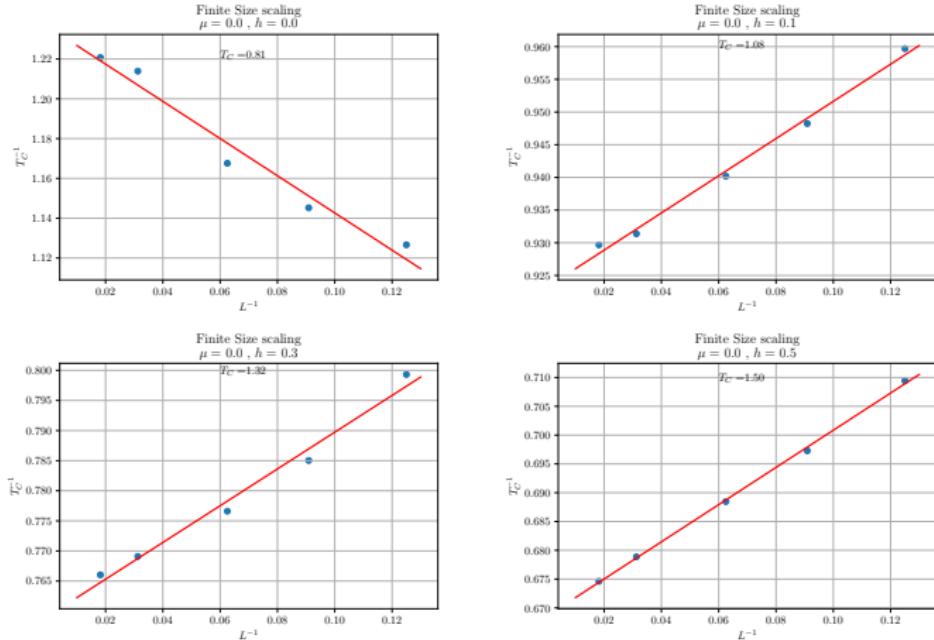


Figure: Finite size scaling following Ibarra and others for several values of h , with $\mu = 0.0$. Notice how stoichiometric alloy has a different lattice size scaling than non-stoichiometric alloys. Critical temperature for stoichiometric alloy, and inflection temperature for non-stoichiometric alloys, are determined by the inverse of the intercept of linear fits [4].

Finite Size Scaling According to Ibarra and others [4]

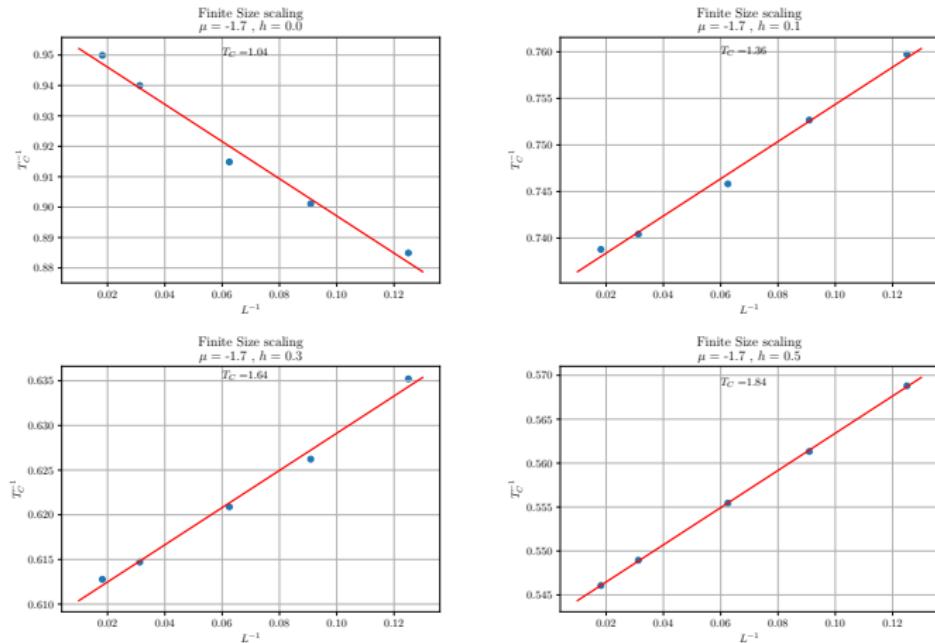


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Discussion of Results

SO1 - Derivation of Alloy Hamiltonian

Statistical considerations lead to a study of a BEG Hamiltonian in the presence of a staggered magnetic field. The case study $K = 0$ is of capital importance since it would lead to a better account of lattice phenomena and even the presence of impurities [7].

SO2 - Landau Theory of BEG Hamiltonian

In the limit of very low vacancy concentration, results from Porta and Castán are recovered [4]. However, it has been shown that increasing vacancy concentration decreases the critical temperature of ordering transitions. See figure 34.

SO3 - Markov Chain Monte Carlo Simulations

Critical temperatures computed using MCMC, for stoichiometric alloys, follow the tendency of Mean Field computations. As expected, numerical values are not consistent due to thermal fluctuations. Non stoichiometric alloys present a rather weak inflection point, which seems to be independent of lattice size.

SO4 - Computation of Critical Points on $h - T$ plane

Non-stoichiometric present a rather weird size scaling which needs to be addressed for further work

Comparison of Mean Field Curves on x – T Plane

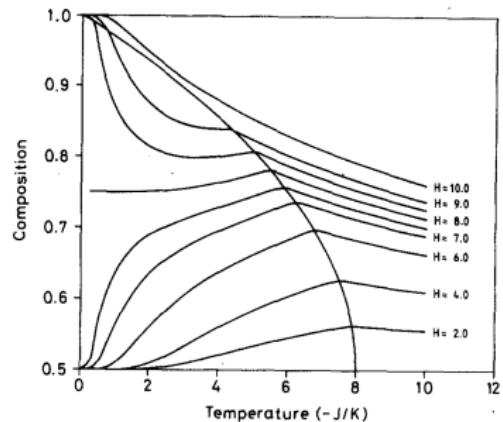
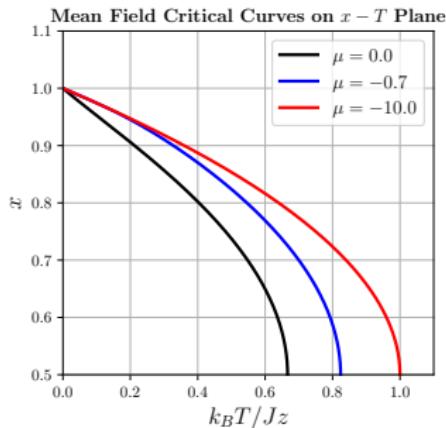


Figure: Temperature profile of order parameter, for a stoichiometric binary alloy, for different values of vacancy chemical potential. The more negative the chemical potential, the smaller the vacancy concentration.

Thermalisation of System

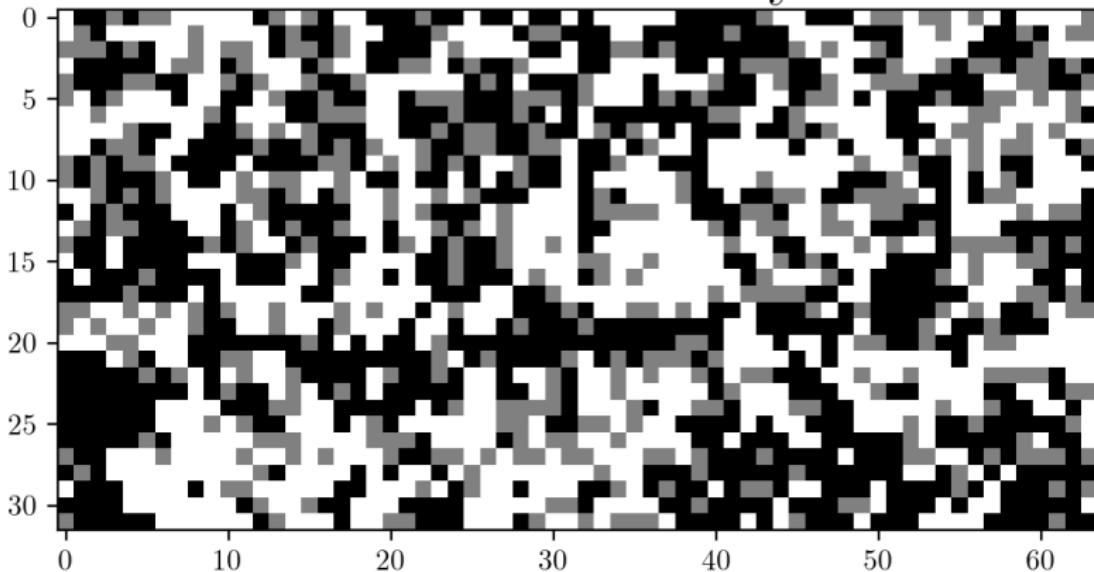


Figure: Alloy Thermalisation simulated using MCMC. A type atoms are represented by black sites, B type, by white sites, and vacancies by gray sites. Notice that vacancies tend to interact strongly with domain borders.

Conclusions

- It has been proven that a substitutional binary alloy can be modeled using a Spin-1 antiferromagnetic BEG Model. The approximation $K = 0$, however should be abandoned to give better count of lattice vibrations and even the presence of impurities in the alloy.
- Mean field calculations are consistent with Porta and Castán's results in the limit of very low vacancy concentration. Results have been generalised though, showing that increasing vacancy concentration leads to a reduction of critical temperature.
- Results are promising for stoichiometric binary alloys with proportions 1 : 1. In this case, experimental results can determine the validity of the presented model.
- Non-stoichiometric alloys present a rather weak inflection point where ordering accelerates. Size scaling suggest that long range correlations are not the dominant factor for ordering in this systems. Further study is needed to confirm the results obtained in this area.

Appendix

All codes, analytical calculations and datasets are available on a public repository on Github under name [InvTeor](#), from user [diegoherrera262](#).

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